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Supplementary data for the manuscript:

Rotational Spectra and Structures of Phenyl Isocyanate and Phenyl Isothiocyanate

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Appendix I: Equilibrium Structures from MP2/aug-cc-pVTZ, B3LYP/aug-cc-pVTZ and B3LYP-D3BJ/aug-cc-pVTZ

Appendix II: Assigned Transitions for PhNCO and PhNCS and Their Minor Isotopologues

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Appendix I: Equilibrium Structures from MP2/aug-cc-pVTZ and B3LYP/aug-cc-pVTZ

Table S1. Cartesian coordinates for the equilibrium structure of PhNCO obtained at the MP2/aug-cc-pVTZ level of theory.

Cartesian Coordinates (Angstroms)			
Atom	X	Y	Z
C	0.043025	-1.099645	0.000000
C	-0.000000	0.297220	0.000000
C	-1.225006	0.964097	0.000000
C	-2.408089	0.230813	0.000000
C	-2.373585	-1.162737	0.000000
C	-1.145613	-1.823328	0.000000
H	1.000027	-1.606502	0.000000
H	-1.234067	2.045589	0.000000
H	-3.357098	0.750377	0.000000
H	-3.294710	-1.729569	0.000000
H	-1.109814	-2.904797	0.000000
N	1.166703	1.068491	0.000000
C	2.362166	0.856864	0.000000
O	3.538919	0.798220	0.000000

Table S2. Cartesian coordinates for the equilibrium structure of PhNCS obtained at the MP2/aug-cc-pVTZ level of theory.

Cartesian Coordinates (Angstroms)			
Atom	X	Y	Z
C	1.346340	0.135298	0.000000
C	0.000000	0.516750	0.000000
C	-0.358841	1.866031	0.000000
C	0.637527	2.837126	0.000000
C	1.982201	2.467899	0.000000
C	2.331278	1.117264	0.000000
H	1.600646	-0.916758	0.000000
H	-1.406801	2.133290	0.000000
H	0.362457	3.883401	0.000000
H	2.753001	3.226616	0.000000
H	3.373272	0.825693	0.000000
N	-0.998091	-0.443079	0.000000
C	-1.263335	-1.619406	0.000000
S	-1.734185	-3.123529	0.000000

Table S3. Cartesian coordinates for the equilibrium structure of PhNCO obtained at the B3LYP/aug-cc-pVTZ level of theory.

Cartesian Coordinates (Angstroms)			
Atom	X	Y	Z
C	0.047422	-1.124452	0.000000
C	-0.000000	0.271579	0.000000
C	-1.230823	0.925675	0.000000
C	-2.405798	0.186156	0.000000
C	-2.363618	-1.203450	0.000000
C	-1.133467	-1.853022	0.000000
H	1.003912	-1.629317	0.000000
H	-1.252305	2.005950	0.000000
H	-3.357417	0.699903	0.000000
H	-3.280459	-1.776184	0.000000
H	-1.090376	-2.933713	0.000000
N	1.162408	1.044877	0.000000
C	2.357028	0.928641	0.000000
O	3.526915	0.941557	0.000000

Table S4. Cartesian coordinates for the equilibrium structure of PhNCS obtained at the B3LYP/aug-cc-pVTZ level of theory.

Cartesian Coordinates (Angstroms)			
Atom	X	Y	Z
C	1.384408	0.292529	0.000000
C	0.000000	0.493787	0.000000
C	-0.520303	1.789064	0.000000
C	0.342508	2.875601	0.000000
C	1.719557	2.681255	0.000000
C	2.234156	1.388254	0.000000
H	1.776527	-0.714584	0.000000
H	-1.591864	1.927143	0.000000
H	-0.063709	3.877712	0.000000
H	2.388027	3.530840	0.000000
H	3.304057	1.230423	0.000000
N	-0.866388	-0.582228	0.000000
C	-1.098487	-1.747718	0.000000
S	-1.507460	-3.275785	0.000000

Table S5. Cartesian coordinates for the equilibrium structure of PhNCO obtained at the B3LYP-D3BJ/aug-cc-pVTZ level of theory.

Cartesian Coordinates (Angstroms)			
Atom	X	Y	Z
C	0.045366	-1.113655	0.000000
C	-0.000000	0.281591	0.000000
C	-1.227893	0.938772	0.000000
C	-2.403970	0.201959	0.000000
C	-2.364503	-1.187219	0.000000
C	-1.136240	-1.839576	0.000000
H	1.001418	-1.618670	0.000000
H	-1.245637	2.018695	0.000000
H	-3.354307	0.717239	0.000000
H	-3.282247	-1.757762	0.000000
H	-1.095785	-2.919968	0.000000
N	1.164756	1.050751	0.000000
C	2.356594	0.904014	0.000000
O	3.525893	0.886236	0.000000

Table S6. Cartesian coordinates for the equilibrium structure of PhNCS obtained at the B3LYP-D3BJ/aug-cc-pVTZ level of theory.

Cartesian Coordinates (Angstroms)			
Atom	X	Y	Z
C	1.361804	0.189726	0.000000
C	0.000000	0.505610	0.000000
C	-0.412504	1.837532	0.000000
C	0.536739	2.848905	0.000000
C	1.892469	2.541372	0.000000
C	2.298901	1.210700	0.000000
H	1.667021	-0.846742	0.000000
H	-1.468977	2.061785	0.000000
H	0.215081	3.880858	0.000000
H	2.628523	3.332595	0.000000
H	3.351838	0.965566	0.000000
N	-0.951619	-0.496867	0.000000
C	-1.211934	-1.657849	0.000000
S	-1.657813	-3.173248	0.000000

Appendix II: Assigned Transitions for PhNCO and PhNCS and Their Minor Isotopologues

Table S7. Assigned transitions for PhNCO (parent).

J'	K _a '	K _c '	F'	J''	K _a ''	K _c ''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}$
3	1	3	4	2	1	2	3	5144.7475	0.0000
3	1	3	3	2	1	2	2	5144.9897	0.0003
3	0	3	4	2	0	2	3	5360.5834	0.0000
3	0	3	3	2	0	2	2	5360.6138	0.0001
3	0	3	2	2	0	2	1	5360.7524	0.0000
3	2	2	2	2	2	1	1	5376.2382	-0.0006
3	2	2	4	2	2	1	3	5376.7266	0.0015
3	2	2	3	2	2	1	2	5377.6010	0.0001
3	2	1	2	2	2	0	1	5392.5363	0.0000
3	2	1	4	2	2	0	3	5393.0244	0.0012
3	2	1	3	2	2	0	2	5393.9014	0.0003
3	1	2	4	2	1	1	3	5603.8365	-0.0001
3	1	2	2	2	1	1	1	5603.8489	0.0020
3	1	2	3	2	1	1	2	5604.0805	0.0000
4	1	4	5	3	1	3	4	6855.1107	0.0001
4	1	4	3	3	1	3	2	6855.1432	-0.0003
4	1	4	4	3	1	3	3	6855.2175	-0.0001
4	0	4	5	3	0	3	4	7128.5700	0.0000
4	0	4	4	3	0	3	3	7128.5877	0.0000
4	0	4	3	3	0	3	2	7128.6492	-0.0002
4	2	3	3	3	2	2	2	7165.8507	0.0000
4	2	3	5	3	2	2	4	7165.9462	0.0000
4	2	3	4	3	2	2	3	7166.3175	0.0001
4	3	2	3	3	3	1	2	7176.6756	0.0007
4	3	2	5	3	3	1	4	7176.9901	0.0015
4	3	1	3	3	3	0	2	7177.0829	0.0003
4	3	1	5	3	3	0	4	7177.3975	0.0013
4	3	2	4	3	3	1	3	7177.8004	0.0011
4	3	1	4	3	3	0	3	7178.2075	0.0004
4	2	2	3	3	2	1	2	7206.4691	0.0000
4	2	2	5	3	2	1	4	7206.5651	0.0000
4	2	2	4	3	2	1	3	7206.9390	0.0000
4	1	3	5	3	1	2	4	7466.9099	-0.0001
4	1	3	3	3	1	2	2	7466.9484	0.0004
4	1	3	4	3	1	2	3	7467.0182	0.0000
5	1	5	6	4	1	4	5	8561.7046	-0.0001
5	1	5	4	4	1	4	3	8561.7336	0.0000
5	1	5	5	4	1	4	4	8561.7628	0.0000
5	0	5	6	4	0	4	5	8880.7625	-0.0002
5	0	5	5	4	0	4	4	8880.7741	0.0008
5	0	5	4	4	0	4	3	8880.8096	-0.0002

5	2	4	4	4	2	3	3	8952.3684	-0.0002
5	2	4	6	4	2	3	5	8952.3886	0.0001
5	2	4	5	4	2	3	4	8952.5822	0.0001
5	3	3	4	4	3	2	3	8974.6271	0.0001
5	3	3	6	4	3	2	5	8974.7297	0.0000
5	3	3	5	4	3	2	4	8975.1496	-0.0001
5	3	2	4	4	3	1	3	8976.0527	0.0001
5	3	2	6	4	3	1	5	8976.1553	0.0000
5	3	2	5	4	3	1	4	8976.5756	0.0001
5	2	3	4	4	2	2	3	9033.0833	-0.0003
5	2	3	6	4	2	2	5	9033.1039	0.0002
5	2	3	5	4	2	2	4	9033.3011	-0.0001
5	1	4	6	4	1	3	5	9325.5328	0.0000
5	1	4	4	4	1	3	3	9325.5639	-0.0006
5	1	4	5	4	1	3	4	9325.5921	0.0005
6	1	6	5	5	1	5	5	10262.8840	-0.0006
6	1	6	7	5	1	5	6	10263.8460	0.0003
6	1	6	5	5	1	5	4	10263.8666	-0.0015
6	1	6	6	5	1	5	5	10263.8810	0.0000
6	1	6	6	5	1	5	6	10264.6978	-0.0003
6	0	6	5	5	0	5	5	10613.0032	-0.0004
6	0	6	7	5	0	5	6	10614.0941	-0.0006
6	0	6	6	5	0	5	5	10614.1019	0.0009
6	0	6	5	5	0	5	4	10614.1262	0.0000
6	0	6	6	5	0	5	6	10615.0333	-0.0002
4	1	4	4	3	0	3	3	10719.2898	0.0003
4	1	4	5	3	0	3	4	10719.4346	-0.0001
4	1	4	3	3	0	3	2	10719.5556	-0.0005
6	2	5	5	5	2	4	5	10734.7306	-0.0002
6	2	5	7	5	2	4	6	10735.4106	0.0002
6	2	5	6	5	2	4	5	10735.5248	0.0000
6	2	5	6	5	2	4	6	10736.0896	-0.0002
6	5	1	5	5	5	0	4	10763.7102	-0.0004
6	5	2	5	5	5	1	4	10763.7102	-0.0002
6	5	1	7	5	5	0	6	10763.8728	0.0005
6	5	2	7	5	5	1	6	10763.8728	0.0006
6	5	1	6	5	5	0	5	10764.5381	0.0000
6	5	2	6	5	5	1	5	10764.5381	0.0001
6	3	4	5	5	3	3	4	10774.2725	0.0007
6	3	4	7	5	3	3	6	10774.3098	-0.0003
6	3	4	6	5	3	3	5	10774.5569	0.0001
6	3	3	5	5	3	2	4	10778.0674	0.0008
6	3	3	7	5	3	2	6	10778.1046	-0.0002
6	3	3	6	5	3	2	5	10778.3520	0.0000
10	2	8	10	10	1	9	10	10798.7438	-0.0006
10	2	8	11	10	1	9	11	10798.8143	-0.0005

10	2	8	9	10	1	9	9	10798.8229	0.0009
6	2	4	5	5	2	3	5	10874.3585	-0.0013
6	2	4	7	5	2	3	6	10875.0521	0.0000
6	2	4	6	5	2	3	5	10875.1709	0.0000
6	2	4	6	5	2	3	6	10875.7456	-0.0005
6	1	5	5	5	1	4	5	11177.3162	-0.0005
6	1	5	7	5	1	4	6	11178.3469	0.0002
6	1	5	5	5	1	4	4	11178.3702	-0.0009
6	1	5	6	5	1	4	5	11178.3830	0.0006
6	1	5	6	5	1	4	6	11179.2582	-0.0001
7	2	5	7	7	1	6	7	11334.3155	0.0002
7	2	5	8	7	1	6	8	11334.4781	0.0001
7	2	5	6	7	1	6	6	11334.5023	0.0008
8	0	8	9	7	1	7	8	11461.5791	-0.0012
8	0	8	7	7	1	7	6	11461.5881	0.0002
8	0	8	8	7	1	7	7	11461.6479	-0.0001
6	2	4	6	6	1	5	6	11624.3312	0.0007
6	2	4	7	6	1	5	7	11624.5489	0.0007
6	2	4	5	6	1	5	5	11624.5831	-0.0018
5	2	3	5	5	1	4	5	11927.5419	0.0000
5	2	3	6	5	1	4	6	11927.8426	-0.0001
7	1	7	6	6	1	6	6	11960.0128	0.0000
7	1	7	8	6	1	6	7	11960.9908	-0.0007
7	1	7	6	6	1	6	5	11961.0084	-0.0007
7	1	7	7	6	1	6	6	11961.0158	0.0011
7	1	7	7	6	1	6	7	11961.8668	-0.0004
5	1	5	5	4	0	4	4	12152.4644	-0.0001
5	1	5	6	4	0	4	5	12152.5698	0.0003
5	1	5	4	4	0	4	3	12152.6405	0.0002
7	0	7	8	6	0	6	7	12326.5453	-0.0007
7	0	7	7	6	0	6	6	12326.5485	-0.0007
7	0	7	6	6	0	6	5	12326.5698	0.0012
7	2	6	6	6	2	5	6	12513.5677	-0.0003
7	2	6	8	6	2	5	7	12514.3554	-0.0005
7	2	6	6	6	2	5	5	12514.3627	0.0005
7	2	6	7	6	2	5	6	12514.4299	0.0003
7	2	6	7	6	2	5	7	12515.1086	-0.0003
7	6	1	6	6	6	0	5	12557.3007	0.0008
7	6	2	6	6	6	1	5	12557.3007	0.0008
7	6	1	8	6	6	0	7	12557.4245	0.0004
7	6	2	8	6	6	1	7	12557.4245	0.0004
7	6	1	7	6	6	0	6	12558.0292	-0.0007
7	6	2	7	6	6	1	6	12558.0292	-0.0007
7	5	3	6	6	5	2	5	12560.4145	-0.0005
7	5	2	6	6	5	1	5	12560.4145	-0.0012
7	5	3	8	6	5	2	7	12560.4951	0.0005

7	5	2	8	6	5	1	7	12560.4951	0.0000
7	5	3	7	6	5	2	6	12560.9180	0.0001
7	5	2	7	6	5	1	6	12560.9180	-0.0004
7	4	4	6	6	4	3	5	12566.2472	0.0010
7	4	4	8	6	4	3	7	12566.2893	0.0003
7	4	3	6	6	4	2	5	12566.3591	0.0003
7	4	3	8	6	4	2	7	12566.4009	-0.0006
7	4	4	7	6	4	3	6	12566.5630	0.0000
7	4	3	7	6	4	2	6	12566.6755	0.0000
7	3	5	6	6	3	4	5	12575.7702	-0.0009
7	3	5	8	6	3	4	7	12575.7862	0.0007
7	3	5	7	6	3	4	6	12575.9434	0.0000
7	3	4	6	6	3	3	5	12584.2832	-0.0014
7	3	4	8	6	3	3	7	12584.3000	0.0009
7	3	4	7	6	3	3	6	12584.4574	0.0000
7	2	5	6	6	2	4	6	12732.9344	-0.0007
7	2	5	8	6	2	4	7	12733.7400	-0.0005
7	2	5	6	6	2	4	5	12733.7464	0.0002
7	2	5	7	6	2	4	6	12733.8195	0.0007
7	2	5	7	6	2	4	7	12734.5125	-0.0004
7	1	6	6	6	1	5	6	13022.7639	-0.0002
7	1	6	8	6	1	5	7	13023.8101	-0.0005
7	1	6	6	6	1	5	5	13023.8296	0.0000
7	1	6	7	6	1	5	6	13023.8346	0.0006
7	1	6	7	6	1	5	7	13024.7455	-0.0001
9	0	9	10	8	1	8	9	13497.2280	-0.0003
9	0	9	8	8	1	8	7	13497.2359	0.0007
9	0	9	9	8	1	8	8	13497.2800	0.0000
6	1	6	6	5	0	5	5	13535.5716	-0.0005
6	1	6	7	5	0	5	6	13535.6522	-0.0001
6	1	6	5	5	0	5	4	13535.6988	0.0003
8	1	8	7	7	1	7	7	13651.7769	0.0001
8	1	8	9	7	1	7	8	13652.7640	-0.0006
8	1	8	8	7	1	7	7	13652.7806	-0.0001
8	1	8	8	7	1	7	8	13653.6558	-0.0005
4	2	3	5	4	1	4	5	13689.3137	0.0001
4	2	3	3	4	1	4	3	13689.4125	-0.0009
8	0	8	7	7	0	7	7	14016.5225	-0.0001
8	0	8	9	7	0	7	8	14017.5839	0.0005
8	0	8	7	7	0	7	6	14017.6015	0.0009
8	0	8	8	7	0	7	8	14018.5264	-0.0003
5	2	4	6	5	1	5	6	14079.9978	0.0005
5	2	4	4	5	1	5	4	14080.0484	-0.0002
8	2	7	9	7	2	6	8	14288.5758	-0.0001
8	2	7	7	7	2	6	6	14288.5845	0.0010
8	2	7	8	7	2	6	7	14288.6257	-0.0003

8	5	3	7	7	5	2	6	14358.2316	-0.0006
8	5	4	9	7	5	3	8	14358.2725	0.0007
8	4	5	7	7	4	4	6	14366.8143	-0.0022
8	4	5	9	7	4	4	8	14366.8387	0.0013
8	4	5	8	7	4	4	7	14367.0232	0.0001
8	4	4	7	7	4	3	6	14367.1226	-0.0030
8	4	4	9	7	4	3	8	14367.1478	0.0012
8	4	4	8	7	4	3	7	14367.3322	0.0000
8	3	6	9	7	3	5	8	14379.0315	0.0001
8	3	6	8	7	3	5	7	14379.1390	0.0001
8	3	5	9	7	3	4	8	14395.9824	0.0001
8	3	5	8	7	3	4	7	14396.0904	0.0000
8	2	6	9	7	2	5	8	14608.9861	-0.0001
8	2	6	7	7	2	5	6	14608.9945	0.0011
8	2	6	8	7	2	5	7	14609.0406	-0.0006
8	1	7	9	7	1	6	8	14860.1751	-0.0013
8	1	7	8	7	1	6	7	14860.1922	0.0000
9	1	9	8	8	1	8	8	15337.9692	0.0013
9	1	9	10	8	1	8	9	15338.9596	-0.0009
9	1	9	9	8	1	8	8	15338.9725	0.0004
9	0	9	8	8	0	8	8	15687.3633	-0.0006
9	0	9	10	8	0	8	9	15688.4125	-0.0001
9	0	9	8	8	0	8	7	15688.4274	0.0014
9	0	9	9	8	0	8	9	15689.3556	-0.0004
9	2	8	10	8	2	7	9	16057.4399	-0.0001
9	2	8	8	8	2	7	7	16057.4492	0.0017
9	2	8	9	8	2	7	8	16057.4748	-0.0008
9	6	3	8	8	6	2	7	16150.8693	0.0007
9	6	4	8	8	6	3	7	16150.8693	0.0008
9	6	3	10	8	6	2	9	16150.9063	-0.0014
9	6	4	10	8	6	3	9	16150.9063	-0.0014
9	6	3	9	8	6	2	8	16151.1972	-0.0001
9	6	4	9	8	6	3	8	16151.1972	-0.0001
9	4	6	9	8	4	5	8	16169.5721	0.0005
9	4	5	9	8	4	4	8	16170.3126	0.0004
8	1	8	8	7	0	7	7	16208.7193	0.0018
8	1	8	9	7	0	7	8	16208.7659	-0.0018
8	1	8	7	7	0	7	6	16208.7911	-0.0002
9	2	7	10	8	2	6	9	16498.8348	-0.0002
9	2	7	8	8	2	6	7	16498.8435	0.0011
9	2	7	9	8	2	6	8	16498.8755	-0.0001
9	1	8	10	8	1	7	9	16685.4692	-0.0013
9	1	8	8	8	1	7	7	16685.4829	0.0001
10	1	10	9	9	1	9	9	17018.5505	-0.0004
10	1	10	11	9	1	9	10	17019.5445	-0.0013
10	1	10	9	9	1	9	8	17019.5554	0.0003

10	1	10	10	9	1	9	10	17020.4588	0.0012
10	0	10	11	9	0	9	10	17341.8641	-0.0005
10	0	10	9	9	0	9	8	17341.8776	0.0021
9	1	9	9	8	0	8	8	17530.1048	0.0000
9	1	9	10	8	0	8	9	17530.1453	0.0004
9	1	9	8	8	0	8	7	17530.1619	-0.0007
10	2	9	11	9	2	8	10	17820.3484	-0.0003
10	2	9	9	9	2	8	8	17820.3571	0.0014
10	2	9	10	9	2	8	9	17820.3739	-0.0008
10	3	8	11	9	3	7	10	17989.4470	0.0007
10	3	8	10	9	3	7	9	17989.5036	0.0006
10	3	7	11	9	3	6	10	18041.8792	0.0012
10	2	8	11	9	2	7	10	18399.6616	0.0000
10	2	8	9	9	2	7	8	18399.6701	0.0017
10	2	8	10	9	2	7	9	18399.6916	-0.0009
10	1	9	11	9	1	8	10	18497.4981	-0.0011
10	1	9	9	9	1	8	8	18497.5094	0.0000
11	1	11	12	10	1	10	11	18694.6452	-0.0010
11	1	11	10	10	1	10	9	18694.6541	0.0001

Table S8. Assigned transitions for PhNCO ($^{13}\text{C1}$).

J'	K _a '	K _c '	F'	J''	K _a ''	K _c ''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}$
8	1	8	9	7	1	7	8	13651.8312	-0.0008
8	1	8	8	7	1	7	7	13651.8485	-0.0006
8	0	8	9	7	0	7	8	14016.5578	0.0007
9	1	9	10	8	1	8	9	15337.8731	-0.0001
9	1	9	9	8	1	8	8	15337.8854	0.0000
9	0	9	10	8	0	8	9	15687.1287	0.0001
9	0	9	8	8	0	8	7	15687.1442	0.0010
9	2	8	10	8	2	7	9	16056.8826	-0.0002
9	2	8	8	8	2	7	7	16056.8923	0.0014
9	2	8	9	8	2	7	8	16056.9196	-0.0017
10	1	10	11	9	1	9	10	17018.2944	-0.0013
10	1	10	10	9	1	9	9	17018.3061	0.0014
10	0	10	11	9	0	9	10	17340.3216	-0.0009
10	0	10	9	9	0	9	8	17340.3357	0.0014
10	2	9	11	9	2	8	10	17819.6828	0.0001
11	1	11	11	10	1	10	10	18693.2349	0.0013
11	0	11	12	10	0	10	11	18980.0900	-0.0022
11	0	11	10	10	0	10	9	18980.1024	0.0004

Table S9. Assigned transitions for PhNCO ($^{13}\text{C}2$).

J'	K _a '	K _c '	F'	J''	K _a ''	K _c ''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
3	1	2	4	2	1	1	3	5600.2896	-0.0002
3	1	2	3	2	1	1	2	5600.5327	-0.0005
4	1	4	5	3	1	3	4	6844.5516	0.0000
4	1	4	3	3	1	3	2	6844.5835	-0.0010
4	1	4	4	3	1	3	3	6844.6583	-0.0001
4	0	4	5	3	0	3	4	7119.7917	-0.0002
4	0	4	4	3	0	3	3	7119.8095	0.0000
4	0	4	3	3	0	3	2	7119.8711	-0.0001
4	1	3	5	3	1	2	4	7462.0162	0.0000
4	1	3	3	3	1	2	2	7462.0555	0.0014
4	1	3	4	3	1	2	3	7462.1242	-0.0001
5	1	5	6	4	1	4	5	8548.2810	-0.0002
5	1	5	4	4	1	4	3	8548.3100	0.0000
5	1	5	5	4	1	4	4	8548.3392	0.0000
5	0	5	6	4	0	4	5	8868.8416	-0.0006
5	0	5	5	4	0	4	4	8868.8536	0.0008
5	0	5	4	4	0	4	3	8868.8886	-0.0007
5	1	4	6	4	1	3	5	9319.1389	-0.0002
5	1	4	4	4	1	3	3	9319.1709	0.0000
5	1	4	5	4	1	3	4	9319.1981	0.0002
6	1	6	7	5	1	5	6	10247.4274	-0.0002
6	1	6	5	5	1	5	4	10247.4487	-0.0015
6	1	6	6	5	1	5	5	10247.4633	0.0003
6	0	6	7	5	0	5	6	10598.4855	-0.0010
6	0	6	6	5	0	5	5	10598.4934	0.0007
6	0	6	5	5	0	5	4	10598.5182	0.0001
6	2	5	7	5	2	4	6	10723.6206	-0.0001
6	2	5	6	5	2	4	5	10723.7353	0.0002
6	2	4	7	5	2	3	6	10867.6787	-0.0001
6	2	4	6	5	2	3	5	10867.7974	-0.0003
6	1	5	7	5	1	4	6	11170.2474	0.0002
6	1	5	5	5	1	4	4	11170.2707	-0.0010
6	1	5	6	5	1	4	5	11170.2832	0.0003
7	1	7	8	6	1	6	7	11941.4407	-0.0010
7	1	7	6	6	1	6	5	11941.4584	-0.0009
7	1	7	7	6	1	6	6	11941.4657	0.0008
7	0	7	8	6	0	6	7	12306.7255	0.0005
7	0	7	6	6	0	6	5	12306.7491	0.0015
7	2	6	8	6	2	5	7	12500.2662	-0.0005
7	2	6	6	6	2	5	5	12500.2743	0.0014
7	2	6	7	6	2	5	6	12500.3396	-0.0006
7	2	5	8	6	2	4	7	12726.4089	-0.0005
7	2	5	6	6	2	4	5	12726.4165	0.0013

7	2	5	7	6	2	4	6	12726.4886	0.0008
7	1	6	8	6	1	5	7	13013.7355	-0.0011
7	1	6	6	6	1	5	5	13013.7545	-0.0011
7	1	6	7	6	1	5	6	13013.7606	0.0008
8	1	8	9	7	1	7	8	13629.9479	0.0013
8	1	8	7	7	1	7	6	13629.9614	0.0009
8	0	8	9	7	0	7	8	13993.1369	0.0006
8	2	7	9	7	2	6	8	14272.0341	-0.0015
8	2	7	7	7	2	6	6	14272.0440	0.0009
8	2	7	8	7	2	6	7	14272.0860	0.0004
9	1	9	10	8	1	8	9	15312.7452	-0.0010
9	1	9	9	8	1	8	8	15312.7583	0.0005
9	0	9	10	8	0	8	9	15659.1202	-0.0003
9	0	9	8	8	0	8	7	15659.1359	0.0019
9	2	8	10	8	2	7	9	16038.2777	-0.0010
9	2	8	8	8	2	7	7	16038.2877	0.0016
9	2	8	9	8	2	7	8	16038.3132	-0.0009
10	1	10	11	9	1	9	10	16989.8216	-0.0016
10	1	10	9	9	1	9	8	16989.8335	0.0009
10	0	10	11	9	0	9	10	17307.7400	-0.0008
11	1	11	12	10	1	10	11	18661.3250	0.0007
11	1	11	10	10	1	10	9	18661.3320	0.0000

Table S10. Assigned transitions for PhNCO ($^{13}\text{C}3$).

J'	K _a '	K _c '	F'	J''	K _a ''	K _c ''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
3	1	2	4	2	1	1	3	5569.6926	-0.0171
3	1	2	3	2	1	1	2	5569.9365	-0.0169
4	1	4	5	3	1	3	4	6805.7001	0.0217
4	1	4	3	3	1	3	2	6805.7314	0.0192
4	1	4	4	3	1	3	3	6805.8073	0.0214
4	0	4	5	3	0	3	4	7079.8922	-0.0009
4	0	4	4	3	0	3	3	7079.9100	-0.0013
4	0	4	3	3	0	3	2	7079.9708	-0.0016
4	1	3	5	3	1	2	4	7421.2082	-0.0229
4	1	3	3	3	1	2	2	7421.2463	-0.0221
4	1	3	4	3	1	2	3	7421.3164	-0.0230
5	1	5	6	4	1	4	5	8499.7037	0.0263
5	1	5	4	4	1	4	3	8499.7329	0.0264
5	1	5	5	4	1	4	4	8499.7614	0.0257
5	0	5	6	4	0	4	5	8818.9079	-0.0030
5	0	5	5	4	0	4	4	8818.9196	-0.0025
5	0	5	4	4	0	4	3	8818.9544	-0.0037
5	1	4	6	4	1	3	5	9268.1083	-0.0296
5	1	4	4	4	1	3	3	9268.1392	-0.0300
5	1	4	5	4	1	3	4	9268.1677	-0.0291
6	1	6	7	5	1	5	6	10189.1178	0.0305
6	1	6	5	5	1	5	4	10189.1388	0.0287
6	1	6	6	5	1	5	5	10189.1525	0.0297
6	0	6	7	5	0	5	6	10538.4931	-0.0057
6	0	6	6	5	0	5	5	10538.5010	-0.0047
6	0	6	5	5	0	5	4	10538.5245	-0.0057
6	2	5	7	5	2	4	6	10663.8647	-0.0032
6	2	5	6	5	2	4	5	10663.9782	-0.0045
6	2	4	7	5	2	3	6	10808.1973	-0.0002
6	2	4	6	5	2	3	5	10808.3157	-0.0001
6	1	5	7	5	1	4	6	11108.9773	-0.0363
6	1	5	5	5	1	4	4	11108.9997	-0.0381
6	1	5	6	5	1	4	5	11109.0126	-0.0368
7	1	7	8	6	1	6	7	11873.3940	0.0337
7	1	7	6	6	1	6	5	11873.4112	0.0330
7	1	7	7	6	1	6	6	11873.4189	0.0351
7	0	7	8	6	0	6	7	12236.6651	-0.0074
7	0	7	6	6	0	6	5	12236.6891	-0.0060

7	2	6	8	6	2	5	7	12430.5279	-0.0064
7	2	6	6	6	2	5	5	12430.5360	-0.0044
7	2	6	7	6	2	5	6	12430.6017	-0.0062
7	2	5	8	6	2	4	7	12657.0575	-0.0030
7	1	6	8	6	1	5	7	12942.2024	-0.0456
7	1	6	6	6	1	5	5	12942.2209	-0.0460
7	1	6	7	6	1	5	6	12942.2269	-0.0446
8	1	8	9	7	1	7	8	13552.1603	0.0382
8	1	8	7	7	1	7	6	13552.1743	0.0380
8	0	8	9	7	0	7	8	13913.0310	-0.0092
8	0	8	7	7	0	7	6	13913.0448	-0.0124
8	2	7	9	7	2	6	8	14192.3044	-0.0098
8	2	7	7	7	2	6	6	14192.3139	-0.0078
8	2	7	8	7	2	6	7	14192.3562	-0.0082
9	1	9	10	8	1	8	9	15225.2186	0.0385
9	1	9	8	8	1	8	7	15225.2316	0.0401
9	0	9	10	8	0	8	9	15569.0280	-0.0122
9	0	9	8	8	0	8	7	15569.0439	-0.0097
9	2	8	10	8	2	7	9	15948.5452	-0.0132
9	2	8	8	8	2	7	7	15948.5548	-0.0110
9	2	8	9	8	2	7	8	15948.5809	-0.0133
10	1	10	11	9	1	9	10	16892.5604	0.0400
10	1	10	9	9	1	9	8	16892.5722	0.0425
10	0	10	11	9	0	9	10	17207.7592	-0.0144
10	0	10	9	9	0	9	8	17207.7733	-0.0110

Table S11. Assigned transitions for PhNCO ($^{13}\text{C4}$).

J'	K _a '	K _c '	F'	J''	K _a ''	K _c ''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
3	1	2	4	2	1	1	3	5530.0518	-0.0176
3	1	2	3	2	1	1	2	5530.2971	-0.0168
4	1	4	5	3	1	3	4	6771.4650	0.0228
4	1	4	3	3	1	3	2	6771.4982	0.0227
4	1	4	4	3	1	3	3	6771.5719	0.0223
4	0	4	5	3	0	3	4	7039.2168	-0.0007
4	0	4	4	3	0	3	3	7039.2348	-0.0008
4	0	4	3	3	0	3	2	7039.2958	-0.0013
4	1	3	5	3	1	2	4	7368.7692	-0.0235
4	1	3	3	3	1	2	2	7368.8092	-0.0212
4	1	3	4	3	1	2	3	7368.8775	-0.0238
5	1	5	6	4	1	4	5	8457.4808	0.0278
5	1	5	4	4	1	4	3	8457.5086	0.0265
5	1	5	5	4	1	4	4	8457.5384	0.0270
5	0	5	6	4	0	4	5	8770.4706	-0.0018
5	0	5	5	4	0	4	4	8770.4828	-0.0008
5	0	5	4	4	0	4	3	8770.5172	-0.0024
5	1	4	6	4	1	3	5	9203.2559	-0.0291
5	1	4	4	4	1	3	3	9203.2863	-0.0303
5	1	4	5	4	1	3	4	9203.3150	-0.0290
6	1	6	7	5	1	5	6	10139.2414	0.0335
6	1	6	5	5	1	5	4	10139.2614	0.0308
6	1	6	6	5	1	5	5	10139.2757	0.0322
6	0	6	7	5	0	5	6	10483.6952	-0.0031
6	0	6	6	5	0	5	5	10483.7032	-0.0019
6	0	6	5	5	0	5	4	10483.7280	-0.0019
6	2	5	7	5	2	4	6	10599.3633	-0.0013
6	2	5	6	5	2	4	5	10599.4779	-0.0018
6	2	4	7	5	2	3	6	10732.4829	-0.0003
6	2	4	6	5	2	3	5	10732.6022	0.0002
6	1	5	7	5	1	4	6	11032.2263	-0.0353
6	1	5	5	5	1	4	4	11032.2490	-0.0370
6	1	5	6	5	1	4	5	11032.2614	-0.0362
7	1	7	8	6	1	6	7	11816.2176	0.0368
7	1	7	6	6	1	6	5	11816.2356	0.0371
7	0	7	8	6	0	6	7	12176.8857	-0.0027
7	0	7	6	6	0	6	5	12176.9094	-0.0017
7	2	6	8	6	2	5	7	12356.1232	-0.0033

7	2	6	6	6	2	5	5	12356.1315	-0.0011
7	2	6	7	6	2	5	6	12356.1973	-0.0031
7	2	5	8	6	2	4	7	12565.4354	-0.0016
7	2	5	7	6	2	4	6	12565.5151	0.0000
7	1	6	8	6	1	5	7	12854.2242	-0.0433
7	1	6	6	6	1	5	5	12854.2437	-0.0428
7	1	6	7	6	1	5	6	12854.2493	-0.0417
8	1	8	9	7	1	7	8	13488.0420	0.0428
8	1	8	7	7	1	7	6	13488.0559	0.0425
8	0	8	9	7	0	7	8	13849.4045	-0.0032
8	0	8	7	7	0	7	6	13849.4192	-0.0056
8	2	7	9	7	2	6	8	14108.3803	-0.0054
8	2	7	7	7	2	6	6	14108.3902	-0.0029
8	2	7	8	7	2	6	7	14108.4327	-0.0034
9	1	9	10	8	1	8	9	15154.4981	0.0451
9	1	9	9	8	1	8	8	15154.5114	0.0466
9	0	9	10	8	0	8	9	15502.2456	-0.0038
9	0	9	8	8	0	8	7	15502.2614	-0.0014
9	2	8	10	8	2	7	9	15855.5337	-0.0063
9	2	8	8	8	2	7	7	15855.5428	-0.0046
9	2	8	9	8	2	7	8	15855.5694	-0.0064
10	1	10	11	9	1	9	10	16815.5427	0.0491
10	1	10	9	9	1	9	8	16815.5546	0.0516
10	0	10	11	9	0	9	10	17137.9621	-0.0033

Table S12. Assigned transitions for PhNCO ($^{13}\text{C5}$).

J'	K _a '	K _c '	F'	J''	K _a ''	K _c ''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
3	1	2	4	2	1	1	3	5548.1958	-0.0187
3	1	2	3	2	1	1	2	5548.4418	-0.0173
4	1	4	5	3	1	3	4	6787.5302	0.0219
4	1	4	3	3	1	3	2	6787.5628	0.0208
4	1	4	4	3	1	3	3	6787.6367	0.0207
4	0	4	5	3	0	3	4	7058.1231	-0.0010
4	0	4	4	3	0	3	3	7058.1408	-0.0016
4	0	4	3	3	0	3	2	7058.2029	-0.0009
4	1	3	5	3	1	2	4	7392.7864	-0.0232
4	1	3	3	3	1	2	2	7392.8253	-0.0218
4	1	3	4	3	1	2	3	7392.8948	-0.0234
5	1	5	6	4	1	4	5	8477.3193	0.0271
5	1	5	4	4	1	4	3	8477.3483	0.0269
5	1	5	5	4	1	4	4	8477.3776	0.0269
5	0	5	6	4	0	4	5	8793.0759	-0.0026
5	0	5	5	4	0	4	4	8793.0879	-0.0018
5	0	5	4	4	0	4	3	8793.1228	-0.0030
5	1	4	6	4	1	3	5	9232.9816	-0.0289
5	1	4	4	4	1	3	3	9233.0126	-0.0294
5	1	4	5	4	1	3	4	9233.0408	-0.0288
6	1	6	7	5	1	5	6	10162.7085	0.0309
6	1	6	5	5	1	5	4	10162.7302	0.0298
6	1	6	6	5	1	5	5	10162.7434	0.0301
6	0	6	7	5	0	5	6	10509.3981	-0.0048
6	0	6	6	5	0	5	5	10509.4059	-0.0039
6	0	6	5	5	0	5	4	10509.4299	-0.0045
6	2	5	7	5	2	4	6	10629.2080	-0.0025
6	2	5	6	5	2	4	5	10629.3225	-0.0031
6	2	4	7	5	2	3	6	10767.1179	0.0003
6	2	4	6	5	2	3	5	10767.2363	0.0000
6	1	5	7	5	1	4	6	11067.4417	-0.0352
6	1	5	5	5	1	4	4	11067.4642	-0.0370
6	1	5	6	5	1	4	5	11067.4775	-0.0353
7	1	7	8	6	1	6	7	11843.1631	0.0341
7	1	7	6	6	1	6	5	11843.1805	0.0337
7	1	7	7	6	1	6	6	11843.1880	0.0355
7	0	7	8	6	0	6	7	12205.0912	-0.0048
7	0	7	6	6	0	6	5	12205.1156	-0.0031

7	2	6	8	6	2	5	7	12390.5822	-0.0043
7	2	6	6	6	2	5	5	12390.5907	-0.0019
7	2	6	7	6	2	5	6	12390.6569	-0.0036
7	2	5	8	6	2	4	7	12607.2586	-0.0012
7	2	5	6	6	2	4	5	12607.2673	0.0017
7	2	5	7	6	2	4	6	12607.3387	0.0009
7	1	6	8	6	1	5	7	12894.6452	-0.0429
7	1	6	6	6	1	5	5	12894.6638	-0.0433
7	1	6	7	6	1	5	6	12894.6699	-0.0418
8	1	8	9	7	1	7	8	13518.3117	0.0392
8	1	8	7	7	1	7	6	13518.3260	0.0393
8	0	8	9	7	0	7	8	13879.6143	-0.0070
8	0	8	7	7	0	7	6	13879.6292	-0.0092
8	2	7	9	7	2	6	8	14147.2896	-0.0067
8	2	7	7	7	2	6	6	14147.2994	-0.0043
8	2	7	8	7	2	6	7	14147.3416	-0.0051
9	1	9	10	8	1	8	9	15187.9446	0.0396
9	1	9	9	8	1	8	8	15187.9581	0.0412
9	0	9	10	8	0	8	9	15534.1477	-0.0096
9	0	9	8	8	0	8	7	15534.1637	-0.0070
10	1	10	11	9	1	9	10	16852.0341	0.0417
10	1	10	9	9	1	9	8	16852.0466	0.0447
10	0	10	11	9	0	9	10	17171.4779	-0.0105
10	0	10	9	9	0	9	8	17171.4921	-0.0071

Table S13. Assigned transitions for PhNCO ($^{13}\text{C6}$).

J'	K _a '	K _c '	F'	J''	K _a ''	K _c ''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
3	1	2	4	2	1	1	3	5591.4094	-0.0015
3	1	2	3	2	1	1	2	5591.6559	-0.0004
4	1	4	5	3	1	3	4	6831.4692	0.0004
4	1	4	3	3	1	3	2	6831.5012	-0.0011
4	1	4	4	3	1	3	3	6831.5764	-0.0003
4	0	4	5	3	0	3	4	7106.9695	0.0003
4	0	4	4	3	0	3	3	7106.9872	0.0001
4	0	4	3	3	0	3	2	7107.0489	-0.0002
4	1	3	5	3	1	2	4	7450.1257	0.0004
4	1	3	4	3	1	2	3	7450.2336	-0.0005
5	1	5	6	4	1	4	5	8531.8569	0.0000
5	1	5	4	4	1	4	3	8531.8864	0.0003
5	1	5	5	4	1	4	4	8531.9151	-0.0004
5	0	5	6	4	0	4	5	8852.5123	-0.0004
5	0	5	5	4	0	4	4	8852.5244	0.0008
5	0	5	4	4	0	4	3	8852.5596	-0.0005
5	1	4	6	4	1	3	5	9304.1871	0.0002
5	1	4	4	4	1	3	3	9304.2190	0.0004
5	1	4	5	4	1	3	4	9304.2463	0.0003
6	1	6	7	5	1	5	6	10227.6217	0.0003
6	1	6	5	5	1	5	4	10227.6437	-0.0004
6	1	6	6	5	1	5	5	10227.6570	0.0000
6	0	6	7	5	0	5	6	10578.4795	-0.0009
6	0	6	6	5	0	5	5	10578.4873	0.0004
6	0	6	5	5	0	5	4	10578.5120	-0.0001
6	2	5	7	5	2	4	6	10704.8288	0.0004
6	2	5	6	5	2	4	5	10704.9441	0.0004
6	2	4	7	5	2	3	6	10850.2905	0.0003
6	2	4	6	5	2	3	5	10850.4092	-0.0004
6	1	5	7	5	1	4	6	11152.1673	0.0005
6	1	5	5	5	1	4	4	11152.1903	-0.0010
6	1	5	6	5	1	4	5	11152.2031	0.0004
7	1	7	8	6	1	6	7	11918.2102	-0.0007
7	1	7	6	6	1	6	5	11918.2278	-0.0009
7	1	7	7	6	1	6	6	11918.2357	0.0012
7	0	7	8	6	0	6	7	12282.8842	0.0007
7	0	7	6	6	0	6	5	12282.9072	0.0009
7	2	6	8	6	2	5	7	12478.2350	-0.0010
7	2	6	6	6	2	5	5	12478.2436	0.0015
7	2	6	7	6	2	5	6	12478.3092	-0.0008
7	2	5	8	6	2	4	7	12706.5150	-0.0005
7	2	5	7	6	2	4	6	12706.5960	0.0017
7	1	6	8	6	1	5	7	12992.4411	0.0005

7	1	6	6	6	1	5	5	12992.4581	-0.0015
7	1	6	7	6	1	5	6	12992.4646	0.0005
8	1	8	9	7	1	7	8	13603.2508	0.0008
8	1	8	7	7	1	7	6	13603.2651	0.0010
8	0	8	9	7	0	7	8	13965.3442	0.0005
8	0	8	7	7	0	7	6	13965.3590	-0.0018
8	2	7	9	7	2	6	8	14246.7165	-0.0016
8	2	7	7	7	2	6	6	14246.7269	0.0011
8	2	7	8	7	2	6	7	14246.7693	0.0006
9	1	9	10	8	1	8	9	15282.5449	-0.0013
9	1	9	9	8	1	8	8	15282.5584	0.0004
9	0	9	10	8	0	8	9	15627.3298	-0.0011
9	0	9	8	8	0	8	7	15627.3458	0.0013
9	2	8	10	8	2	7	9	16009.6201	-0.0009
9	2	8	8	8	2	7	7	16009.6295	0.0010
9	2	8	9	8	2	7	8	16009.6557	-0.0011
10	1	10	11	9	1	9	10	16956.0865	-0.0015
10	1	10	9	9	1	9	8	16956.0984	0.0010
10	0	10	11	9	0	9	10	17271.9868	-0.0015
10	0	10	9	9	0	9	8	17272.0014	0.0023

Table S14. Assigned transitions for PhNCO ($^{13}\text{C7}$).

J'	K _a '	K _c '	F'	J''	K _a ''	K _c ''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
3	1	2	4	2	1	1	3	5543.5192	-0.0175
3	1	2	3	2	1	1	2	5543.7644	-0.0166
4	1	4	5	3	1	3	4	6787.3604	0.0222
4	1	4	3	3	1	3	2	6787.3933	0.0213
4	1	4	4	3	1	3	3	6787.4677	0.0217
4	0	4	5	3	0	3	4	7055.9560	-0.0007
4	0	4	4	3	0	3	3	7055.9738	-0.0013
4	0	4	3	3	0	3	2	7056.0350	-0.0012
4	1	3	5	3	1	2	4	7386.6991	-0.0232
4	1	3	3	3	1	2	2	7386.7379	-0.0216
4	1	3	4	3	1	2	3	7386.8077	-0.0231
5	0	5	6	4	0	4	5	8791.2360	-0.0018
5	0	5	5	4	0	4	4	8791.2484	-0.0009
5	0	5	4	4	0	4	3	8791.2827	-0.0023
5	1	4	6	4	1	3	5	9225.6240	-0.0285
5	1	4	4	4	1	3	3	9225.6538	-0.0300
5	1	4	5	4	1	3	4	9225.6830	-0.0284
6	1	6	7	5	1	5	6	10162.9859	0.0320
6	1	6	5	5	1	5	4	10163.0071	0.0303
6	1	6	6	5	1	5	5	10163.0211	0.0314
6	0	6	7	5	0	5	6	10508.3908	-0.0034
6	0	6	6	5	0	5	5	10508.3985	-0.0029
6	0	6	5	5	0	5	4	10508.4224	-0.0033
6	2	5	7	5	2	4	6	10624.6989	-0.0011
6	2	5	6	5	2	4	5	10624.8121	-0.0029
6	2	4	7	5	2	3	6	10758.5585	0.0004
6	2	4	6	5	2	3	5	10758.6770	0.0005
6	1	5	7	5	1	4	6	11058.9994	-0.0349
6	1	5	5	5	1	4	4	11059.0224	-0.0362
6	1	5	6	5	1	4	5	11059.0356	-0.0349
7	1	7	8	6	1	6	7	11843.8509	0.0350
7	1	7	6	6	1	6	5	11843.8686	0.0349
7	1	7	7	6	1	6	6	11843.8761	0.0366
7	0	7	8	6	0	6	7	12205.4108	-0.0043
7	0	7	6	6	0	6	5	12205.4356	-0.0021
7	2	6	8	6	2	5	7	12385.6260	-0.0034
7	2	6	6	6	2	5	5	12385.6341	-0.0013
7	2	6	7	6	2	5	6	12385.6998	-0.0035
7	2	5	8	6	2	4	7	12596.0858	-0.0015
7	2	5	6	6	2	4	5	12596.0941	0.0009
7	2	5	7	6	2	4	6	12596.1660	0.0010
7	1	6	8	6	1	5	7	12885.3630	-0.0409
7	1	6	6	6	1	5	5	12885.3794	-0.0433

7	1	6	7	6	1	5	6	12885.3861	-0.0415
8	1	8	9	7	1	7	8	13519.5382	0.0405
8	1	8	7	7	1	7	6	13519.5529	0.0411
8	0	8	9	7	0	7	8	13881.6689	-0.0044
8	0	8	7	7	0	7	6	13881.6833	-0.0070
8	2	7	9	7	2	6	8	14142.0253	-0.0055
8	2	7	7	7	2	6	6	14142.0351	-0.0033
8	2	7	8	7	2	6	7	14142.0774	-0.0040
9	1	9	10	8	1	8	9	15189.8314	0.0420
9	1	9	9	8	1	8	8	15189.8449	0.0435
9	0	9	10	8	0	8	9	15538.1751	-0.0062
9	0	9	8	8	0	8	7	15538.1907	-0.0039
9	2	8	10	8	2	7	9	15893.2925	-0.0068
9	2	8	8	8	2	7	7	15893.3017	-0.0050
9	2	8	9	8	2	7	8	15893.3281	-0.0071
10	1	10	11	9	1	9	10	16854.6883	0.0444
10	1	10	9	9	1	9	8	16854.7002	0.0469
10	0	10	11	9	0	9	10	17177.5123	-0.0064
10	0	10	9	9	0	9	8	17177.5260	-0.0034

Table S15. Assigned transitions for PhNCO (^{14}N).

J'	K_a'	K_c'	F'	J''	K_a''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
3	1	3	2	1	2	5126.0267	0.0171
3	0	3	2	0	2	5341.1969	-0.0005
3	1	2	2	1	1	5583.8429	-0.0173
4	1	4	3	1	3	6830.0974	0.0222
4	0	4	3	0	3	7102.7163	-0.0009
4	2	3	3	2	2	7140.1392	-0.0002
4	2	2	3	2	1	7180.7233	0.0011
4	1	3	3	1	2	7440.1985	-0.0231
5	1	5	4	1	4	8530.4213	0.0274
5	0	5	4	0	4	8848.4630	-0.0022
5	1	4	4	1	3	9292.1246	-0.0294
6	1	6	5	1	5	10226.3030	0.0312
6	0	6	5	0	5	10575.3728	-0.0050
6	2	5	5	2	4	10696.6025	-0.0008
6	3	3	5	3	2	10739.3008	0.0018
6	2	4	5	2	3	10836.1107	0.0003
6	1	5	5	1	4	11138.2527	-0.0364
7	1	7	6	1	6	11917.1995	0.0345
7	0	7	6	0	6	12281.4362	-0.0059
7	2	6	6	2	5	12469.0701	-0.0041
7	3	5	6	3	4	12530.4653	-0.0005
7	3	4	6	3	3	12538.9871	0.0000
7	2	5	6	2	4	12688.2330	0.0001
7	1	6	6	1	5	12977.0389	-0.0437
8	1	8	7	1	7	13602.7336	0.0378
8	0	8	7	0	7	13966.1269	-0.0081
8	2	7	7	2	6	14236.8243	-0.0048
8	1	7	7	1	6	14806.7330	-0.0520
9	1	9	8	1	8	15282.7017	0.0415
9	0	9	8	0	8	15630.6632	-0.0096

Table S16. Assigned transitions for PhNCO (^{18}O).

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
4	1	4	5	3	1	3	4	6580.7967	0.0251
4	1	4	3	3	1	3	2	6580.8282	0.0233
4	1	4	4	3	1	3	3	6580.9038	0.0254
4	0	4	5	3	0	3	4	6835.1533	0.0007
4	0	4	4	3	0	3	3	6835.1714	0.0004
4	0	4	3	3	0	3	2	6835.2325	0.0009
4	1	3	5	3	1	2	4	7144.2631	-0.0240
4	1	3	3	3	1	2	2	7144.3020	-0.0223
4	1	3	4	3	1	2	3	7144.3717	-0.0233
5	1	5	6	4	1	4	5	8219.9092	0.0313
5	1	5	4	4	1	4	3	8219.9380	0.0313
5	1	5	5	4	1	4	4	8219.9673	0.0314
5	0	5	6	4	0	4	5	8518.6005	0.0017
5	0	5	5	4	0	4	4	8518.6124	0.0022
5	0	5	4	4	0	4	3	8518.6478	0.0023
6	1	6	7	5	1	5	6	9855.2211	0.0397
6	1	6	5	5	1	5	4	9855.2393	0.0353
6	1	6	6	5	1	5	5	9855.2559	0.0390
6	0	6	7	5	0	5	6	10185.9399	0.0027
6	0	6	6	5	0	5	5	10185.9481	0.0037
6	0	6	5	5	0	5	4	10185.9701	0.0015
6	2	5	7	5	2	4	6	10288.6467	0.0031
6	2	5	6	5	2	4	5	10288.7616	0.0038
6	2	4	7	5	2	3	6	10406.8138	0.0025
6	2	4	6	5	2	3	5	10406.9311	0.0024
6	1	5	7	5	1	4	6	10697.9478	-0.0329
6	1	5	5	5	1	4	4	10697.9708	-0.0341
6	1	5	6	5	1	4	5	10697.9836	-0.0329
7	1	7	8	6	1	6	7	11486.2416	0.0469
7	1	7	6	6	1	6	5	11486.2562	0.0438
7	1	7	7	6	1	6	6	11486.2645	0.0464
7	0	7	8	6	0	6	7	11835.2222	0.0062
7	0	7	7	6	0	6	6	11835.2262	0.0059
7	0	7	6	6	0	6	5	11835.2426	0.0042
8	1	8	9	7	1	7	8	13112.6146	0.0554
8	1	8	7	7	1	7	6	13112.6274	0.0541
8	0	8	9	7	0	7	8	13465.6097	0.0097
8	0	8	7	7	0	7	6	13465.6249	0.0079
8	2	7	9	7	2	6	8	13696.8408	0.0067
8	2	7	7	7	2	6	6	13696.8492	0.0076

8	2	7	8	7	2	6	7	13696.8911	0.0069
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Table S17. Assigned transitions for PhNCS (parent).

J'	K _a '	K _c '	F'	J''	K _a ''	K _c ''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
4	1	4	5	3	1	3	4	4661.1923	-0.0001
4	1	4	3	3	1	3	2	4661.2041	0.0003
4	1	4	4	3	1	3	3	4661.2642	-0.0002
4	0	4	5	3	0	3	4	4792.7090	-0.0001
4	0	4	4	3	0	3	3	4792.7191	0.0004
4	0	4	3	3	0	3	2	4792.7654	-0.0006
4	2	3	3	3	2	2	2	4799.6784	0.0000
4	2	3	5	3	2	2	4	4799.7459	-0.0001
4	2	3	4	3	2	2	3	4800.0097	0.0003
4	2	2	3	3	2	1	2	4807.3641	0.0000
4	2	2	5	3	2	1	4	4807.4325	0.0000
4	2	2	4	3	2	1	3	4807.7010	0.0000
4	1	3	5	3	1	2	4	4936.4966	0.0000
4	1	3	3	3	1	2	2	4936.5360	0.0000
4	1	3	4	3	1	2	3	4936.5759	-0.0001
5	1	5	6	4	1	4	5	5825.0927	-0.0002
5	1	5	4	4	1	4	3	5825.1067	0.0005
5	1	5	5	4	1	4	4	5825.1307	-0.0002
5	0	5	6	4	0	4	5	5985.1374	-0.0005
5	0	5	5	4	0	4	4	5985.1421	0.0005
5	0	5	4	4	0	4	3	5985.1717	-0.0001
5	2	4	4	4	2	3	3	5998.7454	-0.0003
5	2	4	6	4	2	3	5	5998.7597	0.0000
5	2	4	5	4	2	3	4	5998.8967	0.0000
5	2	3	4	4	2	2	3	6014.1006	-0.0003
5	2	3	6	4	2	2	5	6014.1156	0.0001
5	2	3	5	4	2	2	4	6014.2591	0.0000
5	1	4	6	4	1	3	5	6169.1517	0.0000
5	1	4	4	4	1	3	3	6169.1816	0.0000
5	1	4	5	4	1	3	4	6169.1950	0.0002
6	1	6	7	5	1	5	6	6988.0759	0.0000
6	1	6	5	5	1	5	4	6988.0872	0.0000
6	1	6	6	5	1	5	5	6988.0982	0.0000
6	0	6	7	5	0	5	6	7173.7660	0.0000
6	0	6	5	5	0	5	4	7173.7879	-0.0009

6	2	5	7	5	2	4	6	7197.1125	0.0000
6	2	5	6	5	2	4	5	7197.1931	0.0000
6	5	2	5	5	5	1	4	7202.3112	0.0005
6	5	2	7	5	5	1	6	7202.4243	-0.0013
6	5	2	6	5	5	1	5	7202.8989	-0.0001
6	4	3	5	5	4	2	4	7203.0829	0.0005
6	4	3	7	5	4	2	6	7203.1480	0.0000
6	4	2	6	5	4	1	5	7203.4547	-0.0004
6	3	4	5	5	3	3	4	7204.6116	0.0005
6	3	4	7	5	3	3	6	7204.6379	-0.0004
6	3	4	6	5	3	3	5	7204.8145	0.0000
6	3	3	5	5	3	2	4	7204.9123	0.0005
6	3	3	7	5	3	2	6	7204.9388	-0.0003
6	3	3	6	5	3	2	5	7205.1153	0.0000
6	2	4	7	5	2	3	6	7223.9300	-0.0001
6	2	4	6	5	2	3	5	7224.0187	0.0000
6	1	5	7	5	1	4	6	7400.7796	0.0006
6	1	5	5	5	1	4	4	7400.8006	-0.0007
6	1	5	6	5	1	4	5	7400.8050	0.0001
7	1	7	8	6	1	6	7	8149.9890	-0.0007
7	1	7	6	6	1	6	5	8149.9988	-0.0001
7	1	7	7	6	1	6	6	8150.0045	0.0008
7	0	7	7	6	0	6	6	8357.8968	-0.0004
7	0	7	8	6	0	6	7	8357.9013	0.0006
7	0	7	6	6	0	6	5	8357.9164	-0.0007
7	2	6	8	6	2	5	7	8394.6833	-0.0005
7	2	6	6	6	2	5	5	8394.6891	0.0008
7	2	6	7	6	2	5	6	8394.7358	0.0006
7	5	3	6	6	5	2	5	8403.3060	-0.0006
7	5	3	8	6	5	2	7	8403.3640	0.0008
7	5	3	7	6	5	2	6	8403.6638	-0.0005
7	3	5	6	6	3	4	5	8406.7061	-0.0010
7	3	5	8	6	3	4	7	8406.7181	0.0006
7	3	5	7	6	3	4	6	8406.8303	0.0000
7	3	4	6	6	3	3	5	8407.3822	-0.0012
7	3	4	8	6	3	3	7	8407.3942	0.0005
7	3	4	7	6	3	3	6	8407.5068	0.0000
7	2	5	8	6	2	4	7	8437.4469	-0.0002
7	2	5	6	6	2	4	5	8437.4511	0.0002
7	2	5	7	6	2	4	6	8437.5078	0.0001

7	1	6	8	6	1	5	7	8631.1472	0.0005
7	1	6	7	6	1	5	6	8631.1632	0.0001
4	1	4	5	3	0	3	4	9076.7662	-0.0003
8	1	8	9	7	1	7	8	9310.6962	-0.0006
8	1	8	8	7	1	7	7	9310.7057	0.0000
8	0	8	8	7	0	7	7	9536.9096	-0.0008
8	0	8	9	7	0	7	8	9536.9167	0.0004
8	0	8	7	7	0	7	6	9536.9307	0.0018
8	2	7	9	7	2	6	8	9591.3473	-0.0012
8	2	7	7	7	2	6	6	9591.3547	0.0007
8	2	7	8	7	2	6	7	9591.3840	0.0009
8	4	5	7	7	4	4	6	9606.1258	0.0008
8	4	5	9	7	4	4	8	9606.1377	-0.0020
8	4	4	9	7	4	3	8	9606.1490	-0.0011
8	3	6	7	7	3	5	6	9609.3049	-0.0002
8	3	6	9	7	3	5	8	9609.3082	0.0000
8	3	6	8	7	3	5	7	9609.3861	0.0005
8	3	5	9	7	3	4	8	9610.6583	-0.0016
8	3	5	8	7	3	4	7	9610.7378	0.0002
8	2	6	9	7	2	5	8	9655.1636	-0.0005
8	2	6	7	7	2	5	6	9655.1701	0.0012
8	2	6	8	7	2	5	7	9655.2088	-0.0002
8	1	7	9	7	1	6	8	9860.0047	0.0000
8	1	7	8	7	1	6	7	9860.0151	-0.0002
8	1	7	7	7	1	6	6	9860.0184	0.0002
9	1	9	10	8	1	8	9	10470.0752	-0.0008
9	1	9	9	8	1	8	8	10470.0825	0.0009
9	0	9	9	8	0	8	8	10710.2802	-0.0003
9	0	9	10	8	0	8	9	10710.2892	0.0008
9	0	9	8	8	0	8	7	10710.2975	-0.0008
9	2	8	10	8	2	7	9	10786.9802	-0.0004
9	2	8	8	8	2	7	7	10786.9872	0.0012
9	2	8	9	8	2	7	8	10787.0040	-0.0006
9	3	7	10	8	3	6	9	10812.4377	0.0000
9	3	7	9	8	3	6	8	10812.4928	-0.0003
9	3	6	10	8	3	5	9	10814.9127	0.0000
9	3	6	9	8	3	5	8	10814.9677	-0.0010
9	2	7	10	8	2	6	9	10877.4737	-0.0007
9	2	7	8	8	2	6	7	10877.4799	0.0007
9	2	7	9	8	2	6	8	10877.5109	0.0008

9	1	8	10	8	1	7	9	11087.0812	-0.0019
9	1	8	9	8	1	7	8	11087.0900	0.0000
9	1	8	8	8	1	7	7	11087.0953	0.0012
6	1	6	6	5	0	5	5	11111.8894	-0.0007
6	1	6	7	5	0	5	6	11112.0876	-0.0007
6	1	6	5	5	0	5	4	11112.1457	0.0010
10	1	10	11	9	1	9	10	11628.0241	-0.0003
10	1	10	9	9	1	9	8	11628.0295	0.0000
10	0	10	10	9	0	9	9	11877.6217	0.0000
10	0	10	11	9	0	9	10	11877.6306	-0.0004
10	0	10	9	9	0	9	8	11877.6397	0.0006
10	2	9	11	9	2	8	10	11981.4535	-0.0006
10	2	9	9	9	2	8	8	11981.4604	0.0013
10	3	8	11	9	3	7	10	12016.1121	0.0002
10	3	8	10	9	3	7	9	12016.1539	0.0008
10	3	7	11	9	3	6	10	12020.3479	0.0000
10	3	7	10	9	3	6	9	12020.3911	0.0010
7	1	7	7	6	0	6	6	12088.1286	0.0003
7	1	7	8	6	0	6	7	12088.3104	-0.0017
7	1	7	6	6	0	6	5	12088.3563	0.0015
10	2	8	11	9	2	7	10	12104.6301	-0.0006
10	2	8	9	9	2	7	8	12104.6361	0.0010
10	2	8	10	9	2	7	9	12104.6606	0.0003
10	1	9	11	9	1	8	10	12312.0878	-0.0015
10	1	9	10	9	1	8	9	12312.0924	-0.0010
10	1	9	9	9	1	8	8	12312.0999	0.0015
11	0	11	11	10	0	10	10	13038.7231	-0.0005
11	0	11	12	10	0	10	11	13038.7331	-0.0011
11	0	11	10	10	0	10	9	13038.7424	0.0014
8	1	8	8	7	0	7	7	13040.9374	0.0007
8	1	8	9	7	0	7	8	13041.1085	0.0001
8	1	8	7	7	0	7	6	13041.1419	0.0000
11	2	10	12	10	2	9	11	13174.6438	-0.0010
11	2	10	10	10	2	9	9	13174.6495	0.0002
11	2	10	11	10	2	9	10	13174.6593	0.0019
6	2	4	6	6	1	5	6	13192.5678	-0.0001
6	2	4	7	6	1	5	7	13192.8539	-0.0002
11	3	9	12	10	3	8	11	13220.3171	0.0009
11	3	9	11	10	3	8	10	13220.3474	-0.0004
11	3	8	12	10	3	7	11	13227.1859	0.0008

11	3	8	11	10	3	7	10	13227.2183	0.0003
11	2	9	12	10	2	8	11	13336.7075	0.0002
11	2	9	10	10	2	8	9	13336.7112	0.0000
11	2	9	11	10	2	8	10	13336.7318	-0.0010
5	2	3	5	5	1	4	5	13369.3548	0.0006
5	2	3	6	5	1	4	6	13369.7034	0.0004
4	2	2	5	4	1	3	5	13524.7390	-0.0001
11	1	10	12	10	1	9	11	13534.7059	-0.0003
11	1	10	10	10	1	9	9	13534.7154	0.0017
12	1	12	13	11	1	11	12	13939.3193	0.0004
9	1	9	9	8	0	8	8	13974.1077	-0.0002
9	1	9	10	8	0	8	9	13974.2682	0.0001
9	1	9	8	8	0	8	7	13974.2928	-0.0022
3	2	2	4	3	1	3	4	14062.8919	0.0000
4	2	3	4	4	1	4	4	14201.3143	-0.0012
4	2	3	5	4	1	4	5	14201.4450	-0.0006
5	2	4	5	5	1	5	5	14375.0821	0.0008
5	2	4	6	5	1	5	6	14375.1128	0.0003
12	3	10	13	11	3	9	12	14425.0143	-0.0008
12	3	10	11	11	3	9	10	14425.0176	0.0002
12	3	10	12	11	3	9	11	14425.0405	0.0003
12	3	9	13	11	3	8	12	14435.6704	0.0009
12	3	9	12	11	3	8	11	14435.6961	0.0000
12	2	10	13	11	2	9	12	14573.5716	0.0007
12	2	10	11	11	2	9	10	14573.5754	0.0010
12	2	10	12	11	2	9	11	14573.5918	-0.0017
12	1	11	13	11	1	10	12	14754.5892	-0.0004
12	1	11	11	11	1	10	10	14754.5961	0.0000
13	1	13	14	12	1	12	13	15092.5609	-0.0015
13	1	13	12	12	1	12	11	15092.5648	-0.0007
13	0	13	12	12	0	12	11	15342.4240	0.0010
13	2	12	14	12	2	11	13	15556.6893	-0.0007
13	2	12	12	12	2	11	11	15556.6935	-0.0001
13	2	12	13	12	2	11	12	15556.6965	0.0000
13	3	11	14	12	3	10	13	15630.1522	0.0007
13	3	10	14	12	3	9	13	15646.0751	0.0008
13	3	10	13	12	3	9	12	15646.0937	-0.0026
13	2	11	14	12	2	10	13	15814.8659	0.0000
13	2	11	13	12	2	10	12	15814.8874	0.0010
13	1	12	14	12	1	11	13	15971.3671	-0.0012

13	1	12	12	12	1	11	11	15971.3740	0.0002
2	2	1	3	1	1	0	2	16221.7267	-0.0006
14	1	14	15	13	1	13	14	16244.1708	0.0005
14	0	14	14	13	0	13	13	16485.6228	-0.0007
14	0	14	15	13	0	13	14	16485.6377	0.0018
14	0	14	13	13	0	13	12	16485.6408	0.0007
14	3	12	15	13	3	11	14	16835.6475	0.0006
14	3	11	15	13	3	10	14	16858.6997	0.0003
14	2	12	15	13	2	11	14	17060.0205	0.0006
14	1	13	15	13	1	12	14	17184.6400	-0.0029
14	1	13	13	13	1	12	12	17184.6476	-0.0001
3	2	2	4	2	1	1	3	17352.9851	0.0003
15	1	15	16	14	1	14	15	17394.1447	0.0012
15	0	15	15	14	0	14	14	17623.8361	-0.0036
15	0	15	14	14	0	14	13	17623.8555	-0.0001
15	2	14	16	14	2	13	15	17932.1759	0.0018
15	3	12	16	14	3	11	15	18073.8700	0.0001
15	2	13	16	14	2	12	15	18308.2725	0.0004
15	1	14	16	14	1	13	15	18393.9886	-0.0002

Table S18. Assigned transitions for PhNCS ($^{13}\text{C}1$).

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}$
5	1	5	6	4	1	4	5	5823.1223	-0.0008
5	1	5	4	4	1	4	3	5823.1373	0.0003
5	1	5	5	4	1	4	4	5823.1606	-0.0009
5	0	5	6	4	0	4	5	5983.1718	0.0000
5	0	5	5	4	0	4	4	5983.1757	-0.0002
5	0	5	4	4	0	4	3	5983.2059	0.0001
5	1	4	6	4	1	3	5	6167.2139	0.0003
5	1	4	4	4	1	3	3	6167.2432	0.0002
5	1	4	5	4	1	3	4	6167.2581	0.0014
6	1	6	7	5	1	5	6	6985.7091	-0.0013
6	1	6	5	5	1	5	4	6985.7206	-0.0015
6	1	6	6	5	1	5	5	6985.7319	-0.0012
6	0	6	7	5	0	5	6	7171.3986	-0.0001
6	0	6	5	5	0	5	4	7171.4205	-0.0010
6	2	5	7	5	2	4	6	7194.7685	0.0000
6	2	5	6	5	2	4	5	7194.8489	-0.0005
6	2	4	7	5	2	3	6	7221.6128	-0.0002
6	2	4	6	5	2	3	5	7221.7019	0.0006
6	1	5	7	5	1	4	6	7398.4537	0.0026
6	1	5	5	5	1	4	4	7398.4732	0.0001
6	1	5	6	5	1	4	5	7398.4781	0.0010
7	1	7	8	6	1	6	7	8147.2267	-0.0011
7	1	7	6	6	1	6	5	8147.2334	-0.0039
7	1	7	7	6	1	6	6	8147.2414	-0.0006
7	0	7	7	6	0	6	6	8355.1238	-0.0013
7	0	7	8	6	0	6	7	8355.1281	0.0001
7	0	7	6	6	0	6	5	8355.1445	0.0000
7	2	6	8	6	2	5	7	8391.9468	-0.0006
7	2	6	6	6	2	5	5	8391.9524	0.0004
7	2	6	7	6	2	5	6	8391.9989	-0.0001

Table S19. Assigned transitions for PhNCS ($^{13}\text{C}2$).

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
5	1	5	6	4	1	4	5	5814.4876	0.0016
5	1	5	5	4	1	4	4	5814.5259	0.0020
5	0	5	6	4	0	4	5	5975.6500	0.0000
5	0	5	5	4	0	4	4	5975.6536	0.0002
5	0	5	4	4	0	4	3	5975.6843	0.0005
5	1	4	6	4	1	3	5	6161.5139	-0.0017
5	1	4	5	4	1	3	4	6161.5573	-0.0014
6	1	6	7	5	1	5	6	6975.2890	0.0026
6	1	6	5	5	1	5	4	6975.3006	0.0030
6	1	6	6	5	1	5	5	6975.3118	0.0031
6	0	6	7	5	0	5	6	7162.1263	0.0005
6	0	6	5	5	0	5	4	7162.1478	-0.0007
6	2	5	7	5	2	4	6	7186.1828	-0.0010
6	2	5	6	5	2	4	5	7186.2631	-0.0013
6	2	4	7	5	2	3	6	7213.8184	-0.0008
6	2	4	6	5	2	3	5	7213.9072	-0.0007
6	1	5	7	5	1	4	6	7391.5451	-0.0007
6	1	5	5	5	1	4	4	7391.5657	-0.0025
6	1	5	6	5	1	4	5	7391.5703	-0.0014
7	1	7	8	6	1	6	7	8134.9910	0.0040
7	1	7	7	6	1	6	6	8135.0059	0.0051
7	0	7	7	6	0	6	6	8343.9720	-0.0002
7	0	7	8	6	0	6	7	8343.9780	0.0020
7	0	7	6	6	0	6	5	8343.9936	0.0011
7	2	6	8	6	2	5	7	8381.8721	-0.0013
7	2	6	6	6	2	5	5	8381.8788	0.0009
7	2	6	7	6	2	5	6	8381.9256	0.0008

Table S20. Assigned transitions for PhNCS ($^{13}\text{C}3$).

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
5	1	5	6	4	1	4	5	5782.4710	-0.0010
5	1	5	4	4	1	4	3	5782.4868	0.0010
5	1	5	5	4	1	4	4	5782.5094	-0.0007
5	0	5	6	4	0	4	5	5943.1446	0.0000
5	0	5	5	4	0	4	4	5943.1484	0.0000
5	0	5	4	4	0	4	3	5943.1775	-0.0008
5	1	4	6	4	1	3	5	6128.6073	0.0004
5	1	4	4	4	1	3	3	6128.6364	0.0003
5	1	4	5	4	1	3	4	6128.6510	0.0013
6	1	6	7	5	1	5	6	6936.8626	-0.0010
6	1	6	5	5	1	5	4	6936.8742	-0.0010
6	1	6	6	5	1	5	5	6936.8850	-0.0010
6	0	6	7	5	0	5	6	7123.0904	0.0001
6	0	6	5	5	0	5	4	7123.1114	-0.0015
6	2	5	7	5	2	4	6	7147.2337	0.0005
6	2	5	6	5	2	4	5	7147.3137	0.0000
6	2	4	7	5	2	3	6	7174.9657	-0.0004
6	2	4	6	5	2	3	5	7175.0549	0.0007
6	1	5	7	5	1	4	6	7352.0482	0.0010
6	1	5	5	5	1	4	4	7352.0696	0.0003
6	1	5	6	5	1	4	5	7352.0738	0.0008
7	1	7	8	6	1	6	7	8090.1525	0.0000
7	1	7	6	6	1	6	5	8090.1576	-0.0042
7	1	7	7	6	1	6	6	8090.1659	-0.0005
7	0	7	7	6	0	6	6	8298.3917	-0.0010
7	0	7	8	6	0	6	7	8298.3964	0.0005
7	0	7	6	6	0	6	5	8298.4125	0.0001
7	2	6	8	6	2	5	7	8336.4242	-0.0007
7	2	6	6	6	2	5	5	8336.4300	0.0006
7	2	6	7	6	2	5	6	8336.4758	-0.0004

Table S21. Assigned transitions for PhNCS ($^{13}\text{C4}$).

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
5	1	5	6	4	1	4	5	5756.0871	-0.0019
5	1	5	4	4	1	4	3	5756.1020	-0.0011
5	1	5	5	4	1	4	4	5756.1254	-0.0023
5	0	5	6	4	0	4	5	5912.7879	0.0004
5	0	5	5	4	0	4	4	5912.7917	-0.0002
5	0	5	4	4	0	4	3	5912.8212	-0.0002
5	1	4	6	4	1	3	5	6092.3982	0.0017
5	1	4	4	4	1	3	3	6092.4271	0.0014
5	1	4	5	4	1	3	4	6092.4425	0.0027
6	1	6	7	5	1	5	6	6905.3578	-0.0027
6	1	6	5	5	1	5	4	6905.3681	-0.0043
6	1	6	6	5	1	5	5	6905.3805	-0.0027
6	0	6	7	5	0	5	6	7087.3149	0.0001
6	0	6	5	5	0	5	4	7087.3360	-0.0015
6	2	5	7	5	2	4	6	7109.6339	0.0016
6	2	5	6	5	2	4	5	7109.7140	0.0005
6	2	4	7	5	2	3	6	7135.2681	-0.0001
6	2	4	6	5	2	3	5	7135.3568	0.0004
6	1	5	7	5	1	4	6	7308.7749	0.0023
6	1	5	5	5	1	4	4	7308.7959	0.0014
6	1	5	6	5	1	4	5	7308.8005	0.0018
7	1	7	8	6	1	6	7	8053.6037	-0.0046
7	1	7	6	6	1	6	5	8053.6108	-0.0071
7	1	7	7	6	1	6	6	8053.6193	-0.0034
7	0	7	7	6	0	6	6	8257.5381	-0.0016
7	0	7	8	6	0	6	7	8257.5422	0.0001
7	0	7	6	6	0	6	5	8257.5563	-0.0022
7	2	6	8	6	2	5	7	8292.7100	-0.0007
7	2	6	6	6	2	5	5	8292.7161	0.0009
7	2	6	7	6	2	5	6	8292.7637	0.0011

Table S22. Assigned transitions for PhNCS ($^{13}\text{C5}$).

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
5	1	5	6	4	1	4	5	5767.7870	0.0013
5	1	5	4	4	1	4	3	5767.8011	0.0015
5	1	5	5	4	1	4	4	5767.8252	0.0013
5	0	5	6	4	0	4	5	5926.1068	-0.0003
5	0	5	5	4	0	4	4	5926.1115	0.0002
5	0	5	4	4	0	4	3	5926.1411	0.0003
5	1	4	6	4	1	3	5	6108.0771	-0.0021
5	1	4	4	4	1	3	3	6108.1061	-0.0021
5	1	4	5	4	1	3	4	6108.1215	-0.0005
6	1	6	7	5	1	5	6	6919.3361	0.0025
6	1	6	5	5	1	5	4	6919.3479	0.0027
6	1	6	6	5	1	5	5	6919.3588	0.0028
6	0	6	7	5	0	5	6	7103.0406	0.0008
6	0	6	5	5	0	5	4	7103.0617	-0.0007
6	2	5	7	5	2	4	6	7126.0747	-0.0017
6	2	5	6	5	2	4	5	7126.1555	-0.0012
6	2	4	7	5	2	3	6	7152.5380	-0.0002
6	2	4	6	5	2	3	5	7152.6257	0.0000
6	1	5	7	5	1	4	6	7327.5203	-0.0004
6	1	5	5	5	1	4	4	7327.5416	-0.0008
6	1	5	6	5	1	4	5	7327.5453	-0.0012
7	1	7	8	6	1	6	7	8069.8299	0.0040
7	1	7	6	6	1	6	5	8069.8373	0.0019
7	1	7	7	6	1	6	6	8069.8455	0.0055
7	0	7	7	6	0	6	6	8275.5357	0.0006
7	0	7	6	6	0	6	5	8275.5558	0.0017
7	2	6	8	6	2	5	7	8311.8321	-0.0013
7	2	6	6	6	2	5	5	8311.8388	0.0009
7	2	6	7	6	2	5	6	8311.8833	-0.0012

Table S23. Assigned transitions for PhNCS ($^{13}\text{C6}$).

J'	K _a '	K _c '	F'	J''	K _a ''	K _c ''	F''	v _{obs} /MHz	v _{obs} - calc
5	1	5	6	4	1	4	5	5802.6100	0.0004
5	1	5	5	4	1	4	4	5802.6484	0.0007
5	0	5	6	4	0	4	5	5963.8879	0.0000
5	0	5	5	4	0	4	4	5963.8916	-0.0001
5	0	5	4	4	0	4	3	5963.9226	0.0007
5	1	4	6	4	1	3	5	6150.0642	-0.0010
5	1	4	4	4	1	3	3	6150.0931	-0.0017
5	1	4	5	4	1	3	4	6150.1084	0.0001
6	1	6	7	5	1	5	6	6961.0202	0.0011
6	1	6	5	5	1	5	4	6961.0316	0.0010
6	1	6	6	5	1	5	5	6961.0425	0.0010
6	0	6	7	5	0	5	6	7147.9440	0.0003
6	0	6	5	5	0	5	4	7147.9653	-0.0011
6	2	5	7	5	2	4	6	7172.1923	-0.0007
6	2	5	6	5	2	4	5	7172.2727	-0.0009
6	2	4	7	5	2	3	6	7200.0487	0.0004
6	2	4	6	5	2	3	5	7200.1365	0.0000
6	1	5	7	5	1	4	6	7377.7878	0.0008
6	1	5	5	5	1	4	4	7377.8081	-0.0009
6	1	5	6	5	1	4	5	7377.8128	0.0000
7	1	7	8	6	1	6	7	8118.3227	0.0019
7	1	7	6	6	1	6	5	8118.3301	0.0000
7	1	7	7	6	1	6	6	8118.3378	0.0030
7	0	7	7	6	0	6	6	8327.3351	-0.0005
7	0	7	8	6	0	6	7	8327.3397	0.0007
7	0	7	6	6	0	6	5	8327.3572	0.0018
7	2	6	8	6	2	5	7	8365.5334	-0.0020
7	2	6	6	6	2	5	5	8365.5407	0.0008
7	2	6	7	6	2	5	6	8365.5864	-0.0004

Table S24. Assigned transitions for PhNCS ($^{13}\text{C}7$).

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
5	1	5	6	4	1	4	5	5799.7380	-0.0008
5	1	5	4	4	1	4	3	5799.7544	0.0013
5	1	5	5	4	1	4	4	5799.7764	-0.0010
5	0	5	6	4	0	4	5	5958.5494	-0.0002
5	0	5	5	4	0	4	4	5958.5537	-0.0002
5	0	5	4	4	0	4	3	5958.5841	0.0006
5	1	4	6	4	1	3	5	6140.9353	0.0001
5	1	4	4	4	1	3	3	6140.9644	0.0002
5	1	4	5	4	1	3	4	6140.9794	0.0012
6	1	6	7	5	1	5	6	6957.6834	-0.0007
6	1	6	5	5	1	5	4	6957.6948	-0.0012
6	1	6	6	5	1	5	5	6957.7051	-0.0018
6	0	6	7	5	0	5	6	7141.9978	0.0003
6	0	6	5	5	0	5	4	7142.0185	-0.0017
6	2	5	7	5	2	4	6	7164.9613	0.0005
6	2	5	6	5	2	4	5	7165.0415	-0.0001
6	2	4	7	5	2	3	6	7191.3380	-0.0002
6	2	4	6	5	2	3	5	7191.4267	0.0006
6	1	5	7	5	1	4	6	7366.9574	0.0013
6	1	5	5	5	1	4	4	7366.9775	-0.0003
6	1	5	6	5	1	4	5	7366.9828	0.0007
7	1	7	8	6	1	6	7	8114.5767	-0.0005
7	1	7	6	6	1	6	5	8114.5837	-0.0031
7	1	7	7	6	1	6	6	8114.5915	0.0000
7	0	7	7	6	0	6	6	8321.0202	-0.0012
7	0	7	8	6	0	6	7	8321.0248	0.0008
7	0	7	6	6	0	6	5	8321.0406	0.0001

Table S25. Assigned transitions for PhNCS (^{14}N).

J'	K _a '	K _c '	F'	J''	K _a ''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
5	1	5	4	1	4	5818.8966	0.0002
5	0	5	4	0	4	5979.2250	-0.0006
5	1	4	4	1	3	6163.7694	-0.0005
6	1	6	5	1	5	6980.6130	0.0000
6	0	6	5	0	5	7166.5871	-0.0006
6	2	5	5	2	4	7190.1772	0.0010
6	2	4	5	2	3	7217.2512	0.0011
6	1	5	5	1	4	7394.2877	-0.0011
7	1	7	6	1	6	8141.2539	0.0005
7	0	7	6	0	6	8349.4166	0.0000
7	2	6	6	2	5	8386.5616	0.0012
7	1	6	6	1	5	8623.5375	-0.0005
8	1	8	7	1	7	9300.6770	-0.0006
8	0	8	7	0	7	9527.0834	0.0014
8	1	7	7	1	6	9851.2631	-0.0007
9	1	9	8	1	8	10458.7649	0.0013
9	0	9	8	0	8	10699.0580	0.0002
9	1	8	8	1	7	11077.1907	-0.0014
10	1	10	9	1	9	11615.4093	0.0015
10	0	10	9	0	9	11864.9602	0.0010

Table S26. Assigned transitions for PhNCS (^{34}S).

J'	K _a '	K _c '	F'	J''	K _a ''	K _c ''	F''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
5	1	5	6	4	1	4	5	5670.4318	-0.0006
5	1	5	4	4	1	4	3	5670.4458	0.0005
5	1	5	5	4	1	4	4	5670.4699	-0.0006
5	0	5	6	4	0	4	5	5822.6205	-0.0005
5	0	5	5	4	0	4	4	5822.6251	0.0004
5	0	5	4	4	0	4	3	5822.6548	-0.0003
5	1	4	6	4	1	3	5	5996.2496	0.0001
5	1	4	4	4	1	3	3	5996.2797	-0.0004
5	1	4	5	4	1	3	4	5996.2933	0.0004
6	1	6	7	5	1	5	6	6802.6940	-0.0007
6	1	6	5	5	1	5	4	6802.7053	-0.0003
6	1	6	6	5	1	5	5	6802.7163	-0.0007
6	0	6	7	5	0	5	6	6979.6262	-0.0002
6	0	6	5	5	0	5	4	6979.6480	-0.0013
6	2	5	7	5	2	4	6	7000.5147	0.0005
6	2	5	6	5	2	4	5	7000.5950	-0.0002
6	1	5	7	5	1	4	6	7193.5344	0.0008
6	1	5	5	5	1	4	4	7193.5556	-0.0007
6	1	5	6	5	1	4	5	7193.5601	0.0004
7	1	7	8	6	1	6	7	7933.9942	-0.0016
7	1	7	6	6	1	6	5	7934.0036	-0.0011
7	1	7	7	6	1	6	6	7934.0097	0.0000
7	0	7	7	6	0	6	6	8132.5966	-0.0001
7	0	7	8	6	0	6	7	8132.6001	-0.0001
7	0	7	6	6	0	6	5	8132.6175	0.0006
7	2	6	8	6	2	5	7	8165.5244	-0.0007
7	2	6	6	6	2	5	5	8165.5304	0.0007
7	2	6	7	6	2	5	6	8165.5779	0.0010
7	3	5	6	6	3	4	5	8176.2921	-0.0002
7	3	5	8	6	3	4	7	8176.3044	0.0017
7	3	5	7	6	3	4	6	8176.4168	0.0005
7	3	4	6	6	3	3	5	8176.8623	-0.0013
7	3	4	8	6	3	3	7	8176.8759	0.0019
7	3	4	7	6	3	3	6	8176.9880	0.0001
7	2	5	8	6	2	4	7	8203.7996	0.0004
7	2	5	6	6	2	4	5	8203.8039	0.0009
7	2	5	7	6	2	4	6	8203.8595	-0.0006
7	1	6	8	6	1	5	7	8389.6960	0.0009

7	1	6	7	6	1	5	6	8389.7124	0.0006
8	1	8	9	7	1	7	8	9064.2079	-0.0022
8	1	8	8	7	1	7	7	9064.2176	-0.0013
8	0	8	8	7	0	7	7	9280.9634	-0.0004
8	0	8	9	7	0	7	8	9280.9704	0.0005
8	0	8	7	7	0	7	6	9280.9813	-0.0011
8	2	7	9	7	2	6	8	9329.7236	-0.0008
8	2	7	7	7	2	6	6	9329.7307	0.0008
8	2	7	8	7	2	6	7	9329.7596	0.0004
8	2	6	9	7	2	5	8	9386.8719	0.0001
8	2	6	8	7	2	5	7	9386.9168	-0.0001
9	1	9	10	8	1	8	9	10193.2222	-0.0037
9	1	9	9	8	1	8	8	10193.2306	-0.0009
9	0	9	9	8	0	8	8	10424.2343	-0.0016
9	0	9	10	8	0	8	9	10424.2452	0.0013
9	0	9	8	8	0	8	7	10424.2525	-0.0014
9	2	8	10	8	2	7	9	10492.9972	-0.0018
9	2	8	8	8	2	7	7	10493.0063	0.0019
9	2	8	9	8	2	7	8	10493.0235	0.0002
9	1	8	10	8	1	7	9	10777.7512	0.0002
9	1	8	9	8	1	7	8	10777.7593	0.0014
9	1	8	8	8	1	7	7	10777.7634	0.0015
10	1	10	11	9	1	9	10	11320.9443	-0.0028
10	1	10	10	9	1	9	9	11320.9485	-0.0020
10	0	10	10	9	0	9	9	11562.0314	-0.0035
10	0	10	11	9	0	9	10	11562.0431	-0.0014
10	0	10	9	9	0	9	8	11562.0543	0.0016

Appendix III: Kraitchman Coordinates for PhNCO and PhNCS

Table S27. r_s coordinates for PhNCO

13C1			

	a	b	
PLANAR:	0.13179*i+- 0.00204	0.27253 +- 0.00069	
+Costain err.	0.13179*i+- 0.01156	0.27253 +- 0.00555	
	a	b	c
NONPLANAR:	0.13144*i+- 0.00137	0.27270 +- 0.00066	0.00962*i+- 0.01878
+Costain err.	0.13144*i+- 0.01149	0.27270 +- 0.00554	0.00962*i+- 0.15704

13C2			

	a	b	
PLANAR:	0.34435 +- 0.00006	1.06190 +- 0.00006	
+Costain err.	0.34435 +- 0.00436	1.06190 +- 0.00141	
	a	b	c
NONPLANAR:	0.34353 +- 0.00010	1.06163 +- 0.00003	0.02395 +- 0.00152
+Costain err.	0.34353 +- 0.00437	1.06163 +- 0.00141	0.02395 +- 0.06265

13C3			

	a	b	
PLANAR:	1.71020 +- 0.00001	1.38965 +- 0.00006	
+Costain err.	1.71020 +- 0.00088	1.38965 +- 0.00108	
	a	b	c
NONPLANAR:	1.71058 +- 0.00003	1.39013 +- 0.00003	0.03632*i+- 0.00133
+Costain err.	1.71058 +- 0.00088	1.39013 +- 0.00108	0.03632*i+- 0.04133

13C4			

	a	b	
PLANAR:	2.68253 +- 0.00001	0.38201 +- 0.00023	
+Costain err.	2.68253 +- 0.00056	0.38201 +- 0.00393	
	a	b	c
NONPLANAR:	2.68242 +- 0.00002	0.38120 +- 0.00012	0.02481 +- 0.00186
+Costain err.	2.68242 +- 0.00056	0.38120 +- 0.00394	0.02481 +- 0.06049

13C5			

	a	b	
PLANAR:	2.28964 +- 0.00001	0.95159 +- 0.00009	

+Costain err.	2.28964 +- 0.00066	0.95159 +- 0.00158	
	a	b	c
NONPLANAR:	2.28957 +- 0.00002	0.95144 +- 0.00005	0.01727 +- 0.00276
+Costain err.	2.28957 +- 0.00066	0.95144 +- 0.00158	0.01727 +- 0.08689

13C6

	a	b	
PLANAR:	0.93201 +- 0.00003	1.29111 +- 0.00006	
+Costain err.	0.93201 +- 0.00161	1.29111 +- 0.00116	
	a	b	c
NONPLANAR:	0.93276 +- 0.00005	1.29167 +- 0.00003	0.03780*i+- 0.00115
+Costain err.	0.93276 +- 0.00161	1.29167 +- 0.00116	0.03780*i+- 0.03970

15N

	a	b	
PLANAR:	1.36718 +- 0.00001	0.66711 +- 0.00007	
+Costain err.	1.36718 +- 0.00110	0.66711 +- 0.00225	
	a	b	c
NONPLANAR:	1.36662 +- 0.00002	0.66594 +- 0.00004	0.03934 +- 0.00070
+Costain err.	1.36662 +- 0.00110	0.66594 +- 0.00225	0.03934 +- 0.03814

13C7

	a	b	
PLANAR:	2.42724 +- 0.00001	0.09466 +- 0.00091	
+Costain err.	2.42724 +- 0.00062	0.09466 +- 0.01587	
	a	b	c
NONPLANAR:	2.42722 +- 0.00002	0.09402 +- 0.00049	0.01101 +- 0.00417
+Costain err.	2.42722 +- 0.00062	0.09402 +- 0.01596	0.01101 +- 0.13629

18O

	a	b	
PLANAR:	3.51291 +- 0.00000	0.35767 +- 0.00028	
+Costain err.	3.51291 +- 0.00043	0.35767 +- 0.00420	
	a	b	c
NONPLANAR:	3.51294 +- 0.00001	0.35799 +- 0.00015	0.01497*i+- 0.00346
+Costain err.	3.51294 +- 0.00043	0.35799 +- 0.00419	0.01497*i+- 0.10024

Table S28. r_s coordinates for PhNCS

13C1			

	a	b	
PLANAR:	0.49163 +- 0.00009	0.27160 +- 0.00172	
+Costain err.	0.49163 +- 0.00305	0.27160 +- 0.00578	
	a	b	c
NONPLANAR:	0.49129 +- 0.00048	0.27097 +- 0.00087	0.01841 +- 0.01284
+Costain err.	0.49129 +- 0.00309	0.27097 +- 0.00560	0.01841 +- 0.08248

13C2			

	a	b	
PLANAR:	0.87262 +- 0.00006	1.06872 +- 0.00045	
+Costain err.	0.87262 +- 0.00172	1.06872 +- 0.00147	
	a	b	c
NONPLANAR:	0.87323 +- 0.00028	1.06923 +- 0.00023	0.03302*i+- 0.00745
+Costain err.	0.87323 +- 0.00174	1.06923 +- 0.00142	0.03302*i+- 0.04604

13C3			

	a	b	
PLANAR:	2.23191 +- 0.00002	1.40654 +- 0.00035	
+Costain err.	2.23191 +- 0.00067	1.40654 +- 0.00112	
	a	b	c
NONPLANAR:	2.23204 +- 0.00011	1.40677 +- 0.00018	0.02500*i+- 0.01010
+Costain err.	2.23204 +- 0.00068	1.40677 +- 0.00108	0.02500*i+- 0.06085

13C4			

	a	b	
PLANAR:	3.21122 +- 0.00002	0.41088 +- 0.00162	
+Costain err.	3.21122 +- 0.00047	0.41088 +- 0.00399	
	a	b	c
NONPLANAR:	3.21066 +- 0.00010	0.40643 +- 0.00083	0.06025 +- 0.00557
+Costain err.	3.21066 +- 0.00048	0.40643 +- 0.00378	0.06025 +- 0.02551

13C5			

	a	b	
PLANAR:	2.83052 +- 0.00002	0.93132 +- 0.00072	
+Costain err.	2.83052 +- 0.00053	0.93132 +- 0.00176	
	a	b	c

NONPLANAR:	2.83091 +- 0.00012	0.93254 +- 0.00036	0.04753*i+- 0.00719
+Costain err.	2.83091 +- 0.00054	0.93254 +- 0.00165	0.04753*i+- 0.03237

13C6

	a	b	
PLANAR:	1.47490 +- 0.00003	1.28391 +- 0.00045	
+Costain err.	1.47490 +- 0.00102	1.28391 +- 0.00125	
	a	b	c
NONPLANAR:	1.47625 +- 0.00020	1.28550 +- 0.00023	0.06384*i+- 0.00467
+Costain err.	1.47625 +- 0.00104	1.28550 +- 0.00119	0.06384*i+- 0.02396

15N

	a	b	
PLANAR:	0.79359 +- 0.00004	0.65170 +- 0.00044	
+Costain err.	0.79359 +- 0.00189	0.65170 +- 0.00234	
	a	b	c
NONPLANAR:	0.79289 +- 0.00018	0.65085 +- 0.00022	0.03331 +- 0.00436
+Costain err.	0.79289 +- 0.00190	0.65085 +- 0.00232	0.03331 +- 0.04525

13C7

	a	b	
PLANAR:	1.93952 +- 0.00002	0.24201 +- 0.00232	
+Costain err.	1.93952 +- 0.00077	0.24201 +- 0.00662	
	a	b	c
NONPLANAR:	1.93933 +- 0.00015	0.24050 +- 0.00118	0.02695 +- 0.01057
+Costain err.	1.93933 +- 0.00079	0.24050 +- 0.00635	0.02695 +- 0.05665

34S

	a	b	
PLANAR:	3.46212 +- 0.00000	0.19870 +- 0.00049	
+Costain err.	3.46212 +- 0.00043	0.19870 +- 0.00757	
	a	b	c
NONPLANAR:	3.46219 +- 0.00001	0.20003 +- 0.00025	0.02301*i+- 0.00219
+Costain err.	3.46219 +- 0.00043	0.20003 +- 0.00750	0.02301*i+- 0.06522

Appendix IV: NBO Output for PhNCO and PhNCS

```
***** NBO 6.0 *****
      N A T U R A L   A T O M I C   O R B I T A L   A N D
      N A T U R A L   B O N D   O R B I T A L   A N A L Y S I S
***** University of Manitoba (100811) *****
(c) Copyright 1996-2015 Board of Regents of the University of Wisconsin System
    on behalf of the Theoretical Chemistry Institute. All rights reserved.
```

Cite this program as:

NBO 6.0. E. D. Glendening, J. K. Badenhoop, A. E. Reed,
J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis,
and F. Weinhold (Theoretical Chemistry Institute, University
of Wisconsin, Madison, WI, 2013); <http://nb06.chem.wisc.edu/>

/AONBO / : Checkpoint the AO to NBO transformation

Filename set to /scratch/12026589.yak.local/Gau-10440

Job title: Title Card Required

Interatomic linear dependence detected; p-type subshell on C 3 discarded
FIXDM: density matrix trace differs from integer value by -0.00001e; fixed

NATURAL POPULATIONS: Natural atomic orbital occupancies

NAO	Atom	No	lang	Type(AO)	Occupancy	Energy
1	C	1	s	Cor(1s)	1.99999	-10.19659
2	C	1	s	Val(2s)	0.97276	-0.12841
3	C	1	s	Ryd(3s)	0.00100	2.15856
4	C	1	s	Ryd(4s)	0.00007	3.43568
5	C	1	s	Ryd(5s)	0.00003	1.24977
6	C	1	px	Val(2p)	1.15027	-0.05619
7	C	1	px	Ryd(3p)	0.00349	1.78988
8	C	1	px	Ryd(4p)	0.00010	1.40599
9	C	1	px	Ryd(5p)	0.00002	2.10304
10	C	1	py	Val(2p)	1.05661	-0.03634
11	C	1	py	Ryd(3p)	0.00268	1.86639
12	C	1	py	Ryd(4p)	0.00006	1.02673
13	C	1	py	Ryd(5p)	0.00003	2.13197
14	C	1	pz	Val(2p)	1.02316	-0.12925
15	C	1	pz	Ryd(3p)	0.00073	0.93865
16	C	1	pz	Ryd(4p)	0.00020	0.71344
17	C	1	pz	Ryd(5p)	0.00000	1.76338
18	C	1	dxxy	Ryd(3d)	0.00096	3.49075
19	C	1	dxxy	Ryd(5d)	0.00027	1.54920
20	C	1	dxxy	Ryd(4d)	0.00033	4.28221
21	C	1	dxz	Ryd(3d)	0.00013	1.74378
22	C	1	dxz	Ryd(4d)	0.00012	1.11821
23	C	1	dxz	Ryd(5d)	0.00001	3.10271
24	C	1	dyz	Ryd(4d)	0.00014	1.84865
25	C	1	dyz	Ryd(3d)	0.00018	1.06222
26	C	1	dyz	Ryd(5d)	0.00002	3.13491
27	C	1	dx2y2	Ryd(3d)	0.00193	4.22181
28	C	1	dx2y2	Ryd(5d)	0.00011	1.54051
29	C	1	dx2y2	Ryd(4d)	0.00026	4.19892
30	C	1	dz2	Ryd(3d)	0.00129	2.78789
31	C	1	dz2	Ryd(4d)	0.00020	1.63443
32	C	1	dz2	Ryd(5d)	0.00003	4.08950

33	C	1	f(0)	Ryd(4f)	0.00038	2.10955
34	C	1	f(0)	Ryd(5f)	0.00004	2.95529
35	C	1	f(c1)	Ryd(4f)	0.00050	2.55404
36	C	1	f(c1)	Ryd(5f)	0.00005	3.25796
37	C	1	f(s1)	Ryd(4f)	0.00037	2.71456
38	C	1	f(s1)	Ryd(5f)	0.00007	3.23909
39	C	1	f(c2)	Ryd(5f)	0.00003	2.24653
40	C	1	f(c2)	Ryd(4f)	0.00004	2.98826
41	C	1	f(s2)	Ryd(4f)	0.00006	2.34633
42	C	1	f(s2)	Ryd(5f)	0.00005	2.95779
43	C	1	f(c3)	Ryd(4f)	0.00074	2.71415
44	C	1	f(c3)	Ryd(5f)	0.00025	3.85901
45	C	1	f(s3)	Ryd(4f)	0.00055	4.77545
46	C	1	f(s3)	Ryd(5f)	0.00014	3.90223
47	C	2	s	Cor(1s)	1.99999	-10.24779
48	C	2	s	Val(2s)	0.87294	-0.08852
49	C	2	s	Ryd(3s)	0.00194	1.80506
50	C	2	s	Ryd(4s)	0.00009	2.86585
51	C	2	s	Ryd(5s)	0.00006	2.51140
52	C	2	px	Val(2p)	0.93630	-0.03750
53	C	2	px	Ryd(3p)	0.00527	1.42439
54	C	2	px	Ryd(4p)	0.00019	1.64798
55	C	2	px	Ryd(5p)	0.00007	1.89433
56	C	2	py	Val(2p)	1.02922	-0.03595
57	C	2	py	Ryd(3p)	0.00708	1.65518
58	C	2	py	Ryd(4p)	0.00028	1.82337
59	C	2	py	Ryd(5p)	0.00009	1.53176
60	C	2	pz	Val(2p)	1.02789	-0.13660
61	C	2	pz	Ryd(3p)	0.00136	0.76494
62	C	2	pz	Ryd(4p)	0.00039	1.17645
63	C	2	pz	Ryd(5p)	0.00002	1.41766
64	C	2	dxy	Ryd(3d)	0.00285	2.01814
65	C	2	dxy	Ryd(4d)	0.00053	4.28960
66	C	2	dxy	Ryd(5d)	0.00043	3.19155
67	C	2	dxz	Ryd(3d)	0.00100	0.76927
68	C	2	dxz	Ryd(4d)	0.00057	2.84251
69	C	2	dxz	Ryd(5d)	0.00012	2.27091
70	C	2	dyz	Ryd(3d)	0.00082	0.86348
71	C	2	dyz	Ryd(4d)	0.00036	2.84094
72	C	2	dyz	Ryd(5d)	0.00002	2.22941
73	C	2	dx2y2	Ryd(3d)	0.00510	2.29503
74	C	2	dx2y2	Ryd(4d)	0.00072	4.57025
75	C	2	dx2y2	Ryd(5d)	0.00012	3.28498
76	C	2	dz2	Ryd(3d)	0.00134	1.15507
77	C	2	dz2	Ryd(4d)	0.00037	4.29878
78	C	2	dz2	Ryd(5d)	0.00006	2.98818
79	C	2	f(0)	Ryd(4f)	0.00031	1.71207
80	C	2	f(0)	Ryd(5f)	0.00014	3.62861
81	C	2	f(c1)	Ryd(4f)	0.00047	2.27191
82	C	2	f(c1)	Ryd(5f)	0.00008	3.72894
83	C	2	f(s1)	Ryd(4f)	0.00048	2.41286
84	C	2	f(s1)	Ryd(5f)	0.00014	3.69819
85	C	2	f(c2)	Ryd(4f)	0.00015	1.79776
86	C	2	f(c2)	Ryd(5f)	0.00002	3.58667
87	C	2	f(s2)	Ryd(4f)	0.00043	1.76704
88	C	2	f(s2)	Ryd(5f)	0.00005	3.68913
89	C	2	f(c3)	Ryd(4f)	0.00358	2.36388
90	C	2	f(c3)	Ryd(5f)	0.00012	4.84450
91	C	2	f(s3)	Ryd(4f)	0.00078	5.21596
92	C	2	f(s3)	Ryd(5f)	0.00018	4.20929
93	C	3	s	Cor(1s)	1.99999	-10.19305

94	C	3	s	Val(2s)	0.97331	-0.12793
95	C	3	s	Ryd(3s)	0.00057	1.94455
96	C	3	s	Ryd(4s)	0.00014	3.26398
97	C	3	s	Ryd(5s)	0.00004	1.16990
98	C	3	px	Val(2p)	1.00660	-0.02963
99	C	3	px	Ryd(3p)	0.00135	2.17298
100	C	3	px	Ryd(4p)	0.00004	1.11661
101	C	3	py	Val(2p)	1.15129	-0.04439
102	C	3	py	Ryd(3p)	0.00076	2.15526
103	C	3	py	Ryd(4p)	0.00004	1.23928
104	C	3	pz	Val(2p)	0.99080	-0.12853
105	C	3	pz	Ryd(4p)	0.00003	1.54318
106	C	3	pz	Ryd(3p)	0.00005	1.06502
107	C	3	dxxy	Ryd(3d)	0.00400	3.60346
108	C	3	dxxy	Ryd(5d)	0.00012	3.27303
109	C	3	dxxy	Ryd(4d)	0.00015	2.69007
110	C	3	dxz	Ryd(3d)	0.00014	1.43769
111	C	3	dxz	Ryd(4d)	0.00013	2.34645
112	C	3	dxz	Ryd(5d)	0.00002	2.25864
113	C	3	dyz	Ryd(3d)	0.00092	1.27286
114	C	3	dyz	Ryd(5d)	0.00001	2.46629
115	C	3	dyz	Ryd(4d)	0.00003	2.09337
116	C	3	dx2y2	Ryd(4d)	0.00045	2.74203
117	C	3	dx2y2	Ryd(3d)	0.00067	3.02661
118	C	3	dx2y2	Ryd(5d)	0.00036	3.39879
119	C	3	dz2	Ryd(3d)	0.00120	2.21566
120	C	3	dz2	Ryd(4d)	0.00018	3.32184
121	C	3	dz2	Ryd(5d)	0.00005	2.88540
122	C	3	f(0)	Ryd(4f)	0.00117	1.76633
123	C	3	f(0)	Ryd(5f)	0.00000	3.18208
124	C	3	f(c1)	Ryd(4f)	0.00081	2.39692
125	C	3	f(c1)	Ryd(5f)	0.00002	3.44596
126	C	3	f(s1)	Ryd(4f)	0.00121	2.14729
127	C	3	f(s1)	Ryd(5f)	0.00001	3.37962
128	C	3	f(c2)	Ryd(4f)	0.00003	2.09393
129	C	3	f(c2)	Ryd(5f)	0.00001	3.13343
130	C	3	f(s2)	Ryd(4f)	0.00006	1.97406
131	C	3	f(s2)	Ryd(5f)	0.00003	3.26680
132	C	3	f(c3)	Ryd(4f)	0.00097	2.40435
133	C	3	f(c3)	Ryd(5f)	0.00012	4.04677
134	C	3	f(s3)	Ryd(4f)	0.00053	4.72134
135	C	3	f(s3)	Ryd(5f)	0.00021	3.86846
136	C	4	s	Cor(1s)	1.99999	-10.19465
137	C	4	s	Val(2s)	0.97863	-0.13109
138	C	4	s	Ryd(3s)	0.00209	1.82386
139	C	4	s	Ryd(4s)	0.00003	3.07547
140	C	4	s	Ryd(5s)	0.00003	1.51079
141	C	4	px	Val(2p)	1.13556	-0.04499
142	C	4	px	Ryd(3p)	0.00517	1.46635
143	C	4	px	Ryd(4p)	0.00007	1.42764
144	C	4	px	Ryd(5p)	0.00002	1.97624
145	C	4	py	Val(2p)	1.07924	-0.03240
146	C	4	py	Ryd(3p)	0.00710	1.45755
147	C	4	py	Ryd(4p)	0.00016	1.58821
148	C	4	py	Ryd(5p)	0.00004	1.67875
149	C	4	pz	Val(2p)	0.99205	-0.12455
150	C	4	pz	Ryd(3p)	0.00102	0.77516
151	C	4	pz	Ryd(4p)	0.00015	1.05471
152	C	4	pz	Ryd(5p)	0.00001	1.61077
153	C	4	dxxy	Ryd(3d)	0.00198	2.85771
154	C	4	dxxy	Ryd(4d)	0.00029	2.96187
155	C	4	dxxy	Ryd(5d)	0.00020	3.39599

156	C	4	dxz	Ryd(4d)	0.00013	1.23509
157	C	4	dxz	Ryd(3d)	0.00074	2.19539
158	C	4	dxz	Ryd(5d)	0.00005	2.44474
159	C	4	dyz	Ryd(3d)	0.00023	1.34460
160	C	4	dyz	Ryd(4d)	0.00017	2.18006
161	C	4	dyz	Ryd(5d)	0.00000	2.48621
162	C	4	dx2y2	Ryd(3d)	0.00236	3.83014
163	C	4	dx2y2	Ryd(4d)	0.00054	2.88856
164	C	4	dx2y2	Ryd(5d)	0.00007	3.13759
165	C	4	dz2	Ryd(3d)	0.00178	2.23388
166	C	4	dz2	Ryd(4d)	0.00022	2.94616
167	C	4	dz2	Ryd(5d)	0.00003	3.28042
168	C	4	f(0)	Ryd(4f)	0.00037	2.10829
169	C	4	f(0)	Ryd(5f)	0.00004	2.93655
170	C	4	f(c1)	Ryd(4f)	0.00064	2.47314
171	C	4	f(c1)	Ryd(5f)	0.00002	3.14702
172	C	4	f(s1)	Ryd(4f)	0.00046	2.64781
173	C	4	f(s1)	Ryd(5f)	0.00005	3.13306
174	C	4	f(c2)	Ryd(4f)	0.00005	2.28965
175	C	4	f(c2)	Ryd(5f)	0.00004	2.94252
176	C	4	f(s2)	Ryd(5f)	0.00005	2.33473
177	C	4	f(s2)	Ryd(4f)	0.00005	2.90963
178	C	4	f(c3)	Ryd(4f)	0.00073	2.75789
179	C	4	f(c3)	Ryd(5f)	0.00021	3.73341
180	C	4	f(s3)	Ryd(4f)	0.00071	4.48499
181	C	4	f(s3)	Ryd(5f)	0.00011	3.68884
182	C	5	s	Cor(1s)	1.99999	-10.19095
183	C	5	s	Val(2s)	0.97530	-0.13091
184	C	5	s	Ryd(3s)	0.00085	2.11000
185	C	5	s	Ryd(4s)	0.00003	1.61576
186	C	5	s	Ryd(5s)	0.00001	2.60582
187	C	5	px	Val(2p)	1.13271	-0.04483
188	C	5	px	Ryd(3p)	0.00425	1.60075
189	C	5	px	Ryd(4p)	0.00005	0.93341
190	C	5	px	Ryd(5p)	0.00001	2.20903
191	C	5	py	Val(2p)	1.07856	-0.03100
192	C	5	py	Ryd(3p)	0.00339	1.77502
193	C	5	py	Ryd(4p)	0.00006	0.84686
194	C	5	py	Ryd(5p)	0.00002	2.05781
195	C	5	pz	Val(2p)	1.00790	-0.12211
196	C	5	pz	Ryd(3p)	0.00093	0.91086
197	C	5	pz	Ryd(4p)	0.00015	0.51820
198	C	5	pz	Ryd(5p)	0.00000	1.91995
199	C	5	dxy	Ryd(3d)	0.00151	3.12347
200	C	5	dxy	Ryd(4d)	0.00031	3.23627
201	C	5	dxy	Ryd(5d)	0.00019	2.73103
202	C	5	dxz	Ryd(3d)	0.00017	1.65402
203	C	5	dxz	Ryd(4d)	0.00010	2.45309
204	C	5	dxz	Ryd(5d)	0.00003	1.75995
205	C	5	dyz	Ryd(3d)	0.00018	1.72266
206	C	5	dyz	Ryd(4d)	0.00008	2.38608
207	C	5	dyz	Ryd(5d)	0.00002	1.86131
208	C	5	dx2y2	Ryd(3d)	0.00186	4.27525
209	C	5	dx2y2	Ryd(4d)	0.00015	3.49176
210	C	5	dx2y2	Ryd(5d)	0.00008	2.19539
211	C	5	dz2	Ryd(3d)	0.00126	2.83965
212	C	5	dz2	Ryd(4d)	0.00018	3.05271
213	C	5	dz2	Ryd(5d)	0.00005	2.56483
214	C	5	f(0)	Ryd(4f)	0.00029	2.20414
215	C	5	f(0)	Ryd(5f)	0.00004	2.83137
216	C	5	f(c1)	Ryd(4f)	0.00048	2.58018
217	C	5	f(c1)	Ryd(5f)	0.00004	3.04040

218	C	5	f(s1)	Ryd(4f)	0.00044	2.71823
219	C	5	f(s1)	Ryd(5f)	0.00005	3.02027
220	C	5	f(c2)	Ryd(5f)	0.00003	2.37030
221	C	5	f(c2)	Ryd(4f)	0.00004	2.84327
222	C	5	f(s2)	Ryd(5f)	0.00004	2.44200
223	C	5	f(s2)	Ryd(4f)	0.00004	2.77806
224	C	5	f(c3)	Ryd(4f)	0.00069	2.82504
225	C	5	f(c3)	Ryd(5f)	0.00027	3.59030
226	C	5	f(s3)	Ryd(4f)	0.00054	4.41339
227	C	5	f(s3)	Ryd(5f)	0.00011	3.67921
228	C	6	s	Cor(1s)	1.99999	-10.19585
229	C	6	s	Val(2s)	0.97535	-0.13358
230	C	6	s	Ryd(3s)	0.00093	2.09378
231	C	6	s	Ryd(4s)	0.00002	2.78397
232	C	6	s	Ryd(5s)	0.00002	1.26076
233	C	6	px	Val(2p)	1.04303	-0.02204
234	C	6	px	Ryd(3p)	0.00277	1.79841
235	C	6	px	Ryd(4p)	0.00005	1.08303
236	C	6	px	Ryd(5p)	0.00002	1.73063
237	C	6	py	Val(2p)	1.16481	-0.05337
238	C	6	py	Ryd(3p)	0.00509	1.53760
239	C	6	py	Ryd(4p)	0.00004	1.13399
240	C	6	py	Ryd(5p)	0.00000	2.15279
241	C	6	pz	Val(2p)	0.98736	-0.12392
242	C	6	pz	Ryd(3p)	0.00080	0.88318
243	C	6	pz	Ryd(4p)	0.00013	0.71192
244	C	6	pz	Ryd(5p)	0.00000	1.73074
245	C	6	dxy	Ryd(3d)	0.00173	4.57802
246	C	6	dxy	Ryd(4d)	0.00015	3.83983
247	C	6	dxy	Ryd(5d)	0.00005	1.74014
248	C	6	dxz	Ryd(3d)	0.00031	1.81770
249	C	6	dxz	Ryd(4d)	0.00002	2.49121
250	C	6	dxz	Ryd(5d)	0.00000	1.72179
251	C	6	dyz	Ryd(3d)	0.00013	1.69316
252	C	6	dyz	Ryd(4d)	0.00008	2.65085
253	C	6	dyz	Ryd(5d)	0.00005	1.49296
254	C	6	dx2y2	Ryd(3d)	0.00127	2.98847
255	C	6	dx2y2	Ryd(4d)	0.00035	3.33505
256	C	6	dx2y2	Ryd(5d)	0.00025	2.62480
257	C	6	dz2	Ryd(3d)	0.00118	3.03789
258	C	6	dz2	Ryd(4d)	0.00013	3.19263
259	C	6	dz2	Ryd(5d)	0.00007	2.26400
260	C	6	f(0)	Ryd(4f)	0.00028	2.15670
261	C	6	f(0)	Ryd(5f)	0.00005	2.90204
262	C	6	f(c1)	Ryd(4f)	0.00041	2.77418
263	C	6	f(c1)	Ryd(5f)	0.00006	3.08368
264	C	6	f(s1)	Ryd(4f)	0.00053	2.44821
265	C	6	f(s1)	Ryd(5f)	0.00002	3.12020
266	C	6	f(c2)	Ryd(4f)	0.00006	2.43440
267	C	6	f(c2)	Ryd(5f)	0.00004	2.85185
268	C	6	f(s2)	Ryd(5f)	0.00004	2.29000
269	C	6	f(s2)	Ryd(4f)	0.00004	2.92709
270	C	6	f(c3)	Ryd(4f)	0.00080	2.79991
271	C	6	f(c3)	Ryd(5f)	0.00025	3.68265
272	C	6	f(s3)	Ryd(4f)	0.00052	4.48550
273	C	6	f(s3)	Ryd(5f)	0.00011	3.70621
274	H	7	s	Val(1s)	0.78644	0.03617
275	H	7	s	Ryd(2s)	0.00028	1.28845
276	H	7	s	Ryd(3s)	0.00009	2.13756
277	H	7	s	Ryd(4s)	0.00003	1.56906
278	H	7	px	Ryd(2p)	0.00036	1.45255

279	H	7	px	Ryd(3p)	0.00014	4.76439
280	H	7	px	Ryd(4p)	0.00009	2.78418
281	H	7	py	Ryd(2p)	0.00033	1.32787
282	H	7	py	Ryd(3p)	0.00006	3.91196
283	H	7	py	Ryd(4p)	0.00002	2.53504
284	H	7	pz	Ryd(2p)	0.00031	0.90220
285	H	7	pz	Ryd(3p)	0.00010	3.57967
286	H	7	pz	Ryd(4p)	0.00001	1.99065
287	H	7	dxy	Ryd(3d)	0.00004	2.10713
288	H	7	dxy	Ryd(4d)	0.00002	4.68126
289	H	7	dxz	Ryd(3d)	0.00004	1.41757
290	H	7	dxz	Ryd(4d)	0.00000	4.23967
291	H	7	dyz	Ryd(3d)	0.00001	1.37055
292	H	7	dyz	Ryd(4d)	0.00000	3.91104
293	H	7	dx2y2	Ryd(3d)	0.00005	1.99217
294	H	7	dx2y2	Ryd(4d)	0.00001	4.70586
295	H	7	dz2	Ryd(3d)	0.00001	1.97030
296	H	7	dz2	Ryd(4d)	0.00001	4.18483
297	H	8	s	Val(1s)	0.78562	0.05801
298	H	8	s	Ryd(2s)	0.00076	1.50572
299	H	8	s	Ryd(3s)	0.00002	1.44517
300	H	8	s	Ryd(4s)	0.00001	1.51850
301	H	8	px	Ryd(2p)	0.00271	1.12718
302	H	8	px	Ryd(4p)	0.00001	3.36919
303	H	8	px	Ryd(3p)	0.00002	2.76828
304	H	8	py	Ryd(2p)	0.00031	1.31205
305	H	8	py	Ryd(3p)	0.00025	4.98517
306	H	8	py	Ryd(4p)	0.00003	2.98333
307	H	8	pz	Ryd(2p)	0.00109	0.74592
308	H	8	pz	Ryd(3p)	0.00005	3.32003
309	H	8	pz	Ryd(4p)	0.00001	2.30246
310	H	8	dxy	Ryd(3d)	0.00003	1.81499
311	H	8	dxy	Ryd(4d)	0.00000	4.69588
312	H	8	dxz	Ryd(3d)	0.00001	1.38366
313	H	8	dxz	Ryd(4d)	0.00000	3.72954
314	H	8	dyz	Ryd(3d)	0.00005	1.51843
315	H	8	dyz	Ryd(4d)	0.00001	4.33618
316	H	8	dx2y2	Ryd(3d)	0.00006	2.49629
317	H	8	dx2y2	Ryd(4d)	0.00002	4.55348
318	H	8	dz2	Ryd(3d)	0.00003	2.07936
319	H	8	dz2	Ryd(4d)	0.00001	4.11532
320	H	9	s	Val(1s)	0.78763	0.04782
321	H	9	s	Ryd(2s)	0.00054	0.96608
322	H	9	s	Ryd(3s)	0.00009	2.22629
323	H	9	s	Ryd(4s)	0.00001	1.21565
324	H	9	px	Ryd(2p)	0.00058	1.22690
325	H	9	px	Ryd(3p)	0.00011	4.73125
326	H	9	px	Ryd(4p)	0.00007	2.98427
327	H	9	py	Ryd(2p)	0.00070	1.30731
328	H	9	py	Ryd(4p)	0.00004	3.77056
329	H	9	py	Ryd(3p)	0.00004	2.74428
330	H	9	pz	Ryd(2p)	0.00016	0.90298
331	H	9	pz	Ryd(3p)	0.00010	3.38185
332	H	9	pz	Ryd(4p)	0.00003	2.27519
333	H	9	dxy	Ryd(4d)	0.00003	2.47992
334	H	9	dxy	Ryd(3d)	0.00003	4.21517
335	H	9	dxz	Ryd(3d)	0.00002	1.71835
336	H	9	dxz	Ryd(4d)	0.00000	3.90784
337	H	9	dyz	Ryd(3d)	0.00002	1.64718
338	H	9	dyz	Ryd(4d)	0.00000	3.58468
339	H	9	dx2y2	Ryd(3d)	0.00004	2.31773

340	H	9	dx2y2	Ryd(4d)	0.00001	4.27464
341	H	9	dz2	Ryd(4d)	0.00001	2.27515
342	H	9	dz2	Ryd(3d)	0.00001	3.75343
343	H	10	s	Val(1s)	0.78784	0.04901
344	H	10	s	Ryd(2s)	0.00027	0.85676
345	H	10	s	Ryd(3s)	0.00011	2.25573
346	H	10	s	Ryd(4s)	0.00000	1.32345
347	H	10	px	Ryd(2p)	0.00045	1.19934
348	H	10	px	Ryd(3p)	0.00011	4.80624
349	H	10	px	Ryd(4p)	0.00007	2.80760
350	H	10	py	Ryd(2p)	0.00048	1.21430
351	H	10	py	Ryd(3p)	0.00005	4.08076
352	H	10	py	Ryd(4p)	0.00005	2.58705
353	H	10	pz	Ryd(2p)	0.00035	0.83351
354	H	10	pz	Ryd(3p)	0.00009	3.75632
355	H	10	pz	Ryd(4p)	0.00002	1.97563
356	H	10	dxy	Ryd(3d)	0.00004	2.90561
357	H	10	dxy	Ryd(4d)	0.00003	3.81165
358	H	10	dxz	Ryd(3d)	0.00002	2.04516
359	H	10	dxz	Ryd(4d)	0.00000	3.54949
360	H	10	dyz	Ryd(3d)	0.00001	1.98002
361	H	10	dyz	Ryd(4d)	0.00000	3.29450
362	H	10	dx2y2	Ryd(3d)	0.00005	2.63440
363	H	10	dx2y2	Ryd(4d)	0.00001	3.92381
364	H	10	dz2	Ryd(4d)	0.00001	2.61099
365	H	10	dz2	Ryd(3d)	0.00002	3.41681
366	H	11	s	Val(1s)	0.78783	0.04659
367	H	11	s	Ryd(2s)	0.00037	1.06403
368	H	11	s	Ryd(3s)	0.00012	2.18064
369	H	11	s	Ryd(4s)	0.00000	1.26673
370	H	11	px	Ryd(2p)	0.00045	1.14960
371	H	11	px	Ryd(4p)	0.00001	3.66444
372	H	11	px	Ryd(3p)	0.00002	2.44239
373	H	11	py	Ryd(2p)	0.00047	1.34690
374	H	11	py	Ryd(3p)	0.00015	5.21844
375	H	11	py	Ryd(4p)	0.00008	2.73568
376	H	11	pz	Ryd(2p)	0.00028	0.83838
377	H	11	pz	Ryd(3p)	0.00009	3.61419
378	H	11	pz	Ryd(4p)	0.00001	2.06909
379	H	11	dxy	Ryd(3d)	0.00005	2.29131
380	H	11	dxy	Ryd(4d)	0.00000	4.14526
381	H	11	dxz	Ryd(3d)	0.00000	1.79557
382	H	11	dxz	Ryd(4d)	0.00000	3.29792
383	H	11	dyz	Ryd(3d)	0.00003	1.91890
384	H	11	dyz	Ryd(4d)	0.00000	3.87369
385	H	11	dx2y2	Ryd(4d)	0.00002	2.97445
386	H	11	dx2y2	Ryd(3d)	0.00003	3.92912
387	H	11	dz2	Ryd(3d)	0.00002	2.53131
388	H	11	dz2	Ryd(4d)	0.00001	3.56831
389	N	12	s	Cor(1s)	1.99999	-14.36215
390	N	12	s	Val(2s)	1.26951	-0.38907
391	N	12	s	Ryd(3s)	0.00071	2.06845
392	N	12	s	Ryd(4s)	0.00022	2.45058
393	N	12	s	Ryd(5s)	0.00001	10.58395
394	N	12	px	Val(2p)	1.24786	-0.17618
395	N	12	px	Ryd(3p)	0.00212	3.23034
396	N	12	px	Ryd(4p)	0.00038	1.49028
397	N	12	px	Ryd(5p)	0.00006	4.15399
398	N	12	py	Val(2p)	1.51303	-0.23981
399	N	12	py	Ryd(3p)	0.00386	1.04591

400	N 12	py	Ryd(4p)	0.00020	1.25914
401	N 12	py	Ryd(5p)	0.00002	3.67816
402	N 12	pz	Val(2p)	1.46809	-0.23951
403	N 12	pz	Ryd(3p)	0.00235	0.84584
404	N 12	pz	Ryd(4p)	0.00023	0.92526
405	N 12	pz	Ryd(5p)	0.00001	3.17076
406	N 12	dxy	Ryd(3d)	0.00361	3.07423
407	N 12	dxy	Ryd(4d)	0.00022	2.09856
408	N 12	dxy	Ryd(5d)	0.00005	5.74090
409	N 12	dxz	Ryd(3d)	0.00150	2.01376
410	N 12	dxz	Ryd(4d)	0.00013	1.42606
411	N 12	dxz	Ryd(5d)	0.00004	5.32193
412	N 12	dyz	Ryd(3d)	0.00187	1.55685
413	N 12	dyz	Ryd(4d)	0.00005	1.04724
414	N 12	dyz	Ryd(5d)	0.00000	4.94086
415	N 12	dx2y2	Ryd(3d)	0.00292	3.48935
416	N 12	dx2y2	Ryd(4d)	0.00020	1.63126
417	N 12	dx2y2	Ryd(5d)	0.00005	6.65929
418	N 12	dz2	Ryd(3d)	0.00231	2.67887
419	N 12	dz2	Ryd(4d)	0.00022	1.89277
420	N 12	dz2	Ryd(5d)	0.00001	5.77553
421	N 12	f(0)	Ryd(4f)	0.00067	2.13970
422	N 12	f(0)	Ryd(5f)	0.00002	4.64949
423	N 12	f(c1)	Ryd(4f)	0.00074	3.13182
424	N 12	f(c1)	Ryd(5f)	0.00002	5.11982
425	N 12	f(s1)	Ryd(4f)	0.00024	2.17265
426	N 12	f(s1)	Ryd(5f)	0.00001	4.45911
427	N 12	f(c2)	Ryd(4f)	0.00061	2.30619
428	N 12	f(c2)	Ryd(5f)	0.00002	4.87910
429	N 12	f(s2)	Ryd(4f)	0.00007	2.13988
430	N 12	f(s2)	Ryd(5f)	0.00001	4.63263
431	N 12	f(c3)	Ryd(4f)	0.00108	3.25200
432	N 12	f(c3)	Ryd(5f)	0.00007	5.39872
433	N 12	f(s3)	Ryd(4f)	0.00142	3.02564
434	N 12	f(s3)	Ryd(5f)	0.00005	5.51646
435	C 13	s	Cor(1s)	1.99999	-10.32492
436	C 13	s	Val(2s)	0.71404	-0.05515
437	C 13	s	Ryd(3s)	0.00117	2.66702
438	C 13	s	Ryd(4s)	0.00008	3.37563
439	C 13	s	Ryd(5s)	0.00002	2.02712
440	C 13	px	Val(2p)	0.84215	0.14741
441	C 13	px	Ryd(3p)	0.01174	1.64844
442	C 13	px	Ryd(4p)	0.00007	1.59286
443	C 13	px	Ryd(5p)	0.00002	0.75028
444	C 13	py	Val(2p)	0.75574	-0.12704
445	C 13	py	Ryd(3p)	0.00232	1.25179
446	C 13	py	Ryd(4p)	0.00005	1.29037
447	C 13	py	Ryd(5p)	0.00002	0.66833
448	C 13	pz	Val(2p)	0.82100	-0.13458
449	C 13	pz	Ryd(3p)	0.00064	1.18930
450	C 13	pz	Ryd(4p)	0.00006	1.10673
451	C 13	pz	Ryd(5p)	0.00001	0.46586
452	C 13	dxy	Ryd(3d)	0.00213	3.56564
453	C 13	dxy	Ryd(4d)	0.00013	1.13103
454	C 13	dxy	Ryd(5d)	0.00002	2.56721
455	C 13	dxz	Ryd(3d)	0.00250	3.42568
456	C 13	dxz	Ryd(4d)	0.00017	0.94878
457	C 13	dxz	Ryd(5d)	0.00002	2.19037
458	C 13	dyz	Ryd(4d)	0.00002	2.63761
459	C 13	dyz	Ryd(3d)	0.00003	0.57835
460	C 13	dyz	Ryd(5d)	0.00000	1.96425
461	C 13	dx2y2	Ryd(3d)	0.00073	4.15029

462	C 13	dx2y2	Ryd(4d)	0.00003	1.20938
463	C 13	dx2y2	Ryd(5d)	0.00003	4.32456
464	C 13	dz2	Ryd(3d)	0.00026	3.18382
465	C 13	dz2	Ryd(4d)	0.00006	0.86375
466	C 13	dz2	Ryd(5d)	0.00002	3.14129
467	C 13	f(0)	Ryd(4f)	0.00016	2.86482
468	C 13	f(0)	Ryd(5f)	0.00005	2.04315
469	C 13	f(c1)	Ryd(4f)	0.00072	3.72526
470	C 13	f(c1)	Ryd(5f)	0.00006	2.77029
471	C 13	f(s1)	Ryd(4f)	0.00003	2.61640
472	C 13	f(s1)	Ryd(5f)	0.00002	1.90707
473	C 13	f(c2)	Ryd(4f)	0.00026	3.07893
474	C 13	f(c2)	Ryd(5f)	0.00007	2.21499
475	C 13	f(s2)	Ryd(4f)	0.00004	2.96262
476	C 13	f(s2)	Ryd(5f)	0.00003	1.91570
477	C 13	f(c3)	Ryd(4f)	0.00106	4.06506
478	C 13	f(c3)	Ryd(5f)	0.00009	2.90226
479	C 13	f(s3)	Ryd(4f)	0.00032	3.53231
480	C 13	f(s3)	Ryd(5f)	0.00014	2.71864
481	O 14	s	Cor(1s)	2.00000	-19.19067
482	O 14	s	Val(2s)	1.71337	-0.71165
483	O 14	s	Ryd(3s)	0.00025	2.20100
484	O 14	s	Ryd(4s)	0.00003	1.15737
485	O 14	s	Ryd(5s)	0.00000	13.55738
486	O 14	px	Val(2p)	1.52369	-0.30655
487	O 14	px	Ryd(3p)	0.00062	1.13091
488	O 14	px	Ryd(4p)	0.00007	0.65015
489	O 14	px	Ryd(5p)	0.00005	6.09363
490	O 14	py	Val(2p)	1.57727	-0.31012
491	O 14	py	Ryd(3p)	0.00129	0.90569
492	O 14	py	Ryd(4p)	0.00002	0.68838
493	O 14	py	Ryd(5p)	0.00000	4.79435
494	O 14	pz	Val(2p)	1.64016	-0.31279
495	O 14	pz	Ryd(3p)	0.00217	0.85280
496	O 14	pz	Ryd(4p)	0.00001	0.61920
497	O 14	pz	Ryd(5p)	0.00000	4.70816
498	O 14	dxy	Ryd(3d)	0.00642	1.83774
499	O 14	dxy	Ryd(5d)	0.00001	3.14527
500	O 14	dxy	Ryd(4d)	0.00001	5.20052
501	O 14	dxz	Ryd(3d)	0.00645	1.74227
502	O 14	dxz	Ryd(4d)	0.00002	3.00138
503	O 14	dxz	Ryd(5d)	0.00001	5.29075
504	O 14	dyz	Ryd(3d)	0.00002	1.48862
505	O 14	dyz	Ryd(4d)	0.00000	2.59600
506	O 14	dyz	Ryd(5d)	0.00000	5.33144
507	O 14	dx2y2	Ryd(3d)	0.00817	2.16817
508	O 14	dx2y2	Ryd(4d)	0.00002	3.49670
509	O 14	dx2y2	Ryd(5d)	0.00001	7.21904
510	O 14	dz2	Ryd(3d)	0.00272	1.76727
511	O 14	dz2	Ryd(4d)	0.00001	3.08321
512	O 14	dz2	Ryd(5d)	0.00000	5.92459
513	O 14	f(0)	Ryd(4f)	0.00021	2.65951
514	O 14	f(0)	Ryd(5f)	0.00000	5.88299
515	O 14	f(c1)	Ryd(4f)	0.00029	3.12236
516	O 14	f(c1)	Ryd(5f)	0.00000	6.06608
517	O 14	f(s1)	Ryd(4f)	0.00004	2.48499
518	O 14	f(s1)	Ryd(5f)	0.00000	5.67632
519	O 14	f(c2)	Ryd(4f)	0.00034	2.78887
520	O 14	f(c2)	Ryd(5f)	0.00000	6.05764
521	O 14	f(s2)	Ryd(4f)	0.00000	2.92134
522	O 14	f(s2)	Ryd(5f)	0.00000	5.88528
523	O 14	f(c3)	Ryd(4f)	0.00046	3.21714

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524   O 14  f(c3)  Ryd( 5f)    0.00000    6.18333
525   O 14  f(s3)  Ryd( 4f)    0.00047    2.98135
526   O 14  f(s3)  Ryd( 5f)    0.00000    6.34965

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Population inversion found on atom C 1
Population inversion found on atom C 2
Population inversion found on atom C 3
Population inversion found on atom C 4
Population inversion found on atom C 5
Population inversion found on atom C 6
Population inversion found on atom H 7
Population inversion found on atom H 8
Population inversion found on atom H 9
Population inversion found on atom H 10
Population inversion found on atom H 11
Population inversion found on atom N 12
Population inversion found on atom C 13
Population inversion found on atom O 14

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Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
C 1	-0.22045	1.99999	4.20280	0.01766	6.22045
C 2	0.09547	1.99999	3.86635	0.03820	5.90453
C 3	-0.13861	1.99999	4.12201	0.01662	6.13861
C 4	-0.21372	1.99999	4.18549	0.02824	6.21372
C 5	-0.21349	1.99999	4.19447	0.01903	6.21349
C 6	-0.18939	1.99999	4.17055	0.01885	6.18939
H 7	0.21153	0.00000	0.78644	0.00202	0.78847
H 8	0.20889	0.00000	0.78562	0.00549	0.79111
H 9	0.20972	0.00000	0.78763	0.00265	0.79028
H 10	0.20992	0.00000	0.78784	0.00224	0.79008
H 11	0.20997	0.00000	0.78783	0.00220	0.79003
N 12	-0.52683	1.99999	5.49850	0.02834	7.52683
C 13	0.84167	1.99999	3.13293	0.02541	5.15833
O 14	-0.48470	2.00000	6.45448	0.03021	8.48470
=====					
* Total *	0.00000	17.99990	43.76293	0.23716	62.00000

Natural Population		
Core	17.99990	(99.9995% of 18)
Valence	43.76293	(99.4612% of 44)
Natural Minimal Basis	61.76284	(99.6175% of 62)
Natural Rydberg Basis	0.23716	(0.3825% of 62)

Atom No	Natural Electron Configuration
C 1	[core]2s(0.97)2p(3.23)3p(0.01)
C 2	[core]2s(0.87)2p(2.99)3p(0.01)3d(0.01)4f(0.01)
C 3	[core]2s(0.97)2p(3.15)3d(0.01)
C 4	[core]2s(0.98)2p(3.21)3p(0.01)3d(0.01)
C 5	[core]2s(0.98)2p(3.22)3p(0.01)
C 6	[core]2s(0.98)2p(3.20)3p(0.01)
H 7	1s(0.79)
H 8	1s(0.79)
H 9	1s(0.79)
H 10	1s(0.79)


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H 11          1s( 0.79)
N 12    [core]2s( 1.27)2p( 4.23)3p( 0.01)3d( 0.01)
C 13    [core]2s( 0.71)2p( 2.42)3p( 0.01)3d( 0.01)
O 14    [core]2s( 1.71)2p( 4.74)3d( 0.02)

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NATURAL BOND ORBITAL ANALYSIS:

Cycle	Max Ctr	Occ Thresh	Occupancies		Lewis Structure				Low occ (L)	High occ (NL)
			Lewis	non-Lewis	CR	BD	nC	LP		
1	2	1.90	57.89803	4.10197	9	16	0	6	5	5
2	2	1.68	58.55641	3.44359	9	17	0	5	4	5
3	2	1.66	59.21156	2.78844	9	18	0	4	3	5
4	2	1.65	59.21021	2.78979	9	18	0	4	3	5
5	2	1.64	59.87685	2.12315	9	19	0	3	0	5
6	2	1.59	59.87685	2.12315	9	19	0	3	0	5
7	2	1.58	59.47373	2.52627	9	18	0	4	0	5
8	2	1.64	59.87685	2.12315	9	19	0	3	0	5

Structure accepted: No low occupancy Lewis orbitals

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Core                17.99990 ( 99.999% of 18)
Valence Lewis      41.87695 ( 95.175% of 44)
=====
Total Lewis        59.87685 ( 96.576% of 62)
-----
Valence non-Lewis  1.99506 (  3.218% of 62)
Rydberg non-Lewis  0.12809 (  0.207% of 62)
=====
Total non-Lewis    2.12315 (  3.424% of 62)
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(Occupancy)  Bond orbital / Coefficients / Hybrids
----- Lewis -----
1. (1.99999) CR ( 1) C 1          s(100.00%)
    1.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000
2. (1.99999) CR ( 1) C 2          s(100.00%)
    1.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000  0.0000  0.0000  0.0000  0.0000
    0.0000
3. (1.99999) CR ( 1) C 3          s(100.00%)
    1.0000  0.0000  0.0000  0.0000  0.0000

```


9. (2.00000) CR (1) O 14 s(100.00%)
1.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000

10. (1.64584) LP (1) N 12 s(24.33%)p 3.10(75.45%)d 0.01(0.19%)
f 0.00(0.03%)
0.0000 0.4932 -0.0008 0.0061 -0.0002
-0.1740 -0.0066 -0.0032 -0.0010 0.8508
0.0148 0.0012 -0.0005 0.0000 0.0000
0.0000 0.0000 0.0259 -0.0050 -0.0004
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0272 -0.0053 -0.0030 0.0183
0.0088 0.0010 0.0000 0.0000 0.0018
-0.0005 -0.0071 -0.0003 0.0000 0.0000
0.0000 0.0000 -0.0055 0.0009 0.0148
0.0011

11. (1.97764) LP (1) O 14 s(62.72%)p 0.59(37.16%)d 0.00(0.11%)
f 0.00(0.00%)
0.0000 0.7920 0.0039 0.0015 0.0000
0.6080 0.0068 -0.0005 0.0037 -0.0431
-0.0008 0.0001 -0.0003 0.0000 0.0000
0.0000 0.0000 0.0038 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0288 -0.0033 0.0012 0.0162
0.0023 -0.0009 0.0000 0.0000 -0.0042
0.0002 0.0003 0.0000 0.0000 0.0000
0.0000 0.0000 0.0053 -0.0003 -0.0011
0.0001

12. (1.64719) LP (2) O 14 s(0.00%)p 1.00(99.58%)d 0.00(0.39%)
f 0.00(0.03%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.9979 0.0056
-0.0002 -0.0004 0.0000 0.0000 0.0000
-0.0625 0.0024 -0.0006 0.0027 -0.0001
0.0001 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0112 -0.0003 0.0000
0.0000 0.0000 0.0000 0.0139 0.0003
-0.0016 0.0000 0.0000 0.0000 0.0000
0.0000

13. (1.97683) BD (1) C 1- C 2
(48.77%) 0.6983* C 1 s(34.89%)p 1.86(64.90%)d 0.00(0.16%)
f 0.00(0.05%)
0.0000 0.5906 -0.0019 0.0029 0.0004
0.0050 0.0205 0.0019 0.0000 0.8053
0.0103 0.0008 0.0017 0.0000 0.0000
0.0000 0.0000 -0.0060 0.0046 0.0029
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0329 -0.0025 -0.0027 -0.0218
-0.0015 -0.0011 0.0000 0.0000 0.0012
0.0012 -0.0148 0.0053 0.0000 0.0000
0.0000 0.0000 0.0021 0.0039 -0.0140
0.0051
(51.23%) 0.7158* C 2 s(36.38%)p 1.74(63.45%)d 0.00(0.10%)
f 0.00(0.06%)
0.0000 0.6030 0.0131 -0.0009 0.0034

0.0588 0.0145 0.0019 0.0012 -0.7942
0.0080 -0.0050 -0.0025 0.0000 0.0000
0.0000 0.0000 0.0090 -0.0013 0.0025
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0190 -0.0186 0.0037 0.0091
-0.0111 0.0004 0.0000 0.0000 -0.0011
-0.0001 0.0156 0.0092 0.0000 0.0000
0.0000 0.0000 -0.0019 -0.0015 0.0143
0.0086

14. (1.97777) BD (1) C 1- C 6
(50.47%) 0.7104* C 1 s(36.53%)p 1.73(63.26%)d 0.00(0.16%)
f 0.00(0.06%)

0.0000 0.6042 -0.0157 0.0007 0.0007
-0.6626 0.0058 -0.0019 -0.0021 -0.4388
-0.0313 -0.0030 -0.0018 0.0000 0.0000
0.0000 0.0000 0.0210 0.0077 0.0063
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0203 0.0005 -0.0008 -0.0244
0.0021 -0.0022 0.0000 0.0000 0.0138
-0.0043 0.0066 -0.0037 0.0000 0.0000
0.0000 0.0000 -0.0013 -0.0046 -0.0164
0.0055

(49.53%) 0.7038* C 6 s(35.70%)p 1.80(64.09%)d 0.00(0.15%)
f 0.00(0.06%)

0.0000 0.5974 -0.0099 -0.0002 0.0010
0.6959 0.0295 0.0017 -0.0003 0.3942
-0.0193 -0.0010 0.0001 0.0000 0.0000
0.0000 0.0000 0.0282 0.0024 -0.0004
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0103 -0.0013 0.0055 -0.0238
0.0037 0.0013 0.0000 0.0000 -0.0131
0.0045 -0.0095 0.0014 0.0000 0.0000
0.0000 0.0000 -0.0042 -0.0044 0.0153
-0.0050

15. (1.68239) BD (2) C 1- C 6
(51.33%) 0.7164* C 1 s(0.00%)p 1.00(99.92%)d 0.00(0.03%)
f 0.00(0.05%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.9996 -0.0062
0.0030 -0.0012 0.0000 0.0000 0.0000
-0.0102 -0.0116 0.0012 0.0008 0.0066
0.0034 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0189 0.0059 0.0000
0.0000 0.0000 0.0000 0.0004 0.0013
-0.0065 -0.0078 0.0000 0.0000 0.0000
0.0000

(48.67%) 0.6977* C 6 s(0.00%)p 1.00(99.93%)d 0.00(0.03%)
f 0.00(0.04%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.9996 -0.0093
0.0001 0.0005 0.0000 0.0000 0.0000
0.0079 0.0019 -0.0002 0.0105 0.0094
-0.0068 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0167 0.0067 0.0000
0.0000 0.0000 0.0000 -0.0052 -0.0063
-0.0029 -0.0028 0.0000 0.0000 0.0000
0.0000

16. (1.97779) BD (1) C 1- H 7
(60.63%) 0.7786* C 1 s(28.42%)p 2.52(71.47%)d 0.00(0.08%)
f 0.00(0.04%)

0.0000 0.5329 0.0137 -0.0036 -0.0013

0.7474 -0.0147 -0.0034 -0.0021 -0.3949
-0.0016 0.0022 0.0005 0.0000 0.0000
0.0000 0.0000 -0.0166 0.0042 -0.0045
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0155 -0.0026 0.0013 -0.0121
-0.0071 -0.0016 0.0000 0.0000 -0.0145
0.0035 0.0072 -0.0021 0.0000 0.0000
0.0000 0.0000 0.0021 -0.0007 -0.0072
0.0054

(39.37%) 0.6275* H 7 s(99.96%)p 0.00(0.03%)d 0.00(0.01%)
0.9998 -0.0008 0.0010 0.0000 0.0088
-0.0125 0.0047 -0.0006 0.0078 -0.0015
0.0000 0.0000 0.0000 0.0009 -0.0047
0.0000 0.0000 0.0000 0.0000 -0.0021
0.0037 0.0005 -0.0035

17. (1.97129) BD (1) C 2- C 3
(52.00%) 0.7211* C 2 s(36.08%)p 1.76(63.60%)d 0.01(0.23%)
f 0.00(0.10%)

0.0000 0.6006 -0.0062 0.0000 -0.0023
-0.6863 0.0149 -0.0071 0.0025 0.4053
0.0227 0.0047 -0.0011 0.0000 0.0000
0.0000 0.0000 -0.0195 -0.0175 0.0032
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0233 0.0111 -0.0010 0.0270
-0.0127 0.0004 0.0000 0.0000 0.0170
0.0067 -0.0095 -0.0042 0.0000 0.0000
0.0000 0.0000 -0.0039 0.0013 0.0213
0.0071

(48.00%) 0.6928* C 3 s(34.91%)p 1.85(64.73%)d 0.01(0.28%)
f 0.00(0.09%)

0.0000 0.5908 -0.0048 0.0058 -0.0006
0.7179 0.0110 0.0038 -0.3630 -0.0008
0.0000 0.0000 0.0000 0.0000 -0.0455
0.0044 0.0053 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0101 0.0036
-0.0036 -0.0215 -0.0064 -0.0024 0.0000
0.0000 -0.0202 0.0023 0.0123 0.0002
0.0000 0.0000 0.0000 0.0000 0.0111
0.0001 -0.0094 0.0091

18. (1.64084) BD (2) C 2- C 3
(51.43%) 0.7172* C 2 s(0.00%)p 1.00(99.78%)d 0.00(0.17%)
f 0.00(0.05%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.9987 0.0016
-0.0197 -0.0012 0.0000 0.0000 0.0000
0.0255 -0.0137 -0.0093 -0.0281 0.0026
0.0039 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0176 -0.0112 0.0000
0.0000 0.0000 0.0000 0.0013 -0.0008
0.0062 -0.0039 0.0000 0.0000 0.0000
0.0000

(48.57%) 0.6969* C 3 s(0.00%)p 1.00(99.78%)d 0.00(0.10%)
f 0.00(0.12%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9989 0.0006 -0.0035 0.0000
0.0000 0.0000 0.0085 0.0049 0.0009
-0.0300 -0.0011 -0.0051 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 -0.0337
-0.0006 0.0000 0.0000 0.0000 0.0000
0.0010 -0.0034 0.0029 0.0019 0.0000
0.0000 0.0000 0.0000

19. (1.96572) BD (1) C 2- N 12
 (38.85%) 0.6233* C 2 s(27.28%)p 2.66(72.65%)d 0.00(0.04%)
 f 0.00(0.03%)
 0.0000 0.5221 -0.0143 0.0015 -0.0015
 0.7237 0.0018 0.0041 0.0024 0.4499
 0.0176 0.0053 0.0015 0.0000 0.0000
 0.0000 0.0000 -0.0021 0.0094 -0.0105
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0027 0.0071 -0.0012 0.0033
 -0.0111 0.0002 0.0000 0.0000 -0.0091
 -0.0059 -0.0023 -0.0044 0.0000 0.0000
 0.0000 0.0000 0.0073 -0.0021 0.0051
 0.0058
 (61.15%) 0.7820* N 12 s(38.17%)p 1.61(61.59%)d 0.00(0.14%)
 f 0.00(0.10%)
 0.0000 0.6177 0.0107 -0.0034 0.0006
 -0.6176 0.0000 0.0023 -0.0005 -0.4841
 0.0020 0.0031 0.0025 0.0000 0.0000
 0.0000 0.0000 0.0288 -0.0006 0.0018
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 -0.0079 -0.0060 -0.0005 -0.0225
 0.0030 0.0005 0.0000 0.0000 0.0137
 0.0021 0.0104 0.0012 0.0000 0.0000
 0.0000 0.0000 -0.0046 0.0001 -0.0261
 -0.0030

20. (1.97362) BD (1) C 3- C 4
 (49.72%) 0.7051* C 3 s(36.27%)p 1.75(63.41%)d 0.01(0.23%)
 f 0.00(0.10%)
 0.0000 0.6021 0.0105 0.0026 0.0010
 -0.6922 -0.0133 -0.0023 -0.3934 0.0031
 0.0016 0.0000 0.0000 0.0000 0.0403
 -0.0042 -0.0063 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 -0.0028 0.0052
 -0.0039 -0.0233 -0.0029 -0.0008 0.0000
 0.0000 0.0190 -0.0027 0.0155 0.0003
 0.0000 0.0000 0.0000 0.0000 -0.0064
 -0.0009 -0.0156 0.0084
 (50.28%) 0.7091* C 4 s(35.62%)p 1.80(64.01%)d 0.01(0.29%)
 f 0.00(0.09%)
 0.0000 0.5964 -0.0230 0.0015 0.0002
 0.6640 -0.0073 0.0027 -0.0027 0.4438
 0.0454 0.0061 -0.0009 0.0000 0.0000
 0.0000 0.0000 0.0335 0.0041 -0.0028
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0213 0.0060 0.0028 -0.0349
 0.0012 -0.0008 0.0000 0.0000 -0.0180
 -0.0014 -0.0090 0.0025 0.0000 0.0000
 0.0000 0.0000 0.0015 0.0051 0.0206
 -0.0020

21. (1.97082) BD (1) C 3- H 8
 (60.46%) 0.7775* C 3 s(28.66%)p 2.48(71.19%)d 0.00(0.07%)
 f 0.00(0.08%)
 0.0000 0.5353 -0.0036 -0.0074 -0.0010
 -0.0134 -0.0027 -0.0016 0.8435 -0.0146
 0.0006 0.0000 0.0000 0.0000 0.0057
 -0.0026 -0.0005 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 -0.0095 -0.0201
 -0.0026 -0.0099 -0.0091 -0.0043 0.0000
 0.0000 0.0004 0.0004 -0.0258 0.0012
 0.0000 0.0000 0.0000 0.0000 -0.0007
 0.0000 -0.0098 0.0044
 (39.54%) 0.6288* H 8 s(99.95%)p 0.00(0.04%)d 0.00(0.01%)
 0.9998 -0.0028 0.0001 -0.0001 0.0046

-0.0001 -0.0002 -0.0077 -0.0174 0.0032
0.0000 0.0000 0.0000 -0.0014 0.0005
0.0000 0.0000 0.0000 0.0000 -0.0050
-0.0043 -0.0046 -0.0017

22. (1.98304) BD (1) C 4- C 5
(50.13%) 0.7080* C 4 s(36.20%)p 1.76(63.58%)d 0.00(0.16%)
f 0.00(0.06%)

0.0000 0.6016 -0.0033 -0.0036 0.0009
-0.0074 -0.0287 -0.0029 -0.0013 -0.7967
-0.0106 -0.0053 -0.0022 0.0000 0.0000
0.0000 0.0000 -0.0071 -0.0042 -0.0040
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0310 -0.0050 0.0051 -0.0225
-0.0051 -0.0006 0.0000 0.0000 -0.0013
0.0005 0.0158 -0.0055 0.0000 0.0000
0.0000 0.0000 -0.0034 -0.0042 0.0148
-0.0065

(49.87%) 0.7062* C 5 s(35.81%)p 1.79(63.97%)d 0.00(0.16%)
f 0.00(0.06%)

0.0000 0.5983 -0.0097 0.0010 -0.0002
-0.0494 -0.0308 0.0010 0.0008 0.7975
0.0151 -0.0015 0.0015 0.0000 0.0000
0.0000 0.0000 0.0039 0.0019 -0.0045
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0320 -0.0001 -0.0039 -0.0233
0.0013 0.0003 0.0000 0.0000 -0.0004
-0.0011 -0.0160 0.0050 0.0000 0.0000
0.0000 0.0000 -0.0016 -0.0056 -0.0157
0.0042

23. (1.66387) BD (2) C 4- C 5
(49.42%) 0.7030* C 4 s(0.00%)p 1.00(99.89%)d 0.00(0.06%)
f 0.00(0.05%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.9994 -0.0087
-0.0028 0.0014 0.0000 0.0000 0.0000
-0.0066 0.0174 0.0055 -0.0156 -0.0032
0.0015 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0183 0.0064 0.0000
0.0000 0.0000 0.0000 0.0073 0.0073
-0.0032 -0.0044 0.0000 0.0000 0.0000
0.0000

(50.58%) 0.7112* C 5 s(0.00%)p 1.00(99.93%)d 0.00(0.03%)
f 0.00(0.04%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.9996 -0.0109
0.0030 0.0004 0.0000 0.0000 0.0000
0.0031 0.0098 -0.0056 0.0090 0.0090
-0.0037 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0174 0.0062 0.0000
0.0000 0.0000 0.0000 0.0043 0.0053
0.0033 0.0046 0.0000 0.0000 0.0000
0.0000

24. (1.97998) BD (1) C 4- H 9
(60.63%) 0.7786* C 4 s(28.03%)p 2.56(71.83%)d 0.00(0.10%)
f 0.00(0.04%)

0.0000 0.5289 0.0230 0.0020 -0.0010
-0.7439 0.0193 0.0018 0.0003 0.4055
-0.0103 -0.0009 0.0001 0.0000 0.0000
0.0000 0.0000 -0.0224 -0.0096 0.0008
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0149 0.0050 -0.0015 -0.0056

					-0.0116	-0.0030	0.0000	0.0000	0.0156
					0.0031	-0.0083	0.0020	0.0000	0.0000
					0.0000	0.0000	-0.0010	0.0004	0.0064
					-0.0052				
(39.37%)	0.6275* H	9	s(99.96%)p	0.00(0.04%)d	0.00(0.01%)				
					0.9998	-0.0008	-0.0010	0.0001	-0.0130
					0.0101	-0.0068	0.0042	-0.0064	0.0039
					0.0000	0.0000	0.0000	-0.0005	-0.0056
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0030	0.0004	-0.0038		
25. (1.98145)	BD (1) C	5- C	6						
(49.81%)	0.7057* C	5	s(35.73%)p	1.79(64.05%)d	0.00(0.17%)				
				f	0.00(0.06%)				
					0.0000	0.5977	-0.0095	0.0005	-0.0002
					0.6894	-0.0010	0.0007	-0.0005	-0.4050
					-0.0348	0.0018	-0.0005	0.0000	0.0000
					0.0000	0.0000	-0.0244	0.0015	-0.0057
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0219	0.0020	-0.0016	-0.0233
					0.0012	0.0003	0.0000	0.0000	-0.0144
					0.0040	0.0067	-0.0033	0.0000	0.0000
					0.0000	0.0000	0.0043	0.0046	-0.0147
					0.0054				
(50.19%)	0.7085* C	6	s(36.13%)p	1.76(63.67%)d	0.00(0.14%)				
				f	0.00(0.06%)				
					0.0000	0.6010	-0.0095	0.0014	-0.0002
					-0.7151	-0.0271	-0.0033	-0.0018	0.3523
					-0.0203	-0.0012	-0.0003	0.0000	0.0000
					0.0000	0.0000	-0.0268	-0.0014	-0.0013
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0126	-0.0024	0.0070	-0.0224
					0.0023	0.0004	0.0000	0.0000	0.0134
					-0.0054	-0.0083	0.0016	0.0000	0.0000
					0.0000	0.0000	0.0006	0.0051	0.0155
					-0.0049				
26. (1.97963)	BD (1) C	5- H	10						
(60.61%)	0.7785* C	5	s(28.31%)p	2.53(71.55%)d	0.00(0.10%)				
				f	0.00(0.04%)				
					0.0000	0.5318	0.0164	-0.0017	0.0004
					-0.7205	0.0133	-0.0017	-0.0014	-0.4430
					0.0082	-0.0009	0.0011	0.0000	0.0000
					0.0000	0.0000	0.0252	0.0045	-0.0004
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0126	0.0019	0.0001	-0.0095
					-0.0073	0.0045	0.0000	0.0000	0.0144
					-0.0030	0.0089	-0.0017	0.0000	0.0000
					0.0000	0.0000	0.0009	-0.0002	-0.0078
					0.0045				
(39.39%)	0.6276* H	10	s(99.96%)p	0.00(0.04%)d	0.00(0.01%)				
					0.9998	-0.0003	-0.0012	0.0001	-0.0106
					0.0114	-0.0050	-0.0056	0.0074	-0.0030
					0.0000	0.0000	0.0000	0.0011	-0.0056
					0.0000	0.0000	0.0000	0.0000	0.0001
					-0.0028	0.0000	-0.0040		
27. (1.97891)	BD (1) C	6- H	11						
(60.59%)	0.7784* C	6	s(28.02%)p	2.56(71.85%)d	0.00(0.10%)				
				f	0.00(0.04%)				
					0.0000	0.5291	0.0166	-0.0012	-0.0009
					0.0266	-0.0014	0.0001	-0.0003	-0.8470
					0.0163	0.0041	0.0011	0.0000	0.0000
					0.0000	0.0000	-0.0026	-0.0005	0.0006
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	-0.0277	-0.0044	0.0008	-0.0102

				-0.0067	-0.0054	0.0000	0.0000	-0.0009
				-0.0001	0.0173	-0.0036	0.0000	0.0000
				0.0000	0.0000	-0.0001	0.0006	0.0072
				-0.0047				
(39.41%)	0.6278*	H 11	s(99.96%)p 0.00(0.04%)d 0.00(0.01%)					
				0.9998	-0.0008	-0.0011	0.0001	0.0006
				-0.0003	0.0004	-0.0129	0.0125	-0.0059
				0.0000	0.0000	0.0000	0.0001	-0.0005
				0.0000	0.0000	0.0000	0.0000	-0.0003
				-0.0059	0.0009	-0.0038		
28. (1.98926)	BD (1)	N 12- C 13						
(59.06%)	0.7685*	N 12	s(37.31%)p 1.67(62.24%)d 0.01(0.34%)					
			f 0.00(0.11%)					
				0.0000	0.6107	-0.0110	-0.0039	-0.0004
				0.7638	-0.0139	0.0028	0.0048	-0.1970
				-0.0048	-0.0016	0.0012	0.0000	0.0000
				0.0000	0.0000	-0.0332	-0.0005	-0.0014
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0361	-0.0031	0.0017	-0.0309
				-0.0013	-0.0009	0.0000	0.0000	-0.0193
				-0.0005	0.0018	0.0004	0.0000	0.0000
				0.0000	0.0000	0.0254	0.0008	-0.0058
				-0.0007				
(40.94%)	0.6399*	C 13	s(53.60%)p 0.86(46.25%)d 0.00(0.06%)					
			f 0.00(0.10%)					
				0.0000	0.7320	-0.0139	0.0004	-0.0004
				-0.6775	0.0182	-0.0028	-0.0038	0.0511
				-0.0218	0.0021	-0.0012	0.0000	0.0000
				0.0000	0.0000	0.0026	-0.0037	0.0008
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	-0.0208	0.0023	-0.0019	0.0128
				-0.0008	0.0007	0.0000	0.0000	0.0199
				0.0007	-0.0019	0.0003	0.0000	0.0000
				0.0000	0.0000	-0.0225	-0.0009	0.0072
				-0.0010				
29. (1.92962)	BD (2)	N 12- C 13						
(70.80%)	0.8414*	N 12	s(0.00%)p 1.00(99.74%)d 0.00(0.19%)					
			f 0.00(0.07%)					
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.9986	-0.0104
				0.0010	-0.0012	0.0000	0.0000	0.0000
				0.0274	-0.0036	0.0013	-0.0338	-0.0045
				0.0007	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	-0.0190	-0.0021	0.0000
				0.0000	0.0000	0.0000	0.0171	0.0023
				0.0055	-0.0001	0.0000	0.0000	0.0000
				0.0000				
(29.20%)	0.5404*	C 13	s(0.00%)p 1.00(99.77%)d 0.00(0.16%)					
			f 0.00(0.07%)					
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.9987	0.0155
				-0.0019	-0.0027	0.0000	0.0000	0.0000
				0.0387	0.0088	-0.0042	-0.0053	0.0028
				-0.0005	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	-0.0143	0.0057	0.0000
				0.0000	0.0000	0.0000	0.0195	-0.0053
				0.0038	0.0072	0.0000	0.0000	0.0000
				0.0000				
30. (1.99368)	BD (1)	C 13- O 14						
(35.20%)	0.5933*	C 13	s(39.43%)p 1.53(60.40%)d 0.00(0.08%)					
			f 0.00(0.09%)					

0.0000 0.6278 0.0109 -0.0017 -0.0005
 0.6440 -0.0446 -0.0082 -0.0007 -0.4327
 -0.0070 -0.0023 0.0003 0.0000 0.0000
 0.0000 0.0000 0.0172 -0.0042 0.0009
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 -0.0174 -0.0018 -0.0040 0.0109
 0.0007 0.0023 0.0000 0.0000 -0.0182
 -0.0045 0.0033 -0.0016 0.0000 0.0000
 0.0000 0.0000 0.0198 0.0044 -0.0100
 0.0055
 (64.80%) 0.8050* O 14 s(31.03%)p 2.20(68.29%)d 0.02(0.64%)
 f 0.00(0.05%)
 0.0000 0.5570 -0.0071 -0.0025 0.0001
 -0.7463 0.0179 0.0018 0.0030 -0.3543
 0.0014 -0.0005 0.0001 0.0000 0.0000
 0.0000 0.0000 0.0179 0.0004 0.0001
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0679 0.0004 0.0009 -0.0381
 -0.0009 -0.0002 0.0000 0.0000 0.0127
 -0.0002 0.0012 0.0001 0.0000 0.0000
 0.0000 0.0000 -0.0171 0.0002 -0.0038
 -0.0004

31. (1.98974) BD (2) C 13- O 14
 (26.58%) 0.5155* C 13 s(6.84%)p13.59(92.91%)d 0.03(0.18%)
 f 0.01(0.07%)
 0.0000 0.2611 0.0142 0.0001 0.0026
 0.3485 -0.0133 -0.0016 -0.0007 0.8984
 0.0198 0.0059 -0.0011 0.0000 0.0000
 0.0000 0.0000 -0.0382 0.0099 -0.0037
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 -0.0131 -0.0019 -0.0033 0.0077
 0.0028 0.0008 0.0000 0.0000 -0.0048
 -0.0010 -0.0054 0.0044 0.0000 0.0000
 0.0000 0.0000 0.0149 0.0023 0.0140
 -0.0147
 (73.42%) 0.8569* O 14 s(6.16%)p15.16(93.37%)d 0.07(0.44%)
 f 0.01(0.03%)
 0.0000 0.2481 -0.0043 -0.0017 0.0000
 -0.2553 0.0089 0.0007 0.0014 0.9319
 -0.0053 0.0017 0.0000 0.0000 0.0000
 0.0000 0.0000 -0.0602 0.0006 -0.0003
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0227 0.0002 0.0002 -0.0165
 -0.0005 0.0002 0.0000 0.0000 0.0056
 -0.0001 -0.0044 -0.0001 0.0000 0.0000
 0.0000 0.0000 -0.0043 0.0000 0.0155
 0.0008

----- non-Lewis -----

32. (0.02833) BD*(1) C 1- C 2
 (51.23%) 0.7158* C 1 s(34.89%)p 1.86(64.90%)d 0.00(0.16%)
 f 0.00(0.05%)
 0.0000 0.5906 -0.0019 0.0029 0.0004
 0.0050 0.0205 0.0019 0.0000 0.8053
 0.0103 0.0008 0.0017 0.0000 0.0000
 0.0000 0.0000 -0.0060 0.0046 0.0029
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 -0.0329 -0.0025 -0.0027 -0.0218
 -0.0015 -0.0011 0.0000 0.0000 0.0012
 0.0012 -0.0148 0.0053 0.0000 0.0000
 0.0000 0.0000 0.0021 0.0039 -0.0140
 0.0051
 (48.77%) -0.6983* C 2 s(36.38%)p 1.74(63.45%)d 0.00(0.10%)
 f 0.00(0.06%)

0.0000 0.6030 0.0131 -0.0009 0.0034
0.0588 0.0145 0.0019 0.0012 -0.7942
0.0080 -0.0050 -0.0025 0.0000 0.0000
0.0000 0.0000 0.0090 -0.0013 0.0025
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0190 -0.0186 0.0037 0.0091
-0.0111 0.0004 0.0000 0.0000 -0.0011
-0.0001 0.0156 0.0092 0.0000 0.0000
0.0000 0.0000 -0.0019 -0.0015 0.0143
0.0086

33. (0.01267) BD*(1) C 1- C 6
(49.53%) 0.7038* C 1 s(36.53%)p 1.73(63.26%)d 0.00(0.16%)
f 0.00(0.06%)

0.0000 0.6042 -0.0157 0.0007 0.0007
-0.6626 0.0058 -0.0019 -0.0021 -0.4388
-0.0313 -0.0030 -0.0018 0.0000 0.0000
0.0000 0.0000 0.0210 0.0077 0.0063
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0203 0.0005 -0.0008 -0.0244
0.0021 -0.0022 0.0000 0.0000 0.0138
-0.0043 0.0066 -0.0037 0.0000 0.0000
0.0000 0.0000 -0.0013 -0.0046 -0.0164
0.0055

(50.47%) -0.7104* C 6 s(35.70%)p 1.80(64.09%)d 0.00(0.15%)
f 0.00(0.06%)

0.0000 0.5974 -0.0099 -0.0002 0.0010
0.6959 0.0295 0.0017 -0.0003 0.3942
-0.0193 -0.0010 0.0001 0.0000 0.0000
0.0000 0.0000 0.0282 0.0024 -0.0004
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0103 -0.0013 0.0055 -0.0238
0.0037 0.0013 0.0000 0.0000 -0.0131
0.0045 -0.0095 0.0014 0.0000 0.0000
0.0000 0.0000 -0.0042 -0.0044 0.0153
-0.0050

34. (0.32958) BD*(2) C 1- C 6
(48.67%) 0.6977* C 1 s(0.00%)p 1.00(99.92%)d 0.00(0.03%)
f 0.00(0.05%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 -0.9996 0.0062
-0.0030 0.0012 0.0000 0.0000 0.0000
0.0102 0.0116 -0.0012 -0.0008 -0.0066
-0.0034 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0189 -0.0059 0.0000
0.0000 0.0000 0.0000 -0.0004 -0.0013
0.0065 0.0078 0.0000 0.0000 0.0000
0.0000

(51.33%) -0.7164* C 6 s(0.00%)p 1.00(99.93%)d 0.00(0.03%)
f 0.00(0.04%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 -0.9996 0.0093
-0.0001 -0.0005 0.0000 0.0000 0.0000
-0.0079 -0.0019 0.0002 -0.0105 -0.0094
0.0068 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0167 -0.0067 0.0000
0.0000 0.0000 0.0000 0.0052 0.0063
0.0029 0.0028 0.0000 0.0000 0.0000
0.0000

35. (0.01320) BD*(1) C 1- H 7
(39.37%) 0.6275* C 1 s(28.42%)p 2.52(71.47%)d 0.00(0.08%)
f 0.00(0.04%)

				0.0000	-0.5329	-0.0137	0.0036	0.0013
				-0.7474	0.0147	0.0034	0.0021	0.3949
				0.0016	-0.0022	-0.0005	0.0000	0.0000
				0.0000	0.0000	0.0166	-0.0042	0.0045
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	-0.0155	0.0026	-0.0013	0.0121
				0.0071	0.0016	0.0000	0.0000	0.0145
				-0.0035	-0.0072	0.0021	0.0000	0.0000
				0.0000	0.0000	-0.0021	0.0007	0.0072
				-0.0054				
	(60.63%)	-0.7786* H	7	s(99.96%)	p 0.00(0.03%)	d 0.00(0.01%)		
				-0.9998	0.0008	-0.0010	0.0000	-0.0088
				0.0125	-0.0047	0.0006	-0.0078	0.0015
				0.0000	0.0000	0.0000	-0.0009	0.0047
				0.0000	0.0000	0.0000	0.0000	0.0021
				-0.0037	-0.0005	0.0035		
36.	(0.02201)	BD*(1) C	2- C	3				
	(48.00%)	0.6928* C	2	s(36.08%)	p 1.76(63.60%)	d 0.01(0.23%)		
				f 0.00(0.10%)				
				0.0000	-0.6006	0.0062	0.0000	0.0023
				0.6863	-0.0149	0.0071	-0.0025	-0.4053
				-0.0227	-0.0047	0.0011	0.0000	0.0000
				0.0000	0.0000	0.0195	0.0175	-0.0032
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	-0.0233	-0.0111	0.0010	-0.0270
				0.0127	-0.0004	0.0000	0.0000	-0.0170
				-0.0067	0.0095	0.0042	0.0000	0.0000
				0.0000	0.0000	0.0039	-0.0013	-0.0213
				-0.0071				
	(52.00%)	-0.7211* C	3	s(34.91%)	p 1.85(64.73%)	d 0.01(0.28%)		
				f 0.00(0.09%)				
				0.0000	-0.5908	0.0048	-0.0058	0.0006
				-0.7179	-0.0110	-0.0038	0.3630	0.0008
				0.0000	0.0000	0.0000	0.0000	0.0455
				-0.0044	-0.0053	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	-0.0101	-0.0036
				0.0036	0.0215	0.0064	0.0024	0.0000
				0.0000	0.0202	-0.0023	-0.0123	-0.0002
				0.0000	0.0000	0.0000	0.0000	-0.0111
				-0.0001	0.0094	-0.0091		
37.	(0.38091)	BD*(2) C	2- C	3				
	(48.57%)	0.6969* C	2	s(0.00%)	p 1.00(99.78%)	d 0.00(0.17%)		
				f 0.00(0.05%)				
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	-0.9987	-0.0016
				0.0197	0.0012	0.0000	0.0000	0.0000
				-0.0255	0.0137	0.0093	0.0281	-0.0026
				-0.0039	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0176	0.0112	0.0000
				0.0000	0.0000	0.0000	-0.0013	0.0008
				-0.0062	0.0039	0.0000	0.0000	0.0000
				0.0000				
	(51.43%)	-0.7172* C	3	s(0.00%)	p 1.00(99.78%)	d 0.00(0.10%)		
				f 0.00(0.12%)				
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	-0.9989	-0.0006	0.0035	0.0000
				0.0000	0.0000	-0.0085	-0.0049	-0.0009
				0.0300	0.0011	0.0051	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0337
				0.0006	0.0000	0.0000	0.0000	0.0000
				-0.0010	0.0034	-0.0029	-0.0019	0.0000

0.0000 0.0000 0.0000

38. (0.03169) BD*(1) C 2- N 12
 (61.15%) 0.7820* C 2 s(27.28%)p 2.66(72.65%)d 0.00(0.04%)
 f 0.00(0.03%)
 0.0000 0.5221 -0.0143 0.0015 -0.0015
 0.7237 0.0018 0.0041 0.0024 0.4499
 0.0176 0.0053 0.0015 0.0000 0.0000
 0.0000 0.0000 -0.0021 0.0094 -0.0105
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0027 0.0071 -0.0012 0.0033
 -0.0111 0.0002 0.0000 0.0000 -0.0091
 -0.0059 -0.0023 -0.0044 0.0000 0.0000
 0.0000 0.0000 0.0073 -0.0021 0.0051
 0.0058
 (38.85%) -0.6233* N 12 s(38.17%)p 1.61(61.59%)d 0.00(0.14%)
 f 0.00(0.10%)
 0.0000 0.6177 0.0107 -0.0034 0.0006
 -0.6176 0.0000 0.0023 -0.0005 -0.4841
 0.0020 0.0031 0.0025 0.0000 0.0000
 0.0000 0.0000 0.0288 -0.0006 0.0018
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 -0.0079 -0.0060 -0.0005 -0.0225
 0.0030 0.0005 0.0000 0.0000 0.0137
 0.0021 0.0104 0.0012 0.0000 0.0000
 0.0000 0.0000 -0.0046 0.0001 -0.0261
 -0.0030

39. (0.01143) BD*(1) C 3- C 4
 (50.28%) 0.7091* C 3 s(36.27%)p 1.75(63.41%)d 0.01(0.23%)
 f 0.00(0.10%)
 0.0000 0.6021 0.0105 0.0026 0.0010
 -0.6922 -0.0133 -0.0023 -0.3934 0.0031
 0.0016 0.0000 0.0000 0.0000 0.0403
 -0.0042 -0.0063 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 -0.0028 0.0052
 -0.0039 -0.0233 -0.0029 -0.0008 0.0000
 0.0000 0.0190 -0.0027 0.0155 0.0003
 0.0000 0.0000 0.0000 0.0000 -0.0064
 -0.0009 -0.0156 0.0084
 (49.72%) -0.7051* C 4 s(35.62%)p 1.80(64.01%)d 0.01(0.29%)
 f 0.00(0.09%)
 0.0000 0.5964 -0.0230 0.0015 0.0002
 0.6640 -0.0073 0.0027 -0.0027 0.4438
 0.0454 0.0061 -0.0009 0.0000 0.0000
 0.0000 0.0000 0.0335 0.0041 -0.0028
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0213 0.0060 0.0028 -0.0349
 0.0012 -0.0008 0.0000 0.0000 -0.0180
 -0.0014 -0.0090 0.0025 0.0000 0.0000
 0.0000 0.0000 0.0015 0.0051 0.0206
 -0.0020

40. (0.01101) BD*(1) C 3- H 8
 (39.54%) 0.6288* C 3 s(28.66%)p 2.48(71.19%)d 0.00(0.07%)
 f 0.00(0.08%)
 0.0000 -0.5353 0.0036 0.0074 0.0010
 0.0134 0.0027 0.0016 -0.8435 0.0146
 -0.0006 0.0000 0.0000 0.0000 -0.0057
 0.0026 0.0005 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0095 0.0201
 0.0026 0.0099 0.0091 0.0043 0.0000
 0.0000 -0.0004 -0.0004 0.0258 -0.0012
 0.0000 0.0000 0.0000 0.0000 0.0007
 0.0000 0.0098 -0.0044
 (60.46%) -0.7775* H 8 s(99.95%)p 0.00(0.04%)d 0.00(0.01%)

-0.9998 0.0028 -0.0001 0.0001 -0.0046
0.0001 0.0002 0.0077 0.0174 -0.0032
0.0000 0.0000 0.0000 0.0014 -0.0005
0.0000 0.0000 0.0000 0.0000 0.0050
0.0043 0.0046 0.0017

41. (0.01461) BD*(1) C 4- C 5
(49.87%) 0.7062* C 4 s(36.20%)p 1.76(63.58%)d 0.00(0.16%)
f 0.00(0.06%)

0.0000 0.6016 -0.0033 -0.0036 0.0009
-0.0074 -0.0287 -0.0029 -0.0013 -0.7967
-0.0106 -0.0053 -0.0022 0.0000 0.0000
0.0000 0.0000 -0.0071 -0.0042 -0.0040
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0310 -0.0050 0.0051 -0.0225
-0.0051 -0.0006 0.0000 0.0000 -0.0013
0.0005 0.0158 -0.0055 0.0000 0.0000
0.0000 0.0000 -0.0034 -0.0042 0.0148
-0.0065

(50.13%) -0.7080* C 5 s(35.81%)p 1.79(63.97%)d 0.00(0.16%)
f 0.00(0.06%)

0.0000 0.5983 -0.0097 0.0010 -0.0002
-0.0494 -0.0308 0.0010 0.0008 0.7975
0.0151 -0.0015 0.0015 0.0000 0.0000
0.0000 0.0000 0.0039 0.0019 -0.0045
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0320 -0.0001 -0.0039 -0.0233
0.0013 0.0003 0.0000 0.0000 -0.0004
-0.0011 -0.0160 0.0050 0.0000 0.0000
0.0000 0.0000 -0.0016 -0.0056 -0.0157
0.0042

42. (0.33812) BD*(2) C 4- C 5
(50.58%) 0.7112* C 4 s(0.00%)p 1.00(99.89%)d 0.00(0.06%)
f 0.00(0.05%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.9994 -0.0087
-0.0028 0.0014 0.0000 0.0000 0.0000
-0.0066 0.0174 0.0055 -0.0156 -0.0032
0.0015 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0183 0.0064 0.0000
0.0000 0.0000 0.0000 0.0073 0.0073
-0.0032 -0.0044 0.0000 0.0000 0.0000
0.0000

(49.42%) -0.7030* C 5 s(0.00%)p 1.00(99.93%)d 0.00(0.03%)
f 0.00(0.04%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.9996 -0.0109
0.0030 0.0004 0.0000 0.0000 0.0000
0.0031 0.0098 -0.0056 0.0090 0.0090
-0.0037 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0174 0.0062 0.0000
0.0000 0.0000 0.0000 0.0043 0.0053
0.0033 0.0046 0.0000 0.0000 0.0000
0.0000

43. (0.01394) BD*(1) C 4- H 9
(39.37%) 0.6275* C 4 s(28.03%)p 2.56(71.83%)d 0.00(0.10%)
f 0.00(0.04%)

0.0000 -0.5289 -0.0230 -0.0020 0.0010
0.7439 -0.0193 -0.0018 -0.0003 -0.4055
0.0103 0.0009 -0.0001 0.0000 0.0000
0.0000 0.0000 0.0224 0.0096 -0.0008
0.0000 0.0000 0.0000 0.0000 0.0000

				0.0000	-0.0149	-0.0050	0.0015	0.0056
				0.0116	0.0030	0.0000	0.0000	-0.0156
				-0.0031	0.0083	-0.0020	0.0000	0.0000
				0.0000	0.0000	0.0010	-0.0004	-0.0064
				0.0052				
	(60.63%)	-0.7786*	H 9	s(99.96%)	p 0.00(0.04%)	d 0.00(0.01%)		
				-0.9998	0.0008	0.0010	-0.0001	0.0130
				-0.0101	0.0068	-0.0042	0.0064	-0.0039
				0.0000	0.0000	0.0000	0.0005	0.0056
				0.0000	0.0000	0.0000	0.0000	0.0000
				-0.0030	-0.0004	0.0038		
44.	(0.01409)	BD*(1)	C 5- C 6					
	(50.19%)	0.7085*	C 5	s(35.73%)	p 1.79(64.05%)	d 0.00(0.17%)		
				f 0.00(0.06%)				
				0.0000	-0.5977	0.0095	-0.0005	0.0002
				-0.6894	0.0010	-0.0007	0.0005	0.4050
				0.0348	-0.0018	0.0005	0.0000	0.0000
				0.0000	0.0000	0.0244	-0.0015	0.0057
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	-0.0219	-0.0020	0.0016	0.0233
				-0.0012	-0.0003	0.0000	0.0000	0.0144
				-0.0040	-0.0067	0.0033	0.0000	0.0000
				0.0000	0.0000	-0.0043	-0.0046	0.0147
				-0.0054				
	(49.81%)	-0.7057*	C 6	s(36.13%)	p 1.76(63.67%)	d 0.00(0.14%)		
				f 0.00(0.06%)				
				0.0000	-0.6010	0.0095	-0.0014	0.0002
				0.7151	0.0271	0.0033	0.0018	-0.3523
				0.0203	0.0012	0.0003	0.0000	0.0000
				0.0000	0.0000	0.0268	0.0014	0.0013
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	-0.0126	0.0024	-0.0070	0.0224
				-0.0023	-0.0004	0.0000	0.0000	-0.0134
				0.0054	0.0083	-0.0016	0.0000	0.0000
				0.0000	0.0000	-0.0006	-0.0051	-0.0155
				0.0049				
45.	(0.01388)	BD*(1)	C 5- H 10					
	(39.39%)	0.6276*	C 5	s(28.31%)	p 2.53(71.55%)	d 0.00(0.10%)		
				f 0.00(0.04%)				
				0.0000	-0.5318	-0.0164	0.0017	-0.0004
				0.7205	-0.0133	0.0017	0.0014	0.4430
				-0.0082	0.0009	-0.0011	0.0000	0.0000
				0.0000	0.0000	-0.0252	-0.0045	0.0004
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	-0.0126	-0.0019	-0.0001	0.0095
				0.0073	-0.0045	0.0000	0.0000	-0.0144
				0.0030	-0.0089	0.0017	0.0000	0.0000
				0.0000	0.0000	-0.0009	0.0002	0.0078
				-0.0045				
	(60.61%)	-0.7785*	H 10	s(99.96%)	p 0.00(0.04%)	d 0.00(0.01%)		
				-0.9998	0.0003	0.0012	-0.0001	0.0106
				-0.0114	0.0050	0.0056	-0.0074	0.0030
				0.0000	0.0000	0.0000	-0.0011	0.0056
				0.0000	0.0000	0.0000	0.0000	-0.0001
				0.0028	0.0000	0.0040		
46.	(0.01354)	BD*(1)	C 6- H 11					
	(39.41%)	0.6278*	C 6	s(28.02%)	p 2.56(71.85%)	d 0.00(0.10%)		
				f 0.00(0.04%)				
				0.0000	-0.5291	-0.0166	0.0012	0.0009
				-0.0266	0.0014	-0.0001	0.0003	0.8470
				-0.0163	-0.0041	-0.0011	0.0000	0.0000
				0.0000	0.0000	0.0026	0.0005	-0.0006
				0.0000	0.0000	0.0000	0.0000	0.0000

			0.0000	0.0277	0.0044	-0.0008	0.0102
			0.0067	0.0054	0.0000	0.0000	0.0009
			0.0001	-0.0173	0.0036	0.0000	0.0000
			0.0000	0.0000	0.0001	-0.0006	-0.0072
			0.0047				
(60.59%)	-0.7784*	H 11	s(99.96%)	p 0.00(0.04%)	d 0.00(0.01%)		
			-0.9998	0.0008	0.0011	-0.0001	-0.0006
			0.0003	-0.0004	0.0129	-0.0125	0.0059
			0.0000	0.0000	0.0000	-0.0001	0.0005
			0.0000	0.0000	0.0000	0.0000	0.0003
			0.0059	-0.0009	0.0038		
47. (0.02079)	BD*(1)	N 12- C 13					
(40.94%)	0.6399*	N 12	s(37.31%)	p 1.67(62.24%)	d 0.01(0.34%)		
			f 0.00(0.11%)				
			0.0000	-0.6107	0.0110	0.0039	0.0004
			-0.7638	0.0139	-0.0028	-0.0048	0.1970
			0.0048	0.0016	-0.0012	0.0000	0.0000
			0.0000	0.0000	0.0332	0.0005	0.0014
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	-0.0361	0.0031	-0.0017	0.0309
			0.0013	0.0009	0.0000	0.0000	0.0193
			0.0005	-0.0018	-0.0004	0.0000	0.0000
			0.0000	0.0000	-0.0254	-0.0008	0.0058
			0.0007				
(59.06%)	-0.7685*	C 13	s(53.60%)	p 0.86(46.25%)	d 0.00(0.06%)		
			f 0.00(0.10%)				
			0.0000	-0.7320	0.0139	-0.0004	0.0004
			0.6775	-0.0182	0.0028	0.0038	-0.0511
			0.0218	-0.0021	0.0012	0.0000	0.0000
			0.0000	0.0000	-0.0026	0.0037	-0.0008
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0208	-0.0023	0.0019	-0.0128
			0.0008	-0.0007	0.0000	0.0000	-0.0199
			-0.0007	0.0019	-0.0003	0.0000	0.0000
			0.0000	0.0000	0.0225	0.0009	-0.0072
			0.0010				
48. (0.36343)	BD*(2)	N 12- C 13					
(29.20%)	0.5404*	N 12	s(0.00%)	p 1.00(99.74%)	d 0.00(0.19%)		
			f 0.00(0.07%)				
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	-0.9986	0.0104
			-0.0010	0.0012	0.0000	0.0000	0.0000
			-0.0274	0.0036	-0.0013	0.0338	0.0045
			-0.0007	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0190	0.0021	0.0000
			0.0000	0.0000	0.0000	-0.0171	-0.0023
			-0.0055	0.0001	0.0000	0.0000	0.0000
			0.0000				
(70.80%)	-0.8414*	C 13	s(0.00%)	p 1.00(99.77%)	d 0.00(0.16%)		
			f 0.00(0.07%)				
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	-0.9987	-0.0155
			0.0019	0.0027	0.0000	0.0000	0.0000
			-0.0387	-0.0088	0.0042	0.0053	-0.0028
			0.0005	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0143	-0.0057	0.0000
			0.0000	0.0000	0.0000	-0.0195	0.0053
			-0.0038	-0.0072	0.0000	0.0000	0.0000
			0.0000				
49. (0.07943)	BD*(1)	C 13- O 14					
(64.80%)	0.8050*	C 13	s(39.43%)	p 1.53(60.40%)	d 0.00(0.08%)		

f 0.00(0.09%)
0.0000 0.6278 0.0109 -0.0017 -0.0005
0.6440 -0.0446 -0.0082 -0.0007 -0.4327
-0.0070 -0.0023 0.0003 0.0000 0.0000
0.0000 0.0000 0.0172 -0.0042 0.0009
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0174 -0.0018 -0.0040 0.0109
0.0007 0.0023 0.0000 0.0000 -0.0182
-0.0045 0.0033 -0.0016 0.0000 0.0000
0.0000 0.0000 0.0198 0.0044 -0.0100
0.0055

(35.20%) -0.5933* O 14 s(31.03%)p 2.20(68.29%)d 0.02(0.64%)
f 0.00(0.05%)

0.0000 0.5570 -0.0071 -0.0025 0.0001
-0.7463 0.0179 0.0018 0.0030 -0.3543
0.0014 -0.0005 0.0001 0.0000 0.0000
0.0000 0.0000 0.0179 0.0004 0.0001
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0679 0.0004 0.0009 -0.0381
-0.0009 -0.0002 0.0000 0.0000 0.0127
-0.0002 0.0012 0.0001 0.0000 0.0000
0.0000 0.0000 -0.0171 0.0002 -0.0038
-0.0004

50. (0.28242) BD*(2) C 13- O 14

(73.42%) 0.8569* C 13 s(6.84%)p13.59(92.91%)d 0.03(0.18%)
f 0.01(0.07%)

0.0000 0.2611 0.0142 0.0001 0.0026
0.3485 -0.0133 -0.0016 -0.0007 0.8984
0.0198 0.0059 -0.0011 0.0000 0.0000
0.0000 0.0000 -0.0382 0.0099 -0.0037
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0131 -0.0019 -0.0033 0.0077
0.0028 0.0008 0.0000 0.0000 -0.0048
-0.0010 -0.0054 0.0044 0.0000 0.0000
0.0000 0.0000 0.0149 0.0023 0.0140
-0.0147

(26.58%) -0.5155* O 14 s(6.16%)p15.16(93.37%)d 0.07(0.44%)
f 0.01(0.03%)

0.0000 0.2481 -0.0043 -0.0017 0.0000
-0.2553 0.0089 0.0007 0.0014 0.9319
-0.0053 0.0017 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0602 0.0006 -0.0003
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0227 0.0002 0.0002 -0.0165
-0.0005 0.0002 0.0000 0.0000 0.0056
-0.0001 -0.0044 -0.0001 0.0000 0.0000
0.0000 0.0000 -0.0043 0.0000 0.0155
0.0008

51. (0.00423) RY (1) C 1

s(1.38%)p61.74(84.94%)d 8.16(11.23%)
f 1.79(2.46%)

0.0000 -0.0079 0.1126 0.0319 0.0004
0.0180 0.7853 -0.0076 0.0115 -0.0044
-0.4783 -0.0193 0.0542 0.0000 0.0000
0.0000 0.0000 -0.0420 -0.0359 0.2003
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0299 0.0090 -0.1904 0.1368
-0.1098 0.0334 0.0000 0.0000 0.0039
0.0171 -0.0333 -0.0095 0.0000 0.0000
0.0000 0.0000 -0.1275 -0.0541 0.0407
0.0474

52. (0.00175) RY (2) C 1

s(0.06%)p99.99(49.42%)d99.99(8.71%)
f99.99(41.81%)

0.0000 -0.0038 0.0211 0.0094 -0.0091

	0.0078	-0.4424	-0.0770	0.0187	0.0265
	-0.5362	-0.0389	0.0489	0.0000	0.0000
	0.0000	0.0000	0.1367	0.0688	-0.1648
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0627	0.0819	-0.1587	0.0149
	-0.0197	0.0098	0.0000	0.0000	-0.0639
	-0.0470	-0.0838	-0.0675	0.0000	0.0000
	0.0000	0.0000	-0.5488	-0.3132	-0.0294
	-0.0038				
53. (0.00092) RY (3) C 1	s(0.00%)	p 1.00(84.82%)	d 0.15(12.55%)		
		f 0.03(2.64%)			
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0020	0.8147
	-0.4293	0.0159	0.0000	0.0000	0.0000
	-0.1542	-0.0164	-0.0773	0.1882	0.2449
	0.0070	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	-0.0294	-0.0178	0.0000
	0.0000	0.0000	0.0000	0.1262	0.0681
	-0.0670	0.0108	0.0000	0.0000	0.0000
	0.0000				
54. (0.00071) RY (4) C 1	s(60.39%)	p 0.10(5.74%)	d 0.47(28.21%)		
		f 0.09(5.66%)			
	0.0000	0.0102	0.7710	0.0929	0.0268
	-0.0239	0.0286	0.0439	0.0184	-0.0026
	0.2279	0.0419	-0.0023	0.0000	0.0000
	0.0000	0.0000	-0.0442	-0.3486	-0.2679
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0440	0.2199	0.0207	0.0672
	-0.1715	-0.0469	0.0000	0.0000	-0.0001
	0.0167	0.1062	0.0762	0.0000	0.0000
	0.0000	0.0000	-0.1541	-0.0462	-0.1081
	-0.0409				
55. (0.00050) RY (5) C 1	s(11.38%)	p 2.49(28.30%)	d 2.55(29.03%)		
		f 2.75(31.29%)			
	0.0000	0.0049	0.3059	0.1212	0.0744
	-0.0081	-0.2668	-0.0272	-0.0029	0.0051
	-0.4559	-0.0381	-0.0400	0.0000	0.0000
	0.0000	0.0000	-0.0762	0.1306	0.0099
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.2648	-0.1724	0.2444	0.2533
	-0.1912	0.0841	0.0000	0.0000	0.0649
	0.0280	0.0829	0.0246	0.0000	0.0000
	0.0000	0.0000	0.4454	0.1357	0.1678
	0.2356				
56. (0.00038) RY (6) C 1	s(0.00%)	p 1.00(15.00%)	d 4.15(62.29%)		
		f 1.51(22.71%)			
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0050	-0.3124
	-0.2285	-0.0127	0.0000	0.0000	0.0000
	0.3907	0.1497	-0.1351	0.5110	0.3450
	-0.2225	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	-0.0319	-0.0182	0.0000
	0.0000	0.0000	0.0000	0.2023	0.2733
	0.2657	0.1987	0.0000	0.0000	0.0000
	0.0000				
57. (0.00028) RY (7) C 1	s(5.63%)	p 5.46(30.71%)	d 7.71(43.39%)		
		f 3.60(20.28%)			
	0.0000	0.0075	0.0812	0.1865	-0.1219
	-0.0027	0.0169	0.4034	0.0040	-0.0140
	0.2771	0.2589	0.0053	0.0000	0.0000
	0.0000	0.0000	0.1329	0.4499	0.0259

		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	-0.1983	-0.2480	-0.2602	0.1319
		-0.1542	0.0582	0.0000	0.0000	0.1684
		0.1244	0.1061	0.1109	0.0000	0.0000
		0.0000	0.0000	-0.2363	-0.1399	0.2160
		0.1156				
58.	(0.00015) RY (8) C 1	s(24.99%)p	0.17(4.28%)d	2.14(53.49%)		
		f	0.69(17.24%)			
		0.0000	-0.0218	0.3952	-0.2777	0.1272
		0.0019	-0.0191	0.0583	-0.0597	-0.0002
		-0.1475	0.1095	-0.0420	0.0000	0.0000
		0.0000	0.0000	-0.1560	0.3059	0.1688
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	-0.0085	-0.1962	-0.0665	-0.4248
		0.3582	-0.1916	0.0000	0.0000	0.2291
		0.0569	-0.0819	0.0362	0.0000	0.0000
		0.0000	0.0000	0.0928	-0.0821	-0.2187
		-0.2131				
59.	(0.00010) RY (9) C 1	s(10.35%)p	1.02(10.55%)d	6.74(69.76%)		
		f	0.90(9.34%)			
60.	(0.00006) RY (10) C 1	s(2.16%)p	13.60(29.43%)d	24.23(52.44%)		
		f	7.38(15.97%)			
61.	(0.00004) RY (11) C 1	s(0.00%)p	1.00(37.53%)d	0.87(32.75%)		
		f	0.79(29.72%)			
62.	(0.00003) RY (12) C 1	s(3.88%)p	14.15(54.96%)d	6.38(24.78%)		
		f	4.22(16.37%)			
63.	(0.00002) RY (13) C 1	s(9.60%)p	2.19(21.03%)d	3.48(33.37%)		
		f	3.75(36.00%)			
64.	(0.00001) RY (14) C 1	s(13.39%)p	3.21(43.00%)d	0.71(9.44%)		
		f	2.55(34.17%)			
65.	(0.00001) RY (15) C 1	s(0.00%)p	1.00(6.23%)d	12.24(76.24%)		
		f	2.81(17.53%)			
66.	(0.00001) RY (16) C 1	s(14.54%)p	0.50(7.32%)d	2.21(32.19%)		
		f	3.16(45.95%)			
67.	(0.00000) RY (17) C 1	s(10.70%)p	1.18(12.62%)d	3.56(38.09%)		
		f	3.61(38.59%)			
68.	(0.00000) RY (18) C 1	s(1.25%)p	18.57(23.20%)d	38.56(48.17%)		
		f	21.91(27.38%)			
69.	(0.00000) RY (19) C 1	s(18.42%)p	0.58(10.60%)d	2.45(45.22%)		
		f	1.40(25.75%)			
70.	(0.00000) RY (20) C 1	s(6.18%)p	0.81(5.01%)d	8.61(53.23%)		
		f	5.76(35.59%)			
71.	(0.00000) RY (21) C 1	s(0.00%)p	1.00(34.42%)d	1.27(43.63%)		
		f	0.64(21.95%)			
72.	(0.00000) RY (22) C 1	s(0.00%)p	1.00(11.37%)d	7.19(81.68%)		
		f	0.61(6.95%)			
73.	(0.00000) RY (23) C 1	s(1.58%)p	10.88(17.23%)d	19.70(31.20%)		
		f	31.56(49.99%)			
74.	(0.00000) RY (24) C 1	s(0.00%)p	1.00(8.38%)d	8.03(67.29%)		
		f	2.90(24.33%)			
75.	(0.00000) RY (25) C 1	s(0.00%)p	1.00(3.12%)d	19.84(61.99%)		
		f	11.17(34.89%)			
76.	(0.00000) RY (26) C 1	s(5.69%)p	3.65(20.74%)d	1.27(7.25%)		
		f	11.66(66.33%)			
77.	(0.00000) RY (27) C 1	s(0.00%)p	1.00(64.63%)d	0.23(14.68%)		
		f	0.32(20.69%)			
78.	(0.00000) RY (28) C 1	s(2.18%)p	2.23(4.88%)d	33.86(73.97%)		
		f	8.68(18.96%)			
79.	(0.00000) RY (29) C 1	s(2.76%)p	6.42(17.70%)d	11.36(31.31%)		
		f	17.50(48.24%)			
80.	(0.00000) RY (30) C 1	s(0.00%)p	1.00(3.36%)d	16.00(53.77%)		
		f	12.76(42.87%)			
81.	(0.00000) RY (31) C 1	s(0.00%)p	1.00(0.62%)d	13.26(8.16%)		

					f99.99(91.22%)
82.	(0.00000)	RY (32)	C 1	s(2.77%)	p 5.88(16.32%)d 5.43(15.07%)
					f23.73(65.84%)
83.	(0.00000)	RY (33)	C 1	s(15.73%)	p 0.83(13.00%)d 1.28(20.18%)
					f 3.25(51.09%)
84.	(0.00000)	RY (34)	C 1	s(26.23%)	p 1.16(30.41%)d 0.89(23.46%)
					f 0.76(19.90%)
85.	(0.00000)	RY (35)	C 1	s(0.00%)	p 1.00(1.29%)d 8.30(10.74%)
					f68.00(87.97%)
86.	(0.00000)	RY (36)	C 1	s(0.00%)	p 1.00(4.27%)d 7.03(30.01%)
					f15.41(65.73%)
87.	(0.00000)	RY (37)	C 1	s(0.00%)	p 1.00(2.53%)d12.53(31.69%)
					f26.01(65.78%)
88.	(0.00000)	RY (38)	C 1	s(0.00%)	p 1.00(22.52%)d 0.56(12.50%)
					f 2.88(64.97%)
89.	(0.00000)	RY (39)	C 1	s(38.03%)	p 0.77(29.41%)d 0.25(9.43%)
					f 0.61(23.13%)
90.	(0.00000)	RY (40)	C 1	s(5.34%)	p 0.53(2.83%)d13.15(70.17%)
					f 4.06(21.66%)
91.	(0.00000)	RY (41)	C 1	s(5.55%)	p 4.82(26.75%)d 6.63(36.82%)
					f 5.56(30.87%)
92.	(0.01245)	RY (1)	C 2	s(0.57%)	p99.44(56.38%)d67.64(38.35%)
					f 8.31(4.71%)
					0.0000 -0.0231 0.0712 0.0039 0.0072
					0.0105 0.3937 -0.0251 0.0187 -0.0092
					0.6367 -0.0459 -0.0079 0.0000 0.0000
					0.0000 0.0000 0.3201 -0.0738 0.0219
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.5170 -0.0238 0.0107 -0.0838
					0.0079 0.0001 0.0000 0.0000 -0.0245
					0.0000 0.0445 -0.0110 0.0000 0.0000
					0.0000 0.0000 -0.2076 0.0318 0.0159
					0.0065
93.	(0.00554)	RY (2)	C 2	s(9.95%)	p 6.34(63.09%)d 2.37(23.57%)
					f 0.34(3.40%)
					0.0000 0.0076 0.3147 -0.0182 -0.0074
					-0.0032 0.6762 0.0656 -0.0457 0.0262
					-0.3969 -0.0835 0.0448 0.0000 0.0000
					0.0000 0.0000 0.3654 -0.0330 0.1372
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 -0.2572 0.0012 -0.0369 -0.1208
					0.0026 -0.0139 0.0000 0.0000 0.0461
					-0.0193 -0.0890 0.0280 0.0000 0.0000
					0.0000 0.0000 0.1397 -0.0102 -0.0534
					0.0166
94.	(0.00390)	RY (3)	C 2	s(4.83%)	p 2.17(10.50%)d 2.42(11.67%)
					f15.12(73.00%)
					0.0000 0.0022 0.2048 -0.0702 -0.0375
					-0.0097 -0.2433 0.0304 0.0067 0.0033
					0.1990 0.0675 -0.0242 0.0000 0.0000
					0.0000 0.0000 0.1903 0.0493 0.0675
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0999 -0.1290 0.0543 -0.2087
					0.0193 -0.0009 0.0000 0.0000 0.0945
					-0.0196 0.0630 -0.0258 0.0000 0.0000
					0.0000 0.0000 0.8231 -0.1475 0.1283
					-0.0190
95.	(0.00254)	RY (4)	C 2	s(0.00%)	p 1.00(29.59%)d 2.01(59.51%)
					f 0.37(10.90%)
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 -0.0386 0.4419
					-0.3131 0.0328 0.0000 0.0000 0.0000

	0.5737	-0.3647	-0.1960	-0.2401	0.1882
	0.0387	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	-0.0729	0.0182	0.0000
	0.0000	0.0000	0.0000	-0.1272	0.0609
	0.2766	-0.0835	0.0000	0.0000	0.0000
	0.0000				
96. (0.00214) RY (5) C 2	s(38.31%)	p 0.62(23.58%)	d 0.68(25.96%)		
	f 0.32(12.15%)				
	0.0000	0.0197	0.6153	0.0476	-0.0426
	0.0000	-0.2951	-0.0403	-0.0551	0.0170
	-0.2805	-0.2185	-0.1318	0.0000	0.0000
	0.0000	0.0000	-0.0056	0.1462	-0.0637
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.2967	-0.2203	0.1093	-0.2762
	-0.0228	-0.0941	0.0000	0.0000	0.0337
	-0.0043	0.0963	0.0030	0.0000	0.0000
	0.0000	0.0000	-0.3268	-0.0078	0.0615
	-0.0210				
97. (0.00166) RY (6) C 2	s(0.00%)	p 1.00(48.27%)	d 0.68(32.65%)		
	f 0.40(19.08%)				
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	-0.0074	-0.6932
	0.0096	-0.0454	0.0000	0.0000	0.0000
	0.2080	-0.3929	-0.0821	0.2485	-0.2448
	0.0204	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	-0.1330	0.0353	0.0000
	0.0000	0.0000	0.0000	-0.1039	-0.0371
	0.3785	-0.1282	0.0000	0.0000	0.0000
	0.0000				
98. (0.00052) RY (7) C 2	s(15.89%)	p 1.26(20.08%)	d 3.50(55.64%)		
	f 0.53(8.39%)				
	0.0000	0.0000	0.3388	0.1437	0.1533
	-0.0112	-0.1857	-0.0361	0.0085	0.0065
	0.1597	0.3144	0.2011	0.0000	0.0000
	0.0000	0.0000	0.3214	-0.1662	-0.4895
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.3089	0.2459	-0.1269	0.0336
	-0.0503	-0.1010	0.0000	0.0000	-0.2436
	0.0500	0.0110	0.0032	0.0000	0.0000
	0.0000	0.0000	-0.0901	0.0189	0.0795
	-0.0845				
99. (0.00043) RY (8) C 2	s(0.00%)	p 1.00(21.50%)	d 2.49(53.53%)		
	f 1.16(24.97%)				
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	-0.0078	-0.4343
	-0.0857	-0.1378	0.0000	0.0000	0.0000
	-0.0167	-0.0085	0.0531	-0.3081	0.6549
	0.0911	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0690	-0.0084	0.0000
	0.0000	0.0000	0.0000	-0.3980	0.1435
	-0.2554	-0.0240	0.0000	0.0000	0.0000
	0.0000				
100. (0.00039) RY (9) C 2	s(19.93%)	p 1.19(23.78%)	d 2.57(51.30%)		
	f 0.25(4.99%)				
	0.0000	-0.0137	0.3922	0.1565	-0.1444
	0.0161	-0.0315	-0.3566	0.1924	0.0015
	0.2596	-0.0170	-0.0679	0.0000	0.0000
	0.0000	0.0000	-0.2155	-0.0473	0.4524
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.2077	-0.0461	-0.3508	0.2702
	-0.0660	-0.1181	0.0000	0.0000	0.0338

				0.0380	-0.1726	-0.0647	0.0000	0.0000
				0.0000	0.0000	0.0054	0.0924	-0.0266
				0.0638				
101.	(0.00028)	RY (10)	C 2	s(11.14%)	p 0.95(10.60%)	d 6.03(67.18%)		
				f 0.99(11.08%)				
				0.0000	0.0012	-0.2063	0.2514	-0.0751
				0.0021	-0.2568	0.0379	-0.0700	0.0036
				-0.1818	0.0232	-0.0079	0.0000	0.0000
				0.0000	0.0000	0.5979	0.0709	0.3443
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0960	0.0183	0.0263	0.3699
				-0.1425	-0.1528	0.0000	0.0000	0.1444
				-0.0170	0.0946	-0.0296	0.0000	0.0000
				0.0000	0.0000	-0.0958	0.0444	0.1533
				-0.2125				
102.	(0.00019)	RY (11)	C 2	s(8.67%)	p 3.53(30.59%)	d 4.74(41.12%)		
				f 2.26(19.62%)				
				0.0000	-0.0209	0.1467	0.2343	0.0992
				0.0125	0.2522	0.4124	-0.2343	-0.0110
				-0.0222	0.1281	0.0108	0.0000	0.0000
				0.0000	0.0000	-0.4210	0.0402	-0.0572
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.2014	0.0680	-0.0663	0.2353
				-0.1531	-0.3174	0.0000	0.0000	0.0151
				-0.0061	0.0764	-0.0682	0.0000	0.0000
				0.0000	0.0000	0.1404	0.0635	0.3483
				-0.2009				
103.	(0.00010)	RY (12)	C 2	s(0.00%)	p 1.00(3.76%)	d20.83(78.38%)		
				f 4.74(17.86%)				
104.	(0.00008)	RY (13)	C 2	s(13.93%)	p 1.39(19.31%)	d 3.56(49.52%)		
				f 1.24(17.24%)				
105.	(0.00004)	RY (14)	C 2	s(12.64%)	p 1.97(24.90%)	d 2.52(31.82%)		
				f 2.42(30.64%)				
106.	(0.00003)	RY (15)	C 2	s(5.21%)	p 1.98(10.31%)	d11.07(57.71%)		
				f 5.14(26.77%)				
107.	(0.00001)	RY (16)	C 2	s(10.70%)	p 1.80(19.24%)	d 3.10(33.18%)		
				f 3.45(36.88%)				
108.	(0.00001)	RY (17)	C 2	s(3.27%)	p 2.90(9.48%)	d16.87(55.09%)		
				f 9.85(32.16%)				
109.	(0.00001)	RY (18)	C 2	s(14.79%)	p 1.39(20.52%)	d 2.39(35.40%)		
				f 1.98(29.29%)				
110.	(0.00000)	RY (19)	C 2	s(24.42%)	p 0.42(10.28%)	d 0.96(23.40%)		
				f 1.72(41.90%)				
111.	(0.00000)	RY (20)	C 2	s(0.05%)	p99.99(22.52%)	d99.99(70.00%)		
				f99.99(7.44%)				
112.	(0.00000)	RY (21)	C 2	s(4.68%)	p 9.79(45.84%)	d 5.11(23.92%)		
				f 5.46(25.56%)				
113.	(0.00000)	RY (22)	C 2	s(0.00%)	p 1.00(8.22%)	d 3.95(32.47%)		
				f 7.21(59.31%)				
114.	(0.00000)	RY (23)	C 2	s(0.00%)	p 1.00(30.22%)	d 1.62(49.08%)		
				f 0.68(20.70%)				
115.	(0.00000)	RY (24)	C 2	s(0.00%)	p 1.00(63.94%)	d 0.42(27.00%)		
				f 0.14(9.07%)				
116.	(0.00000)	RY (25)	C 2	s(0.00%)	p 1.00(10.76%)	d 8.01(86.23%)		
				f 0.28(3.00%)				
117.	(0.00000)	RY (26)	C 2	s(0.00%)	p 1.00(56.64%)	d 0.60(34.12%)		
				f 0.16(9.24%)				
118.	(0.00000)	RY (27)	C 2	s(2.47%)	p 6.83(16.90%)	d19.66(48.62%)		
				f12.94(32.00%)				
119.	(0.00000)	RY (28)	C 2	s(8.10%)	p 2.02(16.33%)	d 4.87(39.45%)		
				f 4.46(36.12%)				
120.	(0.00000)	RY (29)	C 2	s(0.00%)	p 1.00(10.99%)	d 3.65(40.06%)		
				f 4.46(48.96%)				

121. (0.00000) RY (30) C 2 s(0.00%)p 1.00(1.20%)d 0.81(0.97%)
f81.47(97.83%)

122. (0.00000) RY (31) C 2 s(17.76%)p 1.49(26.49%)d 1.60(28.44%)
f 1.54(27.31%)

123. (0.00000) RY (32) C 2 s(3.59%)p 7.93(28.44%)d 1.04(3.75%)
f17.91(64.23%)

124. (0.00000) RY (33) C 2 s(0.35%)p12.70(4.42%)d48.77(16.96%)
f99.99(78.28%)

125. (0.00000) RY (34) C 2 s(2.37%)p 5.62(13.31%)d 1.80(4.26%)
f33.82(80.06%)

126. (0.00000) RY (35) C 2 s(0.00%)p 1.00(7.23%)d 5.03(36.34%)
f 7.81(56.44%)

127. (0.00000) RY (36) C 2 s(0.00%)p 1.00(0.27%)d 8.74(2.33%)
f99.99(97.41%)

128. (0.00000) RY (37) C 2 s(0.00%)p 1.00(5.73%)d10.31(59.10%)
f 6.14(35.17%)

129. (0.00000) RY (38) C 2 s(0.00%)p 1.00(1.90%)d 4.26(8.07%)
f47.50(90.04%)

130. (0.00000) RY (39) C 2 s(53.08%)p 0.42(22.18%)d 0.15(8.09%)
f 0.31(16.65%)

131. (0.00000) RY (40) C 2 s(3.26%)p 6.70(21.84%)d 5.64(18.39%)
f17.33(56.51%)

132. (0.00000) RY (41) C 2 s(10.31%)p 2.85(29.41%)d 3.58(36.86%)
f 2.27(23.42%)

133. (0.00139) RY (1) C 3 s(1.31%)p22.90(29.92%)d12.52(16.36%)
f40.11(52.41%)
0.0000 -0.0015 0.1109 -0.0111 0.0253
-0.0111 0.5355 -0.0548 0.0001 -0.0902
-0.0348 0.0000 0.0000 0.0000 -0.2453
0.1880 -0.1618 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0336 -0.1023
0.1262 -0.1018 0.0624 0.0117 0.0000
0.0000 0.1132 0.0486 0.0156 0.0013
0.0000 0.0000 0.0000 0.0000 -0.6548
-0.2589 -0.1049 -0.0425

134. (0.00119) RY (2) C 3 s(5.43%)p12.17(66.04%)d 2.54(13.81%)
f 2.71(14.73%)
0.0000 -0.0077 0.2105 -0.0302 0.0948
0.0229 -0.7625 0.0003 -0.0048 -0.2776
-0.0379 0.0000 0.0000 0.0000 0.0162
-0.0131 -0.1444 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.1183 -0.1983
0.1742 -0.1316 0.1102 0.0605 0.0000
0.0000 0.0638 0.0068 0.0187 0.0024
0.0000 0.0000 0.0000 0.0000 -0.3661
-0.0742 -0.0547 0.0150

135. (0.00077) RY (3) C 3 s(28.79%)p 0.71(20.42%)d 1.49(42.87%)
f 0.28(7.92%)
0.0000 0.0044 0.5305 -0.0703 -0.0391
0.0117 -0.1391 0.0548 0.0114 0.4179
0.0832 0.0000 0.0000 0.0000 -0.0216
0.1104 -0.0685 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 -0.3086 0.1576
-0.5255 0.1181 -0.0134 0.0316 0.0000
0.0000 -0.0496 -0.0360 0.1393 0.0772
0.0000 0.0000 0.0000 0.0000 -0.1881
-0.0771 0.0928 0.0134

136. (0.00049) RY (4) C 3 s(17.11%)p 2.91(49.84%)d 0.83(14.13%)
f 1.11(18.93%)
0.0000 0.0058 0.3683 0.1475 -0.1166
-0.0003 0.1745 -0.0917 -0.0071 -0.6770
0.0339 0.0000 0.0000 0.0000 0.0839
0.0255 0.1313 0.0000 0.0000 0.0000

		0.0000	0.0000	0.0000	0.0115	-0.0650
		-0.1369	0.2681	-0.1075	0.0990	0.0000
		0.0000	-0.0240	-0.0508	0.0722	0.0633
		0.0000	0.0000	0.0000	0.0000	0.0709
		0.0730	0.3390	0.2271		
137.	(0.00036) RY (5) C 3	s(0.00%)	p 1.00(1.54%)	d43.40(66.89%)		
		f20.49(31.57%)				
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	-0.0095	-0.0891	0.0859	0.0000
		0.0000	0.0000	0.4898	0.6275	-0.1839
		-0.0281	0.0005	-0.0254	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0065
		-0.0106	0.0000	0.0000	0.0000	0.0000
		-0.0617	-0.0499	0.4506	0.3260	0.0000
		0.0000	0.0000	0.0000		
138.	(0.00033) RY (6) C 3	s(15.68%)	p 0.52(8.19%)	d 4.22(66.14%)		
		f 0.64(10.00%)				
		0.0000	-0.0103	0.3833	-0.0507	0.0848
		-0.0202	0.1337	0.0901	0.0078	0.1818
		-0.1498	0.0000	0.0000	0.0000	-0.1987
		-0.0842	0.0933	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.5070	-0.4708
		-0.1214	-0.3171	0.0961	-0.0532	0.0000
		0.0000	-0.0609	0.0266	0.1031	0.0273
		0.0000	0.0000	0.0000	0.0000	0.2619
		0.1047	0.0524	-0.0431		
139.	(0.00025) RY (7) C 3	s(10.58%)	p 1.39(14.69%)	d 6.26(66.18%)		
		f 0.81(8.54%)				
		0.0000	0.0046	0.2833	0.0289	-0.1572
		0.0465	0.1116	-0.0981	-0.0019	0.1806
		-0.3001	0.0000	0.0000	0.0000	0.6796
		0.0486	0.0902	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	-0.1502	-0.0902
		0.3862	-0.0866	-0.0255	-0.0387	0.0000
		0.0000	0.1152	-0.0310	0.0545	-0.0002
		0.0000	0.0000	0.0000	0.0000	-0.0264
		0.0122	0.0972	-0.2407		
140.	(0.00013) RY (8) C 3	s(14.35%)	p 0.83(11.86%)	d 3.83(54.91%)		
		f 1.32(18.88%)				
		0.0000	0.0160	-0.2143	0.3023	0.0769
		0.0061	-0.0790	0.0268	-0.0003	0.3308
		0.0466	0.0000	0.0000	0.0000	0.1591
		0.0731	0.0088	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.4439	-0.1853
		-0.0204	0.4346	-0.2896	-0.1177	0.0000
		0.0000	0.0465	-0.0022	-0.0287	0.0701
		0.0000	0.0000	0.0000	0.0000	-0.2600
		-0.0823	0.2875	0.1547		
141.	(0.00013) RY (9) C 3	s(0.00%)	p 1.00(22.07%)	d 2.73(60.25%)		
		f 0.80(17.67%)				
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0265	0.2688	-0.3844	0.0000
		0.0000	0.0000	-0.0944	0.1756	-0.0315
		0.6940	0.1802	0.2184	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.1937
		-0.0534	0.0000	0.0000	0.0000	0.0000
		0.3630	-0.0053	0.0675	0.0072	0.0000
		0.0000	0.0000	0.0000		
142.	(0.00008) RY (10) C 3	s(0.00%)	p 1.00(12.73%)	d 4.60(58.58%)		
		f 2.25(28.69%)				
143.	(0.00004) RY (11) C 3	s(22.85%)	p 0.37(8.55%)	d 2.41(55.13%)		

					f 0.59(13.47%)
144.	(0.00004)	R	Y (12)	C 3	s(0.00%)p 1.00(51.41%)d 0.68(34.99%)
					f 0.26(13.60%)
145.	(0.00002)	R	Y (13)	C 3	s(13.79%)p 0.80(10.99%)d 4.52(62.35%)
					f 0.93(12.87%)
146.	(0.00001)	R	Y (14)	C 3	s(0.85%)p12.42(10.62%)d46.75(39.97%)
					f56.80(48.56%)
147.	(0.00001)	R	Y (15)	C 3	s(18.88%)p 0.16(3.09%)d 0.49(9.30%)
					f 3.64(68.73%)
148.	(0.00000)	R	Y (16)	C 3	s(12.03%)p 1.55(18.63%)d 4.47(53.75%)
					f 1.30(15.59%)
149.	(0.00000)	R	Y (17)	C 3	s(32.22%)p 0.25(8.13%)d 1.01(32.48%)
					f 0.84(27.17%)
150.	(0.00000)	R	Y (18)	C 3	s(0.00%)p 1.00(10.76%)d 7.51(80.86%)
					f 0.78(8.38%)
151.	(0.00000)	R	Y (19)	C 3	s(0.00%)p 1.00(2.86%)d11.05(31.64%)
					f22.88(65.50%)
152.	(0.00000)	R	Y (20)	C 3	s(0.00%)p 1.00(10.51%)d 7.09(74.49%)
					f 1.43(15.00%)
153.	(0.00000)	R	Y (21)	C 3	s(0.00%)p 1.00(10.71%)d 7.90(84.60%)
					f 0.44(4.69%)
154.	(0.00000)	R	Y (22)	C 3	s(0.00%)p 1.00(0.61%)d 9.46(5.76%)
					f99.99(93.63%)
155.	(0.00000)	R	Y (23)	C 3	s(15.50%)p 0.52(7.98%)d 2.29(35.50%)
					f 2.65(41.02%)
156.	(0.00000)	R	Y (24)	C 3	s(28.70%)p 0.05(1.43%)d 0.67(19.12%)
					f 1.77(50.75%)
157.	(0.00000)	R	Y (25)	C 3	s(10.21%)p 3.56(36.33%)d 1.28(13.06%)
					f 3.96(40.40%)
158.	(0.00000)	R	Y (26)	C 3	s(7.75%)p 0.53(4.10%)d10.05(77.86%)
					f 1.33(10.30%)
159.	(0.00000)	R	Y (27)	C 3	s(0.00%)p 1.00(17.03%)d 0.68(11.55%)
					f 4.20(71.42%)
160.	(0.00000)	R	Y (28)	C 3	s(0.00%)p 1.00(1.11%)d 1.52(1.69%)
					f87.56(97.20%)
161.	(0.00000)	R	Y (29)	C 3	s(0.61%)p 3.66(2.24%)d21.95(13.40%)
					f99.99(83.75%)
162.	(0.00000)	R	Y (30)	C 3	s(11.33%)p 0.47(5.28%)d 3.30(37.44%)
					f 4.06(45.95%)
163.	(0.00000)	R	Y (31)	C 3	s(0.49%)p14.06(6.85%)d99.99(54.42%)
					f78.49(38.24%)
164.	(0.00000)	R	Y (32)	C 3	s(14.44%)p 0.19(2.69%)d 1.47(21.28%)
					f 4.27(61.60%)
165.	(0.00000)	R	Y (33)	C 3	s(0.00%)p 1.00(56.49%)d 0.65(36.81%)
					f 0.12(6.69%)
166.	(0.00000)	R	Y (34)	C 3	s(0.00%)p 1.00(0.28%)d77.72(21.59%)
					f99.99(78.14%)
167.	(0.00000)	R	Y (35)	C 3	s(0.00%)p 1.00(2.11%)d14.34(30.20%)
					f32.15(67.70%)
168.	(0.00000)	R	Y (36)	C 3	s(9.94%)p 1.75(17.37%)d 3.93(39.05%)
					f 3.38(33.64%)
169.	(0.00000)	R	Y (37)	C 3	s(4.01%)p11.68(46.83%)d 9.37(37.55%)
					f 2.90(11.62%)
170.	(0.00000)	R	Y (38)	C 3	s(3.34%)p 2.58(8.62%)d 7.00(23.38%)
					f19.37(64.66%)
171.	(0.00833)	R	Y (1)	C 4	s(0.25%)p99.99(86.88%)d44.70(11.19%)
					f 6.71(1.68%)

0.0000	-0.0160	-0.0197	0.0209	0.0377
-0.0383	-0.5850	0.0253	-0.0299	-0.0064
0.7197	-0.0660	-0.0337	0.0000	0.0000
0.0000	0.0000	-0.0572	0.1031	-0.0799
0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.1980	-0.2097	0.0485	0.0737

		-0.0238	0.0093	0.0000	0.0000	-0.0091
		0.0020	0.0369	0.0153	0.0000	0.0000
		0.0000	0.0000	0.1005	0.0422	0.0558
		0.0109				
172. (0.00293) RY (2) C 4	s(12.72%)p 5.11(65.06%)d 0.78(9.98%)					
	f 0.96(12.24%)					
		0.0000	0.0072	0.3563	-0.0123	0.0093
		0.0266	-0.6522	-0.1058	0.0170	0.0372
		-0.4556	-0.0403	0.0503	0.0000	0.0000
		0.0000	0.0000	-0.1502	0.1153	-0.1249
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	-0.1413	0.0673	-0.0043	0.1355
		-0.0721	-0.0169	0.0000	0.0000	-0.0134
		0.0158	-0.0546	-0.0373	0.0000	0.0000
		0.0000	0.0000	-0.2847	-0.1705	-0.0727
		-0.0467				
173. (0.00139) RY (3) C 4	s(0.00%)p 1.00(73.20%)d 0.31(22.98%)					
	f 0.05(3.82%)					
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	-0.0034	0.8067
		-0.2796	0.0557	0.0000	0.0000	0.0000
		-0.0939	0.3742	0.0822	-0.0702	0.2595
		-0.0442	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	-0.0653	-0.0365	0.0000
		0.0000	0.0000	0.0000	0.0261	-0.0337
		-0.1489	-0.0931	0.0000	0.0000	0.0000
		0.0000				
174. (0.00115) RY (4) C 4	s(34.97%)p 0.17(6.11%)d 0.66(23.00%)					
	f 1.03(35.93%)					
		0.0000	0.0095	0.5859	-0.0322	0.0723
		0.0340	0.0797	-0.0542	0.0319	-0.0068
		-0.1740	-0.1292	-0.0507	0.0000	0.0000
		0.0000	0.0000	-0.1021	0.0406	0.2534
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.2648	-0.2472	0.0391	0.1024
		-0.0915	-0.0457	0.0000	0.0000	0.1312
		-0.0660	0.0791	0.0021	0.0000	0.0000
		0.0000	0.0000	0.5143	0.2079	0.1140
		0.1034				
175. (0.00052) RY (5) C 4	s(34.12%)p 1.04(35.58%)d 0.42(14.21%)					
	f 0.47(16.08%)					
		0.0000	-0.0025	0.5802	0.0078	-0.0670
		0.0119	0.3070	-0.0397	0.0306	-0.0142
		0.4174	0.2653	0.1187	0.0000	0.0000
		0.0000	0.0000	-0.1171	0.1833	-0.0050
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	-0.1784	0.1185	-0.1645	-0.0547
		-0.0657	-0.1206	0.0000	0.0000	0.0159
		-0.0335	-0.0233	0.0319	0.0000	0.0000
		0.0000	0.0000	-0.3704	-0.0929	0.0578
		0.0932				
176. (0.00039) RY (6) C 4	s(0.00%)p 1.00(24.24%)d 2.72(65.96%)					
	f 0.40(9.80%)					
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	-0.0033	-0.4303
		-0.2010	-0.1299	0.0000	0.0000	0.0000
		-0.2733	0.3969	0.0176	0.3998	0.5143
		-0.0526	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	-0.0493	-0.0331	0.0000
		0.0000	0.0000	0.0000	-0.2202	-0.1774
		0.0068	-0.1202	0.0000	0.0000	0.0000

0.0000

177.	(0.00009)	RY (7)	C	4	s(3.59%)	p 2.14(7.68%)	d19.41(69.76%)
					f 5.28(18.97%)		
178.	(0.00005)	RY (8)	C	4	s(8.60%)	p 1.54(13.22%)	d 7.90(67.94%)
					f 1.19(10.24%)		
179.	(0.00003)	RY (9)	C	4	s(15.77%)	p 1.55(24.51%)	d 3.03(47.79%)
					f 0.76(11.93%)		
180.	(0.00002)	RY (10)	C	4	s(3.12%)	p 3.25(10.13%)	d15.65(48.80%)
					f12.17(37.95%)		
181.	(0.00002)	RY (11)	C	4	s(0.00%)	p 1.00(6.47%)	d14.14(91.58%)
					f 0.30(1.95%)		
182.	(0.00001)	RY (12)	C	4	s(4.96%)	p 6.63(32.90%)	d 2.88(14.29%)
					f 9.65(47.85%)		
183.	(0.00000)	RY (13)	C	4	s(6.72%)	p 1.08(7.24%)	d 8.14(54.71%)
					f 4.66(31.32%)		
184.	(0.00000)	RY (14)	C	4	s(18.98%)	p 0.76(14.38%)	d 1.42(26.93%)
					f 2.09(39.72%)		
185.	(0.00000)	RY (15)	C	4	s(0.00%)	p 1.00(17.86%)	d 3.03(54.17%)
					f 1.57(27.97%)		
186.	(0.00000)	RY (16)	C	4	s(0.00%)	p 1.00(55.63%)	d 0.45(25.29%)
					f 0.34(19.08%)		
187.	(0.00000)	RY (17)	C	4	s(8.01%)	p 2.97(23.78%)	d 3.13(25.04%)
					f 5.39(43.16%)		
188.	(0.00000)	RY (18)	C	4	s(22.92%)	p 0.77(17.65%)	d 1.58(36.31%)
					f 1.01(23.11%)		
189.	(0.00000)	RY (19)	C	4	s(0.00%)	p 1.00(22.79%)	d 1.64(37.33%)
					f 1.75(39.88%)		
190.	(0.00000)	RY (20)	C	4	s(6.73%)	p 8.11(54.59%)	d 1.55(10.45%)
					f 4.20(28.23%)		
191.	(0.00000)	RY (21)	C	4	s(0.00%)	p 1.00(27.58%)	d 1.81(49.80%)
					f 0.82(22.62%)		
192.	(0.00000)	RY (22)	C	4	s(0.00%)	p 1.00(13.96%)	d 4.91(68.60%)
					f 1.25(17.44%)		
193.	(0.00000)	RY (23)	C	4	s(0.00%)	p 1.00(16.65%)	d 3.14(52.33%)
					f 1.86(31.02%)		
194.	(0.00000)	RY (24)	C	4	s(13.80%)	p 0.37(5.08%)	d 4.21(58.10%)
					f 1.67(23.02%)		
195.	(0.00000)	RY (25)	C	4	s(9.56%)	p 2.03(19.42%)	d 4.50(43.05%)
					f 2.93(27.98%)		
196.	(0.00000)	RY (26)	C	4	s(19.64%)	p 0.87(17.17%)	d 2.33(45.85%)
					f 0.88(17.34%)		
197.	(0.00000)	RY (27)	C	4	s(1.28%)	p 8.05(10.27%)	d55.07(70.27%)
					f14.25(18.18%)		
198.	(0.00000)	RY (28)	C	4	s(37.25%)	p 0.17(6.20%)	d 0.70(26.17%)
					f 0.82(30.38%)		
199.	(0.00000)	RY (29)	C	4	s(0.00%)	p 1.00(4.73%)	d 2.44(11.52%)
					f17.71(83.75%)		
200.	(0.00000)	RY (30)	C	4	s(0.00%)	p 1.00(7.09%)	d 4.82(34.15%)
					f 8.29(58.76%)		
201.	(0.00000)	RY (31)	C	4	s(1.00%)	p 7.71(7.73%)	d34.42(34.51%)
					f56.61(56.76%)		
202.	(0.00000)	RY (32)	C	4	s(11.25%)	p 1.25(14.04%)	d 2.37(26.73%)
					f 4.26(47.98%)		
203.	(0.00000)	RY (33)	C	4	s(16.90%)	p 2.84(48.04%)	d 0.50(8.50%)
					f 1.57(26.56%)		
204.	(0.00000)	RY (34)	C	4	s(2.17%)	p 4.07(8.83%)	d 6.92(15.01%)
					f34.13(73.99%)		
205.	(0.00000)	RY (35)	C	4	s(0.00%)	p 1.00(3.91%)	d 9.90(38.73%)
					f14.66(57.36%)		
206.	(0.00000)	RY (36)	C	4	s(0.00%)	p 1.00(6.40%)	d 1.91(12.21%)
					f12.72(81.39%)		
207.	(0.00000)	RY (37)	C	4	s(0.00%)	p 1.00(10.53%)	d 2.21(23.26%)
					f 6.29(66.21%)		

208.	(0.00000)	RY (38)	C	4	s(0.00%)p 1.00(9.08%)d 1.33(12.03%) f 8.69(78.89%)
209.	(0.00000)	RY (39)	C	4	s(0.87%)p 2.17(1.88%)d38.66(33.51%) f73.53(63.74%)
210.	(0.00000)	RY (40)	C	4	s(1.85%)p 7.95(14.75%)d23.88(44.30%) f21.07(39.09%)
211.	(0.00000)	RY (41)	C	4	s(3.11%)p15.25(47.46%)d10.62(33.05%) f 5.26(16.38%)
212.	(0.00501)	RY (1)	C	5	s(2.38%)p36.47(86.65%)d 4.39(10.43%) f 0.23(0.54%) 0.0000 -0.0077 0.1520 -0.0026 -0.0241 -0.0168 -0.7773 -0.0017 -0.0150 -0.0105 -0.5107 0.0076 0.0274 0.0000 0.0000 0.0000 0.0000 0.0463 -0.2021 -0.1162 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0198 -0.0600 -0.0591 0.1502 -0.1276 0.0392 0.0000 0.0000 -0.0142 -0.0165 -0.0068 -0.0040 0.0000 0.0000 0.0000 0.0000 -0.0155 -0.0163 0.0377 0.0544
213.	(0.00154)	RY (2)	C	5	s(0.79%)p55.65(44.01%)d15.32(12.11%) f54.49(43.09%) 0.0000 0.0006 0.0878 0.0125 -0.0060 0.0225 -0.3198 0.0939 -0.0115 -0.0309 0.5647 -0.0891 -0.0229 0.0000 0.0000 0.0000 0.0000 0.1084 -0.1213 -0.0302 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 -0.1815 0.2190 0.1122 -0.0079 -0.0049 0.0127 0.0000 0.0000 -0.0668 -0.0418 0.1241 0.0829 0.0000 0.0000 0.0000 0.0000 -0.5376 -0.3324 -0.0455 -0.0301
214.	(0.00096)	RY (3)	C	5	s(0.00%)p 1.00(86.67%)d 0.13(10.99%) f 0.03(2.34%) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0017 0.8488 0.3823 0.0079 0.0000 0.0000 0.0000 0.1343 0.0454 -0.0828 0.2343 0.1221 -0.1146 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0287 -0.0122 0.0000 0.0000 0.0000 0.0000 0.0918 0.0545 0.1050 -0.0025 0.0000 0.0000 0.0000 0.0000
215.	(0.00071)	RY (4)	C	5	s(0.52%)p99.99(52.21%)d23.10(11.97%) f68.16(35.30%) 0.0000 -0.0004 0.0689 0.0108 0.0177 0.0141 -0.3881 0.0228 0.0698 -0.0177 0.5883 -0.0773 0.1165 0.0000 0.0000 0.0000 0.0000 0.0022 0.0257 0.1389 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.1294 -0.2430 -0.1543 -0.0067 0.0033 0.0076 0.0000 0.0000 0.0238 -0.0238 -0.0293 0.0453 0.0000 0.0000 0.0000 0.0000 0.5509 0.2127 0.0141 -0.0037
216.	(0.00042)	RY (5)	C	5	s(0.00%)p 1.00(10.65%)d 6.77(72.10%) f 1.62(17.26%) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0112 -0.2420 0.2184 0.0096 0.0000 0.0000 0.0000 -0.5388 -0.0089 -0.0681 0.5827 0.2925

		-0.0269	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	-0.0356	-0.0157	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.1983	0.2573	0.0000	0.0000
		-0.1923	-0.1689	0.0000	0.0000	0.0000	0.0000	0.0000
217.	(0.00035) RY (6) C 5	s(51.25%)	p 0.07(3.77%)	d 0.66(33.96%)				
		f 0.22(11.02%)						
		0.0000	-0.0037	0.6892	0.1819	0.0660	0.0000	0.0000
		0.0128	0.1239	-0.0341	-0.0102	0.0171	0.0000	0.0000
		-0.0657	0.1268	-0.0145	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.1022	-0.2630	0.3516	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.1434	-0.1154	0.1648	-0.2033	0.0000	0.0000
		0.0492	0.1776	0.0000	0.0000	0.0472	0.0000	0.0000
		0.0486	-0.0010	-0.0071	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	-0.0257	-0.0001	-0.2421	0.0000	0.0000
		-0.2153						
218.	(0.00015) RY (7) C 5	s(22.06%)	p 0.45(10.04%)	d 2.89(63.85%)				
		f 0.18(4.04%)						
		0.0000	0.0080	0.3761	0.2541	-0.1207	0.0000	0.0000
		-0.0046	0.0171	0.2701	0.0061	0.0063	0.0000	0.0000
		-0.0202	-0.1623	-0.0166	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	-0.4965	0.4474	0.0792	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	-0.1216	0.1952	0.0083	0.2719	0.0000	0.0000
		-0.2377	0.0470	0.0000	0.0000	0.0586	0.0000	0.0000
		0.0223	0.1279	0.0390	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0303	0.0217	0.0375	0.0000	0.0000
		0.1259						
219.	(0.00011) RY (8) C 5	s(5.27%)	p 7.49(39.48%)	d 8.16(42.99%)				
		f 2.33(12.26%)						
		0.0000	-0.0136	0.1814	-0.1398	-0.0101	0.0000	0.0000
		-0.0096	0.0200	0.4328	-0.0105	0.0025	0.0000	0.0000
		-0.0709	-0.4414	-0.0841	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	-0.0187	0.0593	-0.4783	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0697	-0.0958	-0.1212	-0.3412	0.0000	0.0000
		0.2280	-0.0072	0.0000	0.0000	-0.1798	0.0000	0.0000
		-0.0128	-0.0063	-0.0168	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0049	0.0856	-0.0749	0.0000	0.0000
		-0.2773						
220.	(0.00004) RY (9) C 5	s(7.41%)	p 2.34(17.38%)	d 6.26(46.39%)				
		f 3.89(28.82%)						
221.	(0.00002) RY (10) C 5	s(0.00%)	p 1.00(11.77%)	d 6.61(77.81%)				
		f 0.89(10.42%)						
222.	(0.00001) RY (11) C 5	s(9.38%)	p 3.87(36.29%)	d 3.65(34.24%)				
		f 2.14(20.09%)						
223.	(0.00001) RY (12) C 5	s(13.12%)	p 3.00(39.40%)	d 0.98(12.88%)				
		f 2.64(34.60%)						
224.	(0.00000) RY (13) C 5	s(8.67%)	p 3.83(33.20%)	d 4.65(40.25%)				
		f 2.06(17.89%)						
225.	(0.00000) RY (14) C 5	s(32.70%)	p 0.12(4.04%)	d 0.81(26.52%)				
		f 1.12(36.74%)						
226.	(0.00000) RY (15) C 5	s(0.00%)	p 1.00(47.10%)	d 0.73(34.24%)				
		f 0.40(18.66%)						
227.	(0.00000) RY (16) C 5	s(17.37%)	p 0.67(11.60%)	d 1.74(30.22%)				
		f 2.35(40.82%)						
228.	(0.00000) RY (17) C 5	s(5.90%)	p 1.11(6.53%)	d 7.74(45.64%)				
		f 7.11(41.93%)						
229.	(0.00000) RY (18) C 5	s(0.73%)	p77.89(56.64%)	d41.17(29.94%)				
		f17.45(12.69%)						
230.	(0.00000) RY (19) C 5	s(0.00%)	p 1.00(6.14%)	d14.57(89.45%)				
		f 0.72(4.41%)						

231.	(0.00000)	RY (20)	C	5	s(0.00%)p 1.00(8.21%)d 6.88(56.49%)
					f 4.30(35.30%)
232.	(0.00000)	RY (21)	C	5	s(0.00%)p 1.00(18.59%)d 2.76(51.29%)
					f 1.62(30.11%)
233.	(0.00000)	RY (22)	C	5	s(0.00%)p 1.00(41.20%)d 1.03(42.51%)
					f 0.40(16.29%)
234.	(0.00000)	RY (23)	C	5	s(8.82%)p 1.86(16.44%)d 4.54(40.03%)
					f 3.93(34.70%)
235.	(0.00000)	RY (24)	C	5	s(15.09%)p 1.21(18.31%)d 1.62(24.49%)
					f 2.79(42.11%)
236.	(0.00000)	RY (25)	C	5	s(2.06%)p 2.39(4.91%)d36.89(75.93%)
					f 8.31(17.11%)
237.	(0.00000)	RY (26)	C	5	s(7.41%)p 3.59(26.57%)d 1.16(8.61%)
					f 7.75(57.41%)
238.	(0.00000)	RY (27)	C	5	s(10.86%)p 0.42(4.59%)d 2.80(30.45%)
					f 4.98(54.10%)
239.	(0.00000)	RY (28)	C	5	s(1.44%)p20.00(28.85%)d25.94(37.42%)
					f22.38(32.29%)
240.	(0.00000)	RY (29)	C	5	s(20.23%)p 0.87(17.64%)d 1.74(35.28%)
					f 1.33(26.85%)
241.	(0.00000)	RY (30)	C	5	s(0.00%)p 1.00(13.77%)d 2.58(35.59%)
					f 3.68(50.64%)
242.	(0.00000)	RY (31)	C	5	s(0.00%)p 1.00(6.62%)d 1.70(11.24%)
					f12.40(82.14%)
243.	(0.00000)	RY (32)	C	5	s(37.47%)p 0.10(3.70%)d 1.02(38.38%)
					f 0.55(20.45%)
244.	(0.00000)	RY (33)	C	5	s(5.54%)p 0.56(3.11%)d 2.32(12.84%)
					f14.18(78.52%)
245.	(0.00000)	RY (34)	C	5	s(6.19%)p 1.28(7.90%)d10.02(62.01%)
					f 3.86(23.91%)
246.	(0.00000)	RY (35)	C	5	s(0.00%)p 1.00(2.04%)d12.27(25.04%)
					f35.73(72.92%)
247.	(0.00000)	RY (36)	C	5	s(0.00%)p 1.00(2.71%)d 1.81(4.92%)
					f34.06(92.37%)
248.	(0.00000)	RY (37)	C	5	s(0.00%)p 1.00(21.67%)d 0.56(12.17%)
					f 3.05(66.16%)
249.	(0.00000)	RY (38)	C	5	s(0.00%)p 1.00(2.31%)d 3.44(7.94%)
					f38.89(89.75%)
250.	(0.00000)	RY (39)	C	5	s(0.00%)p 1.00(20.62%)d 3.31(68.19%)
					f 0.54(11.19%)
251.	(0.00000)	RY (40)	C	5	s(3.36%)p 2.22(7.47%)d17.60(59.18%)
					f 8.92(29.99%)
252.	(0.00000)	RY (41)	C	5	s(4.14%)p 4.76(19.73%)d 8.11(33.57%)
					f10.28(42.56%)
253.	(0.00476)	RY (1)	C	6	s(0.94%)p95.41(89.93%)d 9.39(8.85%)
					f 0.29(0.28%)
					0.0000 -0.0112 0.0951 -0.0023 0.0157
					-0.0007 0.0572 -0.0313 -0.0017 -0.0240
					-0.9457 0.0076 0.0076 0.0000 0.0000
					0.0000 0.0000 -0.0012 0.0151 0.0075
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 -0.0372 0.2329 0.1276 0.0966
					-0.0793 -0.0266 0.0000 0.0000 0.0038
					0.0044 -0.0302 -0.0192 0.0000 0.0000
					0.0000 0.0000 -0.0049 0.0091 -0.0070
					-0.0361
254.	(0.00180)	RY (2)	C	6	s(0.62%)p88.99(54.82%)d 7.34(4.52%)
					f65.00(40.04%)
					0.0000 0.0014 0.0781 0.0041 0.0070
					0.0337 -0.7338 -0.0524 0.0680 0.0041
					-0.0331 -0.0031 0.0086 0.0000 0.0000
					0.0000 0.0000 -0.0689 0.1509 0.1297
					0.0000 0.0000 0.0000 0.0000 0.0000

		0.0000	0.0173	-0.0047	-0.0094	0.0121
		-0.0126	-0.0133	0.0000	0.0000	-0.1324
		-0.0848	0.0046	-0.0016	0.0000	0.0000
		0.0000	0.0000	0.5321	0.3039	0.0076
		0.0107				
255.	(0.00088) RY (3) C 6	s(0.00%)	p 1.00(88.22%)	d 0.08(7.20%)		
		f 0.05(4.58%)				
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0020	0.8549
		-0.3874	0.0354	0.0000	0.0000	0.0000
		0.0530	0.0244	-0.0083	0.1868	0.1059
		-0.1498	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	-0.0128	-0.0317	0.0000
		0.0000	0.0000	0.0000	-0.1976	-0.0608
		-0.0385	-0.0210	0.0000	0.0000	0.0000
		0.0000				
256.	(0.00078) RY (4) C 6	s(0.48%)	p86.42(41.14%)	d43.75(20.83%)		
		f78.86(37.55%)				
		0.0000	-0.0019	0.0330	-0.0073	0.0601
		0.0145	-0.6219	-0.1118	-0.1024	0.0000
		-0.0369	0.0093	0.0012	0.0000	0.0000
		0.0000	0.0000	0.2441	-0.3609	-0.1272
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	-0.0144	0.0212	-0.0138	-0.0277
		0.0254	-0.0005	0.0000	0.0000	0.0424
		-0.0333	0.0056	0.0060	0.0000	0.0000
		0.0000	0.0000	-0.5736	-0.2084	-0.0009
		0.0057				
257.	(0.00056) RY (5) C 6	s(64.33%)	p 0.05(2.94%)	d 0.46(29.48%)		
		f 0.05(3.25%)				
		0.0000	0.0036	0.7978	0.0765	0.0321
		-0.0040	0.0709	0.0169	0.0016	0.0252
		0.0949	-0.1195	-0.0109	0.0000	0.0000
		0.0000	0.0000	0.0022	-0.0015	-0.0222
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	-0.1393	0.2638	-0.3995	-0.0732
		-0.0650	-0.1899	0.0000	0.0000	0.0187
		0.0107	0.0448	0.0295	0.0000	0.0000
		0.0000	0.0000	-0.0024	-0.0135	0.1243
		0.1164				
258.	(0.00047) RY (6) C 6	s(0.00%)	p 1.00(1.00%)	d80.35(80.71%)		
		f18.21(18.29%)				
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	-0.0101	-0.0962
		-0.0262	0.0011	0.0000	0.0000	0.0000
		0.8790	0.1525	0.0926	0.0217	0.0212
		-0.0403	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0076	-0.0033	0.0000
		0.0000	0.0000	0.0000	0.0303	0.0271
		-0.2987	-0.3033	0.0000	0.0000	0.0000
		0.0000				
259.	(0.00013) RY (7) C 6	s(8.44%)	p 0.40(3.41%)	d 8.27(69.81%)		
		f 2.17(18.34%)				
		0.0000	0.0130	0.1796	0.2274	0.0152
		0.0154	-0.0110	-0.1641	-0.0537	0.0027
		-0.0410	0.0304	-0.0360	0.0000	0.0000
		0.0000	0.0000	-0.2894	0.0510	-0.0692
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.3692	-0.4243	-0.1739	0.3997
		-0.3167	-0.0178	0.0000	0.0000	0.0598
		-0.0487	0.1304	0.0202	0.0000	0.0000

				0.0000	0.0000	-0.1415	0.0524	-0.1580
				-0.3352				
260.	(0.00008)	RY (8)	C 6	s(2.81%)	p 6.02(16.90%)	d24.66(69.19%)		
				f 3.96(11.10%)				
261.	(0.00005)	RY (9)	C 6	s(14.84%)	p 0.51(7.52%)	d 3.91(58.00%)		
				f 1.32(19.64%)				
262.	(0.00002)	RY (10)	C 6	s(12.53%)	p 1.70(21.25%)	d 2.87(35.95%)		
				f 2.42(30.28%)				
263.	(0.00002)	RY (11)	C 6	s(0.00%)	p 1.00(8.94%)	d 8.54(76.40%)		
				f 1.64(14.66%)				
264.	(0.00002)	RY (12)	C 6	s(2.64%)	p 9.96(26.30%)	d12.80(33.78%)		
				f14.12(37.28%)				
265.	(0.00000)	RY (13)	C 6	s(2.25%)	p17.16(38.57%)	d14.57(32.76%)		
				f11.75(26.42%)				
266.	(0.00000)	RY (14)	C 6	s(51.05%)	p 0.34(17.17%)	d 0.29(14.93%)		
				f 0.33(16.84%)				
267.	(0.00000)	RY (15)	C 6	s(17.96%)	p 0.57(10.28%)	d 2.93(52.58%)		
				f 1.07(19.18%)				
268.	(0.00000)	RY (16)	C 6	s(7.90%)	p 1.61(12.68%)	d 7.86(62.06%)		
				f 2.20(17.35%)				
269.	(0.00000)	RY (17)	C 6	s(0.00%)	p 1.00(39.98%)	d 1.23(49.35%)		
				f 0.27(10.67%)				
270.	(0.00000)	RY (18)	C 6	s(1.33%)	p16.40(21.79%)	d24.34(32.35%)		
				f33.49(44.52%)				
271.	(0.00000)	RY (19)	C 6	s(0.55%)	p48.50(26.89%)	d81.58(45.22%)		
				f49.32(27.34%)				
272.	(0.00000)	RY (20)	C 6	s(8.47%)	p 1.57(13.27%)	d 5.90(49.95%)		
				f 3.34(28.31%)				
273.	(0.00000)	RY (21)	C 6	s(0.00%)	p 1.00(53.03%)	d 0.78(41.61%)		
				f 0.10(5.36%)				
274.	(0.00000)	RY (22)	C 6	s(0.00%)	p 1.00(11.38%)	d 5.89(67.07%)		
				f 1.89(21.54%)				
275.	(0.00000)	RY (23)	C 6	s(0.00%)	p 1.00(3.27%)	d19.64(64.23%)		
				f 9.94(32.50%)				
276.	(0.00000)	RY (24)	C 6	s(0.00%)	p 1.00(30.06%)	d 1.89(56.83%)		
				f 0.44(13.11%)				
277.	(0.00000)	RY (25)	C 6	s(2.14%)	p 0.66(1.41%)	d16.52(35.31%)		
				f28.60(61.14%)				
278.	(0.00000)	RY (26)	C 6	s(12.74%)	p 2.01(25.61%)	d 0.72(9.24%)		
				f 4.11(52.42%)				
279.	(0.00000)	RY (27)	C 6	s(35.46%)	p 1.06(37.71%)	d 0.33(11.65%)		
				f 0.43(15.19%)				
280.	(0.00000)	RY (28)	C 6	s(11.29%)	p 0.76(8.58%)	d 3.15(35.55%)		
				f 3.95(44.58%)				
281.	(0.00000)	RY (29)	C 6	s(0.00%)	p 1.00(4.93%)	d 2.22(10.96%)		
				f17.05(84.11%)				
282.	(0.00000)	RY (30)	C 6	s(0.00%)	p 1.00(8.11%)	d 2.67(21.64%)		
				f 8.66(70.25%)				
283.	(0.00000)	RY (31)	C 6	s(6.24%)	p 2.71(16.94%)	d 7.08(44.16%)		
				f 5.23(32.66%)				
284.	(0.00000)	RY (32)	C 6	s(7.04%)	p 1.17(8.23%)	d 2.80(19.73%)		
				f 9.23(65.00%)				
285.	(0.00000)	RY (33)	C 6	s(14.09%)	p 2.50(35.18%)	d 1.40(19.79%)		
				f 2.20(30.95%)				
286.	(0.00000)	RY (34)	C 6	s(10.24%)	p 1.51(15.43%)	d 2.91(29.76%)		
				f 4.35(44.56%)				
287.	(0.00000)	RY (35)	C 6	s(0.00%)	p 1.00(0.94%)	d42.02(39.65%)		
				f62.95(59.40%)				
288.	(0.00000)	RY (36)	C 6	s(0.00%)	p 1.00(1.30%)	d 8.76(11.39%)		
				f67.17(87.31%)				
289.	(0.00000)	RY (37)	C 6	s(0.00%)	p 1.00(0.39%)	d51.22(19.91%)		
				f99.99(79.70%)				
290.	(0.00000)	RY (38)	C 6	s(0.00%)	p 1.00(2.33%)	d 4.60(10.71%)		

									f37.30(86.96%)
291.	(0.00000)	RY (39)	C	6	s(0.73%)	p47.43(34.82%)	d36.87(27.07%)		
									f50.90(37.37%)
292.	(0.00000)	RY (40)	C	6	s(0.00%)	p 1.00(46.18%)	d 0.92(42.30%)		
									f 0.25(11.52%)
293.	(0.00000)	RY (41)	C	6	s(3.06%)	p 3.80(11.63%)	d15.38(47.08%)		
									f12.50(38.24%)
294.	(0.00049)	RY (1)	H	7	s(38.35%)	p 1.43(54.81%)	d 0.18(6.84%)		
					-0.0005	0.6157	0.0463	0.0482	0.1314
					0.0673	0.0353	-0.7227	0.0317	0.0420
					0.0000	0.0000	0.0000	0.0754	0.0036
					0.0000	0.0000	0.0000	0.0000	0.2236
					0.0380	0.1057	-0.0092		
295.	(0.00040)	RY (2)	H	7	s(13.82%)	p 5.68(78.45%)	d 0.56(7.73%)		
					-0.0060	0.3603	-0.0837	0.0356	0.7937
					-0.0152	-0.0711	0.3778	-0.0797	0.0153
					0.0000	0.0000	0.0000	-0.2264	-0.0675
					0.0000	0.0000	0.0000	0.0000	-0.1421
					0.0212	0.0276	0.0103		
296.	(0.00038)	RY (3)	H	7	s(0.00%)	p 1.00(96.13%)	d 0.04(3.87%)		
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.8883	0.4146	0.0177	0.0000	0.0000
					0.1917	-0.0407	-0.0160	-0.0073	0.0000
					0.0000	0.0000	0.0000		
297.	(0.00017)	RY (4)	H	7	s(45.66%)	p 1.09(49.69%)	d 0.10(4.65%)		
					-0.0020	0.0472	0.6677	-0.0924	0.0618
					0.1261	0.6650	0.0734	-0.0943	-0.1438
					0.0000	0.0000	0.0000	0.0653	0.0175
					0.0000	0.0000	0.0000	0.0000	-0.1728
					-0.0496	0.0272	0.0944		
298.	(0.00010)	RY (5)	H	7	s(54.91%)	p 0.72(39.76%)	d 0.10(5.32%)		
					0.0042	0.6418	-0.1541	-0.3368	-0.4831
					-0.0550	0.0718	0.3700	-0.0609	0.1243
					0.0000	0.0000	0.0000	0.0335	-0.0804
					0.0000	0.0000	0.0000	0.0000	-0.1163
					-0.0156	-0.1780	-0.0142		
299.	(0.00009)	RY (6)	H	7	s(0.00%)	p 1.00(68.43%)	d 0.46(31.57%)		
300.	(0.00003)	RY (7)	H	7	s(19.70%)	p 1.60(31.52%)	d 2.48(48.78%)		
301.	(0.00002)	RY (8)	H	7	s(45.61%)	p 0.76(34.55%)	d 0.44(19.84%)		
302.	(0.00001)	RY (9)	H	7	s(1.24%)	p44.08(54.68%)	d35.53(44.08%)		
303.	(0.00001)	RY (10)	H	7	s(0.00%)	p 1.00(5.58%)	d16.91(94.42%)		
304.	(0.00001)	RY (11)	H	7	s(8.75%)	p 5.21(45.59%)	d 5.22(45.67%)		
305.	(0.00001)	RY (12)	H	7	s(33.34%)	p 1.16(38.80%)	d 0.84(27.86%)		
306.	(0.00000)	RY (13)	H	7	s(5.00%)	p 3.09(15.44%)	d15.92(79.56%)		
307.	(0.00000)	RY (14)	H	7	s(5.03%)	p13.10(65.92%)	d 5.77(29.05%)		
308.	(0.00000)	RY (15)	H	7	s(11.82%)	p 2.95(34.89%)	d 4.51(53.30%)		
309.	(0.00000)	RY (16)	H	7	s(0.00%)	p 1.00(48.27%)	d 1.07(51.73%)		
310.	(0.00000)	RY (17)	H	7	s(0.00%)	p 1.00(46.40%)	d 1.15(53.60%)		
311.	(0.00000)	RY (18)	H	7	s(0.00%)	p 1.00(28.19%)	d 2.55(71.81%)		
312.	(0.00000)	RY (19)	H	7	s(0.00%)	p 1.00(7.00%)	d13.29(93.00%)		
313.	(0.00000)	RY (20)	H	7	s(9.78%)	p 3.20(31.34%)	d 6.02(58.89%)		
314.	(0.00000)	RY (21)	H	7	s(3.35%)	p 5.20(17.42%)	d23.66(79.23%)		
315.	(0.00000)	RY (22)	H	7	s(3.70%)	p 1.92(7.11%)	d24.09(89.19%)		
316.	(0.00274)	RY (1)	H	8	s(0.29%)	p99.99(98.78%)	d 3.19(0.93%)		
					-0.0042	0.0343	-0.0337	0.0242	0.9905
					0.0228	0.0416	0.0642	-0.0013	-0.0145
					0.0000	0.0000	0.0000	-0.0931	-0.0046
					0.0000	0.0000	0.0000	0.0000	-0.0241
					-0.0055	0.0016	0.0014		
317.	(0.00116)	RY (2)	H	8	s(0.00%)	p 1.00(95.88%)	d 0.04(4.12%)		
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0000	0.0000	0.0000	0.0000

				0.9672	-0.1434	-0.0517	0.0000	0.0000
				-0.0110	-0.0010	-0.1956	0.0531	0.0000
				0.0000	0.0000	0.0000		
318.	(0.00097)	RY (3)	H 8	s(77.18%)	p 0.28(21.50%)	d 0.02(1.31%)		
				0.0065	0.8784	0.0041	-0.0120	-0.0586
				0.0243	-0.0005	0.4376	-0.0136	-0.1392
				0.0000	0.0000	0.0000	0.0299	0.0011
				0.0000	0.0000	0.0000	0.0000	-0.0059
				-0.0444	0.0845	-0.0557		
319.	(0.00013)	RY (4)	H 8	s(13.96%)	p 4.48(62.52%)	d 1.68(23.51%)		
				-0.0045	0.3413	-0.0955	0.1183	0.0348
				-0.0376	0.0162	-0.7558	-0.1142	-0.1951
				0.0000	0.0000	0.0000	-0.0481	0.0121
				0.0000	0.0000	0.0000	0.0000	0.4601
				-0.0450	0.0176	-0.1366		
320.	(0.00004)	RY (5)	H 8	s(0.00%)	p 1.00(80.12%)	d 0.25(19.88%)		
321.	(0.00004)	RY (6)	H 8	s(27.66%)	p 1.19(32.86%)	d 1.43(39.48%)		
322.	(0.00003)	RY (7)	H 8	s(37.75%)	p 1.18(44.54%)	d 0.47(17.71%)		
323.	(0.00001)	RY (8)	H 8	s(2.01%)	p35.35(70.97%)	d13.46(27.02%)		
324.	(0.00001)	RY (9)	H 8	s(0.00%)	p 1.00(0.29%)	d99.99(99.71%)		
325.	(0.00001)	RY (10)	H 8	s(12.09%)	p 2.34(28.24%)	d 4.93(59.67%)		
326.	(0.00000)	RY (11)	H 8	s(48.69%)	p 0.82(40.02%)	d 0.23(11.29%)		
327.	(0.00000)	RY (12)	H 8	s(5.46%)	p 3.72(20.33%)	d13.59(74.21%)		
328.	(0.00000)	RY (13)	H 8	s(14.77%)	p 4.15(61.35%)	d 1.62(23.88%)		
329.	(0.00000)	RY (14)	H 8	s(7.62%)	p 5.55(42.27%)	d 6.57(50.10%)		
330.	(0.00000)	RY (15)	H 8	s(0.00%)	p 1.00(46.58%)	d 1.15(53.42%)		
331.	(0.00000)	RY (16)	H 8	s(0.00%)	p 1.00(28.53%)	d 2.50(71.47%)		
332.	(0.00000)	RY (17)	H 8	s(19.71%)	p 0.80(15.80%)	d 3.27(64.49%)		
333.	(0.00000)	RY (18)	H 8	s(0.00%)	p 1.00(42.12%)	d 1.37(57.88%)		
334.	(0.00000)	RY (19)	H 8	s(0.00%)	p 1.00(6.48%)	d14.44(93.52%)		
335.	(0.00000)	RY (20)	H 8	s(3.38%)	p 4.52(15.30%)	d24.04(81.32%)		
336.	(0.00000)	RY (21)	H 8	s(9.35%)	p 3.47(32.41%)	d 6.23(58.24%)		
337.	(0.00000)	RY (22)	H 8	s(20.11%)	p 0.65(13.07%)	d 3.32(66.82%)		
338.	(0.00102)	RY (1)	H 9	s(43.26%)	p 1.26(54.48%)	d 0.05(2.26%)		
				-0.0042	0.6572	0.0048	-0.0266	-0.2328
				-0.1145	-0.0245	0.6858	0.0389	-0.0708
				0.0000	0.0000	0.0000	0.0735	-0.0661
				0.0000	0.0000	0.0000	0.0000	0.0804
				0.0049	0.0783	-0.0135		
339.	(0.00065)	RY (2)	H 9	s(9.83%)	p 8.57(84.28%)	d 0.60(5.89%)		
				-0.0065	0.3128	0.0067	0.0193	-0.7349
				-0.0948	-0.0392	-0.5330	0.0490	0.0757
				0.0000	0.0000	0.0000	-0.1604	-0.0046
				0.0000	0.0000	0.0000	0.0000	-0.1662
				0.0036	0.0742	-0.0008		
340.	(0.00020)	RY (3)	H 9	s(0.00%)	p 1.00(93.24%)	d 0.07(6.76%)		
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.7282	0.6151	0.1537	0.0000	0.0000
				-0.1901	0.0212	0.1708	-0.0433	0.0000
				0.0000	0.0000	0.0000		
341.	(0.00016)	RY (4)	H 9	s(57.19%)	p 0.69(39.51%)	d 0.06(3.31%)		
				-0.0008	-0.1582	0.7377	-0.0516	-0.1974
				0.1635	0.4215	0.0980	-0.0896	-0.3661
				0.0000	0.0000	0.0000	-0.1543	-0.0363
				0.0000	0.0000	0.0000	0.0000	0.0353
				0.0037	-0.0316	-0.0755		
342.	(0.00013)	RY (5)	H 9	s(0.00%)	p 1.00(80.23%)	d 0.25(19.77%)		
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000
				-0.6262	0.4396	0.4657	0.0000	0.0000
				-0.3404	0.0194	0.2854	-0.0034	0.0000
				0.0000	0.0000	0.0000		

343.	(0.00008)	RY (6)	H	9	s(52.86%)p 0.77(40.86%)d 0.12(6.28%)
344.	(0.00002)	RY (7)	H	9	s(1.55%)p12.46(19.29%)d51.16(79.17%)
345.	(0.00001)	RY (8)	H	9	s(3.39%)p24.64(83.64%)d 3.82(12.96%)
346.	(0.00000)	RY (9)	H	9	s(20.01%)p 2.88(57.71%)d 1.11(22.28%)
347.	(0.00000)	RY (10)	H	9	s(0.00%)p 1.00(51.47%)d 0.94(48.53%)
348.	(0.00000)	RY (11)	H	9	s(23.89%)p 1.19(28.43%)d 2.00(47.68%)
349.	(0.00000)	RY (12)	H	9	s(18.05%)p 0.87(15.62%)d 3.68(66.33%)
350.	(0.00000)	RY (13)	H	9	s(19.17%)p 3.08(59.08%)d 1.13(21.74%)
351.	(0.00000)	RY (14)	H	9	s(9.44%)p 7.16(67.61%)d 2.43(22.95%)
352.	(0.00000)	RY (15)	H	9	s(3.34%)p 1.44(4.81%)d27.47(91.85%)
353.	(0.00000)	RY (16)	H	9	s(0.00%)p 1.00(26.35%)d 2.79(73.65%)
354.	(0.00000)	RY (17)	H	9	s(0.00%)p 1.00(27.21%)d 2.68(72.79%)
355.	(0.00000)	RY (18)	H	9	s(0.00%)p 1.00(16.77%)d 4.96(83.23%)
356.	(0.00000)	RY (19)	H	9	s(0.00%)p 1.00(4.73%)d20.12(95.27%)
357.	(0.00000)	RY (20)	H	9	s(28.42%)p 1.10(31.29%)d 1.42(40.29%)
358.	(0.00000)	RY (21)	H	9	s(7.92%)p 1.48(11.74%)d10.15(80.35%)
359.	(0.00000)	RY (22)	H	9	s(1.71%)p 0.95(1.63%)d56.37(96.66%)
360.	(0.00065)	RY (1)	H	10	s(0.03%)p99.99(91.64%)d99.99(8.33%)
					0.0017 0.0049 0.0097 0.0128 0.5683
					-0.0153 -0.0716 -0.7538 0.0536 0.1303
					0.0000 0.0000 0.0000 -0.1281 -0.0099
					0.0000 0.0000 0.0000 0.0000 0.2572
					0.0237 -0.0072 -0.0005
361.	(0.00047)	RY (2)	H	10	s(50.66%)p 0.91(46.08%)d 0.06(3.26%)
					-0.0072 0.7115 0.0111 -0.0137 -0.5255
					-0.0962 -0.1148 -0.3945 -0.0587 -0.0558
					0.0000 0.0000 0.0000 0.1209 -0.0280
					0.0000 0.0000 0.0000 0.0000 0.0582
					-0.0128 0.1140 -0.0252
362.	(0.00042)	RY (3)	H	10	s(0.00%)p 1.00(97.94%)d 0.02(2.06%)
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.9052 0.3960 0.0561 0.0000 0.0000
					-0.1256 0.0490 -0.0492 0.0037 0.0000
					0.0000 0.0000 0.0000
363.	(0.00019)	RY (4)	H	10	s(59.56%)p 0.55(32.72%)d 0.13(7.72%)
					0.0005 -0.0642 0.7690 -0.0116 -0.1120
					0.0942 0.4651 -0.0723 0.0491 0.2860
					0.0000 0.0000 0.0000 0.2406 -0.0041
					0.0000 0.0000 0.0000 0.0000 0.1069
					-0.0069 -0.0560 -0.0684
364.	(0.00007)	RY (5)	H	10	s(0.00%)p 1.00(69.16%)d 0.45(30.84%)
365.	(0.00005)	RY (6)	H	10	s(49.34%)p 0.79(38.84%)d 0.24(11.81%)
366.	(0.00002)	RY (7)	H	10	s(1.90%)p51.20(97.17%)d 0.49(0.94%)
367.	(0.00000)	RY (8)	H	10	s(5.69%)p 4.69(26.70%)d11.89(67.61%)
368.	(0.00000)	RY (9)	H	10	s(8.05%)p 5.44(43.75%)d 5.99(48.21%)
369.	(0.00000)	RY (10)	H	10	s(0.00%)p 1.00(5.12%)d18.52(94.88%)
370.	(0.00000)	RY (11)	H	10	s(12.53%)p 4.01(50.26%)d 2.97(37.21%)
371.	(0.00000)	RY (12)	H	10	s(58.38%)p 0.29(17.03%)d 0.42(24.60%)
372.	(0.00000)	RY (13)	H	10	s(6.52%)p 6.71(43.75%)d 7.63(49.73%)
373.	(0.00000)	RY (14)	H	10	s(4.81%)p12.23(58.80%)d 7.57(36.39%)
374.	(0.00000)	RY (15)	H	10	s(0.00%)p 1.00(85.32%)d 0.17(14.68%)
375.	(0.00000)	RY (16)	H	10	s(3.37%)p 1.45(4.90%)d27.19(91.72%)
376.	(0.00000)	RY (17)	H	10	s(0.00%)p 1.00(31.08%)d 2.22(68.92%)
377.	(0.00000)	RY (18)	H	10	s(0.00%)p 1.00(10.66%)d 8.38(89.34%)
378.	(0.00000)	RY (19)	H	10	s(0.00%)p 1.00(0.72%)d99.99(99.28%)
379.	(0.00000)	RY (20)	H	10	s(26.27%)p 1.14(30.06%)d 1.66(43.67%)
380.	(0.00000)	RY (21)	H	10	s(7.38%)p 1.83(13.48%)d10.73(79.15%)
381.	(0.00000)	RY (22)	H	10	s(5.56%)p 0.86(4.79%)d16.13(89.65%)
382.	(0.00068)	RY (1)	H	11	s(49.57%)p 0.96(47.71%)d 0.05(2.71%)
					-0.0071 0.7031 -0.0342 -0.0120 0.1845
					-0.0101 -0.0311 -0.6528 -0.1214 -0.0344
					0.0000 0.0000 0.0000 0.0255 -0.0084

			0.0000	0.0000	0.0000	0.0000	-0.0938
			-0.0431	0.1230	-0.0251		
383.	(0.00050)	R Y (2) H 11	s(1.32%)	p68.12(90.17%)	d 6.43(8.51%)		
			-0.0012	0.1128	0.0188	0.0124	-0.9239
			0.0780	0.1355	-0.1531	-0.0112	-0.0008
			0.0000	0.0000	0.0000	-0.2905	0.0063
			0.0000	0.0000	0.0000	0.0000	-0.0116
			0.0101	0.0198	-0.0006		
384.	(0.00034)	R Y (3) H 11	s(0.00%)	p 1.00(97.33%)	d 0.03(2.67%)		
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.8810	0.4440	0.0067	0.0000	0.0000
			0.0154	-0.0073	-0.1564	0.0443	0.0000
			0.0000	0.0000	0.0000		
385.	(0.00020)	R Y (4) H 11	s(58.81%)	p 0.63(37.05%)	d 0.07(4.14%)		
			0.0011	0.1011	0.7601	-0.0053	0.0166
			-0.0068	-0.0558	0.0217	0.2384	0.5565
			0.0000	0.0000	0.0000	-0.0119	-0.0048
			0.0000	0.0000	0.0000	0.0000	-0.1747
			-0.0213	-0.0563	-0.0845		
386.	(0.00006)	R Y (5) H 11	s(0.00%)	p 1.00(68.24%)	d 0.47(31.76%)		
387.	(0.00005)	R Y (6) H 11	s(44.67%)	p 0.81(36.19%)	d 0.43(19.13%)		
388.	(0.00001)	R Y (7) H 11	s(0.44%)	p99.99(81.45%)	d41.63(18.12%)		
389.	(0.00001)	R Y (8) H 11	s(12.73%)	p 4.72(60.08%)	d 2.14(27.19%)		
390.	(0.00000)	R Y (9) H 11	s(51.54%)	p 0.19(9.54%)	d 0.75(38.91%)		
391.	(0.00000)	R Y (10) H 11	s(0.00%)	p 1.00(1.58%)	d62.37(98.42%)		
392.	(0.00000)	R Y (11) H 11	s(9.63%)	p 3.90(37.55%)	d 5.48(52.82%)		
393.	(0.00000)	R Y (12) H 11	s(22.67%)	p 1.52(34.48%)	d 1.89(42.85%)		
394.	(0.00000)	R Y (13) H 11	s(1.42%)	p26.55(37.84%)	d42.62(60.74%)		
395.	(0.00000)	R Y (14) H 11	s(14.45%)	p 3.05(44.10%)	d 2.87(41.45%)		
396.	(0.00000)	R Y (15) H 11	s(5.31%)	p 3.63(19.29%)	d14.21(75.40%)		
397.	(0.00000)	R Y (16) H 11	s(0.00%)	p 1.00(95.95%)	d 0.04(4.05%)		
398.	(0.00000)	R Y (17) H 11	s(14.97%)	p 2.07(31.04%)	d 3.61(53.99%)		
399.	(0.00000)	R Y (18) H 11	s(0.00%)	p 1.00(10.91%)	d 8.17(89.09%)		
400.	(0.00000)	R Y (19) H 11	s(0.00%)	p 1.00(6.33%)	d14.80(93.67%)		
401.	(0.00000)	R Y (20) H 11	s(0.00%)	p 1.00(19.66%)	d 4.09(80.34%)		
402.	(0.00000)	R Y (21) H 11	s(5.80%)	p 3.14(18.20%)	d13.11(76.00%)		
403.	(0.00000)	R Y (22) H 11	s(6.70%)	p 2.28(15.27%)	d11.64(78.03%)		
404.	(0.00478)	R Y (1) N 12	s(2.88%)	p31.63(91.12%)	d 0.99(2.86%)		
			f 1.09(3.14%)				
			0.0000	-0.0054	0.1348	0.1030	-0.0036
			0.0089	-0.4844	0.0300	-0.0308	-0.0166
			0.8211	0.0090	-0.0071	0.0000	0.0000
			0.0000	0.0000	-0.0090	-0.1173	-0.0196
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	-0.0487	0.0378	-0.0678	0.0578
			0.0496	0.0115	0.0000	0.0000	0.0234
			-0.0200	-0.0462	0.0268	0.0000	0.0000
			0.0000	0.0000	-0.1340	0.0808	0.0533
			-0.0173				
405.	(0.00278)	R Y (2) N 12	s(0.00%)	p 1.00(84.69%)	d 0.13(10.64%)		
			f 0.06(4.67%)				
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	-0.0030	0.9171
			0.0741	-0.0199	0.0000	0.0000	0.0000
			0.3162	-0.0322	-0.0545	0.0328	-0.0054
			0.0364	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	-0.1233	0.0676	0.0000
			0.0000	0.0000	0.0000	0.1385	-0.0575
			0.0565	-0.0351	0.0000	0.0000	0.0000
			0.0000				
406.	(0.00139)	R Y (3) N 12	s(6.47%)	p10.19(65.94%)	d 1.40(9.08%)		

					f 2.86(18.50%)
		0.0000	0.0090	0.2453	0.0647 -0.0168
		0.0085	0.6594	-0.2446	0.0861 -0.0161
		0.3897	-0.0716	-0.0118	0.0000 0.0000
		0.0000	0.0000	0.0894	0.1927 -0.1313
		0.0000	0.0000	0.0000	0.0000 0.0000
		0.0000	0.0106	-0.0440	-0.0168 0.1223
		0.1050	0.0123	0.0000	0.0000 -0.0838
		0.0419	-0.0702	0.0255	0.0000 0.0000
		0.0000	0.0000	0.2201	-0.1288 0.3014
		-0.1214			
407.	(0.00065)	R Y	(4)	N 12	s(33.52%)p 1.16(38.99%)d 0.54(18.24%)
					f 0.28(9.25%)
		0.0000	-0.0008	0.5259	-0.2415 -0.0180
		0.0159	-0.2065	-0.5542	-0.0969 0.0094
		-0.1438	-0.0844	0.0515	0.0000 0.0000
		0.0000	0.0000	0.0407	0.1111 0.0859
		0.0000	0.0000	0.0000	0.0000 0.0000
		0.0000	-0.1651	-0.3289	-0.0937 0.0571
		0.1132	0.0270	0.0000	0.0000 -0.0876
		0.0051	0.0290	0.0024	0.0000 0.0000
		0.0000	0.0000	-0.0578	0.0262 -0.2748
		0.0667			
408.	(0.00043)	R Y	(5)	N 12	s(0.00%)p 1.00(40.24%)d 1.05(42.06%)
					f 0.44(17.70%)
		0.0000	0.0000	0.0000	0.0000 0.0000
		0.0000	0.0000	0.0000	0.0000 0.0000
		0.0000	0.0000	0.0000	0.0063 -0.0609
		0.6311	0.0186	0.0000	0.0000 0.0000
		0.1783	-0.5370	0.2280	0.2170 0.0359
		0.0062	0.0000	0.0000	0.0000 0.0000
		0.0000	0.0000	0.1785	-0.0466 0.0000
		0.0000	0.0000	0.0000	-0.2942 0.1174
		0.1710	-0.1158	0.0000	0.0000 0.0000
		0.0000			
409.	(0.00032)	R Y	(6)	N 12	s(7.13%)p 4.58(32.64%)d 3.90(27.78%)
					f 4.55(32.45%)
		0.0000	0.0053	0.1446	0.2243 -0.0070
		-0.0051	-0.1761	0.0220	0.0486 0.0001
		-0.1421	0.5179	-0.0638	0.0000 0.0000
		0.0000	0.0000	-0.0538	-0.3320 -0.0857
		0.0000	0.0000	0.0000	0.0000 0.0000
		0.0000	-0.2729	-0.0229	0.0865 0.2047
		0.1772	0.0399	0.0000	0.0000 -0.1235
		0.0989	0.0499	0.0046	0.0000 0.0000
		0.0000	0.0000	0.5043	-0.1808 0.0729
		-0.0680			
410.	(0.00026)	R Y	(7)	N 12	s(13.36%)p 2.09(27.92%)d 3.85(51.38%)
					f 0.55(7.35%)
		0.0000	-0.0248	0.3145	-0.1737 -0.0626
		0.0105	-0.0032	0.1973	-0.0090 0.0049
		0.0676	0.4852	0.0003	0.0000 0.0000
		0.0000	0.0000	0.3891	0.1749 -0.1395
		0.0000	0.0000	0.0000	0.0000 0.0000
		0.0000	0.3923	-0.0282	-0.0611 -0.2706
		-0.2840	0.0004	0.0000	0.0000 0.1462
		-0.0755	0.0272	0.0003	0.0000 0.0000
		0.0000	0.0000	0.1313	-0.0314 -0.1420
		0.0852			
411.	(0.00014)	R Y	(8)	N 12	s(0.00%)p 1.00(33.52%)d 1.71(57.48%)
					f 0.27(9.00%)
		0.0000	0.0000	0.0000	0.0000 0.0000
		0.0000	0.0000	0.0000	0.0000 0.0000

	0.0000	0.0000	0.0000	0.0100	-0.0862
	-0.5579	0.1282	0.0000	0.0000	0.0000
	0.3097	-0.1102	0.2439	0.5754	0.2727
	0.0408	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.1119	-0.0280	0.0000
	0.0000	0.0000	0.0000	0.1233	0.0319
	0.2081	-0.1310	0.0000	0.0000	0.0000
	0.0000				
412. (0.00012) RY (9) N 12	s(25.56%)	p 1.75(44.80%)	d 0.63(15.99%)		
	f 0.53(13.64%)				
	0.0000	0.0072	0.4984	-0.0127	0.0839
	0.0052	-0.0027	0.6005	-0.1408	0.0022
	-0.1743	-0.1592	0.1092	0.0000	0.0000
	0.0000	0.0000	-0.1711	0.0763	-0.0914
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.1020	-0.1524	-0.0709	-0.0362
	0.2520	0.1139	0.0000	0.0000	0.1333
	-0.0033	-0.0830	0.0613	0.0000	0.0000
	0.0000	0.0000	-0.1459	0.0185	0.2633
	-0.1306				
413. (0.00008) RY (10) N 12	s(3.41%)	p 3.93(13.40%)	d14.44(49.26%)		
	f 9.94(33.93%)				
414. (0.00005) RY (11) N 12	s(9.28%)	p 2.33(21.67%)	d 5.36(49.70%)		
	f 2.09(19.35%)				
415. (0.00004) RY (12) N 12	s(0.00%)	p 1.00(3.99%)	d18.35(73.16%)		
	f 5.73(22.85%)				
416. (0.00002) RY (13) N 12	s(9.85%)	p 3.11(30.68%)	d 4.94(48.68%)		
	f 1.10(10.80%)				
417. (0.00001) RY (14) N 12	s(14.62%)	p 3.67(53.66%)	d 1.34(19.54%)		
	f 0.83(12.18%)				
418. (0.00000) RY (15) N 12	s(30.75%)	p 0.59(18.11%)	d 1.31(40.33%)		
	f 0.35(10.81%)				
419. (0.00000) RY (16) N 12	s(5.65%)	p 2.66(15.00%)	d 7.01(39.59%)		
	f 7.04(39.76%)				
420. (0.00000) RY (17) N 12	s(6.22%)	p 1.37(8.50%)	d 5.31(33.02%)		
	f 8.40(52.26%)				
421. (0.00000) RY (18) N 12	s(17.48%)	p 1.23(21.42%)	d 2.12(37.11%)		
	f 1.37(23.98%)				
422. (0.00000) RY (19) N 12	s(6.55%)	p 3.38(22.12%)	d 5.87(38.48%)		
	f 5.01(32.85%)				
423. (0.00000) RY (20) N 12	s(17.67%)	p 0.68(12.09%)	d 1.85(32.73%)		
	f 2.12(37.51%)				
424. (0.00000) RY (21) N 12	s(0.00%)	p 1.00(4.28%)	d13.43(57.54%)		
	f 8.91(38.17%)				
425. (0.00000) RY (22) N 12	s(0.00%)	p 1.00(18.10%)	d 4.05(73.26%)		
	f 0.48(8.65%)				
426. (0.00000) RY (23) N 12	s(0.00%)	p 1.00(3.28%)	d24.72(81.00%)		
	f 4.80(15.72%)				
427. (0.00000) RY (24) N 12	s(0.00%)	p 1.00(5.58%)	d11.44(63.86%)		
	f 5.47(30.55%)				
428. (0.00000) RY (25) N 12	s(0.00%)	p 1.00(90.93%)	d 0.10(8.83%)		
	f 0.00(0.24%)				
429. (0.00000) RY (26) N 12	s(0.70%)	p 1.24(0.87%)	d85.59(59.71%)		
	f55.52(38.73%)				
430. (0.00000) RY (27) N 12	s(2.21%)	p 4.57(10.13%)	d21.81(48.32%)		
	f17.76(39.34%)				
431. (0.00000) RY (28) N 12	s(0.00%)	p 1.00(2.22%)	d17.67(39.19%)		
	f26.42(58.59%)				
432. (0.00000) RY (29) N 12	s(0.00%)	p 1.00(0.27%)	d74.24(20.28%)		
	f99.99(79.45%)				
433. (0.00000) RY (30) N 12	s(6.11%)	p 2.22(13.56%)	d10.90(66.63%)		
	f 2.24(13.70%)				
434. (0.00000) RY (31) N 12	s(1.04%)	p 1.50(1.56%)	d31.86(33.00%)		

					f62.17(64.40%)
435.	(0.00000)	RY (32)	N 12	s(2.12%)p 3.90(8.25%)d23.56(49.91%)	f18.76(39.72%)
436.	(0.00000)	RY (33)	N 12	s(11.18%)p 0.25(2.74%)d 1.19(13.36%)	f 6.50(72.72%)
437.	(0.00000)	RY (34)	N 12	s(0.00%)p 1.00(9.85%)d 4.93(48.53%)	f 4.23(41.62%)
438.	(0.00000)	RY (35)	N 12	s(0.00%)p 1.00(1.22%)d 0.97(1.19%)	f79.71(97.59%)
439.	(0.00000)	RY (36)	N 12	s(0.00%)p 1.00(2.01%)d 9.40(18.86%)	f39.47(79.14%)
440.	(0.00000)	RY (37)	N 12	s(0.00%)p 1.00(0.08%)d51.41(3.93%)	f99.99(95.99%)
441.	(0.00000)	RY (38)	N 12	s(11.66%)p 2.11(24.56%)d 0.77(9.02%)	f 4.70(54.76%)
442.	(0.00000)	RY (39)	N 12	s(3.67%)p 0.72(2.64%)d 9.19(33.72%)	f16.35(59.97%)
443.	(0.00000)	RY (40)	N 12	s(28.64%)p 0.41(11.86%)d 1.07(30.55%)	f 1.01(28.95%)
444.	(0.00000)	RY (41)	N 12	s(22.45%)p 0.29(6.49%)d 1.84(41.34%)	f 1.32(29.72%)
445.	(0.01183)	RY (1)	C 13	s(3.14%)p29.00(90.90%)d 1.05(3.29%)	f 0.85(2.67%)
				0.0000 -0.0126 0.1753 0.0172 -0.0127	
				-0.0554 -0.9371 -0.0051 0.0020 0.0108	
				0.1649 -0.0232 -0.0003 0.0000 0.0000	
				0.0000 0.0000 0.1637 0.0093 -0.0006	
				0.0000 0.0000 0.0000 0.0000 0.0000	
				0.0000 0.0733 0.0072 -0.0069 -0.0212	
				-0.0116 -0.0009 0.0000 0.0000 -0.0985	
				-0.0605 -0.0005 -0.0043 0.0000 0.0000	
				0.0000 0.0000 0.1050 0.0463 0.0046	
				0.0094	
446.	(0.00370)	RY (2)	C 13	s(0.00%)p 1.00(1.08%)d88.79(95.83%)	f 2.86(3.09%)
				0.0000 0.0000 0.0000 0.0000 0.0000	
				0.0000 0.0000 0.0000 0.0000 0.0000	
				0.0000 0.0000 0.0000 -0.0408 0.0230	
				-0.0746 -0.0551 0.0000 0.0000 0.0000	
				0.9756 -0.0096 -0.0333 -0.0686 -0.0015	
				-0.0230 0.0000 0.0000 0.0000 0.0000	
				0.0000 0.0000 -0.0142 -0.0375 0.0000	
				0.0000 0.0000 0.0000 0.0664 0.0812	
				0.1066 0.0831 0.0000 0.0000 0.0000	
				0.0000	
447.	(0.00338)	RY (3)	C 13	s(3.45%)p 1.68(5.78%)d25.06(86.36%)	f 1.28(4.41%)
				0.0000 -0.0003 0.1374 0.1174 0.0424	
				-0.0173 -0.1013 0.0032 0.0132 -0.0459	
				0.2087 0.0338 0.0171 0.0000 0.0000	
				0.0000 0.0000 -0.9153 0.0208 0.0255	
				0.0000 0.0000 0.0000 0.0000 0.0000	
				0.0000 -0.1202 -0.0167 -0.0289 0.0051	
				0.0955 -0.0043 0.0000 0.0000 0.0903	
				0.0491 -0.0273 -0.0005 0.0000 0.0000	
				0.0000 0.0000 0.1187 0.1124 -0.0200	
				-0.0753	
448.	(0.00148)	RY (4)	C 13	s(9.04%)p 8.90(80.51%)d 0.85(7.66%)	f 0.31(2.79%)
				0.0000 -0.0105 0.2996 0.0212 -0.0099	
				0.0053 -0.1345 -0.0015 -0.0052 0.0118	
				-0.8799 0.1116 0.0139 0.0000 0.0000	
				0.0000 0.0000 -0.1779 -0.0589 -0.0345	

	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0976	-0.0483	-0.0206	-0.1210
	-0.1086	0.0398	0.0000	0.0000	-0.0109
	-0.0145	0.0391	0.0133	0.0000	0.0000
	0.0000	0.0000	-0.1185	-0.0249	-0.1028
	-0.0244				
449. (0.00053) RY (5) C 13	s(0.00%)p	1.00(80.28%)d	0.21(16.87%)		
	f	0.04(2.84%)			
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	-0.0164	0.8447
	-0.2750	0.1156	0.0000	0.0000	0.0000
	-0.0134	0.3754	0.1548	-0.0335	-0.0502
	0.0018	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	-0.0399	0.0105	0.0000
	0.0000	0.0000	0.0000	0.0651	0.0069
	-0.1348	-0.0653	0.0000	0.0000	0.0000
	0.0000				
450. (0.00033) RY (6) C 13	s(68.06%)p	0.23(15.65%)d	0.19(13.22%)		
	f	0.05(3.07%)			
	0.0000	0.0157	0.8086	-0.1616	-0.0219
	-0.0125	0.2328	0.0600	-0.0862	-0.0052
	0.2633	-0.1343	0.0610	0.0000	0.0000
	0.0000	0.0000	0.1130	0.1193	0.0509
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.1856	-0.1773	-0.1110	-0.1171
	-0.0075	0.1033	0.0000	0.0000	-0.0229
	0.0356	0.0691	0.0870	0.0000	0.0000
	0.0000	0.0000	-0.0155	-0.0029	-0.1273
	-0.0103				
451. (0.00007) RY (7) C 13	s(18.75%)p	0.25(4.65%)d	2.99(56.04%)		
	f	1.10(20.55%)			
452. (0.00004) RY (8) C 13	s(28.95%)p	0.65(18.74%)d	1.61(46.73%)		
	f	0.19(5.58%)			
453. (0.00004) RY (9) C 13	s(6.01%)p	7.25(43.59%)d	6.28(37.74%)		
	f	2.10(12.65%)			
454. (0.00003) RY (10) C 13	s(0.00%)p	1.00(3.36%)d	27.27(91.76%)		
	f	1.45(4.88%)			
455. (0.00001) RY (11) C 13	s(7.54%)p	4.27(32.23%)d	5.98(45.10%)		
	f	2.01(15.13%)			
456. (0.00001) RY (12) C 13	s(6.19%)p	0.53(3.30%)d	13.82(85.55%)		
	f	0.80(4.96%)			
457. (0.00000) RY (13) C 13	s(0.00%)p	1.00(27.41%)d	1.89(51.79%)		
	f	0.76(20.80%)			
458. (0.00000) RY (14) C 13	s(16.24%)p	1.69(27.41%)d	2.14(34.74%)		
	f	1.33(21.61%)			
459. (0.00000) RY (15) C 13	s(11.41%)p	1.27(14.51%)d	4.17(47.61%)		
	f	2.32(26.48%)			
460. (0.00000) RY (16) C 13	s(3.35%)p	5.32(17.82%)d	1.71(5.74%)		
	f	21.81(73.09%)			
461. (0.00000) RY (17) C 13	s(0.00%)p	1.00(45.37%)d	0.90(40.99%)		
	f	0.30(13.64%)			
462. (0.00000) RY (18) C 13	s(7.82%)p	3.54(27.69%)d	4.68(36.60%)		
	f	3.56(27.88%)			
463. (0.00000) RY (19) C 13	s(23.70%)p	0.76(17.97%)d	1.68(39.79%)		
	f	0.78(18.53%)			
464. (0.00000) RY (20) C 13	s(0.00%)p	1.00(24.30%)d	3.06(74.25%)		
	f	0.06(1.45%)			
465. (0.00000) RY (21) C 13	s(0.00%)p	1.00(0.11%)d	99.99(99.76%)		
	f	1.21(0.13%)			
466. (0.00000) RY (22) C 13	s(17.31%)p	0.32(5.55%)d	2.18(37.75%)		
	f	2.28(39.39%)			
467. (0.00000) RY (23) C 13	s(0.00%)p	1.00(39.79%)d	1.51(59.93%)		

					f 0.01(0.28%)
468.	(0.00000)	RY (24)	C 13	s(13.48%)	p 2.63(35.50%)d 3.03(40.86%)
					f 0.75(10.16%)
469.	(0.00000)	RY (25)	C 13	s(21.78%)	p 1.96(42.72%)d 1.12(24.31%)
					f 0.51(11.20%)
470.	(0.00000)	RY (26)	C 13	s(2.05%)	p 6.31(12.92%)d20.26(41.50%)
					f21.25(43.53%)
471.	(0.00000)	RY (27)	C 13	s(11.87%)	p 0.89(10.52%)d 4.64(55.07%)
					f 1.90(22.55%)
472.	(0.00000)	RY (28)	C 13	s(0.00%)	p 1.00(1.42%)d 2.08(2.96%)
					f67.26(95.62%)
473.	(0.00000)	RY (29)	C 13	s(0.00%)	p 1.00(6.00%)d 1.79(10.72%)
					f13.87(83.27%)
474.	(0.00000)	RY (30)	C 13	s(3.01%)	p 7.49(22.52%)d 3.73(11.22%)
					f21.04(63.25%)
475.	(0.00000)	RY (31)	C 13	s(2.67%)	p 9.13(24.35%)d 8.28(22.10%)
					f19.07(50.88%)
476.	(0.00000)	RY (32)	C 13	s(0.79%)	p 6.89(5.44%)d18.33(14.47%)
					f99.99(79.30%)
477.	(0.00000)	RY (33)	C 13	s(10.09%)	p 0.29(2.92%)d 2.90(29.23%)
					f 5.73(57.76%)
478.	(0.00000)	RY (34)	C 13	s(0.00%)	p 1.00(0.81%)d 6.03(4.88%)
					f99.99(94.31%)
479.	(0.00000)	RY (35)	C 13	s(0.00%)	p 1.00(3.26%)d 2.16(7.03%)
					f27.55(89.71%)
480.	(0.00000)	RY (36)	C 13	s(0.00%)	p 1.00(6.50%)d 0.88(5.72%)
					f13.50(87.78%)
481.	(0.00000)	RY (37)	C 13	s(0.00%)	p 1.00(1.04%)d 4.56(4.76%)
					f90.35(94.20%)
482.	(0.00000)	RY (38)	C 13	s(0.20%)	p25.48(5.07%)d99.99(42.17%)
					f99.99(52.56%)
483.	(0.00000)	RY (39)	C 13	s(1.82%)	p 5.11(9.30%)d 7.83(14.25%)
					f40.98(74.63%)
484.	(0.00000)	RY (40)	C 13	s(1.43%)	p15.93(22.86%)d14.34(20.56%)
					f38.44(55.14%)
485.	(0.00000)	RY (41)	C 13	s(0.00%)	p 1.00(59.49%)d 0.55(32.58%)
					f 0.13(7.93%)
486.	(0.00218)	RY (1)	O 14	s(0.00%)	p 1.00(97.32%)d 0.02(1.60%)
					f 0.01(1.08%)
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 -0.0118 0.9857
					-0.0184 -0.0328 0.0000 0.0000 0.0000
					-0.0701 0.0655 0.0759 -0.0152 -0.0260
					0.0103 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 -0.0545 0.0211 0.0000
					0.0000 0.0000 0.0000 0.0808 -0.0299
					-0.0028 -0.0021 0.0000 0.0000 0.0000
					0.0000
487.	(0.00145)	RY (2)	O 14	s(1.51%)	p62.48(94.36%)d 1.55(2.34%)
					f 1.18(1.79%)
					0.0000 0.0009 0.1186 -0.0322 0.0030
					-0.0015 0.0370 -0.0841 0.0103 -0.0034
					0.9661 -0.0149 -0.0385 0.0000 0.0000
					0.0000 0.0000 -0.1080 0.0588 0.0813
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 -0.0211 0.0302 -0.0060 0.0070
					0.0135 -0.0055 0.0000 0.0000 0.0036
					0.0035 -0.0250 0.0086 0.0000 0.0000
					0.0000 0.0000 -0.0011 0.0032 0.1240
					-0.0419
488.	(0.00025)	RY (3)	O 14	s(52.49%)	p 0.69(36.03%)d 0.18(9.64%)
					f 0.04(1.84%)

0.0000 0.0125 0.6921 -0.2140 -0.0033
 -0.0324 -0.2969 -0.4531 0.0900 -0.0010
 -0.1304 0.1839 0.0825 0.0000 0.0000
 0.0000 0.0000 -0.0190 0.0074 0.0156
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 -0.2608 0.0217 -0.0613 0.1460
 0.0452 0.0115 0.0000 0.0000 0.0768
 -0.0017 -0.0054 0.0035 0.0000 0.0000
 0.0000 0.0000 -0.1088 0.0172 0.0165
 -0.0073

489.	(0.00002)	RY (4)	O 14	s(9.54%)	p 3.31(31.61%)	d 5.74(54.74%)
				f 0.43(4.11%)		
490.	(0.00002)	RY (5)	O 14	s(2.80%)	p24.62(68.98%)	d 7.79(21.83%)
				f 2.28(6.38%)		
491.	(0.00002)	RY (6)	O 14	s(0.00%)	p 1.00(31.58%)	d 2.04(64.52%)
				f 0.12(3.90%)		
492.	(0.00001)	RY (7)	O 14	s(25.78%)	p 1.10(28.29%)	d 1.28(33.09%)
				f 0.50(12.84%)		
493.	(0.00001)	RY (8)	O 14	s(0.00%)	p 1.00(66.05%)	d 0.43(28.51%)
				f 0.08(5.44%)		
494.	(0.00000)	RY (9)	O 14	s(13.78%)	p 1.41(19.45%)	d 4.20(57.89%)
				f 0.64(8.88%)		
495.	(0.00000)	RY (10)	O 14	s(8.58%)	p 4.95(42.48%)	d 3.51(30.07%)
				f 2.20(18.86%)		
496.	(0.00000)	RY (11)	O 14	s(46.41%)	p 0.21(9.59%)	d 0.47(21.88%)
				f 0.48(22.13%)		
497.	(0.00000)	RY (12)	O 14	s(2.06%)	p 1.67(3.44%)	d 8.02(16.57%)
				f37.74(77.93%)		
498.	(0.00000)	RY (13)	O 14	s(6.80%)	p 3.77(25.65%)	d 8.32(56.56%)
				f 1.62(10.98%)		
499.	(0.00000)	RY (14)	O 14	s(17.06%)	p 0.34(5.80%)	d 1.07(18.24%)
				f 3.45(58.90%)		
500.	(0.00000)	RY (15)	O 14	s(10.54%)	p 1.29(13.57%)	d 2.25(23.67%)
				f 4.95(52.22%)		
501.	(0.00000)	RY (16)	O 14	s(0.00%)	p 1.00(93.97%)	d 0.06(6.03%)
				f 0.00(0.00%)		
502.	(0.00000)	RY (17)	O 14	s(8.70%)	p 3.51(30.54%)	d 4.43(38.52%)
				f 2.56(22.24%)		
503.	(0.00000)	RY (18)	O 14	s(5.55%)	p 7.96(44.18%)	d 8.11(45.02%)
				f 0.94(5.24%)		
504.	(0.00000)	RY (19)	O 14	s(0.00%)	p 1.00(1.74%)	d56.47(98.26%)
				f 0.00(0.00%)		
505.	(0.00000)	RY (20)	O 14	s(0.00%)	p 1.00(0.44%)	d99.99(99.47%)
				f 0.21(0.09%)		
506.	(0.00000)	RY (21)	O 14	s(0.00%)	p 1.00(4.58%)	d18.45(84.57%)
				f 2.37(10.85%)		
507.	(0.00000)	RY (22)	O 14	s(0.00%)	p 1.00(1.75%)	d56.16(98.25%)
				f 0.00(0.00%)		
508.	(0.00000)	RY (23)	O 14	s(0.00%)	p 1.00(0.40%)	d99.99(99.42%)
				f 0.44(0.18%)		
509.	(0.00000)	RY (24)	O 14	s(26.06%)	p 0.17(4.53%)	d 1.02(26.51%)
				f 1.65(42.90%)		
510.	(0.00000)	RY (25)	O 14	s(5.32%)	p 6.51(34.66%)	d 7.17(38.20%)
				f 4.10(21.81%)		
511.	(0.00000)	RY (26)	O 14	s(18.53%)	p 0.96(17.77%)	d 2.65(49.16%)
				f 0.78(14.54%)		
512.	(0.00000)	RY (27)	O 14	s(2.21%)	p 1.63(3.59%)	d23.50(51.92%)
				f19.13(42.28%)		
513.	(0.00000)	RY (28)	O 14	s(0.00%)	p 1.00(0.45%)	d25.70(11.50%)
				f99.99(88.06%)		
514.	(0.00000)	RY (29)	O 14	s(0.00%)	p 1.00(0.03%)	d11.01(0.37%)
				f99.99(99.60%)		
515.	(0.00000)	RY (30)	O 14	s(1.71%)	p 8.64(14.80%)	d17.25(29.55%)

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                    f31.50( 53.94%)
516. (0.00000) RY (31) O 14      s( 0.30%)p32.78( 9.79%)d99.99( 55.25%)
                    f99.99( 34.66%)
517. (0.00000) RY (32) O 14      s( 5.99%)p 0.97( 5.80%)d 3.07( 18.41%)
                    f11.66( 69.81%)
518. (0.00000) RY (33) O 14      s( 6.00%)p 1.11( 6.63%)d 4.52( 27.11%)
                    f10.05( 60.27%)
519. (0.00000) RY (34) O 14      s( 13.56%)p 0.61( 8.32%)d 4.54( 61.58%)
                    f 1.22( 16.55%)
520. (0.00000) RY (35) O 14      s( 0.00%)p 1.00( 1.80%)d 2.13( 3.85%)
                    f52.29( 94.35%)
521. (0.00000) RY (36) O 14      s( 0.00%)p 1.00( 0.23%)d 3.19( 0.75%)
                    f99.99( 99.02%)
522. (0.00000) RY (37) O 14      s( 0.00%)p 1.00( 0.03%)d91.34( 2.40%)
                    f99.99( 97.57%)
523. (0.00000) RY (38) O 14      s( 0.00%)p 1.00( 0.04%)d 3.04( 0.13%)
                    f99.99( 99.83%)
524. (0.00000) RY (39) O 14      s( 0.57%)p30.40( 17.41%)d61.17( 35.02%)
                    f82.10( 47.00%)
525. (0.00000) RY (40) O 14      s( 5.70%)p 1.82( 10.39%)d 7.04( 40.15%)
                    f 7.68( 43.76%)
526. (0.00000) RY (41) O 14      s( 2.53%)p 5.35( 13.52%)d14.20( 35.89%)
                    f19.01( 48.06%)

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NHO DIRECTIONALITY AND BOND BENDING (deviation from line of nuclear centers at the position of maximum hybrid amplitude)

[Thresholds for printing: angular deviation > 1.0 degree]
 p- or d-character > 25.0%
 orbital occupancy > 0.10e

NBO	Line of Centers		Hybrid 1			Hybrid 2		
	Theta	Phi	Theta	Phi	Dev	Theta	Phi	Dev
10. LP (1) N 12	--	--	90.0	100.4	--	--	--	--
11. LP (1) O 14	--	--	90.0	355.6	--	--	--	--
12. LP (2) O 14	--	--	1.2	177.5	--	--	--	--
13. BD (1) C 1- C 2	90.0	91.8	90.0	90.1	1.6	90.0	275.2	3.4
14. BD (1) C 1- C 6	90.0	211.3	90.0	213.6	2.3	90.0	29.1	2.2
15. BD (2) C 1- C 6	90.0	211.3	0.8	187.5	89.3	0.8	52.2	89.2
17. BD (1) C 2- C 3	90.0	151.4	90.0	147.2	4.2	90.0	332.5	1.0
18. BD (2) C 2- C 3	90.0	151.4	0.9	156.5	89.1	1.0	312.7	89.1
19. BD (1) C 2- N 12	90.0	33.5	--	--	--	90.0	218.3	4.9
20. BD (1) C 3- C 4	90.0	211.8	90.0	210.0	1.8	90.0	34.5	2.7
22. BD (1) C 4- C 5	90.0	271.4	90.0	269.2	2.2	90.0	93.7	2.3
23. BD (2) C 4- C 5	90.0	271.4	0.8	296.4	89.3	0.8	66.7	89.3
25. BD (1) C 5- C 6	90.0	331.7	90.0	329.3	2.4	90.0	154.0	2.3
28. BD (1) N 12- C 13	90.0	350.0	90.0	346.6	3.3	90.0	174.4	4.4
29. BD (2) N 12- C 13	90.0	350.0	1.2	325.8	88.9	2.8	171.3	87.2
30. BD (1) C 13- O 14	90.0	357.1	90.0	328.8	28.3	90.0	200.6	23.5
31. BD (2) C 13- O 14	90.0	357.1	90.0	62.0	64.8	90.0	110.8	66.4

3-Center, 4-Electron A:-B-:C Hyperbonds (A-B :C <=> A: B-C)
 [threshold for detection: 33.3%]

Hyperbond A:-B-:C	%A-B/%B-C	occ	NBOs		3-center hybrids		
			BD(A-B)	LP(C)	h(A)	h(B)	h(C)
1. N 12:- C 13-: O 14	56.7/43.3	3.9402	29	12	45	46	12

2. O 14:- C 13-: N 12 63.0/37.0 3.9180 31 10 49 50 10

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
=====				
within unit 1				
10. LP (1) N 12	32. BD*(1) C 1- C 2	9.39	0.85	0.080
10. LP (1) N 12	36. BD*(1) C 2- C 3	2.40	0.86	0.040
10. LP (1) N 12	47. BD*(1) N 12- C 13	1.40	1.05	0.034
10. LP (1) N 12	49. BD*(1) C 13- O 14	14.01	0.88	0.099
10. LP (1) N 12	50. BD*(2) C 13- O 14	40.31	0.41	0.115
10. LP (1) N 12	94. RY (3) C 2	0.98	2.54	0.044
10. LP (1) N 12	96. RY (5) C 2	0.80	2.15	0.037
10. LP (1) N 12	444. RY (41) N 12	0.60	5.54	0.051
10. LP (1) N 12	445. RY (1) C 13	2.34	1.74	0.057
10. LP (1) N 12	447. RY (3) C 13	2.42	3.51	0.082
10. LP (1) N 12	450. RY (6) C 13	0.68	3.39	0.043
11. LP (1) O 14	47. BD*(1) N 12- C 13	10.91	1.36	0.109
11. LP (1) O 14	445. RY (1) C 13	9.85	2.05	0.127
12. LP (2) O 14	48. BD*(2) N 12- C 13	115.02	0.33	0.173
12. LP (2) O 14	446. RY (2) C 13	3.63	3.64	0.103
12. LP (2) O 14	449. RY (5) C 13	0.72	1.33	0.028
12. LP (2) O 14	491. RY (6) O 14	0.96	1.50	0.034
12. LP (2) O 14	493. RY (8) O 14	0.51	1.32	0.023
13. BD (1) C 1- C 2	33. BD*(1) C 1- C 6	1.30	1.16	0.035
13. BD (1) C 1- C 2	35. BD*(1) C 1- H 7	0.53	1.02	0.021
13. BD (1) C 1- C 2	36. BD*(1) C 2- C 3	2.38	1.15	0.047
13. BD (1) C 1- C 2	38. BD*(1) C 2- N 12	0.80	1.03	0.026
13. BD (1) C 1- C 2	40. BD*(1) C 3- H 8	1.80	1.06	0.039
13. BD (1) C 1- C 2	46. BD*(1) C 6- H 11	2.14	1.04	0.042
13. BD (1) C 1- C 2	135. RY (3) C 3	1.29	3.99	0.064
13. BD (1) C 1- C 2	136. RY (4) C 3	1.17	4.37	0.064
13. BD (1) C 1- C 2	148. RY (16) C 3	0.75	3.39	0.045
13. BD (1) C 1- C 2	253. RY (1) C 6	1.29	2.42	0.050
13. BD (1) C 1- C 2	254. RY (2) C 6	1.41	2.80	0.056
13. BD (1) C 1- C 2	297. RY (4) H 7	0.57	4.18	0.043
13. BD (1) C 1- C 2	404. RY (1) N 12	1.94	2.37	0.060
13. BD (1) C 1- C 2	406. RY (3) N 12	1.45	3.37	0.062
13. BD (1) C 1- C 2	409. RY (6) N 12	0.67	2.37	0.036
13. BD (1) C 1- C 2	452. RY (8) C 13	0.89	3.32	0.048
14. BD (1) C 1- C 6	32. BD*(1) C 1- C 2	1.35	1.14	0.035
14. BD (1) C 1- C 6	35. BD*(1) C 1- H 7	0.66	1.01	0.023
14. BD (1) C 1- C 6	38. BD*(1) C 2- N 12	3.51	1.02	0.053
14. BD (1) C 1- C 6	44. BD*(1) C 5- C 6	1.20	1.15	0.033
14. BD (1) C 1- C 6	45. BD*(1) C 5- H 10	2.20	1.03	0.042
14. BD (1) C 1- C 6	93. RY (2) C 2	2.76	2.14	0.069
14. BD (1) C 1- C 6	94. RY (3) C 2	0.62	2.83	0.037
14. BD (1) C 1- C 6	96. RY (5) C 2	1.01	2.44	0.044
14. BD (1) C 1- C 6	212. RY (1) C 5	0.92	2.33	0.041
14. BD (1) C 1- C 6	213. RY (2) C 5	1.09	2.73	0.049
14. BD (1) C 1- C 6	382. RY (1) H 11	0.61	1.51	0.027
15. BD (2) C 1- C 6	37. BD*(2) C 2- C 3	22.28	0.27	0.069
15. BD (2) C 1- C 6	42. BD*(2) C 4- C 5	19.04	0.28	0.065
15. BD (2) C 1- C 6	99. RY (8) C 2	1.04	2.26	0.043
15. BD (2) C 1- C 6	214. RY (3) C 5	0.85	1.14	0.028
15. BD (2) C 1- C 6	216. RY (5) C 5	0.50	2.17	0.029
16. BD (1) C 1- H 7	36. BD*(1) C 2- C 3	4.13	1.04	0.058
16. BD (1) C 1- H 7	38. BD*(1) C 2- N 12	0.94	0.91	0.026

16.	BD	(1)	C	1-	H	7	44.	BD*	(1)	C	5-	C	6	3.47	1.04	0.054
16.	BD	(1)	C	1-	H	7	46.	BD*	(1)	C	6-	H	11	0.69	0.92	0.022
16.	BD	(1)	C	1-	H	7	92.	RY	(1)	C	2			0.55	1.84	0.028
16.	BD	(1)	C	1-	H	7	93.	RY	(2)	C	2			1.17	2.04	0.044
16.	BD	(1)	C	1-	H	7	94.	RY	(3)	C	2			2.02	2.72	0.066
16.	BD	(1)	C	1-	H	7	100.	RY	(9)	C	2			0.73	3.02	0.042
16.	BD	(1)	C	1-	H	7	104.	RY	(13)	C	2			0.68	4.45	0.049
16.	BD	(1)	C	1-	H	7	253.	RY	(1)	C	6			1.42	2.30	0.051
16.	BD	(1)	C	1-	H	7	256.	RY	(4)	C	6			1.27	3.74	0.062
16.	BD	(1)	C	1-	H	7	259.	RY	(7)	C	6			0.60	2.89	0.037
17.	BD	(1)	C	2-	C	3	32.	BD*	(1)	C	1-	C	2	1.83	1.15	0.041
17.	BD	(1)	C	2-	C	3	35.	BD*	(1)	C	1-	H	7	2.21	1.02	0.042
17.	BD	(1)	C	2-	C	3	38.	BD*	(1)	C	2-	N	12	0.64	1.02	0.023
17.	BD	(1)	C	2-	C	3	39.	BD*	(1)	C	3-	C	4	0.56	1.16	0.023
17.	BD	(1)	C	2-	C	3	43.	BD*	(1)	C	4-	H	9	2.41	1.03	0.045
17.	BD	(1)	C	2-	C	3	47.	BD*	(1)	N	12-	C	13	2.90	1.35	0.056
17.	BD	(1)	C	2-	C	3	51.	RY	(1)	C	1			0.81	2.41	0.039
17.	BD	(1)	C	2-	C	3	52.	RY	(2)	C	1			1.64	2.94	0.062
17.	BD	(1)	C	2-	C	3	93.	RY	(2)	C	2			0.90	2.15	0.039
17.	BD	(1)	C	2-	C	3	171.	RY	(1)	C	4			3.76	1.98	0.077
17.	BD	(1)	C	2-	C	3	172.	RY	(2)	C	4			0.79	2.18	0.037
17.	BD	(1)	C	2-	C	3	316.	RY	(1)	H	8			1.04	1.88	0.039
17.	BD	(1)	C	2-	C	3	404.	RY	(1)	N	12			2.58	2.36	0.070
18.	BD	(2)	C	2-	C	3	34.	BD*	(2)	C	1-	C	6	19.65	0.28	0.066
18.	BD	(2)	C	2-	C	3	42.	BD*	(2)	C	4-	C	5	21.21	0.28	0.069
18.	BD	(2)	C	2-	C	3	48.	BD*	(2)	N	12-	C	13	14.14	0.28	0.056
18.	BD	(2)	C	2-	C	3	53.	RY	(3)	C	1			1.58	1.14	0.038
18.	BD	(2)	C	2-	C	3	173.	RY	(3)	C	4			2.26	1.21	0.047
18.	BD	(2)	C	2-	C	3	317.	RY	(2)	H	8			0.63	1.36	0.026
18.	BD	(2)	C	2-	C	3	405.	RY	(2)	N	12			1.04	1.30	0.033
19.	BD	(1)	C	2-	N	12	33.	BD*	(1)	C	1-	C	6	1.42	1.27	0.038
19.	BD	(1)	C	2-	N	12	36.	BD*	(1)	C	2-	C	3	0.54	1.26	0.023
19.	BD	(1)	C	2-	N	12	39.	BD*	(1)	C	3-	C	4	0.96	1.27	0.031
19.	BD	(1)	C	2-	N	12	47.	BD*	(1)	N	12-	C	13	1.24	1.45	0.038
19.	BD	(1)	C	2-	N	12	49.	BD*	(1)	C	13-	O	14	2.08	1.28	0.046
19.	BD	(1)	C	2-	N	12	50.	BD*	(2)	C	13-	O	14	6.40	0.81	0.064
19.	BD	(1)	C	2-	N	12	51.	RY	(1)	C	1			0.51	2.51	0.032
19.	BD	(1)	C	2-	N	12	52.	RY	(2)	C	1			0.72	3.04	0.042
19.	BD	(1)	C	2-	N	12	445.	RY	(1)	C	13			0.50	2.14	0.029
19.	BD	(1)	C	2-	N	12	448.	RY	(4)	C	13			1.68	2.41	0.057
20.	BD	(1)	C	3-	C	4	36.	BD*	(1)	C	2-	C	3	0.61	1.14	0.024
20.	BD	(1)	C	3-	C	4	38.	BD*	(1)	C	2-	N	12	3.85	1.01	0.056
20.	BD	(1)	C	3-	C	4	41.	BD*	(1)	C	4-	C	5	1.11	1.15	0.032
20.	BD	(1)	C	3-	C	4	45.	BD*	(1)	C	5-	H	10	2.34	1.02	0.044
20.	BD	(1)	C	3-	C	4	92.	RY	(1)	C	2			5.04	1.94	0.088
20.	BD	(1)	C	3-	C	4	93.	RY	(2)	C	2			0.68	2.14	0.034
20.	BD	(1)	C	3-	C	4	212.	RY	(1)	C	5			1.33	2.32	0.050
20.	BD	(1)	C	3-	C	4	213.	RY	(2)	C	5			0.96	2.72	0.046
20.	BD	(1)	C	3-	C	4	316.	RY	(1)	H	8			0.93	1.87	0.037
21.	BD	(1)	C	3-	H	8	32.	BD*	(1)	C	1-	C	2	4.76	1.03	0.062
21.	BD	(1)	C	3-	H	8	38.	BD*	(1)	C	2-	N	12	1.02	0.90	0.027
21.	BD	(1)	C	3-	H	8	41.	BD*	(1)	C	4-	C	5	4.13	1.04	0.058
21.	BD	(1)	C	3-	H	8	43.	BD*	(1)	C	4-	H	9	0.69	0.91	0.022
21.	BD	(1)	C	3-	H	8	92.	RY	(1)	C	2			4.15	1.83	0.078
21.	BD	(1)	C	3-	H	8	109.	RY	(18)	C	2			0.66	3.95	0.046
21.	BD	(1)	C	3-	H	8	171.	RY	(1)	C	4			2.12	1.86	0.056
21.	BD	(1)	C	3-	H	8	174.	RY	(4)	C	4			0.89	2.42	0.042
22.	BD	(1)	C	4-	C	5	39.	BD*	(1)	C	3-	C	4	1.25	1.16	0.034
22.	BD	(1)	C	4-	C	5	40.	BD*	(1)	C	3-	H	8	1.99	1.05	0.041
22.	BD	(1)	C	4-	C	5	43.	BD*	(1)	C	4-	H	9	0.62	1.03	0.023
22.	BD	(1)	C	4-	C	5	44.	BD*	(1)	C	5-	C	6	1.14	1.15	0.032
22.	BD	(1)	C	4-	C	5	45.	BD*	(1)	C	5-	H	10	0.58	1.03	0.022
22.	BD	(1)	C	4-	C	5	46.	BD*	(1)	C	6-	H	11	2.29	1.02	0.043

22.	BD (1) C 4- C 5	133.	RY (1) C 3	0.95	3.07	0.048
22.	BD (1) C 4- C 5	135.	RY (3) C 3	0.80	3.98	0.050
22.	BD (1) C 4- C 5	253.	RY (1) C 6	1.11	2.40	0.046
22.	BD (1) C 4- C 5	254.	RY (2) C 6	1.19	2.79	0.051
22.	BD (1) C 4- C 5	339.	RY (2) H 9	0.57	1.94	0.030
23.	BD (2) C 4- C 5	34.	BD*(2) C 1- C 6	21.57	0.28	0.069
23.	BD (2) C 4- C 5	37.	BD*(2) C 2- C 3	18.30	0.27	0.063
23.	BD (2) C 4- C 5	255.	RY (3) C 6	1.09	1.13	0.031
24.	BD (1) C 4- H 9	36.	BD*(1) C 2- C 3	3.28	1.03	0.052
24.	BD (1) C 4- H 9	44.	BD*(1) C 5- C 6	3.78	1.04	0.056
24.	BD (1) C 4- H 9	45.	BD*(1) C 5- H 10	0.69	0.92	0.022
24.	BD (1) C 4- H 9	133.	RY (1) C 3	0.87	2.96	0.045
24.	BD (1) C 4- H 9	134.	RY (2) C 3	1.70	2.69	0.060
24.	BD (1) C 4- H 9	143.	RY (11) C 3	0.51	3.02	0.035
24.	BD (1) C 4- H 9	212.	RY (1) C 5	1.77	2.21	0.056
24.	BD (1) C 4- H 9	213.	RY (2) C 5	0.54	2.61	0.033
24.	BD (1) C 4- H 9	215.	RY (4) C 5	0.82	3.17	0.046
25.	BD (1) C 5- C 6	33.	BD*(1) C 1- C 6	1.15	1.15	0.032
25.	BD (1) C 5- C 6	35.	BD*(1) C 1- H 7	2.30	1.01	0.043
25.	BD (1) C 5- C 6	41.	BD*(1) C 4- C 5	1.13	1.15	0.032
25.	BD (1) C 5- C 6	43.	BD*(1) C 4- H 9	2.36	1.02	0.044
25.	BD (1) C 5- C 6	45.	BD*(1) C 5- H 10	0.56	1.03	0.021
25.	BD (1) C 5- C 6	46.	BD*(1) C 6- H 11	0.55	1.02	0.021
25.	BD (1) C 5- C 6	51.	RY (1) C 1	1.40	2.40	0.052
25.	BD (1) C 5- C 6	52.	RY (2) C 1	0.86	2.93	0.045
25.	BD (1) C 5- C 6	54.	RY (4) C 1	0.51	2.93	0.034
25.	BD (1) C 5- C 6	59.	RY (9) C 1	0.66	3.55	0.043
25.	BD (1) C 5- C 6	172.	RY (2) C 4	1.63	2.17	0.053
26.	BD (1) C 5- H 10	33.	BD*(1) C 1- C 6	3.72	1.04	0.056
26.	BD (1) C 5- H 10	39.	BD*(1) C 3- C 4	3.77	1.04	0.056
26.	BD (1) C 5- H 10	43.	BD*(1) C 4- H 9	0.66	0.91	0.022
26.	BD (1) C 5- H 10	46.	BD*(1) C 6- H 11	0.66	0.91	0.022
26.	BD (1) C 5- H 10	171.	RY (1) C 4	0.87	1.86	0.036
26.	BD (1) C 5- H 10	172.	RY (2) C 4	1.06	2.06	0.042
26.	BD (1) C 5- H 10	175.	RY (5) C 4	1.47	3.62	0.065
26.	BD (1) C 5- H 10	253.	RY (1) C 6	1.59	2.29	0.054
26.	BD (1) C 5- H 10	256.	RY (4) C 6	1.02	3.73	0.055
26.	BD (1) C 5- H 10	260.	RY (8) C 6	0.89	3.79	0.052
27.	BD (1) C 6- H 11	32.	BD*(1) C 1- C 2	3.61	1.03	0.054
27.	BD (1) C 6- H 11	35.	BD*(1) C 1- H 7	0.64	0.90	0.021
27.	BD (1) C 6- H 11	41.	BD*(1) C 4- C 5	3.71	1.04	0.056
27.	BD (1) C 6- H 11	45.	BD*(1) C 5- H 10	0.69	0.92	0.022
27.	BD (1) C 6- H 11	51.	RY (1) C 1	1.92	2.29	0.059
27.	BD (1) C 6- H 11	54.	RY (4) C 1	0.81	2.82	0.043
27.	BD (1) C 6- H 11	55.	RY (5) C 1	1.08	3.15	0.052
27.	BD (1) C 6- H 11	212.	RY (1) C 5	1.27	2.21	0.047
27.	BD (1) C 6- H 11	215.	RY (4) C 5	1.07	3.17	0.052
28.	BD (1) N 12- C 13	36.	BD*(1) C 2- C 3	1.37	1.39	0.039
28.	BD (1) N 12- C 13	38.	BD*(1) C 2- N 12	1.63	1.27	0.041
28.	BD (1) N 12- C 13	49.	BD*(1) C 13- O 14	3.54	1.41	0.063
28.	BD (1) N 12- C 13	92.	RY (1) C 2	0.64	2.19	0.033
28.	BD (1) N 12- C 13	93.	RY (2) C 2	1.66	2.39	0.056
28.	BD (1) N 12- C 13	94.	RY (3) C 2	2.69	3.08	0.081
28.	BD (1) N 12- C 13	488.	RY (3) O 14	0.54	2.59	0.033
29.	BD (2) N 12- C 13	37.	BD*(2) C 2- C 3	15.92	0.39	0.070
29.	BD (2) N 12- C 13	48.	BD*(2) N 12- C 13	3.16	0.39	0.031
29.	BD (2) N 12- C 13	97.	RY (6) C 2	1.93	1.85	0.053
29.	BD (2) N 12- C 13	486.	RY (1) O 14	1.73	1.33	0.043
30.	BD (1) C 13- O 14	47.	BD*(1) N 12- C 13	3.31	1.64	0.066
30.	BD (1) C 13- O 14	50.	BD*(2) C 13- O 14	1.60	1.00	0.036
31.	BD (2) C 13- O 14	38.	BD*(1) C 2- N 12	2.75	0.93	0.045
31.	BD (2) C 13- O 14	47.	BD*(1) N 12- C 13	2.98	1.26	0.055
31.	BD (2) C 13- O 14	49.	BD*(1) C 13- O 14	1.99	1.08	0.041

31. BD (2) C 13- O 14	50. BD*(2) C 13- O 14	2.40	0.62	0.034
31. BD (2) C 13- O 14	406. RY (3) N 12	1.10	3.27	0.054

NATURAL BOND ORBITALS (Summary):

NBO	Occupancy	Energy	Principal Delocalizations (geminal,vicinal,remote)
=====			
Molecular unit 1 (C7H5NO)			
----- Lewis -----			
1. CR (1) C 1	1.99999	-10.19659	
2. CR (1) C 2	1.99999	-10.24779	
3. CR (1) C 3	1.99999	-10.19305	
4. CR (1) C 4	1.99999	-10.19465	
5. CR (1) C 5	1.99999	-10.19095	
6. CR (1) C 6	1.99999	-10.19585	
7. CR (1) N 12	1.99999	-14.36215	
8. CR (1) C 13	1.99999	-10.32492	
9. CR (1) O 14	2.00000	-19.19067	
10. LP (1) N 12	1.64584	-0.31668	50(v),49(v),32(v),447(v) 36(v),445(v),47(g),94(v) 96(v),450(v),444(g)
11. LP (1) O 14	1.97764	-0.62629	47(v),445(v)
12. LP (2) O 14	1.64719	-0.31645	48(v),446(v),491(g),449(v) 493(g)
13. BD (1) C 1- C 2	1.97683	-0.61514	36(g),46(v),404(v),40(v) 406(v),254(v),33(g),253(v) 135(v),136(v),452(r),38(g) 148(v),409(v),297(v),35(g)
14. BD (1) C 1- C 6	1.97777	-0.60492	38(v),93(v),45(v),32(g) 44(g),213(v),96(v),212(v) 35(g),94(v),382(v)
15. BD (2) C 1- C 6	1.68239	-0.26725	37(v),42(v),99(v),214(v) 216(v)
16. BD (1) C 1- H 7	1.97779	-0.49824	36(v),44(v),94(v),253(v) 256(v),93(v),38(v),100(v) 46(v),104(v),259(v),92(v)
17. BD (1) C 2- C 3	1.97129	-0.60903	171(v),47(v),404(v),43(v) 35(v),32(g),52(v),316(v) 93(g),51(v),172(v),38(g) 39(g)
18. BD (2) C 2- C 3	1.64084	-0.26858	42(v),34(v),48(v),173(v) 53(v),405(v),317(v)
19. BD (1) C 2- N 12	1.96572	-0.71745	50(v),49(v),448(v),33(v) 47(g),39(v),52(v),36(g) 51(v),445(v)
20. BD (1) C 3- C 4	1.97362	-0.59994	92(v),38(v),45(v),212(v) 41(g),213(v),316(v),93(v) 36(g)
21. BD (1) C 3- H 8	1.97082	-0.48845	32(v),92(v),41(v),171(v) 38(v),174(v),43(v),109(v)
22. BD (1) C 4- C 5	1.98304	-0.60300	46(v),40(v),39(g),254(v) 44(g),253(v),133(v),135(v) 43(g),45(g),339(v)
23. BD (2) C 4- C 5	1.66387	-0.26400	34(v),37(v),255(v)
24. BD (1) C 4- H 9	1.97998	-0.49263	44(v),36(v),212(v),134(v) 133(v),215(v),45(v),213(v) 143(v)
25. BD (1) C 5- C 6	1.98145	-0.60212	43(v),35(v),172(v),51(v) 33(g),41(g),52(v),59(v) 45(g),46(g),54(v)
26. BD (1) C 5- H 10	1.97963	-0.49067	39(v),33(v),253(v),175(v)

				172(v), 256(v), 260(v), 171(v)
				46(v), 43(v)
27.	BD (1) C 6- H 11	1.97891	-0.49318	41(v), 32(v), 51(v), 212(v)
				55(v), 215(v), 54(v), 45(v)
				35(v)
28.	BD (1) N 12- C 13	1.98926	-0.85365	49(g), 94(v), 93(v), 38(g)
				36(v), 92(v), 488(v)
29.	BD (2) N 12- C 13	1.92962	-0.38258	37(v), 48(g), 97(v), 486(v)
30.	BD (1) C 13- O 14	1.99368	-0.90038	47(g), 50(g)
31.	BD (2) C 13- O 14	1.98974	-0.52051	47(g), 38(v), 50(g), 49(g)
				406(v)
----- non-Lewis -----				
32.	BD*(1) C 1- C 2	0.02833	0.53807	
33.	BD*(1) C 1- C 6	0.01267	0.54837	
34.	BD*(2) C 1- C 6	0.32958	0.01176	
35.	BD*(1) C 1- H 7	0.01320	0.40891	
36.	BD*(1) C 2- C 3	0.02201	0.53894	
37.	BD*(2) C 2- C 3	0.38091	0.00411	
38.	BD*(1) C 2- N 12	0.03169	0.41138	
39.	BD*(1) C 3- C 4	0.01143	0.55240	
40.	BD*(1) C 3- H 8	0.01101	0.44514	
41.	BD*(1) C 4- C 5	0.01461	0.54876	
42.	BD*(2) C 4- C 5	0.33812	0.01402	
43.	BD*(1) C 4- H 9	0.01394	0.42250	
44.	BD*(1) C 5- C 6	0.01409	0.54664	
45.	BD*(1) C 5- H 10	0.01388	0.42309	
46.	BD*(1) C 6- H 11	0.01354	0.42123	
47.	BD*(1) N 12- C 13	0.02079	0.73655	
48.	BD*(2) N 12- C 13	0.36343	0.00923	
49.	BD*(1) C 13- O 14	0.07943	0.55891	
50.	BD*(2) C 13- O 14	0.28242	0.09728	
51.	RY (1) C 1	0.00423	1.79600	
52.	RY (2) C 1	0.00175	2.32691	
53.	RY (3) C 1	0.00092	0.87215	
54.	RY (4) C 1	0.00071	2.33107	
55.	RY (5) C 1	0.00050	2.66182	
56.	RY (6) C 1	0.00038	2.26389	
57.	RY (7) C 1	0.00028	1.77037	
58.	RY (8) C 1	0.00015	2.42335	
59.	RY (9) C 1	0.00010	2.95251	
60.	RY (10) C 1	0.00006	1.94978	
61.	RY (11) C 1	0.00004	1.52870	
62.	RY (12) C 1	0.00003	2.27860	
63.	RY (13) C 1	0.00002	3.82390	
64.	RY (14) C 1	0.00001	2.75761	
65.	RY (15) C 1	0.00001	1.43970	
66.	RY (16) C 1	0.00001	2.25903	
67.	RY (17) C 1	0.00000	2.81561	
68.	RY (18) C 1	0.00000	3.28189	
69.	RY (19) C 1	0.00000	3.07062	
70.	RY (20) C 1	0.00000	3.99700	
71.	RY (21) C 1	0.00000	1.27446	
72.	RY (22) C 1	0.00000	1.81378	
73.	RY (23) C 1	0.00000	2.81931	
74.	RY (24) C 1	0.00000	2.09669	
75.	RY (25) C 1	0.00000	1.54312	
76.	RY (26) C 1	0.00000	3.50007	
77.	RY (27) C 1	0.00000	1.61359	
78.	RY (28) C 1	0.00000	3.30173	
79.	RY (29) C 1	0.00000	3.17967	
80.	RY (30) C 1	0.00000	2.53436	
81.	RY (31) C 1	0.00000	3.16666	
82.	RY (32) C 1	0.00000	2.97514	

83.	RY (33)	C	1	0.00000	2.20115
84.	RY (34)	C	1	0.00000	2.72983
85.	RY (35)	C	1	0.00000	3.28626
86.	RY (36)	C	1	0.00000	2.40331
87.	RY (37)	C	1	0.00000	3.29639
88.	RY (38)	C	1	0.00000	1.89767
89.	RY (39)	C	1	0.00000	2.05225
90.	RY (40)	C	1	0.00000	3.75269
91.	RY (41)	C	1	0.00000	2.93888
92.	RY (1)	C	2	0.01245	1.34054
93.	RY (2)	C	2	0.00554	1.53964
94.	RY (3)	C	2	0.00390	2.22513
95.	RY (4)	C	2	0.00254	1.05651
96.	RY (5)	C	2	0.00214	1.83027
97.	RY (6)	C	2	0.00166	1.46454
98.	RY (7)	C	2	0.00052	2.12784
99.	RY (8)	C	2	0.00043	1.99737
100.	RY (9)	C	2	0.00039	2.52639
101.	RY (10)	C	2	0.00028	2.36151
102.	RY (11)	C	2	0.00019	2.69101
103.	RY (12)	C	2	0.00010	1.11723
104.	RY (13)	C	2	0.00008	3.94705
105.	RY (14)	C	2	0.00004	3.09851
106.	RY (15)	C	2	0.00003	2.28300
107.	RY (16)	C	2	0.00001	2.89890
108.	RY (17)	C	2	0.00001	3.63958
109.	RY (18)	C	2	0.00001	3.46339
110.	RY (19)	C	2	0.00000	5.33695
111.	RY (20)	C	2	0.00000	4.19487
112.	RY (21)	C	2	0.00000	2.49159
113.	RY (22)	C	2	0.00000	1.77989
114.	RY (23)	C	2	0.00000	1.65416
115.	RY (24)	C	2	0.00000	1.11037
116.	RY (25)	C	2	0.00000	2.36350
117.	RY (26)	C	2	0.00000	1.96585
118.	RY (27)	C	2	0.00000	3.06420
119.	RY (28)	C	2	0.00000	2.62194
120.	RY (29)	C	2	0.00000	2.29266
121.	RY (30)	C	2	0.00000	3.56327
122.	RY (31)	C	2	0.00000	3.04854
123.	RY (32)	C	2	0.00000	3.10565
124.	RY (33)	C	2	0.00000	3.01103
125.	RY (34)	C	2	0.00000	3.70207
126.	RY (35)	C	2	0.00000	1.58126
127.	RY (36)	C	2	0.00000	3.56608
128.	RY (37)	C	2	0.00000	2.54255
129.	RY (38)	C	2	0.00000	3.30241
130.	RY (39)	C	2	0.00000	2.07212
131.	RY (40)	C	2	0.00000	3.27118
132.	RY (41)	C	2	0.00000	2.08049
133.	RY (1)	C	3	0.00139	2.46320
134.	RY (2)	C	3	0.00119	2.19978
135.	RY (3)	C	3	0.00077	3.37944
136.	RY (4)	C	3	0.00049	3.75586
137.	RY (5)	C	3	0.00036	2.55747
138.	RY (6)	C	3	0.00033	1.41654
139.	RY (7)	C	3	0.00025	3.24594
140.	RY (8)	C	3	0.00013	1.68775
141.	RY (9)	C	3	0.00013	1.42367
142.	RY (10)	C	3	0.00008	1.36444
143.	RY (11)	C	3	0.00004	2.52915
144.	RY (12)	C	3	0.00004	1.62495
145.	RY (13)	C	3	0.00002	2.29138

146.	RY	(14)	C	3	0.00001	3.42023
147.	RY	(15)	C	3	0.00001	3.22660
148.	RY	(16)	C	3	0.00000	2.77911
149.	RY	(17)	C	3	0.00000	3.03846
150.	RY	(18)	C	3	0.00000	1.86976
151.	RY	(19)	C	3	0.00000	2.27943
152.	RY	(20)	C	3	0.00000	2.03599
153.	RY	(21)	C	3	0.00000	1.59351
154.	RY	(22)	C	3	0.00000	3.52030
155.	RY	(23)	C	3	0.00000	2.54667
156.	RY	(24)	C	3	0.00000	2.77469
157.	RY	(25)	C	3	0.00000	2.42136
158.	RY	(26)	C	3	0.00000	3.58772
159.	RY	(27)	C	3	0.00000	1.57714
160.	RY	(28)	C	3	0.00000	3.41115
161.	RY	(29)	C	3	0.00000	2.62930
162.	RY	(30)	C	3	0.00000	3.50257
163.	RY	(31)	C	3	0.00000	3.22437
164.	RY	(32)	C	3	0.00000	2.76902
165.	RY	(33)	C	3	0.00000	1.20610
166.	RY	(34)	C	3	0.00000	3.38257
167.	RY	(35)	C	3	0.00000	2.05220
168.	RY	(36)	C	3	0.00000	2.47712
169.	RY	(37)	C	3	0.00000	2.63776
170.	RY	(38)	C	3	0.00000	2.57460
171.	RY	(1)	C	4	0.00833	1.37336
172.	RY	(2)	C	4	0.00293	1.57127
173.	RY	(3)	C	4	0.00139	0.93981
174.	RY	(4)	C	4	0.00115	1.93651
175.	RY	(5)	C	4	0.00052	3.12875
176.	RY	(6)	C	4	0.00039	1.84635
177.	RY	(7)	C	4	0.00009	2.31981
178.	RY	(8)	C	4	0.00005	3.23638
179.	RY	(9)	C	4	0.00003	2.97800
180.	RY	(10)	C	4	0.00002	2.30353
181.	RY	(11)	C	4	0.00002	1.27460
182.	RY	(12)	C	4	0.00001	2.17241
183.	RY	(13)	C	4	0.00000	3.80125
184.	RY	(14)	C	4	0.00000	4.19154
185.	RY	(15)	C	4	0.00000	1.24910
186.	RY	(16)	C	4	0.00000	1.38559
187.	RY	(17)	C	4	0.00000	2.40094
188.	RY	(18)	C	4	0.00000	2.80333
189.	RY	(19)	C	4	0.00000	1.75963
190.	RY	(20)	C	4	0.00000	2.77312
191.	RY	(21)	C	4	0.00000	2.49014
192.	RY	(22)	C	4	0.00000	2.10456
193.	RY	(23)	C	4	0.00000	2.43529
194.	RY	(24)	C	4	0.00000	2.26973
195.	RY	(25)	C	4	0.00000	2.59734
196.	RY	(26)	C	4	0.00000	2.68376
197.	RY	(27)	C	4	0.00000	2.97456
198.	RY	(28)	C	4	0.00000	3.02807
199.	RY	(29)	C	4	0.00000	2.81618
200.	RY	(30)	C	4	0.00000	2.20008
201.	RY	(31)	C	4	0.00000	3.03385
202.	RY	(32)	C	4	0.00000	2.73641
203.	RY	(33)	C	4	0.00000	2.36517
204.	RY	(34)	C	4	0.00000	2.67170
205.	RY	(35)	C	4	0.00000	2.17362
206.	RY	(36)	C	4	0.00000	2.98779
207.	RY	(37)	C	4	0.00000	2.20456
208.	RY	(38)	C	4	0.00000	2.98252

209.	RY (39)	C	4	0.00000	2.97150
210.	RY (40)	C	4	0.00000	2.55807
211.	RY (41)	C	4	0.00000	2.68740
212.	RY (1)	C	5	0.00501	1.72086
213.	RY (2)	C	5	0.00154	2.12183
214.	RY (3)	C	5	0.00096	0.87634
215.	RY (4)	C	5	0.00071	2.67464
216.	RY (5)	C	5	0.00042	1.90231
217.	RY (6)	C	5	0.00035	3.03525
218.	RY (7)	C	5	0.00015	1.88378
219.	RY (8)	C	5	0.00011	1.74979
220.	RY (9)	C	5	0.00004	2.25011
221.	RY (10)	C	5	0.00002	0.86474
222.	RY (11)	C	5	0.00001	2.36093
223.	RY (12)	C	5	0.00001	2.12554
224.	RY (13)	C	5	0.00000	2.51168
225.	RY (14)	C	5	0.00000	4.06182
226.	RY (15)	C	5	0.00000	1.62615
227.	RY (16)	C	5	0.00000	2.77972
228.	RY (17)	C	5	0.00000	2.29251
229.	RY (18)	C	5	0.00000	2.33230
230.	RY (19)	C	5	0.00000	3.23413
231.	RY (20)	C	5	0.00000	1.31470
232.	RY (21)	C	5	0.00000	1.35049
233.	RY (22)	C	5	0.00000	1.30310
234.	RY (23)	C	5	0.00000	2.47496
235.	RY (24)	C	5	0.00000	2.99230
236.	RY (25)	C	5	0.00000	4.57369
237.	RY (26)	C	5	0.00000	2.85171
238.	RY (27)	C	5	0.00000	2.99611
239.	RY (28)	C	5	0.00000	2.14825
240.	RY (29)	C	5	0.00000	2.50420
241.	RY (30)	C	5	0.00000	2.34362
242.	RY (31)	C	5	0.00000	3.02916
243.	RY (32)	C	5	0.00000	2.74294
244.	RY (33)	C	5	0.00000	3.36999
245.	RY (34)	C	5	0.00000	2.64663
246.	RY (35)	C	5	0.00000	2.49887
247.	RY (36)	C	5	0.00000	3.25815
248.	RY (37)	C	5	0.00000	1.81749
249.	RY (38)	C	5	0.00000	3.08098
250.	RY (39)	C	5	0.00000	2.15663
251.	RY (40)	C	5	0.00000	2.95594
252.	RY (41)	C	5	0.00000	2.93981
253.	RY (1)	C	6	0.00476	1.80073
254.	RY (2)	C	6	0.00180	2.18386
255.	RY (3)	C	6	0.00088	0.86583
256.	RY (4)	C	6	0.00078	3.23889
257.	RY (5)	C	6	0.00056	2.46597
258.	RY (6)	C	6	0.00047	1.98015
259.	RY (7)	C	6	0.00013	2.38780
260.	RY (8)	C	6	0.00008	3.29588
261.	RY (9)	C	6	0.00005	2.82365
262.	RY (10)	C	6	0.00002	2.36711
263.	RY (11)	C	6	0.00002	1.73401
264.	RY (12)	C	6	0.00002	2.26571
265.	RY (13)	C	6	0.00000	2.04814
266.	RY (14)	C	6	0.00000	2.96133
267.	RY (15)	C	6	0.00000	2.70270
268.	RY (16)	C	6	0.00000	3.81231
269.	RY (17)	C	6	0.00000	0.85559
270.	RY (18)	C	6	0.00000	2.14951
271.	RY (19)	C	6	0.00000	2.86855

272.	RY	(20)	C	6	0.00000	3.25482
273.	RY	(21)	C	6	0.00000	1.08674
274.	RY	(22)	C	6	0.00000	1.81778
275.	RY	(23)	C	6	0.00000	2.47943
276.	RY	(24)	C	6	0.00000	1.84620
277.	RY	(25)	C	6	0.00000	2.86374
278.	RY	(26)	C	6	0.00000	3.05344
279.	RY	(27)	C	6	0.00000	2.70506
280.	RY	(28)	C	6	0.00000	2.06143
281.	RY	(29)	C	6	0.00000	2.29695
282.	RY	(30)	C	6	0.00000	2.82697
283.	RY	(31)	C	6	0.00000	2.67056
284.	RY	(32)	C	6	0.00000	3.17685
285.	RY	(33)	C	6	0.00000	2.64468
286.	RY	(34)	C	6	0.00000	2.63805
287.	RY	(35)	C	6	0.00000	2.43295
288.	RY	(36)	C	6	0.00000	3.29689
289.	RY	(37)	C	6	0.00000	2.31520
290.	RY	(38)	C	6	0.00000	3.16920
291.	RY	(39)	C	6	0.00000	2.08863
292.	RY	(40)	C	6	0.00000	1.75301
293.	RY	(41)	C	6	0.00000	2.71390
294.	RY	(1)	H	7	0.00049	1.23943
295.	RY	(2)	H	7	0.00040	1.53639
296.	RY	(3)	H	7	0.00038	0.60031
297.	RY	(4)	H	7	0.00017	3.56923
298.	RY	(5)	H	7	0.00010	1.81990
299.	RY	(6)	H	7	0.00009	2.39884
300.	RY	(7)	H	7	0.00003	1.88414
301.	RY	(8)	H	7	0.00002	1.85312
302.	RY	(9)	H	7	0.00001	2.18020
303.	RY	(10)	H	7	0.00001	1.30134
304.	RY	(11)	H	7	0.00001	3.45240
305.	RY	(12)	H	7	0.00001	2.36078
306.	RY	(13)	H	7	0.00000	4.77902
307.	RY	(14)	H	7	0.00000	3.55479
308.	RY	(15)	H	7	0.00000	2.96204
309.	RY	(16)	H	7	0.00000	2.94350
310.	RY	(17)	H	7	0.00000	2.49278
311.	RY	(18)	H	7	0.00000	3.76798
312.	RY	(19)	H	7	0.00000	3.90660
313.	RY	(20)	H	7	0.00000	3.26578
314.	RY	(21)	H	7	0.00000	3.62138
315.	RY	(22)	H	7	0.00000	3.33023
316.	RY	(1)	H	8	0.00274	1.26627
317.	RY	(2)	H	8	0.00116	1.09041
318.	RY	(3)	H	8	0.00097	1.15014
319.	RY	(4)	H	8	0.00013	1.68799
320.	RY	(5)	H	8	0.00004	2.01570
321.	RY	(6)	H	8	0.00004	2.03501
322.	RY	(7)	H	8	0.00003	1.76172
323.	RY	(8)	H	8	0.00001	4.11101
324.	RY	(9)	H	8	0.00001	1.18940
325.	RY	(10)	H	8	0.00001	1.60108
326.	RY	(11)	H	8	0.00000	2.31748
327.	RY	(12)	H	8	0.00000	3.92782
328.	RY	(13)	H	8	0.00000	3.66279
329.	RY	(14)	H	8	0.00000	3.52867
330.	RY	(15)	H	8	0.00000	2.70868
331.	RY	(16)	H	8	0.00000	2.69309
332.	RY	(17)	H	8	0.00000	3.47824
333.	RY	(18)	H	8	0.00000	3.48099
334.	RY	(19)	H	8	0.00000	4.15795

335.	RY (20)	H	8	0.00000	3.47604
336.	RY (21)	H	8	0.00000	3.64478
337.	RY (22)	H	8	0.00000	3.11448
338.	RY (1)	H	9	0.00102	1.01289
339.	RY (2)	H	9	0.00065	1.33995
340.	RY (3)	H	9	0.00020	0.97240
341.	RY (4)	H	9	0.00016	2.94723
342.	RY (5)	H	9	0.00013	1.50561
343.	RY (6)	H	9	0.00008	1.92577
344.	RY (7)	H	9	0.00002	2.69513
345.	RY (8)	H	9	0.00001	2.93054
346.	RY (9)	H	9	0.00000	2.70252
347.	RY (10)	H	9	0.00000	3.02774
348.	RY (11)	H	9	0.00000	2.69130
349.	RY (12)	H	9	0.00000	3.18607
350.	RY (13)	H	9	0.00000	2.82525
351.	RY (14)	H	9	0.00000	4.27469
352.	RY (15)	H	9	0.00000	3.27296
353.	RY (16)	H	9	0.00000	1.80220
354.	RY (17)	H	9	0.00000	3.26939
355.	RY (18)	H	9	0.00000	2.62632
356.	RY (19)	H	9	0.00000	4.21441
357.	RY (20)	H	9	0.00000	2.96289
358.	RY (21)	H	9	0.00000	2.28397
359.	RY (22)	H	9	0.00000	3.43447
360.	RY (1)	H	10	0.00065	1.45206
361.	RY (2)	H	10	0.00047	0.93176
362.	RY (3)	H	10	0.00042	0.57961
363.	RY (4)	H	10	0.00019	3.52132
364.	RY (5)	H	10	0.00007	2.33897
365.	RY (6)	H	10	0.00005	1.64751
366.	RY (7)	H	10	0.00002	2.33508
367.	RY (8)	H	10	0.00000	3.22278
368.	RY (9)	H	10	0.00000	3.06753
369.	RY (10)	H	10	0.00000	1.41910
370.	RY (11)	H	10	0.00000	3.59150
371.	RY (12)	H	10	0.00000	1.97829
372.	RY (13)	H	10	0.00000	3.81438
373.	RY (14)	H	10	0.00000	4.20904
374.	RY (15)	H	10	0.00000	3.16479
375.	RY (16)	H	10	0.00000	2.40688
376.	RY (17)	H	10	0.00000	1.78106
377.	RY (18)	H	10	0.00000	4.26168
378.	RY (19)	H	10	0.00000	3.88942
379.	RY (20)	H	10	0.00000	2.40182
380.	RY (21)	H	10	0.00000	1.97957
381.	RY (22)	H	10	0.00000	3.87199
382.	RY (1)	H	11	0.00068	0.90397
383.	RY (2)	H	11	0.00050	1.33646
384.	RY (3)	H	11	0.00034	0.65380
385.	RY (4)	H	11	0.00020	3.71600
386.	RY (5)	H	11	0.00006	2.22037
387.	RY (6)	H	11	0.00005	1.61401
388.	RY (7)	H	11	0.00001	2.09365
389.	RY (8)	H	11	0.00001	3.23135
390.	RY (9)	H	11	0.00000	2.25087
391.	RY (10)	H	11	0.00000	1.19730
392.	RY (11)	H	11	0.00000	2.93060
393.	RY (12)	H	11	0.00000	2.00706
394.	RY (13)	H	11	0.00000	4.01227
395.	RY (14)	H	11	0.00000	3.10268
396.	RY (15)	H	11	0.00000	3.61678
397.	RY (16)	H	11	0.00000	3.12808

398.	RY (17)	H 11	0.00000	3.17719
399.	RY (18)	H 11	0.00000	3.68178
400.	RY (19)	H 11	0.00000	4.30690
401.	RY (20)	H 11	0.00000	2.21950
402.	RY (21)	H 11	0.00000	3.31506
403.	RY (22)	H 11	0.00000	3.19753
404.	RY (1)	N 12	0.00478	1.75068
405.	RY (2)	N 12	0.00278	1.03006
406.	RY (3)	N 12	0.00139	2.75092
407.	RY (4)	N 12	0.00065	1.78162
408.	RY (5)	N 12	0.00043	1.84020
409.	RY (6)	N 12	0.00032	1.75892
410.	RY (7)	N 12	0.00026	2.96696
411.	RY (8)	N 12	0.00014	1.54498
412.	RY (9)	N 12	0.00012	1.64540
413.	RY (10)	N 12	0.00008	2.75922
414.	RY (11)	N 12	0.00005	2.61923
415.	RY (12)	N 12	0.00004	1.84344
416.	RY (13)	N 12	0.00002	2.72362
417.	RY (14)	N 12	0.00001	3.73542
418.	RY (15)	N 12	0.00000	3.73083
419.	RY (16)	N 12	0.00000	4.58226
420.	RY (17)	N 12	0.00000	4.47241
421.	RY (18)	N 12	0.00000	4.70160
422.	RY (19)	N 12	0.00000	6.01926
423.	RY (20)	N 12	0.00000	4.12898
424.	RY (21)	N 12	0.00000	3.35774
425.	RY (22)	N 12	0.00000	1.48806
426.	RY (23)	N 12	0.00000	1.80196
427.	RY (24)	N 12	0.00000	3.20562
428.	RY (25)	N 12	0.00000	3.57974
429.	RY (26)	N 12	0.00000	3.37706
430.	RY (27)	N 12	0.00000	3.39398
431.	RY (28)	N 12	0.00000	2.72637
432.	RY (29)	N 12	0.00000	3.34154
433.	RY (30)	N 12	0.00000	2.72175
434.	RY (31)	N 12	0.00000	4.46295
435.	RY (32)	N 12	0.00000	4.45368
436.	RY (33)	N 12	0.00000	4.89194
437.	RY (34)	N 12	0.00000	3.09479
438.	RY (35)	N 12	0.00000	4.87229
439.	RY (36)	N 12	0.00000	3.38849
440.	RY (37)	N 12	0.00000	4.88035
441.	RY (38)	N 12	0.00000	5.31061
442.	RY (39)	N 12	0.00000	4.25164
443.	RY (40)	N 12	0.00000	4.84734
444.	RY (41)	N 12	0.00000	5.21865
445.	RY (1)	C 13	0.01183	1.42547
446.	RY (2)	C 13	0.00370	3.31921
447.	RY (3)	C 13	0.00338	3.19239
448.	RY (4)	C 13	0.00148	1.68973
449.	RY (5)	C 13	0.00053	1.00871
450.	RY (6)	C 13	0.00033	3.07813
451.	RY (7)	C 13	0.00007	3.24895
452.	RY (8)	C 13	0.00004	2.70398
453.	RY (9)	C 13	0.00004	1.02009
454.	RY (10)	C 13	0.00003	0.58925
455.	RY (11)	C 13	0.00001	2.48180
456.	RY (12)	C 13	0.00001	4.69688
457.	RY (13)	C 13	0.00000	0.72627
458.	RY (14)	C 13	0.00000	2.42940
459.	RY (15)	C 13	0.00000	2.55163
460.	RY (16)	C 13	0.00000	4.02155

461.	RY	(17)	C	13	0.00000	1.51178
462.	RY	(18)	C	13	0.00000	2.47356
463.	RY	(19)	C	13	0.00000	2.14981
464.	RY	(20)	C	13	0.00000	2.10236
465.	RY	(21)	C	13	0.00000	2.63436
466.	RY	(22)	C	13	0.00000	2.69277
467.	RY	(23)	C	13	0.00000	1.38779
468.	RY	(24)	C	13	0.00000	1.59654
469.	RY	(25)	C	13	0.00000	1.29700
470.	RY	(26)	C	13	0.00000	2.30102
471.	RY	(27)	C	13	0.00000	1.96474
472.	RY	(28)	C	13	0.00000	2.74035
473.	RY	(29)	C	13	0.00000	1.85083
474.	RY	(30)	C	13	0.00000	2.85750
475.	RY	(31)	C	13	0.00000	1.48887
476.	RY	(32)	C	13	0.00000	2.75211
477.	RY	(33)	C	13	0.00000	1.82438
478.	RY	(34)	C	13	0.00000	2.96223
479.	RY	(35)	C	13	0.00000	2.21949
480.	RY	(36)	C	13	0.00000	2.69949
481.	RY	(37)	C	13	0.00000	1.97135
482.	RY	(38)	C	13	0.00000	2.86696
483.	RY	(39)	C	13	0.00000	2.70064
484.	RY	(40)	C	13	0.00000	2.09538
485.	RY	(41)	C	13	0.00000	1.86285
486.	RY	(1)	O	14	0.00218	0.94944
487.	RY	(2)	O	14	0.00145	1.11461
488.	RY	(3)	O	14	0.00025	1.73602
489.	RY	(4)	O	14	0.00002	1.78015
490.	RY	(5)	O	14	0.00002	1.37645
491.	RY	(6)	O	14	0.00002	1.18587
492.	RY	(7)	O	14	0.00001	1.88372
493.	RY	(8)	O	14	0.00001	1.00327
494.	RY	(9)	O	14	0.00000	2.41663
495.	RY	(10)	O	14	0.00000	3.88569
496.	RY	(11)	O	14	0.00000	3.16838
497.	RY	(12)	O	14	0.00000	6.03490
498.	RY	(13)	O	14	0.00000	2.59224
499.	RY	(14)	O	14	0.00000	5.02319
500.	RY	(15)	O	14	0.00000	5.48534
501.	RY	(16)	O	14	0.00000	4.58073
502.	RY	(17)	O	14	0.00000	3.96079
503.	RY	(18)	O	14	0.00000	3.47532
504.	RY	(19)	O	14	0.00000	2.82475
505.	RY	(20)	O	14	0.00000	5.42990
506.	RY	(21)	O	14	0.00000	2.29698
507.	RY	(22)	O	14	0.00000	2.34943
508.	RY	(23)	O	14	0.00000	5.31946
509.	RY	(24)	O	14	0.00000	5.15424
510.	RY	(25)	O	14	0.00000	5.31609
511.	RY	(26)	O	14	0.00000	4.66911
512.	RY	(27)	O	14	0.00000	5.47027
513.	RY	(28)	O	14	0.00000	2.59560
514.	RY	(29)	O	14	0.00000	5.92176
515.	RY	(30)	O	14	0.00000	4.38688
516.	RY	(31)	O	14	0.00000	5.46786
517.	RY	(32)	O	14	0.00000	4.11983
518.	RY	(33)	O	14	0.00000	3.89355
519.	RY	(34)	O	14	0.00000	3.52040
520.	RY	(35)	O	14	0.00000	2.57291
521.	RY	(36)	O	14	0.00000	6.08745
522.	RY	(37)	O	14	0.00000	2.82695
523.	RY	(38)	O	14	0.00000	5.88539

524. RY (39) O 14 0.00000 4.88129
525. RY (40) O 14 0.00000 5.35922
526. RY (41) O 14 0.00000 4.92070

Total Lewis 59.87685 (96.5756%)
Valence non-Lewis 1.99506 (3.2178%)
Rydberg non-Lewis 0.12809 (0.2066%)

Total unit 1 62.00000 (100.0000%)
Charge unit 1 0.00000

\$CHOOSE

LONE 12 1 14 2 END

BOND S 1 2 D 1 6 S 1 7 D 2 3 S 2 12 S 3 4 S 3 8 D 4 5 S 4 9 S 5 6 S 5 10
S 6 11 D 12 13 D 13 14 END

\$END

Maximum scratch memory used by NBO was 2589519 words
Maximum scratch memory used by G09NBO was 1825014 words

Read Unf file /scratch/12026589.yak.local/Gau-10440.EUF:

Label Gaussian matrix elements

IVers= 1 NLab=

2 Version=ES64L-G09RevE.01

Title Title Card Required

NAtoms= 14 NBasis= 529 NBSUse= 529 ICharg= 0 Multip= 1 NE= 62

Len12L=8 Len4L=8

Label GAUSSIAN SCALARS

NI= 1 NR= 1

NTot= 1 LenBuf= 2000 N= 1000 1 1 1 1

Label ALPHA ORBITAL ENERGIES

NI= 0 NR= 1

NTot= 529 LenBuf= 4000 N= 529 0 0 0 0

Label ALPHA MO COEFFICIENTS

NI= 0 NR= 1

NTot= 279841 LenBuf= 4000 N= 529 529 0 0 0

Store file 524 Len= 279841.

Label NPA CHARGES

NI= 0 NR= 1

NTot= 14 LenBuf= 4000 N= 14 0 0 0 0

Recovered energy= -399.882763712 dipole= 0.000000000000 0.000000000000

0.000000000000

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996,0.\C,0,0.,0.2972,0.\C,0,-1.225,0.9641,0.\C,0,-2.4081,0.2308,0.\C,0
, -2.3736,-1.1627,0.\C,0,-1.1456,-1.8233,0.\H,0,1.,-1.6065,0.\H,0,-1.23
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7651,-1.6358937,0.,0.\PG=CS [SG(C7H5N1O1)]\@

A MAN SHOULD NEVER BE ASHAMED TO OWN HE HAS BEEN IN THE WRONG
WHICH IS BUT SAYING IN OTHER WORDS,
THAT HE IS WISER TODAY THAN HE WAS YESTERDAY.

-- JONATHAN SWIFT

Job cpu time: 0 days 1 hours 48 minutes 36.6 seconds.

File lengths (MBytes): RWF= 148 Int= 0 D2E= 0 Chk= 15 Scr= 1

Normal termination of Gaussian 09 at Fri Nov 30 12:29:51 2018.

***** NBO 6.0 *****

N A T U R A L A T O M I C O R B I T A L A N D
N A T U R A L B O N D O R B I T A L A N A L Y S I S

***** University of Manitoba (100811) *****
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Cite this program as:

NBO 6.0. E. D. Glendening, J. K. Badenhoop, A. E. Reed,
J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis,
and F. Weinhold (Theoretical Chemistry Institute, University
of Wisconsin, Madison, WI, 2013); <http://nbo6.chem.wisc.edu/>

/AONBO / : Checkpoint the AO to NBO transformation

Filename set to /scratch/12026604.yak.local/Gau-1709

Job title: Title Card Required

Interatomic linear dependence detected; p-type subshell on C 3 discarded
Interatomic linear dependence detected; s-type subshell on H 10 discarded
FIXDM: density matrix trace differs from integer value by -0.00001e; fixed

NATURAL POPULATIONS: Natural atomic orbital occupancies

NAO	Atom	No	lang	Type(AO)	Occupancy	Energy
1	C	1	s	Cor(1s)	1.99999	-10.19948
2	C	1	s	Val(2s)	0.97477	-0.13189
3	C	1	s	Ryd(3s)	0.00106	2.09381
4	C	1	s	Ryd(4s)	0.00007	3.43248
5	C	1	s	Ryd(5s)	0.00002	1.16053
6	C	1	px	Val(2p)	1.03574	-0.03262
7	C	1	px	Ryd(3p)	0.00252	1.90604
8	C	1	px	Ryd(4p)	0.00010	1.13034
9	C	1	px	Ryd(5p)	0.00005	1.88069
10	C	1	py	Val(2p)	1.16787	-0.06085
11	C	1	py	Ryd(3p)	0.00374	1.73226
12	C	1	py	Ryd(4p)	0.00009	1.34579
13	C	1	py	Ryd(5p)	0.00001	2.08102
14	C	1	pz	Val(2p)	1.00942	-0.13040
15	C	1	pz	Ryd(3p)	0.00073	0.93624
16	C	1	pz	Ryd(4p)	0.00020	0.74848
17	C	1	pz	Ryd(5p)	0.00000	1.72901
18	C	1	dxxy	Ryd(3d)	0.00145	4.19997
19	C	1	dxxy	Ryd(5d)	0.00016	1.40942
20	C	1	dxxy	Ryd(4d)	0.00019	4.34820
21	C	1	dxz	Ryd(3d)	0.00016	1.84936
22	C	1	dxz	Ryd(4d)	0.00014	0.98075
23	C	1	dxz	Ryd(5d)	0.00003	3.21378
24	C	1	dyz	Ryd(4d)	0.00015	1.71322
25	C	1	dyz	Ryd(3d)	0.00016	1.07633
26	C	1	dyz	Ryd(5d)	0.00001	3.15159
27	C	1	dx2y2	Ryd(3d)	0.00145	3.57138
28	C	1	dx2y2	Ryd(5d)	0.00027	1.55179
29	C	1	dx2y2	Ryd(4d)	0.00042	4.29877
30	C	1	dz2	Ryd(3d)	0.00130	2.74370
31	C	1	dz2	Ryd(4d)	0.00019	1.60646
32	C	1	dz2	Ryd(5d)	0.00003	4.20459
33	C	1	f(0)	Ryd(4f)	0.00037	2.10748
34	C	1	f(0)	Ryd(5f)	0.00003	2.94747
35	C	1	f(c1)	Ryd(4f)	0.00035	2.77470
36	C	1	f(c1)	Ryd(5f)	0.00007	3.25158
37	C	1	f(s1)	Ryd(4f)	0.00051	2.48444

38	C	1	f(s1)	Ryd(5f)	0.00004	3.24286
39	C	1	f(c2)	Ryd(5f)	0.00004	2.30446
40	C	1	f(c2)	Ryd(4f)	0.00004	2.94099
41	C	1	f(s2)	Ryd(4f)	0.00005	2.27281
42	C	1	f(s2)	Ryd(5f)	0.00005	3.02153
43	C	1	f(c3)	Ryd(4f)	0.00064	3.89509
44	C	1	f(c3)	Ryd(5f)	0.00018	3.87016
45	C	1	f(s3)	Ryd(4f)	0.00062	3.70150
46	C	1	f(s3)	Ryd(5f)	0.00021	3.77309
47	C	2	s	Cor(1s)	1.99999	-10.25074
48	C	2	s	Val(2s)	0.86898	-0.08270
49	C	2	s	Ryd(3s)	0.00204	1.86976
50	C	2	s	Ryd(4s)	0.00015	3.51933
51	C	2	s	Ryd(5s)	0.00004	1.85670
52	C	2	px	Val(2p)	0.97639	-0.03013
53	C	2	px	Ryd(3p)	0.00749	1.58918
54	C	2	px	Ryd(4p)	0.00031	1.79808
55	C	2	px	Ryd(5p)	0.00012	1.48240
56	C	2	py	Val(2p)	0.99479	-0.04114
57	C	2	py	Ryd(3p)	0.00597	1.58649
58	C	2	py	Ryd(4p)	0.00028	1.78370
59	C	2	py	Ryd(5p)	0.00007	1.66329
60	C	2	pz	Val(2p)	1.03736	-0.13982
61	C	2	pz	Ryd(3p)	0.00165	0.72509
62	C	2	pz	Ryd(4p)	0.00052	1.27536
63	C	2	pz	Ryd(5p)	0.00001	1.30297
64	C	2	dxy	Ryd(3d)	0.00533	1.75167
65	C	2	dxy	Ryd(5d)	0.00032	4.19943
66	C	2	dxy	Ryd(4d)	0.00040	3.42579
67	C	2	dxz	Ryd(3d)	0.00050	0.83368
68	C	2	dxz	Ryd(4d)	0.00035	2.76013
69	C	2	dxz	Ryd(5d)	0.00001	2.33203
70	C	2	dyz	Ryd(3d)	0.00219	0.74259
71	C	2	dyz	Ryd(4d)	0.00044	2.74118
72	C	2	dyz	Ryd(5d)	0.00013	2.42310
73	C	2	dx2y2	Ryd(3d)	0.00373	2.26513
74	C	2	dx2y2	Ryd(4d)	0.00084	4.90375
75	C	2	dx2y2	Ryd(5d)	0.00028	3.45898
76	C	2	dz2	Ryd(3d)	0.00145	1.10167
77	C	2	dz2	Ryd(4d)	0.00042	4.03557
78	C	2	dz2	Ryd(5d)	0.00008	3.30389
79	C	2	f(0)	Ryd(4f)	0.00028	1.74502
80	C	2	f(0)	Ryd(5f)	0.00014	3.64731
81	C	2	f(c1)	Ryd(4f)	0.00038	2.45798
82	C	2	f(c1)	Ryd(5f)	0.00012	3.76597
83	C	2	f(s1)	Ryd(4f)	0.00052	2.42616
84	C	2	f(s1)	Ryd(5f)	0.00008	3.77546
85	C	2	f(c2)	Ryd(4f)	0.00018	1.90538
86	C	2	f(c2)	Ryd(5f)	0.00002	3.51737
87	C	2	f(s2)	Ryd(4f)	0.00029	1.83637
88	C	2	f(s2)	Ryd(5f)	0.00003	3.70068
89	C	2	f(c3)	Ryd(4f)	0.00174	3.81727
90	C	2	f(c3)	Ryd(5f)	0.00016	4.60170
91	C	2	f(s3)	Ryd(4f)	0.00169	4.30566
92	C	2	f(s3)	Ryd(5f)	0.00018	4.51029
93	C	3	s	Cor(1s)	1.99999	-10.19766
94	C	3	s	Val(2s)	0.97371	-0.13199
95	C	3	s	Ryd(3s)	0.00054	1.96573
96	C	3	s	Ryd(4s)	0.00012	1.58394
97	C	3	s	Ryd(5s)	0.00010	2.77645
98	C	3	px	Val(2p)	1.14851	-0.04659

99	C	3	px	Ryd(3p)	0.00084	2.15505
100	C	3	px	Ryd(4p)	0.00008	1.26411
101	C	3	py	Val(2p)	1.00587	-0.03326
102	C	3	py	Ryd(3p)	0.00126	2.07361
103	C	3	py	Ryd(4p)	0.00007	1.13352
104	C	3	pz	Val(2p)	0.98501	-0.13182
105	C	3	pz	Ryd(4p)	0.00004	1.50296
106	C	3	pz	Ryd(3p)	0.00006	1.10779
107	C	3	dxy	Ryd(3d)	0.00301	3.44270
108	C	3	dxy	Ryd(4d)	0.00024	3.18479
109	C	3	dxy	Ryd(5d)	0.00018	2.93948
110	C	3	dxz	Ryd(3d)	0.00077	1.28932
111	C	3	dxz	Ryd(5d)	0.00001	2.50742
112	C	3	dxz	Ryd(4d)	0.00003	2.06927
113	C	3	dyz	Ryd(3d)	0.00028	1.40539
114	C	3	dyz	Ryd(4d)	0.00010	2.41764
115	C	3	dyz	Ryd(5d)	0.00002	2.17767
116	C	3	dx2y2	Ryd(3d)	0.00211	2.81609
117	C	3	dx2y2	Ryd(4d)	0.00045	3.15348
118	C	3	dx2y2	Ryd(5d)	0.00038	3.21041
119	C	3	dz2	Ryd(3d)	0.00125	2.13049
120	C	3	dz2	Ryd(4d)	0.00018	3.52059
121	C	3	dz2	Ryd(5d)	0.00006	2.76185
122	C	3	f(0)	Ryd(4f)	0.00107	1.79551
123	C	3	f(0)	Ryd(5f)	0.00001	3.16655
124	C	3	f(c1)	Ryd(4f)	0.00116	2.20281
125	C	3	f(c1)	Ryd(5f)	0.00001	3.39625
126	C	3	f(s1)	Ryd(4f)	0.00078	2.42626
127	C	3	f(s1)	Ryd(5f)	0.00002	3.45625
128	C	3	f(c2)	Ryd(4f)	0.00004	2.07739
129	C	3	f(c2)	Ryd(5f)	0.00002	3.14517
130	C	3	f(s2)	Ryd(4f)	0.00005	2.04866
131	C	3	f(s2)	Ryd(5f)	0.00003	3.22833
132	C	3	f(c3)	Ryd(4f)	0.00078	3.48322
133	C	3	f(c3)	Ryd(5f)	0.00018	3.91736
134	C	3	f(s3)	Ryd(4f)	0.00066	3.81464
135	C	3	f(s3)	Ryd(5f)	0.00014	3.96411
136	C	4	s	Cor(1s)	1.99999	-10.19755
137	C	4	s	Val(2s)	0.97934	-0.13423
138	C	4	s	Ryd(3s)	0.00204	1.79956
139	C	4	s	Ryd(4s)	0.00004	2.74098
140	C	4	s	Ryd(5s)	0.00003	1.70626
141	C	4	px	Val(2p)	1.05867	-0.03076
142	C	4	px	Ryd(3p)	0.00552	1.51959
143	C	4	px	Ryd(4p)	0.00020	1.44027
144	C	4	px	Ryd(5p)	0.00003	1.48791
145	C	4	py	Val(2p)	1.15727	-0.05296
146	C	4	py	Ryd(3p)	0.00642	1.42223
147	C	4	py	Ryd(4p)	0.00006	1.37736
148	C	4	py	Ryd(5p)	0.00002	2.06438
149	C	4	pz	Val(2p)	0.99287	-0.12745
150	C	4	pz	Ryd(3p)	0.00099	0.77111
151	C	4	pz	Ryd(4p)	0.00016	0.95836
152	C	4	pz	Ryd(5p)	0.00001	1.66477
153	C	4	dxy	Ryd(3d)	0.00222	3.79761
154	C	4	dxy	Ryd(4d)	0.00025	2.97281
155	C	4	dxy	Ryd(5d)	0.00011	2.97552
156	C	4	dxz	Ryd(4d)	0.00026	1.33471
157	C	4	dxz	Ryd(3d)	0.00033	2.20390
158	C	4	dxz	Ryd(5d)	0.00001	2.50102
159	C	4	dyz	Ryd(4d)	0.00006	1.24625
160	C	4	dyz	Ryd(3d)	0.00055	2.24369

161	C	4	dyz	Ryd(5d)	0.00005	2.33571
162	C	4	dx2y2	Ryd(3d)	0.00205	2.92693
163	C	4	dx2y2	Ryd(4d)	0.00067	2.98338
164	C	4	dx2y2	Ryd(5d)	0.00015	3.37122
165	C	4	dz2	Ryd(3d)	0.00174	2.27597
166	C	4	dz2	Ryd(4d)	0.00022	2.95531
167	C	4	dz2	Ryd(5d)	0.00003	3.21963
168	C	4	f(0)	Ryd(4f)	0.00037	2.13270
169	C	4	f(0)	Ryd(5f)	0.00003	2.91906
170	C	4	f(c1)	Ryd(4f)	0.00046	2.72108
171	C	4	f(c1)	Ryd(5f)	0.00005	3.12129
172	C	4	f(s1)	Ryd(4f)	0.00063	2.44348
173	C	4	f(s1)	Ryd(5f)	0.00002	3.13169
174	C	4	f(c2)	Ryd(4f)	0.00007	2.37921
175	C	4	f(c2)	Ryd(5f)	0.00006	2.87952
176	C	4	f(s2)	Ryd(5f)	0.00002	2.29911
177	C	4	f(s2)	Ryd(4f)	0.00003	2.92772
178	C	4	f(c3)	Ryd(4f)	0.00079	3.60356
179	C	4	f(c3)	Ryd(5f)	0.00022	3.64313
180	C	4	f(s3)	Ryd(4f)	0.00057	3.78201
181	C	4	f(s3)	Ryd(5f)	0.00011	3.66371
182	C	5	s	Cor(1s)	1.99999	-10.19470
183	C	5	s	Val(2s)	0.97693	-0.13545
184	C	5	s	Ryd(3s)	0.00075	2.06547
185	C	5	s	Ryd(4s)	0.00002	2.00485
186	C	5	s	Ryd(5s)	0.00002	2.10368
187	C	5	px	Val(2p)	1.10777	-0.04426
188	C	5	px	Ryd(3p)	0.00382	1.61851
189	C	5	px	Ryd(4p)	0.00005	0.91483
190	C	5	px	Ryd(5p)	0.00002	2.02434
191	C	5	py	Val(2p)	1.10490	-0.04334
192	C	5	py	Ryd(3p)	0.00351	1.60400
193	C	5	py	Ryd(4p)	0.00008	0.92284
194	C	5	py	Ryd(5p)	0.00001	2.05316
195	C	5	pz	Val(2p)	1.00095	-0.12479
196	C	5	pz	Ryd(3p)	0.00098	0.92180
197	C	5	pz	Ryd(4p)	0.00015	0.57340
198	C	5	pz	Ryd(5p)	0.00000	1.84225
199	C	5	dxy	Ryd(3d)	0.00103	2.88699
200	C	5	dxy	Ryd(4d)	0.00051	3.01888
201	C	5	dxy	Ryd(5d)	0.00023	3.05646
202	C	5	dxz	Ryd(3d)	0.00018	1.75563
203	C	5	dxz	Ryd(4d)	0.00009	2.35227
204	C	5	dxz	Ryd(5d)	0.00002	1.81006
205	C	5	dyz	Ryd(3d)	0.00021	1.75589
206	C	5	dyz	Ryd(4d)	0.00007	2.34055
207	C	5	dyz	Ryd(5d)	0.00002	1.80582
208	C	5	dx2y2	Ryd(3d)	0.00184	4.55484
209	C	5	dx2y2	Ryd(4d)	0.00015	3.57506
210	C	5	dx2y2	Ryd(5d)	0.00004	2.01776
211	C	5	dz2	Ryd(3d)	0.00125	2.95179
212	C	5	dz2	Ryd(4d)	0.00015	3.00730
213	C	5	dz2	Ryd(5d)	0.00004	2.57519
214	C	5	f(0)	Ryd(4f)	0.00029	2.21227
215	C	5	f(0)	Ryd(5f)	0.00004	2.81903
216	C	5	f(c1)	Ryd(4f)	0.00046	2.65056
217	C	5	f(c1)	Ryd(5f)	0.00004	3.00589
218	C	5	f(s1)	Ryd(4f)	0.00045	2.64368
219	C	5	f(s1)	Ryd(5f)	0.00004	3.01450
220	C	5	f(c2)	Ryd(5f)	0.00003	2.35579
221	C	5	f(c2)	Ryd(4f)	0.00004	2.84458
222	C	5	f(s2)	Ryd(5f)	0.00004	2.47934

223	C	5	f(s2)	Ryd(4f)	0.00004	2.75107
224	C	5	f(c3)	Ryd(4f)	0.00060	3.62508
225	C	5	f(c3)	Ryd(5f)	0.00019	3.59044
226	C	5	f(s3)	Ryd(4f)	0.00060	3.71314
227	C	5	f(s3)	Ryd(5f)	0.00018	3.59621
228	C	6	s	Cor(1s)	1.99999	-10.19823
229	C	6	s	Val(2s)	0.97597	-0.13581
230	C	6	s	Ryd(3s)	0.00089	2.08569
231	C	6	s	Ryd(4s)	0.00003	1.82856
232	C	6	s	Ryd(5s)	0.00001	2.06964
233	C	6	px	Val(2p)	1.15454	-0.05311
234	C	6	px	Ryd(3p)	0.00485	1.56449
235	C	6	px	Ryd(4p)	0.00004	1.11325
236	C	6	px	Ryd(5p)	0.00001	2.12002
237	C	6	py	Val(2p)	1.05401	-0.02758
238	C	6	py	Ryd(3p)	0.00285	1.81488
239	C	6	py	Ryd(4p)	0.00007	1.08511
240	C	6	py	Ryd(5p)	0.00002	1.56035
241	C	6	pz	Val(2p)	0.98737	-0.12630
242	C	6	pz	Ryd(3p)	0.00077	0.89227
243	C	6	pz	Ryd(4p)	0.00012	0.71186
244	C	6	pz	Ryd(5p)	0.00000	1.71945
245	C	6	dxy	Ryd(3d)	0.00183	4.09175
246	C	6	dxy	Ryd(4d)	0.00021	3.84496
247	C	6	dxy	Ryd(5d)	0.00007	1.87107
248	C	6	dxz	Ryd(3d)	0.00015	1.66349
249	C	6	dxz	Ryd(4d)	0.00007	2.77570
250	C	6	dxz	Ryd(5d)	0.00006	1.41543
251	C	6	dyz	Ryd(3d)	0.00027	1.76364
252	C	6	dyz	Ryd(4d)	0.00002	2.68996
253	C	6	dyz	Ryd(5d)	0.00000	1.58184
254	C	6	dx2y2	Ryd(3d)	0.00144	3.34559
255	C	6	dx2y2	Ryd(4d)	0.00027	3.66551
256	C	6	dx2y2	Ryd(5d)	0.00020	2.28370
257	C	6	dz2	Ryd(3d)	0.00121	2.90642
258	C	6	dz2	Ryd(4d)	0.00012	3.45360
259	C	6	dz2	Ryd(5d)	0.00007	2.09807
260	C	6	f(0)	Ryd(4f)	0.00028	2.15120
261	C	6	f(0)	Ryd(5f)	0.00005	2.90640
262	C	6	f(c1)	Ryd(4f)	0.00052	2.47685
263	C	6	f(c1)	Ryd(5f)	0.00002	3.12648
264	C	6	f(s1)	Ryd(4f)	0.00041	2.75742
265	C	6	f(s1)	Ryd(5f)	0.00006	3.09902
266	C	6	f(c2)	Ryd(4f)	0.00005	2.39684
267	C	6	f(c2)	Ryd(5f)	0.00004	2.88730
268	C	6	f(s2)	Ryd(4f)	0.00004	2.31480
269	C	6	f(s2)	Ryd(5f)	0.00004	2.89809
270	C	6	f(c3)	Ryd(4f)	0.00061	3.68291
271	C	6	f(c3)	Ryd(5f)	0.00018	3.67439
272	C	6	f(s3)	Ryd(4f)	0.00067	3.68786
273	C	6	f(s3)	Ryd(5f)	0.00020	3.64517
274	H	7	s	Val(1s)	0.78062	0.03998
275	H	7	s	Ryd(2s)	0.00027	1.13596
276	H	7	s	Ryd(3s)	0.00010	2.21327
277	H	7	s	Ryd(4s)	0.00001	1.51968
278	H	7	px	Ryd(2p)	0.00037	1.25781
279	H	7	px	Ryd(3p)	0.00002	3.69596
280	H	7	px	Ryd(4p)	0.00002	2.52007
281	H	7	py	Ryd(2p)	0.00022	1.51836
282	H	7	py	Ryd(3p)	0.00017	4.99282
283	H	7	py	Ryd(4p)	0.00010	2.79991

284	H	7	pz	Ryd(2p)	0.00026	0.90772
285	H	7	pz	Ryd(3p)	0.00010	3.60028
286	H	7	pz	Ryd(4p)	0.00001	2.00595
287	H	7	dxz	Ryd(3d)	0.00007	1.65538
288	H	7	dxz	Ryd(4d)	0.00001	4.87480
289	H	7	dxz	Ryd(3d)	0.00001	1.21460
290	H	7	dxz	Ryd(4d)	0.00000	3.91062
291	H	7	dyz	Ryd(3d)	0.00006	1.28796
292	H	7	dyz	Ryd(4d)	0.00000	4.44609
293	H	7	dx2y2	Ryd(3d)	0.00003	2.05141
294	H	7	dx2y2	Ryd(4d)	0.00003	4.80981
295	H	7	dz2	Ryd(3d)	0.00001	1.79446
296	H	7	dz2	Ryd(4d)	0.00001	4.32346
297	H	8	s	Val(1s)	0.78428	0.05483
298	H	8	s	Ryd(2s)	0.00076	1.48768
299	H	8	s	Ryd(3s)	0.00003	1.05188
300	H	8	s	Ryd(4s)	0.00003	1.78831
301	H	8	px	Ryd(2p)	0.00056	1.27141
302	H	8	px	Ryd(3p)	0.00025	4.86788
303	H	8	px	Ryd(4p)	0.00003	2.97152
304	H	8	py	Ryd(2p)	0.00219	1.13526
305	H	8	py	Ryd(3p)	0.00003	3.45935
306	H	8	py	Ryd(4p)	0.00002	2.80918
307	H	8	pz	Ryd(2p)	0.00092	0.74060
308	H	8	pz	Ryd(3p)	0.00005	3.32852
309	H	8	pz	Ryd(4p)	0.00001	2.29496
310	H	8	dxz	Ryd(3d)	0.00006	1.95770
311	H	8	dxz	Ryd(4d)	0.00001	4.64762
312	H	8	dxz	Ryd(3d)	0.00005	1.52233
313	H	8	dxz	Ryd(4d)	0.00000	4.27909
314	H	8	dyz	Ryd(3d)	0.00001	1.39892
315	H	8	dyz	Ryd(4d)	0.00000	3.75379
316	H	8	dx2y2	Ryd(3d)	0.00004	2.33908
317	H	8	dx2y2	Ryd(4d)	0.00002	4.57618
318	H	8	dz2	Ryd(3d)	0.00003	2.04035
319	H	8	dz2	Ryd(4d)	0.00001	4.11327
320	H	9	s	Val(1s)	0.78712	0.04540
321	H	9	s	Ryd(2s)	0.00055	0.98623
322	H	9	s	Ryd(3s)	0.00010	2.21666
323	H	9	s	Ryd(4s)	0.00001	1.19891
324	H	9	px	Ryd(2p)	0.00059	1.24071
325	H	9	px	Ryd(4p)	0.00001	3.43495
326	H	9	px	Ryd(3p)	0.00002	2.77783
327	H	9	py	Ryd(2p)	0.00057	1.29190
328	H	9	py	Ryd(3p)	0.00012	4.94721
329	H	9	py	Ryd(4p)	0.00010	3.02027
330	H	9	pz	Ryd(2p)	0.00015	0.87998
331	H	9	pz	Ryd(3p)	0.00011	3.24754
332	H	9	pz	Ryd(4p)	0.00002	2.41328
333	H	9	dxz	Ryd(3d)	0.00005	2.10626
334	H	9	dxz	Ryd(4d)	0.00001	4.40922
335	H	9	dxz	Ryd(3d)	0.00001	1.53551
336	H	9	dxz	Ryd(4d)	0.00000	3.58419
337	H	9	dyz	Ryd(3d)	0.00003	1.63725
338	H	9	dyz	Ryd(4d)	0.00000	4.10685
339	H	9	dx2y2	Ryd(4d)	0.00002	2.51011
340	H	9	dx2y2	Ryd(3d)	0.00002	4.29789
341	H	9	dz2	Ryd(3d)	0.00001	2.23347
342	H	9	dz2	Ryd(4d)	0.00001	3.84901
343	H	10	s	Val(1s)	0.78469	0.03609

344	H 10	s	Ryd(2s)	0.00020	2.11461
345	H 10	s	Ryd(3s)	0.00004	0.65713
346	H 10	px	Ryd(2p)	0.00043	0.78755
347	H 10	px	Ryd(3p)	0.00012	4.74961
348	H 10	px	Ryd(4p)	0.00006	2.79593
349	H 10	py	Ryd(2p)	0.00041	0.80277
350	H 10	py	Ryd(3p)	0.00012	4.73433
351	H 10	py	Ryd(4p)	0.00006	2.78392
352	H 10	pz	Ryd(2p)	0.00037	0.48655
353	H 10	pz	Ryd(3p)	0.00004	4.14467
354	H 10	pz	Ryd(4p)	0.00003	1.93983
355	H 10	dxxy	Ryd(3d)	0.00003	3.39246
356	H 10	dxxy	Ryd(4d)	0.00003	3.44167
357	H 10	dxz	Ryd(3d)	0.00002	2.30670
358	H 10	dxz	Ryd(4d)	0.00000	3.13179
359	H 10	dyz	Ryd(3d)	0.00001	2.30191
360	H 10	dyz	Ryd(4d)	0.00000	3.12441
361	H 10	dx2y2	Ryd(3d)	0.00006	2.83623
362	H 10	dx2y2	Ryd(4d)	0.00000	3.63926
363	H 10	dz2	Ryd(4d)	0.00001	2.92541
364	H 10	dz2	Ryd(3d)	0.00001	3.13351
365	H 11	s	Val(1s)	0.78662	0.04517
366	H 11	s	Ryd(2s)	0.00035	1.05934
367	H 11	s	Ryd(3s)	0.00011	2.16804
368	H 11	s	Ryd(4s)	0.00001	1.19513
369	H 11	px	Ryd(2p)	0.00054	1.36738
370	H 11	px	Ryd(3p)	0.00013	5.06829
371	H 11	px	Ryd(4p)	0.00007	2.75213
372	H 11	py	Ryd(2p)	0.00046	1.26360
373	H 11	py	Ryd(4p)	0.00002	3.71259
374	H 11	py	Ryd(3p)	0.00002	2.45500
375	H 11	pz	Ryd(2p)	0.00024	0.89070
376	H 11	pz	Ryd(3p)	0.00009	3.57694
377	H 11	pz	Ryd(4p)	0.00001	2.06399
378	H 11	dxxy	Ryd(3d)	0.00005	2.50527
379	H 11	dxxy	Ryd(4d)	0.00001	4.03034
380	H 11	dxz	Ryd(3d)	0.00002	1.96692
381	H 11	dxz	Ryd(4d)	0.00000	3.77061
382	H 11	dyz	Ryd(3d)	0.00000	1.85459
383	H 11	dyz	Ryd(4d)	0.00000	3.28037
384	H 11	dx2y2	Ryd(3d)	0.00002	2.85534
385	H 11	dx2y2	Ryd(4d)	0.00002	3.91921
386	H 11	dz2	Ryd(3d)	0.00002	2.57333
387	H 11	dz2	Ryd(4d)	0.00001	3.51465
388	N 12	s	Cor(1s)	1.99999	-14.36830
389	N 12	s	Val(2s)	1.21270	-0.37258
390	N 12	s	Ryd(3s)	0.00222	1.73906
391	N 12	s	Ryd(4s)	0.00021	5.04084
392	N 12	s	Ryd(5s)	0.00001	7.14131
393	N 12	px	Val(2p)	1.42572	-0.22394
394	N 12	px	Ryd(3p)	0.00617	1.39284
395	N 12	px	Ryd(4p)	0.00033	1.46219
396	N 12	px	Ryd(5p)	0.00003	3.80190
397	N 12	py	Val(2p)	1.34763	-0.20049
398	N 12	py	Ryd(3p)	0.00392	2.91914
399	N 12	py	Ryd(4p)	0.00114	2.99524
400	N 12	py	Ryd(5p)	0.00005	3.90695
401	N 12	pz	Val(2p)	1.40763	-0.23920
402	N 12	pz	Ryd(3p)	0.00480	0.75232
403	N 12	pz	Ryd(4p)	0.00019	1.09909
404	N 12	pz	Ryd(5p)	0.00002	3.24976

405	N 12	dxy	Ryd(3d)	0.00222	2.76593
406	N 12	dxy	Ryd(4d)	0.00048	2.14697
407	N 12	dxy	Ryd(5d)	0.00005	5.79381
408	N 12	dxz	Ryd(3d)	0.00050	1.68537
409	N 12	dxz	Ryd(4d)	0.00009	1.13119
410	N 12	dxz	Ryd(5d)	0.00000	4.97203
411	N 12	dyz	Ryd(3d)	0.00133	1.81362
412	N 12	dyz	Ryd(4d)	0.00045	1.27829
413	N 12	dyz	Ryd(5d)	0.00002	5.26030
414	N 12	dx2y2	Ryd(3d)	0.00304	3.35930
415	N 12	dx2y2	Ryd(4d)	0.00052	2.24652
416	N 12	dx2y2	Ryd(5d)	0.00004	6.31609
417	N 12	dz2	Ryd(3d)	0.00154	2.54180
418	N 12	dz2	Ryd(4d)	0.00026	2.23825
419	N 12	dz2	Ryd(5d)	0.00002	5.55048
420	N 12	f(0)	Ryd(4f)	0.00078	2.04628
421	N 12	f(0)	Ryd(5f)	0.00002	4.66452
422	N 12	f(c1)	Ryd(4f)	0.00047	2.30718
423	N 12	f(c1)	Ryd(5f)	0.00001	4.67642
424	N 12	f(s1)	Ryd(4f)	0.00118	3.02244
425	N 12	f(s1)	Ryd(5f)	0.00002	5.28130
426	N 12	f(c2)	Ryd(4f)	0.00037	2.21687
427	N 12	f(c2)	Ryd(5f)	0.00002	4.83024
428	N 12	f(s2)	Ryd(4f)	0.00065	2.06788
429	N 12	f(s2)	Ryd(5f)	0.00002	4.78074
430	N 12	f(c3)	Ryd(4f)	0.00212	3.33054
431	N 12	f(c3)	Ryd(5f)	0.00008	5.52671
432	N 12	f(s3)	Ryd(4f)	0.00217	3.03778
433	N 12	f(s3)	Ryd(5f)	0.00005	5.48014
434	C 13	s	Cor(1s)	1.99999	-10.29100
435	C 13	s	Val(2s)	0.93534	-0.17520
436	C 13	s	Ryd(3s)	0.00131	1.75871
437	C 13	s	Ryd(4s)	0.00003	3.69059
438	C 13	s	Ryd(5s)	0.00002	1.71473
439	C 13	px	Val(2p)	0.89127	-0.14643
440	C 13	px	Ryd(3p)	0.00357	0.87245
441	C 13	px	Ryd(4p)	0.00010	2.20821
442	C 13	px	Ryd(5p)	0.00001	0.63366
443	C 13	py	Val(2p)	1.00184	0.00429
444	C 13	py	Ryd(3p)	0.00619	1.45777
445	C 13	py	Ryd(4p)	0.00064	2.09936
446	C 13	py	Ryd(5p)	0.00004	0.72695
447	C 13	pz	Val(2p)	0.92807	-0.15449
448	C 13	pz	Ryd(3p)	0.00223	0.77922
449	C 13	pz	Ryd(4p)	0.00010	1.86248
450	C 13	pz	Ryd(5p)	0.00002	0.50579
451	C 13	dxy	Ryd(3d)	0.00185	2.92567
452	C 13	dxy	Ryd(4d)	0.00019	3.49443
453	C 13	dxy	Ryd(5d)	0.00008	0.99454
454	C 13	dxz	Ryd(3d)	0.00025	1.88694
455	C 13	dxz	Ryd(5d)	0.00001	2.65617
456	C 13	dxz	Ryd(4d)	0.00005	0.55724
457	C 13	dyz	Ryd(3d)	0.00171	2.36259
458	C 13	dyz	Ryd(4d)	0.00020	2.87147
459	C 13	dyz	Ryd(5d)	0.00012	0.74497
460	C 13	dx2y2	Ryd(3d)	0.00155	3.35537
461	C 13	dx2y2	Ryd(4d)	0.00020	4.10847
462	C 13	dx2y2	Ryd(5d)	0.00011	0.82999
463	C 13	dz2	Ryd(3d)	0.00054	2.47938
464	C 13	dz2	Ryd(4d)	0.00009	3.51585
465	C 13	dz2	Ryd(5d)	0.00007	0.74638
466	C 13	f(0)	Ryd(4f)	0.00119	1.74000

467	C 13	f(0)	Ryd(5f)	0.00001	2.91207
468	C 13	f(c1)	Ryd(4f)	0.00041	1.69181
469	C 13	f(c1)	Ryd(5f)	0.00001	2.86905
470	C 13	f(s1)	Ryd(4f)	0.00227	2.47621
471	C 13	f(s1)	Ryd(5f)	0.00004	3.46675
472	C 13	f(c2)	Ryd(4f)	0.00128	1.77153
473	C 13	f(c2)	Ryd(5f)	0.00002	3.02949
474	C 13	f(s2)	Ryd(4f)	0.00066	1.79642
475	C 13	f(s2)	Ryd(5f)	0.00000	2.85493
476	C 13	f(c3)	Ryd(4f)	0.00364	2.35636
477	C 13	f(c3)	Ryd(5f)	0.00005	3.59217
478	C 13	f(s3)	Ryd(4f)	0.00313	2.40992
479	C 13	f(s3)	Ryd(5f)	0.00003	3.59866
480	S 14	s	Cor(1s)	2.00000	-81.53444
481	S 14	s	Cor(2s)	2.00000	-15.31373
482	S 14	s	Val(3s)	1.75535	-0.52939
483	S 14	s	Ryd(4s)	0.00439	0.93846
484	S 14	s	Ryd(5s)	0.00000	1.25707
485	S 14	s	Ryd(6s)	0.00000	5.74110
486	S 14	px	Cor(2p)	2.00000	-5.90945
487	S 14	px	Val(3p)	1.50538	-0.22176
488	S 14	px	Ryd(4p)	0.00134	0.63456
489	S 14	px	Ryd(5p)	0.00002	1.43545
490	S 14	px	Ryd(6p)	0.00000	1.05368
491	S 14	py	Cor(2p)	2.00000	-5.91402
492	S 14	py	Val(3p)	1.07716	-0.15915
493	S 14	py	Ryd(4p)	0.00171	0.63509
494	S 14	py	Ryd(5p)	0.00006	1.35597
495	S 14	py	Ryd(6p)	0.00001	1.18953
496	S 14	pz	Cor(2p)	2.00000	-5.90822
497	S 14	pz	Val(3p)	1.60673	-0.23006
498	S 14	pz	Ryd(4p)	0.00223	0.62634
499	S 14	pz	Ryd(5p)	0.00002	1.27572
500	S 14	pz	Ryd(6p)	0.00000	1.06824
501	S 14	dxxy	Ryd(3d)	0.00430	1.30646
502	S 14	dxxy	Ryd(4d)	0.00026	0.63955
503	S 14	dxxy	Ryd(5d)	0.00000	2.10383
504	S 14	dxz	Ryd(3d)	0.00030	0.71440
505	S 14	dxz	Ryd(4d)	0.00002	0.51013
506	S 14	dxz	Ryd(5d)	0.00000	1.69720
507	S 14	dyyz	Ryd(3d)	0.00307	1.18948
508	S 14	dyyz	Ryd(4d)	0.00038	0.61046
509	S 14	dyyz	Ryd(5d)	0.00000	1.75770
510	S 14	dx2y2	Ryd(3d)	0.00554	1.30999
511	S 14	dx2y2	Ryd(4d)	0.00018	0.69127
512	S 14	dx2y2	Ryd(5d)	0.00000	2.49591
513	S 14	dz2	Ryd(3d)	0.00218	0.90589
514	S 14	dz2	Ryd(4d)	0.00005	0.57496
515	S 14	dz2	Ryd(5d)	0.00000	2.20289
516	S 14	f(0)	Ryd(4f)	0.00009	1.78378
517	S 14	f(0)	Ryd(5f)	0.00000	1.42497
518	S 14	f(c1)	Ryd(4f)	0.00003	1.68303
519	S 14	f(c1)	Ryd(5f)	0.00000	1.34977
520	S 14	f(s1)	Ryd(4f)	0.00014	2.02887
521	S 14	f(s1)	Ryd(5f)	0.00000	1.51626
522	S 14	f(c2)	Ryd(4f)	0.00009	1.93223
523	S 14	f(c2)	Ryd(5f)	0.00000	1.48744
524	S 14	f(s2)	Ryd(4f)	0.00004	1.92222
525	S 14	f(s2)	Ryd(5f)	0.00000	1.46977
526	S 14	f(c3)	Ryd(4f)	0.00022	2.12512
527	S 14	f(c3)	Ryd(5f)	0.00000	1.63699
528	S 14	f(s3)	Ryd(4f)	0.00021	2.08944

529 S 14 f(s3) Ryd(5f) 0.00000 1.63917

Population inversion found on atom C 1
 Population inversion found on atom C 2
 Population inversion found on atom C 3
 Population inversion found on atom C 4
 Population inversion found on atom C 5
 Population inversion found on atom C 6
 Population inversion found on atom H 7
 Population inversion found on atom H 8
 Population inversion found on atom H 9
 Population inversion found on atom H 10
 Population inversion found on atom H 11
 Population inversion found on atom N 12
 Population inversion found on atom C 13
 Population inversion found on atom S 14

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
C 1	-0.20569	1.99999	4.18780	0.01790	6.20569
C 2	0.08155	1.99999	3.87752	0.04094	5.91845
C 3	-0.13023	1.99999	4.11312	0.01712	6.13023
C 4	-0.21580	1.99999	4.18815	0.02766	6.21580
C 5	-0.20882	1.99999	4.19055	0.01828	6.20882
C 6	-0.19067	1.99999	4.17189	0.01880	6.19067
H 7	0.21751	0.00000	0.78062	0.00188	0.78249
H 8	0.21063	0.00000	0.78428	0.00510	0.78937
H 9	0.21035	0.00000	0.78712	0.00253	0.78965
H 10	0.21325	0.00000	0.78469	0.00206	0.78675
H 11	0.21115	0.00000	0.78662	0.00223	0.78885
N 12	-0.43124	1.99999	5.39367	0.03757	7.43124
C 13	0.20952	1.99999	3.75651	0.03398	5.79048
S 14	0.02850	9.99999	5.94462	0.02688	15.97150
=====					
* Total *	0.00000	25.99990	43.74717	0.25293	70.00000

Natural Population	
Core	25.99990 (99.9996% of 26)
Valence	43.74717 (99.4254% of 44)
Natural Minimal Basis	69.74707 (99.6387% of 70)
Natural Rydberg Basis	0.25293 (0.3613% of 70)

Atom No	Natural Electron Configuration
C 1	[core]2s(0.97)2p(3.21)3p(0.01)
C 2	[core]2s(0.87)2p(3.01)3p(0.02)3d(0.01)4f(0.01)
C 3	[core]2s(0.97)2p(3.14)3d(0.01)
C 4	[core]2s(0.98)2p(3.21)3p(0.01)3d(0.01)
C 5	[core]2s(0.98)2p(3.21)3p(0.01)
C 6	[core]2s(0.98)2p(3.20)3p(0.01)
H 7	1s(0.78)
H 8	1s(0.78)
H 9	1s(0.79)
H 10	1s(0.78)
H 11	1s(0.79)
N 12	[core]2s(1.21)2p(4.18)3p(0.01)3d(0.01)4f(0.01)

				0.0000	0.0000	-0.1280	0.0013	0.0006
				0.0002	0.0000	-0.4200	0.0043	0.0013
				0.0010	0.0000	0.0000	0.0000	0.0000
				0.0000	-0.0101	-0.0030	0.0001	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0149	0.0045	-0.0003	0.0097	0.0031
				-0.0005	0.0000	0.0000	0.0002	0.0001
				0.0008	0.0002	0.0000	0.0000	0.0000
				0.0000	0.0008	0.0003	0.0005	0.0001
15.	(1.60967)	LP (2) S 14		s(0.00%)	p 1.00(99.84%)	d 0.00(0.15%)		
				f 0.00(0.01%)				
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.9991	0.0141	-0.0006
				0.0002	0.0000	0.0000	0.0000	0.0110
				-0.0035	-0.0005	0.0342	-0.0141	0.0004
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	-0.0073	-0.0004	0.0000	0.0000
				0.0000	0.0000	-0.0072	-0.0001	0.0047
				0.0001	0.0000	0.0000	0.0000	0.0000
16.	(1.97245)	BD (1) C 1- C 2		s(34.57%)	p 1.89(65.21%)	d 0.00(0.17%)		
	(48.61%)	0.6972* C 1		f 0.00(0.05%)				
				0.0000	0.5880	-0.0015	-0.0020	0.0008
				-0.7839	-0.0141	-0.0015	-0.0016	0.1929
				0.0162	-0.0013	0.0007	0.0000	0.0000
				0.0000	0.0000	-0.0204	0.0042	0.0010
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0266	-0.0044	0.0036	-0.0222
				-0.0001	-0.0006	0.0000	0.0000	0.0140
				-0.0050	-0.0049	0.0002	0.0000	0.0000
				0.0000	0.0000	-0.0093	0.0062	0.0117
				-0.0001				
	(51.39%)	0.7169* C 2		s(37.29%)	p 1.68(62.56%)	d 0.00(0.09%)		
				f 0.00(0.06%)				
				0.0000	0.6105	0.0122	0.0019	0.0030
				0.7487	-0.0102	0.0052	0.0022	-0.2544
				-0.0108	-0.0036	-0.0025	0.0000	0.0000
				0.0000	0.0000	-0.0021	-0.0094	0.0044
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0164	0.0160	-0.0026	0.0102
				-0.0118	0.0007	0.0000	0.0000	-0.0147
				-0.0081	0.0055	0.0021	0.0000	0.0000
				0.0000	0.0000	0.0093	0.0062	-0.0117
				-0.0068				
17.	(1.64561)	BD (2) C 1- C 2		s(0.00%)	p 1.00(99.91%)	d 0.00(0.04%)		
	(48.85%)	0.6990* C 1		f 0.00(0.05%)				
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.9995	-0.0029
				-0.0038	-0.0012	0.0000	0.0000	0.0000
				-0.0087	-0.0103	0.0003	0.0090	0.0121
				0.0013	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	-0.0188	0.0057	0.0000
				0.0000	0.0000	0.0000	-0.0055	-0.0074
				-0.0008	-0.0017	0.0000	0.0000	0.0000
				0.0000				
	(51.15%)	0.7152* C 2		s(0.00%)	p 1.00(99.90%)	d 0.00(0.05%)		
				f 0.00(0.05%)				
				0.0000	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000

0.0000 0.0000 0.0000 0.9994 -0.0085
-0.0106 -0.0017 0.0000 0.0000 0.0000
0.0070 0.0116 0.0002 -0.0175 0.0002
0.0052 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0156 -0.0114 0.0000
0.0000 0.0000 0.0000 -0.0063 0.0028
0.0057 -0.0029 0.0000 0.0000 0.0000
0.0000

18. (1.97780) BD (1) C 1- C 6
(50.44%) 0.7102* C 1 s(36.48%)p 1.74(63.31%)d 0.00(0.16%)
f 0.00(0.06%)

0.0000 0.6038 -0.0160 -0.0010 0.0006
0.5850 0.0301 0.0040 0.0030 0.5383
0.0128 0.0018 0.0010 0.0000 0.0000
0.0000 0.0000 0.0278 0.0070 0.0052
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0090 -0.0027 0.0037 -0.0246
0.0023 -0.0022 0.0000 0.0000 -0.0094
0.0046 -0.0122 0.0030 0.0000 0.0000
0.0000 0.0000 -0.0121 0.0014 0.0106
-0.0072

(49.56%) 0.7040* C 6 s(35.70%)p 1.79(64.08%)d 0.00(0.16%)
f 0.00(0.06%)

0.0000 0.5975 -0.0093 -0.0015 -0.0002
-0.5483 0.0115 -0.0009 0.0001 -0.5822
-0.0328 -0.0018 0.0006 0.0000 0.0000
0.0000 0.0000 0.0308 0.0018 0.0018
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0051 0.0011 -0.0049 -0.0239
0.0028 0.0011 0.0000 0.0000 0.0124
-0.0021 0.0103 -0.0040 0.0000 0.0000
0.0000 0.0000 0.0088 -0.0068 -0.0131
0.0000

19. (1.97775) BD (1) C 1- H 7
(60.90%) 0.7804* C 1 s(28.78%)p 2.47(71.11%)d 0.00(0.08%)
f 0.00(0.04%)

0.0000 0.5363 0.0133 0.0029 -0.0014
0.2002 0.0035 -0.0012 0.0014 -0.8190
-0.0135 0.0046 0.0024 0.0000 0.0000
0.0000 0.0000 -0.0081 0.0012 -0.0033
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0208 -0.0054 -0.0035 -0.0121
-0.0074 -0.0015 0.0000 0.0000 -0.0034
0.0011 0.0158 -0.0039 0.0000 0.0000
0.0000 0.0000 -0.0051 0.0032 0.0056
-0.0044

(39.10%) 0.6253* H 7 s(99.97%)p 0.00(0.03%)d 0.00(0.01%)

0.9998 0.0006 0.0011 0.0000 0.0010
-0.0039 0.0002 -0.0076 0.0140 -0.0051
0.0000 0.0000 0.0000 -0.0009 -0.0022
0.0000 0.0000 0.0000 0.0000 0.0028
-0.0052 0.0013 -0.0032

20. (1.97058) BD (1) C 2- C 3
(52.19%) 0.7224* C 2 s(35.46%)p 1.81(64.24%)d 0.01(0.20%)
f 0.00(0.09%)

0.0000 0.5955 -0.0077 -0.0005 -0.0027
-0.2247 -0.0244 -0.0031 0.0004 0.7689
-0.0088 0.0097 -0.0034 0.0000 0.0000
0.0000 0.0000 -0.0036 -0.0105 0.0028
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0249 -0.0180 0.0021 0.0267
-0.0141 0.0000 0.0000 0.0000 0.0051
0.0023 -0.0189 -0.0068 0.0000 0.0000

				0.0000	0.0000	0.0139	0.0060	-0.0155	
				-0.0051					
(47.81%)	0.6914* C	3	s(34.74%)p 1.87(64.87%)d 0.01(0.31%)						
				f 0.00(0.08%)					
				0.0000	0.5893	-0.0053	0.0007	-0.0050	
				0.1818	-0.0021	-0.0015	-0.7846	-0.0101	
				-0.0041	0.0000	0.0000	0.0000	-0.0376	
				0.0056	0.0033	0.0000	0.0000	0.0000	
				0.0000	0.0000	0.0000	-0.0324	-0.0012	
				0.0056	-0.0215	-0.0066	-0.0030	0.0000	
				0.0000	-0.0069	-0.0006	0.0226	-0.0014	
				0.0000	0.0000	0.0000	0.0000	-0.0004	
				0.0066	0.0144	-0.0058			
21. (1.98421)	BD (1) C	2- N 12							
(38.26%)	0.6185* C	2	s(27.02%)p 2.70(72.92%)d 0.00(0.04%)						
				f 0.00(0.02%)					
				0.0000	0.5198	-0.0080	-0.0014	-0.0010	
				-0.6221	-0.0115	-0.0037	-0.0024	-0.5847	
				0.0118	-0.0021	-0.0028	0.0000	0.0000	
				0.0000	0.0000	-0.0012	0.0095	-0.0092	
				0.0000	0.0000	0.0000	0.0000	0.0000	
				0.0000	-0.0077	0.0000	-0.0051	-0.0060	
				-0.0099	0.0005	0.0000	0.0000	0.0022	
				0.0057	0.0056	0.0045	0.0000	0.0000	
				0.0000	0.0000	0.0094	0.0019	0.0040	
				-0.0053					
(61.74%)	0.7858* N 12	s(47.73%)p 1.09(52.00%)d 0.00(0.14%)							
				f 0.00(0.12%)					
				0.0000	0.6907	-0.0164	-0.0029	0.0014	
				0.4537	0.0007	-0.0011	-0.0027	0.5604	
				0.0097	-0.0049	0.0006	0.0000	0.0000	
				0.0000	0.0000	0.0302	-0.0023	0.0003	
				0.0000	0.0000	0.0000	0.0000	0.0000	
				0.0000	0.0152	0.0055	0.0014	-0.0156	
				0.0037	0.0005	0.0000	0.0000	-0.0140	
				-0.0009	-0.0161	-0.0008	0.0000	0.0000	
				0.0000	0.0000	-0.0249	-0.0013	0.0130	
				0.0013					
22. (1.97411)	BD (1) C	3- C 4							
(49.71%)	0.7051* C	3	s(36.32%)p 1.74(63.33%)d 0.01(0.26%)						
				f 0.00(0.09%)					
				0.0000	0.6025	0.0112	0.0023	-0.0012	
				0.5477	0.0000	-0.0005	0.5772	0.0135	
				0.0035	0.0000	0.0000	0.0000	0.0370	
				-0.0013	-0.0073	0.0000	0.0000	0.0000	
				0.0000	0.0000	0.0000	0.0234	-0.0070	
				0.0003	-0.0242	-0.0032	-0.0017	0.0000	
				0.0000	-0.0192	0.0007	-0.0141	0.0029	
				0.0000	0.0000	0.0000	0.0000	-0.0148	
				0.0061	0.0063	-0.0056			
(50.29%)	0.7091* C	4	s(35.62%)p 1.80(64.04%)d 0.01(0.26%)						
				f 0.00(0.08%)					
				0.0000	0.5964	-0.0228	-0.0011	0.0013	
				-0.5909	-0.0423	-0.0070	0.0019	-0.5376	
				0.0177	-0.0011	0.0027	0.0000	0.0000	
				0.0000	0.0000	0.0366	0.0080	-0.0008	
				0.0000	0.0000	0.0000	0.0000	0.0000	
				0.0000	-0.0038	-0.0029	-0.0041	-0.0342	
				0.0009	-0.0004	0.0000	0.0000	0.0128	
				-0.0026	0.0151	-0.0005	0.0000	0.0000	
				0.0000	0.0000	0.0153	0.0016	-0.0128	
				0.0053					
23. (1.66197)	BD (2) C	3- C 4							

(49.74%) 0.7052* C 3 s(0.00%)p 1.00(99.79%)d 0.00(0.10%)
f 0.00(0.11%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9989 0.0022 -0.0046 0.0000
0.0000 0.0000 0.0290 0.0024 0.0040
-0.0089 0.0050 -0.0046 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 -0.0326
-0.0005 0.0000 0.0000 0.0000 0.0000
-0.0022 0.0011 -0.0028 -0.0039 0.0000
0.0000 0.0000 0.0000

(50.26%) 0.7090* C 4 s(0.00%)p 1.00(99.82%)d 0.00(0.12%)
f 0.00(0.06%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.9991 0.0011
-0.0104 0.0011 0.0000 0.0000 0.0000
0.0149 -0.0148 -0.0020 0.0060 -0.0256
-0.0075 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0203 0.0051 0.0000
0.0000 0.0000 0.0000 -0.0068 -0.0073
-0.0029 -0.0046 0.0000 0.0000 0.0000
0.0000

24. (1.97067) BD (1) C 3- H 8
(60.52%) 0.7779* C 3 s(28.78%)p 2.47(71.07%)d 0.00(0.07%)
f 0.00(0.08%)
0.0000 0.5364 -0.0041 -0.0037 0.0052
-0.8154 0.0147 0.0009 0.2135 -0.0008
0.0013 0.0000 0.0000 0.0000 -0.0002
-0.0107 -0.0018 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0127 0.0150
0.0019 -0.0097 -0.0089 -0.0050 0.0000
0.0000 0.0245 -0.0013 -0.0064 -0.0001
0.0000 0.0000 0.0000 0.0000 -0.0076
0.0030 0.0064 -0.0029

(39.48%) 0.6283* H 8 s(99.95%)p 0.00(0.04%)d 0.00(0.01%)
0.9998 0.0027 -0.0001 -0.0001 -0.0055
0.0175 -0.0027 -0.0059 -0.0046 0.0005
0.0000 0.0000 0.0000 -0.0034 -0.0018
0.0000 0.0000 0.0000 0.0000 0.0037
0.0041 -0.0047 -0.0016

25. (1.98300) BD (1) C 4- C 5
(50.19%) 0.7084* C 4 s(36.17%)p 1.76(63.61%)d 0.00(0.17%)
f 0.00(0.06%)
0.0000 0.6014 -0.0036 0.0013 -0.0034
0.7751 0.0174 0.0057 0.0026 -0.1852
0.0254 0.0018 0.0010 0.0000 0.0000
0.0000 0.0000 -0.0201 -0.0063 -0.0009
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0254 0.0017 -0.0068 -0.0225
-0.0045 -0.0001 0.0000 0.0000 -0.0149
0.0054 0.0051 -0.0007 0.0000 0.0000
0.0000 0.0000 0.0087 -0.0078 -0.0120
0.0011

(49.81%) 0.7058* C 5 s(35.84%)p 1.78(63.94%)d 0.00(0.16%)
f 0.00(0.06%)
0.0000 0.5986 -0.0086 -0.0008 0.0006
-0.7621 -0.0050 -0.0017 -0.0016 0.2396
0.0338 0.0014 0.0009 0.0000 0.0000
0.0000 0.0000 -0.0127 0.0036 -0.0065
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0290 0.0011 0.0013 -0.0223
0.0018 0.0002 0.0000 0.0000 0.0157

					-0.0045	-0.0034	0.0024	0.0000	0.0000
					0.0000	0.0000	-0.0123	-0.0004	0.0093
					-0.0071				
26.	(1.97981)	BD (1) C	4- H 9						
	(60.65%)		0.7788* C	4 s(28.07%)p	2.56(71.79%)d	0.00(0.10%)			
					f 0.00(0.04%)				
					0.0000	0.5293	0.0231	-0.0003	0.0020
					-0.2139	0.0055	0.0004	-0.0006	0.8196
					-0.0213	-0.0020	-0.0005	0.0000	0.0000
					0.0000	0.0000	-0.0134	-0.0063	-0.0002
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	-0.0231	-0.0096	0.0015	-0.0060
					-0.0115	-0.0030	0.0000	0.0000	0.0043
					-0.0010	-0.0172	0.0034	0.0000	0.0000
					0.0000	0.0000	0.0038	-0.0037	-0.0051
					0.0038				
	(39.35%)		0.6273* H	9 s(99.96%)p	0.00(0.04%)d	0.00(0.01%)			
					0.9998	-0.0009	-0.0010	0.0002	-0.0019
					0.0032	-0.0025	0.0129	-0.0102	0.0085
					0.0000	0.0000	0.0000	-0.0003	-0.0034
					0.0000	0.0000	0.0000	0.0000	0.0005
					-0.0051	0.0011	-0.0037		
27.	(1.98158)	BD (1) C	5- C 6						
	(49.81%)		0.7058* C	5 s(35.79%)p	1.79(64.00%)d	0.00(0.15%)			
					f 0.00(0.06%)				
					0.0000	0.5982	-0.0086	-0.0003	0.0003
					0.2287	0.0343	0.0012	0.0001	-0.7659
					-0.0051	-0.0013	-0.0009	0.0000	0.0000
					0.0000	0.0000	-0.0113	0.0030	-0.0062
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	-0.0287	-0.0016	-0.0009	-0.0224
					0.0015	0.0001	0.0000	0.0000	-0.0031
					0.0023	0.0157	-0.0044	0.0000	0.0000
					0.0000	0.0000	-0.0084	0.0073	0.0126
					-0.0002				
	(50.19%)		0.7084* C	6 s(36.10%)p	1.76(63.68%)d	0.00(0.16%)			
					f 0.00(0.06%)				
					0.0000	0.6008	-0.0100	0.0004	-0.0011
					-0.1726	0.0261	-0.0015	0.0010	0.7784
					0.0214	0.0032	0.0017	0.0000	0.0000
					0.0000	0.0000	-0.0199	-0.0009	0.0012
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	-0.0246	0.0013	-0.0074	-0.0229
					0.0020	0.0004	0.0000	0.0000	0.0049
					-0.0002	-0.0149	0.0055	0.0000	0.0000
					0.0000	0.0000	0.0119	-0.0004	-0.0095
					0.0074				
28.	(1.65134)	BD (2) C	5- C 6						
	(50.52%)		0.7108* C	5 s(0.00%)p	1.00(99.93%)d	0.00(0.03%)			
					f 0.00(0.04%)				
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0000	0.0000	0.9996	-0.0121
					0.0032	0.0002	0.0000	0.0000	0.0000
					-0.0022	-0.0062	0.0037	-0.0112	-0.0085
					0.0032	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0000	-0.0169	0.0062	0.0000
					0.0000	0.0000	0.0000	0.0022	0.0026
					0.0056	0.0069	0.0000	0.0000	0.0000
					0.0000				
	(49.48%)		0.7034* C	6 s(0.00%)p	1.00(99.93%)d	0.00(0.03%)			
					f 0.00(0.04%)				
					0.0000	0.0000	0.0000	0.0000	0.0000

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.9996 -0.0086
0.0008 0.0001 0.0000 0.0000 0.0000
-0.0081 -0.0081 0.0071 0.0091 0.0029
0.0004 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0170 0.0067 0.0000
0.0000 0.0000 0.0000 0.0059 0.0071
-0.0005 -0.0009 0.0000 0.0000 0.0000
0.0000

29. (1.97972) BD (1) C 5- H 10
(60.77%) 0.7796* C 5 s(28.18%)p 2.54(71.70%)d 0.00(0.08%)
f 0.00(0.04%)

0.0000 0.5306 0.0146 0.0013 -0.0009
0.6032 -0.0078 -0.0037 -0.0014 0.5942
-0.0075 -0.0032 -0.0015 0.0000 0.0000
0.0000 0.0000 0.0230 0.0095 -0.0018
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0004 0.0002 0.0000 -0.0128
-0.0039 -0.0032 0.0000 0.0000 -0.0118
0.0023 -0.0116 0.0023 0.0000 0.0000
0.0000 0.0000 -0.0064 0.0025 0.0066
-0.0027

(39.23%) 0.6263* H 10 s(99.96%)p 0.00(0.03%)d 0.00(0.01%)
0.9998 -0.0013 0.0002 -0.0053 -0.0114
0.0038 -0.0051 -0.0112 0.0037 0.0000
0.0000 0.0000 0.0027 -0.0058 0.0000
0.0000 0.0000 0.0000 0.0001 -0.0001
-0.0009 -0.0037

30. (1.97870) BD (1) C 6- H 11
(60.65%) 0.7788* C 6 s(28.04%)p 2.56(71.82%)d 0.00(0.10%)
f 0.00(0.04%)

0.0000 0.5293 0.0165 0.0010 0.0014
0.8164 -0.0156 0.0035 -0.0005 -0.2268
0.0047 0.0008 0.0007 0.0000 0.0000
0.0000 0.0000 -0.0160 -0.0022 0.0012
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0235 0.0035 -0.0002 -0.0097
-0.0066 -0.0060 0.0000 0.0000 -0.0165
0.0036 0.0050 -0.0005 0.0000 0.0000
0.0000 0.0000 0.0050 -0.0033 -0.0049
0.0034

(39.35%) 0.6273* H 11 s(99.96%)p 0.00(0.04%)d 0.00(0.01%)
0.9998 -0.0008 -0.0011 0.0001 0.0136
-0.0118 0.0056 -0.0039 0.0035 -0.0017
0.0000 0.0000 0.0000 -0.0009 -0.0031
0.0000 0.0000 0.0000 0.0000 0.0004
0.0051 0.0007 -0.0039

31. (1.98444) BD (1) N 12- C 13
(61.58%) 0.7847* N 12 s(49.54%)p 1.01(50.02%)d 0.01(0.27%)
f 0.00(0.17%)

0.0000 0.7035 0.0222 -0.0001 -0.0013
-0.2518 0.0037 -0.0014 -0.0008 -0.6608
0.0069 -0.0023 -0.0031 0.0000 0.0000
0.0000 0.0000 0.0089 -0.0031 0.0001
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0460 -0.0008 -0.0016 -0.0226
0.0007 -0.0008 0.0000 0.0000 0.0083
0.0000 0.0237 0.0005 0.0000 0.0000
0.0000 0.0000 0.0275 0.0005 0.0186
0.0005

(38.42%) 0.6199* C 13 s(45.04%)p 1.21(54.30%)d 0.01(0.48%)
f 0.00(0.18%)

0.0000 0.6710 0.0115 0.0004 0.0053

0.1099 -0.0739 -0.0067 0.0045 0.7244
0.0164 0.0186 -0.0049 0.0000 0.0000
0.0000 0.0000 -0.0399 0.0045 -0.0078
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0502 0.0137 0.0132 -0.0063
0.0110 0.0084 0.0000 0.0000 -0.0096
0.0005 -0.0076 -0.0066 0.0000 0.0000
0.0000 0.0000 -0.0395 0.0020 -0.0025
-0.0059

32. (1.93740) BD (2) N 12- C 13
(65.67%) 0.8104* N 12 s(0.00%)p 1.00(99.81%)d 0.00(0.10%)
f 0.00(0.09%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.9987 -0.0274
0.0019 0.0001 0.0000 0.0000 0.0000
0.0156 0.0068 -0.0006 -0.0246 0.0093
-0.0009 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0205 -0.0027 0.0000
0.0000 0.0000 0.0000 -0.0117 -0.0030
0.0194 0.0015 0.0000 0.0000 0.0000
0.0000

(34.33%) 0.5859* C 13 s(0.00%)p 1.00(99.76%)d 0.00(0.06%)
f 0.00(0.18%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.9985 0.0220
0.0073 -0.0046 0.0000 0.0000 0.0000
0.0067 -0.0006 0.0033 0.0162 -0.0167
0.0023 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0254 -0.0030 0.0000
0.0000 0.0000 0.0000 -0.0227 -0.0047
0.0253 -0.0004 0.0000 0.0000 0.0000
0.0000

33. (1.75862) BD (3) N 12- C 13
(84.94%) 0.9216* N 12 s(2.56%)p37.93(97.24%)d 0.04(0.11%)
f 0.03(0.09%)

0.0000 0.1599 -0.0066 0.0061 -0.0001
-0.8535 0.0023 -0.0019 0.0012 0.4938
0.0024 0.0035 0.0012 0.0000 0.0000
0.0000 0.0000 0.0204 -0.0126 -0.0009
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0011 -0.0063 0.0021 0.0202
0.0077 0.0013 0.0000 0.0000 0.0072
0.0015 -0.0063 0.0005 0.0000 0.0000
0.0000 0.0000 -0.0005 0.0039 -0.0276
-0.0024

(15.06%) 0.3880* C 13 s(2.56%)p29.87(76.36%)d 6.86(17.54%)
f 1.39(3.55%)

0.0000 -0.1315 -0.0860 -0.0028 0.0295
-0.7087 -0.4619 -0.0603 0.0218 0.1429
-0.1510 0.0266 -0.0003 0.0000 0.0000
0.0000 0.0000 -0.3372 0.0550 -0.0553
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.2248 0.0087 0.0491 0.0337
0.0215 0.0307 0.0000 0.0000 -0.0242
0.0120 0.0878 -0.0101 0.0000 0.0000
0.0000 0.0000 -0.1219 0.0399 0.1019
-0.0085

34. (1.82991) BD (1) C 13- S 14
(47.56%) 0.6897* C 13 s(37.82%)p 1.41(53.22%)d 0.17(6.44%)
f 0.07(2.52%)

0.0000 0.6118 -0.0609 -0.0019 0.0155

0.1616 -0.2857 -0.0282 0.0130 -0.6442
-0.0864 0.0322 0.0004 0.0000 0.0000
0.0000 0.0000 -0.1877 0.0250 -0.0339
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.1607 -0.0019 0.0336 0.0036
0.0103 0.0184 0.0000 0.0000 -0.0159
0.0056 0.0824 -0.0086 0.0000 0.0000
0.0000 0.0000 -0.0645 0.0181 0.1161
-0.0053

(52.44%) 0.7241* S 14 s(14.28%)p 5.95(84.93%)d 0.05(0.75%)
f 0.00(0.04%)

0.0000 0.0000 0.3734 -0.0574 -0.0005
-0.0001 0.0000 0.7214 -0.0092 0.0012
0.0006 0.0000 0.5722 -0.0367 0.0044
-0.0001 0.0000 0.0000 0.0000 0.0000
0.0000 0.0607 0.0003 0.0008 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
-0.0445 -0.0098 -0.0019 -0.0419 -0.0050
0.0004 0.0000 0.0000 -0.0051 -0.0003
-0.0102 0.0002 0.0000 0.0000 0.0000
0.0000 -0.0150 0.0003 -0.0043 0.0004

35. (1.76441) BD (2) C 13- S 14

(27.44%) 0.5239* C 13 s(15.92%)p 4.17(66.45%)d 0.82(13.08%)
f 0.29(4.55%)

0.0000 0.3934 0.0626 0.0015 -0.0223
-0.6752 0.4022 0.0477 -0.0167 -0.1834
0.1023 -0.0141 0.0009 0.0000 0.0000
0.0000 0.0000 0.2998 -0.0300 0.0422
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.1842 -0.0039 -0.0450 -0.0370
-0.0189 -0.0224 0.0000 0.0000 0.0442
-0.0102 -0.0511 0.0048 0.0000 0.0000
0.0000 0.0000 0.1633 -0.0299 -0.1150
0.0041

(72.56%) 0.8518* S 14 s(5.42%)p17.36(94.11%)d 0.08(0.44%)
f 0.00(0.02%)

0.0000 0.0000 0.2297 -0.0382 0.0008
0.0000 0.0000 -0.6780 -0.0077 0.0020
-0.0001 0.0000 0.6934 -0.0237 0.0022
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0083 0.0112 0.0012 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
-0.0597 0.0006 -0.0004 -0.0257 -0.0028
0.0005 0.0000 0.0000 0.0008 0.0003
-0.0076 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0009 0.0004 -0.0130 0.0003

----- non-Lewis -----

36. (0.02774) BD*(1) C 1- C 2

(51.39%) 0.7169* C 1 s(34.57%)p 1.89(65.21%)d 0.00(0.17%)
f 0.00(0.05%)

0.0000 -0.5880 0.0015 0.0020 -0.0008
0.7839 0.0141 0.0015 0.0016 -0.1929
-0.0162 0.0013 -0.0007 0.0000 0.0000
0.0000 0.0000 0.0204 -0.0042 -0.0010
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0266 0.0044 -0.0036 0.0222
0.0001 0.0006 0.0000 0.0000 -0.0140
0.0050 0.0049 -0.0002 0.0000 0.0000
0.0000 0.0000 0.0093 -0.0062 -0.0117
0.0001

(48.61%) -0.6972* C 2 s(37.29%)p 1.68(62.56%)d 0.00(0.09%)
f 0.00(0.06%)

0.0000 -0.6105 -0.0122 -0.0019 -0.0030

-0.7487	0.0102	-0.0052	-0.0022	0.2544
0.0108	0.0036	0.0025	0.0000	0.0000
0.0000	0.0000	0.0021	0.0094	-0.0044
0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	-0.0164	-0.0160	0.0026	-0.0102
0.0118	-0.0007	0.0000	0.0000	0.0147
0.0081	-0.0055	-0.0021	0.0000	0.0000
0.0000	0.0000	-0.0093	-0.0062	0.0117
0.0068				

37. (0.40310) BD*(2) C 1- C 2
 (51.15%) 0.7152* C 1 s(0.00%)p 1.00(99.91%)d 0.00(0.04%)
 f 0.00(0.05%)

0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.9995	-0.0029
-0.0038	-0.0012	0.0000	0.0000	0.0000
-0.0087	-0.0103	0.0003	0.0090	0.0121
0.0013	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	-0.0188	0.0057	0.0000
0.0000	0.0000	0.0000	-0.0055	-0.0074
-0.0008	-0.0017	0.0000	0.0000	0.0000
0.0000				

(48.85%) -0.6990* C 2 s(0.00%)p 1.00(99.90%)d 0.00(0.05%)
 f 0.00(0.05%)

0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.9994	-0.0085
-0.0106	-0.0017	0.0000	0.0000	0.0000
0.0070	0.0116	0.0002	-0.0175	0.0002
0.0052	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	-0.0156	-0.0114	0.0000
0.0000	0.0000	0.0000	-0.0063	0.0028
0.0057	-0.0029	0.0000	0.0000	0.0000
0.0000				

38. (0.01217) BD*(1) C 1- C 6
 (49.56%) 0.7040* C 1 s(36.48%)p 1.74(63.31%)d 0.00(0.16%)
 f 0.00(0.06%)

0.0000	0.6038	-0.0160	-0.0010	0.0006
0.5850	0.0301	0.0040	0.0030	0.5383
0.0128	0.0018	0.0010	0.0000	0.0000
0.0000	0.0000	0.0278	0.0070	0.0052
0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	-0.0090	-0.0027	0.0037	-0.0246
0.0023	-0.0022	0.0000	0.0000	-0.0094
0.0046	-0.0122	0.0030	0.0000	0.0000
0.0000	0.0000	-0.0121	0.0014	0.0106
-0.0072				

(50.44%) -0.7102* C 6 s(35.70%)p 1.79(64.08%)d 0.00(0.16%)
 f 0.00(0.06%)

0.0000	0.5975	-0.0093	-0.0015	-0.0002
-0.5483	0.0115	-0.0009	0.0001	-0.5822
-0.0328	-0.0018	0.0006	0.0000	0.0000
0.0000	0.0000	0.0308	0.0018	0.0018
0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0051	0.0011	-0.0049	-0.0239
0.0028	0.0011	0.0000	0.0000	0.0124
-0.0021	0.0103	-0.0040	0.0000	0.0000
0.0000	0.0000	0.0088	-0.0068	-0.0131
0.0000				

39. (0.01258) BD*(1) C 1- H 7
 (39.10%) 0.6253* C 1 s(28.78%)p 2.47(71.11%)d 0.00(0.08%)
 f 0.00(0.04%)

0.0000	-0.5363	-0.0133	-0.0029	0.0014
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-0.2002 -0.0035 0.0012 -0.0014 0.8190
 0.0135 -0.0046 -0.0024 0.0000 0.0000
 0.0000 0.0000 0.0081 -0.0012 0.0033
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0208 0.0054 0.0035 0.0121
 0.0074 0.0015 0.0000 0.0000 0.0034
 -0.0011 -0.0158 0.0039 0.0000 0.0000
 0.0000 0.0000 0.0051 -0.0032 -0.0056
 0.0044
 (60.90%) -0.7804* H 7 s(99.97%)p 0.00(0.03%)d 0.00(0.01%)
 -0.9998 -0.0006 -0.0011 0.0000 -0.0010
 0.0039 -0.0002 0.0076 -0.0140 0.0051
 0.0000 0.0000 0.0000 0.0009 0.0022
 0.0000 0.0000 0.0000 0.0000 -0.0028
 0.0052 -0.0013 0.0032
 40. (0.02243) BD*(1) C 2- C 3
 (47.81%) 0.6914* C 2 s(35.46%)p 1.81(64.24%)d 0.01(0.20%)
 f 0.00(0.09%)
 0.0000 -0.5955 0.0077 0.0005 0.0027
 0.2247 0.0244 0.0031 -0.0004 -0.7689
 0.0088 -0.0097 0.0034 0.0000 0.0000
 0.0000 0.0000 0.0036 0.0105 -0.0028
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0249 0.0180 -0.0021 -0.0267
 0.0141 0.0000 0.0000 0.0000 -0.0051
 -0.0023 0.0189 0.0068 0.0000 0.0000
 0.0000 0.0000 -0.0139 -0.0060 0.0155
 0.0051
 (52.19%) -0.7224* C 3 s(34.74%)p 1.87(64.87%)d 0.01(0.31%)
 f 0.00(0.08%)
 0.0000 -0.5893 0.0053 -0.0007 0.0050
 -0.1818 0.0021 0.0015 0.7846 0.0101
 0.0041 0.0000 0.0000 0.0000 0.0376
 -0.0056 -0.0033 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0324 0.0012
 -0.0056 0.0215 0.0066 0.0030 0.0000
 0.0000 0.0069 0.0006 -0.0226 0.0014
 0.0000 0.0000 0.0000 0.0000 0.0004
 -0.0066 -0.0144 0.0058
 41. (0.03370) BD*(1) C 2- N 12
 (61.74%) 0.7858* C 2 s(27.02%)p 2.70(72.92%)d 0.00(0.04%)
 f 0.00(0.02%)
 0.0000 -0.5198 0.0080 0.0014 0.0010
 0.6221 0.0115 0.0037 0.0024 0.5847
 -0.0118 0.0021 0.0028 0.0000 0.0000
 0.0000 0.0000 0.0012 -0.0095 0.0092
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0077 0.0000 0.0051 0.0060
 0.0099 -0.0005 0.0000 0.0000 -0.0022
 -0.0057 -0.0056 -0.0045 0.0000 0.0000
 0.0000 0.0000 -0.0094 -0.0019 -0.0040
 0.0053
 (38.26%) -0.6185* N 12 s(47.73%)p 1.09(52.00%)d 0.00(0.14%)
 f 0.00(0.12%)
 0.0000 -0.6907 0.0164 0.0029 -0.0014
 -0.4537 -0.0007 0.0011 0.0027 -0.5604
 -0.0097 0.0049 -0.0006 0.0000 0.0000
 0.0000 0.0000 -0.0302 0.0023 -0.0003
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 -0.0152 -0.0055 -0.0014 0.0156
 -0.0037 -0.0005 0.0000 0.0000 0.0140
 0.0009 0.0161 0.0008 0.0000 0.0000
 0.0000 0.0000 0.0249 0.0013 -0.0130

-0.0013

42. (0.01133) BD*(1) C 3- C 4
 (50.29%) 0.7091* C 3 s(36.32%)p 1.74(63.33%)d 0.01(0.26%)
 f 0.00(0.09%)
 0.0000 0.6025 0.0112 0.0023 -0.0012
 0.5477 0.0000 -0.0005 0.5772 0.0135
 0.0035 0.0000 0.0000 0.0000 0.0370
 -0.0013 -0.0073 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0234 -0.0070
 0.0003 -0.0242 -0.0032 -0.0017 0.0000
 0.0000 -0.0192 0.0007 -0.0141 0.0029
 0.0000 0.0000 0.0000 0.0000 -0.0148
 0.0061 0.0063 -0.0056
 (49.71%) -0.7051* C 4 s(35.62%)p 1.80(64.04%)d 0.01(0.26%)
 f 0.00(0.08%)
 0.0000 0.5964 -0.0228 -0.0011 0.0013
 -0.5909 -0.0423 -0.0070 0.0019 -0.5376
 0.0177 -0.0011 0.0027 0.0000 0.0000
 0.0000 0.0000 0.0366 0.0080 -0.0008
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 -0.0038 -0.0029 -0.0041 -0.0342
 0.0009 -0.0004 0.0000 0.0000 0.0128
 -0.0026 0.0151 -0.0005 0.0000 0.0000
 0.0000 0.0000 0.0153 0.0016 -0.0128
 0.0053

43. (0.31902) BD*(2) C 3- C 4
 (50.26%) 0.7090* C 3 s(0.00%)p 1.00(99.79%)d 0.00(0.10%)
 f 0.00(0.11%)
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.9989 0.0022 -0.0046 0.0000
 0.0000 0.0000 0.0290 0.0024 0.0040
 -0.0089 0.0050 -0.0046 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0000 -0.0326
 -0.0005 0.0000 0.0000 0.0000 0.0000
 -0.0022 0.0011 -0.0028 -0.0039 0.0000
 0.0000 0.0000 0.0000
 (49.74%) -0.7052* C 4 s(0.00%)p 1.00(99.82%)d 0.00(0.12%)
 f 0.00(0.06%)
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.9991 0.0011
 -0.0104 0.0011 0.0000 0.0000 0.0000
 0.0149 -0.0148 -0.0020 0.0060 -0.0256
 -0.0075 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 -0.0203 0.0051 0.0000
 0.0000 0.0000 0.0000 -0.0068 -0.0073
 -0.0029 -0.0046 0.0000 0.0000 0.0000
 0.0000

44. (0.01093) BD*(1) C 3- H 8
 (39.48%) 0.6283* C 3 s(28.78%)p 2.47(71.07%)d 0.00(0.07%)
 f 0.00(0.08%)
 0.0000 -0.5364 0.0041 0.0037 -0.0052
 0.8154 -0.0147 -0.0009 -0.2135 0.0008
 -0.0013 0.0000 0.0000 0.0000 0.0002
 0.0107 0.0018 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 -0.0127 -0.0150
 -0.0019 0.0097 0.0089 0.0050 0.0000
 0.0000 -0.0245 0.0013 0.0064 0.0001
 0.0000 0.0000 0.0000 0.0000 0.0076
 -0.0030 -0.0064 0.0029
 (60.52%) -0.7779* H 8 s(99.95%)p 0.00(0.04%)d 0.00(0.01%)
 -0.9998 -0.0027 0.0001 0.0001 0.0055

-0.0175 0.0027 0.0059 0.0046 -0.0005
0.0000 0.0000 0.0000 0.0034 0.0018
0.0000 0.0000 0.0000 0.0000 -0.0037
-0.0041 0.0047 0.0016

45. (0.01454) BD*(1) C 4- C 5
(49.81%) 0.7058* C 4 s(36.17%)p 1.76(63.61%)d 0.00(0.17%)
f 0.00(0.06%)
0.0000 0.6014 -0.0036 0.0013 -0.0034
0.7751 0.0174 0.0057 0.0026 -0.1852
0.0254 0.0018 0.0010 0.0000 0.0000
0.0000 0.0000 -0.0201 -0.0063 -0.0009
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0254 0.0017 -0.0068 -0.0225
-0.0045 -0.0001 0.0000 0.0000 -0.0149
0.0054 0.0051 -0.0007 0.0000 0.0000
0.0000 0.0000 0.0087 -0.0078 -0.0120
0.0011
(50.19%) -0.7084* C 5 s(35.84%)p 1.78(63.94%)d 0.00(0.16%)
f 0.00(0.06%)
0.0000 0.5986 -0.0086 -0.0008 0.0006
-0.7621 -0.0050 -0.0017 -0.0016 0.2396
0.0338 0.0014 0.0009 0.0000 0.0000
0.0000 0.0000 -0.0127 0.0036 -0.0065
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0290 0.0011 0.0013 -0.0223
0.0018 0.0002 0.0000 0.0000 0.0157
-0.0045 -0.0034 0.0024 0.0000 0.0000
0.0000 0.0000 -0.0123 -0.0004 0.0093
-0.0071

46. (0.01387) BD*(1) C 4- H 9
(39.35%) 0.6273* C 4 s(28.07%)p 2.56(71.79%)d 0.00(0.10%)
f 0.00(0.04%)
0.0000 -0.5293 -0.0231 0.0003 -0.0020
0.2139 -0.0055 -0.0004 0.0006 -0.8196
0.0213 0.0020 0.0005 0.0000 0.0000
0.0000 0.0000 0.0134 0.0063 0.0002
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0231 0.0096 -0.0015 0.0060
0.0115 0.0030 0.0000 0.0000 -0.0043
0.0010 0.0172 -0.0034 0.0000 0.0000
0.0000 0.0000 -0.0038 0.0037 0.0051
-0.0038
(60.65%) -0.7788* H 9 s(99.96%)p 0.00(0.04%)d 0.00(0.01%)
-0.9998 0.0009 0.0010 -0.0002 0.0019
-0.0032 0.0025 -0.0129 0.0102 -0.0085
0.0000 0.0000 0.0000 0.0003 0.0034
0.0000 0.0000 0.0000 0.0000 -0.0005
0.0051 -0.0011 0.0037

47. (0.01412) BD*(1) C 5- C 6
(50.19%) 0.7084* C 5 s(35.79%)p 1.79(64.00%)d 0.00(0.15%)
f 0.00(0.06%)
0.0000 -0.5982 0.0086 0.0003 -0.0003
-0.2287 -0.0343 -0.0012 -0.0001 0.7659
0.0051 0.0013 0.0009 0.0000 0.0000
0.0000 0.0000 0.0113 -0.0030 0.0062
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0287 0.0016 0.0009 0.0224
-0.0015 -0.0001 0.0000 0.0000 0.0031
-0.0023 -0.0157 0.0044 0.0000 0.0000
0.0000 0.0000 0.0084 -0.0073 -0.0126
0.0002
(49.81%) -0.7058* C 6 s(36.10%)p 1.76(63.68%)d 0.00(0.16%)
f 0.00(0.06%)

0.0000 -0.6008 0.0100 -0.0004 0.0011
0.1726 -0.0261 0.0015 -0.0010 -0.7784
-0.0214 -0.0032 -0.0017 0.0000 0.0000
0.0000 0.0000 0.0199 0.0009 -0.0012
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0246 -0.0013 0.0074 0.0229
-0.0020 -0.0004 0.0000 0.0000 -0.0049
0.0002 0.0149 -0.0055 0.0000 0.0000
0.0000 0.0000 -0.0119 0.0004 0.0095
-0.0074

48. (0.33844) BD*(2) C 5- C 6
(49.48%) 0.7034* C 5 s(0.00%)p 1.00(99.93%)d 0.00(0.03%)
f 0.00(0.04%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 -0.9996 0.0121
-0.0032 -0.0002 0.0000 0.0000 0.0000
0.0022 0.0062 -0.0037 0.0112 0.0085
-0.0032 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0169 -0.0062 0.0000
0.0000 0.0000 0.0000 -0.0022 -0.0026
-0.0056 -0.0069 0.0000 0.0000 0.0000
0.0000

(50.52%) -0.7108* C 6 s(0.00%)p 1.00(99.93%)d 0.00(0.03%)
f 0.00(0.04%)

0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 -0.9996 0.0086
-0.0008 -0.0001 0.0000 0.0000 0.0000
0.0081 0.0081 -0.0071 -0.0091 -0.0029
-0.0004 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0170 -0.0067 0.0000
0.0000 0.0000 0.0000 -0.0059 -0.0071
0.0005 0.0009 0.0000 0.0000 0.0000
0.0000

49. (0.01387) BD*(1) C 5- H 10
(39.23%) 0.6263* C 5 s(28.18%)p 2.54(71.70%)d 0.00(0.08%)
f 0.00(0.04%)

0.0000 -0.5306 -0.0146 -0.0013 0.0009
-0.6032 0.0078 0.0037 0.0014 -0.5942
0.0075 0.0032 0.0015 0.0000 0.0000
0.0000 0.0000 -0.0230 -0.0095 0.0018
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0004 -0.0002 0.0000 0.0128
0.0039 0.0032 0.0000 0.0000 0.0118
-0.0023 0.0116 -0.0023 0.0000 0.0000
0.0000 0.0000 0.0064 -0.0025 -0.0066
0.0027

(60.77%) -0.7796* H 10 s(99.96%)p 0.00(0.03%)d 0.00(0.01%)

-0.9998 0.0013 -0.0002 0.0053 0.0114
-0.0038 0.0051 0.0112 -0.0037 0.0000
0.0000 0.0000 -0.0027 0.0058 0.0000
0.0000 0.0000 0.0000 -0.0001 0.0001
0.0009 0.0037

50. (0.01373) BD*(1) C 6- H 11
(39.35%) 0.6273* C 6 s(28.04%)p 2.56(71.82%)d 0.00(0.10%)
f 0.00(0.04%)

0.0000 -0.5293 -0.0165 -0.0010 -0.0014
-0.8164 0.0156 -0.0035 0.0005 0.2268
-0.0047 -0.0008 -0.0007 0.0000 0.0000
0.0000 0.0000 0.0160 0.0022 -0.0012
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0235 -0.0035 0.0002 0.0097

			0.0066	0.0060	0.0000	0.0000	0.0165
			-0.0036	-0.0050	0.0005	0.0000	0.0000
			0.0000	0.0000	-0.0050	0.0033	0.0049
			-0.0034				
(60.65%)	-0.7788*	H 11	s(99.96%)	p 0.00(0.04%)	d 0.00(0.01%)		
			-0.9998	0.0008	0.0011	-0.0001	-0.0136
			0.0118	-0.0056	0.0039	-0.0035	0.0017
			0.0000	0.0000	0.0000	0.0009	0.0031
			0.0000	0.0000	0.0000	0.0000	-0.0004
			-0.0051	-0.0007	0.0039		
51. (0.03013)	BD*(1)	N 12- C 13					
(38.42%)	0.6199*	N 12	s(49.54%)	p 1.01(50.02%)	d 0.01(0.27%)		
			f 0.00(0.17%)				
			0.0000	-0.7035	-0.0222	0.0001	0.0013
			0.2518	-0.0037	0.0014	0.0008	0.6608
			-0.0069	0.0023	0.0031	0.0000	0.0000
			0.0000	0.0000	-0.0089	0.0031	-0.0001
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0460	0.0008	0.0016	0.0226
			-0.0007	0.0008	0.0000	0.0000	-0.0083
			0.0000	-0.0237	-0.0005	0.0000	0.0000
			0.0000	0.0000	-0.0275	-0.0005	-0.0186
			-0.0005				
(61.58%)	-0.7847*	C 13	s(45.04%)	p 1.21(54.30%)	d 0.01(0.48%)		
			f 0.00(0.18%)				
			0.0000	-0.6710	-0.0115	-0.0004	-0.0053
			-0.1099	0.0739	0.0067	-0.0045	-0.7244
			-0.0164	-0.0186	0.0049	0.0000	0.0000
			0.0000	0.0000	0.0399	-0.0045	0.0078
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0502	-0.0137	-0.0132	0.0063
			-0.0110	-0.0084	0.0000	0.0000	0.0096
			-0.0005	0.0076	0.0066	0.0000	0.0000
			0.0000	0.0000	0.0395	-0.0020	0.0025
			0.0059				
52. (0.40258)	BD*(2)	N 12- C 13					
(34.33%)	0.5859*	N 12	s(0.00%)	p 1.00(99.81%)	d 0.00(0.10%)		
			f 0.00(0.09%)				
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	-0.9987	0.0274
			-0.0019	-0.0001	0.0000	0.0000	0.0000
			-0.0156	-0.0068	0.0006	0.0246	-0.0093
			0.0009	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0205	0.0027	0.0000
			0.0000	0.0000	0.0000	0.0117	0.0030
			-0.0194	-0.0015	0.0000	0.0000	0.0000
			0.0000				
(65.67%)	-0.8104*	C 13	s(0.00%)	p 1.00(99.76%)	d 0.00(0.06%)		
			f 0.00(0.18%)				
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0000	-0.9985	-0.0220
			-0.0073	0.0046	0.0000	0.0000	0.0000
			-0.0067	0.0006	-0.0033	-0.0162	0.0167
			-0.0023	0.0000	0.0000	0.0000	0.0000
			0.0000	0.0000	0.0254	0.0030	0.0000
			0.0000	0.0000	0.0000	0.0227	0.0047
			-0.0253	0.0004	0.0000	0.0000	0.0000
			0.0000				
53. (0.22649)	BD*(3)	N 12- C 13					
(15.06%)	0.3880*	N 12	s(2.56%)	p37.93(97.24%)	d 0.04(0.11%)		
			f 0.03(0.09%)				

0.0000 0.1599 -0.0066 0.0061 -0.0001
-0.8535 0.0023 -0.0019 0.0012 0.4938
0.0024 0.0035 0.0012 0.0000 0.0000
0.0000 0.0000 0.0204 -0.0126 -0.0009
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0011 -0.0063 0.0021 0.0202
0.0077 0.0013 0.0000 0.0000 0.0072
0.0015 -0.0063 0.0005 0.0000 0.0000
0.0000 0.0000 -0.0005 0.0039 -0.0276
-0.0024

(84.94%) -0.9216* C 13 s(2.56%)p29.87(76.36%)d 6.86(17.54%)
f 1.39(3.55%)

0.0000 -0.1315 -0.0860 -0.0028 0.0295
-0.7087 -0.4619 -0.0603 0.0218 0.1429
-0.1510 0.0266 -0.0003 0.0000 0.0000
0.0000 0.0000 -0.3372 0.0550 -0.0553
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.2248 0.0087 0.0491 0.0337
0.0215 0.0307 0.0000 0.0000 -0.0242
0.0120 0.0878 -0.0101 0.0000 0.0000
0.0000 0.0000 -0.1219 0.0399 0.1019
-0.0085

54. (0.14736) BD*(1) C 13- S 14

(52.44%) 0.7241* C 13 s(37.82%)p 1.41(53.22%)d 0.17(6.44%)
f 0.07(2.52%)

0.0000 0.6118 -0.0609 -0.0019 0.0155
0.1616 -0.2857 -0.0282 0.0130 -0.6442
-0.0864 0.0322 0.0004 0.0000 0.0000
0.0000 0.0000 -0.1877 0.0250 -0.0339
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.1607 -0.0019 0.0336 0.0036
0.0103 0.0184 0.0000 0.0000 -0.0159
0.0056 0.0824 -0.0086 0.0000 0.0000
0.0000 0.0000 -0.0645 0.0181 0.1161
-0.0053

(47.56%) -0.6897* S 14 s(14.28%)p 5.95(84.93%)d 0.05(0.75%)
f 0.00(0.04%)

0.0000 0.0000 0.3734 -0.0574 -0.0005
-0.0001 0.0000 0.7214 -0.0092 0.0012
0.0006 0.0000 0.5722 -0.0367 0.0044
-0.0001 0.0000 0.0000 0.0000 0.0000
0.0000 0.0607 0.0003 0.0008 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
-0.0445 -0.0098 -0.0019 -0.0419 -0.0050
0.0004 0.0000 0.0000 -0.0051 -0.0003
-0.0102 0.0002 0.0000 0.0000 0.0000
0.0000 -0.0150 0.0003 -0.0043 0.0004

55. (0.24443) BD*(2) C 13- S 14

(72.56%) 0.8518* C 13 s(15.92%)p 4.17(66.45%)d 0.82(13.08%)
f 0.29(4.55%)

0.0000 0.3934 0.0626 0.0015 -0.0223
-0.6752 0.4022 0.0477 -0.0167 -0.1834
0.1023 -0.0141 0.0009 0.0000 0.0000
0.0000 0.0000 0.2998 -0.0300 0.0422
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.1842 -0.0039 -0.0450 -0.0370
-0.0189 -0.0224 0.0000 0.0000 0.0442
-0.0102 -0.0511 0.0048 0.0000 0.0000
0.0000 0.0000 0.1633 -0.0299 -0.1150
0.0041

(27.44%) -0.5239* S 14 s(5.42%)p17.36(94.11%)d 0.08(0.44%)
f 0.00(0.02%)

0.0000 0.0000 0.2297 -0.0382 0.0008

	0.0000	0.0000	-0.6780	-0.0077	0.0020
	-0.0001	0.0000	0.6934	-0.0237	0.0022
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.0083	0.0112	0.0012	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	-0.0597	0.0006	-0.0004	-0.0257	-0.0028
	0.0005	0.0000	0.0000	0.0008	0.0003
	-0.0076	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.0009	0.0004	-0.0130	0.0003
56. (0.00409) RY (1) C 1	s(1.41%)p59.52(83.85%)d 8.45(11.91%)	f 2.01(2.83%)			
	0.0000	-0.0072	0.1134	-0.0344	0.0010
	-0.0034	0.2979	0.0145	-0.0622	-0.0182
	0.8632	0.0121	0.0063	0.0000	0.0000
	0.0000	0.0000	0.0003	-0.0151	0.0766
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.0755	0.0352	0.2764	0.1352
	-0.1006	0.0361	0.0000	0.0000	0.0370
	0.0121	-0.0125	-0.0161	0.0000	0.0000
	0.0000	0.0000	-0.0583	-0.0083	-0.1300
	-0.0774				
57. (0.00179) RY (2) C 1	s(0.58%)p99.99(64.80%)d10.38(6.07%)	f48.79(28.54%)			
	0.0000	-0.0055	0.0751	-0.0133	-0.0018
	-0.0274	0.7151	0.0556	-0.0454	-0.0012
	-0.3548	0.0678	-0.0180	0.0000	0.0000
	0.0000	0.0000	0.1127	0.1182	-0.1709
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0357	0.0136	0.0577	0.0003
	-0.0044	0.0079	0.0000	0.0000	0.0745
	0.0542	0.0202	0.0169	0.0000	0.0000
	0.0000	0.0000	-0.3185	-0.1765	-0.3147
	-0.2112				
58. (0.00099) RY (3) C 1	s(0.00%)p 1.00(82.59%)d 0.17(13.86%)	f 0.04(3.56%)			
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	-0.0073	0.7925
	-0.4441	0.0233	0.0000	0.0000	0.0000
	-0.2039	-0.2336	0.0513	0.1741	0.0550
	0.0801	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	-0.0089	-0.0062	0.0000
	0.0000	0.0000	0.0000	-0.1567	-0.0771
	0.0289	0.0643	0.0000	0.0000	0.0000
	0.0000				
59. (0.00073) RY (4) C 1	s(51.53%)p 0.19(9.84%)d 0.27(13.67%)	f 0.48(24.96%)			
	0.0000	0.0059	0.7083	-0.0968	0.0642
	0.0024	0.2929	-0.0259	0.0277	0.0169
	-0.1040	-0.0002	-0.0073	0.0000	0.0000
	0.0000	0.0000	-0.1610	-0.0828	0.0770
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0997	0.0366	-0.1915	0.1565
	-0.1596	0.0133	0.0000	0.0000	-0.1369
	-0.1066	-0.0547	-0.0446	0.0000	0.0000
	0.0000	0.0000	0.3066	0.2129	0.2660
	0.0666				
60. (0.00068) RY (5) C 1	s(24.37%)p 0.67(16.24%)d 1.39(33.94%)	f 1.04(25.46%)			
	0.0000	0.0050	0.4936	0.0042	0.0037
	0.0063	-0.3966	-0.0496	0.0056	0.0141
	0.0457	-0.0172	-0.0027	0.0000	0.0000
	0.0000	0.0000	0.1277	-0.1826	-0.3060

	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.1072	0.4038	-0.0629	-0.0709
	-0.0743	-0.0834	0.0000	0.0000	-0.0204
	-0.0144	0.0531	0.0291	0.0000	0.0000
	0.0000	0.0000	-0.4254	-0.2183	-0.1449
	-0.0261				
61. (0.00037) RY (6) C 1	s(0.00%)p 1.00(17.10%)d 3.56(60.81%)				
	f 1.29(22.09%)				
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0080	0.3726
	0.1791	0.0031	0.0000	0.0000	0.0000
	0.5730	0.3483	-0.2698	0.2756	0.0633
	-0.0753	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0046	0.0037	0.0000
	0.0000	0.0000	0.0000	0.0558	0.1521
	-0.3250	-0.2983	0.0000	0.0000	0.0000
	0.0000				
62. (0.00031) RY (7) C 1	s(7.28%)p 4.50(32.74%)d 6.06(44.11%)				
	f 2.18(15.87%)				
	0.0000	-0.0045	-0.1762	0.1953	0.0602
	-0.0151	0.2084	0.4124	0.0176	0.0001
	0.0162	0.3349	-0.0298	0.0000	0.0000
	0.0000	0.0000	-0.0358	-0.2133	0.1331
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.2910	0.4995	-0.1890	-0.0486
	0.0559	-0.0342	0.0000	0.0000	0.1417
	0.1233	0.1092	0.0689	0.0000	0.0000
	0.0000	0.0000	0.0057	0.0091	0.2845
	0.1602				
63. (0.00016) RY (8) C 1	s(16.37%)p 0.15(2.51%)d 3.97(64.95%)				
	f 0.99(16.16%)				
	0.0000	-0.0205	0.2582	0.3109	-0.0021
	-0.0052	0.0759	-0.0824	0.0780	-0.0030
	0.0011	-0.0471	0.0651	0.0000	0.0000
	0.0000	0.0000	-0.0943	0.2641	0.1773
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.2666	-0.1026	0.2513	-0.4391
	0.4122	-0.1789	0.0000	0.0000	-0.0107
	-0.1198	-0.2397	-0.1071	0.0000	0.0000
	0.0000	0.0000	-0.0791	-0.1429	0.1561
	0.1649				
64. (0.00009) RY (9) C 1	s(7.46%)p 1.21(9.04%)d10.14(75.65%)				
	f 1.05(7.86%)				
65. (0.00008) RY (10) C 1	s(4.59%)p 6.69(30.74%)d 9.77(44.91%)				
	f 4.30(19.75%)				
66. (0.00007) RY (11) C 1	s(0.00%)p 1.00(26.00%)d 2.43(63.30%)				
	f 0.41(10.71%)				
67. (0.00005) RY (12) C 1	s(11.86%)p 0.57(6.81%)d 4.96(58.88%)				
	f 1.89(22.45%)				
68. (0.00004) RY (13) C 1	s(0.00%)p 1.00(16.54%)d 4.01(66.29%)				
	f 1.04(17.17%)				
69. (0.00003) RY (14) C 1	s(8.48%)p 6.46(54.73%)d 3.04(25.73%)				
	f 1.31(11.06%)				
70. (0.00002) RY (15) C 1	s(14.74%)p 0.86(12.60%)d 3.50(51.59%)				
	f 1.43(21.07%)				
71. (0.00001) RY (16) C 1	s(14.90%)p 1.00(14.97%)d 2.83(42.11%)				
	f 1.88(28.02%)				
72. (0.00000) RY (17) C 1	s(9.62%)p 3.56(34.26%)d 1.70(16.32%)				
	f 4.14(39.80%)				
73. (0.00000) RY (18) C 1	s(14.81%)p 0.71(10.57%)d 2.54(37.59%)				
	f 2.50(37.03%)				
74. (0.00000) RY (19) C 1	s(17.63%)p 0.28(4.98%)d 3.02(53.29%)				

					f 1.37(24.10%)
75.	(0.00000)	RY (20)	C 1	s(4.76%)	p 2.06(9.80%)d 6.82(32.45%)
					f11.14(52.99%)
76.	(0.00000)	RY (21)	C 1	s(8.89%)	p 4.76(42.34%)d 2.92(25.97%)
					f 2.56(22.80%)
77.	(0.00000)	RY (22)	C 1	s(4.82%)	p 6.15(29.64%)d 2.59(12.48%)
					f11.02(53.07%)
78.	(0.00000)	RY (23)	C 1	s(0.00%)	p 1.00(31.87%)d 1.36(43.18%)
					f 0.78(24.95%)
79.	(0.00000)	RY (24)	C 1	s(0.00%)	p 1.00(15.12%)d 4.78(72.32%)
					f 0.83(12.55%)
80.	(0.00000)	RY (25)	C 1	s(0.00%)	p 1.00(3.90%)d24.27(94.61%)
					f 0.38(1.50%)
81.	(0.00000)	RY (26)	C 1	s(0.00%)	p 1.00(19.19%)d 2.57(49.25%)
					f 1.64(31.56%)
82.	(0.00000)	RY (27)	C 1	s(0.00%)	p 1.00(59.63%)d 0.53(31.36%)
					f 0.15(9.01%)
83.	(0.00000)	RY (28)	C 1	s(2.36%)	p 5.97(14.06%)d 2.03(4.79%)
					f33.43(78.79%)
84.	(0.00000)	RY (29)	C 1	s(5.86%)	p 0.72(4.23%)d 7.91(46.37%)
					f 7.43(43.54%)
85.	(0.00000)	RY (30)	C 1	s(0.00%)	p 1.00(2.69%)d11.89(32.01%)
					f24.25(65.29%)
86.	(0.00000)	RY (31)	C 1	s(0.00%)	p 1.00(7.13%)d 0.77(5.46%)
					f12.26(87.41%)
87.	(0.00000)	RY (32)	C 1	s(5.23%)	p 3.12(16.31%)d 3.82(20.00%)
					f11.18(58.47%)
88.	(0.00000)	RY (33)	C 1	s(5.07%)	p 5.51(27.93%)d 6.41(32.49%)
					f 6.81(34.51%)
89.	(0.00000)	RY (34)	C 1	s(26.00%)	p 0.30(7.84%)d 1.34(34.80%)
					f 1.21(31.37%)
90.	(0.00000)	RY (35)	C 1	s(0.00%)	p 1.00(12.26%)d 1.95(23.97%)
					f 5.20(63.77%)
91.	(0.00000)	RY (36)	C 1	s(0.00%)	p 1.00(0.81%)d 6.55(5.28%)
					f99.99(93.92%)
92.	(0.00000)	RY (37)	C 1	s(0.00%)	p 1.00(4.70%)d 6.07(28.56%)
					f14.19(66.74%)
93.	(0.00000)	RY (38)	C 1	s(0.00%)	p 1.00(0.57%)d16.96(9.70%)
					f99.99(89.73%)
94.	(0.00000)	RY (39)	C 1	s(2.26%)	p 7.75(17.54%)d18.10(40.99%)
					f17.31(39.20%)
95.	(0.00000)	RY (40)	C 1	s(9.02%)	p 1.68(15.17%)d 5.10(46.02%)
					f 3.30(29.78%)
96.	(0.00000)	RY (41)	C 1	s(20.28%)	p 1.32(26.82%)d 1.11(22.52%)
					f 1.50(30.38%)
97.	(0.01399)	RY (1)	C 2	s(0.41%)	p99.99(55.48%)d99.19(40.47%)
					f 8.95(3.65%)
					0.0000 -0.0183 0.0606 -0.0087 -0.0001
					0.0011 -0.6495 0.0635 -0.0039 -0.0145
					-0.3586 0.0033 -0.0072 0.0000 0.0000
					0.0000 0.0000 0.5791 -0.0427 0.0371
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 -0.2477 -0.0310 0.0127 -0.0600
					0.0087 0.0025 0.0000 0.0000 -0.0230
					0.0097 0.0175 0.0025 0.0000 0.0000
					0.0000 0.0000 -0.1093 0.0343 -0.1473
					0.0270
98.	(0.00622)	RY (2)	C 2	s(1.20%)	p60.24(72.58%)d20.27(24.43%)
					f 1.48(1.79%)
					0.0000 0.0089 0.1083 0.0151 -0.0044
					-0.0237 0.2736 0.0474 -0.0200 0.0016
					-0.7973 -0.0963 0.0530 0.0000 0.0000
					0.0000 0.0000 0.0057 0.0013 0.0709

	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.4708	-0.0368	0.1251	0.0126
	-0.0138	-0.0151	0.0000	0.0000	0.0985
	-0.0233	-0.0493	0.0239	0.0000	0.0000
	0.0000	0.0000	-0.0332	0.0115	0.0567
	-0.0135				
99. (0.00373) RY (3) C 2	s(28.23%)	p 0.10(2.89%)	d 0.96(26.96%)		
	f 1.49(41.93%)				
	0.0000	0.0085	0.5266	0.0587	-0.0378
	-0.0068	0.0641	-0.0055	0.0353	0.0192
	0.1515	-0.0075	-0.0076	0.0000	0.0000
	0.0000	0.0000	0.3258	-0.0091	0.1024
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.1022	0.1532	-0.0475	-0.3391
	0.0393	-0.0143	0.0000	0.0000	-0.0548
	0.0101	-0.0622	0.0094	0.0000	0.0000
	0.0000	0.0000	0.4807	-0.1048	0.3970
	-0.1119				
100. (0.00273) RY (4) C 2	s(0.00%)	p 1.00(20.53%)	d 3.45(70.85%)		
	f 0.42(8.62%)				
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	-0.0154	0.2943
	-0.3439	0.0143	0.0000	0.0000	0.0000
	0.0676	-0.0783	0.0027	-0.7373	0.3534
	0.1710	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	-0.0771	0.0126	0.0000
	0.0000	0.0000	0.0000	0.1959	-0.0754
	0.1840	-0.0463	0.0000	0.0000	0.0000
	0.0000				
101. (0.00203) RY (5) C 2	s(0.00%)	p 1.00(65.39%)	d 0.41(27.10%)		
	f 0.11(7.51%)				
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0143	0.8081
	-0.0074	0.0267	0.0000	0.0000	0.0000
	0.3459	-0.2814	0.0120	0.2167	-0.1539
	-0.0373	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.1135	-0.0254	0.0000
	0.0000	0.0000	0.0000	-0.0722	-0.0279
	-0.2186	0.0879	0.0000	0.0000	0.0000
	0.0000				
102. (0.00199) RY (6) C 2	s(29.57%)	p 0.69(20.54%)	d 0.41(12.11%)		
	f 1.28(37.77%)				
	0.0000	0.0148	0.5351	-0.0947	0.0126
	-0.0122	0.3579	0.2489	0.1115	0.0090
	0.0471	-0.0202	0.0097	0.0000	0.0000
	0.0000	0.0000	0.0714	0.0554	-0.0635
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.1833	0.1149	-0.1444	-0.1763
	-0.0332	-0.0954	0.0000	0.0000	-0.0269
	-0.0108	0.0879	-0.0066	0.0000	0.0000
	0.0000	0.0000	-0.4323	0.0583	-0.4192
	0.0554				
103. (0.00079) RY (7) C 2	s(1.84%)	p 8.03(14.76%)	d41.10(75.58%)		
	f 4.25(7.82%)				
	0.0000	0.0106	-0.0918	-0.0102	0.0987
	-0.0023	0.0261	-0.1859	-0.1821	0.0130
	0.2477	0.1312	-0.0216	0.0000	0.0000
	0.0000	0.0000	0.3791	-0.0884	-0.3898
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.5890	-0.2388	-0.1685	-0.1317
	0.0306	0.0416	0.0000	0.0000	-0.0581

		-0.0117	0.0271	0.0048	0.0000	0.0000
		0.0000	0.0000	-0.1074	-0.0432	-0.2036
		0.1380				
104.	(0.00053) RY (8) C 2	s(0.00%)	p 1.00(21.08%)	d 2.56(53.97%)		
		f 1.18(24.94%)				
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	-0.0049	0.4442
		0.0154	0.1153	0.0000	0.0000	0.0000
		-0.3678	0.6144	0.0661	0.0684	-0.1314
		0.0253	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	-0.0887	0.0105	0.0000
		0.0000	0.0000	0.0000	-0.2011	0.1317
		0.4263	-0.0447	0.0000	0.0000	0.0000
		0.0000				
105.	(0.00047) RY (9) C 2	s(30.62%)	p 0.77(23.63%)	d 1.25(38.28%)		
		f 0.24(7.47%)				
		0.0000	-0.0123	0.4708	-0.2900	0.0167
		0.0012	-0.3022	-0.1220	-0.1803	-0.0100
		0.0476	0.2854	-0.1173	0.0000	0.0000
		0.0000	0.0000	-0.3073	-0.0608	-0.1358
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0958	-0.2038	0.3834	0.1231
		-0.1110	-0.2028	0.0000	0.0000	0.2280
		0.0230	0.1174	-0.0371	0.0000	0.0000
		0.0000	0.0000	0.0308	0.0755	0.0016
		0.0190				
106.	(0.00032) RY (10) C 2	s(16.26%)	p 0.69(11.21%)	d 3.06(49.69%)		
		f 1.40(22.84%)				
		0.0000	0.0091	0.0708	0.3961	0.0252
		0.0022	-0.2105	0.1783	-0.0731	0.0092
		-0.0702	0.1261	-0.0988	0.0000	0.0000
		0.0000	0.0000	-0.3235	-0.1251	-0.1984
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0128	-0.0725	-0.1754	-0.3834
		0.2399	0.3107	0.0000	0.0000	0.1243
		-0.0704	0.0826	0.0064	0.0000	0.0000
		0.0000	0.0000	-0.2757	0.1572	0.2488
		-0.1961				
107.	(0.00028) RY (11) C 2	s(2.61%)	p13.96(36.44%)	d19.14(49.96%)		
		f 4.21(10.98%)				
		0.0000	-0.0088	0.1214	0.0231	0.1037
		0.0054	-0.0085	-0.3279	0.0238	-0.0004
		-0.2208	-0.3928	0.2307	0.0000	0.0000
		0.0000	0.0000	-0.1750	-0.1147	-0.5525
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	-0.2765	-0.0901	-0.2416	-0.0142
		-0.0130	-0.0853	0.0000	0.0000	-0.0488
		-0.0395	0.1273	-0.0089	0.0000	0.0000
		0.0000	0.0000	0.2782	-0.0756	-0.0585
		0.0552				
108.	(0.00023) RY (12) C 2	s(0.00%)	p 1.00(3.69%)	d19.12(70.47%)		
		f 7.01(25.85%)				
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	-0.0006	0.0016
		-0.1851	-0.0509	0.0000	0.0000	0.0000
		0.4269	0.3168	-0.2223	0.4563	0.3978
		-0.0787	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	-0.1191	0.0217	0.0000
		0.0000	0.0000	0.0000	0.4274	-0.0793
		0.2087	-0.1063	0.0000	0.0000	0.0000
		0.0000				

109.	(0.00014)	RY	(13)	C	2	s(7.97%)p 3.86(30.77%)d 6.21(49.49%) f 1.48(11.77%) 0.0000 -0.0125 0.0887 0.2678 -0.0036 -0.0177 -0.1846 -0.0961 0.4440 0.0011 -0.0099 0.2396 0.0971 0.0000 0.0000 0.0000 0.0000 -0.0886 -0.0935 -0.2519 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.2269 0.5456 0.1186 0.2226 -0.0445 -0.0029 0.0000 0.0000 -0.2373 0.1002 -0.1412 -0.1162 0.0000 0.0000 0.0000 0.0000 -0.0226 0.0230 -0.1191 -0.0517
110.	(0.00006)	RY	(14)	C	2	s(1.53%)p10.53(16.13%)d35.70(54.69%) f18.04(27.64%)
111.	(0.00004)	RY	(15)	C	2	s(3.81%)p10.02(38.24%)d 8.19(31.25%) f 7.00(26.70%)
112.	(0.00001)	RY	(16)	C	2	s(29.77%)p 1.07(31.88%)d 0.59(17.70%) f 0.69(20.65%)
113.	(0.00001)	RY	(17)	C	2	s(7.98%)p 3.58(28.58%)d 5.58(44.48%) f 2.38(18.96%)
114.	(0.00001)	RY	(18)	C	2	s(5.58%)p 2.62(14.60%)d 8.80(49.06%) f 5.51(30.76%)
115.	(0.00000)	RY	(19)	C	2	s(2.59%)p 6.17(15.97%)d24.79(64.19%) f 6.66(17.25%)
116.	(0.00000)	RY	(20)	C	2	s(16.84%)p 0.38(6.46%)d 1.46(24.59%) f 3.09(52.11%)
117.	(0.00000)	RY	(21)	C	2	s(2.36%)p 5.08(11.98%)d 4.26(10.05%) f32.05(75.62%)
118.	(0.00000)	RY	(22)	C	2	s(0.00%)p 1.00(26.08%)d 2.63(68.50%) f 0.21(5.42%)
119.	(0.00000)	RY	(23)	C	2	s(30.57%)p 0.64(19.55%)d 0.94(28.71%) f 0.69(21.17%)
120.	(0.00000)	RY	(24)	C	2	s(0.00%)p 1.00(40.42%)d 1.14(46.21%) f 0.33(13.36%)
121.	(0.00000)	RY	(25)	C	2	s(0.00%)p 1.00(3.66%)d15.54(56.97%) f10.74(39.37%)
122.	(0.00000)	RY	(26)	C	2	s(0.00%)p 1.00(36.69%)d 1.07(39.11%) f 0.66(24.19%)
123.	(0.00000)	RY	(27)	C	2	s(13.49%)p 1.73(23.31%)d 1.87(25.17%) f 2.82(38.04%)
124.	(0.00000)	RY	(28)	C	2	s(13.23%)p 0.93(12.26%)d 3.71(49.10%) f 1.92(25.41%)
125.	(0.00000)	RY	(29)	C	2	s(0.00%)p 1.00(6.52%)d 4.74(30.90%) f 9.59(62.58%)
126.	(0.00000)	RY	(30)	C	2	s(0.00%)p 1.00(0.91%)d 1.84(1.68%) f99.99(97.41%)
127.	(0.00000)	RY	(31)	C	2	s(2.41%)p 3.44(8.32%)d 9.45(22.82%) f27.51(66.44%)
128.	(0.00000)	RY	(32)	C	2	s(0.92%)p17.82(16.36%)d21.87(20.07%) f68.25(62.65%)
129.	(0.00000)	RY	(33)	C	2	s(31.39%)p 0.56(17.53%)d 0.61(19.17%) f 1.02(31.91%)
130.	(0.00000)	RY	(34)	C	2	s(7.08%)p 4.12(29.20%)d 5.95(42.14%) f 3.05(21.58%)
131.	(0.00000)	RY	(35)	C	2	s(0.00%)p 1.00(6.58%)d 6.23(40.95%) f 7.98(52.47%)
132.	(0.00000)	RY	(36)	C	2	s(0.00%)p 1.00(1.38%)d 5.58(7.68%) f66.09(90.94%)
133.	(0.00000)	RY	(37)	C	2	s(0.00%)p 1.00(24.29%)d 1.72(41.82%) f 1.39(33.88%)
134.	(0.00000)	RY	(38)	C	2	s(0.00%)p 1.00(5.03%)d 1.47(7.40%) f17.42(87.58%)
135.	(0.00000)	RY	(39)	C	2	s(1.69%)p 5.48(9.24%)d 1.60(2.70%)

					f51.25(86.37%)
136. (0.00000) RY (40) C 2	s(0.00%)	p 1.00(37.83%)	d 0.96(36.33%)		f 0.68(25.84%)
137. (0.00000) RY (41) C 2	s(10.27%)	p 3.15(32.36%)	d 2.61(26.81%)		f 2.98(30.56%)
138. (0.00142) RY (1) C 3	s(0.54%)	p63.02(33.86%)	d37.62(20.21%)		f84.46(45.38%)
				0.0000	-0.0008 0.0642 0.0354 -0.0008
				0.0051	0.0128 0.0381 0.0174 -0.5778
				0.0529	0.0000 0.0000 0.0000 -0.2286
				0.1237	-0.0483 0.0000 0.0000 0.0000
				0.0000	0.0000 0.0000 -0.1900 0.1940
				-0.2085	-0.1051 0.0613 0.0157 0.0000
				0.0000	-0.0227 -0.0058 -0.1023 -0.0478
				0.0000	0.0000 0.0000 0.0000 -0.4853
				-0.1930	-0.3775 -0.1591
139. (0.00120) RY (2) C 3	s(4.45%)	p14.71(65.48%)	d 4.03(17.92%)		f 2.73(12.16%)
				0.0000	-0.0079 0.1293 0.1457 0.0806
				0.0009	0.4968 0.0398 -0.0190 0.6371
				-0.0149	0.0000 0.0000 0.0000 0.0440
				-0.1022	-0.0301 0.0000 0.0000 0.0000
				0.0000	0.0000 0.0000 -0.1164 0.1614
				-0.2952	-0.1541 0.1086 0.0598 0.0000
				0.0000	-0.0025 0.0084 -0.0605 -0.0149
				0.0000	0.0000 0.0000 0.0000 -0.2697
				-0.0402	-0.1972 -0.0658
140. (0.00077) RY (3) C 3	s(27.19%)	p 0.47(12.88%)	d 1.59(43.12%)		f 0.62(16.81%)
				0.0000	0.0063 0.5118 -0.0862 0.0499
				-0.0101	-0.2323 -0.1211 -0.0117 0.2435
				-0.0250	0.0000 0.0000 0.0000 -0.1651
				0.1619	-0.3392 0.0000 0.0000 0.0000
				0.0000	0.0000 0.0000 0.2585 -0.0477
				0.3987	0.1778 -0.0262 0.0483 0.0000
				0.0000	-0.1191 -0.0585 0.0563 0.0437
				0.0000	0.0000 0.0000 0.0000 -0.1139
				-0.0476	-0.3420 -0.1148
141. (0.00050) RY (4) C 3	s(19.78%)	p 2.75(54.33%)	d 0.40(7.91%)		f 0.91(17.98%)
				0.0000	0.0027 0.3854 -0.1254 -0.1832
				0.0064	0.6472 0.0294 0.0019 -0.3168
				0.1520	0.0000 0.0000 0.0000 0.0476
				-0.0259	0.1140 0.0000 0.0000 0.0000
				0.0000	0.0000 0.0000 -0.0280 0.0379
				0.1508	0.1490 -0.0535 0.1147 0.0000
				0.0000	-0.0513 -0.0389 0.0456 0.0533
				0.0000	0.0000 0.0000 0.0000 0.3260
				0.2298	-0.0865 -0.0645
142. (0.00040) RY (5) C 3	s(7.96%)	p 1.20(9.52%)	d 9.18(73.10%)		f 1.18(9.41%)
				0.0000	-0.0104 0.0520 0.2445 0.1305
				0.0045	0.0274 -0.2554 0.0505 0.0062
				-0.1631	0.0000 0.0000 0.0000 -0.3994
				-0.0912	-0.1421 0.0000 0.0000 0.0000
				0.0000	0.0000 0.0000 -0.5811 0.1426
				0.3658	-0.1921 0.1195 0.0084 0.0000
				0.0000	0.0475 0.0072 0.1296 -0.0155
				0.0000	0.0000 0.0000 0.0000 0.1016
				0.1058	0.2301 -0.0171
143. (0.00036) RY (6) C 3	s(0.00%)	p 1.00(0.39%)	d99.99(70.01%)		f75.37(29.60%)
				0.0000	0.0000 0.0000 0.0000 0.0000

	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.0086	0.0045	-0.0619	0.0000
	0.0000	0.0000	0.2166	0.1257	-0.0578
	0.5593	0.5364	-0.1829	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	-0.0338
	0.0207	0.0000	0.0000	0.0000	0.0000
	-0.2163	-0.1898	-0.3794	-0.2602	0.0000
	0.0000	0.0000	0.0000		
144. (0.00028) RY (7) C 3	s(25.59%)p	1.01(25.79%)d	1.57(40.19%)		
	f	0.33(8.43%)			
	0.0000	-0.0047	0.5045	0.0121	0.0336
	-0.0108	-0.3392	0.3644	-0.0122	-0.0416
	-0.0898	0.0000	0.0000	0.0000	0.3183
	-0.2182	0.1285	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	-0.1512	0.3484
	-0.0499	-0.2878	0.0392	-0.0732	0.0000
	0.0000	-0.1408	-0.0551	-0.0165	-0.0089
	0.0000	0.0000	0.0000	0.0000	0.1673
	-0.0856	0.0249	0.1586		
145. (0.00015) RY (8) C 3	s(0.00%)p	1.00(31.41%)d	1.64(51.63%)		
	f	0.54(16.96%)			
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.0254	-0.3354	0.4483	0.0000
	0.0000	0.0000	0.6175	0.1677	0.2453
	-0.2067	0.0130	-0.0616	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	-0.2224
	0.0913	0.0000	0.0000	0.0000	0.0000
	0.2960	0.0054	-0.1460	0.0535	0.0000
	0.0000	0.0000	0.0000		
146. (0.00013) RY (9) C 3	s(19.73%)p	0.15(2.94%)d	2.93(57.84%)		
	f	0.99(19.49%)			
	0.0000	0.0147	-0.2171	0.3370	-0.1908
	-0.0004	-0.1518	-0.0122	-0.0030	0.0785
	0.0033	0.0000	0.0000	0.0000	0.3588
	-0.0335	0.0062	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	-0.3591	0.1870
	0.1158	0.4340	-0.2694	-0.1013	0.0000
	0.0000	0.0045	-0.0701	-0.0310	0.0290
	0.0000	0.0000	0.0000	0.0000	0.0513
	0.1301	-0.3592	-0.1990		
147. (0.00006) RY (10) C 3	s(0.00%)p	1.00(42.13%)d	0.19(8.00%)		
	f	1.18(49.86%)			
148. (0.00006) RY (11) C 3	s(37.08%)p	0.16(6.10%)d	1.43(53.06%)		
	f	0.10(3.76%)			
149. (0.00003) RY (12) C 3	s(0.00%)p	1.00(4.16%)d	20.57(85.65%)		
	f	2.45(10.18%)			
150. (0.00002) RY (13) C 3	s(8.64%)p	1.28(11.05%)d	4.43(38.24%)		
	f	4.87(42.07%)			
151. (0.00001) RY (14) C 3	s(23.04%)p	0.29(6.76%)d	2.34(53.81%)		
	f	0.71(16.39%)			
152. (0.00001) RY (15) C 3	s(13.29%)p	0.39(5.20%)d	2.16(28.75%)		
	f	3.97(52.76%)			
153. (0.00000) RY (16) C 3	s(7.44%)p	2.79(20.77%)d	6.82(50.72%)		
	f	2.83(21.08%)			
154. (0.00000) RY (17) C 3	s(0.92%)p	8.96(8.20%)d	56.77(51.95%)		
	f	42.54(38.93%)			
155. (0.00000) RY (18) C 3	s(17.57%)p	0.50(8.72%)d	2.94(51.71%)		
	f	1.25(21.99%)			
156. (0.00000) RY (19) C 3	s(14.20%)p	0.38(5.35%)d	3.84(54.47%)		
	f	1.83(25.99%)			
157. (0.00000) RY (20) C 3	s(0.00%)p	1.00(4.54%)d	20.21(91.71%)		
	f	0.83(3.76%)			

158. (0.00000) RY (21) C 3 s(2.79%)p 4.63(12.91%)d14.51(40.50%)
f15.70(43.80%)

159. (0.00000) RY (22) C 3 s(0.00%)p 1.00(1.35%)d72.38(97.79%)
f 0.63(0.86%)

160. (0.00000) RY (23) C 3 s(0.00%)p 1.00(27.05%)d 2.10(56.86%)
f 0.60(16.09%)

161. (0.00000) RY (24) C 3 s(0.00%)p 1.00(39.16%)d 0.24(9.46%)
f 1.31(51.38%)

162. (0.00000) RY (25) C 3 s(2.70%)p 6.09(16.44%)d 8.49(22.94%)
f21.45(57.92%)

163. (0.00000) RY (26) C 3 s(3.16%)p 8.21(25.98%)d14.62(46.25%)
f 7.78(24.61%)

164. (0.00000) RY (27) C 3 s(39.34%)p 0.15(5.83%)d 0.74(28.94%)
f 0.66(25.89%)

165. (0.00000) RY (28) C 3 s(0.00%)p 1.00(4.84%)d 0.07(0.36%)
f19.58(94.80%)

166. (0.00000) RY (29) C 3 s(6.47%)p 0.03(0.20%)d 3.40(22.00%)
f11.03(71.34%)

167. (0.00000) RY (30) C 3 s(2.52%)p 5.17(13.01%)d 8.67(21.84%)
f24.86(62.63%)

168. (0.00000) RY (31) C 3 s(5.96%)p 2.90(17.29%)d 3.80(22.61%)
f 9.09(54.14%)

169. (0.00000) RY (32) C 3 s(0.00%)p 1.00(10.59%)d 1.62(17.20%)
f 6.82(72.21%)

170. (0.00000) RY (33) C 3 s(0.00%)p 1.00(3.95%)d 2.60(10.27%)
f21.70(85.78%)

171. (0.00000) RY (34) C 3 s(0.00%)p 1.00(2.14%)d10.46(22.43%)
f35.18(75.43%)

172. (0.00000) RY (35) C 3 s(0.00%)p 1.00(4.00%)d 1.99(7.98%)
f21.98(88.01%)

173. (0.00000) RY (36) C 3 s(2.20%)p13.87(30.52%)d12.03(26.47%)
f18.54(40.81%)

174. (0.00000) RY (37) C 3 s(0.00%)p 1.00(24.47%)d 2.88(70.56%)
f 0.20(4.96%)

175. (0.00000) RY (38) C 3 s(7.62%)p 0.21(1.59%)d 3.26(24.81%)
f 8.66(65.97%)

176. (0.00814) RY (1) C 4 s(0.38%)p99.99(84.87%)d34.68(13.06%)
f 4.50(1.70%)

0.0000 0.0156 0.0309 0.0498 0.0097
-0.0162 0.5432 -0.0471 -0.0415 -0.0355
-0.7382 0.0522 -0.0205 0.0000 0.0000
0.0000 0.0000 -0.0428 -0.0003 0.0428
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.2336 -0.2468 0.0834 -0.0639
0.0170 -0.0101 0.0000 0.0000 0.0330
0.0164 -0.0188 -0.0061 0.0000 0.0000
0.0000 0.0000 -0.1107 -0.0395 -0.0304
-0.0217

177. (0.00285) RY (2) C 4 s(11.30%)p 5.88(66.40%)d 0.87(9.82%)
f 1.10(12.48%)

0.0000 0.0061 0.3357 -0.0031 -0.0162
-0.0422 0.5996 0.0619 -0.0370 -0.0143
0.5390 0.0826 0.0017 0.0000 0.0000
0.0000 0.0000 -0.1761 0.1271 -0.1108
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0917 -0.0236 -0.0559 0.1400
-0.0810 -0.0222 0.0000 0.0000 0.0493
0.0378 0.0027 0.0098 0.0000 0.0000
0.0000 0.0000 -0.2481 -0.1558 -0.1594
-0.0982

178. (0.00146) RY (3) C 4 s(0.00%)p 1.00(73.53%)d 0.30(22.39%)
f 0.06(4.08%)

0.0000 0.0000 0.0000 0.0000 0.0000

	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	-0.0215	0.8029
	-0.2975	0.0403	0.0000	0.0000	0.0000
	0.0974	-0.3526	0.0212	0.0364	-0.2830
	-0.0906	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	-0.0610	-0.0358	0.0000
	0.0000	0.0000	0.0000	-0.0945	-0.0168
	-0.1262	-0.1033	0.0000	0.0000	0.0000
	0.0000				
179. (0.00117) RY (4) C 4	s(36.99%)	p 0.19(7.02%)	d 0.64(23.58%)		
	f 0.88(32.42%)				
	0.0000	0.0111	0.6066	-0.0088	-0.0411
	-0.0011	0.1583	0.1589	0.0330	-0.0352
	-0.1120	0.0642	-0.0300	0.0000	0.0000
	0.0000	0.0000	0.0759	-0.1188	0.2169
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.2795	0.2286	0.0784	0.1274
	-0.1152	-0.0530	0.0000	0.0000	-0.0959
	-0.0138	-0.1083	-0.0627	0.0000	0.0000
	0.0000	0.0000	0.4002	0.2047	0.2977
	0.0919				
180. (0.00049) RY (5) C 4	s(30.15%)	p 1.09(32.95%)	d 0.61(18.48%)		
	f 0.61(18.43%)				
	0.0000	-0.0043	0.5477	-0.0317	0.0211
	0.0108	-0.4184	-0.3373	-0.0919	-0.0143
	-0.1753	0.0341	0.0026	0.0000	0.0000
	0.0000	0.0000	-0.2298	0.2785	-0.0466
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0443	0.0329	0.1603	-0.0886
	-0.0423	-0.1177	0.0000	0.0000	-0.0122
	-0.0523	-0.0164	-0.0236	0.0000	0.0000
	0.0000	0.0000	-0.1676	0.0223	-0.3557
	-0.1595				
181. (0.00035) RY (6) C 4	s(0.00%)	p 1.00(23.73%)	d 2.79(66.31%)		
	f 0.42(9.96%)				
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0154	0.4360
	0.1814	0.1187	0.0000	0.0000	0.0000
	0.2808	0.6256	-0.0359	-0.3444	0.2665
	0.0427	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0521	0.0329	0.0000
	0.0000	0.0000	0.0000	-0.2027	-0.1046
	0.0947	0.1867	0.0000	0.0000	0.0000
	0.0000				
182. (0.00012) RY (7) C 4	s(7.21%)	p 1.19(8.58%)	d 9.39(67.71%)		
	f 2.29(16.49%)				
	0.0000	0.0106	0.1584	0.2149	-0.0263
	-0.0082	-0.2487	0.0524	0.0487	0.0031
	0.0734	-0.0386	0.1092	0.0000	0.0000
	0.0000	0.0000	0.0732	-0.0975	0.1163
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.6074	-0.1953	0.2198	0.4172
	-0.1033	0.0928	0.0000	0.0000	0.0569
	0.0613	-0.1257	-0.0065	0.0000	0.0000
	0.0000	0.0000	0.0181	-0.2228	0.1689
	0.2522				
183. (0.00004) RY (8) C 4	s(7.25%)	p 2.03(14.69%)	d 9.17(66.53%)		
	f 1.59(11.52%)				
184. (0.00004) RY (9) C 4	s(30.68%)	p 0.61(18.61%)	d 1.31(40.06%)		
	f 0.35(10.65%)				
185. (0.00002) RY (10) C 4	s(4.19%)	p 5.34(22.36%)	d10.36(43.39%)		
	f 7.17(30.06%)				

186.	(0.00001)	RY (11)	C	4	s(0.00%)	p 1.00(15.53%)	d 5.18(80.40%)
					f 0.26(4.07%)		
187.	(0.00001)	RY (12)	C	4	s(9.10%)	p 1.61(14.63%)	d 2.99(27.18%)
					f 5.39(49.08%)		
188.	(0.00000)	RY (13)	C	4	s(3.94%)	p 2.63(10.37%)	d12.33(48.55%)
					f 9.44(37.14%)		
189.	(0.00000)	RY (14)	C	4	s(18.37%)	p 0.39(7.20%)	d 1.76(32.37%)
					f 2.29(42.06%)		
190.	(0.00000)	RY (15)	C	4	s(0.00%)	p 1.00(57.24%)	d 0.18(10.47%)
					f 0.56(32.29%)		
191.	(0.00000)	RY (16)	C	4	s(7.97%)	p 1.53(12.19%)	d 4.20(33.46%)
					f 5.81(46.37%)		
192.	(0.00000)	RY (17)	C	4	s(0.00%)	p 1.00(52.79%)	d 0.41(21.58%)
					f 0.49(25.64%)		
193.	(0.00000)	RY (18)	C	4	s(18.19%)	p 1.85(33.74%)	d 1.13(20.48%)
					f 1.52(27.59%)		
194.	(0.00000)	RY (19)	C	4	s(0.00%)	p 1.00(9.75%)	d 7.94(77.46%)
					f 1.31(12.79%)		
195.	(0.00000)	RY (20)	C	4	s(0.00%)	p 1.00(3.93%)	d21.28(83.63%)
					f 3.17(12.44%)		
196.	(0.00000)	RY (21)	C	4	s(0.00%)	p 1.00(4.19%)	d16.31(68.33%)
					f 6.56(27.48%)		
197.	(0.00000)	RY (22)	C	4	s(0.00%)	p 1.00(6.44%)	d 6.74(43.37%)
					f 7.80(50.19%)		
198.	(0.00000)	RY (23)	C	4	s(4.61%)	p 1.06(4.88%)	d 6.04(27.84%)
					f13.59(62.67%)		
199.	(0.00000)	RY (24)	C	4	s(4.62%)	p 1.53(7.08%)	d12.04(55.67%)
					f 7.06(32.62%)		
200.	(0.00000)	RY (25)	C	4	s(12.05%)	p 1.84(22.23%)	d 1.76(21.23%)
					f 3.69(44.49%)		
201.	(0.00000)	RY (26)	C	4	s(4.10%)	p 7.81(32.04%)	d 6.70(27.48%)
					f 8.87(36.38%)		
202.	(0.00000)	RY (27)	C	4	s(10.73%)	p 1.99(21.35%)	d 5.14(55.22%)
					f 1.18(12.70%)		
203.	(0.00000)	RY (28)	C	4	s(3.52%)	p 8.06(28.34%)	d13.60(47.83%)
					f 5.77(20.31%)		
204.	(0.00000)	RY (29)	C	4	s(0.00%)	p 1.00(5.48%)	d 4.94(27.07%)
					f12.31(67.45%)		
205.	(0.00000)	RY (30)	C	4	s(0.00%)	p 1.00(4.54%)	d 2.15(9.77%)
					f18.86(85.69%)		
206.	(0.00000)	RY (31)	C	4	s(12.06%)	p 2.46(29.63%)	d 2.19(26.44%)
					f 2.64(31.87%)		
207.	(0.00000)	RY (32)	C	4	s(6.20%)	p 6.51(40.35%)	d 7.08(43.93%)
					f 1.53(9.52%)		
208.	(0.00000)	RY (33)	C	4	s(6.87%)	p 2.94(20.21%)	d 3.80(26.08%)
					f 6.82(46.84%)		
209.	(0.00000)	RY (34)	C	4	s(7.68%)	p 1.39(10.67%)	d 2.34(17.95%)
					f 8.30(63.70%)		
210.	(0.00000)	RY (35)	C	4	s(0.00%)	p 1.00(28.07%)	d 0.67(18.81%)
					f 1.89(53.12%)		
211.	(0.00000)	RY (36)	C	4	s(0.00%)	p 1.00(3.61%)	d 0.73(2.65%)
					f25.97(93.74%)		
212.	(0.00000)	RY (37)	C	4	s(0.00%)	p 1.00(5.84%)	d 4.45(25.98%)
					f11.68(68.18%)		
213.	(0.00000)	RY (38)	C	4	s(0.00%)	p 1.00(5.51%)	d 7.56(41.66%)
					f 9.58(52.83%)		
214.	(0.00000)	RY (39)	C	4	s(8.07%)	p 2.60(20.94%)	d 2.26(18.20%)
					f 6.54(52.79%)		
215.	(0.00000)	RY (40)	C	4	s(30.35%)	p 0.74(22.54%)	d 0.49(14.91%)
					f 1.06(32.20%)		
216.	(0.00000)	RY (41)	C	4	s(3.56%)	p 1.88(6.70%)	d20.23(72.01%)
					f 4.98(17.73%)		
217.	(0.00492)	RY (1)	C	5	s(2.51%)	p33.76(84.79%)	d 4.87(12.23%)

					f 0.18(0.46%)
					0.0000 -0.0105 0.1534 0.0041 0.0383
					0.0128 0.6745 0.0125 -0.0317 0.0135
					0.6256 -0.0019 -0.0036 0.0000 0.0000
					0.0000 0.0000 0.0535 -0.2445 -0.1239
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0259 -0.0322 0.0026 0.1460
					-0.1398 -0.0421 0.0000 0.0000 0.0076
					0.0081 0.0105 0.0143 0.0000 0.0000
					0.0000 0.0000 0.0216 0.0312 -0.0312
					-0.0422
218. (0.00148) RY (2) C 5					s(0.98%)p47.84(46.81%)d10.12(9.90%)
					f43.25(42.32%)
					0.0000 0.0009 0.0973 -0.0177 0.0020
					0.0231 -0.4798 -0.0603 0.0178 -0.0270
					0.4679 0.1160 -0.0151 0.0000 0.0000
					0.0000 0.0000 -0.0072 0.0084 0.0192
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.1723 -0.2360 -0.1103 0.0082
					-0.0213 -0.0206 0.0000 0.0000 -0.1047
					-0.0724 0.0894 0.0615 0.0000 0.0000
					0.0000 0.0000 -0.3818 -0.2498 -0.3644
					-0.2328
219. (0.00095) RY (3) C 5					s(0.00%)p 1.00(88.11%)d 0.11(9.41%)
					f 0.03(2.48%)
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0068 0.8724
					-0.3456 0.0226 0.0000 0.0000 0.0000
					-0.2094 -0.0605 0.1045 -0.1852 -0.0100
					0.0360 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 -0.0228 -0.0108 0.0000
					0.0000 0.0000 0.0000 0.0050 -0.0051
					0.1513 0.0343 0.0000 0.0000 0.0000
					0.0000
220. (0.00071) RY (4) C 5					s(0.43%)p99.99(50.22%)d32.93(14.27%)
					f80.92(35.08%)
					0.0000 0.0002 0.0640 -0.0028 -0.0154
					0.0126 -0.4749 -0.0603 -0.0929 -0.0155
					0.5030 0.0492 0.0924 0.0000 0.0000
					0.0000 0.0000 0.0435 -0.0678 0.0353
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 -0.1462 0.2859 0.1783 -0.0072
					0.0031 -0.0072 0.0000 0.0000 0.0283
					-0.0359 -0.0355 0.0342 0.0000 0.0000
					0.0000 0.0000 0.3809 0.1482 0.3919
					0.1601
221. (0.00044) RY (5) C 5					s(0.00%)p 1.00(7.30%)d10.19(74.38%)
					f 2.51(18.32%)
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0059 -0.0963
					-0.2498 0.0353 0.0000 0.0000 0.0000
					-0.5019 -0.2469 0.0254 0.6500 0.0558
					0.0684 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 -0.0337 -0.0150 0.0000
					0.0000 0.0000 0.0000 -0.2768 -0.3195
					-0.0511 -0.0242 0.0000 0.0000 0.0000
					0.0000
222. (0.00039) RY (6) C 5					s(42.44%)p 0.09(3.89%)d 1.01(42.80%)
					f 0.26(10.87%)
					0.0000 0.0003 0.6433 -0.0839 -0.0592
					-0.0187 -0.0093 0.1043 0.0400 -0.0082

						-0.1526	-0.0498	0.0104	0.0000	0.0000
						0.0000	0.0000	0.2396	-0.3988	0.3606
						0.0000	0.0000	0.0000	0.0000	0.0000
						0.0000	-0.0804	0.0005	0.0012	-0.2172
						0.0795	-0.1469	0.0000	0.0000	-0.0065
						-0.0068	-0.0460	-0.0531	0.0000	0.0000
						0.0000	0.0000	-0.1945	-0.1656	0.1331
						0.1439				
223.	(0.00017)	RY (7)	C	5	s(28.82%)	p 0.14(4.14%)	d 2.18(62.76%)			
						f 0.15(4.29%)				
						0.0000	0.0074	0.4667	-0.2548	0.0734
						-0.0079	0.0469	-0.0217	-0.0017	0.0023
						-0.0510	0.1896	0.0079	0.0000	0.0000
						0.0000	0.0000	-0.4505	0.4532	0.1893
						0.0000	0.0000	0.0000	0.0000	0.0000
						0.0000	-0.1098	0.0188	0.0385	0.2861
						-0.2841	-0.0831	0.0000	0.0000	-0.1323
						-0.0496	-0.0650	-0.0271	0.0000	0.0000
						0.0000	0.0000	0.0461	0.0998	0.0130
						-0.0753				
224.	(0.00010)	RY (8)	C	5	s(6.70%)	p 6.69(44.80%)	d 5.67(37.98%)			
						f 1.57(10.52%)				
225.	(0.00004)	RY (9)	C	5	s(6.84%)	p 3.09(21.14%)	d 6.74(46.07%)			
						f 3.80(25.95%)				
226.	(0.00001)	RY (10)	C	5	s(0.00%)	p 1.00(14.70%)	d 5.04(74.02%)			
						f 0.77(11.27%)				
227.	(0.00001)	RY (11)	C	5	s(32.07%)	p 0.47(14.92%)	d 1.00(32.08%)			
						f 0.65(20.93%)				
228.	(0.00001)	RY (12)	C	5	s(4.30%)	p11.18(48.02%)	d 4.63(19.89%)			
						f 6.47(27.80%)				
229.	(0.00000)	RY (13)	C	5	s(5.96%)	p 3.09(18.41%)	d 6.24(37.19%)			
						f 6.46(38.44%)				
230.	(0.00000)	RY (14)	C	5	s(23.04%)	p 0.22(5.07%)	d 1.57(36.10%)			
						f 1.55(35.80%)				
231.	(0.00000)	RY (15)	C	5	s(0.00%)	p 1.00(18.28%)	d 4.04(73.83%)			
						f 0.43(7.89%)				
232.	(0.00000)	RY (16)	C	5	s(2.66%)	p 2.32(6.17%)	d21.94(58.31%)			
						f12.37(32.86%)				
233.	(0.00000)	RY (17)	C	5	s(1.40%)	p12.68(17.76%)	d17.39(24.35%)			
						f40.33(56.48%)				
234.	(0.00000)	RY (18)	C	5	s(0.00%)	p 1.00(6.03%)	d 9.03(54.45%)			
						f 6.56(39.52%)				
235.	(0.00000)	RY (19)	C	5	s(0.00%)	p 1.00(45.63%)	d 0.80(36.35%)			
						f 0.39(18.01%)				
236.	(0.00000)	RY (20)	C	5	s(0.00%)	p 1.00(55.46%)	d 0.69(38.50%)			
						f 0.11(6.04%)				
237.	(0.00000)	RY (21)	C	5	s(0.00%)	p 1.00(39.92%)	d 1.11(44.22%)			
						f 0.40(15.86%)				
238.	(0.00000)	RY (22)	C	5	s(0.00%)	p 1.00(8.20%)	d 6.57(53.91%)			
						f 4.62(37.89%)				
239.	(0.00000)	RY (23)	C	5	s(0.52%)	p30.10(15.67%)	d50.49(26.27%)			
						f99.99(57.54%)				
240.	(0.00000)	RY (24)	C	5	s(24.81%)	p 0.69(17.04%)	d 1.13(28.06%)			
						f 1.21(30.09%)				
241.	(0.00000)	RY (25)	C	5	s(0.70%)	p12.18(8.51%)	d60.71(42.40%)			
						f69.29(48.39%)				
242.	(0.00000)	RY (26)	C	5	s(2.23%)	p 3.22(7.17%)	d34.88(77.67%)			
						f 5.81(12.94%)				
243.	(0.00000)	RY (27)	C	5	s(15.20%)	p 1.12(17.01%)	d 2.69(40.88%)			
						f 1.77(26.90%)				
244.	(0.00000)	RY (28)	C	5	s(0.00%)	p 1.00(1.49%)	d55.92(83.50%)			
						f10.05(15.01%)				
245.	(0.00000)	RY (29)	C	5	s(0.00%)	p 1.00(2.30%)	d 4.27(9.81%)			

					f38.29(87.90%)
246.	(0.00000)	R	(30)	C	5
		s	(13.41%)	p	1.60(21.45%)d 3.03(40.60%)
				f	1.83(24.54%)
247.	(0.00000)	R	(31)	C	5
		s	(3.65%)	p	1.77(6.46%)d 8.88(32.39%)
				f	15.77(57.50%)
248.	(0.00000)	R	(32)	C	5
		s	(19.26%)	p	2.10(40.43%)d 0.69(13.23%)
				f	1.41(27.09%)
249.	(0.00000)	R	(33)	C	5
		s	(7.93%)	p	1.92(15.25%)d 2.78(22.06%)
				f	6.90(54.76%)
250.	(0.00000)	R	(34)	C	5
		s	(0.00%)	p	1.00(2.81%)d 8.54(23.97%)
				f	26.09(73.22%)
251.	(0.00000)	R	(35)	C	5
		s	(0.00%)	p	1.00(2.48%)d 6.76(16.80%)
				f	32.49(80.72%)
252.	(0.00000)	R	(36)	C	5
		s	(0.00%)	p	1.00(3.35%)d 0.32(1.08%)
				f	28.53(95.57%)
253.	(0.00000)	R	(37)	C	5
		s	(0.00%)	p	1.00(4.00%)d 1.43(5.74%)
				f	22.54(90.26%)
254.	(0.00000)	R	(38)	C	5
		s	(1.18%)	p	25.98(30.54%)d18.08(21.25%)
				f	40.01(47.03%)
255.	(0.00000)	R	(39)	C	5
		s	(12.15%)	p	1.27(15.43%)d 3.53(42.89%)
				f	2.43(29.53%)
256.	(0.00000)	R	(40)	C	5
		s	(29.96%)	p	0.60(18.11%)d 0.89(26.54%)
				f	0.85(25.39%)
257.	(0.00000)	R	(41)	C	5
		s	(11.06%)	p	1.91(21.15%)d 4.65(51.44%)
				f	1.48(16.35%)
258.	(0.00464)	R	(1)	C	6
		s	(0.74%)	p	99.99(90.78%)d11.03(8.17%)
				f	0.42(0.31%)
					0.0000 -0.0116 0.0812 -0.0252 -0.0062
					0.0239 0.9186 0.0141 -0.0048 -0.0067
					-0.2505 0.0167 0.0116 0.0000 0.0000
					0.0000 0.0000 -0.0159 0.1251 0.0527
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0221 -0.1903 -0.1048 0.0979
					-0.0703 -0.0279 0.0000 0.0000 0.0330
					0.0192 -0.0143 -0.0112 0.0000 0.0000
					0.0000 0.0000 0.0013 -0.0167 0.0000
					0.0322
259.	(0.00177)	R	(2)	C	6
		s	(0.40%)	p	99.99(53.24%)d17.17(6.88%)
				f	98.48(39.48%)
					0.0000 0.0008 0.0499 -0.0384 -0.0064
					-0.0111 0.1882 -0.0040 -0.0294 -0.0341
					0.6988 0.0528 -0.0609 0.0000 0.0000
					0.0000 0.0000 -0.0944 0.1566 0.0956
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 -0.0899 0.1237 0.0529 -0.0023
					0.0070 -0.0031 0.0000 0.0000 0.0243
					0.0213 0.1236 0.0779 0.0000 0.0000
					0.0000 0.0000 0.3575 0.2166 0.3869
					0.2191
260.	(0.00084)	R	(3)	C	6
		s	(0.00%)	p	1.00(88.38%)d 0.08(6.63%)
				f	0.06(4.99%)
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0020 0.8632
					-0.3697 0.0447 0.0000 0.0000 0.0000
					-0.1779 -0.0669 0.1338 0.0971 0.0468
					-0.0262 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 -0.0191 -0.0347 0.0000
					0.0000 0.0000 0.0000 0.1871 0.0722
					-0.0895 -0.0080 0.0000 0.0000 0.0000
					0.0000
261.	(0.00075)	R	(4)	C	6
		s	(2.20%)	p	19.85(43.70%)d 8.27(18.19%)
				f	16.32(35.91%)

		0.0000	0.0005	0.1463	-0.0113	-0.0219
		-0.0071	0.1602	-0.0768	0.0217	-0.0131
		0.6036	0.1875	0.0724	0.0000	0.0000
		0.0000	0.0000	0.1886	-0.3049	-0.1070
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.1089	-0.1655	-0.0355	0.0008
		-0.0152	-0.0347	0.0000	0.0000	-0.0189
		-0.0008	-0.0186	0.0422	0.0000	0.0000
		0.0000	0.0000	-0.3921	-0.1358	-0.4026
		-0.1495				
262.	(0.00050) RY (5) C 6	s(66.36%)	p 0.05(3.03%)	d 0.37(24.80%)		
			f 0.09(5.81%)			
		0.0000	0.0021	0.8092	-0.0443	-0.0825
		-0.0207	-0.0865	-0.0959	0.0076	0.0103
		-0.0946	-0.0637	0.0082	0.0000	0.0000
		0.0000	0.0000	-0.0504	0.1051	-0.1950
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0636	-0.1420	0.3636	-0.0541
		-0.0476	-0.1864	0.0000	0.0000	-0.0505
		-0.0275	-0.0177	-0.0094	0.0000	0.0000
		0.0000	0.0000	0.1802	0.1129	-0.0593
		-0.0752				
263.	(0.00045) RY (6) C 6	s(0.00%)	p 1.00(1.10%)	d 73.83(80.95%)		
			f 16.38(17.96%)			
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	-0.0069	0.0000
		0.1035	-0.0141	0.0000	0.0000	0.0000
		0.2842	0.0486	-0.0423	0.8282	0.1887
		0.0557	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	-0.0066	0.0066	0.0000
		0.0000	0.0000	0.0000	0.1354	0.1537
		0.2647	0.2597	0.0000	0.0000	0.0000
		0.0000				
264.	(0.00019) RY (7) C 6	s(8.86%)	p 0.79(6.97%)	d 7.58(67.14%)		
			f 1.92(17.03%)			
		0.0000	0.0149	0.1628	0.2066	-0.1385
		-0.0076	-0.0015	-0.0895	0.0531	-0.0125
		-0.0701	0.2313	0.0161	0.0000	0.0000
		0.0000	0.0000	-0.1242	-0.1261	-0.0579
		0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	-0.4492	0.3616	0.0493	0.4327
		-0.3352	-0.0455	0.0000	0.0000	-0.1166
		-0.0061	0.0123	0.0651	0.0000	0.0000
		0.0000	0.0000	-0.2056	-0.2118	0.0747
		0.2441				
265.	(0.00009) RY (8) C 6	s(4.00%)	p 2.99(11.95%)	d 17.55(70.25%)		
			f 3.45(13.79%)			
266.	(0.00004) RY (9) C 6	s(17.12%)	p 0.31(5.29%)	d 3.94(67.52%)		
			f 0.59(10.08%)			
267.	(0.00002) RY (10) C 6	s(14.32%)	p 1.68(24.07%)	d 2.34(33.53%)		
			f 1.96(28.09%)			
268.	(0.00002) RY (11) C 6	s(0.00%)	p 1.00(19.10%)	d 3.38(64.61%)		
			f 0.85(16.29%)			
269.	(0.00001) RY (12) C 6	s(4.85%)	p 5.78(28.04%)	d 7.21(34.94%)		
			f 6.63(32.17%)			
270.	(0.00001) RY (13) C 6	s(30.52%)	p 0.69(21.15%)	d 0.78(23.67%)		
			f 0.81(24.67%)			
271.	(0.00000) RY (14) C 6	s(22.33%)	p 0.63(14.14%)	d 1.57(35.08%)		
			f 1.27(28.44%)			
272.	(0.00000) RY (15) C 6	s(1.93%)	p 10.83(20.89%)	d 27.89(53.81%)		
			f 12.11(23.37%)			
273.	(0.00000) RY (16) C 6	s(41.37%)	p 0.55(22.76%)	d 0.36(14.81%)		

					f 0.51(21.07%)
274.	(0.00000)	RY (17)	C	6	s(10.55%)p 1.71(18.06%)d 3.74(39.51%)
					f 3.02(31.88%)
275.	(0.00000)	RY (18)	C	6	s(3.52%)p 5.66(19.94%)d16.52(58.17%)
					f 5.22(18.37%)
276.	(0.00000)	RY (19)	C	6	s(0.00%)p 1.00(13.74%)d 2.80(38.45%)
					f 3.48(47.81%)
277.	(0.00000)	RY (20)	C	6	s(0.00%)p 1.00(21.20%)d 3.49(74.00%)
					f 0.23(4.80%)
278.	(0.00000)	RY (21)	C	6	s(0.00%)p 1.00(13.12%)d 5.29(69.44%)
					f 1.33(17.44%)
279.	(0.00000)	RY (22)	C	6	s(0.00%)p 1.00(8.18%)d 8.77(71.69%)
					f 2.46(20.13%)
280.	(0.00000)	RY (23)	C	6	s(1.98%)p12.56(24.88%)d14.81(29.33%)
					f22.12(43.81%)
281.	(0.00000)	RY (24)	C	6	s(2.12%)p14.73(31.18%)d11.62(24.59%)
					f19.89(42.11%)
282.	(0.00000)	RY (25)	C	6	s(16.55%)p 0.89(14.69%)d 1.45(24.04%)
					f 2.70(44.72%)
283.	(0.00000)	RY (26)	C	6	s(22.00%)p 1.13(24.93%)d 1.17(25.64%)
					f 1.25(27.44%)
284.	(0.00000)	RY (27)	C	6	s(5.13%)p 0.58(2.99%)d11.87(60.91%)
					f 6.04(30.97%)
285.	(0.00000)	RY (28)	C	6	s(1.63%)p17.83(29.15%)d17.53(28.65%)
					f24.82(40.57%)
286.	(0.00000)	RY (29)	C	6	s(0.00%)p 1.00(1.73%)d 4.59(7.93%)
					f52.27(90.34%)
287.	(0.00000)	RY (30)	C	6	s(0.00%)p 1.00(6.47%)d 5.51(35.62%)
					f 8.95(57.91%)
288.	(0.00000)	RY (31)	C	6	s(4.38%)p 7.21(31.57%)d 6.36(27.85%)
					f 8.27(36.20%)
289.	(0.00000)	RY (32)	C	6	s(2.76%)p 3.77(10.40%)d12.50(34.50%)
					f18.97(52.34%)
290.	(0.00000)	RY (33)	C	6	s(4.02%)p 5.21(20.92%)d 9.21(36.97%)
					f 9.49(38.10%)
291.	(0.00000)	RY (34)	C	6	s(0.00%)p 1.00(45.06%)d 0.48(21.84%)
					f 0.73(33.10%)
292.	(0.00000)	RY (35)	C	6	s(4.89%)p 3.59(17.54%)d 2.58(12.60%)
					f13.29(64.97%)
293.	(0.00000)	RY (36)	C	6	s(0.00%)p 1.00(6.08%)d 8.67(52.72%)
					f 6.77(41.20%)
294.	(0.00000)	RY (37)	C	6	s(0.00%)p 1.00(2.46%)d 4.14(10.18%)
					f35.56(87.37%)
295.	(0.00000)	RY (38)	C	6	s(0.00%)p 1.00(1.66%)d25.51(42.46%)
					f33.57(55.88%)
296.	(0.00000)	RY (39)	C	6	s(0.00%)p 1.00(1.97%)d 5.40(10.63%)
					f44.39(87.40%)
297.	(0.00000)	RY (40)	C	6	s(5.64%)p 1.45(8.16%)d 6.75(38.05%)
					f 8.54(48.15%)
298.	(0.00000)	RY (41)	C	6	s(0.00%)p 1.00(69.83%)d 0.18(12.82%)
					f 0.25(17.35%)
299.	(0.00052)	RY (1)	H	7	s(28.67%)p 2.22(63.68%)d 0.27(7.65%)
					0.0006 0.5327 -0.0478 -0.0249 -0.7806
					0.0198 0.0610 0.1086 0.0576 0.0910
					0.0000 0.0000 0.0000 -0.2127 -0.0325
					0.0000 0.0000 0.0000 0.0000 0.1470
					0.0266 -0.0891 -0.0016
300.	(0.00033)	RY (2)	H	7	s(0.00%)p 1.00(93.27%)d 0.07(6.73%)
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.8423 0.4684 0.0622 0.0000 0.0000
					-0.0193 0.0082 -0.2546 0.0455 0.0000
					0.0000 0.0000 0.0000

301.	(0.00027)	RY (3)	H	7	s(29.92%)p 1.84(55.09%)d 0.50(14.99%)
					0.0046 0.5413 0.0722 -0.0310 0.3508
					-0.1410 -0.0010 0.6384 0.0064 0.0219
					0.0000 0.0000 0.0000 0.3674 0.0518
					0.0000 0.0000 0.0000 0.0000 -0.0561
					0.0722 -0.0616 -0.0076
302.	(0.00019)	RY (4)	H	7	s(47.91%)p 1.01(48.30%)d 0.08(3.80%)
					-0.0011 -0.0759 0.6862 -0.0493 -0.1268
					0.0555 0.0057 0.1142 -0.1156 -0.6613
					0.0000 0.0000 0.0000 -0.0232 -0.0013
					0.0000 0.0000 0.0000 0.0000 0.1546
					0.0687 0.0381 0.0858
303.	(0.00011)	RY (5)	H	7	s(42.26%)p 1.30(54.78%)d 0.07(2.97%)
					-0.0048 0.5782 0.2238 0.1954 0.2309
					-0.0570 0.1098 -0.6856 -0.0955 -0.0004
					0.0000 0.0000 0.0000 0.0890 0.0305
					0.0000 0.0000 0.0000 0.0000 -0.0414
					-0.0332 0.1214 0.0571
304.	(0.00010)	RY (6)	H	7	s(0.00%)p 1.00(64.03%)d 0.56(35.97%)
305.	(0.00002)	RY (7)	H	7	s(23.61%)p 1.34(31.71%)d 1.89(44.68%)
306.	(0.00002)	RY (8)	H	7	s(0.07%)p99.99(85.25%)d99.99(14.67%)
307.	(0.00001)	RY (9)	H	7	s(15.33%)p 0.76(11.68%)d 4.76(72.99%)
308.	(0.00001)	RY (10)	H	7	s(25.16%)p 1.65(41.39%)d 1.33(33.45%)
309.	(0.00001)	RY (11)	H	7	s(0.00%)p 1.00(5.51%)d17.15(94.49%)
310.	(0.00001)	RY (12)	H	7	s(35.31%)p 1.01(35.59%)d 0.82(29.10%)
311.	(0.00000)	RY (13)	H	7	s(20.49%)p 2.40(49.14%)d 1.48(30.37%)
312.	(0.00000)	RY (14)	H	7	s(20.63%)p 1.40(28.82%)d 2.45(50.56%)
313.	(0.00000)	RY (15)	H	7	s(4.80%)p 3.29(15.79%)d16.53(79.41%)
314.	(0.00000)	RY (16)	H	7	s(0.00%)p 1.00(69.93%)d 0.43(30.07%)
315.	(0.00000)	RY (17)	H	7	s(0.00%)p 1.00(10.18%)d 8.83(89.82%)
316.	(0.00000)	RY (18)	H	7	s(0.00%)p 1.00(54.97%)d 0.82(45.03%)
317.	(0.00000)	RY (19)	H	7	s(0.00%)p 1.00(2.12%)d46.21(97.88%)
318.	(0.00000)	RY (20)	H	7	s(0.76%)p30.00(22.85%)d99.99(76.39%)
319.	(0.00000)	RY (21)	H	7	s(4.83%)p 9.28(44.83%)d10.42(50.34%)
320.	(0.00000)	RY (22)	H	7	s(0.30%)p37.30(11.08%)d99.99(88.63%)
321.	(0.00244)	RY (1)	H	8	s(0.27%)p99.99(98.45%)d 4.73(1.28%)
					-0.0038 -0.0199 0.0164 0.0451 0.3324
					-0.0085 0.0093 -0.9331 -0.0190 -0.0520
					0.0000 0.0000 0.0000 -0.1102 -0.0029
					0.0000 0.0000 0.0000 0.0000 -0.0256
					0.0021 0.0045 0.0010
322.	(0.00102)	RY (2)	H	8	s(73.08%)p 0.35(25.59%)d 0.02(1.33%)
					-0.0066 0.8546 0.0157 0.0112 -0.4514
					0.0132 -0.1391 -0.1778 0.0217 0.0241
					0.0000 0.0000 0.0000 -0.0298 0.0149
					0.0000 0.0000 0.0000 0.0000 -0.0237
					-0.0281 -0.0905 0.0517
323.	(0.00099)	RY (3)	H	8	s(0.00%)p 1.00(95.31%)d 0.05(4.69%)
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.9620 -0.1571 -0.0553 0.0000 0.0000
					0.2079 -0.0556 -0.0221 0.0077 0.0000
					0.0000 0.0000 0.0000
324.	(0.00013)	RY (4)	H	8	s(22.96%)p 2.63(60.43%)d 0.72(16.61%)
					0.0047 0.3998 -0.1613 -0.2091 0.7075
					-0.1384 -0.1504 0.2294 -0.0448 0.0855
					0.0000 0.0000 0.0000 -0.1103 0.0200
					0.0000 0.0000 0.0000 0.0000 0.3653
					-0.0690 0.0008 0.1238
325.	(0.00005)	RY (5)	H	8	s(48.50%)p 0.42(20.57%)d 0.64(30.93%)
326.	(0.00004)	RY (6)	H	8	s(0.00%)p 1.00(80.59%)d 0.24(19.41%)
327.	(0.00003)	RY (7)	H	8	s(39.01%)p 0.96(37.38%)d 0.61(23.61%)
328.	(0.00001)	RY (8)	H	8	s(10.97%)p 5.43(59.61%)d 2.68(29.41%)

329.	(0.00001)	RY (9)	H	8	s(36.50%)p 1.41(51.36%)d 0.33(12.13%)
330.	(0.00001)	RY (10)	H	8	s(15.46%)p 2.59(40.08%)d 2.88(44.46%)
331.	(0.00001)	RY (11)	H	8	s(0.00%)p 1.00(0.77%)d99.99(99.23%)
332.	(0.00000)	RY (12)	H	8	s(9.61%)p 5.04(48.43%)d 4.37(41.96%)
333.	(0.00000)	RY (13)	H	8	s(3.96%)p13.24(52.49%)d10.98(43.54%)
334.	(0.00000)	RY (14)	H	8	s(0.00%)p 1.00(49.69%)d 1.01(50.31%)
335.	(0.00000)	RY (15)	H	8	s(12.41%)p 3.56(44.14%)d 3.50(43.45%)
336.	(0.00000)	RY (16)	H	8	s(7.00%)p 2.63(18.39%)d10.66(74.61%)
337.	(0.00000)	RY (17)	H	8	s(0.54%)p48.11(25.90%)d99.99(73.56%)
338.	(0.00000)	RY (18)	H	8	s(0.00%)p 1.00(34.99%)d 1.86(65.01%)
339.	(0.00000)	RY (19)	H	8	s(0.00%)p 1.00(6.24%)d15.03(93.76%)
340.	(0.00000)	RY (20)	H	8	s(0.00%)p 1.00(32.41%)d 2.09(67.59%)
341.	(0.00000)	RY (21)	H	8	s(16.55%)p 0.68(11.22%)d 4.36(72.23%)
342.	(0.00000)	RY (22)	H	8	s(3.22%)p 1.84(5.92%)d28.20(90.86%)
343.	(0.00100)	RY (1)	H	9	s(48.92%)p 1.01(49.35%)d 0.04(1.73%)
					-0.0052 0.6988 0.0054 -0.0287 -0.4927
					-0.0014 0.0713 0.4762 0.1375 -0.0002
					0.0000 0.0000 0.0000 0.0680 -0.0483
					0.0000 0.0000 0.0000 0.0000 -0.0352
					-0.0374 0.0870 -0.0104
344.	(0.00057)	RY (2)	H	9	s(3.89%)p22.71(88.43%)d 1.97(7.67%)
					-0.0049 0.1945 0.0315 0.0099 0.7692
					-0.0429 -0.0652 0.5303 0.0681 0.0250
					0.0000 0.0000 0.0000 -0.2601 -0.0058
					0.0000 0.0000 0.0000 0.0000 0.0675
					0.0042 0.0669 0.0037
345.	(0.00020)	RY (3)	H	9	s(0.00%)p 1.00(91.88%)d 0.09(8.12%)
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.6995 0.6450 0.1162 0.0000 0.0000
					-0.1280 0.0325 0.2512 -0.0257 0.0000
					0.0000 0.0000 0.0000
346.	(0.00018)	RY (4)	H	9	s(52.77%)p 0.85(44.85%)d 0.05(2.38%)
					-0.0005 -0.1742 0.7021 -0.0668 -0.0743
					0.0956 0.2262 0.2077 -0.2545 -0.5242
					0.0000 0.0000 0.0000 -0.0694 -0.0384
					0.0000 0.0000 0.0000 0.0000 -0.1033
					-0.0227 -0.0336 -0.0718
347.	(0.00012)	RY (5)	H	9	s(0.00%)p 1.00(80.98%)d 0.23(19.02%)
					0.0000 0.0000 0.0000 0.0000 0.0000
					0.0000 0.0000 0.0000 0.0000 0.0000
					-0.6590 0.4495 0.4165 0.0000 0.0000
					-0.1974 -0.0091 0.3888 -0.0020 0.0000
					0.0000 0.0000 0.0000
348.	(0.00009)	RY (6)	H	9	s(55.79%)p 0.70(39.13%)d 0.09(5.09%)
349.	(0.00002)	RY (7)	H	9	s(2.17%)p 6.75(14.64%)d38.34(83.19%)
350.	(0.00001)	RY (8)	H	9	s(31.85%)p 1.93(61.39%)d 0.21(6.76%)
351.	(0.00000)	RY (9)	H	9	s(25.67%)p 1.60(41.03%)d 1.30(33.29%)
352.	(0.00000)	RY (10)	H	9	s(0.00%)p 1.00(49.98%)d 1.00(50.02%)
353.	(0.00000)	RY (11)	H	9	s(3.80%)p 9.13(34.70%)d16.19(61.50%)
354.	(0.00000)	RY (12)	H	9	s(22.49%)p 1.97(44.32%)d 1.48(33.19%)
355.	(0.00000)	RY (13)	H	9	s(4.70%)p10.36(48.72%)d 9.90(46.57%)
356.	(0.00000)	RY (14)	H	9	s(1.57%)p30.21(47.32%)d32.64(51.12%)
357.	(0.00000)	RY (15)	H	9	s(22.79%)p 1.08(24.65%)d 2.31(52.56%)
358.	(0.00000)	RY (16)	H	9	s(0.00%)p 1.00(20.96%)d 3.77(79.04%)
359.	(0.00000)	RY (17)	H	9	s(0.00%)p 1.00(29.31%)d 2.41(70.69%)
360.	(0.00000)	RY (18)	H	9	s(0.00%)p 1.00(14.87%)d 5.72(85.13%)
361.	(0.00000)	RY (19)	H	9	s(0.00%)p 1.00(12.01%)d 7.33(87.99%)
362.	(0.00000)	RY (20)	H	9	s(5.74%)p 6.14(35.28%)d10.27(58.98%)
363.	(0.00000)	RY (21)	H	9	s(11.05%)p 2.10(23.24%)d 5.95(65.72%)
364.	(0.00000)	RY (22)	H	9	s(6.84%)p 0.43(2.92%)d13.20(90.24%)
365.	(0.00068)	RY (1)	H	10	s(0.17%)p99.99(91.80%)d47.62(8.03%)
					0.0003 0.0315 0.0263 0.6681 -0.1536

					-0.0792	-0.6410	0.1551	0.0825	0.0000
					0.0000	0.0000	0.0133	0.0001	0.0000
					0.0000	0.0000	0.0000	-0.2789	-0.0484
					0.0031	-0.0033			
366.	(0.00040)	R Y	(2)	H 10	s(0.00%)	p 1.00(98.17%)	d 0.02(1.83%)		
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0000	0.0000	0.0000	0.9570
					0.2008	0.1600	0.0000	0.0000	0.0726
					0.0223	0.0980	0.0541	0.0000	0.0000
					0.0000	0.0000			
367.	(0.00028)	R Y	(3)	H 10	s(30.73%)	p 2.17(66.59%)	d 0.09(2.68%)		
					-0.0015	0.5060	-0.2262	-0.4946	0.0046
					-0.3147	-0.4886	0.0225	-0.2881	0.0000
					0.0000	0.0000	-0.0679	0.0357	0.0000
					0.0000	0.0000	0.0000	-0.0159	-0.0051
					-0.1436	0.0074			
368.	(0.00024)	R Y	(4)	H 10	s(52.22%)	p 0.81(42.23%)	d 0.11(5.55%)		
					0.0050	0.7132	0.1163	0.4083	-0.0209
					-0.1748	0.4411	-0.0469	-0.1668	0.0000
					0.0000	0.0000	0.2176	-0.0041	0.0000
					0.0000	0.0000	0.0000	0.0511	0.0096
					0.0188	-0.0713			
369.	(0.00008)	R Y	(5)	H 10	s(0.00%)	p 1.00(71.18%)	d 0.40(28.82%)		
370.	(0.00005)	R Y	(6)	H 10	s(54.82%)	p 0.50(27.34%)	d 0.33(17.84%)		
371.	(0.00002)	R Y	(7)	H 10	s(2.25%)	p39.61(89.03%)	d 3.88(8.72%)		
372.	(0.00001)	R Y	(8)	H 10	s(28.90%)	p 0.88(25.40%)	d 1.58(45.70%)		
373.	(0.00000)	R Y	(9)	H 10	s(0.00%)	p 1.00(4.70%)	d20.29(95.30%)		
374.	(0.00000)	R Y	(10)	H 10	s(20.45%)	p 2.34(47.91%)	d 1.55(31.64%)		
375.	(0.00000)	R Y	(11)	H 10	s(0.48%)	p99.99(76.08%)	d48.97(23.44%)		
376.	(0.00000)	R Y	(12)	H 10	s(1.81%)	p12.36(22.32%)	d42.00(75.87%)		
377.	(0.00000)	R Y	(13)	H 10	s(2.18%)	p 5.71(12.45%)	d39.15(85.37%)		
378.	(0.00000)	R Y	(14)	H 10	s(3.28%)	p 7.08(23.20%)	d22.44(73.52%)		
379.	(0.00000)	R Y	(15)	H 10	s(0.00%)	p 1.00(41.60%)	d 1.40(58.40%)		
380.	(0.00000)	R Y	(16)	H 10	s(0.84%)	p54.73(46.03%)	d63.17(53.13%)		
381.	(0.00000)	R Y	(17)	H 10	s(0.00%)	p 1.00(55.37%)	d 0.81(44.63%)		
382.	(0.00000)	R Y	(18)	H 10	s(0.00%)	p 1.00(17.13%)	d 4.84(82.87%)		
383.	(0.00000)	R Y	(19)	H 10	s(0.00%)	p 1.00(11.85%)	d 7.44(88.15%)		
384.	(0.00000)	R Y	(20)	H 10	s(0.09%)	p99.99(24.81%)	d99.99(75.10%)		
385.	(0.00000)	R Y	(21)	H 10	s(1.83%)	p 2.61(4.77%)	d51.03(93.40%)		
386.	(0.00069)	R Y	(1)	H 11	s(45.66%)	p 1.12(51.06%)	d 0.07(3.28%)		
					-0.0084	0.6751	-0.0141	-0.0247	0.6958
					0.1239	0.0135	-0.0992	-0.0321	-0.0058
					0.0000	0.0000	0.0000	-0.0935	-0.0183
					0.0000	0.0000	0.0000	0.0000	0.0771
					0.0295	0.1270	-0.0281		
387.	(0.00053)	R Y	(2)	H 11	s(1.21%)	p74.96(90.72%)	d 6.66(8.06%)		
					-0.0003	0.1007	-0.0444	0.0021	-0.2193
					0.0457	0.0696	-0.9142	0.0449	0.1200
					0.0000	0.0000	0.0000	0.2489	-0.0268
					0.0000	0.0000	0.0000	0.0000	0.1334
					0.0102	0.0085	-0.0033		
388.	(0.00031)	R Y	(3)	H 11	s(0.00%)	p 1.00(97.15%)	d 0.03(2.85%)		
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.0000	0.0000	0.0000	0.0000	0.0000
					0.8588	0.4820	0.0396	0.0000	0.0000
					0.1541	-0.0432	-0.0507	0.0191	0.0000
					0.0000	0.0000	0.0000		
389.	(0.00019)	R Y	(4)	H 11	s(60.63%)	p 0.59(35.54%)	d 0.06(3.83%)		
					0.0010	0.0501	0.7769	-0.0146	-0.0090
					-0.2004	-0.5277	-0.0513	0.0605	0.1744
					0.0000	0.0000	0.0000	-0.0691	-0.0076
					0.0000	0.0000	0.0000	0.0000	0.1503
					0.0056	-0.0614	-0.0842		

390.	(0.00006)	RY (5)	H 11	s(0.00%)p 1.00(70.31%)d 0.42(29.69%)
391.	(0.00006)	RY (6)	H 11	s(55.15%)p 0.61(33.56%)d 0.20(11.29%)
392.	(0.00001)	RY (7)	H 11	s(6.72%)p 9.13(61.35%)d 4.75(31.94%)
393.	(0.00001)	RY (8)	H 11	s(5.96%)p12.50(74.55%)d 3.27(19.49%)
394.	(0.00000)	RY (9)	H 11	s(49.12%)p 0.36(17.87%)d 0.67(33.02%)
395.	(0.00000)	RY (10)	H 11	s(17.38%)p 1.86(32.24%)d 2.90(50.37%)
396.	(0.00000)	RY (11)	H 11	s(0.00%)p 1.00(2.11%)d46.42(97.89%)
397.	(0.00000)	RY (12)	H 11	s(26.18%)p 1.52(39.67%)d 1.30(34.16%)
398.	(0.00000)	RY (13)	H 11	s(2.00%)p 9.95(19.91%)d39.01(78.09%)
399.	(0.00000)	RY (14)	H 11	s(8.88%)p 6.72(59.65%)d 3.54(31.47%)
400.	(0.00000)	RY (15)	H 11	s(0.00%)p 1.00(81.17%)d 0.23(18.83%)
401.	(0.00000)	RY (16)	H 11	s(3.20%)p 5.92(18.92%)d24.36(77.88%)
402.	(0.00000)	RY (17)	H 11	s(0.00%)p 1.00(24.49%)d 3.08(75.51%)
403.	(0.00000)	RY (18)	H 11	s(0.00%)p 1.00(21.52%)d 3.65(78.48%)
404.	(0.00000)	RY (19)	H 11	s(0.00%)p 1.00(3.25%)d29.78(96.75%)
405.	(0.00000)	RY (20)	H 11	s(6.09%)p 1.31(7.98%)d14.10(85.92%)
406.	(0.00000)	RY (21)	H 11	s(10.65%)p 4.41(46.92%)d 3.98(42.43%)
407.	(0.00000)	RY (22)	H 11	s(1.22%)p 8.18(10.01%)d72.53(88.76%)
408.	(0.00937)	RY (1)	N 12	s(5.15%)p17.48(90.05%)d 0.32(1.62%) f 0.61(3.17%) 0.0000 -0.0014 0.2202 -0.0548 0.0070 -0.0016 0.7857 -0.0242 -0.0105 0.0152 -0.5306 -0.0107 -0.0254 0.0000 0.0000 0.0000 0.0000 -0.0338 0.0252 0.0555 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0634 -0.0029 -0.0149 -0.0501 -0.0661 -0.0161 0.0000 0.0000 -0.0507 0.0181 0.0232 -0.0099 0.0000 0.0000 0.0000 0.0000 -0.0133 -0.0083 0.1566 -0.0582
409.	(0.00546)	RY (2)	N 12	s(0.00%)p 1.00(89.00%)d 0.08(6.86%) f 0.05(4.14%) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0173 0.9426 -0.0232 0.0275 0.0000 0.0000 0.0000 -0.0334 -0.0121 0.0053 -0.2100 -0.1435 0.0512 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 -0.1212 0.0405 0.0000 0.0000 0.0000 0.0000 -0.1156 0.0351 0.0959 -0.0357 0.0000 0.0000 0.0000 0.0000
410.	(0.00254)	RY (3)	N 12	s(9.79%)p 6.86(67.16%)d 1.50(14.70%) f 0.85(8.36%) 0.0000 0.0080 0.2934 0.1076 0.0110 0.0029 -0.4213 -0.0742 0.0150 0.0106 -0.5469 -0.4271 -0.0820 0.0000 0.0000 0.0000 0.0000 0.1063 0.2934 -0.0307 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0903 0.1656 -0.0949 0.0480 -0.0337 -0.0251 0.0000 0.0000 0.0338 -0.0003 -0.0078 0.0063 0.0000 0.0000 0.0000 0.0000 0.2506 -0.0763 -0.1152 0.0213
411.	(0.00208)	RY (4)	N 12	s(23.15%)p 1.98(45.90%)d 0.92(21.24%) f 0.42(9.70%) 0.0000 -0.0039 0.4692 0.0954 0.0481 0.0031 0.1000 -0.2453 0.0297 0.0030 0.3511 -0.5144 0.0070 0.0000 0.0000 0.0000 0.0000 -0.0692 -0.0763 0.0567 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0275 -0.4254 -0.0132 -0.0131 -0.1222 -0.0403 0.0000 0.0000 -0.0217

	0.0113	-0.1169	0.0684	0.0000	0.0000
	0.0000	0.0000	-0.2222	0.1322	-0.0928
	0.0511				
412. (0.00062) RY (5) N 12	s(0.00%)	p 1.00(13.55%)	d 5.87(79.51%)		
	f 0.51(6.94%)				
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	-0.0105	0.0600
	0.3627	-0.0152	0.0000	0.0000	0.0000
	-0.3174	0.2098	-0.0717	-0.2819	0.7488
	-0.0707	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	-0.0066	0.0380	0.0000
	0.0000	0.0000	0.0000	0.1728	-0.0889
	0.1467	-0.0932	0.0000	0.0000	0.0000
	0.0000				
413. (0.00037) RY (6) N 12	s(13.20%)	p 2.71(35.77%)	d 1.70(22.40%)		
	f 2.17(28.63%)				
	0.0000	-0.0009	0.2722	-0.2400	0.0180
	-0.0061	-0.0806	0.5670	-0.1256	-0.0030
	-0.0111	0.0999	0.0609	0.0000	0.0000
	0.0000	0.0000	0.0745	0.2992	0.1099
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.1709	0.1490	0.1396	-0.1220
	-0.1666	-0.0574	0.0000	0.0000	0.0063
	0.0225	-0.0722	0.0741	0.0000	0.0000
	0.0000	0.0000	-0.4275	0.1865	-0.2298
	0.0684				
414. (0.00026) RY (7) N 12	s(11.92%)	p 2.04(24.28%)	d 4.21(50.13%)		
	f 1.15(13.68%)				
	0.0000	0.0295	0.0752	0.3331	0.0410
	0.0135	0.0867	0.4712	-0.0885	0.0011
	-0.0373	-0.0485	-0.0390	0.0000	0.0000
	0.0000	0.0000	-0.5149	-0.1317	0.0895
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.2224	-0.1166	-0.0013	0.2529
	0.2886	0.0228	0.0000	0.0000	0.1352
	-0.0474	0.1396	-0.0626	0.0000	0.0000
	0.0000	0.0000	0.0851	-0.0910	-0.2575
	0.1050				
415. (0.00021) RY (8) N 12	s(0.00%)	p 1.00(58.22%)	d 0.56(32.79%)		
	f 0.15(9.00%)				
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0036	0.0894
	0.7179	0.2423	0.0000	0.0000	0.0000
	0.4753	0.2291	0.0878	0.1401	-0.1268
	0.0777	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0270	-0.0257	0.0000
	0.0000	0.0000	0.0000	0.1717	0.0045
	-0.2294	0.0801	0.0000	0.0000	0.0000
	0.0000				
416. (0.00016) RY (9) N 12	s(28.49%)	p 1.50(42.60%)	d 0.57(16.22%)		
	f 0.45(12.69%)				
	0.0000	-0.0034	0.5192	0.0629	-0.1064
	0.0060	-0.2517	0.0384	0.1334	0.0331
	-0.0382	0.5465	-0.2051	0.0000	0.0000
	0.0000	0.0000	-0.0521	-0.1041	0.0861
	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	-0.0210	-0.3108	-0.0782	-0.1007
	-0.1552	-0.0621	0.0000	0.0000	-0.0243
	0.0409	0.1665	-0.0499	0.0000	0.0000
	0.0000	0.0000	0.1741	-0.0294	0.2282
	-0.1059				

417.	(0.00007)	RY	(10)	N	12	s(3.04%)	p 6.35(19.29%)	d18.94(57.53%)
						f 6.63(20.14%)		
418.	(0.00005)	RY	(11)	N	12	s(18.68%)	p 0.93(17.45%)	d 2.80(52.29%)
						f 0.62(11.58%)		
419.	(0.00005)	RY	(12)	N	12	s(0.00%)	p 1.00(3.29%)	d23.29(76.64%)
						f 6.10(20.07%)		
420.	(0.00002)	RY	(13)	N	12	s(2.89%)	p 6.26(18.11%)	d19.10(55.24%)
						f 8.21(23.76%)		
421.	(0.00001)	RY	(14)	N	12	s(4.38%)	p 5.49(24.01%)	d12.69(55.54%)
						f 3.67(16.07%)		
422.	(0.00000)	RY	(15)	N	12	s(13.88%)	p 1.31(18.19%)	d 1.80(25.00%)
						f 3.09(42.93%)		
423.	(0.00000)	RY	(16)	N	12	s(8.35%)	p 1.78(14.84%)	d 5.91(49.35%)
						f 3.29(27.45%)		
424.	(0.00000)	RY	(17)	N	12	s(4.95%)	p 2.91(14.42%)	d12.38(61.28%)
						f 3.91(19.35%)		
425.	(0.00000)	RY	(18)	N	12	s(0.00%)	p 1.00(11.28%)	d 7.14(80.47%)
						f 0.73(8.25%)		
426.	(0.00000)	RY	(19)	N	12	s(0.00%)	p 1.00(9.57%)	d 9.25(88.59%)
						f 0.19(1.84%)		
427.	(0.00000)	RY	(20)	N	12	s(0.00%)	p 1.00(0.65%)	d99.99(98.24%)
						f 1.72(1.11%)		
428.	(0.00000)	RY	(21)	N	12	s(5.79%)	p 3.54(20.47%)	d 6.53(37.77%)
						f 6.22(35.97%)		
429.	(0.00000)	RY	(22)	N	12	s(0.00%)	p 1.00(1.37%)	d70.48(96.64%)
						f 1.45(1.99%)		
430.	(0.00000)	RY	(23)	N	12	s(35.10%)	p 0.42(14.73%)	d 0.43(14.97%)
						f 1.00(35.20%)		
431.	(0.00000)	RY	(24)	N	12	s(0.00%)	p 1.00(34.49%)	d 0.38(13.16%)
						f 1.52(52.34%)		
432.	(0.00000)	RY	(25)	N	12	s(8.83%)	p 4.16(36.69%)	d 3.25(28.67%)
						f 2.92(25.80%)		
433.	(0.00000)	RY	(26)	N	12	s(7.83%)	p 1.84(14.39%)	d 3.21(25.17%)
						f 6.72(52.61%)		
434.	(0.00000)	RY	(27)	N	12	s(3.78%)	p 2.54(9.60%)	d15.22(57.51%)
						f 7.71(29.11%)		
435.	(0.00000)	RY	(28)	N	12	s(10.31%)	p 0.19(1.93%)	d 5.23(53.90%)
						f 3.29(33.86%)		
436.	(0.00000)	RY	(29)	N	12	s(0.00%)	p 1.00(1.38%)	d 0.41(0.57%)
						f71.15(98.05%)		
437.	(0.00000)	RY	(30)	N	12	s(0.00%)	p 1.00(37.84%)	d 0.02(0.75%)
						f 1.62(61.41%)		
438.	(0.00000)	RY	(31)	N	12	s(3.07%)	p 2.19(6.75%)	d12.76(39.24%)
						f16.56(50.94%)		
439.	(0.00000)	RY	(32)	N	12	s(4.47%)	p 0.54(2.40%)	d 3.00(13.43%)
						f17.81(79.69%)		
440.	(0.00000)	RY	(33)	N	12	s(6.90%)	p 0.79(5.45%)	d 5.94(40.96%)
						f 6.77(46.69%)		
441.	(0.00000)	RY	(34)	N	12	s(16.34%)	p 0.40(6.54%)	d 1.10(18.05%)
						f 3.62(59.07%)		
442.	(0.00000)	RY	(35)	N	12	s(0.00%)	p 1.00(7.17%)	d 1.33(9.57%)
						f11.61(83.26%)		
443.	(0.00000)	RY	(36)	N	12	s(0.00%)	p 1.00(15.73%)	d 0.13(2.00%)
						f 5.23(82.28%)		
444.	(0.00000)	RY	(37)	N	12	s(0.00%)	p 1.00(10.43%)	d 1.28(13.38%)
						f 7.31(76.19%)		
445.	(0.00000)	RY	(38)	N	12	s(0.00%)	p 1.00(6.23%)	d 0.12(0.73%)
						f14.92(93.03%)		
446.	(0.00000)	RY	(39)	N	12	s(36.56%)	p 0.57(20.71%)	d 0.60(21.86%)
						f 0.57(20.87%)		
447.	(0.00000)	RY	(40)	N	12	s(10.07%)	p 0.80(8.05%)	d 4.72(47.56%)
						f 3.41(34.32%)		
448.	(0.00000)	RY	(41)	N	12	s(3.25%)	p 6.45(20.95%)	d 5.49(17.82%)

449. (0.00608) RY (1) C 13 f17.86(57.98%)
 s(0.00%)p 1.00(49.79%)d 0.82(40.85%)
 f 0.19(9.36%)
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 -0.0180 0.6961
 0.1068 -0.0409 0.0000 0.0000 0.0000
 0.2319 0.0371 -0.0064 0.5902 -0.0671
 0.0220 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 0.1834 -0.0254 0.0000
 0.0000 0.0000 0.0000 0.2397 -0.0325
 -0.0272 -0.0078 0.0000 0.0000 0.0000
 0.0000

450. (0.00589) RY (2) C 13 s(3.55%)p23.21(82.42%)d 1.08(3.84%)
 f 2.87(10.19%)
 0.0000 -0.0078 0.1830 -0.0424 0.0135
 -0.0359 -0.1147 -0.0453 0.0016 -0.0520
 0.8948 -0.0629 -0.0194 0.0000 0.0000
 0.0000 0.0000 -0.1307 0.0015 0.0103
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 -0.0415 0.0803 0.0450 0.0634
 0.0741 0.0386 0.0000 0.0000 -0.0751
 0.0069 -0.1227 0.0006 0.0000 0.0000
 0.0000 0.0000 -0.2719 0.0179 -0.0834
 0.0023

451. (0.00079) RY (3) C 13 s(45.55%)p 0.63(28.80%)d 0.55(25.00%)
 f 0.01(0.65%)
 0.0000 -0.0071 0.6744 0.0056 -0.0246
 -0.0021 -0.4648 0.0964 -0.0404 -0.0112
 -0.1140 0.2090 -0.0652 0.0000 0.0000
 0.0000 0.0000 0.3402 0.0964 0.1356
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.2764 -0.0236 -0.0390 0.1247
 0.0192 0.1103 0.0000 0.0000 0.0210
 -0.0186 0.0562 0.0126 0.0000 0.0000
 0.0000 0.0000 0.0209 -0.0117 -0.0038
 0.0429

452. (0.00036) RY (4) C 13 s(0.00%)p 1.00(30.58%)d 2.07(63.37%)
 f 0.20(6.05%)
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 -0.0126 -0.4479
 0.3223 -0.0345 0.0000 0.0000 0.0000
 0.1238 0.0018 0.2047 0.5185 0.0235
 0.5542 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 -0.1244 0.0436 0.0000
 0.0000 0.0000 0.0000 -0.1694 0.0499
 0.0959 -0.0517 0.0000 0.0000 0.0000
 0.0000

453. (0.00034) RY (5) C 13 s(28.87%)p 1.14(32.81%)d 1.20(34.70%)
 f 0.13(3.62%)
 0.0000 0.0065 0.5297 0.0892 0.0071
 -0.0028 0.4749 -0.1930 -0.0141 -0.0096
 -0.1470 0.1879 -0.0900 0.0000 0.0000
 0.0000 0.0000 -0.4325 0.0298 -0.1511
 0.0000 0.0000 0.0000 0.0000 0.0000
 0.0000 -0.2007 0.0050 -0.2201 0.1815
 0.1166 0.0313 0.0000 0.0000 -0.0565
 0.0541 0.0670 0.0494 0.0000 0.0000
 0.0000 0.0000 -0.0936 0.0681 0.0589
 0.0794

454. (0.00007) RY (6) C 13 s(12.19%)p 1.49(18.17%)d 4.36(53.14%)
 f 1.35(16.50%)

455.	(0.00004)	RY (7)	C 13	s(15.17%)	p 1.03(15.59%)	d 3.06(46.40%)
				f 1.51(22.83%)		
456.	(0.00003)	RY (8)	C 13	s(0.00%)	p 1.00(8.41%)	d 9.31(78.31%)
				f 1.58(13.27%)		
457.	(0.00003)	RY (9)	C 13	s(4.13%)	p 7.69(31.76%)	d13.23(54.62%)
				f 2.30(9.49%)		
458.	(0.00001)	RY (10)	C 13	s(29.99%)	p 0.95(28.35%)	d 1.06(31.74%)
				f 0.33(9.91%)		
459.	(0.00001)	RY (11)	C 13	s(21.58%)	p 0.87(18.83%)	d 1.60(34.58%)
				f 1.16(25.01%)		
460.	(0.00000)	RY (12)	C 13	s(3.11%)	p 3.48(10.82%)	d23.67(73.51%)
				f 4.05(12.57%)		
461.	(0.00000)	RY (13)	C 13	s(9.71%)	p 2.03(19.69%)	d 6.10(59.17%)
				f 1.18(11.44%)		
462.	(0.00000)	RY (14)	C 13	s(0.00%)	p 1.00(22.32%)	d 3.18(70.93%)
				f 0.30(6.75%)		
463.	(0.00000)	RY (15)	C 13	s(0.00%)	p 1.00(90.20%)	d 0.11(9.76%)
				f 0.00(0.04%)		
464.	(0.00000)	RY (16)	C 13	s(1.65%)	p 5.92(9.77%)	d 7.47(12.33%)
				f46.20(76.25%)		
465.	(0.00000)	RY (17)	C 13	s(16.64%)	p 0.87(14.55%)	d 1.03(17.18%)
				f 3.10(51.63%)		
466.	(0.00000)	RY (18)	C 13	s(0.00%)	p 1.00(18.02%)	d 4.55(81.97%)
				f 0.00(0.01%)		
467.	(0.00000)	RY (19)	C 13	s(0.00%)	p 1.00(10.87%)	d 8.20(89.08%)
				f 0.00(0.05%)		
468.	(0.00000)	RY (20)	C 13	s(1.32%)	p18.94(24.94%)	d24.84(32.71%)
				f31.15(41.03%)		
469.	(0.00000)	RY (21)	C 13	s(0.00%)	p 1.00(20.65%)	d 2.87(59.29%)
				f 0.97(20.06%)		
470.	(0.00000)	RY (22)	C 13	s(19.20%)	p 1.26(24.28%)	d 0.66(12.69%)
				f 2.28(43.84%)		
471.	(0.00000)	RY (23)	C 13	s(0.43%)	p39.58(17.11%)	d99.99(68.80%)
				f31.60(13.66%)		
472.	(0.00000)	RY (24)	C 13	s(11.21%)	p 2.73(30.64%)	d 3.77(42.25%)
				f 1.42(15.90%)		
473.	(0.00000)	RY (25)	C 13	s(25.43%)	p 0.70(17.86%)	d 1.63(41.43%)
				f 0.60(15.29%)		
474.	(0.00000)	RY (26)	C 13	s(13.88%)	p 3.22(44.68%)	d 1.85(25.64%)
				f 1.14(15.81%)		
475.	(0.00000)	RY (27)	C 13	s(0.00%)	p 1.00(24.73%)	d 1.80(44.45%)
				f 1.25(30.83%)		
476.	(0.00000)	RY (28)	C 13	s(0.00%)	p 1.00(7.78%)	d 0.64(5.01%)
				f11.21(87.21%)		
477.	(0.00000)	RY (29)	C 13	s(0.00%)	p 1.00(0.55%)	d 0.67(0.37%)
				f99.99(99.07%)		
478.	(0.00000)	RY (30)	C 13	s(0.26%)	p18.12(4.79%)	d50.11(13.26%)
				f99.99(81.68%)		
479.	(0.00000)	RY (31)	C 13	s(3.45%)	p 1.32(4.54%)	d11.03(38.01%)
				f15.67(54.00%)		
480.	(0.00000)	RY (32)	C 13	s(3.12%)	p 1.88(5.86%)	d10.99(34.34%)
				f18.14(56.68%)		
481.	(0.00000)	RY (33)	C 13	s(11.95%)	p 1.71(20.44%)	d 2.30(27.54%)
				f 3.35(40.07%)		
482.	(0.00000)	RY (34)	C 13	s(0.00%)	p 1.00(1.96%)	d21.67(42.40%)
				f28.44(55.64%)		
483.	(0.00000)	RY (35)	C 13	s(0.00%)	p 1.00(0.85%)	d 3.63(3.08%)
				f99.99(96.07%)		
484.	(0.00000)	RY (36)	C 13	s(0.00%)	p 1.00(1.72%)	d 2.14(3.69%)
				f54.88(94.58%)		
485.	(0.00000)	RY (37)	C 13	s(0.00%)	p 1.00(11.81%)	d 0.62(7.37%)
				f 6.85(80.82%)		
486.	(0.00000)	RY (38)	C 13	s(5.05%)	p 2.62(13.22%)	d 4.87(24.60%)

487.	(0.00000)	RY (39)	C 13	f11.33(57.14%) s(3.69%)p 2.36(8.73%)d 7.47(27.59%) f16.24(59.99%)
488.	(0.00000)	RY (40)	C 13	s(7.56%)p 2.78(21.01%)d 3.63(27.40%) f 5.83(44.03%)
489.	(0.00328)	RY (1)	S 14	s(0.00%)p 1.00(58.59%)d 0.70(41.08%) f 0.01(0.33%) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0105 0.7626 0.0652 0.0079 0.0000 0.0000 0.0000 -0.1778 -0.0200 0.0036 -0.6008 -0.1303 0.0286 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0355 0.0069 0.0000 0.0000 0.0000 0.0000 0.0361 0.0101 -0.0240 0.0025 0.0000 0.0000 0.0000 0.0000
490.	(0.00215)	RY (2)	S 14	s(0.13%)p99.99(57.93%)d99.99(41.48%) f 3.41(0.46%) 0.0000 0.0000 -0.0005 0.0355 0.0076 -0.0054 0.0000 -0.0273 -0.7415 -0.0334 0.0141 0.0000 0.0064 0.1570 -0.0525 -0.0050 0.0000 0.0000 0.0000 0.0000 0.0000 0.5282 0.1201 -0.0232 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.3364 0.0848 0.0010 -0.0171 0.0034 -0.0120 0.0000 0.0000 -0.0200 -0.0070 0.0017 0.0081 0.0000 0.0000 0.0000 0.0000 -0.0425 -0.0181 0.0436 0.0061
491.	(0.00022)	RY (3)	S 14	s(73.62%)p 0.19(14.11%)d 0.15(10.90%) f 0.02(1.37%) 0.0000 0.0000 0.0198 0.8550 0.0312 -0.0618 0.0000 0.0236 -0.0520 -0.1492 0.0583 0.0000 0.0739 -0.1202 -0.2844 0.1068 0.0000 0.0000 0.0000 0.0000 0.0000 -0.1619 -0.1798 -0.0297 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0772 0.1276 0.0393 0.0922 0.1301 0.0185 0.0000 0.0000 0.0156 0.0090 0.0646 0.0147 0.0000 0.0000 0.0000 0.0000 0.0600 -0.0085 0.0690 -0.0233
492.	(0.00006)	RY (4)	S 14	s(4.23%)p19.73(83.48%)d 2.58(10.93%) f 0.32(1.35%)
493.	(0.00002)	RY (5)	S 14	s(11.27%)p 5.79(65.26%)d 2.00(22.53%) f 0.08(0.94%)
494.	(0.00001)	RY (6)	S 14	s(15.72%)p 3.08(48.41%)d 1.45(22.80%) f 0.83(13.07%)
495.	(0.00001)	RY (7)	S 14	s(0.00%)p 1.00(49.48%)d 0.83(40.88%) f 0.19(9.64%)
496.	(0.00000)	RY (8)	S 14	s(2.71%)p 6.60(17.88%)d27.48(74.47%) f 1.82(4.93%)
497.	(0.00000)	RY (9)	S 14	s(0.00%)p 1.00(26.04%)d 2.66(69.16%) f 0.18(4.80%)
498.	(0.00000)	RY (10)	S 14	s(46.72%)p 0.43(20.10%)d 0.40(18.63%) f 0.31(14.55%)
499.	(0.00000)	RY (11)	S 14	s(10.18%)p 1.09(11.10%)d 5.99(60.96%) f 1.74(17.76%)
500.	(0.00000)	RY (12)	S 14	s(1.16%)p27.26(31.52%)d50.82(58.74%) f 7.43(8.59%)
501.	(0.00000)	RY (13)	S 14	s(14.91%)p 0.61(9.08%)d 1.77(26.44%) f 3.33(49.57%)
502.	(0.00000)	RY (14)	S 14	s(7.64%)p 9.37(71.65%)d 2.35(17.98%) f 0.36(2.73%)

503.	(0.00000)	RY (15)	S 14	s(0.28%)	p99.99(42.03%)	d99.99(33.95%)	f84.63(23.74%)
504.	(0.00000)	RY (16)	S 14	s(0.00%)	p 1.00(89.05%)	d 0.12(10.63%)	f 0.00(0.32%)
505.	(0.00000)	RY (17)	S 14	s(0.68%)	p10.24(6.99%)	d28.49(19.45%)	f99.99(72.87%)
506.	(0.00000)	RY (18)	S 14	s(0.00%)	p 1.00(19.97%)	d 2.93(58.55%)	f 1.08(21.48%)
507.	(0.00000)	RY (19)	S 14	s(0.00%)	p 1.00(2.08%)	d30.98(64.49%)	f16.06(33.43%)
508.	(0.00000)	RY (20)	S 14	s(0.00%)	p 1.00(39.45%)	d 1.16(45.64%)	f 0.38(14.91%)
509.	(0.00000)	RY (21)	S 14	s(0.00%)	p 1.00(2.14%)	d44.74(95.93%)	f 0.90(1.92%)
510.	(0.00000)	RY (22)	S 14	s(0.00%)	p 1.00(0.47%)	d99.99(88.62%)	f23.42(10.91%)
511.	(0.00000)	RY (23)	S 14	s(5.27%)	p 3.19(16.79%)	d 9.83(51.78%)	f 4.97(26.17%)
512.	(0.00000)	RY (24)	S 14	s(4.68%)	p 2.22(10.39%)	d15.06(70.45%)	f 3.09(14.48%)
513.	(0.00000)	RY (25)	S 14	s(9.39%)	p 1.04(9.78%)	d 2.96(27.82%)	f 5.64(53.00%)
514.	(0.00000)	RY (26)	S 14	s(11.46%)	p 1.81(20.77%)	d 3.47(39.76%)	f 2.44(28.01%)
515.	(0.00000)	RY (27)	S 14	s(3.17%)	p 2.47(7.84%)	d16.05(50.91%)	f12.01(38.09%)
516.	(0.00000)	RY (28)	S 14	s(0.00%)	p 1.00(5.53%)	d 2.44(13.52%)	f14.64(80.95%)
517.	(0.00000)	RY (29)	S 14	s(0.00%)	p 1.00(0.21%)	d 7.93(1.68%)	f99.99(98.11%)
518.	(0.00000)	RY (30)	S 14	s(31.99%)	p 0.27(8.48%)	d 0.64(20.61%)	f 1.22(38.92%)
519.	(0.00000)	RY (31)	S 14	s(1.42%)	p 1.66(2.37%)	d 3.76(5.35%)	f63.82(90.86%)
520.	(0.00000)	RY (32)	S 14	s(16.70%)	p 0.09(1.55%)	d 1.68(28.07%)	f 3.21(53.68%)
521.	(0.00000)	RY (33)	S 14	s(2.65%)	p 4.21(11.15%)	d 6.35(16.81%)	f26.20(69.39%)
522.	(0.00000)	RY (34)	S 14	s(0.00%)	p 1.00(3.32%)	d 2.71(9.01%)	f26.41(87.67%)
523.	(0.00000)	RY (35)	S 14	s(0.00%)	p 1.00(1.02%)	d43.15(43.96%)	f54.01(55.02%)
524.	(0.00000)	RY (36)	S 14	s(0.00%)	p 1.00(2.02%)	d 2.61(5.26%)	f45.97(92.73%)
525.	(0.00000)	RY (37)	S 14	s(0.00%)	p 1.00(0.79%)	d14.48(11.44%)	f99.99(87.77%)
526.	(0.00000)	RY (38)	S 14	s(12.61%)	p 1.05(13.27%)	d 3.15(39.72%)	f 2.73(34.40%)
527.	(0.00000)	RY (39)	S 14	s(2.82%)	p 3.03(8.55%)	d 9.30(26.24%)	f22.11(62.39%)
528.	(0.00000)	RY (40)	S 14	s(6.00%)	p 1.52(9.14%)	d12.55(75.31%)	f 1.59(9.55%)
529.	(0.00000)	RY (41)	S 14	s(2.20%)	p 0.94(2.07%)	d12.13(26.67%)	f31.41(69.06%)

NHO DIRECTIONALITY AND BOND BENDING (deviation from line of nuclear centers at the position of maximum hybrid amplitude)

[Thresholds for printing: angular deviation > 1.0 degree]
p- or d-character > 25.0%
orbital occupancy > 0.10e

NBO	Line of Centers		Hybrid 1			Hybrid 2		
	Theta	Phi	Theta	Phi	Dev	Theta	Phi	Dev
15. LP (2) S 14	--	--	5.6	72.6	--	--	--	--
16. BD (1) C 1- C 2	90.0	164.2	90.0	165.7	1.5	90.0	340.1	4.1
17. BD (2) C 1- C 2	90.0	164.2	0.9	145.5	89.2	0.7	351.2	89.3
18. BD (1) C 1- C 6	90.0	44.9	90.0	42.7	2.2	90.0	227.1	2.2
20. BD (1) C 2- C 3	90.0	104.9	90.0	108.3	3.5	--	--	--
21. BD (1) C 2- N 12	90.0	223.9	90.0	221.4	2.4	90.0	48.6	4.7
22. BD (1) C 3- C 4	90.0	44.3	90.0	46.0	1.7	90.0	221.6	2.7
23. BD (2) C 3- C 4	90.0	44.3	0.9	22.5	89.1	0.9	241.2	89.1
25. BD (1) C 4- C 5	90.0	344.6	90.0	346.8	2.1	90.0	162.3	2.3
27. BD (1) C 5- C 6	90.0	284.5	90.0	286.9	2.4	90.0	102.3	2.2
28. BD (2) C 5- C 6	90.0	284.5	0.8	260.4	89.3	0.8	128.2	89.3
31. BD (1) N 12- C 13	90.0	257.3	90.0	249.9	7.4	90.0	91.2	13.9
32. BD (2) N 12- C 13	90.0	257.3	0.9	281.0	89.2	1.8	77.0	88.2
33. BD (3) N 12- C 13	90.0	257.3	90.0	329.4	72.1	90.0	12.0	65.3
34. BD (1) C 13- S 14	90.0	252.6	90.0	277.8	25.2	90.0	40.9	31.7
35. BD (2) C 13- S 14	90.0	252.6	90.0	211.0	41.6	90.0	126.1	53.5

3-Center, 4-Electron A:-B-:C Hyperbonds (A-B :C <=> A: B-C)
 [threshold for detection: 33.3%]

Hyperbond A:-B-:C	%A-B/%B-C	occ	NBOs		3-center hybrids		
			BD(A-B)	LP(C)	h(A)	h(B)	h(C)
1. N 12:- C 13-: S 14	58.1/41.9	3.9497	32	15	48	49	15

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
within unit 1				
14. LP (1) S 14	51. BD*(1) N 12- C 13	12.45	1.29	0.113
14. LP (1) S 14	55. BD*(2) C 13- S 14	2.49	0.97	0.044
14. LP (1) S 14	450. RY (2) C 13	2.22	1.84	0.057
15. LP (2) S 14	52. BD*(2) N 12- C 13	74.10	0.23	0.116
15. LP (2) S 14	449. RY (1) C 13	0.94	1.76	0.036
15. LP (2) S 14	462. RY (14) C 13	0.54	1.14	0.022
15. LP (2) S 14	489. RY (1) S 14	3.96	0.95	0.055
15. LP (2) S 14	508. RY (20) S 14	1.09	1.08	0.031
16. BD (1) C 1- C 2	38. BD*(1) C 1- C 6	1.28	1.16	0.034
16. BD (1) C 1- C 2	40. BD*(1) C 2- C 3	2.41	1.15	0.047
16. BD (1) C 1- C 2	41. BD*(1) C 2- N 12	1.31	1.04	0.033
16. BD (1) C 1- C 2	44. BD*(1) C 3- H 8	1.66	1.06	0.037
16. BD (1) C 1- C 2	50. BD*(1) C 6- H 11	2.21	1.03	0.043
16. BD (1) C 1- C 2	51. BD*(1) N 12- C 13	1.24	1.36	0.037
16. BD (1) C 1- C 2	53. BD*(3) N 12- C 13	0.91	1.39	0.032
16. BD (1) C 1- C 2	140. RY (3) C 3	1.54	4.30	0.073
16. BD (1) C 1- C 2	141. RY (4) C 3	0.69	3.68	0.045
16. BD (1) C 1- C 2	148. RY (11) C 3	0.51	2.81	0.034
16. BD (1) C 1- C 2	258. RY (1) C 6	1.21	2.41	0.048
16. BD (1) C 1- C 2	259. RY (2) C 6	1.37	2.74	0.055
16. BD (1) C 1- C 2	302. RY (4) H 7	0.52	3.75	0.040
16. BD (1) C 1- C 2	408. RY (1) N 12	1.61	1.69	0.047
16. BD (1) C 1- C 2	410. RY (3) N 12	0.91	2.39	0.042

16.	BD	(1)	C	1-	C	2	411.	RY	(4)	N	12	1.21	4.08	0.063
16.	BD	(1)	C	1-	C	2	413.	RY	(6)	N	12	1.02	2.45	0.045
16.	BD	(1)	C	1-	C	2	416.	RY	(9)	N	12	0.81	4.14	0.052
16.	BD	(1)	C	1-	C	2	455.	RY	(7)	C	13	0.60	4.50	0.047
17.	BD	(2)	C	1-	C	2	43.	BD*	(2)	C	3- C 4	17.18	0.28	0.062
17.	BD	(2)	C	1-	C	2	48.	BD*	(2)	C	5- C 6	20.28	0.29	0.068
17.	BD	(2)	C	1-	C	2	52.	BD*	(2)	N	12- C 13	15.84	0.27	0.059
17.	BD	(2)	C	1-	C	2	260.	RY	(3)	C	6	1.12	1.14	0.032
17.	BD	(2)	C	1-	C	2	409.	RY	(2)	N	12	1.09	1.16	0.032
18.	BD	(1)	C	1-	C	6	36.	BD*	(1)	C	1- C 2	1.26	1.14	0.034
18.	BD	(1)	C	1-	C	6	39.	BD*	(1)	C	1- H 7	0.62	1.02	0.022
18.	BD	(1)	C	1-	C	6	41.	BD*	(1)	C	2- N 12	3.60	1.03	0.054
18.	BD	(1)	C	1-	C	6	47.	BD*	(1)	C	5- C 6	1.19	1.15	0.033
18.	BD	(1)	C	1-	C	6	49.	BD*	(1)	C	5- H 10	2.21	1.01	0.042
18.	BD	(1)	C	1-	C	6	98.	RY	(2)	C	2	2.20	2.07	0.060
18.	BD	(1)	C	1-	C	6	99.	RY	(3)	C	2	0.56	2.50	0.033
18.	BD	(1)	C	1-	C	6	102.	RY	(6)	C	2	0.95	2.87	0.047
18.	BD	(1)	C	1-	C	6	217.	RY	(1)	C	5	0.98	2.32	0.043
18.	BD	(1)	C	1-	C	6	218.	RY	(2)	C	5	1.09	2.74	0.049
19.	BD	(1)	C	1-	H	7	40.	BD*	(1)	C	2- C 3	4.16	1.03	0.058
19.	BD	(1)	C	1-	H	7	41.	BD*	(1)	C	2- N 12	0.95	0.92	0.026
19.	BD	(1)	C	1-	H	7	47.	BD*	(1)	C	5- C 6	3.48	1.04	0.054
19.	BD	(1)	C	1-	H	7	50.	BD*	(1)	C	6- H 11	0.71	0.92	0.023
19.	BD	(1)	C	1-	H	7	97.	RY	(1)	C	2	0.87	1.84	0.036
19.	BD	(1)	C	1-	H	7	98.	RY	(2)	C	2	0.58	1.96	0.030
19.	BD	(1)	C	1-	H	7	99.	RY	(3)	C	2	1.89	2.39	0.060
19.	BD	(1)	C	1-	H	7	102.	RY	(6)	C	2	1.04	2.76	0.048
19.	BD	(1)	C	1-	H	7	106.	RY	(10)	C	2	0.80	3.11	0.044
19.	BD	(1)	C	1-	H	7	109.	RY	(13)	C	2	0.51	4.23	0.041
19.	BD	(1)	C	1-	H	7	113.	RY	(17)	C	2	0.51	4.27	0.042
19.	BD	(1)	C	1-	H	7	258.	RY	(1)	C	6	1.40	2.30	0.051
19.	BD	(1)	C	1-	H	7	261.	RY	(4)	C	6	1.27	3.57	0.060
19.	BD	(1)	C	1-	H	7	264.	RY	(7)	C	6	0.88	2.76	0.044
20.	BD	(1)	C	2-	C	3	36.	BD*	(1)	C	1- C 2	1.79	1.14	0.040
20.	BD	(1)	C	2-	C	3	39.	BD*	(1)	C	1- H 7	2.00	1.02	0.040
20.	BD	(1)	C	2-	C	3	41.	BD*	(1)	C	2- N 12	0.66	1.04	0.023
20.	BD	(1)	C	2-	C	3	42.	BD*	(1)	C	3- C 4	0.52	1.16	0.022
20.	BD	(1)	C	2-	C	3	46.	BD*	(1)	C	4- H 9	2.49	1.03	0.045
20.	BD	(1)	C	2-	C	3	51.	BD*	(1)	N	12- C 13	3.35	1.36	0.060
20.	BD	(1)	C	2-	C	3	56.	RY	(1)	C	1	0.67	2.43	0.036
20.	BD	(1)	C	2-	C	3	57.	RY	(2)	C	1	1.47	2.86	0.058
20.	BD	(1)	C	2-	C	3	60.	RY	(5)	C	1	0.57	3.98	0.042
20.	BD	(1)	C	2-	C	3	98.	RY	(2)	C	2	0.62	2.08	0.032
20.	BD	(1)	C	2-	C	3	176.	RY	(1)	C	4	3.84	2.04	0.079
20.	BD	(1)	C	2-	C	3	177.	RY	(2)	C	4	0.79	2.16	0.037
20.	BD	(1)	C	2-	C	3	321.	RY	(1)	H	8	0.94	1.95	0.038
20.	BD	(1)	C	2-	C	3	408.	RY	(1)	N	12	2.91	1.69	0.062
20.	BD	(1)	C	2-	C	3	411.	RY	(4)	N	12	0.96	4.07	0.056
20.	BD	(1)	C	2-	C	3	414.	RY	(7)	N	12	0.53	4.04	0.041
21.	BD	(1)	C	2-	N	12	38.	BD*	(1)	C	1- C 6	1.15	1.29	0.034
21.	BD	(1)	C	2-	N	12	40.	BD*	(1)	C	2- C 3	0.63	1.28	0.025
21.	BD	(1)	C	2-	N	12	42.	BD*	(1)	C	3- C 4	1.04	1.29	0.033
21.	BD	(1)	C	2-	N	12	51.	BD*	(1)	N	12- C 13	2.41	1.49	0.054
21.	BD	(1)	C	2-	N	12	53.	BD*	(3)	N	12- C 13	0.51	1.52	0.025
21.	BD	(1)	C	2-	N	12	54.	BD*	(1)	C	13- S 14	1.55	1.15	0.038
21.	BD	(1)	C	2-	N	12	55.	BD*	(2)	C	13- S 14	1.23	1.17	0.034
21.	BD	(1)	C	2-	N	12	56.	RY	(1)	C	1	0.51	2.57	0.032
21.	BD	(1)	C	2-	N	12	57.	RY	(2)	C	1	0.56	2.99	0.036
21.	BD	(1)	C	2-	N	12	450.	RY	(2)	C	13	2.56	2.04	0.064
21.	BD	(1)	C	2-	N	12	451.	RY	(3)	C	13	1.26	2.65	0.052
22.	BD	(1)	C	3-	C	4	40.	BD*	(1)	C	2- C 3	0.63	1.14	0.024
22.	BD	(1)	C	3-	C	4	41.	BD*	(1)	C	2- N 12	3.77	1.03	0.056
22.	BD	(1)	C	3-	C	4	45.	BD*	(1)	C	4- C 5	1.12	1.15	0.032

22.	BD	(1)	C	3-	C	4	49.	BD*	(1)	C	5-	H	10	2.27	1.01	0.043
22.	BD	(1)	C	3-	C	4	97.	RY	(1)	C	2			4.79	1.94	0.086
22.	BD	(1)	C	3-	C	4	98.	RY	(2)	C	2			0.87	2.07	0.038
22.	BD	(1)	C	3-	C	4	217.	RY	(1)	C	5			1.15	2.32	0.046
22.	BD	(1)	C	3-	C	4	218.	RY	(2)	C	5			0.94	2.74	0.045
22.	BD	(1)	C	3-	C	4	321.	RY	(1)	H	8			0.83	1.95	0.036
23.	BD	(2)	C	3-	C	4	37.	BD*	(2)	C	1-	C	2	22.26	0.27	0.069
23.	BD	(2)	C	3-	C	4	48.	BD*	(2)	C	5-	C	6	19.95	0.28	0.066
23.	BD	(2)	C	3-	C	4	100.	RY	(4)	C	2			2.14	1.29	0.047
23.	BD	(2)	C	3-	C	4	219.	RY	(3)	C	5			1.25	1.11	0.033
24.	BD	(1)	C	3-	H	8	36.	BD*	(1)	C	1-	C	2	4.60	1.03	0.061
24.	BD	(1)	C	3-	H	8	41.	BD*	(1)	C	2-	N	12	1.14	0.92	0.029
24.	BD	(1)	C	3-	H	8	45.	BD*	(1)	C	4-	C	5	4.09	1.04	0.058
24.	BD	(1)	C	3-	H	8	46.	BD*	(1)	C	4-	H	9	0.68	0.91	0.022
24.	BD	(1)	C	3-	H	8	97.	RY	(1)	C	2			4.76	1.83	0.083
24.	BD	(1)	C	3-	H	8	102.	RY	(6)	C	2			0.67	2.75	0.038
24.	BD	(1)	C	3-	H	8	114.	RY	(18)	C	2			0.61	4.83	0.049
24.	BD	(1)	C	3-	H	8	116.	RY	(20)	C	2			0.54	5.39	0.048
24.	BD	(1)	C	3-	H	8	176.	RY	(1)	C	4			2.15	1.92	0.057
24.	BD	(1)	C	3-	H	8	179.	RY	(4)	C	4			0.92	2.42	0.042
25.	BD	(1)	C	4-	C	5	42.	BD*	(1)	C	3-	C	4	1.26	1.16	0.034
25.	BD	(1)	C	4-	C	5	44.	BD*	(1)	C	3-	H	8	2.00	1.05	0.041
25.	BD	(1)	C	4-	C	5	46.	BD*	(1)	C	4-	H	9	0.61	1.03	0.022
25.	BD	(1)	C	4-	C	5	47.	BD*	(1)	C	5-	C	6	1.10	1.15	0.032
25.	BD	(1)	C	4-	C	5	50.	BD*	(1)	C	6-	H	11	2.28	1.03	0.043
25.	BD	(1)	C	4-	C	5	138.	RY	(1)	C	3			1.10	3.10	0.052
25.	BD	(1)	C	4-	C	5	140.	RY	(3)	C	3			0.72	4.29	0.050
25.	BD	(1)	C	4-	C	5	258.	RY	(1)	C	6			1.17	2.41	0.047
25.	BD	(1)	C	4-	C	5	259.	RY	(2)	C	6			1.06	2.73	0.048
26.	BD	(1)	C	4-	H	9	40.	BD*	(1)	C	2-	C	3	3.26	1.03	0.052
26.	BD	(1)	C	4-	H	9	47.	BD*	(1)	C	5-	C	6	3.76	1.04	0.056
26.	BD	(1)	C	4-	H	9	49.	BD*	(1)	C	5-	H	10	0.69	0.90	0.022
26.	BD	(1)	C	4-	H	9	138.	RY	(1)	C	3			0.98	2.99	0.048
26.	BD	(1)	C	4-	H	9	139.	RY	(2)	C	3			1.74	2.81	0.063
26.	BD	(1)	C	4-	H	9	217.	RY	(1)	C	5			1.64	2.21	0.054
26.	BD	(1)	C	4-	H	9	220.	RY	(4)	C	5			0.88	3.33	0.048
26.	BD	(1)	C	4-	H	9	222.	RY	(6)	C	5			0.54	3.28	0.038
27.	BD	(1)	C	5-	C	6	38.	BD*	(1)	C	1-	C	6	1.16	1.15	0.033
27.	BD	(1)	C	5-	C	6	39.	BD*	(1)	C	1-	H	7	2.29	1.02	0.043
27.	BD	(1)	C	5-	C	6	45.	BD*	(1)	C	4-	C	5	1.11	1.15	0.032
27.	BD	(1)	C	5-	C	6	46.	BD*	(1)	C	4-	H	9	2.31	1.03	0.043
27.	BD	(1)	C	5-	C	6	50.	BD*	(1)	C	6-	H	11	0.58	1.02	0.022
27.	BD	(1)	C	5-	C	6	56.	RY	(1)	C	1			1.47	2.43	0.053
27.	BD	(1)	C	5-	C	6	57.	RY	(2)	C	1			0.81	2.85	0.043
27.	BD	(1)	C	5-	C	6	64.	RY	(9)	C	1			0.64	3.68	0.043
27.	BD	(1)	C	5-	C	6	177.	RY	(2)	C	4			1.60	2.15	0.052
27.	BD	(1)	C	5-	C	6	367.	RY	(3)	H	10			0.55	3.56	0.039
27.	BD	(1)	C	5-	C	6	386.	RY	(1)	H	11			0.55	1.45	0.025
28.	BD	(2)	C	5-	C	6	37.	BD*	(2)	C	1-	C	2	21.07	0.27	0.067
28.	BD	(2)	C	5-	C	6	43.	BD*	(2)	C	3-	C	4	21.33	0.27	0.068
28.	BD	(2)	C	5-	C	6	58.	RY	(3)	C	1			0.54	1.18	0.022
28.	BD	(2)	C	5-	C	6	61.	RY	(6)	C	1			0.72	2.49	0.038
28.	BD	(2)	C	5-	C	6	181.	RY	(6)	C	4			0.84	2.11	0.038
29.	BD	(1)	C	5-	H	10	38.	BD*	(1)	C	1-	C	6	3.70	1.04	0.055
29.	BD	(1)	C	5-	H	10	42.	BD*	(1)	C	3-	C	4	3.72	1.04	0.056
29.	BD	(1)	C	5-	H	10	46.	BD*	(1)	C	4-	H	9	0.68	0.91	0.022
29.	BD	(1)	C	5-	H	10	50.	BD*	(1)	C	6-	H	11	0.69	0.91	0.022
29.	BD	(1)	C	5-	H	10	176.	RY	(1)	C	4			0.94	1.92	0.038
29.	BD	(1)	C	5-	H	10	177.	RY	(2)	C	4			1.05	2.04	0.041
29.	BD	(1)	C	5-	H	10	180.	RY	(5)	C	4			1.30	3.66	0.062
29.	BD	(1)	C	5-	H	10	258.	RY	(1)	C	6			1.62	2.29	0.054
29.	BD	(1)	C	5-	H	10	261.	RY	(4)	C	6			0.80	3.57	0.048
29.	BD	(1)	C	5-	H	10	262.	RY	(5)	C	6			0.60	3.26	0.039

29. BD (1) C 5- H 10	265. RY (8) C 6	0.72	3.78	0.047
29. BD (1) C 5- H 10	370. RY (6) H 10	0.73	2.83	0.041
30. BD (1) C 6- H 11	36. BD*(1) C 1- C 2	3.57	1.03	0.054
30. BD (1) C 6- H 11	39. BD*(1) C 1- H 7	0.62	0.91	0.021
30. BD (1) C 6- H 11	45. BD*(1) C 4- C 5	3.70	1.04	0.055
30. BD (1) C 6- H 11	49. BD*(1) C 5- H 10	0.70	0.90	0.022
30. BD (1) C 6- H 11	56. RY (1) C 1	2.05	2.32	0.062
30. BD (1) C 6- H 11	60. RY (5) C 1	1.40	3.86	0.066
30. BD (1) C 6- H 11	217. RY (1) C 5	1.29	2.21	0.048
30. BD (1) C 6- H 11	220. RY (4) C 5	1.14	3.33	0.055
30. BD (1) C 6- H 11	222. RY (6) C 5	0.58	3.28	0.039
31. BD (1) N 12- C 13	41. BD*(1) C 2- N 12	1.84	1.28	0.043
31. BD (1) N 12- C 13	53. BD*(3) N 12- C 13	10.30	1.63	0.116
31. BD (1) N 12- C 13	54. BD*(1) C 13- S 14	5.45	1.26	0.074
31. BD (1) N 12- C 13	55. BD*(2) C 13- S 14	3.05	1.29	0.056
31. BD (1) N 12- C 13	98. RY (2) C 2	1.65	2.33	0.055
31. BD (1) N 12- C 13	102. RY (6) C 2	1.46	3.12	0.060
31. BD (1) N 12- C 13	411. RY (4) N 12	0.86	4.32	0.054
31. BD (1) N 12- C 13	451. RY (3) C 13	0.70	2.76	0.039
32. BD (2) N 12- C 13	37. BD*(2) C 1- C 2	13.98	0.39	0.066
32. BD (2) N 12- C 13	52. BD*(2) N 12- C 13	1.04	0.39	0.018
32. BD (2) N 12- C 13	101. RY (5) C 2	2.27	1.54	0.053
32. BD (2) N 12- C 13	489. RY (1) S 14	1.90	1.11	0.041
33. BD (3) N 12- C 13	36. BD*(1) C 1- C 2	4.65	0.78	0.054
33. BD (3) N 12- C 13	40. BD*(1) C 2- C 3	6.63	0.78	0.064
33. BD (3) N 12- C 13	41. BD*(1) C 2- N 12	3.94	0.67	0.046
33. BD (3) N 12- C 13	51. BD*(1) N 12- C 13	3.72	0.99	0.054
33. BD (3) N 12- C 13	53. BD*(3) N 12- C 13	69.55	1.01	0.237
33. BD (3) N 12- C 13	54. BD*(1) C 13- S 14	58.29	0.65	0.173
33. BD (3) N 12- C 13	55. BD*(2) C 13- S 14	141.11	0.67	0.275
33. BD (3) N 12- C 13	67. RY (12) C 1	0.63	2.77	0.037
33. BD (3) N 12- C 13	97. RY (1) C 2	1.24	1.58	0.040
33. BD (3) N 12- C 13	98. RY (2) C 2	3.06	1.71	0.065
33. BD (3) N 12- C 13	99. RY (3) C 2	5.53	2.13	0.097
33. BD (3) N 12- C 13	102. RY (6) C 2	1.50	2.50	0.055
33. BD (3) N 12- C 13	109. RY (13) C 2	0.50	3.97	0.040
33. BD (3) N 12- C 13	116. RY (20) C 2	0.88	5.14	0.060
33. BD (3) N 12- C 13	142. RY (5) C 3	0.53	2.15	0.030
33. BD (3) N 12- C 13	148. RY (11) C 3	1.01	2.44	0.044
33. BD (3) N 12- C 13	154. RY (17) C 3	0.61	3.35	0.040
33. BD (3) N 12- C 13	408. RY (1) N 12	0.67	1.32	0.027
33. BD (3) N 12- C 13	410. RY (3) N 12	4.07	2.02	0.081
33. BD (3) N 12- C 13	411. RY (4) N 12	6.67	3.70	0.140
33. BD (3) N 12- C 13	413. RY (6) N 12	1.90	2.08	0.056
33. BD (3) N 12- C 13	416. RY (9) N 12	7.86	3.76	0.154
33. BD (3) N 12- C 13	417. RY (10) N 12	0.57	2.19	0.031
33. BD (3) N 12- C 13	418. RY (11) N 12	2.69	2.88	0.079
33. BD (3) N 12- C 13	420. RY (13) N 12	1.88	3.07	0.068
33. BD (3) N 12- C 13	421. RY (14) N 12	1.89	3.80	0.076
33. BD (3) N 12- C 13	432. RY (25) N 12	1.31	3.52	0.061
33. BD (3) N 12- C 13	433. RY (26) N 12	1.09	4.65	0.064
33. BD (3) N 12- C 13	434. RY (27) N 12	2.20	2.93	0.072
33. BD (3) N 12- C 13	446. RY (39) N 12	1.55	4.98	0.079
33. BD (3) N 12- C 13	447. RY (40) N 12	0.94	4.54	0.058
33. BD (3) N 12- C 13	448. RY (41) N 12	1.05	4.43	0.061
33. BD (3) N 12- C 13	450. RY (2) C 13	0.82	1.54	0.032
33. BD (3) N 12- C 13	451. RY (3) C 13	13.58	2.15	0.152
33. BD (3) N 12- C 13	453. RY (5) C 13	3.17	1.98	0.071
33. BD (3) N 12- C 13	455. RY (7) C 13	0.58	4.13	0.044
33. BD (3) N 12- C 13	458. RY (10) C 13	3.66	2.23	0.081
33. BD (3) N 12- C 13	460. RY (12) C 13	2.30	5.29	0.099
33. BD (3) N 12- C 13	465. RY (17) C 13	2.11	2.75	0.068
33. BD (3) N 12- C 13	473. RY (25) C 13	2.21	2.50	0.066

33.	BD (3) N 12- C 13	474.	RY (26) C 13	0.52	2.33	0.031
33.	BD (3) N 12- C 13	478.	RY (30) C 13	1.11	2.38	0.046
33.	BD (3) N 12- C 13	479.	RY (31) C 13	1.36	3.07	0.058
33.	BD (3) N 12- C 13	481.	RY (33) C 13	5.33	2.34	0.100
33.	BD (3) N 12- C 13	486.	RY (38) C 13	4.71	3.09	0.108
33.	BD (3) N 12- C 13	488.	RY (40) C 13	0.88	2.51	0.042
33.	BD (3) N 12- C 13	490.	RY (2) S 14	6.86	1.02	0.075
33.	BD (3) N 12- C 13	491.	RY (3) S 14	4.54	1.29	0.068
33.	BD (3) N 12- C 13	492.	RY (4) S 14	1.61	1.18	0.039
33.	BD (3) N 12- C 13	494.	RY (6) S 14	2.79	1.91	0.065
33.	BD (3) N 12- C 13	498.	RY (10) S 14	1.52	2.14	0.051
33.	BD (3) N 12- C 13	500.	RY (12) S 14	0.82	1.31	0.029
33.	BD (3) N 12- C 13	514.	RY (26) S 14	1.26	1.84	0.043
33.	BD (3) N 12- C 13	528.	RY (40) S 14	0.56	1.44	0.025
34.	BD (1) C 13- S 14	41.	BD*(1) C 2- N 12	0.81	0.84	0.023
34.	BD (1) C 13- S 14	51.	BD*(1) N 12- C 13	9.11	1.16	0.092
34.	BD (1) C 13- S 14	53.	BD*(3) N 12- C 13	152.14	1.19	0.380
34.	BD (1) C 13- S 14	54.	BD*(1) C 13- S 14	12.61	0.82	0.091
34.	BD (1) C 13- S 14	55.	BD*(2) C 13- S 14	177.54	0.85	0.346
34.	BD (1) C 13- S 14	67.	RY (12) C 1	0.77	2.94	0.043
34.	BD (1) C 13- S 14	72.	RY (17) C 1	0.53	3.73	0.040
34.	BD (1) C 13- S 14	97.	RY (1) C 2	1.43	1.76	0.045
34.	BD (1) C 13- S 14	98.	RY (2) C 2	0.52	1.89	0.028
34.	BD (1) C 13- S 14	99.	RY (3) C 2	1.94	2.31	0.060
34.	BD (1) C 13- S 14	102.	RY (6) C 2	1.69	2.68	0.060
34.	BD (1) C 13- S 14	103.	RY (7) C 2	0.60	2.00	0.031
34.	BD (1) C 13- S 14	109.	RY (13) C 2	0.66	4.15	0.047
34.	BD (1) C 13- S 14	114.	RY (18) C 2	1.24	4.75	0.069
34.	BD (1) C 13- S 14	115.	RY (19) C 2	0.64	5.03	0.051
34.	BD (1) C 13- S 14	116.	RY (20) C 2	1.43	5.31	0.078
34.	BD (1) C 13- S 14	148.	RY (11) C 3	1.10	2.61	0.048
34.	BD (1) C 13- S 14	154.	RY (17) C 3	0.61	3.53	0.041
34.	BD (1) C 13- S 14	303.	RY (5) H 7	0.52	2.53	0.032
34.	BD (1) C 13- S 14	408.	RY (1) N 12	1.70	1.49	0.045
34.	BD (1) C 13- S 14	410.	RY (3) N 12	0.84	2.20	0.038
34.	BD (1) C 13- S 14	411.	RY (4) N 12	15.32	3.88	0.218
34.	BD (1) C 13- S 14	413.	RY (6) N 12	2.16	2.25	0.062
34.	BD (1) C 13- S 14	416.	RY (9) N 12	8.53	3.94	0.164
34.	BD (1) C 13- S 14	417.	RY (10) N 12	1.04	2.37	0.044
34.	BD (1) C 13- S 14	418.	RY (11) N 12	4.40	3.06	0.104
34.	BD (1) C 13- S 14	420.	RY (13) N 12	2.43	3.25	0.079
34.	BD (1) C 13- S 14	421.	RY (14) N 12	2.82	3.97	0.095
34.	BD (1) C 13- S 14	428.	RY (21) N 12	0.59	3.44	0.040
34.	BD (1) C 13- S 14	432.	RY (25) N 12	0.67	3.70	0.045
34.	BD (1) C 13- S 14	433.	RY (26) N 12	2.34	4.83	0.095
34.	BD (1) C 13- S 14	434.	RY (27) N 12	4.61	3.11	0.107
34.	BD (1) C 13- S 14	441.	RY (34) N 12	0.64	6.14	0.056
34.	BD (1) C 13- S 14	446.	RY (39) N 12	2.45	5.16	0.100
34.	BD (1) C 13- S 14	447.	RY (40) N 12	1.32	4.72	0.070
34.	BD (1) C 13- S 14	448.	RY (41) N 12	0.83	4.61	0.055
34.	BD (1) C 13- S 14	450.	RY (2) C 13	1.34	1.72	0.043
34.	BD (1) C 13- S 14	451.	RY (3) C 13	18.26	2.32	0.184
34.	BD (1) C 13- S 14	453.	RY (5) C 13	3.00	2.15	0.072
34.	BD (1) C 13- S 14	455.	RY (7) C 13	0.84	4.31	0.054
34.	BD (1) C 13- S 14	457.	RY (9) C 13	0.53	1.89	0.028
34.	BD (1) C 13- S 14	458.	RY (10) C 13	4.11	2.41	0.089
34.	BD (1) C 13- S 14	460.	RY (12) C 13	2.87	5.47	0.112
34.	BD (1) C 13- S 14	464.	RY (16) C 13	0.67	3.45	0.043
34.	BD (1) C 13- S 14	465.	RY (17) C 13	2.70	2.93	0.079
34.	BD (1) C 13- S 14	471.	RY (23) C 13	0.92	1.73	0.036
34.	BD (1) C 13- S 14	473.	RY (25) C 13	3.56	2.68	0.087
34.	BD (1) C 13- S 14	474.	RY (26) C 13	0.92	2.50	0.043
34.	BD (1) C 13- S 14	478.	RY (30) C 13	1.16	2.55	0.049

34. BD (1) C 13- S 14	479. RY (31) C 13	1.84	3.25	0.069
34. BD (1) C 13- S 14	481. RY (33) C 13	6.89	2.52	0.118
34. BD (1) C 13- S 14	486. RY (38) C 13	5.96	3.27	0.125
34. BD (1) C 13- S 14	488. RY (40) C 13	1.01	2.68	0.047
34. BD (1) C 13- S 14	490. RY (2) S 14	9.11	1.20	0.093
34. BD (1) C 13- S 14	491. RY (3) S 14	3.11	1.47	0.060
34. BD (1) C 13- S 14	492. RY (4) S 14	3.02	1.35	0.057
34. BD (1) C 13- S 14	494. RY (6) S 14	4.33	2.09	0.085
34. BD (1) C 13- S 14	498. RY (10) S 14	2.74	2.31	0.071
34. BD (1) C 13- S 14	500. RY (12) S 14	1.09	1.48	0.036
34. BD (1) C 13- S 14	514. RY (26) S 14	1.14	2.02	0.043
35. BD (2) C 13- S 14	41. BD*(1) C 2- N 12	2.81	0.65	0.038
35. BD (2) C 13- S 14	51. BD*(1) N 12- C 13	0.90	0.97	0.026
35. BD (2) C 13- S 14	53. BD*(3) N 12- C 13	203.70	0.99	0.401
35. BD (2) C 13- S 14	54. BD*(1) C 13- S 14	144.03	0.62	0.268
35. BD (2) C 13- S 14	55. BD*(2) C 13- S 14	50.65	0.65	0.162
35. BD (2) C 13- S 14	67. RY (12) C 1	0.89	2.74	0.044
35. BD (2) C 13- S 14	70. RY (15) C 1	0.59	3.00	0.037
35. BD (2) C 13- S 14	72. RY (17) C 1	0.60	3.53	0.041
35. BD (2) C 13- S 14	73. RY (18) C 1	0.76	4.34	0.051
35. BD (2) C 13- S 14	99. RY (3) C 2	0.89	2.11	0.039
35. BD (2) C 13- S 14	102. RY (6) C 2	1.85	2.48	0.060
35. BD (2) C 13- S 14	103. RY (7) C 2	0.50	1.81	0.027
35. BD (2) C 13- S 14	114. RY (18) C 2	1.22	4.55	0.067
35. BD (2) C 13- S 14	115. RY (19) C 2	1.22	4.83	0.069
35. BD (2) C 13- S 14	116. RY (20) C 2	1.00	5.12	0.064
35. BD (2) C 13- S 14	117. RY (21) C 2	0.54	4.22	0.043
35. BD (2) C 13- S 14	148. RY (11) C 3	1.60	2.42	0.055
35. BD (2) C 13- S 14	154. RY (17) C 3	0.78	3.33	0.046
35. BD (2) C 13- S 14	299. RY (1) H 7	0.54	1.49	0.025
35. BD (2) C 13- S 14	408. RY (1) N 12	1.37	1.30	0.038
35. BD (2) C 13- S 14	410. RY (3) N 12	10.66	2.00	0.130
35. BD (2) C 13- S 14	411. RY (4) N 12	9.30	3.68	0.165
35. BD (2) C 13- S 14	413. RY (6) N 12	3.75	2.06	0.078
35. BD (2) C 13- S 14	414. RY (7) N 12	1.60	3.65	0.068
35. BD (2) C 13- S 14	416. RY (9) N 12	10.39	3.74	0.176
35. BD (2) C 13- S 14	417. RY (10) N 12	2.36	2.17	0.064
35. BD (2) C 13- S 14	418. RY (11) N 12	4.27	2.86	0.099
35. BD (2) C 13- S 14	420. RY (13) N 12	2.82	3.05	0.083
35. BD (2) C 13- S 14	421. RY (14) N 12	2.72	3.78	0.090
35. BD (2) C 13- S 14	428. RY (21) N 12	0.70	3.25	0.043
35. BD (2) C 13- S 14	432. RY (25) N 12	3.14	3.50	0.094
35. BD (2) C 13- S 14	433. RY (26) N 12	1.57	4.63	0.076
35. BD (2) C 13- S 14	434. RY (27) N 12	4.38	2.91	0.101
35. BD (2) C 13- S 14	446. RY (39) N 12	1.34	4.96	0.073
35. BD (2) C 13- S 14	447. RY (40) N 12	1.60	4.52	0.076
35. BD (2) C 13- S 14	448. RY (41) N 12	2.24	4.41	0.089
35. BD (2) C 13- S 14	450. RY (2) C 13	1.06	1.52	0.036
35. BD (2) C 13- S 14	451. RY (3) C 13	20.37	2.13	0.186
35. BD (2) C 13- S 14	453. RY (5) C 13	4.30	1.96	0.082
35. BD (2) C 13- S 14	458. RY (10) C 13	3.97	2.21	0.084
35. BD (2) C 13- S 14	460. RY (12) C 13	3.75	5.27	0.125
35. BD (2) C 13- S 14	464. RY (16) C 13	0.72	3.26	0.043
35. BD (2) C 13- S 14	465. RY (17) C 13	4.02	2.73	0.094
35. BD (2) C 13- S 14	470. RY (22) C 13	0.97	3.04	0.049
35. BD (2) C 13- S 14	471. RY (23) C 13	0.67	1.53	0.029
35. BD (2) C 13- S 14	473. RY (25) C 13	3.02	2.48	0.077
35. BD (2) C 13- S 14	474. RY (26) C 13	0.98	2.30	0.042
35. BD (2) C 13- S 14	478. RY (30) C 13	1.35	2.35	0.050
35. BD (2) C 13- S 14	479. RY (31) C 13	1.93	3.05	0.068
35. BD (2) C 13- S 14	481. RY (33) C 13	8.02	2.32	0.122
35. BD (2) C 13- S 14	486. RY (38) C 13	6.07	3.07	0.122
35. BD (2) C 13- S 14	488. RY (40) C 13	1.95	2.49	0.062

35. BD (2) C 13- S 14	490. RY (2) S 14	9.35	1.00	0.086
35. BD (2) C 13- S 14	491. RY (3) S 14	10.75	1.27	0.104
35. BD (2) C 13- S 14	494. RY (6) S 14	1.85	1.89	0.053
35. BD (2) C 13- S 14	496. RY (8) S 14	0.80	1.88	0.035
35. BD (2) C 13- S 14	498. RY (10) S 14	0.92	2.11	0.039
35. BD (2) C 13- S 14	499. RY (11) S 14	2.37	2.77	0.072
35. BD (2) C 13- S 14	512. RY (24) S 14	0.70	2.08	0.034
35. BD (2) C 13- S 14	514. RY (26) S 14	2.08	1.82	0.055
35. BD (2) C 13- S 14	528. RY (40) S 14	1.78	1.42	0.045

NATURAL BOND ORBITALS (Summary):

NBO	Occupancy	Energy	Principal Delocalizations (geminal,vicinal,remote)
=====			
Molecular unit 1 (C7H5NS)			
----- Lewis -----			
1. CR (1) C 1	1.99999	-10.19948	
2. CR (1) C 2	1.99999	-10.25074	
3. CR (1) C 3	1.99999	-10.19766	
4. CR (1) C 4	1.99999	-10.19755	
5. CR (1) C 5	1.99999	-10.19470	
6. CR (1) C 6	1.99999	-10.19823	
7. CR (1) N 12	1.99999	-14.36830	
8. CR (1) C 13	1.99999	-10.29100	
9. CR (1) S 14	2.00000	-81.53444	
10. CR (2) S 14	2.00000	-15.31373	
11. CR (3) S 14	2.00000	-5.90945	
12. CR (4) S 14	2.00000	-5.91402	
13. CR (5) S 14	2.00000	-5.90822	
14. LP (1) S 14	1.97914	-0.54359	51(v),55(g),450(v)
15. LP (2) S 14	1.60967	-0.22858	52(v),489(g),508(g),449(v) 462(v)
16. BD (1) C 1- C 2	1.97245	-0.61520	40(g),50(v),44(v),408(v) 140(v),259(v),41(g),38(g) 51(v),258(v),411(v),413(v) 410(v),53(v),416(v),141(v) 455(r),302(v),148(v)
17. BD (2) C 1- C 2	1.64561	-0.27598	48(v),43(v),52(v),260(v) 409(v)
18. BD (1) C 1- C 6	1.97780	-0.60789	41(v),49(v),98(v),36(g) 47(g),218(v),217(v),102(v) 39(g),99(v)
19. BD (1) C 1- H 7	1.97775	-0.49869	40(v),47(v),99(v),258(v) 261(v),102(v),41(v),264(v) 97(v),106(v),50(v),98(v) 113(v),109(v)
20. BD (1) C 2- C 3	1.97058	-0.61080	176(v),51(v),408(v),46(v) 39(v),36(g),57(v),411(v) 321(v),177(v),56(v),41(g) 98(g),60(v),414(v),42(g)
21. BD (1) C 2- N 12	1.98421	-0.74457	450(v),51(g),54(v),451(v) 55(v),38(v),42(v),40(g) 57(v),53(g),56(v)
22. BD (1) C 3- C 4	1.97411	-0.60395	97(v),41(v),49(v),217(v) 45(g),218(v),98(v),321(v) 40(g)
23. BD (2) C 3- C 4	1.66197	-0.26549	37(v),48(v),100(v),219(v)
24. BD (1) C 3- H 8	1.97067	-0.49249	97(v),36(v),45(v),176(v) 41(v),179(v),46(v),102(v) 114(v),116(v)
25. BD (1) C 4- C 5	1.98300	-0.60621	50(v),44(v),42(g),258(v)

					138(v), 47(g), 259(v), 140(v) 46(g)
26.	BD (1) C 4- H 9	1.97981	-0.49524	47(v), 40(v), 139(v), 217(v) 138(v), 220(v), 49(v), 222(v)	
27.	BD (1) C 5- C 6	1.98158	-0.60511	46(v), 39(v), 177(v), 56(v) 38(g), 45(g), 57(v), 64(v) 50(g), 386(v), 367(v)	
28.	BD (2) C 5- C 6	1.65134	-0.26560	43(v), 37(v), 181(v), 61(v) 58(v)	
29.	BD (1) C 5- H 10	1.97972	-0.49363	42(v), 38(v), 258(v), 180(v) 177(v), 176(v), 261(v), 370(g) 265(v), 50(v), 46(v), 262(v)	
30.	BD (1) C 6- H 11	1.97870	-0.49515	45(v), 36(v), 56(v), 60(v) 217(v), 220(v), 49(v), 39(v) 222(v)	
31.	BD (1) N 12- C 13	1.98444	-0.85961	53(g), 54(g), 55(g), 41(g) 98(v), 102(v), 411(g), 451(g)	
32.	BD (2) N 12- C 13	1.93740	-0.38741	37(v), 101(v), 489(v), 52(g)	
33.	BD (3) N 12- C 13	1.75862	-0.24259	55(g), 53(g), 54(g), 451(g) 416(g), 490(v), 411(g), 40(v) 99(v), 481(g), 486(g), 36(v) 491(v), 410(g), 41(g), 51(g) 458(g), 453(g), 98(v), 494(v) 418(g), 460(g), 473(g), 434(g) 465(g), 413(g), 421(g), 420(g) 492(v), 446(g), 498(v), 102(v) 479(g), 432(g), 514(v), 97(v) 478(g), 433(g), 448(g), 148(r) 447(g), 116(v), 488(g), 500(v) 450(g), 408(g), 67(r), 154(r) 455(g), 417(g), 528(v), 142(r) 474(g), 109(v)	
34.	BD (1) C 13- S 14	1.82991	-0.41964	55(g), 53(g), 451(g), 411(v) 54(g), 51(g), 490(g), 416(v) 481(g), 486(g), 434(v), 418(v) 494(g), 458(g), 473(g), 491(g) 492(g), 453(g), 460(g), 421(v) 498(g), 465(g), 446(v), 420(v) 433(v), 413(v), 99(r), 479(g) 408(v), 102(r), 97(r), 116(r) 450(g), 447(v), 114(r), 478(g) 514(g), 148(r), 500(g), 417(v) 488(g), 471(g), 474(g), 455(g) 410(v), 448(v), 41(v), 67(r) 432(v), 464(g), 109(r), 441(v) 115(r), 154(r), 103(r), 428(v) 457(g), 72(r), 303(r), 98(r)	
35.	BD (2) C 13- S 14	1.76441	-0.22146	53(g), 54(g), 55(g), 451(g) 491(g), 410(v), 416(v), 490(g) 411(v), 481(g), 486(g), 434(v) 453(g), 418(v), 465(g), 458(g) 413(v), 460(g), 432(v), 473(g) 420(v), 41(v), 421(v), 499(g) 417(v), 448(v), 514(g), 488(g) 479(g), 102(r), 494(g), 528(g) 414(v), 148(r), 447(v), 433(v) 408(v), 478(g), 446(v), 115(r) 114(r), 450(g), 116(r), 474(g) 470(g), 498(g), 51(g), 99(r) 67(r), 496(g), 154(r), 73(r) 464(g), 428(v), 512(g), 471(g) 72(r), 70(r), 117(r), 299(r) 103(r)	

----- non-Lewis -----

36.	BD*(1) C	1- C 2	0.02774	0.53277
37.	BD*(2) C	1- C 2	0.40310	0.00344
38.	BD*(1) C	1- C 6	0.01217	0.54753
39.	BD*(1) C	1- H 7	0.01258	0.41148
40.	BD*(1) C	2- C 3	0.02243	0.53301
41.	BD*(1) C	2- N 12	0.03370	0.42526
42.	BD*(1) C	3- C 4	0.01133	0.55006
43.	BD*(2) C	3- C 4	0.31902	0.00722
44.	BD*(1) C	3- H 8	0.01093	0.44164
45.	BD*(1) C	4- C 5	0.01454	0.54417
46.	BD*(1) C	4- H 9	0.01387	0.42009
47.	BD*(1) C	5- C 6	0.01412	0.54349
48.	BD*(2) C	5- C 6	0.33844	0.01143
49.	BD*(1) C	5- H 10	0.01387	0.40525
50.	BD*(1) C	6- H 11	0.01373	0.41931
51.	BD*(1) N	12- C 13	0.03013	0.74427
52.	BD*(2) N	12- C 13	0.40258	-0.00189
53.	BD*(3) N	12- C 13	0.22649	0.77111
54.	BD*(1) C	13- S 14	0.14736	0.40303
55.	BD*(2) C	13- S 14	0.24443	0.42796
56.	RY (1) C	1	0.00409	1.82331
57.	RY (2) C	1	0.00179	2.24511
58.	RY (3) C	1	0.00099	0.91662
59.	RY (4) C	1	0.00073	1.93773
60.	RY (5) C	1	0.00068	3.36761
61.	RY (6) C	1	0.00037	2.22716
62.	RY (7) C	1	0.00031	1.60331
63.	RY (8) C	1	0.00016	2.08021
64.	RY (9) C	1	0.00009	3.07451
65.	RY (10) C	1	0.00008	2.13274
66.	RY (11) C	1	0.00007	1.01462
67.	RY (12) C	1	0.00005	2.52282
68.	RY (13) C	1	0.00004	1.49558
69.	RY (14) C	1	0.00003	2.53970
70.	RY (15) C	1	0.00002	2.77681
71.	RY (16) C	1	0.00001	3.19731
72.	RY (17) C	1	0.00000	3.31218
73.	RY (18) C	1	0.00000	4.11701
74.	RY (19) C	1	0.00000	3.35098
75.	RY (20) C	1	0.00000	3.47325
76.	RY (21) C	1	0.00000	2.36087
77.	RY (22) C	1	0.00000	2.99647
78.	RY (23) C	1	0.00000	1.50422
79.	RY (24) C	1	0.00000	1.65094
80.	RY (25) C	1	0.00000	3.57576
81.	RY (26) C	1	0.00000	1.24579
82.	RY (27) C	1	0.00000	1.98690
83.	RY (28) C	1	0.00000	3.38402
84.	RY (29) C	1	0.00000	2.55076
85.	RY (30) C	1	0.00000	1.77366
86.	RY (31) C	1	0.00000	2.62933
87.	RY (32) C	1	0.00000	3.21189
88.	RY (33) C	1	0.00000	2.66525
89.	RY (34) C	1	0.00000	2.89877
90.	RY (35) C	1	0.00000	2.06535
91.	RY (36) C	1	0.00000	3.45353
92.	RY (37) C	1	0.00000	2.28773
93.	RY (38) C	1	0.00000	3.16679
94.	RY (39) C	1	0.00000	2.51293
95.	RY (40) C	1	0.00000	2.72368
96.	RY (41) C	1	0.00000	2.79932
97.	RY (1) C	2	0.01399	1.33823

98.	RY (2) C 2	0.00622	1.46597
99.	RY (3) C 2	0.00373	1.88866
100.	RY (4) C 2	0.00273	1.02075
101.	RY (5) C 2	0.00203	1.15497
102.	RY (6) C 2	0.00199	2.25998
103.	RY (7) C 2	0.00079	1.58517
104.	RY (8) C 2	0.00053	1.88972
105.	RY (9) C 2	0.00047	2.83275
106.	RY (10) C 2	0.00032	2.60940
107.	RY (11) C 2	0.00028	3.11965
108.	RY (12) C 2	0.00023	1.41942
109.	RY (13) C 2	0.00014	3.72759
110.	RY (14) C 2	0.00006	1.76526
111.	RY (15) C 2	0.00004	3.19932
112.	RY (16) C 2	0.00001	2.57601
113.	RY (17) C 2	0.00001	3.76870
114.	RY (18) C 2	0.00001	4.33295
115.	RY (19) C 2	0.00000	4.60865
116.	RY (20) C 2	0.00000	4.89467
117.	RY (21) C 2	0.00000	4.00244
118.	RY (22) C 2	0.00000	2.28330
119.	RY (23) C 2	0.00000	2.23877
120.	RY (24) C 2	0.00000	1.43960
121.	RY (25) C 2	0.00000	2.54662
122.	RY (26) C 2	0.00000	1.59268
123.	RY (27) C 2	0.00000	2.86633
124.	RY (28) C 2	0.00000	2.74929
125.	RY (29) C 2	0.00000	1.54563
126.	RY (30) C 2	0.00000	3.61197
127.	RY (31) C 2	0.00000	2.88780
128.	RY (32) C 2	0.00000	3.12256
129.	RY (33) C 2	0.00000	2.41277
130.	RY (34) C 2	0.00000	2.53348
131.	RY (35) C 2	0.00000	2.22813
132.	RY (36) C 2	0.00000	3.46682
133.	RY (37) C 2	0.00000	2.61561
134.	RY (38) C 2	0.00000	3.27731
135.	RY (39) C 2	0.00000	3.57725
136.	RY (40) C 2	0.00000	1.39757
137.	RY (41) C 2	0.00000	2.87353
138.	RY (1) C 3	0.00142	2.49354
139.	RY (2) C 3	0.00120	2.31930
140.	RY (3) C 3	0.00077	3.68377
141.	RY (4) C 3	0.00050	3.06757
142.	RY (5) C 3	0.00040	1.90960
143.	RY (6) C 3	0.00036	2.48999
144.	RY (7) C 3	0.00028	1.99478
145.	RY (8) C 3	0.00015	1.29748
146.	RY (9) C 3	0.00013	1.76176
147.	RY (10) C 3	0.00006	2.04612
148.	RY (11) C 3	0.00006	2.19481
149.	RY (12) C 3	0.00003	1.22475
150.	RY (13) C 3	0.00002	3.24882
151.	RY (14) C 3	0.00001	3.29887
152.	RY (15) C 3	0.00001	3.03412
153.	RY (16) C 3	0.00000	2.10112
154.	RY (17) C 3	0.00000	3.10740
155.	RY (18) C 3	0.00000	2.47982
156.	RY (19) C 3	0.00000	3.98569
157.	RY (20) C 3	0.00000	3.26934
158.	RY (21) C 3	0.00000	2.48416
159.	RY (22) C 3	0.00000	1.73017
160.	RY (23) C 3	0.00000	1.47874

161.	RY (24)	C	3	0.00000	1.80570
162.	RY (25)	C	3	0.00000	3.00356
163.	RY (26)	C	3	0.00000	2.79354
164.	RY (27)	C	3	0.00000	2.87422
165.	RY (28)	C	3	0.00000	3.46849
166.	RY (29)	C	3	0.00000	3.53899
167.	RY (30)	C	3	0.00000	2.36675
168.	RY (31)	C	3	0.00000	3.03964
169.	RY (32)	C	3	0.00000	1.60175
170.	RY (33)	C	3	0.00000	3.05805
171.	RY (34)	C	3	0.00000	2.22262
172.	RY (35)	C	3	0.00000	3.31405
173.	RY (36)	C	3	0.00000	2.82710
174.	RY (37)	C	3	0.00000	0.93036
175.	RY (38)	C	3	0.00000	3.11124
176.	RY (1)	C	4	0.00814	1.42801
177.	RY (2)	C	4	0.00285	1.54962
178.	RY (3)	C	4	0.00146	0.93862
179.	RY (4)	C	4	0.00117	1.93244
180.	RY (5)	C	4	0.00049	3.16197
181.	RY (6)	C	4	0.00035	1.84563
182.	RY (7)	C	4	0.00012	2.24689
183.	RY (8)	C	4	0.00004	3.21388
184.	RY (9)	C	4	0.00004	2.68849
185.	RY (10)	C	4	0.00002	2.17530
186.	RY (11)	C	4	0.00001	1.18634
187.	RY (12)	C	4	0.00001	2.46961
188.	RY (13)	C	4	0.00000	3.73183
189.	RY (14)	C	4	0.00000	4.38339
190.	RY (15)	C	4	0.00000	1.14408
191.	RY (16)	C	4	0.00000	2.78875
192.	RY (17)	C	4	0.00000	2.17789
193.	RY (18)	C	4	0.00000	2.60688
194.	RY (19)	C	4	0.00000	2.15876
195.	RY (20)	C	4	0.00000	1.35515
196.	RY (21)	C	4	0.00000	1.90409
197.	RY (22)	C	4	0.00000	3.26852
198.	RY (23)	C	4	0.00000	2.79276
199.	RY (24)	C	4	0.00000	2.65396
200.	RY (25)	C	4	0.00000	2.36991
201.	RY (26)	C	4	0.00000	3.03588
202.	RY (27)	C	4	0.00000	2.54378
203.	RY (28)	C	4	0.00000	2.68093
204.	RY (29)	C	4	0.00000	1.84487
205.	RY (30)	C	4	0.00000	3.22225
206.	RY (31)	C	4	0.00000	2.73631
207.	RY (32)	C	4	0.00000	2.23993
208.	RY (33)	C	4	0.00000	2.58233
209.	RY (34)	C	4	0.00000	3.25356
210.	RY (35)	C	4	0.00000	1.63683
211.	RY (36)	C	4	0.00000	3.41964
212.	RY (37)	C	4	0.00000	1.86335
213.	RY (38)	C	4	0.00000	2.83130
214.	RY (39)	C	4	0.00000	2.97864
215.	RY (40)	C	4	0.00000	2.10334
216.	RY (41)	C	4	0.00000	2.76374
217.	RY (1)	C	5	0.00492	1.71138
218.	RY (2)	C	5	0.00148	2.13288
219.	RY (3)	C	5	0.00095	0.84257
220.	RY (4)	C	5	0.00071	2.83491
221.	RY (5)	C	5	0.00044	1.93477
222.	RY (6)	C	5	0.00039	2.78416
223.	RY (7)	C	5	0.00017	1.96780

224.	RY (8)	C	5	0.00010	1.70454
225.	RY (9)	C	5	0.00004	2.35659
226.	RY (10)	C	5	0.00001	0.83985
227.	RY (11)	C	5	0.00001	2.16407
228.	RY (12)	C	5	0.00001	2.49603
229.	RY (13)	C	5	0.00000	2.76823
230.	RY (14)	C	5	0.00000	4.52521
231.	RY (15)	C	5	0.00000	1.17073
232.	RY (16)	C	5	0.00000	2.90539
233.	RY (17)	C	5	0.00000	3.33313
234.	RY (18)	C	5	0.00000	2.12450
235.	RY (19)	C	5	0.00000	1.69382
236.	RY (20)	C	5	0.00000	2.04265
237.	RY (21)	C	5	0.00000	1.67537
238.	RY (22)	C	5	0.00000	1.31734
239.	RY (23)	C	5	0.00000	2.78843
240.	RY (24)	C	5	0.00000	2.61623
241.	RY (25)	C	5	0.00000	2.48188
242.	RY (26)	C	5	0.00000	4.47736
243.	RY (27)	C	5	0.00000	2.32088
244.	RY (28)	C	5	0.00000	3.28794
245.	RY (29)	C	5	0.00000	3.02480
246.	RY (30)	C	5	0.00000	2.26150
247.	RY (31)	C	5	0.00000	2.98625
248.	RY (32)	C	5	0.00000	2.61830
249.	RY (33)	C	5	0.00000	2.65542
250.	RY (34)	C	5	0.00000	2.45102
251.	RY (35)	C	5	0.00000	3.18950
252.	RY (36)	C	5	0.00000	2.40277
253.	RY (37)	C	5	0.00000	2.62387
254.	RY (38)	C	5	0.00000	2.88532
255.	RY (39)	C	5	0.00000	2.04272
256.	RY (40)	C	5	0.00000	2.54662
257.	RY (41)	C	5	0.00000	2.39678
258.	RY (1)	C	6	0.00464	1.79913
259.	RY (2)	C	6	0.00177	2.12851
260.	RY (3)	C	6	0.00084	0.86722
261.	RY (4)	C	6	0.00075	3.07256
262.	RY (5)	C	6	0.00050	2.76554
263.	RY (6)	C	6	0.00045	2.01438
264.	RY (7)	C	6	0.00019	2.26233
265.	RY (8)	C	6	0.00009	3.29026
266.	RY (9)	C	6	0.00004	2.10573
267.	RY (10)	C	6	0.00002	2.15604
268.	RY (11)	C	6	0.00002	1.85631
269.	RY (12)	C	6	0.00001	2.55220
270.	RY (13)	C	6	0.00001	3.15408
271.	RY (14)	C	6	0.00000	2.75904
272.	RY (15)	C	6	0.00000	3.38225
273.	RY (16)	C	6	0.00000	2.85421
274.	RY (17)	C	6	0.00000	2.90748
275.	RY (18)	C	6	0.00000	2.79712
276.	RY (19)	C	6	0.00000	2.49687
277.	RY (20)	C	6	0.00000	1.26303
278.	RY (21)	C	6	0.00000	1.57581
279.	RY (22)	C	6	0.00000	1.05907
280.	RY (23)	C	6	0.00000	2.25574
281.	RY (24)	C	6	0.00000	2.80355
282.	RY (25)	C	6	0.00000	2.34106
283.	RY (26)	C	6	0.00000	2.31312
284.	RY (27)	C	6	0.00000	3.23475
285.	RY (28)	C	6	0.00000	2.92871
286.	RY (29)	C	6	0.00000	2.35404

287.	RY	(30)	C	6	0.00000	3.05675
288.	RY	(31)	C	6	0.00000	1.78988
289.	RY	(32)	C	6	0.00000	3.02888
290.	RY	(33)	C	6	0.00000	2.17941
291.	RY	(34)	C	6	0.00000	1.18591
292.	RY	(35)	C	6	0.00000	3.04928
293.	RY	(36)	C	6	0.00000	2.05033
294.	RY	(37)	C	6	0.00000	3.04272
295.	RY	(38)	C	6	0.00000	2.38618
296.	RY	(39)	C	6	0.00000	3.39417
297.	RY	(40)	C	6	0.00000	3.00788
298.	RY	(41)	C	6	0.00000	2.16677
299.	RY	(1)	H	7	0.00052	1.26501
300.	RY	(2)	H	7	0.00033	0.64722
301.	RY	(3)	H	7	0.00027	1.53501
302.	RY	(4)	H	7	0.00019	3.13529
303.	RY	(5)	H	7	0.00011	2.11406
304.	RY	(6)	H	7	0.00010	2.13253
305.	RY	(7)	H	7	0.00002	1.98456
306.	RY	(8)	H	7	0.00002	2.25425
307.	RY	(9)	H	7	0.00001	2.21271
308.	RY	(10)	H	7	0.00001	3.32390
309.	RY	(11)	H	7	0.00001	1.31972
310.	RY	(12)	H	7	0.00001	2.83166
311.	RY	(13)	H	7	0.00000	3.08846
312.	RY	(14)	H	7	0.00000	2.34340
313.	RY	(15)	H	7	0.00000	3.80502
314.	RY	(16)	H	7	0.00000	3.10728
315.	RY	(17)	H	7	0.00000	3.91736
316.	RY	(18)	H	7	0.00000	1.93196
317.	RY	(19)	H	7	0.00000	4.31715
318.	RY	(20)	H	7	0.00000	3.85790
319.	RY	(21)	H	7	0.00000	3.52858
320.	RY	(22)	H	7	0.00000	3.87961
321.	RY	(1)	H	8	0.00244	1.34348
322.	RY	(2)	H	8	0.00102	1.03860
323.	RY	(3)	H	8	0.00099	1.12347
324.	RY	(4)	H	8	0.00013	1.81092
325.	RY	(5)	H	8	0.00005	1.52922
326.	RY	(6)	H	8	0.00004	1.97141
327.	RY	(7)	H	8	0.00003	2.22123
328.	RY	(8)	H	8	0.00001	3.65559
329.	RY	(9)	H	8	0.00001	2.34844
330.	RY	(10)	H	8	0.00001	3.15516
331.	RY	(11)	H	8	0.00001	1.24088
332.	RY	(12)	H	8	0.00000	2.22169
333.	RY	(13)	H	8	0.00000	4.07732
334.	RY	(14)	H	8	0.00000	2.69648
335.	RY	(15)	H	8	0.00000	3.65988
336.	RY	(16)	H	8	0.00000	2.89841
337.	RY	(17)	H	8	0.00000	3.88125
338.	RY	(18)	H	8	0.00000	2.33495
339.	RY	(19)	H	8	0.00000	3.85113
340.	RY	(20)	H	8	0.00000	4.09991
341.	RY	(21)	H	8	0.00000	2.57405
342.	RY	(22)	H	8	0.00000	4.09502
343.	RY	(1)	H	9	0.00100	0.89619
344.	RY	(2)	H	9	0.00057	1.39806
345.	RY	(3)	H	9	0.00020	1.03891
346.	RY	(4)	H	9	0.00018	2.81328
347.	RY	(5)	H	9	0.00012	1.39397
348.	RY	(6)	H	9	0.00009	2.00063
349.	RY	(7)	H	9	0.00002	2.87047

350.	RY (8)	H 9	0.00001	1.85905
351.	RY (9)	H 9	0.00000	3.07226
352.	RY (10)	H 9	0.00000	2.95218
353.	RY (11)	H 9	0.00000	4.27156
354.	RY (12)	H 9	0.00000	2.60237
355.	RY (13)	H 9	0.00000	2.66728
356.	RY (14)	H 9	0.00000	3.86136
357.	RY (15)	H 9	0.00000	3.03539
358.	RY (16)	H 9	0.00000	3.95457
359.	RY (17)	H 9	0.00000	3.87329
360.	RY (18)	H 9	0.00000	2.09288
361.	RY (19)	H 9	0.00000	2.09879
362.	RY (20)	H 9	0.00000	3.30023
363.	RY (21)	H 9	0.00000	2.53913
364.	RY (22)	H 9	0.00000	3.33024
365.	RY (1)	H 10	0.00068	1.36780
366.	RY (2)	H 10	0.00040	0.58195
367.	RY (3)	H 10	0.00028	2.95306
368.	RY (4)	H 10	0.00024	1.47441
369.	RY (5)	H 10	0.00008	2.31886
370.	RY (6)	H 10	0.00005	2.33606
371.	RY (7)	H 10	0.00002	2.44388
372.	RY (8)	H 10	0.00001	2.32848
373.	RY (9)	H 10	0.00000	1.46439
374.	RY (10)	H 10	0.00000	2.28443
375.	RY (11)	H 10	0.00000	3.64844
376.	RY (12)	H 10	0.00000	3.33056
377.	RY (13)	H 10	0.00000	3.46286
378.	RY (14)	H 10	0.00000	3.17594
379.	RY (15)	H 10	0.00000	3.84241
380.	RY (16)	H 10	0.00000	4.02536
381.	RY (17)	H 10	0.00000	3.40664
382.	RY (18)	H 10	0.00000	1.88005
383.	RY (19)	H 10	0.00000	3.94154
384.	RY (20)	H 10	0.00000	3.31834
385.	RY (21)	H 10	0.00000	2.63940
386.	RY (1)	H 11	0.00069	0.84235
387.	RY (2)	H 11	0.00053	1.45908
388.	RY (3)	H 11	0.00031	0.68844
389.	RY (4)	H 11	0.00019	3.59777
390.	RY (5)	H 11	0.00006	2.22790
391.	RY (6)	H 11	0.00006	1.46867
392.	RY (7)	H 11	0.00001	1.93779
393.	RY (8)	H 11	0.00001	3.38235
394.	RY (9)	H 11	0.00000	2.10709
395.	RY (10)	H 11	0.00000	4.28049
396.	RY (11)	H 11	0.00000	1.23847
397.	RY (12)	H 11	0.00000	1.67348
398.	RY (13)	H 11	0.00000	2.67836
399.	RY (14)	H 11	0.00000	4.13338
400.	RY (15)	H 11	0.00000	3.36631
401.	RY (16)	H 11	0.00000	3.31634
402.	RY (17)	H 11	0.00000	3.39946
403.	RY (18)	H 11	0.00000	2.21927
404.	RY (19)	H 11	0.00000	4.26427
405.	RY (20)	H 11	0.00000	3.11938
406.	RY (21)	H 11	0.00000	3.03410
407.	RY (22)	H 11	0.00000	3.40600
408.	RY (1)	N 12	0.00937	1.07457
409.	RY (2)	N 12	0.00546	0.87964
410.	RY (3)	N 12	0.00254	1.77912
411.	RY (4)	N 12	0.00208	3.46109
412.	RY (5)	N 12	0.00062	1.77697

413.	RY (6) N 12	0.00037	1.83417
414.	RY (7) N 12	0.00026	3.42738
415.	RY (8) N 12	0.00021	1.00714
416.	RY (9) N 12	0.00016	3.52128
417.	RY (10) N 12	0.00007	1.94694
418.	RY (11) N 12	0.00005	2.63870
419.	RY (12) N 12	0.00005	1.66719
420.	RY (13) N 12	0.00002	2.82555
421.	RY (14) N 12	0.00001	3.55392
422.	RY (15) N 12	0.00000	3.88408
423.	RY (16) N 12	0.00000	4.47350
424.	RY (17) N 12	0.00000	5.86215
425.	RY (18) N 12	0.00000	1.66841
426.	RY (19) N 12	0.00000	1.11232
427.	RY (20) N 12	0.00000	4.90274
428.	RY (21) N 12	0.00000	3.02509
429.	RY (22) N 12	0.00000	5.13564
430.	RY (23) N 12	0.00000	5.09475
431.	RY (24) N 12	0.00000	4.09881
432.	RY (25) N 12	0.00000	3.28037
433.	RY (26) N 12	0.00000	4.40738
434.	RY (27) N 12	0.00000	2.69000
435.	RY (28) N 12	0.00000	4.82416
436.	RY (29) N 12	0.00000	2.11311
437.	RY (30) N 12	0.00000	4.13655
438.	RY (31) N 12	0.00000	4.37511
439.	RY (32) N 12	0.00000	4.10682
440.	RY (33) N 12	0.00000	4.98928
441.	RY (34) N 12	0.00000	5.71920
442.	RY (35) N 12	0.00000	2.01521
443.	RY (36) N 12	0.00000	4.43210
444.	RY (37) N 12	0.00000	2.08917
445.	RY (38) N 12	0.00000	4.81236
446.	RY (39) N 12	0.00000	4.73948
447.	RY (40) N 12	0.00000	4.29982
448.	RY (41) N 12	0.00000	4.18802
449.	RY (1) C 13	0.00608	1.53207
450.	RY (2) C 13	0.00589	1.29723
451.	RY (3) C 13	0.00079	1.90449
452.	RY (4) C 13	0.00036	1.02839
453.	RY (5) C 13	0.00034	1.73391
454.	RY (6) C 13	0.00007	1.65902
455.	RY (7) C 13	0.00004	3.88820
456.	RY (8) C 13	0.00003	0.85387
457.	RY (9) C 13	0.00003	1.46624
458.	RY (10) C 13	0.00001	1.98672
459.	RY (11) C 13	0.00001	2.12914
460.	RY (12) C 13	0.00000	5.04927
461.	RY (13) C 13	0.00000	1.92194
462.	RY (14) C 13	0.00000	0.91133
463.	RY (15) C 13	0.00000	0.66258
464.	RY (16) C 13	0.00000	3.03428
465.	RY (17) C 13	0.00000	2.51153
466.	RY (18) C 13	0.00000	1.87245
467.	RY (19) C 13	0.00000	2.85022
468.	RY (20) C 13	0.00000	1.93450
469.	RY (21) C 13	0.00000	2.15713
470.	RY (22) C 13	0.00000	2.82283
471.	RY (23) C 13	0.00000	1.30782
472.	RY (24) C 13	0.00000	2.24603
473.	RY (25) C 13	0.00000	2.25774
474.	RY (26) C 13	0.00000	2.08296
475.	RY (27) C 13	0.00000	2.11478

476.	RY (28) C 13	0.00000	1.72401
477.	RY (29) C 13	0.00000	2.94535
478.	RY (30) C 13	0.00000	2.13272
479.	RY (31) C 13	0.00000	2.82803
480.	RY (32) C 13	0.00000	2.34198
481.	RY (33) C 13	0.00000	2.09674
482.	RY (34) C 13	0.00000	2.02293
483.	RY (35) C 13	0.00000	3.13593
484.	RY (36) C 13	0.00000	1.68991
485.	RY (37) C 13	0.00000	2.82706
486.	RY (38) C 13	0.00000	2.85087
487.	RY (39) C 13	0.00000	2.59405
488.	RY (40) C 13	0.00000	2.26484
489.	RY (1) S 14	0.00328	0.72533
490.	RY (2) S 14	0.00215	0.77670
491.	RY (3) S 14	0.00022	1.04956
492.	RY (4) S 14	0.00006	0.93269
493.	RY (5) S 14	0.00002	1.25197
494.	RY (6) S 14	0.00001	1.67056
495.	RY (7) S 14	0.00001	0.83138
496.	RY (8) S 14	0.00000	1.65601
497.	RY (9) S 14	0.00000	0.92221
498.	RY (10) S 14	0.00000	1.89353
499.	RY (11) S 14	0.00000	2.55306
500.	RY (12) S 14	0.00000	1.06348
501.	RY (13) S 14	0.00000	1.76484
502.	RY (14) S 14	0.00000	1.37997
503.	RY (15) S 14	0.00000	1.30591
504.	RY (16) S 14	0.00000	1.58597
505.	RY (17) S 14	0.00000	1.33829
506.	RY (18) S 14	0.00000	1.28180
507.	RY (19) S 14	0.00000	1.63440
508.	RY (20) S 14	0.00000	0.84690
509.	RY (21) S 14	0.00000	0.69272
510.	RY (22) S 14	0.00000	1.69192
511.	RY (23) S 14	0.00000	1.36668
512.	RY (24) S 14	0.00000	1.85472
513.	RY (25) S 14	0.00000	1.68474
514.	RY (26) S 14	0.00000	1.59943
515.	RY (27) S 14	0.00000	1.11702
516.	RY (28) S 14	0.00000	1.48444
517.	RY (29) S 14	0.00000	1.32913
518.	RY (30) S 14	0.00000	2.63262
519.	RY (31) S 14	0.00000	1.88238
520.	RY (32) S 14	0.00000	2.11221
521.	RY (33) S 14	0.00000	1.23914
522.	RY (34) S 14	0.00000	1.64359
523.	RY (35) S 14	0.00000	1.61594
524.	RY (36) S 14	0.00000	1.79436
525.	RY (37) S 14	0.00000	1.38849
526.	RY (38) S 14	0.00000	1.70727
527.	RY (39) S 14	0.00000	1.73200
528.	RY (40) S 14	0.00000	1.19529
529.	RY (41) S 14	0.00000	1.72040

Total Lewis 67.55280 (96.5040%)
Valence non-Lewis 2.31255 (3.3036%)
Rydberg non-Lewis 0.13465 (0.1924%)

Total unit 1 70.00000 (100.0000%)
Charge unit 1 0.00000

\$CHOOSE

LONE 14 2 END
BOND D 1 2 S 1 6 S 1 7 S 2 3 S 2 12 D 3 4 S 3 8 S 4 5 S 4 9 D 5 6 S 5 10
S 6 11 T 12 13 D 13 14 END
\$END

Maximum scratch memory used by NBO was 2647535 words
Maximum scratch memory used by G09NBO was 1852716 words

Read Unf file /scratch/12026604.yak.local/Gau-1709.EUF:
Label Gaussian matrix elements IVer= 1 NLab=
2 Version=ES64L-G09RevE.01
Title Title Card Required
NAtoms= 14 NBasis= 533 NBSUse= 532 ICharg= 0 Multip= 1 NE= 70
Len12L=8 Len4L=8
Label GAUSSIAN SCALARS NI= 1 NR= 1
NTot= 1 LenBuf= 2000 N= 1000 1 1 1 1 NI= 1 NR= 1
Label ALPHA ORBITAL ENERGIES NI= 0 NR= 1
NTot= 532 LenBuf= 4000 N= 532 0 0 0 0 NI= 0 NR= 1
Label ALPHA MO COEFFICIENTS NI= 0 NR= 1
NTot= 283556 LenBuf= 4000 N= 533 532 0 0 0 NI= 0 NR= 1
Store file 524 Len= 283556.
Label NPA CHARGES NI= 0 NR= 1
NTot= 14 LenBuf= 4000 N= 14 0 0 0 0 NI= 0 NR= 1
Recovered energy= -722.844668911 dipole= 0.000000000000 0.000000000000
0.000000000000

This type of calculation cannot be archived.

NECESSARY EVIL: ONE WE LIKE TOO MUCH TO RELINQUISH.

Job cpu time: 0 days 2 hours 35 minutes 30.3 seconds.
File lengths (MBytes): RWF= 150 Int= 0 D2E= 0 Chk= 15 Scr= 1
Normal termination of Gaussian 09 at Fri Nov 30 13:05:23 2018.