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Supplementary Material

Derivation of an accurate geometry of 2-fluoroaniline from rotational spectroscopy and computational chemistry

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Appendix 1: Cartesian coordinates for the 2- Fluoroaniline (2-FAN) structures obtained at the B3LYP/aug-cc-pVTZ and MP2/cc-pVTZ level of theory.

Appendix 2: Kraitchman Coordinates for 2-FAN

Appendix 3: Assigned Transitions for the Parent and Isotopologues of 2-FAN

Appendix 1: Cartesian coordinates for the 2- Fluoroaniline (2-FAN) structures obtained at the B3LYP/aug-cc-pVTZ and MP2/cc-pVTZ level of theory.

Table S1. Cartesian coordinates for the 2-FAN structure obtained at the B3LYP/aug-cc-pVTZ level of theory.

Cartesian Coordinates (Angstroms)			
Atom	X	Y	Z
C	1.921881	-0.714491	-0.002864
C	0.699532	-1.380662	-0.004555
C	-0.464199	-0.643742	-0.000957
C	-0.486266	0.751899	0.002907
C	0.753124	1.399359	0.006540
C	1.938394	0.675572	0.004689
H	2.844107	-1.277103	-0.005936
H	0.637631	-2.459742	-0.005726
H	0.777765	2.481778	0.004414
H	2.881141	1.205140	0.007848
F	-1.664794	-1.286928	0.007685
N	-1.692347	1.437596	-0.053752
H	-2.505087	0.912331	0.223518
H	-1.681776	2.375839	0.309286

Table S2. Cartesian coordinates for the 2-FAN structure obtained at the MP2/cc-pVTZ level of theory.

Cartesian Coordinates (Angstroms)			
Atom	X	Y	Z
C	-1.950940	-0.552894	0.005700
C	-1.825201	0.833655	0.004776
C	-0.565850	1.428141	-0.004322
C	0.596930	0.653782	-0.008267
C	0.433799	-0.732759	-0.004795
C	-0.804042	-1.345970	0.002881
H	-2.926273	-1.016980	0.010958
H	-2.706875	1.458795	0.008601
H	-0.473310	2.506775	-0.014098
H	-0.853027	-2.425268	0.008010
F	1.873930	1.209198	-0.086291
N	1.942649	2.116055	0.347290
H	2.595577	0.589224	0.247211
H	1.555064	-1.488523	0.002248

Table S3. Cartesian coordinates for the transition state for the inversion motion of NH₂ in 2-FAN structure obtained at the MP2/cc-pVTZ level of theory.

Cartesian Coordinates (Angstroms)			
Atom	X	Y	Z
C	1.95347400	-0.55295500	-0.00005600
C	1.82543300	0.83286300	-0.00004800
C	0.56674700	1.42926700	0.00010100
C	-0.59865300	0.65556600	0.00011500
C	-0.43188500	-0.73306000	0.00010100
C	0.80494900	-1.34508800	-0.00000100
H	2.92876700	-1.01678900	-0.00013700
H	2.70633400	1.45932200	-0.00009400
H	0.47711000	2.50815300	0.00021400
H	0.85242500	-2.42455300	-0.00007300
F	-1.86036300	1.19342300	0.00003400
N	-1.99310300	2.18399600	-0.00113700
H	-2.66038600	0.59347800	0.00010900
H	-1.55655500	-1.48634700	-0.00004400

Table S4. Cartesian coordinates for the first transition state for the rotation motion of NH₂ obtained at the MP2/cc-pVTZ level of theory.

Cartesian Coordinates (Angstroms)			
Atom	X	Y	Z
C	-1.95037400	0.54339500	0.00002400
C	-0.80923500	1.34283300	0.00000800
C	0.43229700	0.72928500	0.00000600
C	0.58899600	-0.65705800	-0.00002400
C	-0.56804800	-1.43367100	-0.00004800
C	-1.83042800	-0.84439400	0.00000600
H	-2.92650600	1.00744900	0.00003900
H	-0.86715200	2.42168300	0.00001900
H	-0.44758900	-2.50791400	-0.00011500
H	-2.71489800	-1.46526000	-0.00000300
F	1.54029500	1.49629700	0.00000500
N	1.87256700	-1.29265700	-0.00007800
H	2.40286500	-0.97885500	0.80510300
H	2.40341200	-0.97751500	-0.80437300

Table S5. Cartesian coordinates for the second transition state for the rotation motion of NH₂ obtained at the MP2/cc-pVTZ level of theory.

Cartesian Coordinates (Angstroms)			
Atom	X	Y	Z
C	-1.96591200	0.46973800	-0.00000700
C	-0.85994500	1.31402300	-0.00000100
C	0.41519700	0.76551300	0.00000200
C	0.63145600	-0.61369700	-0.00000400
C	-0.49714700	-1.43849600	0.00000900
C	-1.78558600	-0.91155800	-0.00000500
H	-2.96103200	0.89153200	-0.00000800
H	-0.96512700	2.38927900	0.00000200

H	-0.34682800	-2.51066400	0.00002000
H	-2.63980500	-1.57358100	-0.00000100
F	1.46402100	1.59677400	0.00001100
N	1.97736500	-1.10136900	0.00001400
H	2.13338300	-1.68539200	-0.81156400
H	2.13328500	-1.68570300	0.81138600

Appendix 2: Kraitchman Coordinates for 2-FAN

Table S6. KRA coordinates

Atom	Coordinates (Angstroms)					
C(1)	0.48171	0.00311	0.74347	0.00202	0.00655*i	0.22895
C(2)	0.45587	0.00329	0.63971	0.00235	0.01537	0.09761
C(3)	0.69829	0.00215	1.38455	0.00108	0.00581	0.25833
C(4)	1.92632	0.00078	0.70915	0.00212	0.00700*i	0.21444
C(5)	1.93912	0.00077	0.68256	0.00220	0.01117*i	0.13428
C(6)	0.74225	0.00202	1.40622	0.00107	0.01047	0.14332
N(7)	1.70156	0.00088	1.42939	0.00105	0.04217	0.03558

Planar calculation made from I.a and I.b

C(1)	0.48167	0.00311	0.74344	0.00202	0.00000	0.00000
C(2)	0.45612	0.00329	0.63990	0.00234	0.00000	0.00000
C(3)	0.69831	0.00215	1.38457	0.00108	0.00000	0.00000
C(4)	1.92630	0.00078	0.70911	0.00212	0.00000	0.00000
C(5)	1.93909	0.00077	0.68247	0.00220	0.00000	0.00000
C(6)	0.74232	0.00202	1.40626	0.00107	0.00000	0.00000

N(7) 1.70204 0.00088 1.43005 0.00105 0.00000 0.00000

Appendix 3: Assigned transitions for the Parent and Isotopologues of 2-FAN

Table S7. Assigned transitions for 2-FAN (parent).

J''	K _a ''	K _c ''	F''	J'	K _a '	K _c '	F'	V _{obs} /MHz	V _{obs} - calc
6	3	3	6	6	2	4	6	6427.5692	0.0014
6	3	3	7	6	2	4	7	6428.1457	0.0011
6	3	3	5	6	2	4	5	6428.2423	0.0002
2	0	2	3	1	0	1	2	6732.0019	-0.0001
2	0	2	1	1	0	1	0	6732.3802	-0.0024
2	0	2	2	1	0	1	1	6732.4872	-0.0014
5	2	3	5	5	1	4	5	7101.2085	-0.0001
5	2	3	6	5	1	4	6	7102.3295	-0.0045
5	2	3	4	5	1	4	4	7102.5644	0.0011
2	1	2	1	1	0	1	1	7297.4928	-0.0039
2	1	2	3	1	0	1	2	7298.9473	0.0027
2	1	2	1	1	0	1	0	7299.2183	-0.0012
2	1	2	2	1	0	1	1	7299.6175	-0.0036
2	1	2	2	1	0	1	2	7300.3089	-0.0013
3	2	2	3	3	1	3	3	7470.1168	0.0008
3	2	2	4	3	1	3	3	7470.1168	0.0008
3	2	2	2	3	1	3	3	7470.1168	0.0006
3	2	2	3	3	1	3	4	7471.8376	-0.0031
3	2	2	4	3	1	3	4	7471.8376	-0.003
6	4	2	7	6	3	3	7	7650.4898	-0.0016
3	3	1	3	3	2	2	2	7876.0262	-0.0013
3	3	1	3	3	2	2	3	7876.0262	-0.0015
3	3	1	3	3	2	2	4	7876.0262	-0.0015
3	3	1	4	3	2	2	3	7877.0999	-0.002
3	3	1	4	3	2	2	4	7877.0999	-0.0021
4	3	2	5	4	2	3	5	8690.2742	-0.0013
4	3	2	3	4	2	3	3	8690.5194	-0.0007
3	0	3	2	2	1	2	2	8897.6298	-0.0004
3	0	3	4	2	1	2	3	8899.5678	0.0002
3	0	3	2	2	1	2	1	8899.7551	0.0004
3	0	3	3	2	1	2	2	8899.835	-0.0002
3	0	3	3	2	1	2	3	8901.2004	-0.0005
3	1	3	4	2	1	2	3	9115.3584	0.0035
3	1	3	2	2	1	2	1	9115.5089	-0.0009
3	1	3	3	2	1	2	2	9115.7136	-0.0002
3	0	3	4	2	0	2	3	9466.5099	-0.0001
3	0	3	2	2	0	2	1	9466.5905	-0.0011
3	0	3	3	2	0	2	2	9466.9686	0.0008

3	1	3	2	2	0	2	2	9680.5163	-0.0015
3	1	3	4	2	0	2	3	9682.2974	0.0001
3	1	3	2	2	0	2	1	9682.3471	0.0002
3	1	3	3	2	0	2	2	9682.8458	-0.0005
3	1	3	3	2	0	2	3	9684.0197	-0.0023
6	2	4	6	6	1	5	6	10104.2088	0.0003
6	2	4	7	6	1	5	7	10105.3699	-0.0044
6	2	4	5	6	1	5	5	10105.5731	0.0018
2	2	1	1	1	1	0	0	11259.1063	0.0021
2	2	1	2	1	1	0	2	11259.8660	-0.0013
2	2	1	3	1	1	0	2	11260.6080	0.0021
2	2	1	2	1	1	0	1	11261.1389	-0.0031
3	1	2	2	2	1	1	1	11679.0735	-0.0001
3	1	2	4	2	1	1	3	11679.3359	0.0006
3	1	2	3	2	1	1	2	11679.7139	0.0002
5	2	4	4	5	1	5	5	11809.7660	-0.0010
5	2	4	6	5	1	5	5	11809.9240	0.0023
5	2	4	5	5	1	5	5	11810.6808	-0.0007
5	2	4	6	5	1	5	6	11812.0684	-0.0049
5	2	4	4	5	1	5	4	11812.3580	0.0010
5	2	4	5	5	1	5	6	11812.8350	0.0018
5	2	4	5	5	1	5	4	11813.2738	0.0024
3	2	1	2	2	2	0	1	11822.1636	0.0009
3	2	1	4	2	2	0	3	11822.5118	-0.0005
3	2	1	3	2	2	0	2	11822.8203	-0.0002
4	0	4	3	3	1	3	3	11827.1290	-0.0005
4	0	4	5	3	1	3	4	11829.3540	0.0002
4	0	4	3	3	1	3	2	11829.4576	-0.0004
4	0	4	4	3	1	3	3	11829.5701	-0.0009
6	3	4	6	6	2	5	6	11888.0271	0.0006
6	3	4	5	6	2	5	5	11889.1314	0.0007
4	1	4	5	3	1	3	4	11896.8561	0.0001
4	1	4	3	3	1	3	2	11896.9526	-0.0003
4	1	4	4	3	1	3	3	11897.1015	0.0001
4	0	4	5	3	0	3	4	12045.1412	0.0002
4	0	4	3	3	0	3	2	12045.2110	-0.0021
4	0	4	4	3	0	3	3	12045.4496	0.0000
4	1	4	3	3	0	3	3	12110.5016	-0.0015
4	1	4	5	3	0	3	4	12112.6432	0.0001
4	1	4	3	3	0	3	2	12112.7082	0.0000
4	1	4	4	3	0	3	3	12112.9801	0.0001
4	1	4	4	3	0	3	4	12114.6108	-0.0025
2	2	0	2	1	1	1	1	12512.5363	0.0045
2	2	0	2	1	1	1	2	12513.1139	-0.0032

2	2	0	3	1	1	1	2	12514.2938	0.0009
2	2	0	1	1	1	1	0	12515.8282	0.0037
4	1	3	3	3	2	2	2	12675.7311	0.0012
4	1	3	3	3	2	2	3	12675.7311	0.0010
4	1	3	5	3	2	2	4	12675.7765	-0.0009
4	1	3	4	3	2	2	3	12675.9626	0.0002
4	1	3	4	3	2	2	4	12675.9626	0.0001
4	2	3	3	3	2	2	2	13897.2027	0.0012
4	2	3	3	3	2	2	3	13897.2027	0.0011
4	2	3	5	3	2	2	4	13897.3120	0.0000
4	2	3	4	3	2	2	3	13897.7426	0.0009
4	2	3	4	3	2	2	4	13897.7426	0.0008
3	2	2	2	2	1	1	1	13919.3401	-0.0049
3	2	2	2	2	1	1	1	13919.3401	-0.0049
3	2	2	3	2	1	1	3	13919.6974	0.0035
3	2	2	4	2	1	1	3	13919.6974	0.0036
3	2	2	3	2	1	1	3	13919.6974	0.0035
3	2	2	4	2	1	1	3	13919.6974	0.0036
3	2	2	2	2	1	1	2	13920.3226	0.0012
3	2	2	3	2	1	1	2	13920.3226	0.0014
5	0	5	4	4	1	4	4	14582.3880	-0.0012
5	0	5	6	4	1	4	5	14584.7968	0.0004
5	0	5	4	4	1	4	3	14584.8694	0.0032
5	0	5	5	4	1	4	4	14584.9704	0.0000
5	0	5	5	4	1	4	5	14586.9395	-0.0011
5	1	5	6	4	1	4	5	14603.7129	-0.001
5	1	5	4	4	1	4	3	14603.7853	0.0031
5	1	5	5	4	1	4	4	14603.8960	0.0007
5	0	5	6	4	0	4	5	14652.2992	0.0007
5	0	5	4	4	0	4	3	14652.3612	0.0001
5	0	5	5	4	0	4	4	14652.5005	-0.0002
5	1	5	4	4	0	4	4	14668.8347	-0.001
5	1	5	6	4	0	4	5	14671.2162	0.0001
5	1	5	4	4	0	4	3	14671.2779	0.0007
5	1	5	5	4	0	4	4	14671.4256	0.0000
5	1	5	5	4	0	4	5	14673.3661	-0.0015
4	1	3	5	3	1	2	4	14916.1350	-0.0011
4	2	3	3	3	1	2	2	16137.4723	-0.0005
4	2	3	5	3	1	2	4	16137.6725	0.0019
4	2	3	4	3	1	2	4	16138.1040	0.0037
4	2	3	4	3	1	2	3	16138.3491	0.0000
5	1	4	4	4	2	3	4	16420.2926	0.0004
5	1	4	4	4	2	3	3	16420.8325	0.0002
5	1	4	6	4	2	3	5	16420.8510	0.0007

5	1	4	5	4	2	3	4	16421.0508	0.0002
5	1	4	5	4	2	3	5	16421.4792	-0.0011
8	3	6	8	8	2	7	8	16631.3441	0.0005
5	2	4	4	4	2	3	3	16943.4467	0.0005
5	2	4	6	4	2	3	5	16943.4915	0.0010
5	2	4	5	4	2	3	4	16943.8209	0.0004
7	2	6	7	7	1	7	7	16964.4968	-0.0013
6	0	6	5	5	1	5	5	17270.6465	-0.0004
6	0	6	7	5	1	5	6	17273.1848	0.0002
6	0	6	5	5	1	5	4	17273.2366	-0.0001
6	0	6	6	5	1	5	5	17273.3203	0.0004
6	0	6	6	5	1	5	6	17275.4695	-0.0019
6	1	6	7	5	1	5	6	17278.1427	0.0000
6	1	6	5	5	1	5	4	17278.1948	0.0002
6	1	6	6	5	1	5	5	17278.2804	0.0006
6	0	6	7	5	0	5	6	17292.1035	0.0014
6	0	6	5	5	0	5	4	17292.1524	-0.0003
6	0	6	6	5	0	5	5	17292.2429	-0.0017
6	1	6	7	5	0	5	6	17297.0609	0.0006
6	1	6	5	5	0	5	4	17297.1118	0.0011
6	1	6	6	5	0	5	5	17297.2041	-0.0004
6	1	6	6	5	0	5	6	17299.3465	-0.0022
5	1	4	4	4	1	3	3	17642.3085	0.0046
5	1	4	6	4	1	3	5	17642.3831	-0.0015
5	1	4	5	4	1	3	4	17642.8294	-0.0005
3	2	1	3	2	1	2	2	18127.3901	0.0009
3	2	1	2	2	1	2	2	18128.5614	0.0010
3	2	1	3	2	1	2	3	18128.7503	-0.0045
3	2	1	2	2	1	2	1	18130.6867	0.0018
3	3	1	3	2	2	0	3	18156.1148	0.0015
3	3	1	2	2	2	0	1	18156.9086	-0.0014
3	3	1	4	2	2	0	3	18157.1948	0.0073
3	3	1	3	2	2	0	2	18157.2897	0.0008
3	3	1	2	2	2	0	2	18158.7413	0.0020
5	2	4	4	4	1	3	4	18164.6844	-0.0009
5	2	4	4	4	1	3	3	18164.9141	-0.0035
5	2	4	6	4	1	3	5	18165.0263	0.0013
5	2	4	5	4	1	3	4	18165.5993	-0.0005
3	3	0	3	2	2	1	3	18623.5226	-0.0022
3	3	0	3	2	2	1	2	18624.2631	-0.0002
3	3	0	2	2	2	1	1	18624.6917	0.0011
3	3	0	4	2	2	1	3	18624.6917	-0.0006
3	3	0	2	2	2	1	2	18625.8377	-0.0018

Table S8. Assigned transitions for 2-FAN ($^{13}\text{C1}$).

J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
3	0	3	4	2	1	2	3	8773.1058	0.0018
3	0	3	3	2	1	2	2	8773.3647	-0.0001
3	1	3	4	2	0	2	3	9600.5954	0.0003
3	1	3	2	2	0	2	1	9600.6409	-0.0015
3	1	3	3	2	0	2	2	9601.1514	0.0018
2	2	1	3	1	1	0	2	11215.2133	0.0001
2	2	1	2	1	1	0	1	11215.7471	0.0033
4	0	4	5	3	1	3	4	11686.2480	0.0001
4	0	4	3	3	1	3	2	11686.3518	-0.0016
4	0	4	4	3	1	3	3	11686.4612	-0.0003
4	1	4	5	3	0	3	4	11995.0022	-0.0004
4	1	4	3	3	0	3	2	11995.0668	0.0010
4	1	4	4	3	0	3	3	11995.3468	0.0007
3	2	2	4	2	1	1	3	13845.3132	0.0050
3	2	2	3	2	1	1	2	13845.9259	-0.0042
5	0	5	6	4	1	4	5	14420.2928	0.0000
5	0	5	4	4	1	4	3	14420.3646	0.0015
5	0	5	5	4	1	4	4	14420.4664	0.0005
5	1	5	6	4	0	4	5	14517.5015	0.0000
5	1	5	4	4	0	4	3	14517.5606	-0.0013
5	1	5	5	4	0	4	4	14517.7128	-0.0017
6	0	6	7	5	1	5	6	17083.0645	0.0011
6	0	6	5	5	1	5	4	17083.1128	-0.0028
6	0	6	6	5	1	5	5	17083.1994	0.0006
6	1	6	7	5	0	5	6	17110.7765	-0.0001
6	1	6	5	5	0	5	4	17110.8257	-0.0012
6	1	6	6	5	0	5	5	17110.9248	0.0021
3	3	1	4	2	2	0	3	18090.1153	-0.0020
3	3	1	3	2	2	0	2	18090.2081	0.0002
3	3	0	3	2	2	1	2	18529.1325	-0.0010
3	3	0	4	2	2	1	3	18529.5579	0.0004

Table S9. Assigned transitions for 2-FAN ($^{13}\text{C}_2$).

J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}$
3	0	3	4	2	1	2	3	8866.1737	-0.0034
3	0	3	2	2	1	2	1	8866.3639	0.0028
3	0	3	3	2	1	2	2	8866.4495	-0.0019
3	1	3	4	2	0	2	3	9603.6110	0.0028
3	1	3	2	2	0	2	1	9603.6605	-0.0002
3	1	3	3	2	0	2	2	9604.1520	0.0020
2	2	1	3	1	1	0	2	11130.6120	-0.0050
2	2	1	2	1	1	0	1	11131.1544	0.0024
4	0	4	5	3	1	3	4	11765.8276	-0.0007
4	0	4	3	3	1	3	2	11765.9292	-0.0023
4	0	4	4	3	1	3	3	11766.0488	0.0004
4	1	4	5	3	0	3	4	12026.2686	0.0011
4	1	4	3	3	0	3	2	12026.3327	-0.0015
4	1	4	4	3	0	3	3	12026.5981	-0.0001
3	2	2	4	2	1	1	3	13773.0823	0.0002
3	2	2	3	2	1	1	2	13773.7061	-0.0016
5	0	5	6	4	1	4	5	14497.5763	-0.0012
5	0	5	4	4	1	4	3	14497.6489	0.0019
5	0	5	5	4	1	4	4	14497.7499	-0.0019
5	1	5	6	4	0	4	5	14575.0433	0.0005
5	1	5	4	4	0	4	3	14575.1043	-0.0001
5	1	5	5	4	0	4	4	14575.2502	0.0010
6	0	6	7	5	1	5	6	17166.4786	-0.0004
6	0	6	5	5	1	5	4	17166.5281	-0.0030
6	0	6	6	5	1	5	5	17166.6142	0.0003
6	1	6	7	5	0	5	6	17187.3496	0.0006
6	1	6	5	5	0	5	4	17187.4015	0.0019
6	1	6	6	5	0	5	5	17187.4940	0.0022
3	3	1	4	2	2	0	3	17942.6553	0.0026
3	3	1	3	2	2	0	2	17942.7530	-0.0067
3	3	0	3	2	2	1	2	18425.7067	0.0031
3	3	0	4	2	2	1	3	18426.1395	0.0026

Table S10. Assigned transitions for 2-FAN ($^{13}\text{C3}$).

J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
3	0	3	4	2	1	2	3	8889.1129	0.0027
3	0	3	2	2	1	2	1	8889.2979	0.0011
3	0	3	3	2	1	2	2	8889.3813	-0.001
3	1	3	4	2	0	2	3	9663.5273	-0.0006
3	1	3	2	2	0	2	1	9663.5883	0.0082
3	1	3	3	2	0	2	2	9664.0757	0.0000
2	2	1	1	1	1	0	0	11230.6157	0.0000
2	2	1	3	1	1	0	2	11232.1202	-0.0007
2	2	1	2	1	1	0	1	11232.6525	-0.0011
4	1	4	5	3	0	3	4	12091.2446	0.0000
4	1	4	3	3	0	3	2	12091.3088	-0.0019
4	1	4	4	3	0	3	3	12091.5805	-0.0005
3	2	2	4	2	1	1	3	13886.9230	0.0000
3	2	2	3	2	1	1	2	13887.5509	0.0038
5	0	5	6	4	1	4	5	14561.9929	-0.0008
5	0	5	4	4	1	4	3	14562.0691	0.0051
5	0	5	5	4	1	4	4	14562.1670	-0.0016
5	1	5	6	4	0	4	5	14646.7766	0.0005
5	1	5	4	4	0	4	3	14646.8347	-0.0029
5	1	5	5	4	0	4	4	14646.9852	-0.0004
6	0	6	7	5	1	5	6	17245.5731	-0.0009
6	0	6	5	5	1	5	4	17245.6202	-0.0063
6	0	6	6	5	1	5	5	17245.7107	0.0009
6	1	6	7	5	0	5	6	17268.8986	0.0012
6	1	6	5	5	0	5	4	17268.9501	0.0020
6	1	6	6	5	0	5	5	17269.0410	-0.0009
3	3	1	4	2	2	0	3	18110.4141	-0.0003
3	3	1	3	2	2	0	2	18110.5138	-0.0002
3	3	0	3	2	2	1	2	18579.9343	-0.0004
3	3	0	4	2	2	1	3	18580.3665	-0.0007

Table S11. Assigned transitions for 2-FAN ($^{13}\text{C4}$).

J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
3	0	3	4	2	1	2	3	8887.0419	-0.0005
3	0	3	3	2	1	2	2	8887.3106	0.0011
3	1	3	4	2	0	2	3	9657.8180	0.0008
3	1	3	2	2	0	2	1	9657.8639	-0.0016
3	1	3	3	2	0	2	2	9658.3664	-0.0016
2	2	1	3	1	1	0	2	11222.3657	-0.0002
2	2	1	2	1	1	0	1	11222.9051	-0.0039
4	0	4	5	3	1	3	4	11807.8159	0.0000
4	0	4	3	3	1	3	2	11807.9195	-0.0004
4	0	4	4	3	1	3	3	11808.0336	0.0000
4	1	4	5	3	0	3	4	12085.0767	-0.0003
4	1	4	3	3	0	3	2	12085.1417	-0.0002
4	1	4	4	3	0	3	3	12085.4143	0.0004
3	2	2	4	2	1	1	3	13876.0074	0.0018
3	2	2	3	2	1	1	2	13876.6443	0.0046
5	0	5	6	4	1	4	5	14555.9480	-0.0004
5	0	5	4	4	1	4	3	14556.0204	0.0021
5	0	5	5	4	1	4	4	14556.1224	-0.0003
5	1	5	6	4	0	4	5	14639.9978	0.0018
5	1	5	4	4	0	4	3	14640.0532	-0.0038
5	1	5	5	4	0	4	4	14640.2049	-0.0003
6	0	6	7	5	1	5	6	17238.1323	0.0006
6	0	6	5	5	1	5	4	17238.1818	-0.002
6	0	6	6	5	1	5	5	17238.2693	0.0021
6	1	6	7	5	0	5	6	17261.2080	0.0016
6	1	6	5	5	0	5	4	17261.2566	-0.0001
6	1	6	6	5	0	5	5	17261.3491	-0.0015
3	3	0	3	2	2	1	2	18565.1250	-0.0008
3	3	0	4	2	2	1	3	18565.5556	0.0000

Table S12. Assigned transitions for 2-FAN ($^{13}\text{C5}$).

J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
3	0	3	4	2	1	2	3	8863.5184	-0.0025
3	0	3	2	2	1	2	1	8863.7049	-0.0005
3	0	3	3	2	1	2	2	8863.7920	0.0000
3	1	3	4	2	0	2	3	9600.3580	0.0013
3	1	3	2	2	0	2	1	9600.4074	0.0003
3	1	3	3	2	0	2	2	9600.8996	-0.0016
2	2	1	3	1	1	0	2	11126.5068	0.0042
2	2	1	2	1	1	0	1	11127.0466	0.0020
4	0	4	5	3	1	3	4	11762.1326	-0.0009
4	0	4	3	3	1	3	2	11762.2350	-0.0015
4	0	4	4	3	1	3	3	11762.3527	0.0000
4	1	4	5	3	0	3	4	12022.3073	0.0027
4	1	4	3	3	0	3	2	12022.3674	-0.0033
4	1	4	4	3	0	3	3	12022.6366	0.0003
3	2	2	4	2	1	1	3	13768.1169	-0.0007
3	2	2	3	2	1	1	2	13768.7484	-0.0016
5	0	5	6	4	1	4	5	14492.9460	-0.0008
5	0	5	4	4	1	4	3	14493.0187	0.0025
5	0	5	5	4	1	4	4	14493.1205	-0.0004
5	1	5	6	4	0	4	5	14570.3148	0.0001
5	1	5	4	4	0	4	3	14570.3762	0.0002
5	1	5	5	4	0	4	4	14570.5211	-0.0001
6	0	6	7	5	1	5	6	17160.9670	0.0005
6	0	6	5	5	1	5	4	17161.0152	-0.0031
6	0	6	6	5	1	5	5	17161.1029	0.0017
6	1	6	7	5	0	5	6	17181.8051	-0.0002
6	1	6	5	5	0	5	4	17181.8582	0.0024
6	1	6	6	5	0	5	5	17181.9493	0.0010
3	3	1	4	2	2	0	3	17935.9689	-0.0075
3	3	1	3	2	2	0	2	17936.0888	0.0008
3	3	0	3	2	2	1	2	18419.0471	0.0005
3	3	0	4	2	2	1	3	18419.4823	0.0038

Table S13. Assigned transitions for 2-FAN ($^{13}\text{C6}$).

J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \text{calc}$
3	0	3	4	2	1	2	3	8771.8175	-0.0002
3	0	3	3	2	1	2	2	8772.0709	0.0007
3	1	3	4	2	0	2	3	9601.0929	-0.0015
3	1	3	3	2	0	2	2	9601.6507	-0.0014
2	2	1	3	1	1	0	2	11217.4554	-0.0012
2	2	1	2	1	1	0	1	11217.9995	0.0008
4	0	4	5	3	1	3	4	11685.3816	0.0002
4	0	4	3	3	1	3	2	11685.4860	-0.0002
4	0	4	4	3	1	3	3	11685.5923	0.0003
4	1	4	5	3	0	3	4	11995.1108	-0.0016
4	1	4	3	3	0	3	2	11995.1727	-0.0009
4	1	4	4	3	0	3	3	11995.4586	0.0023
3	2	2	2	2	1	1	1	13847.1123	-0.0035
3	2	2	4	2	1	1	3	13847.4718	0.0044
3	2	2	3	2	1	1	2	13848.0939	-0.0059
5	0	5	6	4	1	4	5	14419.6334	-0.0005
5	0	5	4	4	1	4	3	14419.7058	0.0023
5	0	5	5	4	1	4	4	14419.8055	-0.0001
5	1	5	6	4	0	4	5	14517.2525	0.0010
5	1	5	4	4	0	4	3	14517.3098	-0.0011
5	1	5	5	4	0	4	4	14517.4657	0.0017
6	0	6	7	5	1	5	6	17082.4467	-0.0001
6	0	6	5	5	1	5	4	17082.4969	-0.0017
6	0	6	6	5	1	5	5	17082.5816	0.0001
6	1	6	7	5	0	5	6	17110.3062	0.0005
6	1	6	5	5	0	5	4	17110.3534	-0.0018
6	1	6	6	5	0	5	5	17110.4534	0.0023
3	3	1	4	2	2	0	3	18093.9400	0.0015
3	3	1	3	2	2	0	2	18094.0415	0.0047
3	3	0	3	2	2	1	2	18532.1998	-0.0003
3	3	0	4	2	2	1	3	18532.6158	-0.0026

Table S14. Assigned transitions for 2-FAN (^{15}N).

J''	K_a''	K_c''	J'	K_a'	K_c'	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{obs}} - \nu_{\text{calc}}$
3	0	3	2	1	2	8786.5124	-0.0010
3	1	3	2	0	2	9560.0299	0.0017
2	2	1	1	1	0	11118.8828	-0.0007
4	1	4	3	0	3	11959.3960	-0.0010
2	2	0	1	1	1	12355.9498	-0.0053
4	1	3	3	2	2	12513.6116	0.0030
3	2	2	2	1	1	13744.3559	0.0012
5	0	5	4	1	4	14399.9303	-0.0011
5	1	5	4	0	4	14485.4002	-0.0017
4	2	3	3	1	2	15934.2928	0.0026
6	0	6	5	1	5	17054.2689	-0.0015
6	1	6	5	0	5	17077.8917	-0.0012
3	2	1	2	1	2	17899.2131	-0.0003
3	3	1	2	2	0	17928.6623	0.0003
5	2	4	4	1	3	17935.8164	0.0036
3	3	0	2	2	1	18389.8374	0.0004