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Rotational Spectrum and Quantum Chemical Calculations of Methyl Cyanoacetate: A Compound of Potential Astrochemical Interest

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Table S1. Calculated spectroscopic parameters for the conformers of MCA calculated at the MP2/aug-cc-pVTZ level of theory.

	Conformer Ia/b	Conformer II	Conformer IIIa/b	Conformer IV
A /MHz	5083	9393	3805	6234
B	1851	1420	2278	1638
C	1388	1253	1611	1319
$ \mu_a $ /Debye	2.31	4.48	0.02	4.86
$ \mu_b $	0.63	2.97	1.91	4.80
$ \mu_c $	0.60	0.00	3.30	0.00
Energy ^a /kJ mol ⁻¹	0	0.7	32.3	36.4
Population ^b	57.0%	43.0%	0.0%	0.0%

^aRelative zero point energy corrected. ^bBoltzmann population at 298 K.

Table S2. Internal coordinates for conformer I (observed) calculated at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory.

	Internal Coordinates (Angstroms)		
	X	Y	Z
C	2.013115	1.321934	0.003633
H	1.890094	2.397577	-0.055106
H	2.610280	0.952788	-0.827033
H	2.482060	1.035239	0.942032
O	0.678288	0.781566	-0.067486
C	0.583105	-0.545767	-0.006011
O	1.509206	-1.305317	0.098830
C	-0.857823	-1.036509	-0.109290
H	-0.952448	-1.551000	-1.067811
H	-0.999350	-1.792293	0.663216
C	-1.892343	-0.019271	-0.002047
N	-2.728788	0.762849	0.086455

Table S3. Internal coordinates for conformer II (not observed) calculated at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory.

	Internal Coordinates (Angstroms)		
	X	Y	Z
C	-2.777100	0.108149	0.000064
H	-3.577567	-0.623577	-0.000447
H	-2.825670	0.735662	-0.887009
H	-2.826096	0.734842	0.887699
O	-1.556497	-0.658554	0.000021
C	-0.422387	0.058301	-0.000102
O	-0.363748	1.255412	-0.000036
C	0.766782	-0.894669	-0.000046
H	0.692522	-1.544143	0.873790
H	0.692601	-1.544133	-0.873896
C	2.052050	-0.214871	0.000017
N	3.084152	0.287742	0.000065

Table S4. Internal coordinates for conformer III (not observed) calculated at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory.

	Internal Coordinates (Angstroms)		
	X	Y	Z
C	0.438368	-1.922619	0.165392
H	1.034940	-2.793888	-0.083498
H	-0.503929	-1.954701	-0.376508
H	0.256789	-1.910566	1.239706
O	1.230551	-0.795698	-0.242985
C	0.875221	0.470909	0.018343
O	1.571890	1.380526	-0.328461
C	-0.426257	0.721290	0.800532
H	-0.402009	0.193278	1.755344
H	-0.459532	1.788945	1.003475
C	-1.625087	0.328974	0.074112
N	-2.563538	0.012612	-0.508926

Table S5. Internal coordinates for conformer IV (not observed) calculated at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory.

	Internal Coordinates (Angstroms)		
	X	Y	Z
C	-2.356494	-0.992465	0.000186
H	-3.429488	-0.830940	0.000101
H	-2.080202	-1.551785	0.893996
H	-2.080009	-1.551675	-0.893630
O	-1.774503	0.315854	0.000370
C	-0.439268	0.509448	-0.000123
O	0.008147	1.616529	-0.000188
C	0.426164	-0.754650	-0.000690
H	0.188639	-1.364285	0.873197
H	0.189124	-1.362720	-0.875839
C	1.849489	-0.458910	-0.000041
N	2.982374	-0.273928	0.000522

Table S6. Observed transitions for conformer I of MCA.

J'	K _a '	K _c '	J''	K _a ''	K _c ''	F'	F''	v _{obs} /MHz	v _{obs-calc} /MHz	State
2	0	2	1	0	1	3	2	6408.0131	-0.0005	A
						3	2	6407.9515	0.0013	E
						2	1	6407.8687	0.0002	E
						1	0	6407.6594	0.0016	E
2	1	1	1	1	0	3	2	6912.7204	-0.0011	A
						2	1	6912.3825	0.0018	A
						1	0	6913.4710	-0.0005	A
						3	2	6912.3110	0.0004	E
						2	1	6911.9728	0.0023	E
						1	0	6913.0603	0.0010	E
2	1	2	1	0	1	3	2	9221.3501	-0.0028	A
						3	2	9220.4265	0.0014	E
3	0	3	2	0	2	4	3	9500.9122	0.0005	A
						3	3	9500.3715	-0.0007	A
						2	2	9501.5384	-0.0014	A
						4	3	9500.8097	0.0008	E
						3	2	9500.7092	0.0004	E
						3	3	9500.2684	-0.0010	E
						2	2	9501.4367	-0.0004	E
3	1	2	2	1	1	4	3	10338.9472	0.0006	A
						3	2	10338.8387	0.0019	A
						2	1	10339.0361	-0.0008	A
						4	3	10338.7378	0.0011	E
						3	2	10338.6280	0.0009	E
						2	1	10338.8251	-0.0018	E
3	1	3	2	0	2	4	3	11777.8276	-0.0020	A
						3	2	11777.4940	0.0009	A
						4	3	11777.0029	0.0002	E
						3	2	11776.6657	-0.0006	E
3	1	3	2	1	2	4	3	8964.4925	0.0023	A
						3	2	8964.3538	0.0036	A
						4	3	8964.5254	-0.0025	E
						3	2	8964.3853	-0.0026	E
3	2	1	2	2	0	4	3	9859.7862	-0.0034	A
						3	2	9859.4950	0.0028	A
						2	1	9859.9851	0.0011	A
						4	3	9848.6958	0.0005	E
						3	2	9848.4067	0.0002	E
						2	1	9848.8850	0.0006	E
3	2	2	2	2	1	4	3	9680.3734	-0.0059	A
						3	2	9679.9923	-0.0037	A
						2	1	9680.5926	0.0004	A
						4	3	9691.3247	-0.0015	E

3	2	2	2	2	1	3	2	9690.9351	0.0010	E
						2	1	9691.5459	0.0015	E
4	0	4	3	0	3	5	4	12475.9275	0.0009	A
						4	3	12475.8117	-0.0002	A
						4	4	12475.2714	-0.0010	A
						3	2	12475.9042	-0.0017	A
						3	3	12476.6340	-0.0001	A
						5	4	12475.7793	0.0003	E
						4	3	12475.6644	0.0000	E
						4	4	12475.1243	-0.0007	E
						3	2	12475.7571	-0.0013	E
						3	3	12476.4864	-0.0003	E
4	1	3	3	1	2	5	4	13725.0336	0.0013	A
						4	3	13724.9616	-0.0003	A
						3	2	13725.0568	-0.0068	A
						5	4	13724.8211	0.0015	E
						4	3	13724.7492	-0.0001	E
						3	2	13724.8486	-0.0024	E
4	1	4	3	0	3	5	4	14182.5234	-0.0015	A
						4	3	14182.2066	0.0008	A
						3	2	14182.5585	0.0017	A
						5	4	14181.7690	-0.0018	E
						4	3	14181.4528	0.0011	E
						3	2	14181.8024	-0.0004	E
4	1	4	3	1	3	5	4	11905.6074	0.0005	A
						4	3	11905.5299	0.0055	A
						4	4	11904.7493	0.0009	A
						3	3	11906.6063	0.0027	A
						5	4	11905.5766	-0.0002	E
						4	3	11905.4955	0.0012	E
						4	4	11904.7194	0.0010	E
						3	2	11905.5299	0.0039	E
						3	3	11906.5761	0.0027	E
4	2	2	3	2	1	5	4	13302.4580	0.0026	A
						4	3	13302.3862	0.0018	A
						3	2	13302.4845	-0.0024	A
						5	4	13299.8052	0.0019	E
						4	3	13299.7345	0.0002	E
						3	2	13299.8311	-0.0030	E
4	2	3	3	2	2	5	4	12871.5139	0.0035	A
						4	3	12871.3381	0.0043	A
						3	2	12871.5524	-0.0033	A
						5	4	12873.9748	0.0027	E
						4	3	12873.7981	0.0045	E
						3	2	12874.0152	-0.0030	E
4	3	1	3	3	0	5	4	13007.2363	-0.0019	A

4	3	1	3	3	0	4	3	13006.9108	-0.0063	A
4	3	2	3	3	1	5	4	12990.2750	-0.0036	A
						4	3	12989.9510	0.0024	A
						3	2	12990.4136	0.0025	A
						5	4	12997.7122	-0.0010	E
						4	3	12997.3862	-0.0003	E
						3	2	12997.8456	0.0006	E
5	0	5	4	0	4	6	5	15332.2485	0.0021	A
						5	4	15332.1352	0.0049	A
						4	3	15332.2340	-0.0011	A
						6	5	15332.0578	-0.0001	E
						5	4	15331.9410	-0.0006	E
						4	3	15332.0422	-0.0044	E
5	0	5	4	1	4	6	5	13625.6500	0.0020	A
						5	4	13625.7371	0.0008	A
						6	5	13626.0639	-0.0022	E
						5	4	13626.1494	-0.0049	E
5	1	4	4	1	3	6	5	17050.9326	-0.0011	A
						5	4	17050.8664	-0.0006	A
						4	3	17050.9517	0.0006	A
						6	5	17050.6779	0.0006	E
						5	4	17050.6117	0.0010	E
						4	3	17050.6957	0.0010	E
5	1	5	4	0	4	6	5	16520.6517	0.0024	A
						5	4	16520.3840	0.0013	A
						6	5	16519.9757	-0.0010	E
						5	4	16519.7083	-0.0019	E
						4	3	16519.9915	-0.0046	E
5	1	5	4	1	4	6	5	14814.0529	0.0020	A
						5	4	14813.9858	-0.0029	A
						4	3	14814.0125	-0.0053	A
						6	5	14813.9858	0.0009	E
						5	4	14813.9220	-0.0008	E
						4	3	14813.9478	-0.0040	E
5	2	3	4	2	2	6	5	16832.7340	0.0014	A
						5	4	16832.7340	-0.0006	A
						4	3	16832.7340	-0.0020	A
						6	5	16831.8896	0.0038	E
						5	4	16831.8896	0.0014	E
						4	3	16831.8896	0.0005	E
5	2	4	4	2	3	6	5	16032.4896	-0.0013	A
						5	4	16032.3860	0.0024	A
						4	3	16032.5051	0.0017	A
						6	5	16033.0922	-0.0024	E
						5	4	16032.9867	-0.0001	E
						4	3	16033.1085	0.0015	E

6	0	6	5	0	5	7	6	18101.9315	0.0031	A
						6	5	18101.8254	0.0009	A
						5	4	18101.9189	-0.0002	A
						7	6	18101.7151	0.0010	E
						6	5	18101.6094	-0.0008	E
						5	4	18101.7021	-0.0026	E
6	0	6	5	1	5	7	6	16913.5255	-0.0001	A
						6	5	16913.5728	0.0007	A
						5	4	16913.4860	0.0003	A
						7	6	16913.7934	-0.0018	E
						6	5	16913.8377	-0.0039	E
						5	4	16913.7527	-0.0025	E
6	1	6	5	1	5	7	6	17689.7503	0.0035	A
						6	5	17689.6976	0.0030	A
						5	4	17689.7295	0.0060	A
						7	6	17689.6535	-0.0010	E
						6	5	17689.6014	-0.0009	E
						5	4	17689.6299	-0.0014	E