Shape of the Adduct Formic Acid-Dimethylether: A Rotational Study.

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Supporting Information:

Content:

1) Completion of Ref. [31].
2) Tables of transition frequencies

1) Completion of Reference [31].

M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H.P. Hratchian, A.F. Izmaylov, J. Bloino, G. Zheng, J.L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J.A. Montgomery, Jr., J.E. Peralta, F. Ogliaro, M. Bearpark, J.J. Heyd, E. Brothers, K.N. Kudin, V.N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J.M. Millam, M. Klene, J.E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, R.L. Martin, K. Morokuma, V.G. Zakrzewski, G.A. Voth, P. Salvador, J.J. Dannenberg, S. Dapprich, A.D. Daniels, O. Farkas, J.B. Foresman, J.V. Ortiz, J. Cioslowski, and D.J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, 2013.

2) Tables of transition frequencies

Table S1: Experimental transition frequencies (ν ,MHz) and observed – calculated values (Δν, kHz) of HCOOH-O$(CH_3)_2$ (parent species)

J'	K_a'	K_c'		J''	K_a''	K_c''	ν/MHz	Δν/kHz
2	1	2	←	1	1	1	7249.9245	-6.2
2	0	2	←	1	0	1	7266.3442	-0.7
2	1	1	←	1	1	0	7282.8355	7.7
3	1	3	←	2	1	2	10874.7288	-4.9
3	0	3	←	2	0	2	10899.2424	-1.1
3	2	2	←	2	2	1	10899.3025	-5.3
3	2	1	←	2	2	0	10899.5871	0.6
3	1	2	←	2	1	1	10924.0833	4.3
4	1	4	←	3	1	3	14499.3432	1.0
4	0	4	←	3	0	3	14531.8113	-2.1
4	2	3	←	3	2	2	14532.1133	6.9
4	2	2	←	3	2	1	14532.8022	-0.7
4	1	3	←	3	1	2	14565.1377	2.9
5	1	5	←	4	1	4	18123.7008	9.0
5	0	5	←	4	0	4	18163.9365	-8.6
5	2	4	←	4	2	3	18164.6475	3.2
5	2	3	←	4	2	2	18166.0430	5.7
5	4	2	←	4	4	1	18164.1961	2.5
5	4	1	←	4	4	0	18164.1961	2.5
5	3	3	←	4	3	2	18164.7417	-7.9
5	3	2	←	4	3	1	18164.7417	-12.7
5	1	4	←	4	1	3	18205.9251	-4.3

Table S2: Experimental transition frequencies (ν ,MHz) and observed – calculated values (Δν, kHz) of HCOOH-$^{13}CH_3OCH_3$.

J'	K_a'	K_c'		J''	K_a''	K_c''	ν/MHz	Δν/kHz
2	1	2	←	1	1	1	7171.5749	-5.8
2	0	2	←	1	0	1	7180.2449	3.9
2	1	1	←	1	1	0	7188.8890	-0.5
3	1	3	←	2	1	2	10757.2294	-8.4
3	0	3	←	2	0	2	10770.2013	4.3
3	1	2	←	2	1	1	10783.2035	2.4
4	0	4	←	3	0	3	14359.9607	5.0
5	1	5	←	4	1	4	17928.0273	7.4
5	0	5	←	4	0	4	17949.4431	-8.1
5	1	4	←	4	1	3	17971.2892	-1.3

Table S3: Experimental transition frequencies (ν ,MHz) and observed – calculated values (Δν, kHz) of $H^{13}COOH\text{-}CH_3OCH_3$.

J'	K_a'	K_c'		J''	K_a''	K_c''	ν/MHz	Δν/kHz
2	1	2	←	1	1	1	7152.9134	-2.4
2	0	2	←	1	0	1	7168.8668	3.0
2	1	1	←	1	1	0	7184.8831	8.3
3	1	3	←	2	1	2	10729.2093	-8.5
3	0	3	←	2	0	2	10753.031	-2.3
3	1	2	←	2	1	1	10777.1588	2.7
4	0	4	←	3	0	3	14336.8886	0.3
5	1	5	←	4	1	4	17881.2054	5.9
5	0	5	←	4	0	4	17920.3238	0.1
5	1	4	←	4	1	3	17961.0872	-5.1

Table S4: Experimental transition frequencies (ν ,MHz) and observed – calculated values (Δν, kHz) of $HCOOD\text{-}CH_3OCH_3$.

J'	K_a'	K_c'		J''	K_a''	K_c''	ν/MHz	Δν/kHz
2	0	2	←	1	0	1	7248.3542	-6.4
2	1	1	←	1	1	0	7270.3918	-13.5
3	1	3	←	2	1	2	10839.5227	-7.8
3	0	3	←	2	0	2	10872.1382	-5.4
3	1	2	←	2	1	1	10905.4053	-6.6
4	1	4	←	3	1	3	14452.3564	2.1
4	0	4	←	3	0	3	14495.4502	0.1
4	1	3	←	3	1	2	14540.1829	0.1
5	1	5	←	4	1	4	18064.8825	5.5
5	0	5	←	4	0	4	18118.1186	-3.3
5	1	4	←	4	1	3	18174.6442	5.8
3	2	2	←	2	2	1	10872.4007	1.6
3	2	1	←	2	2	0	10872.8637	-8.4
4	2	3	←	3	2	2	14496.1931	-0.6
4	2	2	←	3	2	1	14497.375	-0.7
5	2	4	←	4	2	3	18119.703	5.0
5	2	3	←	4	2	2	18122.0763	15.2

Table S5: Experimental transition frequencies (ν ,MHz) and observed – calculated values (Δν, kHz) of DCOOH-CH_3OCH_3.

J'	K_a'	K_c'	F'		J''	K_a''	K_c''	F''	ν/MHz	Δν/kHz
2	0	2	2	←	1	0	1	1	7034.1174	-2.8
2	1	1	1	←	1	1	0	0	7049.5451	1.0
2	1	1	3	←	1	1	0	2	7049.6098	12.6
2	1	1	2	←	1	1	0	1	7049.6436	-4.0
2	1	2	3	←	1	1	1	2	7018.677	2.6
2	1	2	2	←	1	1	1	1	7018.7266	1.5
3	0	3	4	←	2	0	2	3	10550.9352	0.6
3	0	3	3	←	2	0	2	2	10550.9506	14.1
3	0	3	2	←	2	0	2	1	10550.9506	6.0
3	1	3	4	←	2	1	2	3	10527.8798	-0.3
3	1	3	2	←	2	1	2	1	10527.8798	-1.0
3	1	3	3	←	2	1	2	2	10527.9013	6.6
3	1	2	4	←	2	1	1	3	10574.2546	-3.2
3	1	2	2	←	2	1	1	1	10574.2546	-3.1
3	1	2	3	←	2	1	1	2	10574.2721	-0.2
3	2	2	4	←	2	2	1	3	10550.9349	-19.4
4	0	4	5	←	3	0	3	4	14067.4579	-1.3
4	0	4	4	←	3	0	3	3	14067.4579	-2.5
4	0	4	3	←	3	0	3	2	14067.4637	-0.2
4	1	3	5	←	3	1	2	4	14098.7372	0.5
4	1	3	3	←	3	1	2	2	14098.7449	6.3
4	1	3	4	←	3	1	2	3	14098.7449	1.8
4	1	4	5	←	3	1	3	4	14036.916	4.0
4	1	4	3	←	3	1	3	2	14036.916	1.6
4	1	4	4	←	3	1	3	3	14036.916	-2.6
4	2	2	5	←	3	2	1	4	14068.2885	-5.3
4	2	2	4	←	3	2	1	3	14068.3112	-4.7
5	0	5	6	←	4	0	4	5	17583.597	3.1
5	0	5	5	←	4	0	4	4	17583.597	2.2
5	0	5	4	←	4	0	4	3	17583.597	0.3
5	1	4	6	←	4	1	3	5	17622.9799	3.3
5	1	4	5	←	4	1	3	4	17622.9799	-0.2
5	1	5	6	←	4	1	4	5	17545.7188	2.3
5	1	5	4	←	4	1	4	3	17545.7188	0.4
5	1	5	5	←	4	1	4	4	17545.7188	-1.3