Oligomers based on a weak hydrogen bond network: a rotational study of the tetramer of difluoromethane

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Supplementary Information

Content:

1) Completion of the Reference 11:

Gaussian 09, Revision A.02, 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, 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, Inc., Wallingford CT, 2009.

2) Experimental details (Reference numbers of the main paper)

Molecular clusters were generated in a supersonic expansion, under conditions optimized for the tetramer formation. Details of the Fourier transform microwave spectrometer,[13] COBRA-type,[14] which covers the range 6.5-18.5 GHz, have been described previously.[15]

A mixture of 1% DFM in He at 0.6 MPa was expanded through a solenoid valve (General Valve, Series 9, nozzle diameter 0.5 mm) into the Fabry-Pérot cavity. The spectral line positions were determined after Fourier transformation of the time-domain signal with 8k data points, recorded with 100 ns sample intervals. Each rotational transition appears as a doublet due to Doppler Effect. The line positions are calculated as the arithmetic mean of the frequencies of the Doppler components. The estimated accuracy of the frequency measurements is better than 3 kHz. Lines separated by more than 7 kHz are resolvable.

3) Table of transition frequencies

Table S1: Experimental and calculated transition frequencies and observed-calculated values $(CH_2F_2)_4$.

$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	ν_{obs}/MHz	ν_{calc}/MHz	$\Delta\nu$/kHz
$11_{0,11}$-$10_{0,10}$	7014.6360	7014.6355	0.5
$11_{1,11}$-$10_{1,10}$	7012.2033	7012.2039	-0.6
$11_{1,10}$-$10_{1,9}$	7508.8188	7508.8189	-0.1
$11_{2,10}$-$10_{2,9}$	7454.8472	7454.8474	-0.2
$11_{2,9}$-$10_{2,8}$	8068.4719	8068.4712	0.7
$11_{3,9}$-$10_{3,8}$	7798.5535	7798.5550	-1.5
$11_{3,8}$-$10_{3,7}$	8310.7136	8310.7134	0.2
$11_{4,8}$-$10_{4,7}$	7947.2066	7947.2080	-1.4
$11_{4,7}$-$10_{4,6}$	8131.7989	8131.7964	2.4
$11_{5,6}$-$10_{5,5}$	7971.4175	7971.4180	-0.5
$12_{0,12}$-$11_{0,11}$	7630.4256	7630.4273	-1.7
$12_{1,12}$-$11_{1,11}$	7629.2262	7629.2270	-0.8
$12_{1,11}$-$11_{1,10}$	8112.1714	8112.1722	-0.8
$12_{2,11}$-$11_{2,10}$	8080.3942	8080.3941	0.1
$12_{2,10}$-$11_{2,9}$	8682.8166	8682.8165	0.1
$12_{3,10}$-$11_{3,9}$	8461.6146	8461.6141	0.5
$12_{3,9}$-$11_{3,8}$	9055.9283	9055.9275	0.8
$13_{0,13}$-$12_{0,12}$	8246.5465	8246.5461	0.4
$13_{1,13}$-$12_{1,12}$	8245.9631	8245.9631	0.0
$13_{1,12}$-$12_{1,11}$	8719.9547	8719.9547	-0.0
$13_{2,12}$-$12_{2,11}$	8702.0741	8702.0742	-0.0
$13_{2,11}$-$12_{2,10}$	9277.2292	9277.2240	5.2
$13_{3,10}$-$12_{3,9}$	9764.9183	9764.9209	-2.6
$13_{4,10}$-$12_{4,9}$	9366.7813	9366.7806	0.7
$13_{4,9}$-$12_{4,8}$	9771.0829	9771.0826	0.3
$14_{0,14}$-$13_{0,13}$	8862.8270	8862.8246	2.4
$14_{1,14}$-$13_{1,13}$	8862.5495	8862.5450	4.4
$14_{1,13}$-$13_{1,12}$	9331.0219	9331.0238	-2.0
$15_{0,15}$-$14_{0,14}$	9479.1708	9479.1725	-1.7
$15_{1,15}$-$14_{1,14}$	9479.0388	9479.0400	-1.2
$15_{1,14}$-$14_{1,13}$	9944.2106	9944.2125	-1.9
$10_{3,7}$-$9_{3,6}$	7535.3315	7535.3338	-2.3
$8_{1,7}$-$7_{0,7}$	8162.7057	8162.7050	0.8
$6_{5,2}$-$5_{4,2}$	8893.2399	8893.2411	-1.2
$6_{5,1}$-$5_{4,1}$	8892.5994	8892.5998	-0.4
$6_{6,1}$-$5_{5,1}$	9916.7954	9916.7964	-1.0
$6_{6,0}$-$5_{5,0}$	9916.7954	9916.7917	3.7
$7_{7,0}$-$6_{6,0}$	11654.4669	11654.4671	-0.2
$7_{7,1}$-$6_{6,1}$	11654.4669	11654.4674	-0.5