Supplementary Material for PCCP

Intermolecular Hydrogen Bond in Molecules with Large Amplitude Motions: Rotational Spectrum of the complex 3,3 Dimethyloxetane···Hydrogen Fluoride

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Supplementary data

3 Tables

Table S1. Rotational transitions (in MHz) measured for the main species of the axial conformer of 3,3-methyloxetane···HF complex.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'	F'	I''	F''	*obs.*	*obs.-cal.*[a]
3	0	3	2	0	2	1	4	1	3	8525.122	-0.001
3	1	3	2	1	2	1	4	1	3	8297.445	0.001
3	1	2	2	1	1	1	4	1	3	8806.380	-0.002
3	2	2	2	2	1	1	4	1	3	8556.985	-0.001
3	2	1	2	2	0	1	3	1	2	8588.704	0.005
3	2	1	2	2	0	1	4	1	3	8588.725	0.000
3	2	1	2	2	0	1	2	1	1	8588.740	0.000
4	0	4	3	0	3	1	5	1	4	11330.345	-0.001
4	1	4	3	1	3	1	5	1	4	11054.327	-0.001
4	1	3	3	1	2	1	5	1	4	11731.732	-0.001
4	2	3	3	2	2	1	4	1	3	11402.886	-0.003
4	2	3	3	2	2	1	5	1	4	11402.902	0.001
4	2	2	3	2	1	1	5	1	4	11481.479	0.000
4	3	2	3	3	1	1	5	1	4	11424.534	0.005
4	3	1	3	3	0	1	5	1	4	11425.934	0.004
5	0	5	4	0	4	1	6	1	5	14106.656	0.000
5	1	5	4	1	4	1	6	1	5	13804.237	-0.002
5	1	4	4	1	3	1	6	1	5	14647.713	0.000
5	2	3	4	2	2	1	6	1	5	14397.450	0.000
5	3	3	4	3	2	1	5	1	4	14286.229	0.000
5	3	3	4	3	2	1	6	1	5	14286.238	-0.005
5	3	2	4	3	1	1	5	1	4	14291.109	-0.005
5	3	2	4	3	1	1	6	1	5	14291.129	0.002
6	0	6	5	0	5	1	7	1	6	16851.429	0.002
6	1	6	5	1	5	1	7	1	6	16546.229	0.000
6	1	5	5	1	4	1	7	1	6	17551.093	0.000
6	2	5	5	2	4	1	7	1	6	17076.980	0.001
6	3	4	5	3	3	1	7	1	6	17150.494	0.000
6	3	3	5	3	2	1	7	1	6	17163.442	0.001
6	4	3	5	4	2	1	7	1	6	17140.383	0.001
6	4	2	5	4	1	1	7	1	6	17140.585	-0.001
2	1	2	1	0	1	1	3	1	2	8160.713	-0.001
3	1	3	2	0	2	1	4	1	3	10761.469	0.001
4	1	4	3	0	3	1	5	1	4	13290.674	0.001
5	1	5	4	0	4	1	6	1	5	15764.564	-0.001

[a]Observed-calculated values from rotational parameters of Table 2.

Table S2. Rotational transitions (in MHz) for the isotopic species of the axial conformer of 3,3dimethyloxetane···HF complex.

						$^{13}C_aC_4H_{10}O\cdots HF$		$^{13}C_bC_4H_{10}O\cdots HF$		$^{13}C_{m1}C_4H_{10}O\cdots HF$		$^{13}C_{m2}C_4H_{10}O\cdots HF$		$C_5H_{10}{}^{18}O\cdots HF$	
J'	K'_{-1}	K'_{+1}	*J''*	K''_{-1}	K''_{+1}	*obs.*	*obs.-cal.*[a]	*obs.*	*obs.-cal.*	*obs.*	*obs.-cal.*	*obs.*	*obs.-cal.*	*obs.*	*obs.-cal.*
3	0	3	2	0	2	8507.652	0.002	8499.672	0.001	8476.986	0.001	8377.167	-0.002	-	-
3	1	2	2	1	1	8782.842	0.000	-	-	8775.945	0.004	8647.800	-0.005	8768.755	-0.005
3	1	3	2	1	2	8284.646	0.001	8273.065	0.000	8239.419	-0.001	8156.127	0.004	8239.958	0.004
4	0	4	3	0	3	11307.985	0.000	11296.848	0.001	11261.009	-0.001	11135.731	0.000	-	-
4	1	3	3	1	2	11700.607	-0.002	11695.608	-0.003	11689.641	0.001	11521.065	-0.002	11680.497	0.000
4	1	4	3	1	3	11037.493	0.000	11021.931	0.000	10975.726	-0.002	10866.548	0.001	-	-
5	0	5	4	0	4	14080.129	-0.001	14065.428	0.000	14012.493	0.000	13867.319	0.001	14012.491	0.000
5	1	4	4	1	3	14609.249	-0.001	14602.776	0.000	14592.497	-0.001	14385.702	0.005	14581.812	0.002
5	1	5	4	1	4	13783.541	0.000	13763.899	0.000	13704.163	-0.001	13570.475	0.000	13706.032	-0.002
6	0	6	5	0	5	16821.484	0.000	16802.761	-0.001	16729.306	0.001	16569.162	-0.001	-	-
6	1	5	5	1	4	17505.629	0.002	17497.514	0.001	17480.700	-0.003	-	-	-	-
6	1	6	5	1	5	16521.861	-0.001	16498.029	-0.001	16423.746	0.003	16266.989	-0.002	-	-

[a]Observed-calculated values from rotational parameters of Table 2.

Table S3. Rotational transitions (in MHz) for the parent and isotopic species of 3,3dimethyloxetane.

						$C_5H_{10}O$		$^{13}C_\alpha C_4H_{10}O$		$^{13}C_\beta C_4H_{10}O$		$^{13}C_m C_4H_{10}O$		$C_5H_{10}{}^{18}O$	
J'	***K'$_{-1}$***	***K'$_{+1}$***	***J''***	***K''$_{-1}$***	***K''$_{+1}$***	***obs.***	***obs.-cal.***[a]	***obs.***	***obs.-cal.***	***obs.***	***obs.-cal.***	***obs.***	***obs.-cal.***	***obs.***	***obs.-cal.***
1	0	1	0	0	0	6017.648	-0.005	5980.103	-0.001	6010.520	0.001	5931.485	0.001	5825.231	0.000
2	0	2	1	0	1	11998.008	-0.002	11927.285	0.000	11983.996	0.000	11820.960	0.000	11618.883	0.000
2	1	1	1	1	0	12363.392	0.002	12265.763	0.000	12348.311	0.000	12208.353	0.000	11958.860	0.000
2	1	2	1	1	1	11706.299	0.002	11653.770	0.001	11692.837	-0.001	11516.670	0.000	11341.035	-0.001
3	0	3	2	0	2	17906.816	0.000	17811.033	0.000	17886.377	0.000	17630.322	0.000	17351.469	0.000
3	1	3	2	1	2	17537.404	0.001	17461.150	0.000	17517.358	0.000	17250.256	0.000	16992.802	0.000

[a]Observed-calculated values from rotational parameters of Table 2

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