Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Hydrated forms of fluoroacetic acid: a rotational study.

Electronic Supplementary Information

Content:

- Tables of experimental transition frequencies of all measured isotopomers of FAA-W.
- Table of MP2/6-311++G(d,p) principal axes coordinates (Å) of of the not observed isomer, *cis-anti* FAA-W.

Table S1: Experimental transition frequencies (ν, MHz) and observed minus calculated values ($\Delta\nu$, kHz) of *trans*-FAA-W

$J'_{Ka'Kc'}$	$J''_{Ka''Kc''}$	H_2O		H_2O^{18}		DOD		DOH	
		ν/MHz	$\Delta\nu$/kHz	ν/MHz	$\Delta\nu$/kHz	ν/MHz	$\Delta\nu$/kHz	ν/MHz	$\Delta\nu$/kHz
3_{13}	2_{12}	8487.9817	-2	8096.3289	-4	7994.593	-5	8286.5524	-2
3_{03}	2_{02}	8809.3698	-0	8390.1234	-6	8289.352	-5	8603.5349	-3
3_{12}	2_{11}	9165.5662	-3	8712.5361	-7	8614.306	-11	8955.6620	-6
3_{22}	2_{21}	8830.0356	3						
3_{21}	2_{20}	8850.6510	-4						
4_{04}	3_{03}	11721.8394	-2	11167.0945	-4	11031.654	0	11447.1756	4
4_{14}	3_{13}	11311.4212	-1	10790.2464	-4	10654.344	0	11042.8013	4
4_{13}	3_{12}	12214.5058	0	11611.5895	-4	11480.336	10	11934.5824	5
4_{23}	3_{22}	11769.3138	7						
4_{22}	3_{21}	11820.7459	-9						
5_{05}	4_{04}	14614.1362	1	13927.4058	0	13756.400	1		
5_{15}	4_{14}	14130.0288	1	13480.1613	-3	13309.880	6	13794.1686	-3
5_{14}	4_{13}	15257.8670	1						
6_{06}	5_{05}	17482.0429	-1	16667.4587	8			17069.1842	-1
6_{16}	5_{15}	16942.8652	-1	16165.2762	4				
6_{15}	5_{14}	18293.9708	1	17394.6561	7				
1_{11}	0_{00}	10245.8852	2	10162.4517	0				
2_{12}	1_{01}	12963.3410	2	12759.3953	-0				
3_{13}	2_{02}	15569.8009	-2						
4_{14}	3_{03}	18071.8527	1						
5_{05}	4_{14}	8264.1227	1						
6_{06}	5_{15}	11616.1366	1						

Table S2: Experimental transition frequencies (ν, MHz) and observed minus calculated values ($\Delta\nu$, kHz) of *cis*-FAA-W

$J'_{Ka'Kc'}$	$J''_{Ka''Kc''}$	H_2O		$H_2{}^{18}O$	
		ν/MHz	$\Delta\nu$/kHz	ν/MHz	$\Delta\nu$/kHz
3_{13}	2_{12}	8660.4889	-2	8261.9525	-3
3_{03}	2_{02}	9017.3176	0	8589.3066	-1
3_{12}	2_{11}	9422.0111	-3	8956.2675	-7
3_{22}	2_{21}	9045.6853	3		
3_{21}	2_{20}	9074.0587	-4		
4_{04}	3_{03}	11990.1769	-2	11425.1292	-2
4_{14}	3_{13}	11539.2816	-1	11009.2583	-4
4_{13}	3_{12}	12554.0515	0	11934.5660	-4
4_{23}	3_{22}	12055.3468	7		
4_{22}	3_{21}	12126.0364	-9		
5_{05}	4_{04}	14935.6160	1		
5_{15}	4_{14}			13751.1177	-2
5_{14}	4_{13}	15678.3108	1	14906.4773	6
6_{06}	5_{05}	17848.4422	-1	17023.7049	-10
6_{16}	5_{15}			16486.5006	1
6_{15}	5_{14}	17276.1003	-1		
1_{11}	0_{00}	9691.1949	2	9590.2055	1
2_{12}	1_{01}	12452.5426	2	12229.6626	-1
3_{13}	2_{02}	15089.6530	-2		
4_{14}	3_{03}	17611.6199	1		
5_{24}	4_{23}	15060.2378	11		
5_{23}	4_{22}	15200.6308	-7		
5_{05}	4_{14}	9314.1839	8		
6_{06}	5_{15}	12751.0651	-4		

Table S3: MP2/6-311++G(d,p) calculated principal axes coordinates (Å) of *cis-anti*-W

atom	X	Y	Z
C	-0.675837	-1.184696	-0.107625
F	0.687789	-1.387928	0.100438
C	-1.079230	0.282628	-0.003276
O	-0.115194	1.198570	0.064967
O	-2.255390	0.561963	-0.005256
H	0.783795	0.813038	0.019863
H	-1.229095	-1.748962	0.643315
H	-0.927959	-1.545709	-1.106610
H	2.884475	-0.212394	0.178882
O	2.574458	0.654070	-0.098332
H	3.185015	1.276968	0.304614