Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information

Weak hydrogen bonds in adducts between freons: the rotational study of CH_2F_2-CH_2ClF

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Content:

.

Table 1: Experimental transition frequencies of CH_2F_2-$CH_2{}^{35}ClF$ and CH_2F_2-$CH_2{}^{37}ClF$

a) CH_2F_2-$CH_2{}^{35}ClF$

N	J'	K_a'	K_c'	F'+1/2	J''	K_a''	K_c''	F''+1/2	ν (MHz)	$\Delta\nu$ (kHz)
1	4	0	4	6	3	0	3	5	7985.4164	0.7
2	4	0	4	5	3	0	3	4	7984.7828	-0.5
3	4	0	4	4	3	0	3	3	7985.9417	-3.2
4	4	0	4	3	3	0	3	2	7986.5639	0.6
5	5	0	5	7	4	0	4	6	9964.0003	1.7
6	5	0	5	6	4	0	4	5	9963.2170	-0.2
7	5	0	5	5	4	0	4	4	9963.9363	-1.7
8	5	0	5	4	4	0	4	3	9964.7064	-0.7
9	6	0	6	8	5	0	5	7	11931.1011	1.5
10	6	0	6	7	5	0	5	6	11930.1695	-0.8
11	6	0	6	6	5	0	5	5	11930.7085	1.5
12	6	0	6	5	5	0	5	4	11931.5804	-1.7
13	7	0	7	9	6	0	6	8	13885.2516	-2.6
14	7	0	7	8	6	0	6	7	13884.6125	-2.2
15	7	0	7	7	6	0	6	6	13884.6641	1.8
16	7	0	7	6	6	0	6	5	13886.1703	-2.3
17	8	0	8	10	7	0	7	9	15825.7186	3.7
18	8	0	8	9	7	0	7	8	15824.3300	0.9
19	8	0	8	8	7	0	7	7	15824.9134	2.3
20	8	0	8	7	7	0	7	6	15825.6077	3.5
21	9	0	9	11	8	0	8	10	17752.6425	0.0
22	9	0	9	10	8	0	8	9	17751.4958	-1.2
23	9	0	9	9	8	0	8	8	17751.7607	-0.6
24	9	0	9	8	8	0	8	7	17752.8672	-2.9
25	4	1	4	6	3	1	3	5	7797.1261	0.8
26	4	1	4	5	3	1	3	4	7797.8692	-0.6
27	4	1	4	4	3	1	3	3	7797.1655	0.7
28	4	1	4	3	3	1	3	2	7796.4614	0.9
29	4	1	3	6	3	1	2	5	8210.8614	-1.3
30	4	1	3	5	3	1	2	4	8211.5658	-1.1
31	4	1	3	4	3	1	2	3	8213.2722	0.9
32	4	1	3	3	3	1	2	2	8212.5017	-2.1
33	4	2	3	6	3	2	2	5	8005.9234	-0.3
34	4	2	3	5	3	2	2	4	8009.3577	1.4
35	4	2	3	4	3	2	2	3	8008.1612	0.0
36	4	2	3	3	3	2	2	2	8004.6960	-3.1
37	4	2	2	6	3	2	1	5	8029.5464	-0.4
38	4	2	2	5	3	2	1	4	8033.6164	1.0
39	4	2	2	4	3	2	1	3	8032.2788	1.1
40	4	2	2	3	3	2	1	2	8028.2030	1.1
41	4	3	2	6	3	3	1	5	8010.7467	-1.8
42	4	3	2	5	3	3	1	4	8018.8153	0.8
43	4	3	2	4	3	3	1	3	8014.7160	-1.7
44	4	3	2	3	3	3	1	2	8006.6642	0.7
45	4	3	1	6	3	3	0	5	8010.9532	1.1
46	4	3	1	5	3	3	0	4	8019.0304	1.3
47	4	3	1	4	3	3	0	3	8014.9275	-1.2
48	4	3	1	3	3	3	0	2	8006.8653	1.7
49	5	1	5	7	4	1	4	6	9742.0872	-1.9
50	5	1	5	6	4	1	4	5	9742.3424	-5.5
51	5	1	5	5	4	1	4	4	9742.0668	-0.2
52	5	1	5	4	4	1	4	3	9741.8146	-1.2
53	5	1	4	7	4	1	3	6	10259.0662	0.4
54	5	1	4	6	4	1	3	5	10259.2977	0.7
55	5	1	4	5	4	1	3	4	10260.4293	-0.1
56	5	1	4	4	4	1	3	3	10260.1902	2.5
57	5	2	4	7	4	2	3	6	10005.0259	0.7
58	5	2	4	6	4	2	3	5	10006.6561	1.2
59	5	2	4	5	4	2	3	4	10006.4467	3.8
60	5	2	4	4	4	2	3	3	10004.7827	0.7
61	5	2	3	7	4	2	2	6	10052.2288	0.2
62	5	2	3	6	4	2	2	5	10054.6324	1.7
63	5	2	3	5	4	2	2	4	10054.2995	-0.6
64	5	2	3	4	4	2	2	3	10051.8614	-0.7
65	5	3	3	7	4	3	2	6	10016.9408	0.1
66	5	3	3	6	4	3	2	5	10021.0164	-2.5
67	5	3	3	5	4	3	2	4	10019.6781	0.1
68	5	3	3	4	4	3	2	3	10015.5920	0.1
69	5	3	2	7	4	3	1	6	10017.6532	-1.0
70	5	3	2	6	4	3	1	5	10021.7581	1.1
71	5	3	2	5	4	3	1	4	10020.4122	-0.4
72	5	3	2	4	4	3	1	3	10016.3068	4.2
73	6	1	6	8	5	1	5	7	11684.2038	0.2
74	6	1	6	7	5	1	5	6	11684.2498	0.7
75	6	1	6	6	5	1	5	5	11684.1077	0.0
76	6	1	6	5	5	1	5	4	11684.0840	1.7
77	6	1	5	8	5	1	4	7	12303.6041	-1.1
78	6	1	5	7	5	1	4	6	12303.5887	-1.5
79	6	1	5	6	5	1	4	5	12304.4056	0.5
80	6	1	5	5	5	1	4	4	12304.3948	-3.1
81	6	2	5	8	5	2	4	7	12001.5089	-0.1

82	6	2	5	7	5	2	4	6	12002.5331	0.1
83	6	2	5	6	5	2	4	5	12002.3213	-1.8
84	6	2	5	5	5	2	4	4	12001.7233	3.5
85	6	2	4	8	5	2	3	7	12083.5510	2.2
86	6	2	4	7	5	2	3	6	12085.4780	0.1
87	6	2	4	6	5	2	3	5	12085.1444	-0.4
88	6	2	4	5	5	2	3	4	12083.6501	3.7
89	6	3	4	8	5	3	3	7	12023.5768	-0.6
90	6	3	4	7	5	3	3	6	12025.9522	-0.9
91	6	3	4	6	5	3	3	5	12025.4526	0.8
92	6	3	4	5	5	3	3	4	12023.0684	1.1
93	6	3	3	8	5	3	2	7	12025.4940	-1.5
94	6	3	3	7	5	3	2	6	12027.9123	-2.1
95	6	3	3	6	5	3	2	5	12027.3999	-1.7
96	6	3	3	5	5	3	2	4	12024.9700	-3.3
97	7	1	7	9	6	1	6	8	13623.1186	-1.1
98	7	1	7	8	6	1	6	7	13623.0331	-0.7
99	7	1	7	7	6	1	6	6	13622.9637	0.2
100	7	1	7	6	6	1	6	5	13623.0486	3.1
101	2	1	2	4	1	0	1	3	7213.3206	-2.7
102	2	1	2	3	1	0	1	2	7198.7154	4.9
103	2	1	2	2	1	0	1	1	7218.7784	1.2
104	3	1	3	5	2	0	2	4	9061.2588	-2.5
105	3	1	3	4	2	0	2	3	9049.1009	0.3
106	3	1	3	3	2	0	2	2	9050.8548	-0.1
107	3	1	3	2	2	0	2	1	9069.0061	0.4
108	4	1	4	6	3	0	6	5	10861.1025	-0.9
109	4	1	4	5	3	0	6	4	10850.1649	-3.8
110	4	1	4	4	3	0	6	3	10854.9416	1.7
111	4	1	4	3	3	0	6	2	10865.8732	-0.7
112	5	1	5	7	4	0	4	6	12617.7785	1.7
113	5	1	5	6	4	0	4	5	12607.7362	2.9
114	5	1	5	5	4	0	4	4	12611.0609	-1.1
115	7	1	7	9	6	0	6	8	16030.0036	1.7
116	7	1	7	8	6	0	6	7	16021.6286	0.0
117	7	1	7	7	6	0	6	6	16023.4857	-2.5
118	7	1	7	6	6	0	6	5	16031.9643	-0.6
119	2	2	1	4	1	1	0	3	14038.2820	3.1
120	2	2	1	3	1	1	0	2	14023.4353	-6.2
121	3	2	2	5	2	1	1	4	15937.2492	3.2
122	3	2	2	4	2	1	1	3	15922.6015	-0.4
123	3	2	2	3	2	1	1	2	15922.6015	-2.5
124	3	2	2	2	2	1	1	1	15947.4429	-2.2
125	4	2	3	6	3	1	2	5	17783.5468	1.1
126	4	2	3	5	3	1	2	4	17770.2858	0.5
127	4	2	3	4	3	1	2	3	17776.9240	2.6
128	4	2	3	3	3	1	2	2	17790.0454	-0.7

b) CH_2F_2-$CH_2{}^{37}ClF$

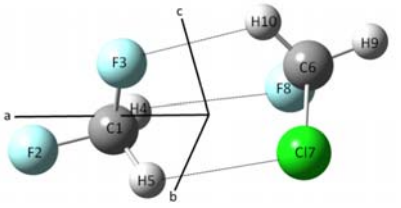
N	J'	K_a'	K_c'	F'+1/2	J''	K_a''	K_c''	F''+1/2	ν (MHz)	$\Delta\nu$ (kHz)
1	4	0	4	6	3	0	3	5	7864.0524	0.1
2	4	0	4	5	3	0	3	4	7863.5451	0.8
3	4	0	4	4	3	0	3	3	7864.4558	0.5
4	4	0	4	3	3	0	3	2	7864.9547	0.4
5	5	0	5	7	4	0	4	6	9811.8864	2.1
6	5	0	5	6	4	0	4	5	9811.2567	-0.7
7	5	0	5	5	4	0	4	4	9811.8242	-1.1
8	5	0	5	4	4	0	4	3	9812.4452	0.9
9	6	0	6	8	5	0	5	7	11748.0223	0.2
10	6	0	6	7	5	0	5	6	11747.2789	-1.0
11	6	0	6	6	5	0	5	5	11747.6994	0.1
12	6	0	6	5	5	0	5	4	11748.4067	-0.8
13	7	0	7	9	6	0	6	8	13670.9980	-1.9
14	7	0	7	8	6	0	6	7	13670.4337	-2.3
15	7	0	7	7	6	0	6	6	13670.5148	-0.8
16	7	0	7	6	6	0	6	5	13671.6558	-1.4
17	9	0	9	11	8	0	8	10	17475.5770	1.5
18	9	0	9	10	8	0	8	9	17474.6680	4.4
19	9	0	9	9	8	0	8	8	17474.8712	1.9
20	9	0	9	8	8	0	8	7	17475.7554	-2.5
21	4	1	4	6	3	1	3	5	7675.5752	1.7
22	4	1	4	5	3	1	3	4	7676.1518	-0.4
23	4	1	4	4	3	1	3	3	7675.5943	-2.7
24	4	1	4	3	3	1	3	2	7675.0437	1.4
25	5	1	5	7	4	1	4	6	9590.0269	-0.7
26	5	1	5	6	4	1	4	5	9590.2266	0.4
27	5	1	5	5	4	1	4	4	9590.0027	-1.2
28	5	1	5	4	4	1	4	3	9589.8091	0.1
29	6	1	6	8	5	1	5	7	11501.5926	-0.6
30	6	1	6	7	5	1	5	6	11501.6245	0.2
31	6	1	6	6	5	1	5	5	11501.5136	1.5
32	6	1	6	5	5	1	5	4	11501.4976	2.0
33	7	1	7	9	6	1	6	8	13409.9118	0.3
34	7	1	7	8	6	1	6	7	13409.8368	-2.8
35	7	1	7	7	6	1	6	6	13409.7828	-0.7
36	7	1	7	6	6	1	6	5	13409.8569	4.9

37	9	1	9	11	8	1	8	10	17215.7700	-2.1
38	9	1	9	10	8	1	8	9	17215.6008	-3.1
39	9	1	9	9	8	1	8	8	17215.5857	2.0
40	9	1	9	8	8	1	8	7	17215.7512	-0.4
41	4	1	3	6	3	1	2	5	8090.7150	-0.7
42	4	1	3	5	3	1	2	4	8091.2659	-1.4
43	4	1	3	4	3	1	2	3	8092.6071	-0.3
44	4	1	3	3	3	1	2	2	8092.0168	0.3
45	4	2	3	6	3	2	2	6	7885.3249	-0.0
46	4	2	3	5	3	2	2	5	7888.0156	0.3
47	4	2	3	4	3	2	2	4	7887.0779	0.4
48	4	2	3	3	3	2	2	3	7884.3703	2.4
49	4	2	2	6	3	2	1	5	7909.5189	-2.5
50	4	2	2	5	3	2	1	4	7912.7211	-1.7
51	4	2	2	4	3	2	1	3	7911.6736	2.2
52	4	2	2	3	3	2	1	2	7908.4702	2.8
53	2	1	2	4	1	0	1	3	7100.0082	1.1
54	3	1	3	5	2	1	2	4	8917.2230	-1.8
55	3	1	3	4	2	1	2	3	8907.6396	1.6
56	3	1	3	3	2	1	2	2	8909.0343	-1.5
57	3	1	3	2	2	1	2	1	8923.3212	-1.4
58	4	1	4	6	3	0	3	5	10686.3093	2.4
59	4	1	4	5	3	0	3	4	10677.6856	0.0
60	4	1	4	4	3	0	3	3	10681.4379	-1.8
61	4	1	4	7	3	0	3	6	10690.0626	2.2
62	5	1	5	7	4	0	4	6	12412.2808	-1.3
63	5	1	5	6	4	0	4	5	12404.3672	-0.3
64	5	1	5	5	4	0	4	4	12406.9869	-1.4
65	5	1	5	4	4	0	4	3	12414.9171	2.0
66	2	2	1	4	1	1	0	3	13821.8292	3.5
67	2	2	1	3	1	1	0	2	13810.1772	0.4
68	2	2	1	2	1	1	0	1	13823.1317	-1.5
69	4	2	3	6	3	1	2	5	17505.7583	-0.4
70	4	2	3	5	3	1	2	4	17495.3110	0.2
71	4	2	3	4	3	1	2	3	17500.5286	-1.5
72	4	2	3	3	3	1	2	2	17510.8924	-0.8

Table 2: MP2/6-311++G(d,p) geometry of the three low energy forms of the complex (see the drawings for atom numbering).

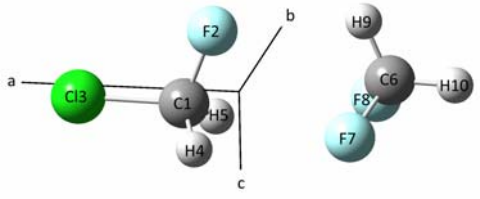
Conformer I (Observed species)

bond lengths/Å		valence angles/°		dihedral angles/°	
F2C1	1.3605				
F3C1	1.3670	F3C1F2	108.1		
H4C1	1.0885	H4C1F2	109.0	H4C1F2F3	-117.7
H5C1	1.0885	H5C1F2	109.0	H5C1F2F3	117.7
C6C1	3.5640	C6C1F3	58.8	C6C1F3H5	-49.2
Cl7C6	1.7642	Cl7C6C1	85.2	Cl7C6C1F3	107.0
F8C6	1.3739	F8C6Cl7	109.8	F8C6Cl7C1	-49.9
H9C6	1.0877	H9C6F8	108.3	H9C6F8Cl7	118.5
H10C6	1.0864	H10C6F8	108.4	H10C6F8Cl7	-118.5



Conformer II

bond lengths/Å		valence angles/°		dihedral angles/°	
F2C1	1.3740				
Cl3C1	1.7639	Cl3C1F2	109.96		
H4C1	1.0869	H4C1Cl3	108.93	H4C1Cl3F2	118.5
H5C1	1.0869	H5C1H4	112.52	H5C1H4Cl3	-120.9
C6C1	3.4891	C6C1F2	59.71	C6C1F2H4	-61.1
F7C6	1.3641	F7C6C1	65.93	F7C6C1F2	117.7
F8C6	1.3641	F8C6C1	65.93	F8C6C1F2	-117.7
H9C6	1.0876	H9C6C1	76.76	H9C6C1F2	0.0
H10C6	1.0895	H10C6H9	114.39	H10C6H9C1	180.0



Conformer III

bond lengths/Å		valence angles/°		dihedral angles/°	
Cl2C1	1.7694				
F3C1	1.3685	F3C1Cl2	109.96		
H4C1	1.0869	H4C1F3	108.94	H4C1F3Cl2	118.5
H5C1	1.0869	H5C1H4	112.46	H5C1H4F3	-120.9
C6C1	3.6349	C6C1Cl2	73.20	C6C1Cl2H4	-61.1
F7C6	1.3632	F7C6C1	62.50	F7C6C1Cl2	114.3
F8C6	1.3632	F8C6C1	62.50	F8C6C1Cl2	-114.3
H9C6	1.0883	H9C6C1	84.61	H9C6C1Cl2	0.0
H10C6	1.0894	H10C6H9	114.16	H10C6H9C1	180.0