Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Weak C-H···N and C-H···F hydrogen bonds and internal rotation in pyridine-CH_3F

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Electronic Supplementary Information (ESI)

Content:

1) Table of experimental transition frequencies of isotopologues (^{14}N)Py-CH_3F, (^{15}N)Py-CH_3F, (^{14}N)Py-CD_3F, (^{15}N)Py-CD_3F of conformer *I*.
2) Ab initio geometry of the observed complex

1) Table 1S: experimental transition frequencies (ν) and their discrepancies with respect to the model calculated values (Δν) of all isotopologues.

a) Pyridine (^{14}N)-CH_3F

N	J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	Sym	ν (MHz)	Δν (kHz)
1	5	0	5	4	4	0	4	3	A	7713.6288	1.9
2	5	0	5	5	4	0	4	4	A	7713.6087	-0.7
3	5	0	5	6	4	0	4	5	A	7713.6730	0.9
4	5	0	5	4	4	0	4	3	E	7700.7647	3.5
5	5	0	5	5	4	0	4	4	E	7700.7448	-1.2
6	5	0	5	6	4	0	4	5	E	7700.8056	-1.0
7	5	1	5	4	4	1	4	3	A	7455.2630	0.3
8	5	1	5	5	4	1	4	4	A	7455.2423	1.5
9	5	1	5	6	4	1	4	5	A	7455.3224	-3.3
10	5	1	5	4	4	1	4	3	E	7450.0798	2.9
11	5	1	5	5	4	1	4	4	E	7450.0548	-0.3
12	5	1	5	6	4	1	4	5	E	7450.1388	-1.2
13	5	1	4	4	4	1	3	3	A	8054.2655	-3.4
14	5	1	4	5	4	1	3	4	A	8054.2046	3.6
15	5	1	4	6	4	1	3	5	A	8054.2655	-2.1
16	5	1	4	4	4	1	3	3	E	8050.0305	-2.8
17	5	1	4	5	4	1	3	4	E	8049.9634	-0.2
18	5	1	4	6	4	1	3	5	E	8050.0305	-1.6
19	5	2	4	4	4	2	3	3	A	7760.4721	0.0
20	5	2	4	5	4	2	3	4	A	7760.2315	-1.3
21	5	2	4	6	4	2	3	5	A	7760.4496	0.0
22	5	2	4	4	4	2	3	3	E	7765.2937	-1.9
23	5	2	4	5	4	2	3	4	E	7765.0444	-2.2
24	5	2	4	6	4	2	3	5	E	7765.2655	-4.9
25	5	2	3	4	4	2	2	3	A	7813.2453	2.9
26	5	2	3	5	4	2	2	4	A	7813.0543	-1.3
27	5	2	3	6	4	2	2	5	A	7813.2252	0.1
28	5	2	3	4	4	2	2	3	E	7797.6623	9.6
29	5	2	3	6	4	2	2	5	E	7797.6390	0.9
30	5	3	3	4	4	3	2	3	A	7775.0829	1.2
31	5	3	3	5	4	3	2	4	A	7774.5270	0.8
32	5	3	3	6	4	3	2	5	A	7774.9712	-0.3
33	5	3	2	4	4	3	1	3	A	7775.8545	0. 5
34	5	3	2	5	4	3	1	4	A	7775.3022	2.2
35	5	3	2	6	4	3	1	5	A	7775.7448	0.8
36	6	0	6	5	5	0	5	4	A	9227.9622	0.4
37	6	0	6	6	5	0	5	5	A	9227.9227	-0.5
38	6	0	6	7	5	0	5	6	A	9227.9907	0.2
39	6	0	6	5	5	0	5	4	E	9215.3264	-2.1
40	6	0	6	6	5	0	5	5	E	9215.2910	-0.8
41	6	0	6	7	5	0	5	6	E	9215.3556	-1.6
42	6	1	6	5	5	1	5	4	A	8939.4824	-3.0
43	6	1	6	6	5	1	5	5	A	8939.4698	-0.9
44	6	1	6	7	5	1	5	6	A	8939.5326	1.9
45	6	1	6	5	5	1	5	4	E	8933.5032	0.1
46	6	1	6	6	5	1	5	5	E	8933.4837	-4.9
47	6	1	6	7	5	1	5	6	E	8933.5477	-0.6
48	6	1	5	5	5	1	4	4	A	9657.1101	3.8
49	6	1	5	6	5	1	4	5	A	9657.0589	-1.6
50	6	1	5	7	5	1	4	6	A	9657.1101	1.5
51	6	1	5	5	5	1	4	4	E	9649.4291	0.3
52	6	1	5	6	5	1	4	5	E	9649.3823	0.1
53	6	1	5	7	5	1	4	6	E	9649.4291	-2.0
54	6	2	5	5	5	2	4	4	A	9307.5366	-2.4
55	6	2	5	6	5	2	4	5	A	9307.4056	1.0
56	6	2	5	7	5	2	4	6	A	9307.5366	-1.5
57	6	2	5	5	5	2	4	4	E	9307.7836	0.1
58	6	2	5	6	5	2	4	5	E	9307.6414	2.9
59	6	2	5	7	5	2	4	6	E	9307.7836	3.0
60	6	2	4	5	5	2	3	4	A	9399.1598	2.8
61	6	2	4	6	5	2	3	5	A	9399.0807	-2.8
62	6	2	4	7	5	2	3	6	A	9399.1598	-1.3
63	6	2	4	5	5	2	3	4	E	9385.9222	1.1
64	6	2	4	6	5	2	3	5	E	9385.8543	-3.8
65	6	2	4	7	5	2	3	6	E	9385.9222	-5.0
66	6	3	4	5	5	3	3	4	A	9332.9422	2.1
67	6	3	4	6	5	3	3	5	A	9332.6370	-3.7
68	6	3	4	7	5	3	3	6	A	9332.8996	0.3
69	6	3	3	5	5	3	2	4	A	9334.9947	-2.7
70	6	3	3	6	5	3	2	5	A	9334.7006	-0.3
71	6	3	3	7	5	3	2	6	A	9334.9570	0.1
72	7	0	7	6	6	0	6	5	A	10727.9589	-1.5
73	7	0	7	7	6	0	6	6	A	10727.9082	0.3
74	7	0	7	8	6	0	6	7	A	10727.9782	-1.7
75	7	0	7	6	6	0	6	5	E	10716.3658	-1.3
76	7	0	7	7	6	0	6	6	E	10716.3164	0.4
77	7	0	7	8	6	0	6	7	E	10716.3901	3.6
78	7	1	7	6	6	1	6	5	A	10420.2998	6.6
79	7	1	7	7	6	1	6	6	A	10420.2752	-4.7
80	7	1	7	8	6	1	6	7	A	10420.3300	3.0

81	7	1	7	6	6	1	6	5	E	10413.6774	0.5
82	7	1	7	7	6	1	6	6	E	10413.6609	-3.0
83	7	1	7	8	6	1	6	7	E	10413.7086	-2.1
84	7	1	6	6	6	1	5	5	A	11255.2478	6.3
85	7	1	6	7	6	1	5	6	A	11255.2050	1.0
86	7	1	6	8	6	1	5	7	A	11255.2478	3.6
87	7	1	6	6	6	1	5	5	E	11243.3827	2.2
88	7	1	6	7	6	1	5	6	E	11243.3463	4.5
89	7	1	6	8	6	1	5	7	E	11243.3827	-0.6
90	7	2	6	6	6	2	5	5	A	10851.9355	5.5
91	7	2	6	7	6	2	5	6	A	10851.8399	-4.2
92	7	2	6	8	6	2	5	7	A	10851.9355	0.1
93	7	2	5	6	6	2	4	5	A	10996.6453	0.2
94	7	2	5	7	6	2	4	6	A	10996.6244	-2.7
95	7	2	5	8	6	2	4	7	A	10996.6591	4.0
96	7	3	5	6	6	3	4	5	A	10892.1749	-6.7
97	7	3	5	7	6	3	4	6	A	10892.0025	-1.4
98	7	3	5	8	6	3	4	7	A	10892.1749	8.4
99	8	0	8	7	7	0	7	6	A	12212.6794	-3.6
100	8	0	8	8	7	0	7	7	A	12212.6192	-2.0
101	8	0	8	9	7	0	7	8	A	12212.6955	-1.6
102	8	0	8	7	7	0	7	6	E	12202.6593	0.4
103	8	0	8	8	7	0	7	7	E	12202.6029	4.9
104	8	0	8	9	7	0	7	8	E	12202.6752	2.4
105	8	1	8	7	7	1	7	6	A	11897.3724	2.1
106	8	1	8	8	7	1	7	7	A	11897.3543	-2.3
107	8	1	8	9	7	1	7	8	A	11897.3988	2.4
108	8	1	8	7	7	1	7	6	E	11890.2680	1.7
109	8	1	8	8	7	1	7	7	E	11890.2510	-1.8
110	8	1	8	9	7	1	7	8	E	11890.2908	-1.5
111	8	1	7	7	7	1	6	6	A	12847.5997	-0.6
112	8	1	7	8	7	1	6	7	A	12847.5628	-2.4
113	8	1	7	9	7	1	6	8	A	12847.5997	-3.0
114	8	1	7	7	7	1	6	6	E	12831.1661	2.9
115	8	1	7	8	7	1	6	7	E	12831.1234	-4.1
116	8	1	7	9	7	1	6	8	E	12831.1661	0.4
117	8	2	7	7	7	2	6	6	A	12393.1927	1.9
118	8	2	7	8	7	2	6	7	A	12393.1264	-3.5
119	8	2	7	9	7	2	6	8	A	12393.1927	-5.1
120	8	2	7	7	7	2	6	6	E	12385.7993	7.1
121	8	2	7	8	7	2	6	7	E	12385.7279	-1.0
122	8	2	7	9	7	2	6	8	E	12385.7993	0.4
123	8	2	6	7	7	2	5	6	A	12606.1515	-4.7
124	8	2	6	8	7	2	5	7	A	12606.1716	3.4
125	8	2	6	9	7	2	5	8	A	12606.1716	4.4
126	8	2	6	7	7	2	5	6	E	12596.0068	-7.1
127	8	2	6	8	7	2	5	7	E	12596.0287	0.6
128	8	2	6	9	7	2	5	8	E	12596.0287	3.5
129	8	3	6	7	7	3	5	6	A	12452.7312	-3.8
130	8	3	6	8	7	3	5	7	A	12452.6232	0.8
131	8	3	6	9	7	3	5	8	A	12452.7312	0.6
132	9	0	9	8	8	0	8	7	A	13682.1502	-5.3
133	9	0	9	9	8	0	8	8	A	13682.0891	0.9
134	9	0	9	10	8	0	8	9	A	13682.1683	2.2
135	9	0	9	8	8	0	8	7	E	13673.9104	-4.6
136	9	0	9	9	8	0	8	8	E	13673.8480	-0.1
137	9	0	9	10	8	0	8	9	E	13673.9255	0.0
138	9	1	9	8	8	1	8	7	A	13370.5101	7.5
139	9	1	9	9	8	1	8	8	A	13370.4873	-0.5
140	9	1	9	10	8	1	8	9	A	13370.5223	-0.9
141	9	1	9	8	8	1	8	7	E	13363.0422	0.0
142	9	1	9	9	8	1	8	8	E	13363.0266	-1.1
143	9	1	9	10	8	1	8	9	E	13363.0651	2.3
144	3	1	3	2	2	0	2	1	A	8357.5180	5.2
145	3	1	3	3	2	0	2	2	A	8357.1688	-0.7
146	3	1	3	4	2	0	2	3	A	8357.5717	1.3
147	3	1	3	2	2	0	2	1	E	8362.2449	-0.9
148	3	1	3	3	2	0	2	2	E	8361.9008	0.4
149	3	1	3	4	2	0	2	3	E	8362.3018	-0.7
150	4	1	4	3	3	0	3	2	A	9676.3647	-9.3
151	4	1	4	4	3	0	3	3	A	9675.8724	4.0
152	4	1	4	4	3	0	3	3	E	9686.6859	-2.1
153	4	1	4	5	3	0	3	4	E	9687.1662	-3.1
154	5	1	5	4	4	0	4	3	E	10962.7390	6.6
155	5	1	5	5	4	0	4	4	E	10962.1756	-2.8
156	5	1	5	6	4	0	4	5	E	10962.6888	2.2
157	2	2	1	1	1	1	0	0	A	15216.7419	-7.6
158	2	2	1	2	1	1	0	1	A	15215.7118	-3.8
159	2	2	1	3	1	1	0	2	A	15215.7737	1.8
160	2	2	0	1	1	1	1	0	A	15337.4842	-0.4
161	2	2	0	2	1	1	1	1	A	15339.2784	-2.7
162	2	2	0	3	1	1	1	2	A	15338.1987	0.1
163	3	2	2	2	2	1	1	1	A	16649.1815	3.4
164	3	2	2	3	2	1	1	2	A	16648.9808	1.6
165	3	2	2	4	2	1	1	3	A	16649.1170	9.9
166	3	2	1	2	2	1	2	1	A	17021.3716	-4.7
167	3	2	1	3	2	1	2	2	A	17023.1073	0.1
168	3	2	1	4	2	1	2	3	A	17021.9879	-0.6

b) Pyridine (^{14}N)-CD_3F

N	J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	*Sym*	ν (MHz)	$\Delta\nu$ (kHz)
1	5	0	5	4	4	0	4	3	A	7310.6998	5.0
2	5	0	5	5	4	0	4	4	A	7310.6880	-0.7
3	5	0	5	6	4	0	4	5	A	7310.7484	1.6
4	5	0	5	4	4	0	4	3	E	7309.7283	2.2
5	5	0	5	5	4	0	4	4	E	7309.7165	-1.5
6	5	0	5	6	4	0	4	5	E	7309.7768	-3.3
7	5	1	5	4	4	1	4	3	A	7074.1254	4.7
8	5	1	5	5	4	1	4	4	A	7074.1021	-1.3
9	5	1	5	6	4	1	4	5	A	7074.1898	-0.6
10	5	1	5	4	4	1	4	3	E	7073.5675	2.7
11	5	1	5	5	4	1	4	4	E	7073.5443	-2.3
12	5	1	5	6	4	1	4	5	E	7073.6319	-1.4
13	5	1	4	4	4	1	3	3	A	7618.2168	-0.4
14	5	1	4	5	4	1	3	4	A	7618.1485	2.6
15	5	1	4	6	4	1	3	5	A	7618.2182	-1.8
16	5	1	4	4	4	1	3	3	E	7616.7610	-3.0
17	5	1	4	5	4	1	3	4	E	7616.6927	0.7
18	5	1	4	6	4	1	3	5	E	7616.7624	-4.4
19	5	2	4	4	4	2	3	3	A	7351.1018	2.2
20	5	2	4	5	4	2	3	4	A	7350.8496	2.0
21	5	2	4	6	4	2	3	5	A	7351.0781	-3.4
22	5	2	4	4	4	2	3	3	E	7350.6029	5.2
23	5	2	4	5	4	2	3	4	E	7350.3488	3.5
24	5	2	4	6	4	2	3	5	E	7350.5789	-6.9
25	5	2	3	4	4	2	2	3	A	7396.5875	7.5
26	5	2	3	5	4	2	2	4	A	7396.3843	-1.5
27	5	2	3	6	4	2	2	5	A	7396.5687	-5.1
28	5	2	3	4	4	2	2	3	E	7394.8723	2.3
29	5	2	3	5	4	2	2	4	E	7394.6709	-2.5
30	5	2	3	6	4	2	2	5	E	7394.8539	2.1
31	6	0	6	5	5	0	5	4	A	8748.3142	2.8
32	6	0	6	6	5	0	5	5	A	8748.2809	0.3
33	6	0	6	7	5	0	5	6	A	8748.3451	0.6
34	6	0	6	5	5	0	5	4	E	8747.2552	-0.8
35	6	0	6	6	5	0	5	5	E	8747.2220	2.2
36	6	0	6	7	5	0	5	6	E	8747.2862	-1.9
37	6	1	6	5	5	1	5	4	A	8483.0469	-0.5
38	6	1	6	6	5	1	5	5	A	8483.0320	-0.8
39	6	1	6	7	5	1	5	6	A	8483.0933	-0.9
40	6	1	6	5	5	1	5	4	E	8482.3979	2.7
41	6	1	6	6	5	1	5	5	E	8482.3831	-1.7
42	6	1	6	7	5	1	5	6	E	8482.4443	-0.1
43	6	1	5	5	5	1	4	4	A	9134.9839	2.3
44	6	1	5	6	5	1	4	5	A	9134.9388	0.3
45	6	1	5	7	5	1	4	6	A	9134.9881	-1.9
46	6	1	5	5	5	1	4	4	E	9133.2375	2.2
47	6	1	5	6	5	1	4	5	E	9133.1924	-2.1
48	6	1	5	7	5	1	4	6	E	9133.2418	-2.1
49	7	0	7	6	6	0	6	5	A	10173.4443	-6.0
50	7	0	7	7	6	0	6	6	A	10173.3969	0.5
51	7	0	7	8	6	0	6	7	A	10173.4655	0.6
52	7	0	7	6	6	0	6	5	E	10172.3438	-7.1
53	7	0	7	7	6	0	6	6	E	10172.2965	1.8
54	7	0	7	8	6	0	6	7	E	10172.3649	-1.5
55	7	1	7	6	6	1	6	5	A	9889.0014	5.4
56	7	1	7	7	6	1	6	6	A	9888.9885	-1.6
57	7	1	7	8	6	1	6	7	A	9889.0361	0.2
58	7	1	7	6	6	1	6	5	E	9888.2722	2.0
59	7	1	7	7	6	1	6	6	E	9888.2594	-3.2
60	7	1	7	8	6	1	6	7	E	9888.3069	0.3
61	7	1	6	6	6	1	5	5	A	10647.7332	5.0
62	7	1	6	7	6	1	5	6	A	10647.6970	-6.0
63	7	1	7	7	6	1	6	6	A	10647.7374	0.8
64	7	1	7	8	6	1	6	7	A	10645.7032	2.8
65	7	1	7	6	6	1	6	5	E	10645.6670	-6.1
66	7	1	7	7	6	1	6	6	E	10645.7075	-1.5
67	8	0	8	7	7	0	7	6	A	11585.1551	-2.9
68	8	0	8	8	7	0	7	7	A	11585.0981	-0.1
69	8	0	8	9	7	0	7	8	A	11585.1703	2.6
70	8	0	8	7	7	0	7	6	E	11584.0554	-0.8
71	8	0	8	8	7	0	7	7	E	11583.9985	0.5
72	8	0	8	9	7	0	7	8	E	11584.0706	-1.1
73	8	1	8	7	7	1	7	6	A	11291.7028	5.5
74	8	1	8	8	7	1	7	7	A	11291.6898	0.9
75	8	1	8	9	7	1	7	8	A	11291.7296	0.0
76	8	1	8	7	7	1	7	6	E	11290.9047	4.9
77	8	1	8	8	7	1	7	7	E	11290.8917	-1.7
78	8	1	8	9	7	1	7	8	E	11290.9315	-1.9
79	8	1	7	7	7	1	6	6	A	12155.5565	5.1
80	8	1	7	8	7	1	6	7	A	12155.5233	-1.7
81	8	1	7	9	7	1	6	8	A	12155.5601	-5.3
82	8	1	7	7	7	1	6	6	E	12153.2568	-0.9
83	8	1	7	8	7	1	6	7	E	12153.2236	6.4

84	8	1	7	9	7	1	6	8	E	12153.2604	6.9
85	9	0	9	8	8	0	8	7	A	12983.2948	-0.5
86	9	0	9	9	8	0	8	8	A	12983.2320	1.5
87	9	0	9	10	8	0	8	9	A	12983.3064	2.3
88	9	0	9	8	8	0	8	7	E	12982.2306	0.6
89	9	0	9	9	8	0	8	8	E	12982.1678	4.6
90	9	0	9	10	8	0	8	9	E	12982.2421	3.7
91	9	1	9	8	8	1	8	7	A	12690.9495	-2.4
92	9	1	9	9	8	1	8	8	A	12690.9356	-4.9
93	9	1	9	10	8	1	8	9	A	12690.9707	0.1
94	9	1	9	8	8	1	8	7	E	12690.0934	3.0
95	9	1	9	9	8	1	8	8	E	12690.0796	-5.7
96	9	1	9	10	8	1	8	9	E	12690.1146	-1.6
97	9	0	9	8	8	0	8	7	A	13657.4432	1.0
98	9	0	9	9	8	0	8	8	A	13657.4098	-3.5
99	9	0	9	10	8	0	8	9	A	13657.4460	-1.8
100	9	0	9	8	8	0	8	7	E	13654.8957	0.1
101	9	0	9	9	8	0	8	8	E	13654.8623	1.4
102	9	0	9	10	8	0	8	9	E	13654.8985	-2.7
103	3	1	3	3	2	0	2	2	A	7972.2975	3.8
104	3	1	3	4	2	0	2	3	A	7972.6751	4.5
105	3	1	3	3	2	0	2	2	E	7972.3470	-2.6
106	3	1	3	4	2	0	2	3	E	7972.7246	0.1
107	4	1	4	3	3	0	3	2	E	9230.9636	0.4
108	4	1	4	4	3	0	3	3	E	9230.4848	1.2
109	4	1	4	5	3	0	3	4	E	9230.9454	0.6
110	5	1	5	5	8	1	8	4	A	10442.1684	-6.6
111	5	1	5	6	8	1	8	5	A	10442.6580	-1.8
112	5	1	5	4	8	1	8	3	E	10443.2398	1.3
113	5	1	5	5	8	1	8	4	E	10442.7113	3.5
114	5	1	5	6	8	1	8	5	E	10443.2009	-4.5

c) Pyridine (^{15}N)-CH_3F

J'	K_a'	K_c'	J''	K_a''	K_c''	*Sym*	ν/MHz	$\Delta\nu$/kHz
5	0	5	4	0	4	A	7709.2912	3.2
5	0	5	4	0	4	E	7696.5261	1.0
6	0	6	5	0	5	A	9222.3232	0.6
6	0	6	5	0	5	E	9209.8194	-0.8
7	0	7	6	0	6	A	10720.8393	-2.2
7	0	7	6	0	6	E	10709.3989	-1.1
8	0	8	7	0	7	A	12203.9140	-0.7
8	0	8	7	0	7	E	12194.0562	1.4
5	1	5	4	1	4	A	7450.2162	0.4
5	1	5	4	1	4	E	7445.0533	0.4
6	1	6	5	1	3	A	8051.8677	0.5
6	1	6	5	1	3	E	8047.6050	-0.3
6	1	5	5	1	4	A	9654.1096	1.6
6	1	5	5	1	4	E	9646.3875	1.1
7	1	7	6	1	6	A	10412.9640	0.8
7	1	7	6	1	6	E	10406.3890	-2.0
7	1	6	6	1	5	A	11251.5643	-0.4
7	1	6	6	1	5	E	11239.6488	-0.6
8	1	8	7	1	7	A	11888.8328	1.4
8	1	8	7	1	7	E	11881.7787	2.0
8	1	7	7	1	6	A	12843.1406	-1.9
8	1	7	7	1	6	E	12826.6522	3.0
6	1	6	5	1	5	A	8933.3194	-1.4
6	1	6	5	1	5	E	8927.3694	-1.8
3	1	3	2	0	2	A	8328.1568	1.3
3	1	3	2	0	2	E	8332.9032	0.0
4	1	4	3	0	3	A	9645.2068	-0.9
4	1	4	3	0	3	E	9656.0099	-0.3

d) Pyridine (^{15}N)-CD_3F

J'	K_a'	K_c'	J''	K_a''	K_c''	*Sym*	ν/MHz	$\Delta\nu$/kHz
5	0	5	4	0	4	A	7306.6767	5.5
5	0	5	4	0	4	E	7305.7106	-13.4
6	0	6	5	0	5	A	8743.1378	7.2
6	0	6	5	0	5	E	8742.0880	-8.6
7	0	7	6	0	6	A	10166.9701	7.4
7	0	7	6	0	6	E	10165.8822	-4.5
8	0	8	7	0	7	A	11577.2456	6.0
8	0	8	7	0	7	E	11576.1624	-0.8
5	1	5	4	1	4	A	7069.4764	3.5
5	1	5	4	1	4	E	7068.9233	0.8
6	1	6	5	1	5	A	8477.3774	1.7
6	1	6	5	1	5	E	8476.7383	2.2
7	1	7	6	1	6	A	9882.2772	-0.4
7	1	7	6	1	6	E	9881.5553	-4.3
8	1	8	7	1	7	A	11283.8913	0.1
8	1	8	7	1	7	E	11283.1016	-4.2
5	1	5	5	1	4	A	9131.9521	-8.1
5	1	5	5	1	4	E	9130.2200	8.7
4	1	4	4	1	3	A	7615.7620	-8.4
4	1	4	4	1	3	E	7614.3200	14.1
6	1	6	6	1	5	A	10644.0631	-1.6
6	1	6	6	1	5	E	10642.0453	3.7
7	1	7	7	1	6	A	12151.1608	-3.0
7	1	7	7	1	6	E	12148.8805	-2.2
3	1	3	2	0	2	A	7947.1509	-9.1
3	1	3	2	0	2	E	7947.1985	6.8
4	1	4	3	0	3	A	9203.6206	-10.7
4	1	4	3	0	3	E	9203.8743	12.9

2) Table 2S: Ab initio geometry of the observed complex (see the drawn for atom numbering), calculated at the MP2/6-311++G(d,p) level.

bond lengths/Å		angles/°		dihedral angles/°	
C2C1	1.3991				
N3C2	1.3467	N3C2C1	123.5		
C4N3	1.3452	C4N3C2	117.0	C4N3C2C1	0.0
C5C4	1.3987	C5C4N3	123.8	C5C4N3C2	0.0
C6C5	1.3974	C6C5C4	118.6	C6C5C4N3	0.0
F7C2	3.4078	F7C2C3	93.2	F7C2N3C4	180.0
C8F7	1.3979	C8F7C2	91.5	C8F7C2C3	0.0
H9C8	1.0912	H9C8F7	108.2	H9C8F7C2	-120.4
H10C4	1.0881	H10C4N3	115.9	H10C4N3C2	180.0
H11C5	1.0860	H11C5C4	120.1	H11C5C4N3	180.0
H12C6	1.0865	H12C6C5	120.8	H12C6C5C4	180.0
H13C1	1.0859	H13C1C2	119.9	H13C1C2N3	180.0
H14C2	1.0873	H14C2N3	115.8	H14C2N3C4	180.0
H15C8	1.0904	H15C8F7	108.5	H15C8F7C2	0.0
H16C8	1.0912	H16C8F7	108.2	H16C8F7C2	120.0