Rotational and Vibrational Spectroscopy of a Weakly Bound Hexafluoroisopropanol···Nitrogen Complex: ^{14}N Hyperfine Splittings, Molecular Geometry, and Experimental Benchmarks

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Table S1. Spectroscopic properties of the most stable HFIP and HFIP···N_2 conformers at the B3LYP-D3(BJ)/def2-QZVP level of theory.

Parameter	H_t	H_tN_H	H_tN_C	H_tN_O	H_tN_F	$H_tN_{F'}$	H_g	H_gN_H	H_gN_C	H_gN_O	H_gN_F	$H_gN_{F'}$	$H_gN_{F''}$
ΔE_e /kJ mol^{-1} [a]	(0.0)	(0.0)	4.6	4.8	7.4	8.4	4.7	5.2	9.6	11.8	12.2	13.1	13.1
ΔE_0 /kJ mol^{-1} [a]	(0.0)	(0.0)	3.3	3.5	5.5	6.2	4.1	4.5	7.6	9.2	9.6	10.3	10.3
A_e /MHz[b]	2089.8	958.2	947.7	1078.3	979.7	1825.4	2093.2	1224.7	956.2	1375.2	987.8	1781.6	1585.9
B_e /MHz[b]	1042.2	743.0	766.8	643.2	830.8	474.5	1043.8	544.9	755.0	575.0	816.5	481.1	505.3
C_e /MHz[b]	922.9	535.7	551.3	502.4	572.1	444.8	923.8	442.4	550.2	480.3	563.0	448.0	451.7
$\lvert\mu_a\rvert$ /Debye[c]	0.0	0.8	0.1	0.5	0.6	0.2	1.1	2.7	0.8	0.4	2.3	1.7	0.0
$\lvert\mu_b\rvert$ /Debye[c]	0.6	0.0[d]	0.0[d]	0.3	0.0[d]	0.6	1.3	0.6	1.2	1.4	0.6	1.2	2.1
$\lvert\mu_c\rvert$ /Debye[c]	0.1	0.4	0.5	0.3	0.2	0.0	1.9	1.4	2.1	2.0	0.8	1.5	1.4
$\chi_{aa}(N_i)$ /MHz[e]	-	-3.040	-3.665	-3.210	2.790	3.016	-	-5.431	-2.792	2.947	2.500	2.979	2.964
$\chi_{bb} - \chi_{cc}(N_i)$ /MHz[e]	-	2.733	2.282	2.762	8.853	5.943	-	0.133	3.012	2.632	2.501	8.486	-8.223
$\chi_{aa}(N_o)$ /MHz[e]	-	-3.222	-3.752	-3.262	2.812	3.011	-	-5.812	-2.856	2.942	2.467	2.977	2.979
$\chi_{bb} - \chi_{cc}(N_o)$ /MHz[e]	-	2.916	2.378	2.858	8.883	5.925	-	0.102	3.130	2.631	2.506	8.476	-8.247
ω_{OH} /cm^{-1} [f]	3789	3753	3790	3789	3788	3789	3827	3797	3829	3829	3827	3826	3827

[a] ΔE_e and ΔE_0 are the relative raw and harmonic vibrational zero-point energy (ZPE) corrected energy in kJ mol^{-1}, respectively. They are relative to H_t and H_tN_H, for the monomer and complex conformers, respectively. [b] Equilibrium rotational constants. [c] Magnitudes of the *a*-, *b*- and *c*-type electric dipole moment components. [d] This dipole moment component is 0 due to symmetry reasons. [e] Nuclear quadrupole coupling constants with N_i and N_o referring to the inner (closer to HFIP) and outer nitrogen, respectively. [f] Harmonic OH stretching wavenumber.

Table S2. Cartesian coordinates (in Å) of the eleven most stable HFIP···N_2 conformers obtained at the B3LYP-D3(BJ)/def2-QZVP geometry optimizations with convergence set to 'verytight' and integration grid to 'SuperFine'.

H_tN_H	a	b	c	H_tN_C	a	b	c
C	0.71978	1.29141	0.02707	C	-0.47634	1.29181	0.12232
C	0.65984	0.00000	-0.81107	C	-0.45328	-0.00001	-0.71559
H	1.54351	0.00000	-1.44798	H	0.48223	0.00001	-1.27056
C	0.71978	-1.29141	0.02707	C	-0.47629	-1.29182	0.12232
F	0.75848	2.35166	-0.79129	F	-0.33836	2.35016	-0.68753
F	-0.36956	1.42154	0.80814	F	-1.64694	1.42868	0.77422
F	1.80215	1.34154	0.81345	F	0.50971	1.33726	1.02658
F	1.80215	-1.34154	0.81345	F	0.50977	-1.33724	1.02657
F	0.75848	-2.35166	-0.79129	F	-0.33828	-2.35017	-0.68753
F	-0.36956	-1.42154	0.80814	F	-1.64688	-1.42873	0.77423
O	-0.45946	0.00000	-1.63975	O	-1.49762	-0.00003	-1.64233
H	-1.26633	0.00000	-1.10927	H	-2.34216	-0.00004	-1.17806
N	-3.16970	0.00000	-0.08008	N	3.99591	0.00004	-0.00610
N	-4.06992	0.00000	0.53277	N	3.05709	0.00006	-0.55899

H_tN_O	a	b	c	H_gN_H	a	b	c
C	-1.39319	-0.85249	-0.11856	C	-1.61780	-0.74936	-0.10529
C	0.02057	-0.26384	0.03903	C	-0.15155	-0.31556	-0.25231
H	0.61686	-0.63764	-0.79099	H	0.11392	-0.48999	-1.29902
C	0.07261	1.27354	-0.02932	C	0.07927	1.18710	0.00230
F	-1.31624	-2.18956	-0.16057	F	-1.74567	-2.02468	-0.50235
F	-2.17714	-0.52362	0.92609	F	-2.05313	-0.66321	1.15332
F	-1.99828	-0.44086	-1.23860	F	-2.41942	0.00109	-0.87883
F	-0.45968	1.75442	-1.15857	F	-0.49409	1.94521	-0.94234
F	1.34915	1.67838	0.02756	F	1.41021	1.42299	-0.04522
F	-0.57613	1.83101	1.01078	F	-0.36074	1.59345	1.19418
O	0.61208	-0.72096	1.21848	O	0.59141	-1.09206	0.63593
H	0.10335	-0.41199	1.97645	H	1.52529	-1.04292	0.40715
N	3.24179	-1.04366	-0.59265	N	3.63448	-0.97362	-0.07668
N	4.14685	-1.05439	0.01378	N	4.70326	-0.85973	-0.25226
H_tN_F	a	b	c	$H_tN_{F'}$	a	b	c
C	0.47597	1.29270	0.15979	C	0.56022	0.27772	-0.24337
C	1.31376	0.00006	0.16826	C	-0.90938	0.66797	-0.48853
H	1.88634	0.00010	1.09447	H	-1.04413	0.73280	-1.56712
C	0.47610	-1.29266	0.15981	C	-1.92792	-0.36528	0.02916
F	1.28923	2.35052	0.27746	F	1.36283	1.18357	-0.81886
F	-0.20060	1.42603	-0.99674	F	0.84611	0.25911	1.07211
F	-0.40589	1.33914	1.16519	F	0.86471	-0.92158	-0.75249
F	-0.40580	-1.33915	1.16518	F	-1.71437	-1.58902	-0.46782
F	1.28945	-2.35040	0.27755	F	-3.16345	0.01231	-0.32523
F	-0.20042	-1.42610	-0.99673	F	-1.89706	-0.44703	1.37276
O	2.22450	0.00009	-0.88916	O	-1.17649	1.92952	0.04517
H	1.74788	0.00005	-1.72693	H	-1.06719	1.90592	1.00249
N	-3.21301	-0.00031	-0.82167	N	4.25625	-0.65290	-0.25410
N	-3.38442	0.00006	0.25467	N	4.21248	-0.19971	0.73618
H_gN_C	a	b	c	H_gN_O	a	b	c
C	-0.16314	1.32588	0.13528	C	-0.32283	1.02909	-0.09691
C	-0.44822	0.07641	-0.71027	C	0.36668	-0.23944	-0.62095
H	0.48485	-0.16328	-1.22537	H	0.55190	-0.07009	-1.68546
C	-0.81201	-1.16746	0.12219	C	1.74262	-0.50931	0.01766
F	0.30955	2.30055	-0.65583	F	-1.42317	1.26962	-0.82672
F	-1.25221	1.78679	0.75316	F	-0.69071	0.92047	1.18062
F	0.76982	1.06772	1.06719	F	0.48661	2.09337	-0.21379
F	0.23144	-1.61059	0.83601	F	2.64897	0.40294	-0.35455
F	-1.16391	-2.15439	-0.73409	F	2.17634	-1.71390	-0.42046
F	-1.83691	-0.96828	0.95215	F	1.70717	-0.55245	1.34998
O	-1.48582	0.41225	-1.58517	O	-0.51191	-1.29936	-0.38322
H	-1.58206	-0.27783	-2.24715	H	-0.19882	-2.08629	-0.83773

N	3.93120	-0.65470	0.04048	N	-3.85552	-0.61884	0.56119
N	3.05651	-0.55796	-0.60193	N	-3.77112	-1.26535	-0.31202

H_gN_F	a	b	c	$H_gN_{F'}$	a	b	c
C	0.23361	1.32887	0.16810	C	-0.55618	-0.36547	-0.19796
C	1.29937	0.22311	0.15596	C	0.92348	-0.70652	-0.42698
H	1.83850	0.30736	1.10410	H	1.04894	-0.81441	-1.50834
C	0.71682	-1.20276	0.11922	C	1.89300	0.40900	0.00845
F	0.82654	2.51671	0.35584	F	-1.32307	-1.31798	-0.74886
F	-0.45755	1.38690	-0.97185	F	-0.86886	-0.28096	1.09633
F	-0.63394	1.13998	1.17589	F	-0.86954	0.80213	-0.78297
F	0.08943	-1.51193	1.25953	F	1.79303	1.48740	-0.77824
F	1.74677	-2.06917	-0.02571	F	3.15491	-0.06565	-0.11278
F	-0.12471	-1.40409	-0.89622	F	1.72550	0.79125	1.27486
O	2.11193	0.46147	-0.95520	O	1.17483	-1.89043	0.27080
H	2.86891	-0.13063	-0.93225	H	2.05501	-2.21027	0.05376
N	-3.45352	-0.14490	-0.68436	N	-4.16159	0.60781	0.73186
N	-3.18818	-0.77344	0.16555	N	-4.24119	0.41599	-0.33811

$H_gN_{F''}$	a	b	c
C	-1.80874	0.53299	-0.00926
C	-1.02084	-0.74278	-0.34204
H	-1.21807	-0.95827	-1.39626
C	0.50604	-0.58125	-0.21563
F	-3.10413	0.34454	-0.30111
F	-1.71957	0.86884	1.27883
F	-1.36897	1.56671	-0.74499
F	0.99778	0.23195	-1.15904
F	1.07028	-1.79755	-0.39400
F	0.89276	-0.12721	0.97764
O	-1.49189	-1.74074	0.51467
H	-1.11745	-2.58787	0.25715
N	4.16491	1.25434	0.33705
N	4.08319	0.19198	0.10781

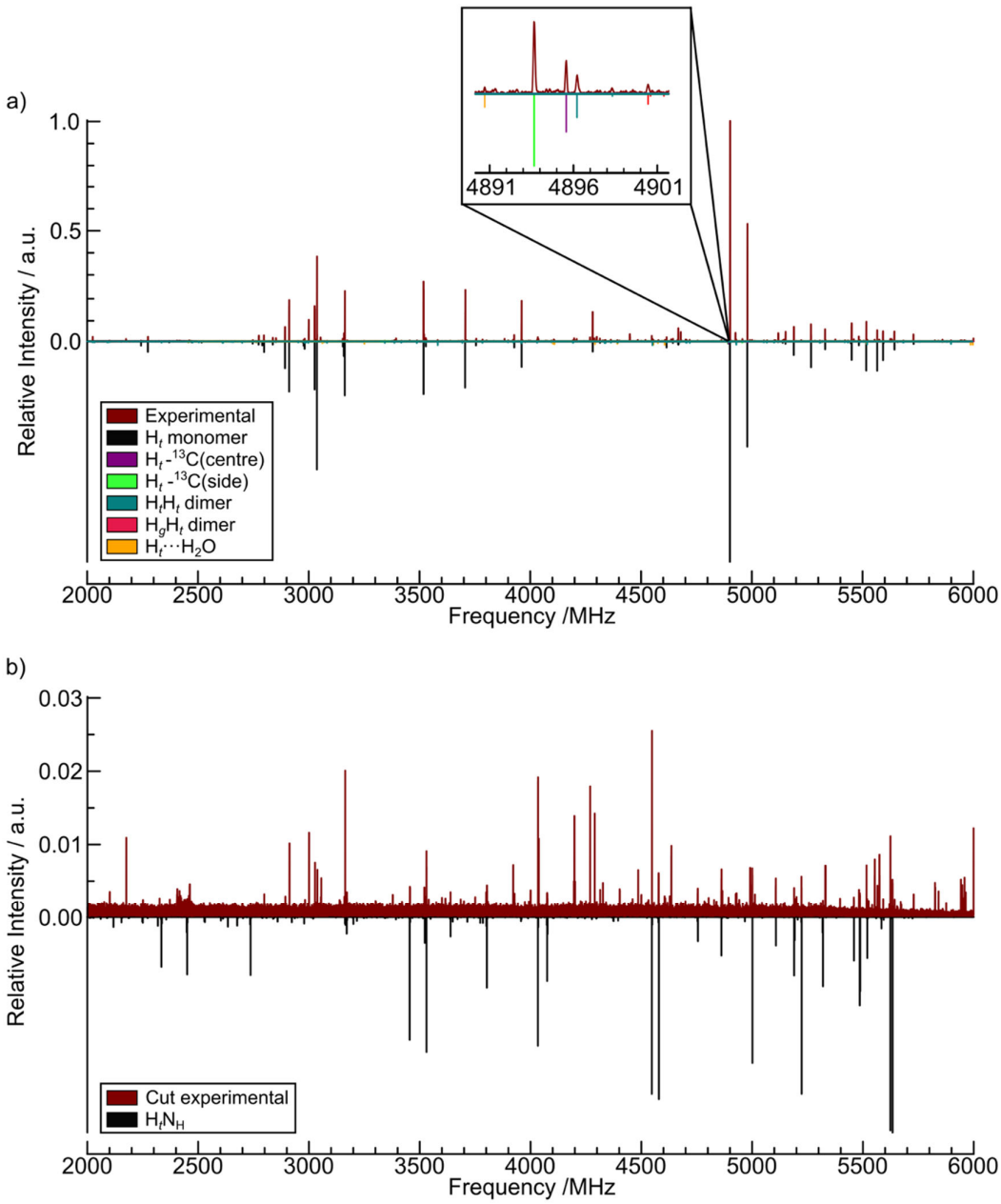

Figure S1. a) The CP-FTMW spectrum (top), recorded with HFIP and N_2 in helium carrier gas, is dominated by strong transitions from previously reported species. These include the *trans*-HFIP monomer and its two ^{13}C isotopologues,[i] the achiral H_tH_t and chiral H_gH_t HFIP dimers,[ii] and the most stable conformer of HFIP$\cdots H_2O$.[iii,iv] The simulated spectrum for these species, based on their known experimental spectroscopic constants and a rotational temperature of 1 K, as well as the theoretical permanent dipole components, are shown in the bottom trace. The insert highlights a small section of the experimental spectrum, alongside the corresponding simulated spectra of multiple species. b) The CP-FTMW spectrum (top) after removing all the transitions of the known species indicated in a). The simulated spectrum (bottom) of H_tN_H based on the experimental spectroscopic constants and a rotational temperature of 1 K, as well as the theoretical permanent dipole components is shown in the bottom trace.

Table S3. Experimentally assigned hypothetical unsplit central transition frequencies of H_tN_H.

J'	Ka'	Kc'		J"	Ka"	Kc"	RSD [a]	ν [b] /MHz	$\Delta\nu$ [c] /MHz
3	1	3	-	2	1	2	2	3455.5582	-0.0002
2	2	0	-	1	1	0	2	3522.8481	0.0050
3	0	3	-	2	0	2	2	3530.2713	-0.0001
2	2	1	-	1	1	1	2	3638.6571	0.0000
3	2	2	-	2	2	1	2	3802.7200	-0.0052
3	2	1	-	2	2	0	2	4075.2456	-0.0003
4	0	4	-	3	0	3	2	4578.4565	-0.0001
3	1	2	-	2	0	2	2	4754.7986	0.0048
3	2	1	-	2	1	1	2	4861.8029	-0.0051
4	2	3	-	3	2	2	2	5000.9404	-0.0002
3	2	2	-	2	1	2	2	5107.2492	-0.0050
4	1	3	-	3	1	2	1	5223.1466	0.0022
4	2	2	-	3	2	1	2	5486.7268	-0.0053
5	1	5	-	4	1	4	2	5624.5241	0.0018
5	1	4	-	4	1	3	1	6297.6518	0.0013
4	1	3	-	3	0	3	1	6447.6655	-0.0013
4	2	3	-	3	1	3	1	6652.6346	-0.0019
6	0	6	-	5	0	5	2	6696.5727	-0.0042
5	2	3	-	4	2	2	1	6811.0406	0.0007
4	3	2	-	3	2	2	1	6907.2423	0.0011
6	1	5	-	5	1	4	1	7328.7583	-0.0005
6	3	4	-	5	3	3	1	7686.0070	0.0014
7	1	7	-	6	1	6	1	7761.0908	-0.0006
7	0	7	-	6	0	6	1	7761.7640	0.0018
6	4	3	-	5	4	2	1	7846.3668	-0.0014
6	2	4	-	5	2	3	1	8007.4720	-0.0002
6	4	2	-	5	4	1	1	8008.8896	0.0021
5	3	2	-	4	2	2	1	8009.8774	0.0002
5	1	4	-	4	0	4	1	8166.8625	0.0019
6	3	3	-	5	3	2	1	8245.1805	-0.0015
7	2	6	-	6	2	5	1	8346.3349	-0.0011
7	1	6	-	6	1	5	1	8370.5503	0.0010
8	1	8	-	7	1	7	1	8827.5562	0.0002
8	0	8	-	7	0	7	1	8827.7180	-0.0012
7	3	5	-	6	3	4	1	8856.4190	0.0002
7	2	5	-	6	2	4	1	9075.2669	-0.0016
8	3	6	-	7	3	5	1	9979.8760	0.0008
8	4	5	-	7	4	4	1	10382.7507	-0.0004
10	1	10	-	9	1	9	1	10960.0021	0.0002
10	0	10	-	9	0	9	1	10960.0106	0.0001

[a] The hypothetical unsplit central frequencies extracted from the cavity-based measurements were given a relative uncertainty of 1, whereas a value of 2 was used for those obtained from the broadband measurements.

[b] Experimental transition frequency

[c] Experimental transition frequency – theoretical transition frequency

Table S4. Experimentally assigned ^{14}N hyperfine components of H_tN_H.

J'	Ka'	Kc'	I_N' [a]	F' [a]		J"	Ka"	Kc"	I_N" [a]	F" [a]	ν [b]/MHz	$\Delta\nu$ [c] /MHz
4	1	3	2	2	-	3	1	2	2	1	5222.8621	0.0033
4	1	3	2	3	-	3	1	2	2	2	5222.9621	0.0023
4	1	3	0	4	-	3	1	2	0	3	5222.9762	0.0012
4	1	3	1	4	-	3	1	2	1	3	5223.0245	0.0022
4	1	3	2	6	-	3	1	2	2	5	5223.0963	0.0016
4	1	3	1	5	-	3	1	2	1	4	5223.1693	0.0013
4	1	3	1	3	-	3	1	2	1	2	5223.2865	0.0037
4	1	3	2	5	-	3	1	2	2	4	5223.3135	0.0016
4	1	3	2	4	-	3	1	2	2	3	5223.3441	0.0027
5	1	4	2	3	-	4	1	3	2	2	6297.4110	0.0003
5	1	4	0	5	-	4	1	3	0	4	6297.4863	0.0004
5	1	4	1	5	-	4	1	3	1	4	6297.5087	0.0036
5	1	4	2	7	-	4	1	3	2	6	6297.5635	0.0002
5	1	4	2	4	-	4	1	3	2	3	6297.5764	0.0024
5	1	4	1	6	-	4	1	3	1	5	6297.6952	0.0018
5	1	4	1	4	-	4	1	3	1	3	6297.7721	0.0028
5	1	4	2	6	-	4	1	3	2	5	6297.8059	0.0013
5	1	4	2	5	-	4	1	3	2	4	6297.9172	0.0011
4	3	2	1	5	-	3	2	2	1	4	6907.2833	0.0004
4	3	2	1	3	-	3	2	2	1	2	6907.3238	0.0024
4	3	2	1	3	-	3	2	2	1	3	6907.3241	0.0021
4	3	2	2	5	-	3	2	2	2	4	6907.3464	-0.0010
4	3	2	2	5	-	3	2	2	2	5	6907.3466	-0.0012
4	3	2	2	4	-	3	2	2	2	3	6907.4637	-0.0005
4	3	2	2	4	-	3	2	2	2	4	6907.4634	-0.0001
6	1	5	2	4	-	5	1	4	2	3	7328.6236	-0.0008
6	1	5	0	6	-	5	1	4	0	5	7328.6616	-0.0008
6	1	5	2	8	-	5	1	4	2	7	7328.7004	-0.0006
6	1	5	2	5	-	5	1	4	2	4	7328.7329	-0.0003
6	1	5	1	7	-	5	1	4	1	6	7328.7892	0.0000
6	1	5	2	7	-	5	1	4	2	6	7328.8487	-0.0010
6	1	5	2	6	-	5	1	4	2	5	7328.9290	0.0000
6	3	4	2	6	-	5	3	3	2	5	7685.7752	0.0019
6	3	4	2	8	-	5	3	3	2	7	7686.1034	0.0016
6	3	4	1	6	-	5	3	3	1	5	7686.1215	0.0020
6	3	4	0	6	-	5	3	3	0	5	7686.1234	0.0000
6	3	4	2	4	-	5	3	3	2	3	7686.1433	0.0012
6	4	3	2	7	-	5	4	2	2	6	7846.0972	0.0029
6	4	3	1	5	-	5	4	2	1	4	7846.1541	0.0014

6	4	3	1	7	-	5	4	2	1	6	7846.2438	0.0031
6	4	3	2	5	-	5	4	2	2	4	7846.3627	0.0016
6	4	3	1	6	-	5	4	2	1	5	7846.6917	0.0009
6	4	3	0	6	-	5	4	2	0	5	7846.7080	0.0032
6	4	3	2	4	-	5	4	2	2	3	7846.7954	0.0034
6	2	4	2	8	-	5	2	3	2	7	8007.4197	0.0003
6	2	4	2	5	-	5	2	3	2	4	8007.4197	0.0002
6	2	4	1	7	-	5	2	3	1	6	8007.4988	-0.0006
6	2	4	1	5	-	5	2	3	1	4	8007.5513	0.0008
6	2	4	2	6	-	5	2	3	2	5	8007.6430	-0.0007
6	4	2	2	7	-	5	4	1	2	6	8008.5352	0.0005
6	4	2	1	5	-	5	4	1	1	4	8008.6083	0.0011
6	4	2	1	7	-	5	4	1	1	6	8008.7209	0.0006
6	4	2	2	5	-	5	4	1	2	4	8008.8675	0.0003
6	4	2	2	8	-	5	4	1	2	7	8009.2253	0.0004
6	4	2	1	6	-	5	4	1	1	5	8009.3164	-0.0001
6	4	2	2	4	-	5	4	1	2	3	8009.4450	0.0005
5	3	2	2	3	-	4	2	2	2	2	8009.6074	0.0008
5	3	2	2	7	-	4	2	2	2	6	8009.7840	0.0010
5	3	2	1	6	-	4	2	2	1	5	8009.9246	-0.0002
5	3	2	1	4	-	4	2	2	1	3	8010.0128	-0.0004
5	3	2	2	6	-	4	2	2	2	5	8010.0509	0.0006
5	3	2	2	5	-	4	2	2	2	4	8010.1675	-0.0011
6	3	3	2	6	-	5	3	2	2	5	8244.8178	-0.0007
6	3	3	2	7	-	5	3	2	2	6	8245.0580	-0.0001
6	3	3	1	7	-	5	3	2	1	6	8245.1024	-0.0026
6	3	3	2	5	-	5	3	2	2	4	8245.1219	0.0007
6	3	3	2	8	-	5	3	2	2	7	8245.3419	-0.0006
6	3	3	1	6	-	5	3	2	1	5	8245.3631	-0.0020
6	3	3	0	6	-	5	3	2	0	5	8245.3626	-0.0015
6	3	3	2	4	-	5	3	2	2	3	8245.3833	-0.0009
7	3	5	2	7	-	6	3	4	2	6	8856.3484	-0.0006
7	3	5	1	8	-	6	3	4	1	7	8856.4014	0.0017
7	3	5	2	8	-	6	3	4	2	7	8856.4021	0.0013
7	3	5	1	6	-	6	3	4	1	5	8856.4032	0.0001
7	3	5	2	9	-	6	3	4	2	8	8856.4535	0.0006
7	2	5	0	7	-	6	2	4	0	6	9075.1325	-0.0016
7	2	5	2	9	-	6	2	4	2	8	9075.1777	0.0002
7	2	5	2	7	-	6	2	4	2	6	9075.5140	0.0000

[a] The coupling scheme used is: $\mathbf{I_{Ni}} + \mathbf{I_{No}} = \mathbf{I_N}$; $\mathbf{I_N} + \mathbf{J} = \mathbf{F}$.

[b] Experimental transition frequency

[c] Experimental transition frequency – theoretical transition frequency

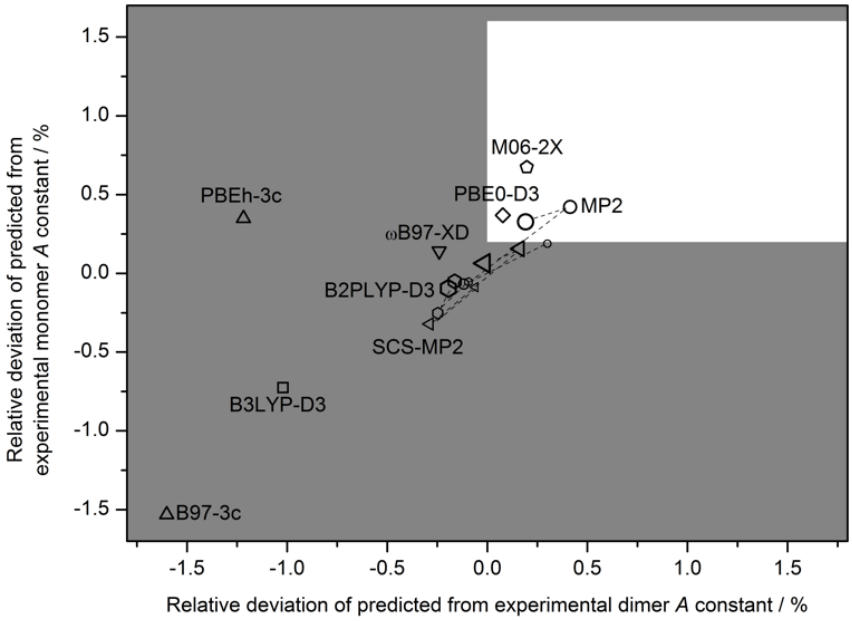

Figure S2. Relative deviation of the theoretically predicted (A_e) from the experimental rotational constant (A_{exp}) for the HFIP monomer and H_tN_H at different levels of electronic structure calculation. Each method is represented by a symbol. For MP2, SCS-MP2 and B2PLYP-D3, four basis sets (VTZ, aVTZ, VQZ, and aVQZ) were used. Increasing basis set size from VTZ to aVQZ is indicated by progressively larger symbols, which are connected by dashed lines for each method. The zone of estimated incompatibility with experiment is grey. Only predictions within the white area are compatible with experiment for both species, using the lower and upper bounds of vibrational effects on rotational constants, ranging from 0.2% to 1.6% for the HFIP monomer and from 0% to 1.8% for H_tN_H. See the main text for further discussion.

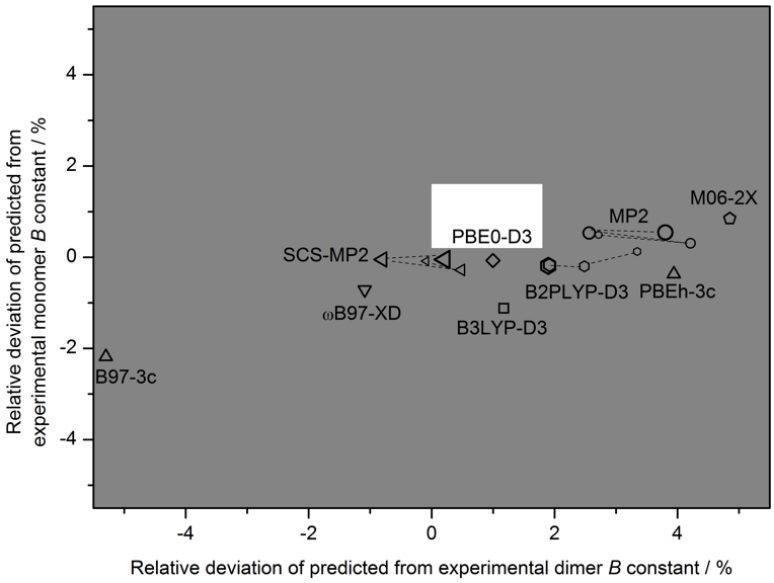

Figure S3. Relative deviation of the theoretically predicted (B_e) from the experimental rotational constant (B_{exp}) for the HFIP monomer and H_tN_H at different levels of electronic structure calculation. Each method is represented by a symbol. For MP2, SCS-MP2 and B2PLYP-D3, four basis sets (VTZ, aVTZ, VQZ, and aVQZ) were used. Increasing basis set size from VTZ to aVQZ is indicated by progressively larger symbols, which are connected by dashed lines for

each method. The zone of estimated incompatibility with experiment is grey. Only predictions within the white area are compatible with experiment for both species, using the lower and upper bounds of vibrational effects on rotational constants, ranging from 0.2% to 1.6% for the HFIP monomer and from 0% to 1.8% for H_tN_H. See the main text for further discussion.

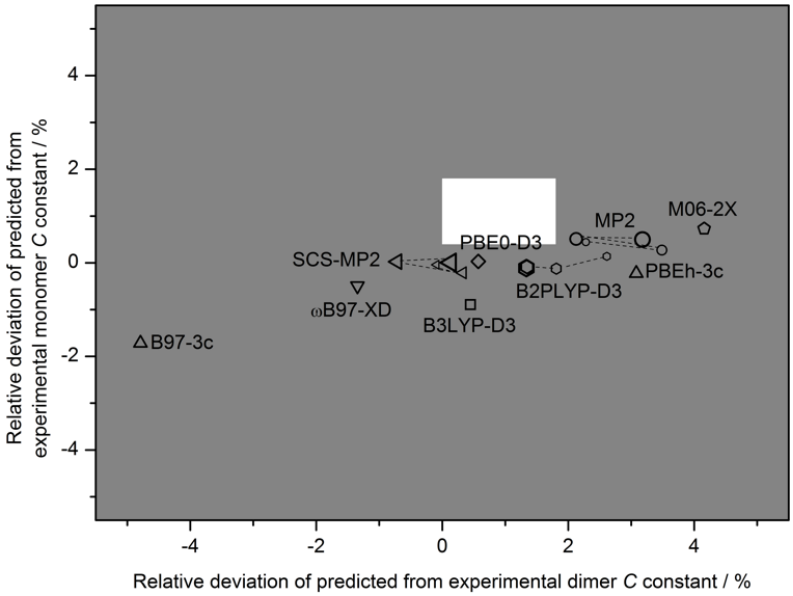

Figure S4. Relative deviation of the theoretically predicted (C_e) from the experimental rotational constant (C_{exp}) for the HFIP monomer and H_tN_H at different levels of electronic structure calculation. Each method is represented by a symbol. For MP2, SCS-MP2 and B2PLYP-D3, four basis sets (VTZ, aVTZ, VQZ, and aVQZ) were used. Increasing basis set size from VTZ to aVQZ is indicated by progressively larger symbols, which are connected by dashed lines for each method. The zone of estimated incompatibility with experiment is grey. Only predictions within the white area are compatible with experiment for both species, using the lower and upper bounds of vibrational effects on rotational constants, ranging from 0.2% to 1.6% for the HFIP monomer and from 0% to 1.8% for H_tN_H. See the main text for further discussion.

Table S5. Theoretically predicted harmonic (ω_{OH}) OH stretching wavenumber, hydrogen bond induced downshift ($\Delta\omega_{OH}$) and lowest predicted wavenumber (ω_1, typically CF_3 torsion in H_t and intermolecular torsion in H_tN_H), in cm^{-1}, IR intensity (S_{OH}) in km mol^{-1}, as well as equilibrium rotational constants (A_e, B_e, C_e) in MHz and magnitudes of the electric dipole moment components ($|\mu_a|$, $|\mu_b|$, $|\mu_c|$) in D calculated at different levels of approximation.

Level of theory	Structure	ω_{OH}	S_{OH}	$\Delta\omega_{OH}$	ω_1	A_e	B_e	C_e	$\|\mu_a\|$	$\|\mu_b\|$	$\|\mu_c\|$
B3LYP-D3/	H_t	3789	63	-	25	2089.8	1042.2	922.9	0.0	0.6	0.1
def2-QZVP	H_tN_H	3753	281	36	18	958.2	743.0	535.7	0.8	0.0	0.4
PBEh-3c	H_t	3895	69	-	34	2112.5	1050.1	930.0	-	-	-
	H_tN_H	3883	240	12	20	956.3	763.3	549.7	-	-	-
B2PLYP-D3/ VTZ	H_t	3807	65	-	26	2104	1055.3	933.8	-	-	-
	H_tN_H	3778	282	29	21	967.2	758.9	547.2	-	-	-
B2PLYP-D3/	H_t	3796	66	-	5	2099.8	1051.9	931.0	-	-	-
aVTZ	H_tN_H	3762	273	34	10	965.7	752.6	542.9	-	-	-
B2PLYP-D3/	H_t	3807	70	-	24	2104.1	1052.2	931.5	-	-	-
VQZ	H_tN_H	3775	280	32	18	966.5	748.4	540.5	-	-	-

B2PLYP-D3/	H_t	3809	65	-	18	2103.1	1052.0	931.2	-	-	-
aVQZ	H_tN_H	3771	278	38	19	966.2	748.2	540.4	-	-	-
B97-3c	H_t	3716	43	-	20	2072.9	1031.0	914.2	-	-	-
	H_tN_H	3688	189	28	14	952.6	695.4	507.7	-	-	-
M06-2X/	H_t	3828	82	-	16	2119.3	1062.9	940.0	0.0	0.6	0.1
aVTZ	H_tN_H	3798	283	30	15	970	769.9	555.4	0.6	0.0	0.4
MP2/	H_t	3818	67	-	28	2109.1	1059.2	937.0	-	-	-
VTZ	H_tN_H	3787	270	31	13	971	754.3	545.4	-	-	-
MP2/	H_t	3794	70	-	15	2103.7	1057.2	935.2	-	-	-
aVTZ	H_tN_H	3758	278	36	11	967	765.2	551.9	-	-	-
MP2/	H_t	3819	73	-	25	2114	1059.6	937.7	-	-	-
VQZ	H_tN_H	3784	275	35	17	972.1	753.1	544.6	-	-	-
MP2/	H_t	3810	73	-	24	2112	1059.7	937.6	-	-	-
aVQZ	H_tN_H	3772	276	38	15	970	762.2	550.2	-	-	-
PBE0-D3/	H_t	3830	65	-	24	2112.9	1053.2	932.6	0.0	0.5	0.1
aVTZ	H_tN_H	3786	274	44	18	968.9	741.7	536.3	0.7	0.0	0.3
SCS-MP2/	H_t	3822	62	-	28	2103.3	1053.1	931.9	-	-	-
VTZ	H_tN_H	3802	232	20	13	967.5	733.7	532.8	-	-	-
SCS-MP2/	H_t	3801	65	-	16	2098.3	1051.1	930.1	-	-	-
aVTZ	H_tN_H	3778	242	23	13	965.3	737.9	535.0	-	-	-
SCS-MP2/	H_t	3827	67	-	26	2108.4	1053.5	932.6	-	-	-
VQZ	H_tN_H	3803	237	24	19	969.7	728.4	529.4	-	-	-
SCS-MP2/ aVQZ	H_t	3818	68	-	24	2106.5	1053.5	932.4	-	-	-
	H_tN_H	3792	241	26	14	968	735.9	534.0	-	-	-
ωB97-XD/	H_t	3860	63	-	21	2108.1	1046.5	927.2	0.0	0.5	0.1
aVTZ	H_tN_H	3816	256	44	17	965.8	726.3	526.1	0.8	0.0	0.3

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