Electronic Supplementary Information

The preferred all-*gauche* conformations in 3-fluoro-1,2-propanediol

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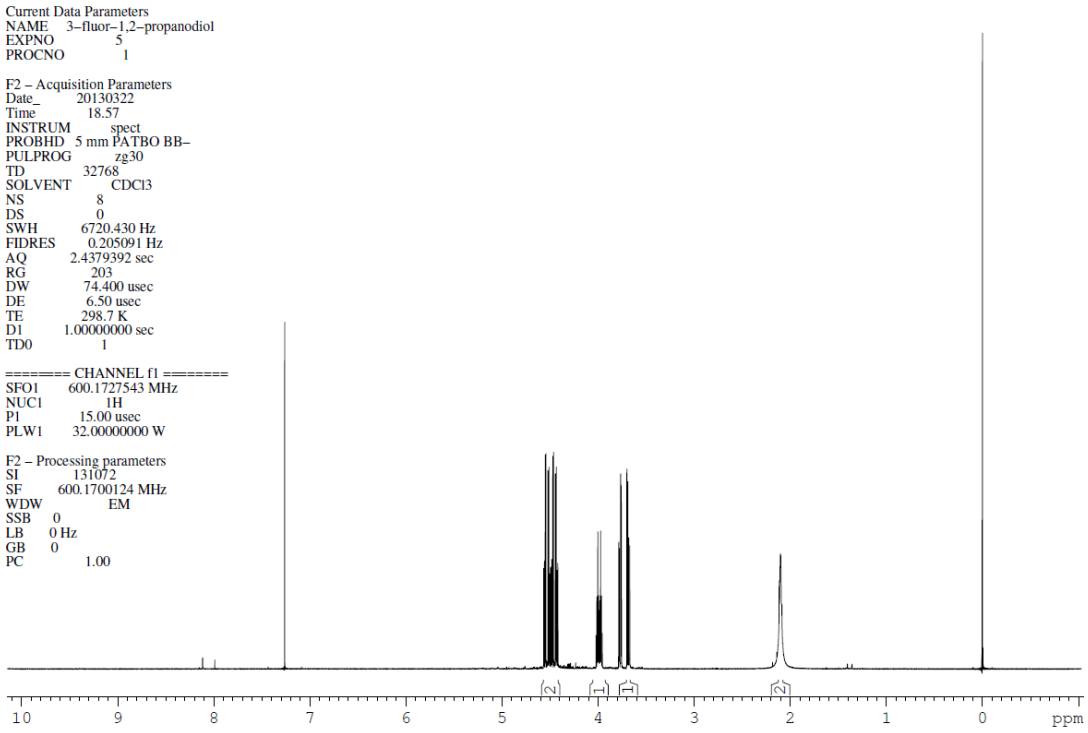


Figure S1. ^{1}H NMR spectrum for 3-fluoro-1,2-propanediol acquired in a Bruker Avance III 600 spectrometer operating at 600.17 MHz, using *ca.* 20 mg mL^{-1} in $CDCl_3$ at 298K.

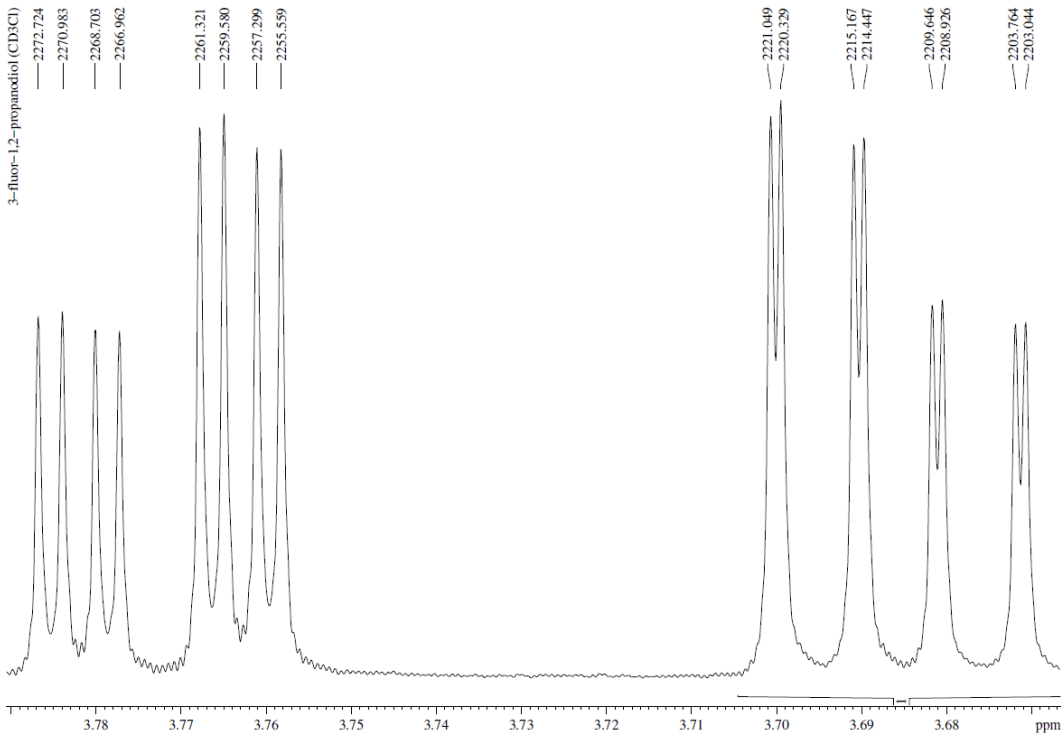


Figure S2. Expansion of the ^{1}H NMR spectrum for 3-fluoro-1,2-propanediol in the region of H1a and H1b, acquired in a Bruker Avance III 600 spectrometer operating at 600.17 MHz, using *ca.* 20 mg mL^{-1} in $CDCl_3$ at 298K.

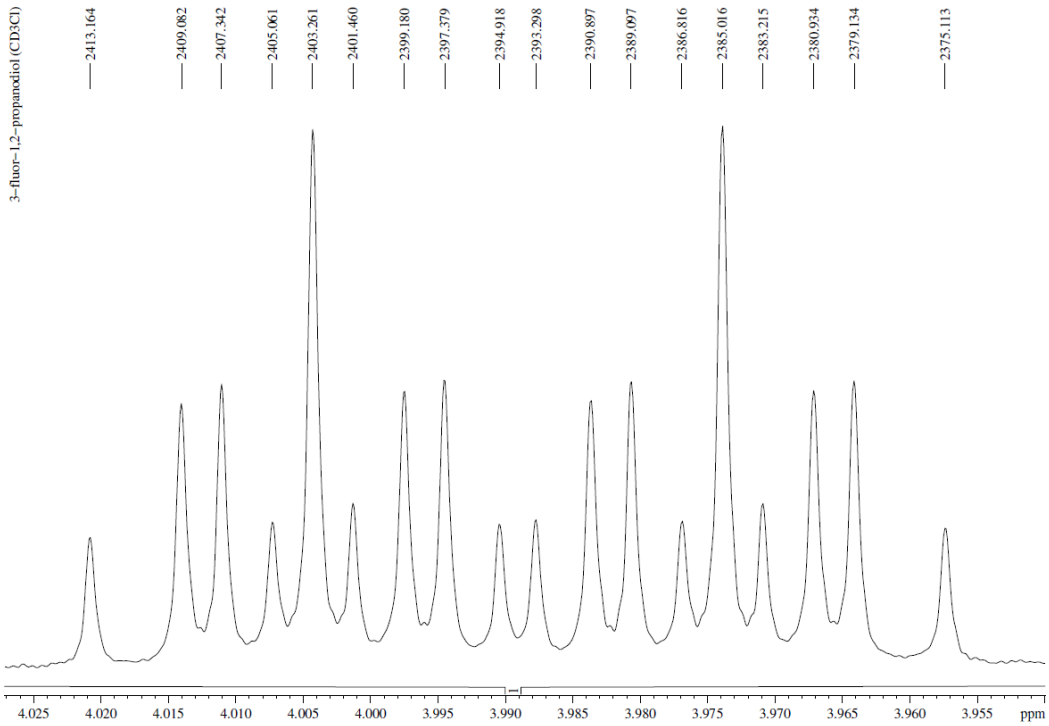


Figure S3. Expansion of the ^{1}H NMR spectrum for 3-fluoro-1,2-propanediol in the region of H2, acquired in a Bruker Avance III 600 spectrometer operating at 600.17 MHz, using *ca.* 20 mg mL^{-1} in $CDCl_3$ at 298K.

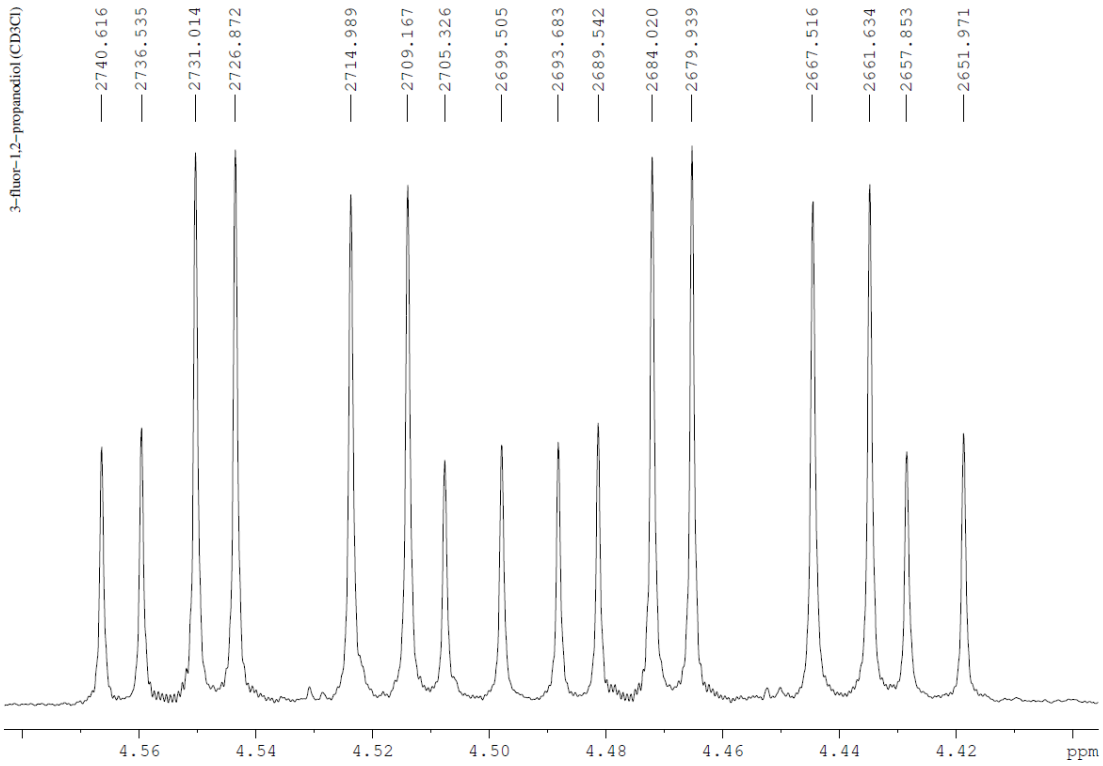


Figure S4. Expansion of the ^{1}H NMR spectrum for 3-fluoro-1,2-propanediol in the region of H3a and H3b, acquired in a Bruker Avance III 600 spectrometer operating at 600.17 MHz, using *ca.* 20 mg mL^{-1} in $CDCl_3$ at 298K.

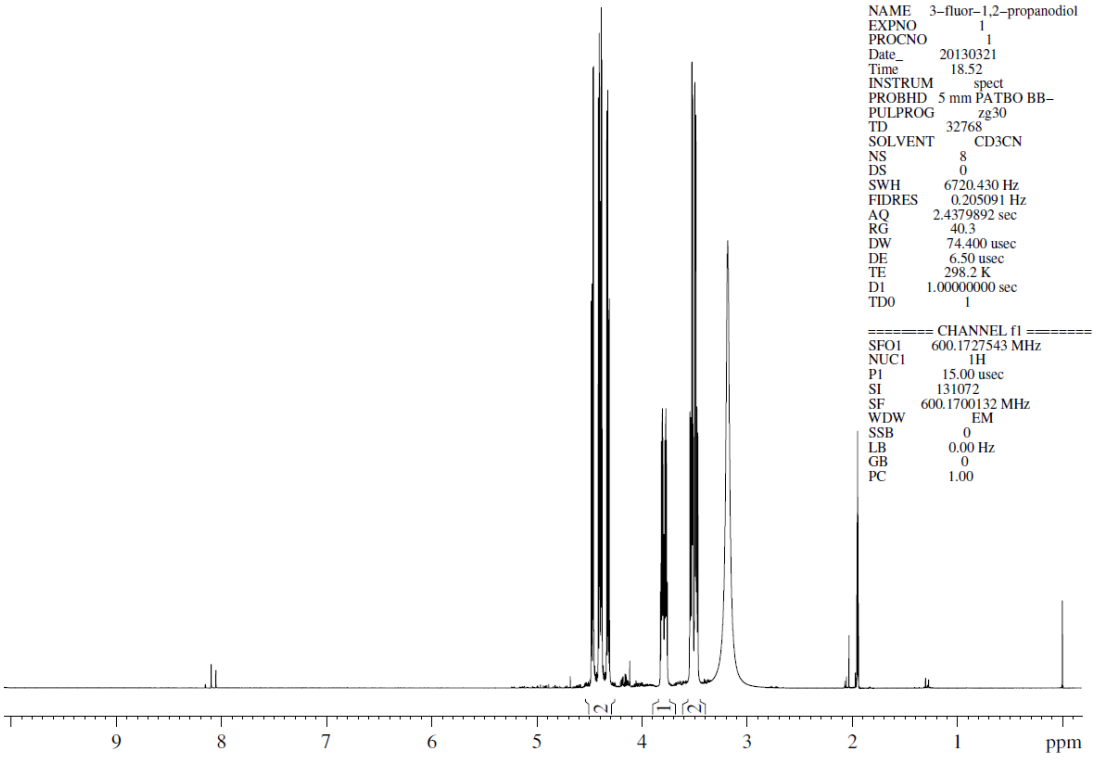


Figure S5. ^{1}H NMR spectrum for 3-fluoro-1,2-propanediol acquired in a Bruker Avance III 600 spectrometer operating at 600.17 MHz, using *ca.* 20 mg mL^{-1} in CD_3CN at 298K.

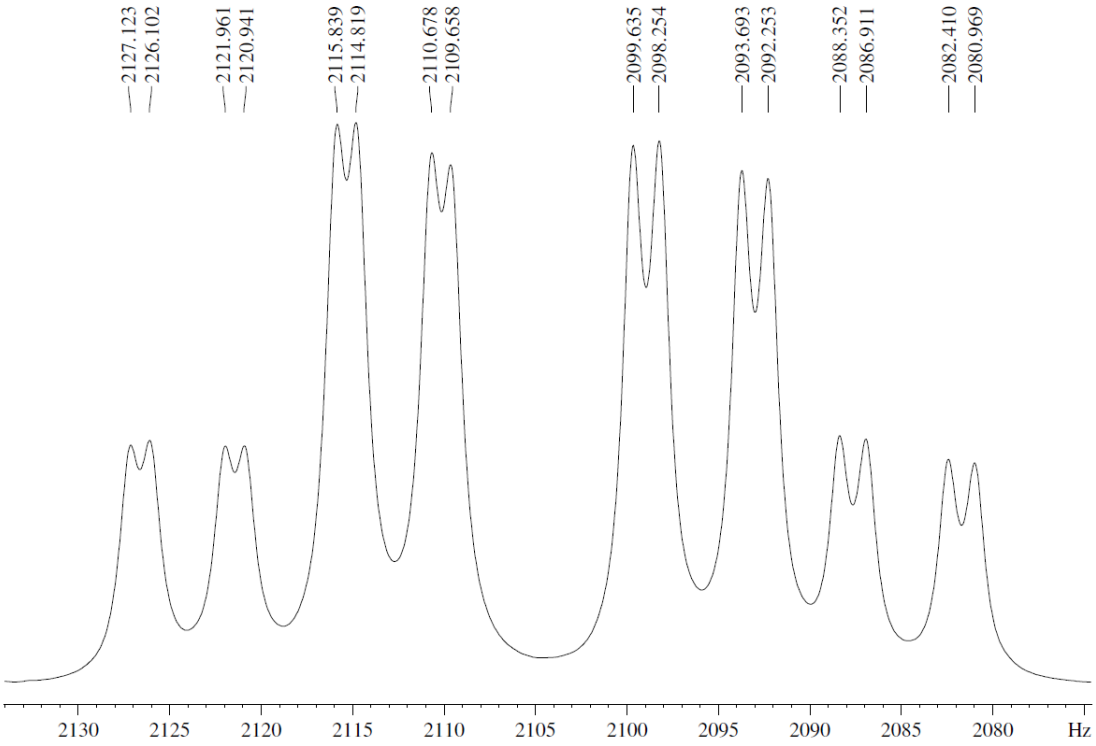


Figure S6. Expansion of the ^{1}H NMR spectrum for 3-fluoro-1,2-propanediol in the region of H1a and H1b, acquired in a Bruker Avance III 600 spectrometer operating at 600.17 MHz, using *ca.* 20 mg mL^{-1} in CD_3CN at 298K.

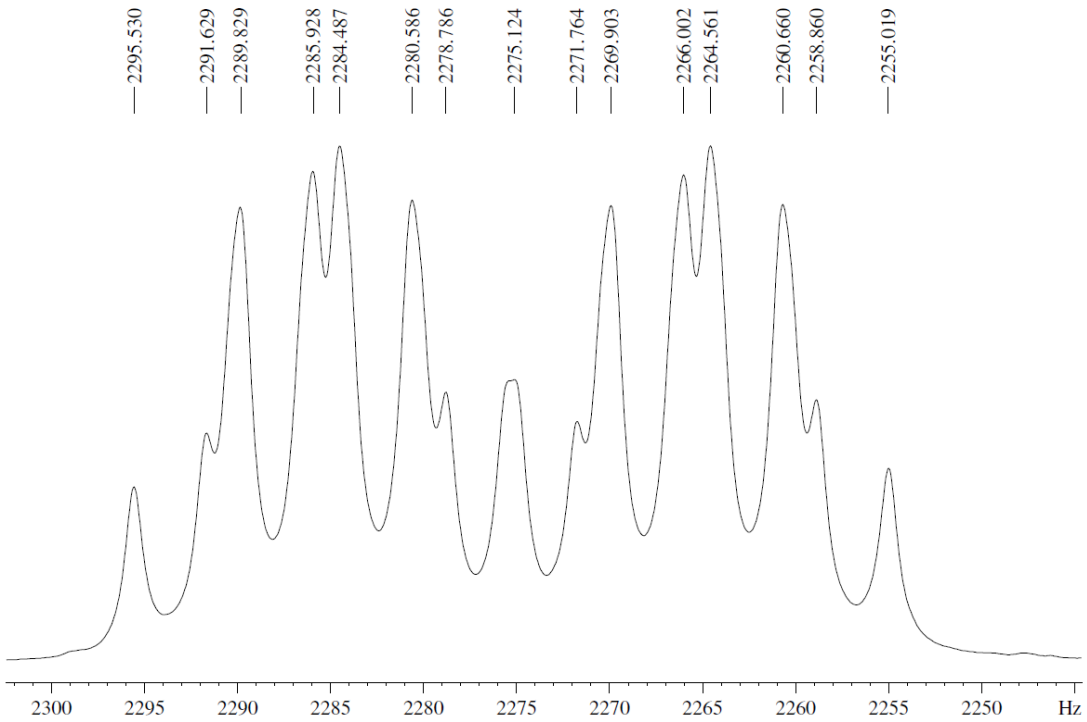


Figure S7. Expansion of the ^{1}H NMR spectrum for 3-fluoro-1,2-propanediol in the region of H2, acquired in a Bruker Avance III 600 spectrometer operating at 600.17 MHz, using *ca.* 20 mg mL^{-1} in CD_3CN at 298K.

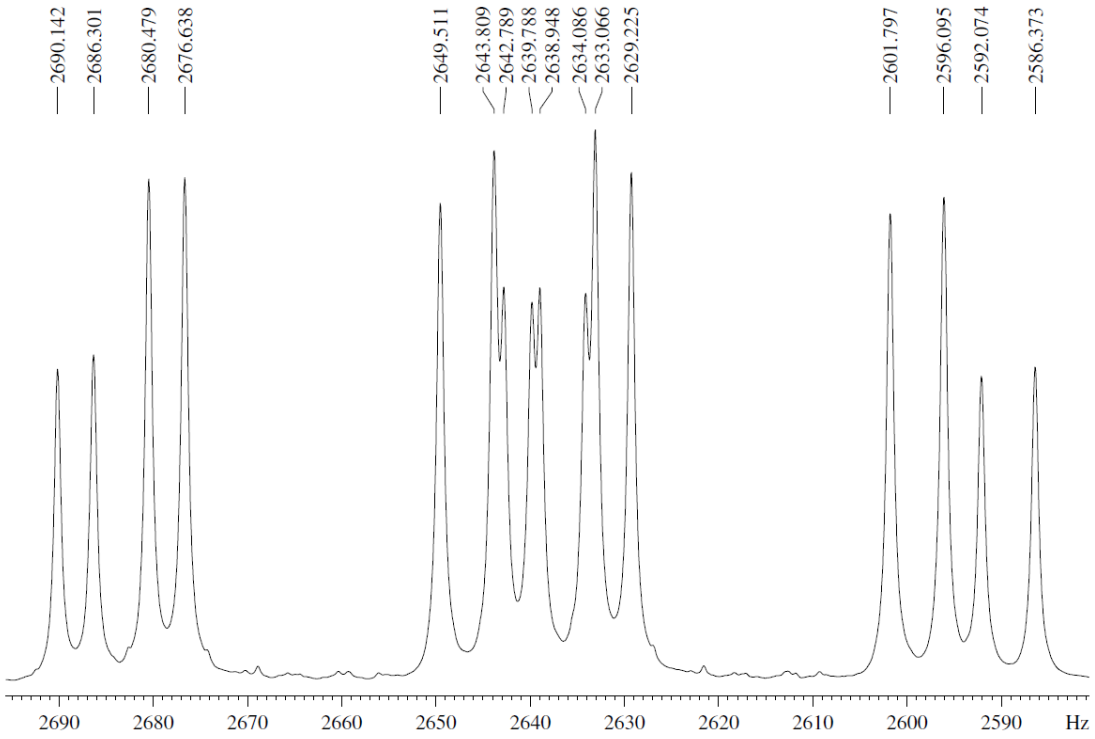


Figure S8. Expansion of the ^{1}H NMR spectrum for 3-fluoro-1,2-propanediol in the region of H3a and H3b, acquired in a Bruker Avance III 600 spectrometer operating at 600.17 MHz, using *ca.* 20 mg mL^{-1} in CD_3CN at 298K.

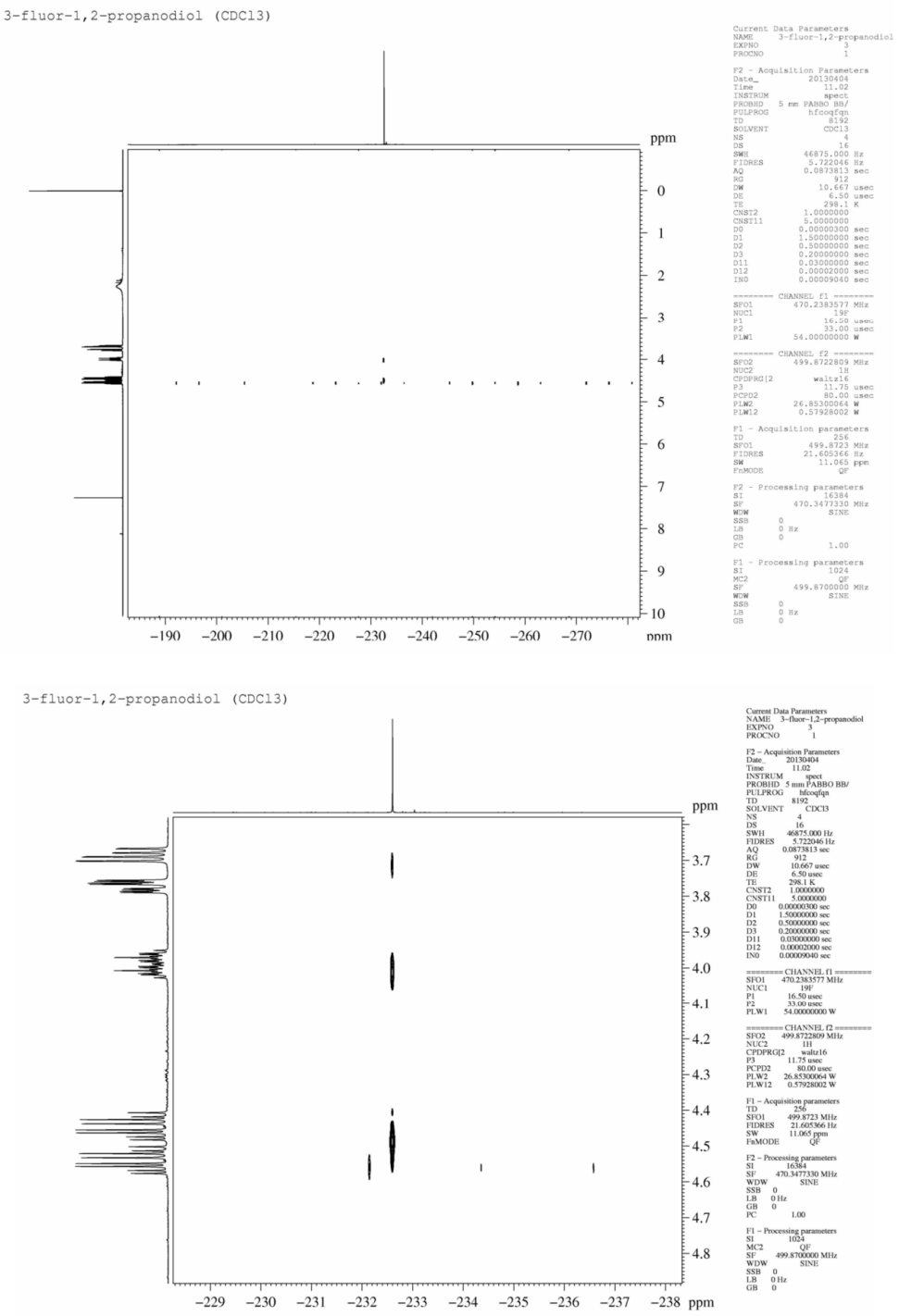


Figure S9. ^{1}H x ^{19}F HETCOR for 3-fluoro-1,2-propanediol in $CDCl_3$, at 499.87 MHz for ^{1}H and 470.35 MHz for ^{19}F, acquired in a Bruker Avance 500 spectrometer using *ca.* 20 mg mL^{-1} in $CDCl_3$at 298K.

Optimized geometries for the 25 main conformers of compound **2** obtained at the B3LYP/6-311++g(d,p) level.

2a Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.954811	-0.794131	-0.069293
2	1	0	0.637354	-1.049596	-1.080427
3	1	0	1.033233	-1.693264	0.546141
4	6	0	0.034690	0.235375	0.563135
5	1	0	0.376867	0.433105	1.589233
6	6	0	-1.416854	-0.236140	0.614080
7	1	0	-2.004599	0.516469	1.153921
8	1	0	-1.489083	-1.179097	1.161230
9	9	0	2.247277	-0.233313	-0.163862
10	8	0	0.036965	1.446301	-0.193626
11	1	0	0.951924	1.690062	-0.374820
12	8	0	-1.952007	-0.470722	-0.679735
13	1	0	-1.846736	0.346887	-1.181171

Rotational constants (GHZ): 6.2470735 2.2060508 1.9450143

2b Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.264777	-0.699002	0.215457
2	1	0	-1.324839	-0.732987	1.305667
3	1	0	-1.342267	-1.705457	-0.203404
4	6	0	-0.005892	0.007273	-0.249672
5	1	0	-0.009925	0.057738	-1.346656
6	6	0	1.263496	-0.706396	0.205208
7	1	0	1.294273	-1.718514	-0.204246
8	1	0	1.265608	-0.774644	1.302081
9	9	0	-2.381087	0.031437	-0.236072
10	8	0	0.067576	1.326965	0.294038
11	1	0	-0.697752	1.828664	-0.007091
12	8	0	2.425160	-0.043438	-0.262082
13	1	0	2.345832	0.882796	-0.003316

Rotational constants (GHZ): 8.1644311 1.9171652 1.6610705

2c Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.388966	0.114470	0.413924
2	1	0	1.688298	-0.229742	1.407960
3	1	0	2.137301	0.795314	0.006069
4	6	0	0.019879	0.778608	0.451097
5	1	0	0.062671	1.513549	1.265406
6	6	0	-1.121057	-0.208241	0.745682
7	1	0	-2.022170	0.350549	1.002138
8	1	0	-0.861937	-0.853811	1.594083
9	9	0	1.371960	-1.029709	-0.420915
10	8	0	-0.247243	1.500843	-0.740312
11	1	0	-0.718748	0.900543	-1.334234
12	8	0	-1.459025	-0.972743	-0.409263
13	1	0	-0.709634	-1.542847	-0.620800

Rotational constants (GHZ): 4.1699277 3.2014358 2.4218741

2d Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.410233	-0.269615	0.614114
2	1	0	1.484518	-1.251784	1.087457
3	1	0	2.043500	0.449593	1.136840
4	6	0	-0.024977	0.217839	0.545895
5	1	0	-0.366708	0.407247	1.568738
6	6	0	-0.983619	-0.779995	-0.107934
7	1	0	-0.995687	-1.716051	0.456698
8	1	0	-0.647982	-1.003441	-1.130006
9	9	0	1.921050	-0.389457	-0.695290
10	8	0	-0.104960	1.481156	-0.121330
11	1	0	0.401622	1.415916	-0.940838
12	8	0	-2.312653	-0.284750	-0.104044
13	1	0	-2.277637	0.623011	-0.430740

Rotational constants (GHZ): 6.2013352 2.1984407 1.9344555

2e Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.189655	0.295012	-0.477325
2	1	0	1.768577	1.211348	-0.601774
3	1	0	0.854343	-0.074577	-1.448551
4	6	0	0.010642	0.543962	0.462897
5	1	0	0.403628	0.844186	1.438503
6	6	0	-0.863152	-0.689753	0.652059
7	1	0	-1.608982	-0.486435	1.428856
8	1	0	-0.244090	-1.540935	0.954934
9	9	0	2.036610	-0.679642	0.080285
10	8	0	-0.752383	1.638679	-0.029887
11	1	0	-1.347719	1.285731	-0.704228
12	8	0	-1.502916	-0.934458	-0.607718
13	1	0	-2.135734	-1.651630	-0.515255

Rotational constants (GHZ): 4.6197834 2.6861889 2.0362485

2f Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.459324	0.348162	0.221950
2	1	0	-2.006554	1.195214	-0.194748
3	1	0	-1.490726	0.391703	1.313689
4	6	0	-0.026615	0.346714	-0.289838
5	1	0	-0.039406	0.223554	-1.381791
6	6	0	0.810099	-0.774519	0.310249
7	1	0	0.400814	-1.746595	0.015696
8	1	0	0.800960	-0.691664	1.404833
9	9	0	-2.104624	-0.829928	-0.180886
10	8	0	0.505399	1.619238	0.058292
11	1	0	1.456728	1.577108	-0.098867
12	8	0	2.137124	-0.593419	-0.198369
13	1	0	2.734654	-1.208667	0.235608

Rotational constants (GHZ): 5.6557412 2.2819323 1.7348390

2g Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.461134	0.351186	0.220660
2	1	0	-2.005831	1.200173	-0.195442
3	1	0	-1.493679	0.392450	1.312341
4	6	0	-0.027701	0.340279	-0.289389
5	1	0	-0.050509	0.189791	-1.380430
6	6	0	0.818257	-0.760964	0.346049
7	1	0	0.418215	-1.748446	0.097037
8	1	0	0.814879	-0.643744	1.432663
9	9	0	-2.108635	-0.825238	-0.186459
10	8	0	0.506438	1.620859	0.018356
11	1	0	1.467801	1.546064	-0.038691
12	8	0	2.187551	-0.630267	-0.053931
13	1	0	2.298395	-1.016884	-0.928668

Rotational constants (GHZ): 5.6285046 2.2567534 1.7245380

2h Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.193974	0.353299	-0.438876
2	1	0	1.795192	1.261113	-0.503493
3	1	0	0.890615	0.048633	-1.444619
4	6	0	-0.017861	0.577983	0.463933
5	1	0	0.330942	0.924390	1.441764
6	6	0	-0.864337	-0.677720	0.668914
7	1	0	-1.651457	-0.458329	1.392936
8	1	0	-0.250693	-1.496847	1.053667
9	9	0	2.004271	-0.668903	0.088404
10	8	0	-0.799805	1.627534	-0.093231
11	1	0	-1.385118	1.223403	-0.748313
12	8	0	-1.531958	-1.044989	-0.545968
13	1	0	-0.984475	-1.663969	-1.037811

Rotational constants (GHZ): 4.4844193 2.7352893 2.0331525

2i Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.839308	-0.751037	0.633405
2	1	0	0.184145	-1.566371	0.941123
3	1	0	1.663224	-0.622000	1.337674
4	6	0	0.067815	0.543857	0.455364
5	1	0	-0.279828	0.860417	1.443741
6	6	0	-1.152939	0.386812	-0.453991
7	1	0	-0.834054	0.032817	-1.442563
8	1	0	-1.623854	1.369239	-0.567309
9	9	0	1.415337	-1.108002	-0.607897
10	8	0	0.912244	1.583020	-0.026127
11	1	0	1.406247	1.238109	-0.779665
12	8	0	-2.035323	-0.548444	0.167754
13	1	0	-2.794394	-0.694595	-0.403611

Rotational constants (GHZ): 4.4781553 2.7589381 2.0524164

2j Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.466714	-0.008986	0.561131
2	1	0	1.640324	-0.713856	1.379231
3	1	0	2.070955	0.888325	0.707174
4	6	0	0.000459	0.364224	0.482494
5	1	0	-0.307087	0.641253	1.504474
6	6	0	-0.877407	-0.794105	0.021592
7	1	0	-0.789026	-1.635629	0.720309
8	1	0	-0.561128	-1.116452	-0.974558
9	9	0	1.904679	-0.626959	-0.618712
10	8	0	-0.140235	1.480883	-0.382448
11	1	0	-1.085305	1.587693	-0.548096
12	8	0	-2.219516	-0.292272	-0.003727
13	1	0	-2.771438	-0.884388	-0.522021

Rotational constants (GHZ): 5.9754799 2.2669008 1.9271733

2k Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.785222	-0.791904	0.329542
2	1	0	-0.832882	-0.694685	1.417380
3	1	0	-0.362679	-1.755640	0.045639
4	6	0	-0.016891	0.360328	-0.291145
5	1	0	-0.016077	0.230501	-1.381796
6	6	0	1.425759	0.408487	0.197685
7	1	0	1.436404	0.530661	1.288502
8	1	0	1.910884	1.281634	-0.251664
9	9	0	-2.113223	-0.743213	-0.146508
10	8	0	-0.598137	1.611769	0.060212
11	1	0	-1.534076	1.577663	-0.166756
12	8	0	2.058792	-0.808652	-0.196010
13	1	0	2.990320	-0.767617	0.037164

Rotational constants (GHZ): 5.5044960 2.3250724 1.7422049

2l Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.813476	-0.772595	0.356046
2	1	0	-0.904224	-0.631251	1.436121
3	1	0	-0.382926	-1.748917	0.131462
4	6	0	-0.013312	0.350642	-0.274394
5	1	0	-0.000245	0.195303	-1.364565
6	6	0	1.426694	0.379878	0.243845
7	1	0	1.425611	0.435319	1.334698
8	1	0	1.913710	1.284307	-0.135088
9	9	0	-2.120607	-0.742570	-0.175371
10	8	0	-0.579432	1.620235	0.030243
11	1	0	-1.516048	1.593207	-0.195856
12	8	0	2.148882	-0.799490	-0.099322
13	1	0	2.394538	-0.758349	-1.028779

Rotational constants (GHZ): 5.4751396 2.2727334 1.7239032

2m Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.449680	0.340732	0.232497
2	1	0	-2.000333	1.199848	-0.159947
3	1	0	-1.478909	0.359818	1.325105
4	6	0	-0.011746	0.336159	-0.277647
5	1	0	-0.008736	0.228570	-1.368640
6	6	0	0.826780	-0.782049	0.327604
7	1	0	0.387051	-1.748932	0.080285
8	1	0	0.828822	-0.670985	1.421663
9	9	0	-2.109669	-0.818584	-0.198188
10	8	0	0.619161	1.567923	0.105920
11	1	0	0.414472	2.251626	-0.538904
12	8	0	2.147944	-0.782345	-0.187078
13	1	0	2.515689	0.093636	-0.021320

Rotational constants (GHZ): 5.4731978 2.2775251 1.7207550

2n Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.166822	0.247363	-0.500487
2	1	0	1.712204	1.170932	-0.717200
3	1	0	0.815944	-0.206534	-1.428442
4	6	0	0.005812	0.508093	0.455809
5	1	0	0.411052	0.790686	1.436424
6	6	0	-0.899859	-0.706281	0.636131
7	1	0	-1.641718	-0.479350	1.412028
8	1	0	-0.304483	-1.559677	0.964693
9	9	0	2.069781	-0.639020	0.104700
10	8	0	-0.827425	1.548184	-0.071354
11	1	0	-0.347419	2.382001	-0.079213
12	8	0	-1.531721	-1.087419	-0.577287
13	1	0	-2.037092	-0.328051	-0.890177

Rotational constants (GHZ): 4.6190088 2.6419825 2.0044739

2o Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.852840	-0.742052	0.639565
2	1	0	0.212745	-1.584985	0.903822
3	1	0	1.642592	-0.602463	1.380133
4	6	0	0.045239	0.529902	0.449160
5	1	0	-0.326388	0.835468	1.434513
6	6	0	-1.154091	0.331794	-0.491213
7	1	0	-0.812390	-0.059518	-1.452030
8	1	0	-1.624205	1.304537	-0.667613
9	9	0	1.489702	-1.054414	-0.582029
10	8	0	0.868691	1.597364	-0.006485
11	1	0	1.391861	1.271829	-0.749066
12	8	0	-2.083941	-0.621799	0.021033
13	1	0	-2.633456	-0.197519	0.687039

Rotational constants (GHZ): 4.5373561 2.6841109 2.0213359

2p Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.174138	0.312121	-0.481796
2	1	0	1.713470	1.248675	-0.631485
3	1	0	0.855952	-0.099378	-1.440893
4	6	0	-0.013797	0.524205	0.448328
5	1	0	0.365881	0.854168	1.423206
6	6	0	-0.862983	-0.733053	0.638726
7	1	0	-1.624530	-0.537596	1.408466
8	1	0	-0.236247	-1.557312	0.984632
9	9	0	2.052889	-0.605443	0.111480
10	8	0	-0.803181	1.556457	-0.167432
11	1	0	-1.264784	2.053309	0.514449
12	8	0	-1.466386	-1.150319	-0.575358
13	1	0	-1.913355	-0.381631	-0.950927

Rotational constants (GHZ): 4.5226418 2.7056883 2.0279810

2q Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.464802	-0.013290	0.573472
2	1	0	1.633314	-0.731756	1.381098
3	1	0	2.066774	0.882159	0.739939
4	6	0	-0.003374	0.356833	0.487044
5	1	0	-0.312655	0.620013	1.515163
6	6	0	-0.878727	-0.796747	-0.006929
7	1	0	-0.808788	-1.653484	0.673736
8	1	0	-0.547907	-1.108781	-0.997113
9	9	0	1.911579	-0.609217	-0.613206
10	8	0	-0.142574	1.487907	-0.357430
11	1	0	-1.064805	1.518779	-0.643341
12	8	0	-2.234503	-0.365370	-0.164389
13	1	0	-2.649738	-0.305048	0.702399

Rotational constants (GHZ): 5.9339541 2.2541519 1.9237323

2r Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.846910	-0.734196	0.655627
2	1	0	0.207917	-1.478824	1.134136
3	1	0	1.761317	-0.592872	1.234260
4	6	0	0.124012	0.583214	0.455591
5	1	0	-0.165701	0.947830	1.446067
6	6	0	-1.141032	0.459640	-0.409831
7	1	0	-0.863106	0.170222	-1.429421
8	1	0	-1.617142	1.440301	-0.456621
9	9	0	1.229667	-1.248679	-0.605175
10	8	0	0.991802	1.573033	-0.089430
11	1	0	1.376473	1.223162	-0.901874
12	8	0	-2.090544	-0.448511	0.145566
13	1	0	-1.956163	-1.319831	-0.237380

Rotational constants (GHZ): 4.2367967 2.8695711 2.0570551

2s Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.305809	-0.555181	0.326532
2	1	0	-1.418292	-0.330530	1.389982
3	1	0	-1.306166	-1.637671	0.167365
4	6	0	-0.035528	0.068996	-0.213655
5	1	0	-0.098832	0.083975	-1.311261
6	6	0	1.193010	-0.747781	0.184136
7	1	0	1.142110	-1.749554	-0.260296
8	1	0	1.241181	-0.839267	1.276598
9	9	0	-2.424799	-0.041270	-0.334403
10	8	0	0.061184	1.391580	0.291944
11	1	0	0.925180	1.730693	0.027230
12	8	0	2.326456	-0.030942	-0.312207
13	1	0	3.126848	-0.367521	0.100030

Rotational constants (GHZ): 7.9171766 1.9037335 1.6620519

2t Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.443830	-0.089355	0.587736
2	1	0	1.564966	-0.885946	1.328982
3	1	0	2.069785	0.762339	0.872212
4	6	0	-0.017566	0.317848	0.487424
5	1	0	-0.351231	0.571144	1.505043
6	6	0	-0.917608	-0.793167	-0.046598
7	1	0	-0.825023	-1.681100	0.582646
8	1	0	-0.600927	-1.053296	-1.062814
9	9	0	1.927796	-0.570700	-0.632169
10	8	0	-0.220785	1.432818	-0.386455
11	1	0	0.137804	2.231972	0.011512
12	8	0	-2.284003	-0.411276	-0.013627
13	1	0	-2.359166	0.406898	-0.518775

Rotational constants (GHZ): 5.9682559 2.2264088 1.9063094

2u Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.991485	-0.712378	-0.154724
2	1	0	0.747843	-0.857869	-1.209223
3	1	0	0.942251	-1.672795	0.367882
4	6	0	0.062510	0.305837	0.498242
5	1	0	0.464860	0.541856	1.488121
6	6	0	-1.346750	-0.255056	0.670147
7	1	0	-1.955837	0.486188	1.198151
8	1	0	-1.324250	-1.181684	1.258033
9	9	0	2.314702	-0.266192	-0.081058
10	8	0	0.032706	1.534968	-0.211741
11	1	0	-0.482079	1.389837	-1.015523
12	8	0	-1.864685	-0.496658	-0.643893
13	1	0	-2.812744	-0.646698	-0.594841

Rotational constants (GHZ): 6.0757749 2.1932232 1.9077887

2v Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.457556	0.361982	0.169985
2	1	0	-2.004455	1.167805	-0.322913
3	1	0	-1.525553	0.485156	1.257071
4	6	0	-0.006550	0.340248	-0.298322
5	1	0	0.021091	0.216165	-1.383424
6	6	0	0.821617	-0.765565	0.347802
7	1	0	0.374771	-1.739246	0.141722
8	1	0	0.827519	-0.621756	1.441724
9	9	0	-2.082635	-0.849145	-0.152453
10	8	0	0.590514	1.622346	-0.058624
11	1	0	0.564643	1.808539	0.888221
12	8	0	2.142730	-0.797663	-0.165321
13	1	0	2.474684	0.108180	-0.175561

Rotational constants (GHZ): 5.3494510 2.3061358 1.7250217

2w Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.310313	-0.552535	0.324878
2	1	0	-1.426313	-0.322963	1.386558
3	1	0	-1.313389	-1.635764	0.169735
4	6	0	-0.035028	0.065474	-0.211808
5	1	0	-0.097741	0.061982	-1.312200
6	6	0	1.197150	-0.739578	0.215134
7	1	0	1.162734	-1.752752	-0.201983
8	1	0	1.239257	-0.810282	1.304488
9	9	0	-2.425435	-0.038394	-0.344192
10	8	0	0.058916	1.397567	0.266908
11	1	0	0.969911	1.686022	0.125372
12	8	0	2.395748	-0.062391	-0.170866
13	1	0	2.546289	-0.202273	-1.111805

Rotational constants (GHZ): 7.9151688 1.8842685 1.6493958

2x Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.378182	1.277311	0.128047
2	1	0	0.951681	1.983974	-0.472667
3	1	0	0.634189	1.390500	1.184021
4	6	0	0.615029	-0.159815	-0.320989
5	1	0	0.467080	-0.232861	-1.405989
6	6	0	-0.324040	-1.167561	0.360698
7	1	0	-0.343560	-0.980563	1.443483
8	1	0	0.075637	-2.173909	0.208442
9	9	0	-0.986194	1.604566	-0.014165
10	8	0	1.979083	-0.401437	0.030066
11	1	0	2.279328	-1.204371	-0.406748
12	8	0	-1.628817	-1.177046	-0.196804
13	1	0	-2.005756	-0.295605	-0.095689

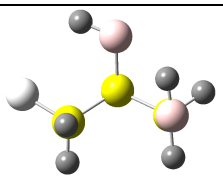
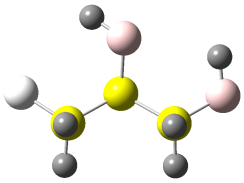
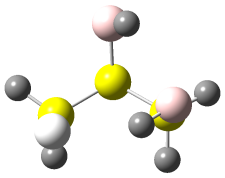
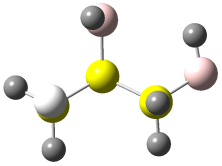
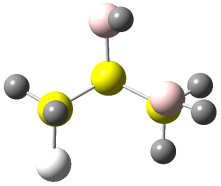
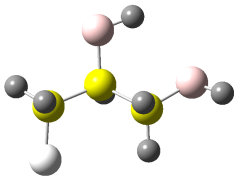
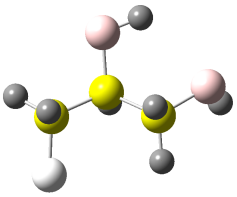
Rotational constants (GHZ): 3.8181534 3.3302455 1.9071258

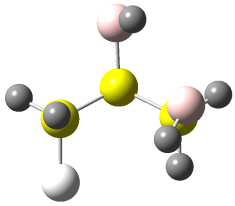
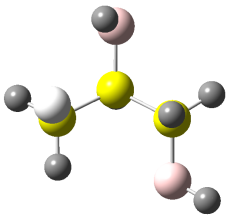
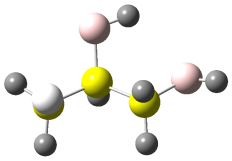
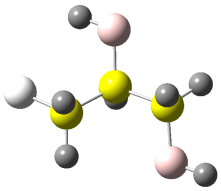
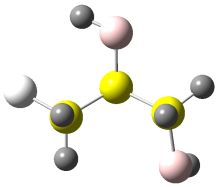
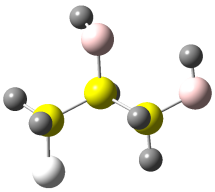
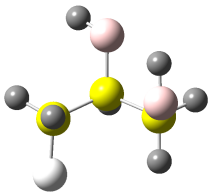
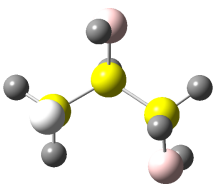
2y Standard orientation:

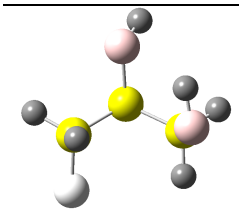
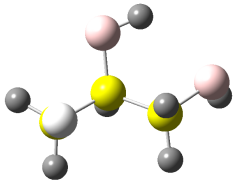
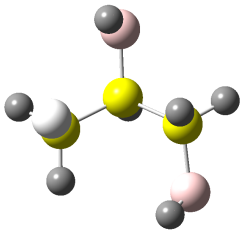
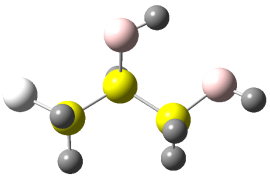
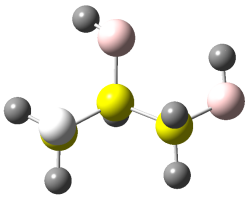
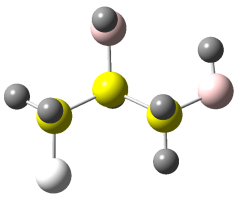
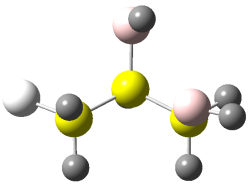
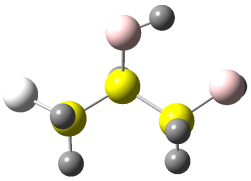
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.281904	-0.623213	0.260113
2	1	0	-1.363580	-0.550381	1.351084
3	1	0	-1.311303	-1.677770	-0.029016
4	6	0	-0.010790	0.031560	-0.245424
5	1	0	-0.032805	0.057323	-1.338306
6	6	0	1.236786	-0.735776	0.206480
7	1	0	1.236266	-1.747515	-0.207138
8	1	0	1.243314	-0.818431	1.305609
9	9	0	-2.410454	-0.004249	-0.280555
10	8	0	0.101176	1.402989	0.149211
11	1	0	-0.182182	1.500168	1.065817
12	8	0	2.415754	-0.103565	-0.255105
13	1	0	2.304385	0.844029	-0.102907

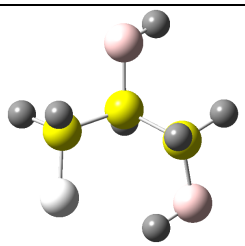
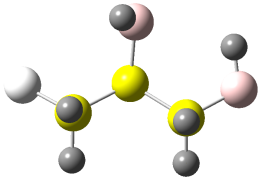
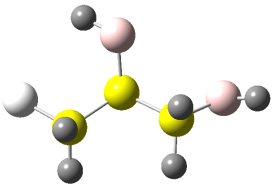
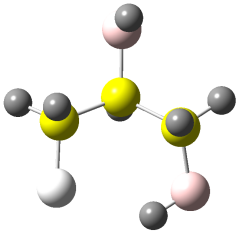
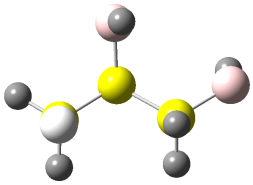
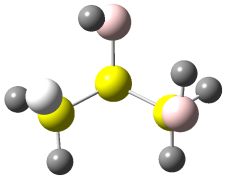
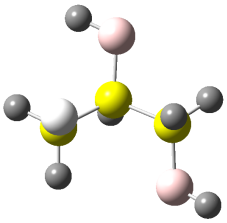
Rotational constants (GHZ): 7.8869468 1.9048022 1.6487450

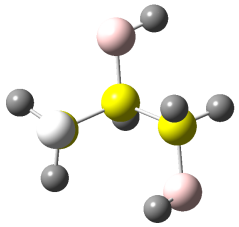
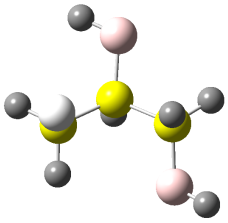
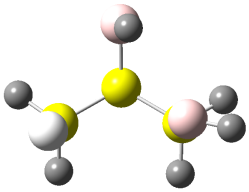
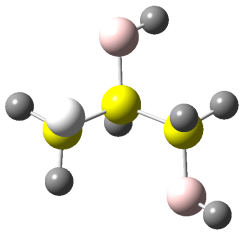
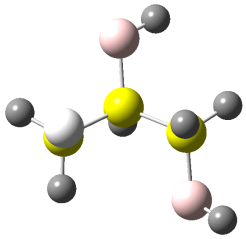
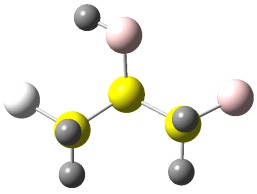
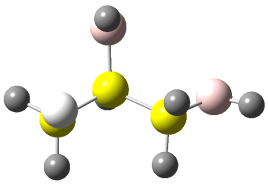
Table S1. Conformers of **2** found at the B3LYP/6-311++g(d,p) level, with respective relative energies (in kcal mol^{-1}) and population (%) in the gas phase and solution ($CHCl_3$ and CH_3CN implicit solvents).

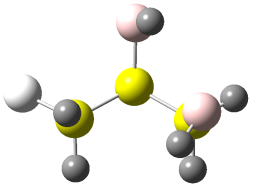
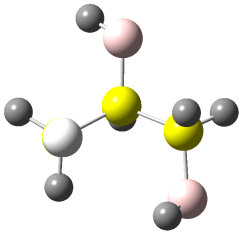
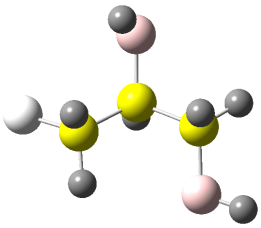
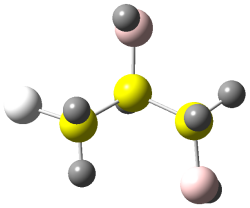
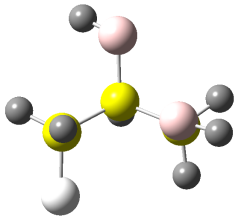
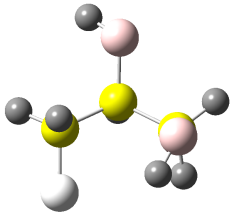
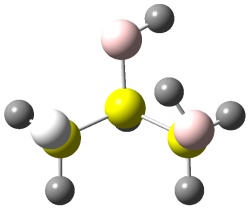
Structure	Conformer	E_{gas}	$\%_{gas}$	E_{CHCl3}	$\%_{CHCl3}$	E_{CH3CN}	$\%_{CH3CN}$
	**2a**	0.0	51	0.0	17	0.1	10
	**2b**	0.6	18	0.1	14	0.0	11
	**2c**	0.7	15	0.3	10	0.3	7
	**2d**	1.1	8	0.4	8	0.2	8
	**2e**	1.3	6	0.9	4	0.9	3
	**2f**	1.5	4	1.2	2	1.2	2
	**2g**	1.7	3	1.2	2	1.1	2

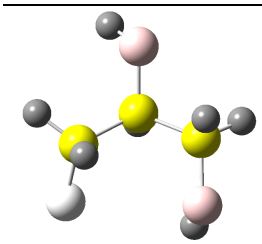
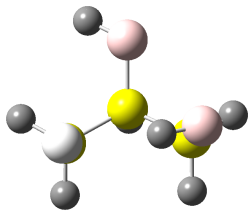
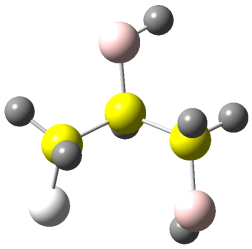
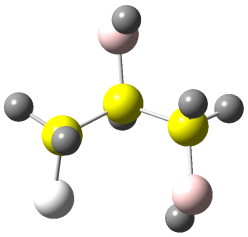
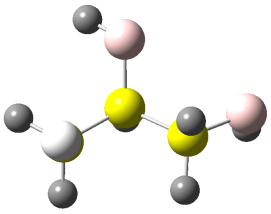
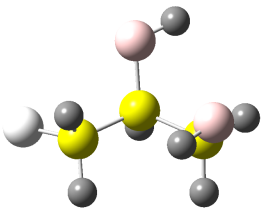
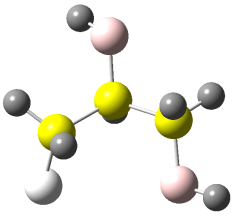
	**2h**	1.7	3	1.2	2	1.1	2
	**2i**	1.9	2	1.4	2	1.3	1
	**2j**	1.9	2	0.6	6	0.3	7
	**2k**	1.9	2	1.5	1	1.4	1
	**2l**	2.1	1	1.3	2	1.2	2
	**2m**	2.1	1	1.1	3	0.8	3
	**2n**	2.2	1	1.4	2	1.1	2
	**2o**	2.4	1	1.4	2	3.1	0

	**2p**	2.5	1	1.5	1	1.2	2
	**2q**	2.6	1	0.8	4	0.3	7
	**2r**	2.7	1	1.8	1	1.6	1
	**2s**	2.9	0	1.1	3	0.5	5
	**2t**	3.0	0	1.1	3	0.5	5
	**2u**	3.2	0	1.3	2	1.5	1
	**2v**	3.1	0	1.8	1	0.8	3
	**2w**	3.3	0	1.1	3	0.4	6

	**2x**	3.4	0	2.8	0	2.6	0
	**2y**	3.8	0	1.6	1	1.0	2
	**2z**	4.0	0	1.6	1	1.0	2
	**2aa**	4.2	0	3.1	0	2.9	0
	**2ab**	4.2	0	2.2	0	1.6	1
	**2ac**	4.2	0	2.8	0	2.5	0
	**2ad**	4.2	0	2.4	0	2.0	0

	**2ae**	4.2	0	2.5	0	2.0	0
	**2af**	4.2	0	2.4	0	2.0	0
	**2ag**	4.3	0	2.4	0	1.9	0
	**2ah**	4.3	0	2.4	0	1.9	0
	**2ai**	4.3	0	2.4	0	1.9	0
	**2aj**	4.4	0	2.1	0	1.4	1
	**2ak**	4.4	0	2.3	0	1.7	1

	**2al**	4.5	0	2.0	1	1.2	2
	**2am**	4.5	0	2.7	0	2.2	0
	**2an**	4.9	0	2.8	0	2.2	0
	**2ao**	4.9	0	2.5	0	1.9	0
	**2ap**	5.3	0	3.1	0	2.5	0
	**2aq**	5.5	0	3.3	0	2.7	0
	**2ar**	5.7	0	3.2	0	2.4	0

	**2as**	6.0	0	4.3	0	3.8	0
	**2at**	6.0	0	3.0	0	2.1	0
	**2au**	6.2	0	4.5	0	4.0	0
	**2av**	6.4	0	4.6	0	4.1	0
	**2aw**	7.0	0	3.2	0	2.0	0
	**2ax**	7.1	0	3.5	0	2.5	0
	**2ay**	7.1	0	4.8	0	4.2	0

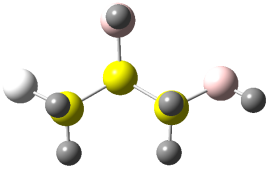
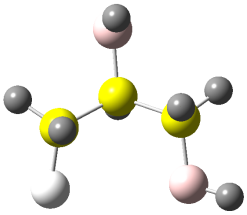
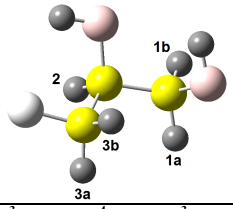
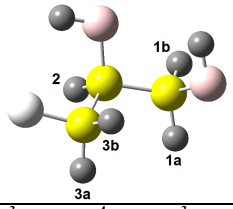
	**2az**	7.6	0	3.6	0	2.5	0
	**2ba**	7.9	0	5.3	0	4.6	0

Table S2. Calculated and experimental chemical shifts (in ppm, relative to TMS, using the calculated isotropic magnetic shielding tensor) and coupling constants (in Hz) for **2**, in $CHCl_3$.



Conformer	δ_{H1a}	δ_{H1b}	δ_{H2}	δ_{H3a}	δ_{H3b}	$^2J_{H1a,H1b}$	$^3J_{H1a,H2}$	$^4J_{H1a,F}$	$^3J_{H1b,H2}$	$^4J_{H1b,F}$	$^3J_{H2,H3a}$	$^3J_{H2,H3b}$	$^3J_{H2,F}$	$^2J_{H3a,H3b}$	$^2J_{H3a,F}$	$^2J_{H3b,F}$
2a	5.0	5.4	5.4	6.2	6.3	-14.0	1.7	-1.5	3.0	6.4	2.2	10.2	15.9	-10.5	49.1	53.3
2b	4.6	4.7	5.4	5.8	5.5	-12.4	10.0	-1.0	2.8	-2.2	2.2	9.9	16.0	-10.4	48.6	52.8
2c	5.5	5.3	4.9	6.3	6.3	-13.5	0.7	-0.1	5.2	-1.1	1.8	1.7	43.2	-10.9	52.4	50.8
2d	5.1	4.9	5.1	6.2	6.0	-12.5	11.2	1.9	3.4	0.6	3.2	0.7	32.7	-11.0	52.4	49.7
2e	5.4	5.3	5.2	6.0	5.9	-10.1	1.0	4.2	3.5	2.8	11.4	5.2	3.3	-9.1	50.5	49.1
2f	4.9	5.4	5.5	5.7	6.1	-9.2	10.1	0.5	2.8	3.3	10.5	4.5	5.7	-9.7	51.6	47.6
2g	4.7	5.5	5.3	5.7	6.1	-12.7	2.7	0.3	2.9	2.7	10.3	4.4	5.7	-9.7	51.4	47.7
2h	5.3	5.0	5.0	5.6	5.8	-13.7	0.7	4.0	3.8	2.5	11.4	5.6	1.7	-10.1	51.4	49.4
2i	5.2	5.2	5.1	6.1	6.4	-8.3	5.3	1.0	11.2	1.2	2.3	1.2	34.5	-10.5	53.1	49.4
2j	5.3	5.3	5.2	6.3	6.0	-9.7	10.3	1.6	2.2	-0.3	1.8	1.9	37.2	-11.4	52.2	50.7
2k	5.3	4.9	5.6	6.4	5.8	-8.9	5.0	5.2	10.5	-1.6	2.5	10.0	13.1	-10.0	48.6	53.3
2l	5.3	4.7	5.4	6.4	5.9	-13.0	4.7	6.7	11.2	-1.9	1.9	9.5	15.7	-10.4	49.1	53.4
2m	4.9	5.2	5.5	5.6	5.9	-13.3	9.6	0.9	2.3	3.7	11.1	4.6	3.4	-9.8	51.0	48.3
2n	5.2	5.3	5.3	6.3	5.7	-13.7	1.5	3.4	2.7	2.2	10.9	4.5	4.5	-9.0	50.1	48.5
2o	5.1	5.0	4.9	6.1	6.5	-12.3	4.8	0.8	11.6	1.1	2.5	1.0	33.4	-10.4	53.1	49.0
2p	5.2	5.1	5.4	6.2	5.9	-13.9	1.1	4.1	2.7	2.9	11.0	5.2	5.2	-9.0	49.5	48.8
2q	5.2	5.3	5.0	6.3	5.9	-13.0	10.8	1.4	2.4	-0.4	1.8	1.8	35.8	-11.5	52.2	50.6
2r	4.9	4.9	4.8	6.0	6.2	-12.6	5.7	0.8	10.7	1.1	2.2	1.1	35.4	-11.4	53.0	50.5
2s	4.7	5.0	5.6	5.8	5.8	-8.9	11.1	-2.1	3.0	-2.1	1.4	9.0	21.0	-10.6	48.7	53.0
2t	5.1	4.8	5.0	5.8	5.8	-12.7	10.1	1.8	2.9	-0.2	2.1	1.2	34.6	-12.2	52.6	50.7
2u	5.2	5.3	5.3	6.0	6.1	-10.4	1.2	-1.3	4.1	4.2	2.2	10.4	16.8	-11.0	49.4	53.0
2v	4.7	5.3	5.3	5.6	6.1	-13.1	10.2	0.7	2.9	4.2	11.3	5.0	3.3	-9.6	50.4	48.4
2w	5.5	5.0	5.4	5.8	5.8	-12.4	11.5	-2.0	3.1	-2.2	1.4	8.8	20.7	-10.7	48.9	52.9
2x	4.8	5.0	5.4	5.2	5.7	-12.7	0.9	-1.6	9.4	0.3	10.5	5.8	0.9	-9.5	50.1	49.9
2y	4.9	4.9	5.6	5.9	5.6	-10.2	8.6	0.2	1.2	-1.4	2.8	11.1	14.5	-9.7	48.4	52.2
Exp.$_{CDCl3}$	3.69	3.77	3.99	4.51	4.47	11.4	5.9	0.7	4.0	1.7	4.0	5.9	18.2	9.6	46.9	47.5

Table S3. Calculated and experimental chemical shifts (in ppm, relative to TMS, using the calculated isotropic magnetic shielding tensor) and coupling constants (in Hz) for **2**, in CH_3CN.



Conformer	δ_{H1a}	δ_{H1b}	δ_{H2}	δ_{H3a}	δ_{H3b}	$^2J_{H1a,H1b}$	$^3J_{H1a,H2}$	$^4J_{H1a,F}$	$^3J_{H1b,H2}$	$^4J_{H1b,F}$	$^3J_{H2,H3a}$	$^3J_{H2,H3b}$	$^3J_{H2,F}$	$^2J_{H3a,H3b}$	$^2J_{H3a,F}$	$^2J_{H3b,F}$
2a	4.8	5.3	5.4	6.1	6.2	-13.6	1.2	-1.4	3.7	6.9	3.0	10.9	12.5	-10.1	48.4	53.1
2b	4.5	4.5	5.3	5.5	5.4	-12.0	10.1	-0.9	2.9	-2.2	2.2	10.0	15.4	-9.9	48.8	52.0
2c	5.5	5.2	4.9	6.3	6.2	-12.9	0.6	-0.1	5.5	-1.3	1.5	1.8	43.6	-10.8	52.2	50.8
2d	5.1	4.9	5.0	6.2	6.0	-12.5	11.2	1.9	3.5	0.6	3.2	0.7	32.9	-11.1	52.3	49.6
2e	5.4	5.3	5.2	6.0	5.9	-10.5	1.1	4.3	3.5	2.8	11.4	5.3	3.2	-9.1	50.5	49.0
2f	4.9	5.4	5.5	5.7	6.1	-9.5	10.2	0.6	2.8	3.3	10.5	4.4	6.5	-9.7	51.5	47.3
2g	4.7	5.5	5.3	5.7	6.1	-12.6	10.6	0.2	2.9	2.7	10.3	4.4	6.0	-9.7	51.3	47.6
2h	5.2	4.9	4.9	5.4	5.7	-13.8	0.7	4.0	3.8	2.4	11.4	5.5	2.2	-10.1	51.1	49.2
2i	5.1	5.1	5.0	6.1	6.4	-8.4	5.4	0.9	11.2	1.2	2.5	0.9	33.3	-10.4	52.9	49.1
2j	5.3	5.0	5.1	6.2	5.6	-9.3	11.1	1.5	3.0	-0.1	2.1	1.7	34.3	-11.5	52.6	51.3
2k	5.3	4.9	5.6	6.4	5.8	-9.0	4.8	5.4	10.6	-1.7	2.4	9.9	13.5	-10.0	48.5	53.2
2l	5.2	4.7	5.4	6.4	5.8	-12.8	4.5	6.8	11.0	-1.8	2.3	9.8	14.0	-10.2	48.6	53.4
2m	4.8	5.2	5.4	5.6	5.9	-0.4	0.3	-2.8	0.1	0.1	0.4	0.2	0.1	-0.3	1.7	1.6
2n	5.1	5.3	5.2	6.2	5.7	-13.4	1.3	3.5	2.9	2.5	10.9	4.6	3.7	-9.1	50.0	48.3
2o	5.0	5.0	4.6	5.9	6.4	-12.7	5.2	0.8	11.9	1.1	2.7	0.9	30.5	-10.3	53.5	49.7
2p	5.2	4.8	5.2	6.1	5.8	-13.8	0.9	4.0	3.1	3.1	11.2	5.5	4.0	-9.3	50.0	50.0
2q	5.3	5.0	4.7	6.2	5.6	-13.1	11.6	1.3	3.1	-0.3	2.1	1.7	32.1	-11.5	52.4	51.0
2r	4.9	4.8	4.8	5.8	6.1	-12.7	5.6	0.7	10.8	1.0	2.3	1.1	35.6	-11.5	53.0	50.3
2s	4.7	5.0	5.6	5.8	5.8	-9.0	11.1	-2.0	3.0	-2.1	1.5	9.2	20.2	-10.6	48.3	52.8
2t	5.2	4.6	4.9	5.6	5.6	-12.6	10.2	1.8	3.0	-0.2	2.1	1.2	35.3	-12.2	52.6	50.7
2u	5.2	5.3	5.3	6.1	6.1	-10.7	1.1	-1.4	4.3	4.5	2.3	10.5	17.0	-10.9	49.1	53.1
2v	4.8	5.3	5.3	5.6	6.1	-13.1	10.2	0.7	2.9	4.2	11.3	5.0	3.7	-9.6	50.4	48.3
2w	4.5	5.0	5.4	5.8	5.8	-12.4	11.5	-2.0	3.1	-2.2	1.6	9.1	19.7	-10.7	48.4	52.7
2x	4.7	5.0	5.3	5.6	6.1	-12.6	3.0	-1.6	9.5	0.2	10.5	5.7	1.1	-9.5	50.0	49.7
2y	4.5	4.7	5.2	5.9	5.5	-12.5	10.7	-1.6	3.2	-2.1	2.4	10.0	15.7	-12.7	49.4	54.7
Exp.$_{CH3CN}$	3.48	3.52	3.80	4.43	4.36	11.3	5.9	1.4	5.1	1.0	3.8	5.7	19.9	9.7	47.3	47.7