Supporting Information

Axial fluorine induced by the endocyclic oxygen in 3-fluorodihydro-2*H*-pyran-4(3*H*)-one

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The electronic (E) and standard free (G) energies for **2** are given in hartrees.

axial(gas_wB97X-D/6-311++G(d,p)) E= -445.005566929, G= -444.916743

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.239702	-1.266869	0.037106
2	6	0	-0.149573	-1.306888	0.701031
3	6	0	-0.479679	1.011636	-0.248387
4	6	0	0.933973	0.901124	-0.809392
5	1	0	-0.558939	-2.317753	0.711689
6	1	0	1.182997	-1.708556	-0.969523
7	1	0	1.958088	-1.840238	0.622451
8	1	0	-1.125197	1.612230	-0.892243
9	1	0	0.864086	0.545025	-1.850040
10	1	0	1.410610	1.882049	-0.805349
11	1	0	-0.056864	-0.933975	1.725119
12	6	0	-1.058269	-0.393390	-0.078419
13	8	0	-2.083233	-0.728179	-0.614468
14	8	0	1.741950	0.048437	-0.037459
15	9	0	-0.429050	1.613942	1.006853

equatorial(gas_wB97X-D/6-311++G(d,p)) E= -445.005943071, G= -444.917065

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.862426	0.283183	-0.285755
2	6	0	-0.919383	1.307632	0.359322
3	6	0	0.800304	-0.540632	0.409106
4	6	0	-0.264183	-1.425755	-0.259767
5	1	0	-1.094347	2.313661	-0.025195
6	1	0	-1.797249	0.352845	-1.381292
7	1	0	-2.895437	0.468532	0.007674
8	1	0	-0.141963	-1.362446	-1.350924
9	1	0	-0.130968	-2.463162	0.045993
10	1	0	-1.088196	1.308237	1.441650
11	6	0	0.519537	0.921487	0.089466
12	8	0	1.346733	1.662829	-0.368002
13	8	0	-1.554065	-1.029860	0.133450
14	9	0	2.045598	-0.919978	-0.025754
15	1	0	0.753346	-0.677107	1.496065

axial(C_6H_6_wB97X-D/6-311++G(d,p)) E= -445.010048368, G= -444.921380

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.249852	-1.263117	0.034593
2	6	0	-0.145469	-1.317160	0.684051
3	6	0	-0.480093	1.008805	-0.252608
4	6	0	0.935902	0.906502	-0.806308
5	1	0	-0.547720	-2.330708	0.679618
6	1	0	1.208419	-1.696248	-0.975418
7	1	0	1.963762	-1.836245	0.624919
8	1	0	-1.123762	1.610958	-0.895886
9	1	0	0.874220	0.547173	-1.845433
10	1	0	1.405700	1.890462	-0.803338
11	1	0	-0.064125	-0.959978	1.714905
12	6	0	-1.056062	-0.397314	-0.082294
13	8	0	-2.093108	-0.724817	-0.603910
14	8	0	1.743160	0.058571	-0.025388
15	9	0	-0.437965	1.608694	1.007824

equatorial(C_6H_6_wB97X-D/6-311++G(d,p)) E= -445.011152801, G= -444.922345

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.861631	0.291173	-0.288892
2	6	0	-0.913232	1.313237	0.352447
3	6	0	0.794932	-0.543568	0.409144
4	6	0	-0.272236	-1.428380	-0.255782
5	1	0	-1.085606	2.317625	-0.036746
6	1	0	-1.795952	0.353422	-1.384099
7	1	0	-2.892385	0.485727	0.004919
8	1	0	-0.153168	-1.371333	-1.347016
9	1	0	-0.141972	-2.463919	0.056767
10	1	0	-1.081771	1.320264	1.434610
11	6	0	0.521386	0.918421	0.089921
12	8	0	1.359979	1.655607	-0.360484
13	8	0	-1.559706	-1.023078	0.138246
14	9	0	2.042001	-0.925418	-0.031935
15	1	0	0.755349	-0.678545	1.495858

axial($CHCl_3$_wB97X-D/6-311++G(d,p)) E= -445.012707793, G= -444.9924112

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.257235	-1.260318	0.032410
2	6	0	-0.142191	-1.324638	0.671647
3	6	0	-0.480185	1.006456	-0.256550
4	6	0	0.938342	0.911239	-0.802606
5	1	0	-0.539610	-2.339865	0.656135
6	1	0	1.226301	-1.686418	-0.980283
7	1	0	1.968169	-1.833912	0.625515
8	1	0	-1.122267	1.609053	-0.900406
9	1	0	0.884913	0.552023	-1.841556
10	1	0	1.402797	1.897618	-0.797076
11	1	0	-0.068627	-0.978670	1.707041
12	6	0	-1.054570	-0.400439	-0.085836
13	8	0	-2.100090	-0.722881	-0.595822
14	8	0	1.744101	0.065613	-0.015738
15	9	0	-0.446172	1.604947	1.007635

equatorial($CHCl_3$_wB97X-D/6-311++G(d,p)) E= -445.014278943, G= -444.9925448

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.861222	0.296311	-0.290729
2	6	0	-0.909162	1.317090	0.347512
3	6	0	0.791466	-0.545576	0.409163
4	6	0	-0.277592	-1.429886	-0.253192
5	1	0	-1.079499	2.320178	-0.045545
6	1	0	-1.795750	0.353544	-1.385741
7	1	0	-2.890399	0.496783	0.003740
8	1	0	-0.160559	-1.376532	-1.344504
9	1	0	-0.149327	-2.464274	0.063568
10	1	0	-1.077769	1.328988	1.429528
11	6	0	0.522792	0.916401	0.090271
12	8	0	1.368890	1.650679	-0.355230
13	8	0	-1.563348	-1.018529	0.141506
14	9	0	2.039415	-0.929123	-0.036118
15	1	0	0.756542	-0.679818	1.495655

axial(CH_2Cl_2_wB97X-D/6-311++G(d,p)) E= -445.014131239, G= -444.925571

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.264684	-1.256632	0.030979
2	6	0	-0.137830	-1.330781	0.661502
3	6	0	-0.481322	1.004106	-0.259640
4	6	0	0.939567	0.916069	-0.798931
5	1	0	-0.530564	-2.347601	0.636691
6	1	0	1.242677	-1.677491	-0.983760
7	1	0	1.974215	-1.829604	0.626197
8	1	0	-1.122685	1.605513	-0.905026
9	1	0	0.893149	0.557362	-1.838021
10	1	0	1.399095	1.904688	-0.790734
11	1	0	-0.071487	-0.993864	1.700536
12	6	0	-1.052965	-0.404121	-0.088926
13	8	0	-2.104672	-0.723782	-0.589084
14	8	0	1.744933	0.072853	-0.007897
15	9	0	-0.455476	1.601842	1.006675

equatorial(CH_2Cl_2_wB97X-D/6-311++G(d,p)) E= -445.015955676, G= -444.927101

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.861234	0.298532	-0.291313
2	6	0	-0.907370	1.318793	0.345300
3	6	0	0.789761	-0.546405	0.409330
4	6	0	-0.279808	-1.430517	-0.252394
5	1	0	-1.076991	2.321186	-0.049675
6	1	0	-1.796447	0.353604	-1.386196
7	1	0	-2.889490	0.501676	0.004102
8	1	0	-0.163742	-1.378281	-1.343714
9	1	0	-0.152220	-2.464437	0.065963
10	1	0	-1.075891	1.332962	1.427257
11	6	0	0.523182	0.915398	0.090506
12	8	0	1.372813	1.648180	-0.353155
13	8	0	-1.564823	-1.016707	0.142857
14	9	0	2.038535	-0.930303	-0.037726
15	1	0	0.756857	-0.680574	1.495614

axial(DMSO_wB97X-D/6-311++G(d,p)) E= -445.015605185, G= -444.927091

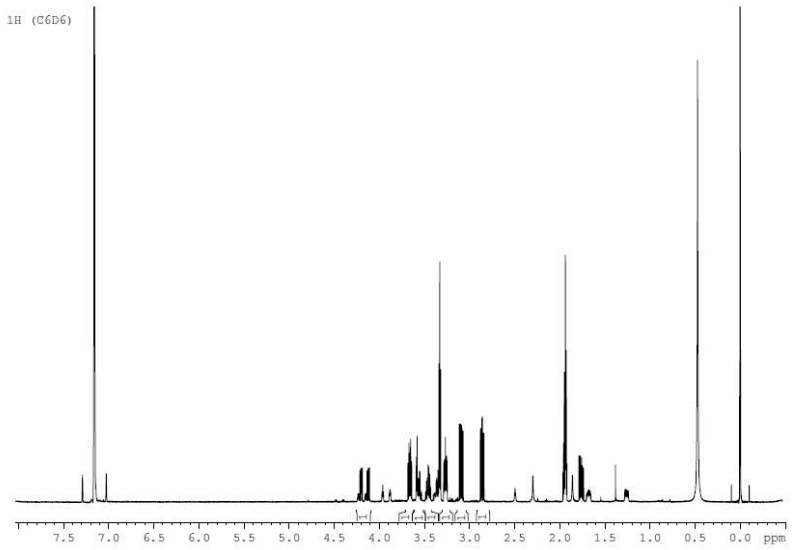
Standard orientation:

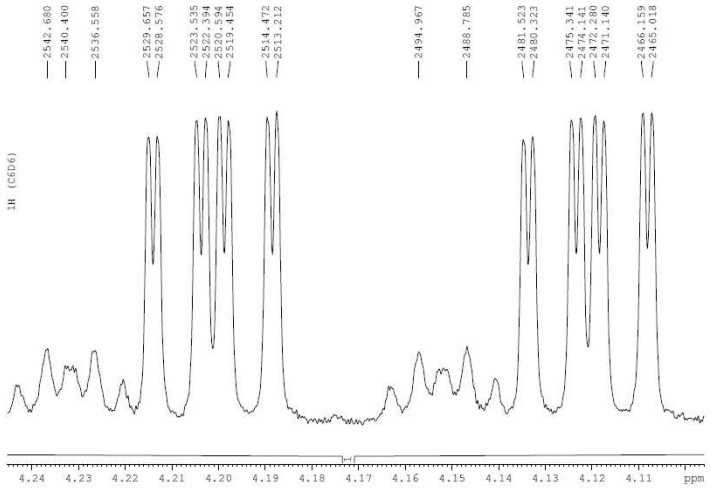
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.272719	-1.252724	0.029365
2	6	0	-0.133097	-1.337504	0.650304
3	6	0	-0.482453	1.001517	-0.263290
4	6	0	0.941076	0.921507	-0.794695
5	1	0	-0.520889	-2.355843	0.615114
6	1	0	1.260434	-1.667677	-0.987524
7	1	0	1.980725	-1.825053	0.626833
8	1	0	-1.123108	1.601601	-0.910245
9	1	0	0.902808	0.564001	-1.834090
10	1	0	1.395189	1.912532	-0.782865
11	1	0	-0.074430	-1.010722	1.693199
12	6	0	-1.051230	-0.408079	-0.092459
13	8	0	-2.109575	-0.724671	-0.581515
14	8	0	1.745621	0.080566	0.000889
15	9	0	-0.465687	1.598410	1.005470

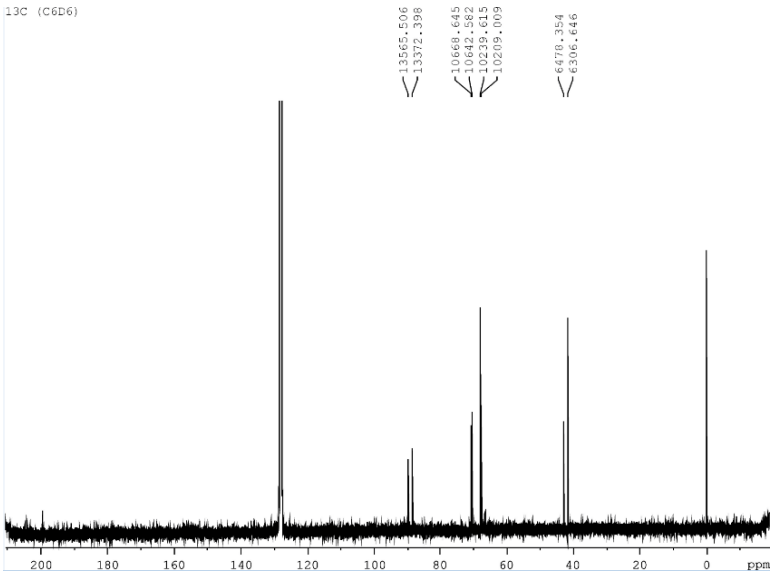
equatorial(DMSO_wB97X-D/6-311++G(d,p)) E= -445.017685480, G= -444.928805

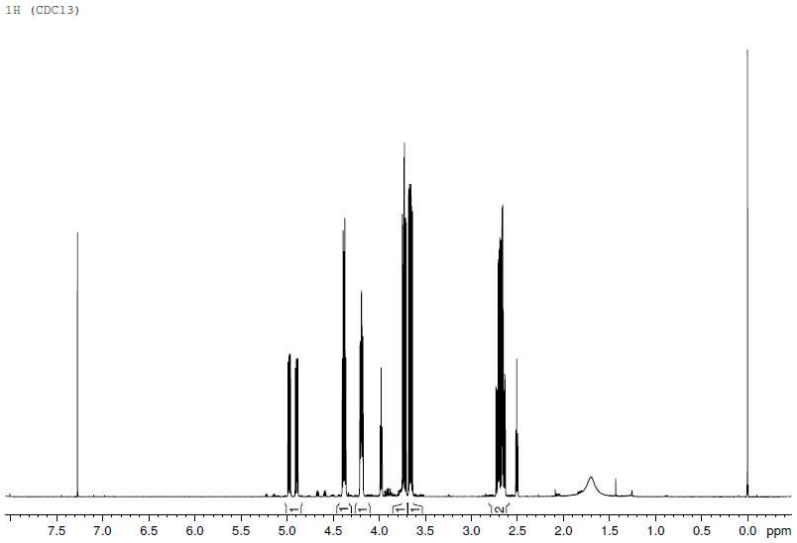
Standard orientation:

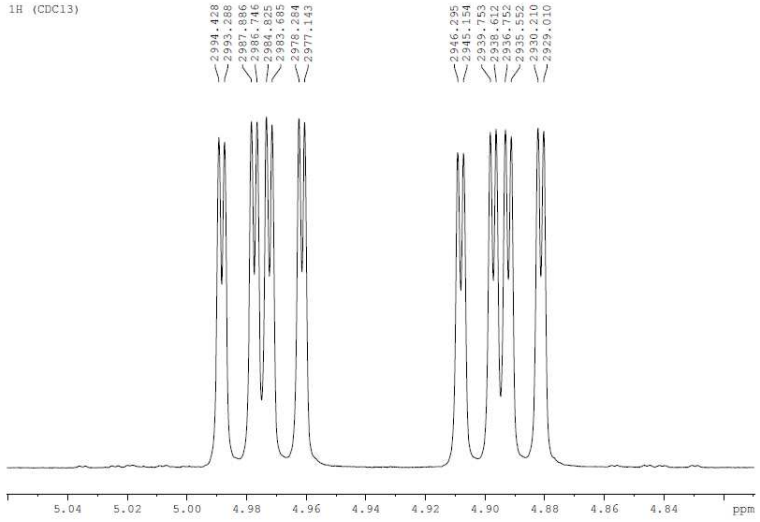
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.861563	0.300152	-0.291401
2	6	0	-0.906026	1.320058	0.343622
3	6	0	0.788223	-0.546962	0.409651
4	6	0	-0.281275	-1.430929	-0.252362
5	1	0	-1.075400	2.321766	-0.053056
6	1	0	-1.798212	0.353665	-1.386135
7	1	0	-2.888790	0.505354	0.005742
8	1	0	-0.166083	-1.378766	-1.343652
9	1	0	-0.153894	-2.464573	0.066756
10	1	0	-1.074228	1.336137	1.425565
11	6	0	0.523141	0.914472	0.090762
12	8	0	1.375756	1.645852	-0.351999
13	8	0	-1.565770	-1.015613	0.143758
14	9	0	2.038336	-0.930536	-0.038505
15	1	0	0.756710	-0.681419	1.495621


1H (C6D6)
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm


2542.680
2540.400
2536.558
2529.657
2528.576
2523.535
2522.394
2520.594
2519.454
2514.472
2513.212
2494.967
2488.785
2481.523
2480.323
2475.341
2474.141
2472.280
2471.140
2466.159
2465.018
1H (C6D6)
4.24 4.23 4.22 4.21 4.20 4.19 4.18 4.17 4.16 4.15 4.14 4.13 4.12 4.11 ppm


13C (C6D6)
13565.506
13372.398
10668.645
10642.582
10239.615
10209.009
6470.354
6306.646
200 180 160 140 120 100 80 60 40 20 0 ppm


1H (CDC13)
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm


1H (CDC13)
2994.428
2993.288
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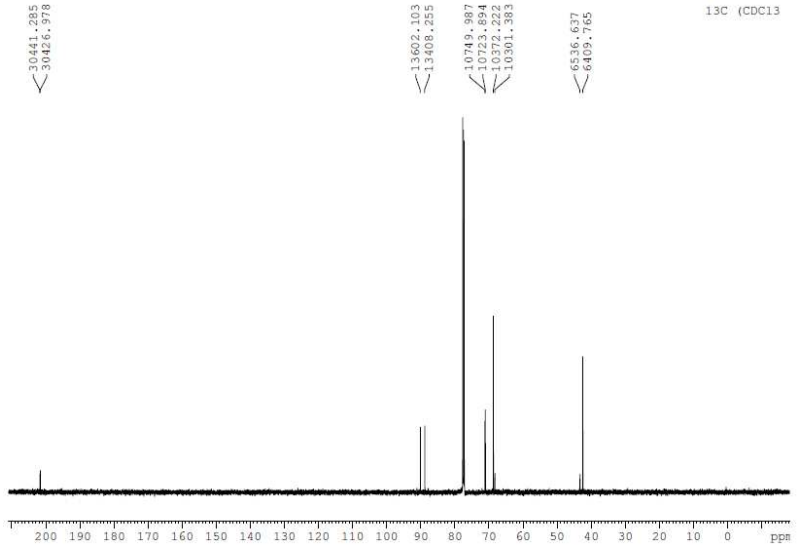
2986.746
2984.825
2983.685
2978.284
2977.143
2946.295
2945.154
2939.753
2938.612
2936.752
2935.552
2930.210
2929.010
5.04 5.02 5.00 4.98 4.96 4.94 4.92 4.90 4.88 4.86 4.84 ppm


13C (CDC13
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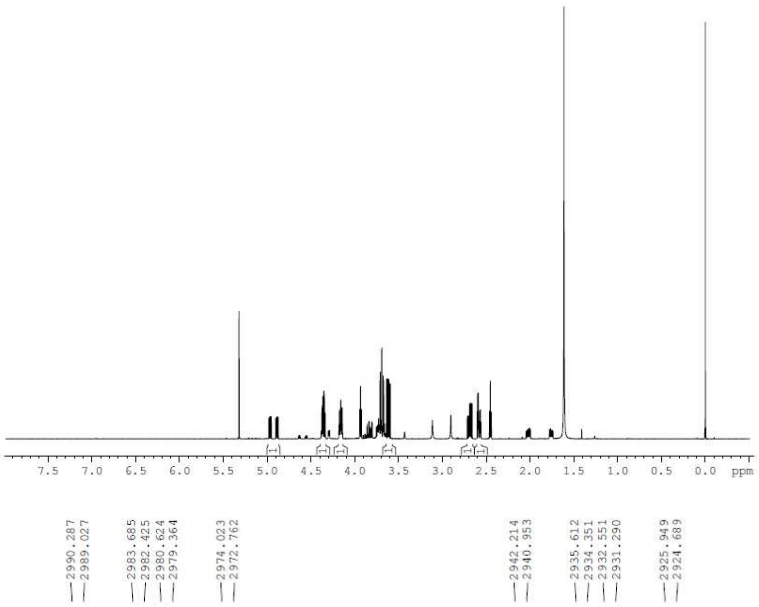
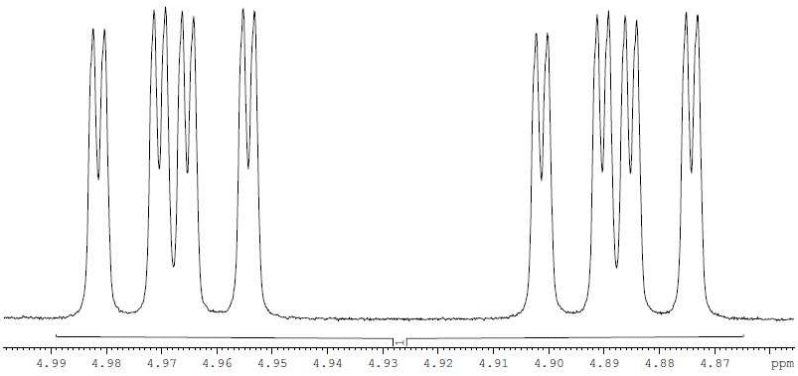
30426.978
13602.103
13408.255
10749.987
10723.894
10372.222
10301.383
6536.637
6409.765
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

1H (CD2C12)



1H (CD2C12)



13C (CD2C12)