Electronic Supplementary Information (ESI)

On the anomeric preference of the isothiocyanato group†

Concepción Sosa,[a,*] Reyes Babiano,[a] Pedro Cintas,[a] Mark E. Light[b] and Juan C. Palacios*

[a]*Departamento de Química Orgánica e Inorgánica, Facultad de Ciencias, and IACYS-Unidad de Química Verde y Desarrollo Sostenible, Universidad de Extremadura, E-06006 Badajoz, Spain*

[b]*Department of Chemistry, Faculty of Natural and Environmental Sciences, The University of Southampton, Southampton SO17 1BJ, U.K.*

E-mail: cososag@unex.es; palacios@unex.es

ORCID:

Concepción Sosa-Gil: 0000-0002-5160-5769

Reyes Babiano: 0000-0003-4853-0484

Pedro Cintas: 0000-0002-2608-3604

Mark E. Light: 0000-0002-0585-0843

Juan Carlos Palacios: 0000-0002-5004-4744

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FT- IR spectra

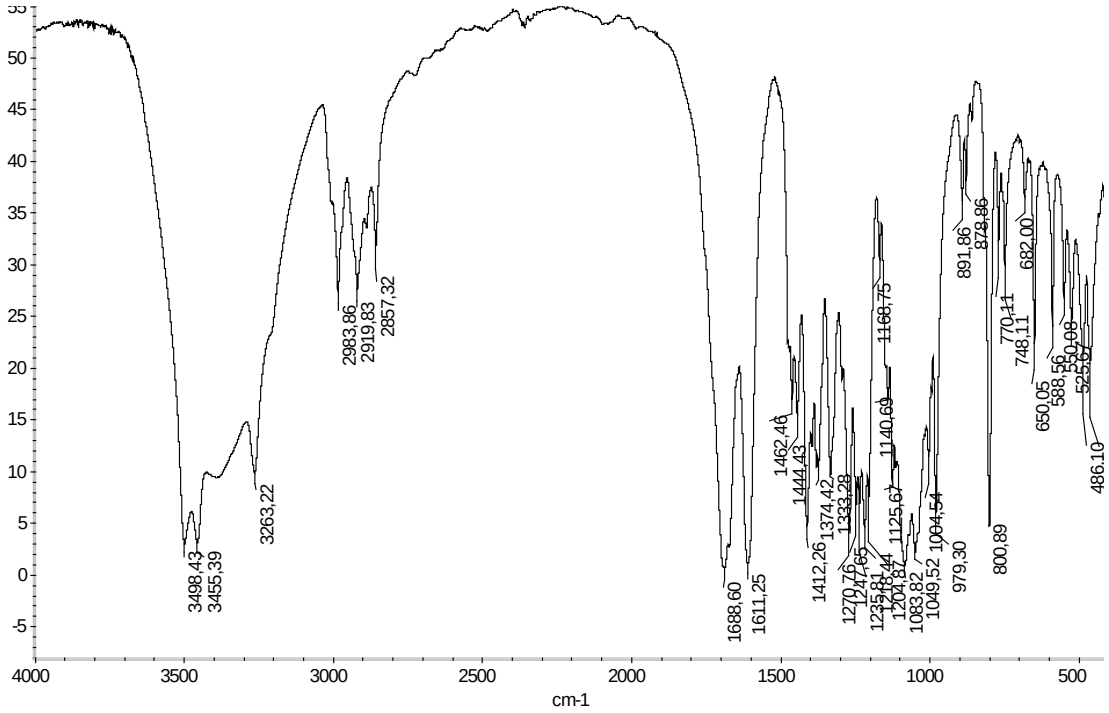


Figure S1. FT-IR spectrum of *N*-[1-(2,2-diethoxycarbonylvinyl)]- β-D-xylopyranosylamine (**3**).

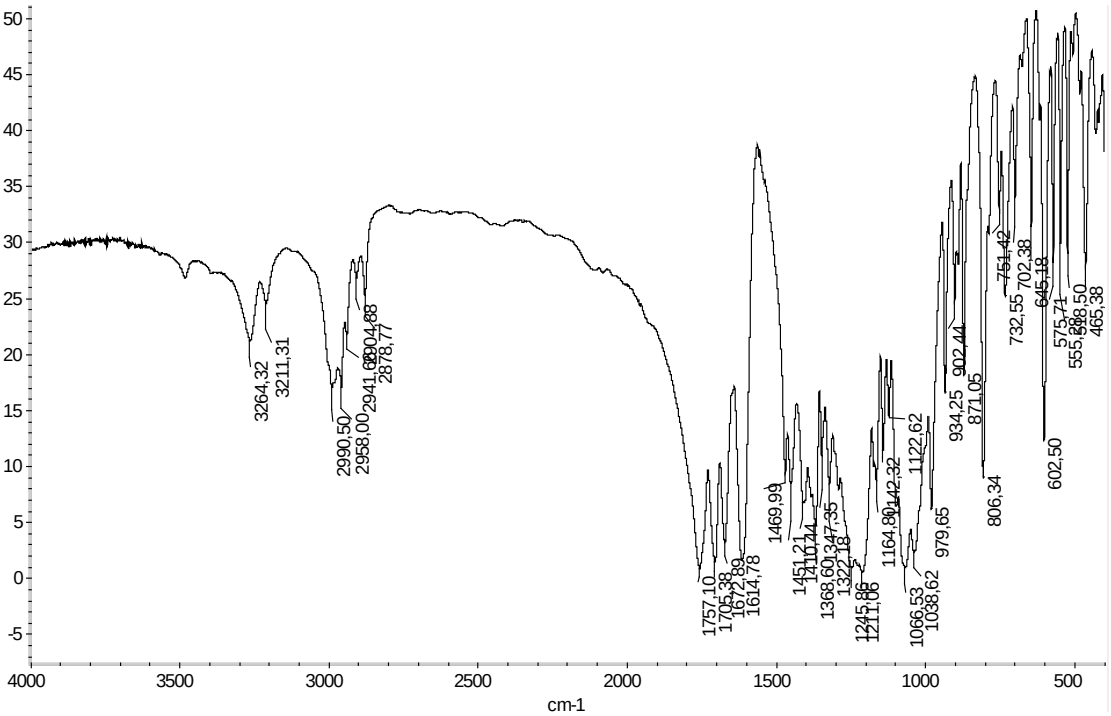


Figure S2. FT-IR spectrum of 2,3,4-tri-*O*-acetyl-*N*-[1-(2,2-diethoxycarbonylvinyl)]-β-D-xylopyranosylamine (**4**).

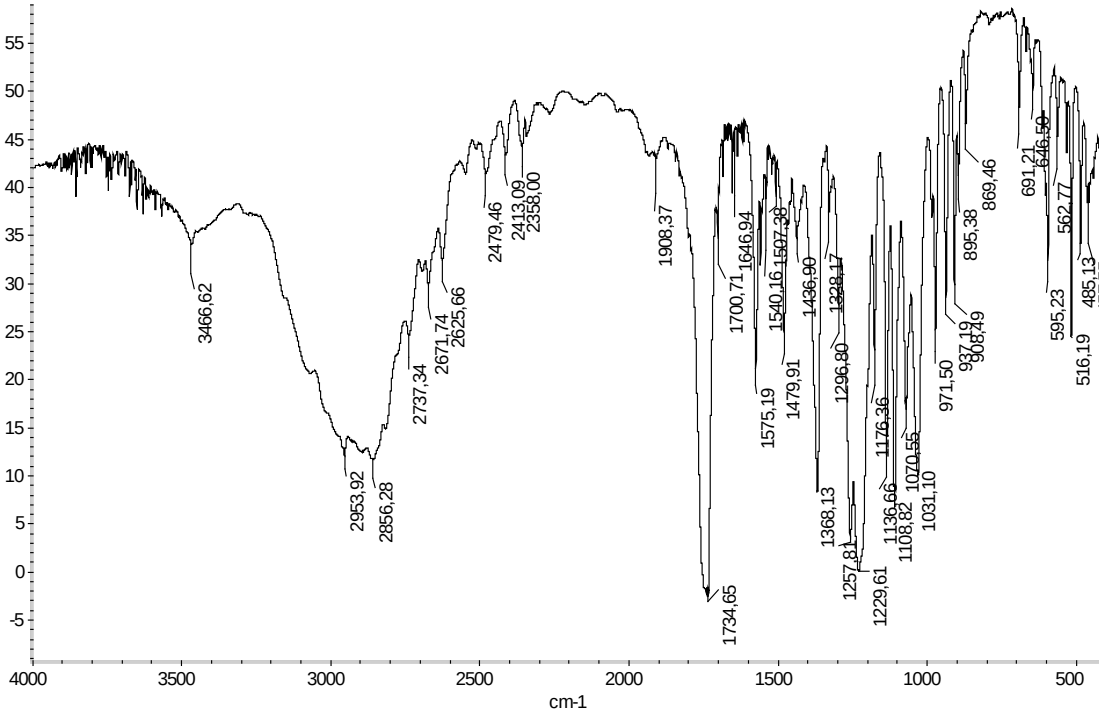


Figure S3. FT-IR spectrum of 2,3,4-tri-*O*-acetyl-β,α-D-xylopyranosylamine hydrobromides (**5** and **8** mixture).

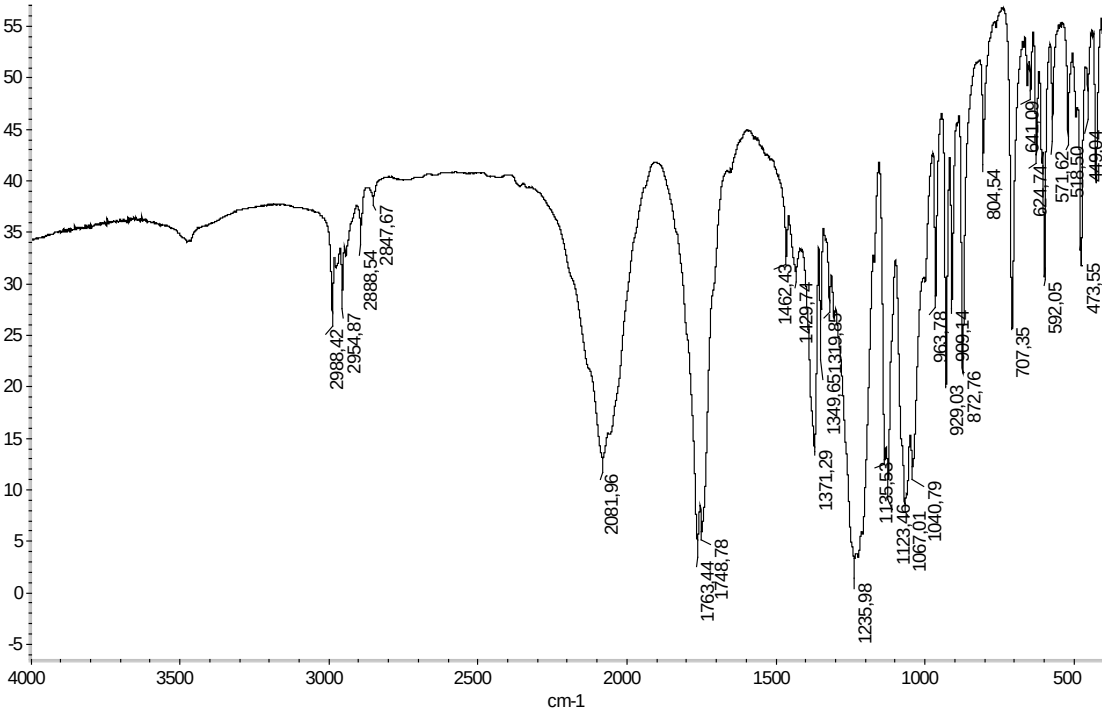


Figure S4. FT-IR spectrum of 2,3,4-tri-*O*-acetyl-α-D-xylopyranosyl isothiocyanate (**17**).

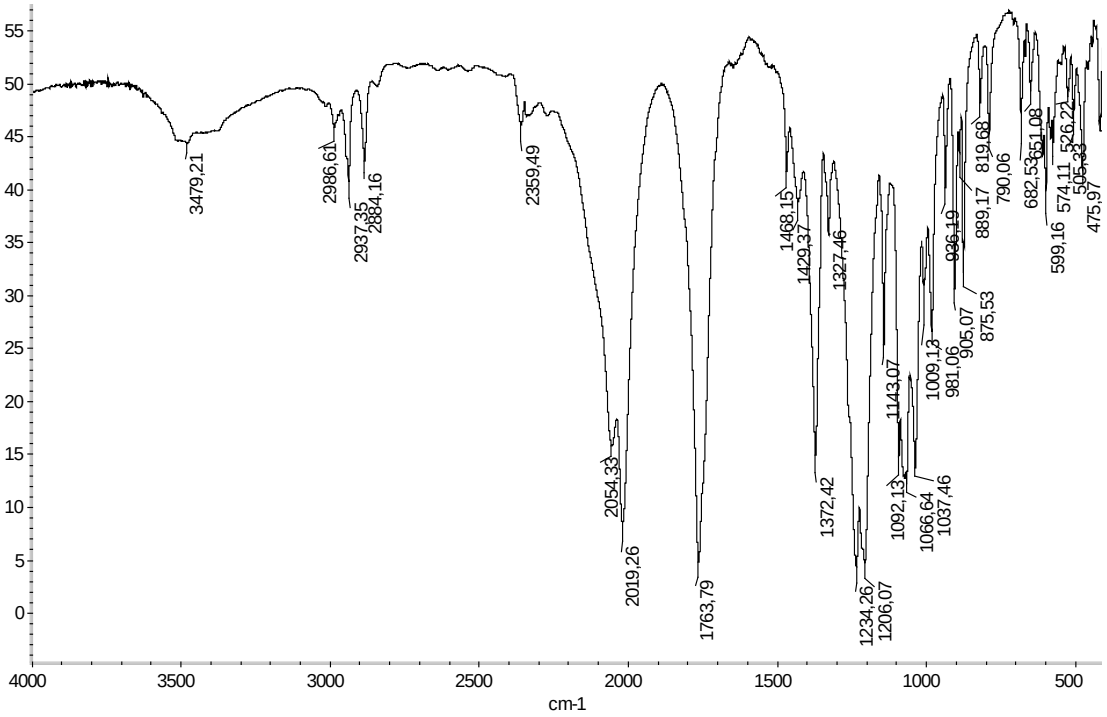


Figure S5. FT-IR spectrum of 2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl isothiocyanate (**6**).

NMR spectra

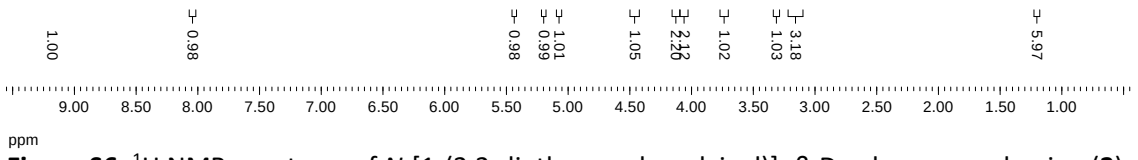


Figure S6. ^{1}H NMR spectrum of *N*-[1-(2,2-diethoxycarbonylvinyl)]- β-D-xylopyranosylamine (**3**).

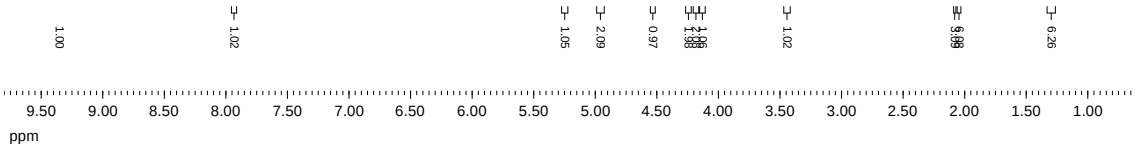


Figure S7. ^{1}H NMR spectrum of 2,3,4-tri-*O*-acetyl-*N*-[1-(2,2-diethoxycarbonylvinyl)]-β-D-xylopyranosylamine (**4**).

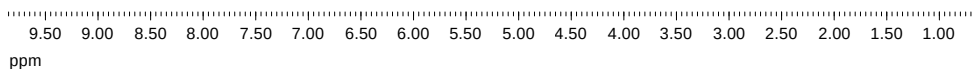


Figure S8. COSY spectrum of 2,3,4-tri-*O*-acetyl-*N*-[1-(2,2-diethoxycarbonylvinyl)]-β-D-xylopyranosylamine (**4**).

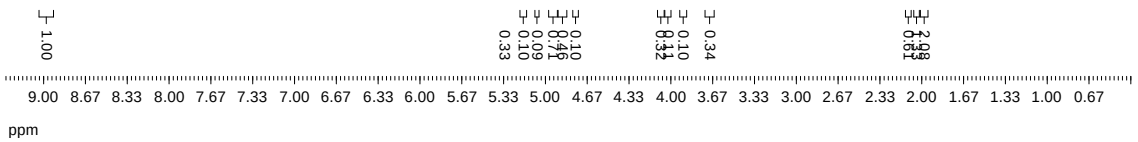


Figure S9. [1]H NMR spectrum of 2,3,4-tri-*O*-acetyl-β,α-D-xylopyranosylamine hydrobromides (**5** and **8** mixture).

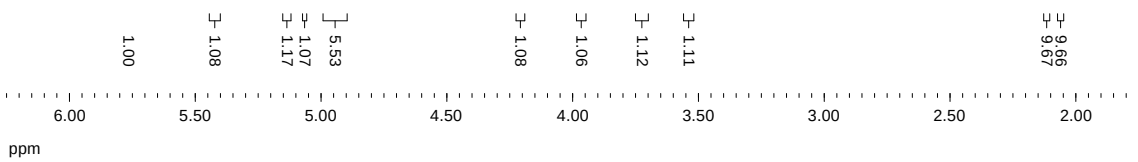


Figure S10. [1]H NMR spectrum of 2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl isothiocyanate (**6**) and 2,3,4-tri-*O*-acetyl-α-D-xylopyranosyl isothiocyanate (**17**).

α-anomer

β-anomer

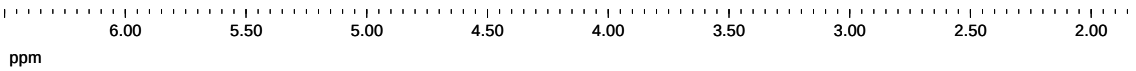


Figure S11. ^{1}H NMR spectra of 2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl isothiocyanate (bottom) and 2,3,4-tri-*O*-acetyl-α-D-xylopyranosyl isothiocyanate (top).

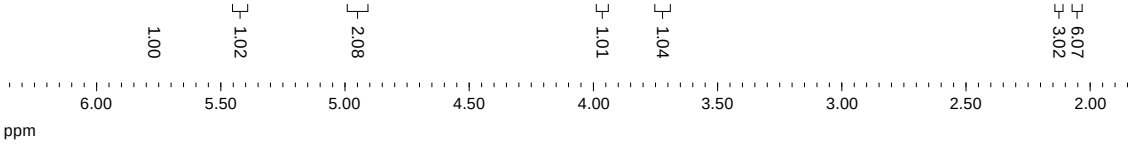


Figure S12. ^{1}H NMR spectrum of 2,3,4-tri-*O*-acetyl-α-D-xylopyranosyl isothiocyanate (**17**).

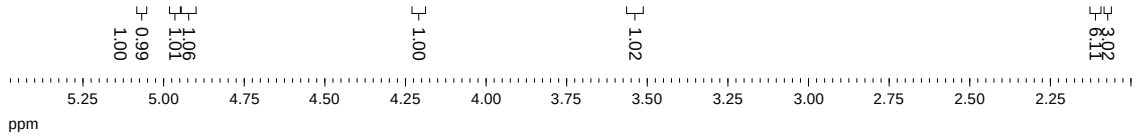


Figure S13. ^{1}H NMR spectrum of 2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl isothiocyanate (**6**).

Figure S14. ^{13}C NMR and DEPT spectra of *N*-[1-(2,2-diethoxycarbonylvinyl)]- β-D-xylopyranosylamine (**3**).

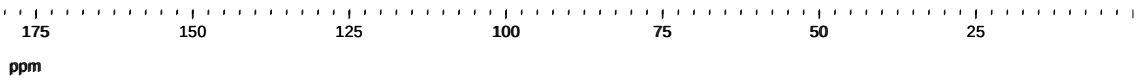


Figure S15. ^{13}C NMR and DEPT spectra of 2,3,4-tri-*O*-acetyl-*N*-[1-(2,2-diethoxycarbonylvinyl)]-β-D-xylopyranosylamine (**4**).

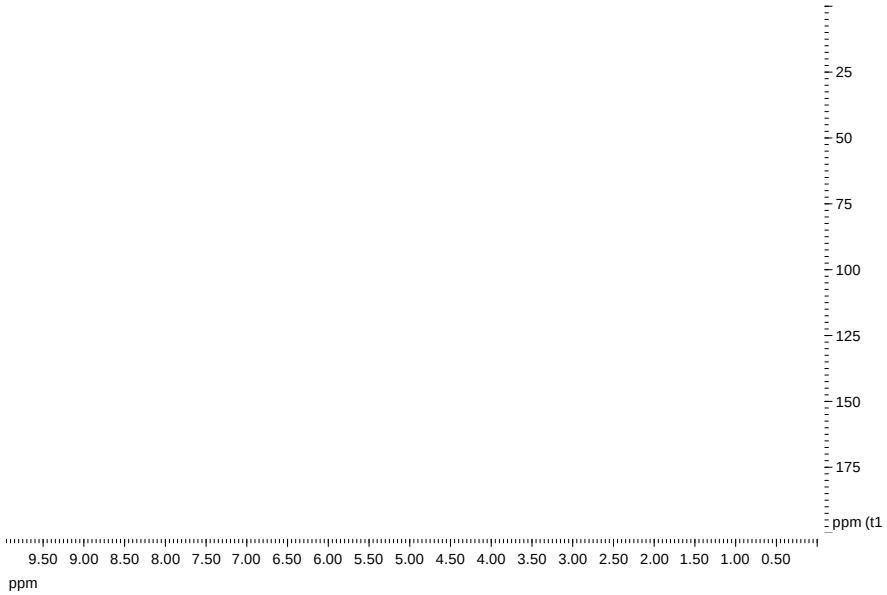


Figure S16. HMQC spectrum of compound 2,3,4-tri-*O*-acetyl-*N*-[1-(2,2-diethoxycarbonylvinyl)]-β-D-xylopyranosylamine (**4**).

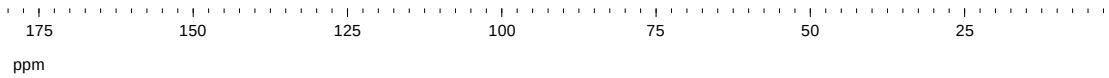


Figure S17. ^{13}C NMR and DEPT spectra of 2,3,4-tri-*O*-acetyl-β,α-D-xylopyranosylamine hydrobromides (**5** and **8** mixture).

α - anomer

β - anomer

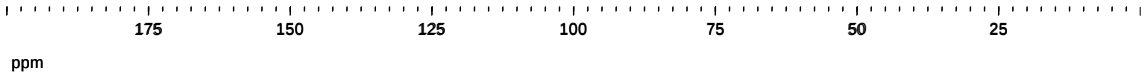


Figure S18. ^{13}C NMR spectra of 2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl isothiocyanate (bottom) and 2,3,4-tri-*O*-acetyl-α-D-xylopyranosyl isothiocyanate (top).

Figure S19. ^{13}C NMR and DEPT spectra of 2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl isothiocyanate (**17**).

Figure S20. ^{13}C NMR and DEPT spectra of 2,3,4-tri-*O*-acetyl-α-D-xylopyranosyl isothiocyanate (**6**).

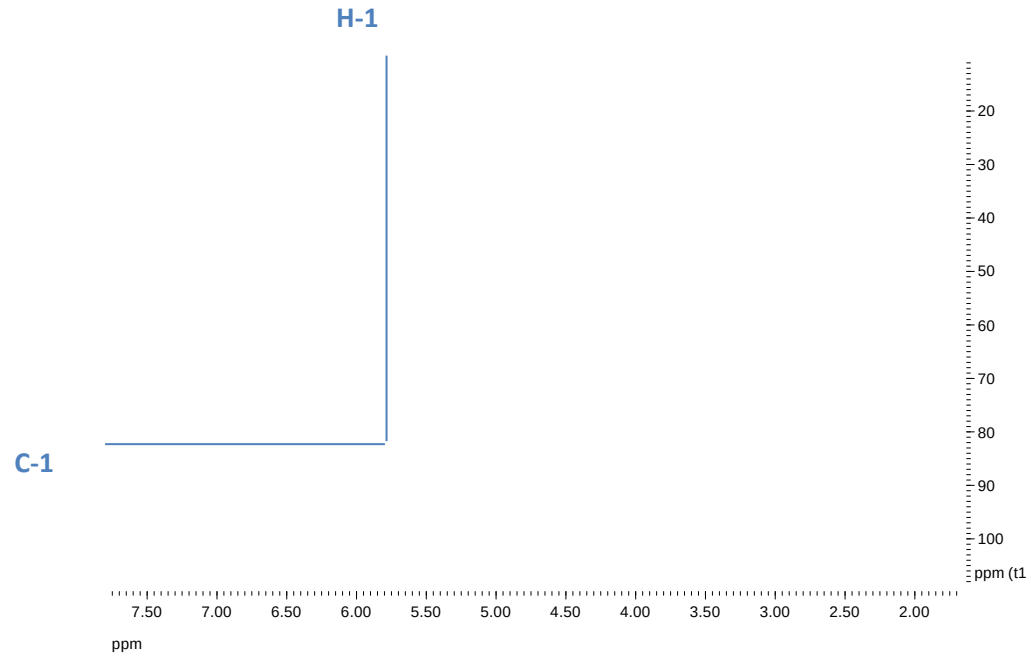


Figure S21. HMQC spectrum of 2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl isothiocyanate (**17**).

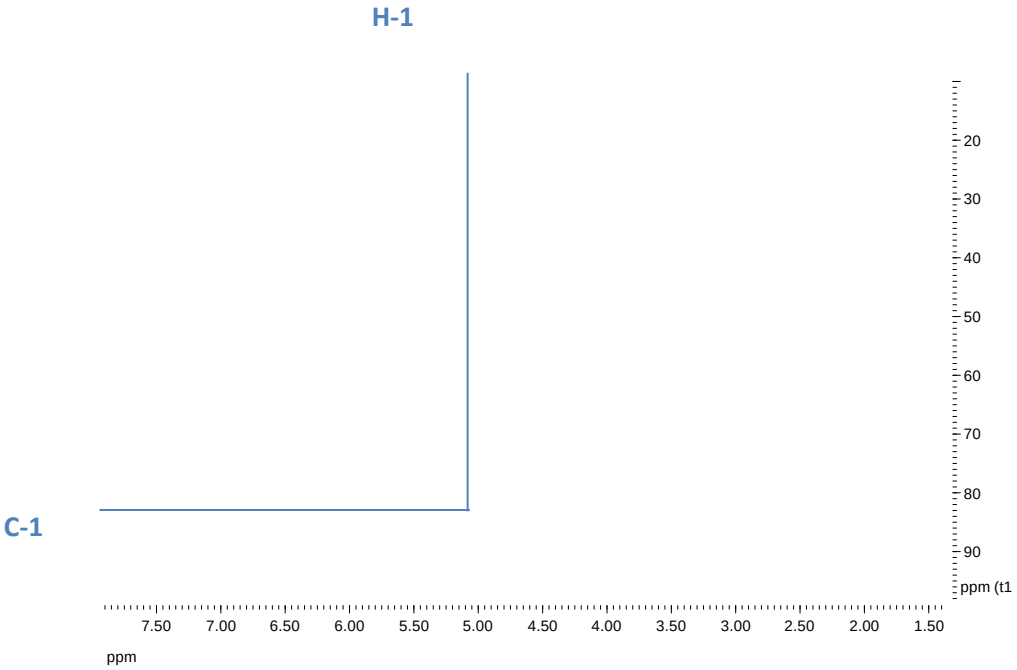


Figure S22. HMQC spectrum of 2,3,4-tri-*O*-acetyl-α-D-xylopyranosyl isothiocyanate (**6**).

Mass spectra

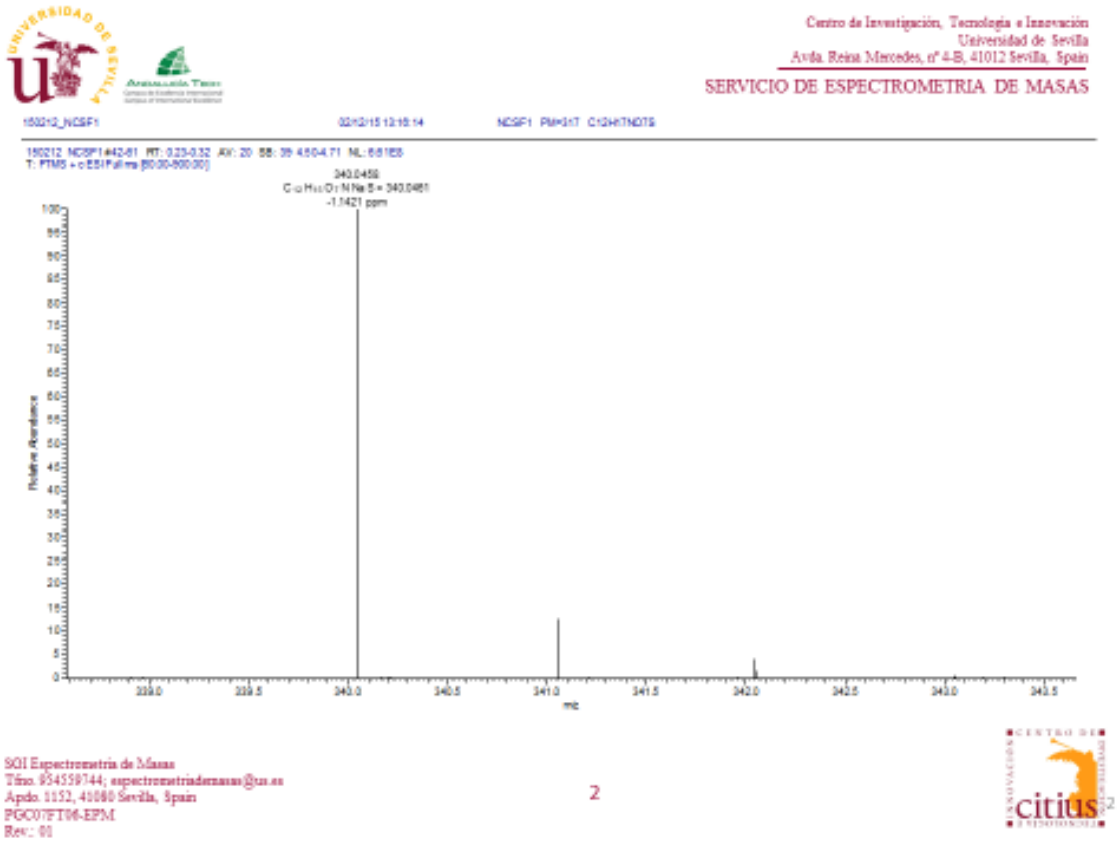


Figure S23. Mass spectrum of 2,3,4-tri-*O*-acetyl-β-D-xylopyranosyl isothiocyanate (**17**).

X-Ray data for compounds 4 and 6

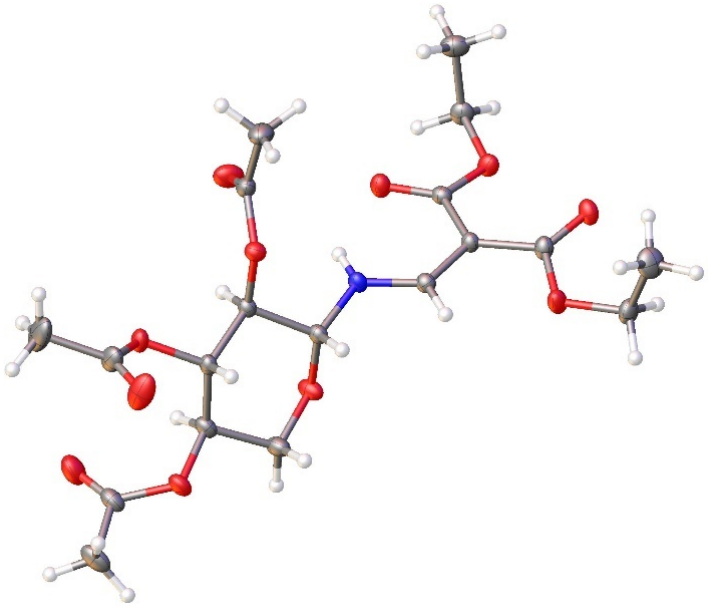


Figure S24. ORTEP diagram for compound **4**; thermal ellipsoids drawn at the 50% probability level. The minor disorder of one acetate group (far right hand side of the molecule) has been omitted for clarity.

Acquisition data. A suitable crystal (0.26×0.20×0.05) was selected and mounted on a MITIGEN holder in perfluoroether oil a Rigaku AFC12 FRE-HF diffractometer. The crystal was kept at T = 100(2) K during data collection. Using Olex2,[1] the structure was solved with the ShelXT structure solution program,[2] using the Direct Methods solution method. The model was refined with version of ShelXL using Least Squares minimisation.[3]

Crystal data. $C_{19}H_{27}NO_{11}$, M_r = 445.41, monoclinic, $P2_1$ (No. 4), a = 10.26472(19) Å, b = 9.99397(19) Å, c = 10.8624(2) Å, β = 92.0775(17)°, $\alpha = \gamma$ = 90°, V = 1113.59(4) Å^3, T = 100(2) K, Z = 2, Z' = 1, μ(Mo K$_\alpha$) = 0.110, 13739 reflections measured, 6383 unique (R_{int} = 0.0152) which were used in all calculations. The final wR_2 was 0.0769 (all data) and R_1 was 0.0300 (I≥2 σ(I)).

Compound 4	Summary
Formula	$C_{19}H_{27}NO_{11}$
$D_{calc.}$/ g cm^{-3}	1.328
μ/mm^{-1}	0.110
Formula Weight	445.41
Colour	clear colourless
Shape	block
Size/mm^3	0.26×0.20×0.05
T/K	100(2)
Crystal System	monoclinic
Flack Parameter	-0.4(2)
Hooft Parameter	-0.45(17)
Space Group	$P2_1$
a/Å	10.26472(19)
b/Å	9.99397(19)
c/Å	10.8624(2)
α/°	90
β/°	92.0775(17)
γ/°	90
V/Å^3	1113.59(4)
Z	2
Z'	1
Wavelength/Å	0.71073
Radiation type	Mo K_α
Θ_{min}/°	1.985
Θ_{max}/°	31.990
Measured Refl's.	13739
Indep't Refl's	6383
Refl's I≥2 σ(I)	6143
R_{int}	0.0152
Parameters	300
Restraints	1
Largest Peak	0.317
Deepest Hole	-0.152
GooF	1.026
wR_2 (all data)	0.0769
wR_2	0.0758
R_1 (all data)	0.0316
R_1	0.0300

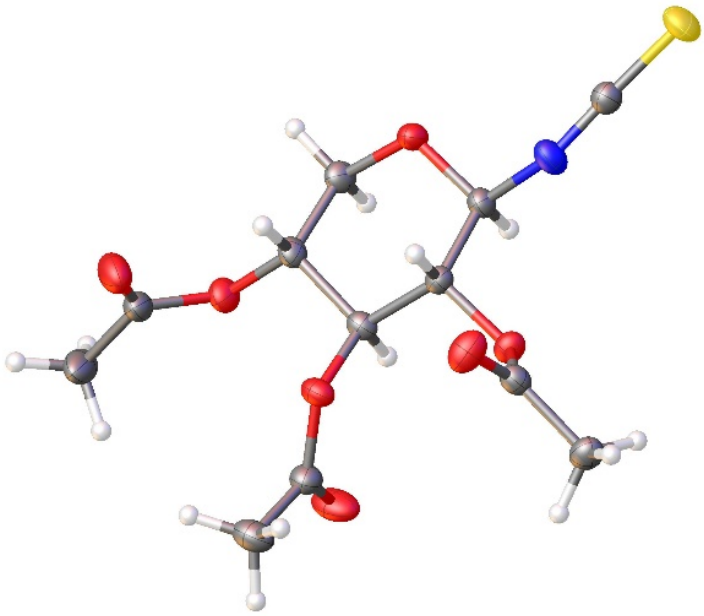


Figure S25. ORTEP diagram for compound **6**; thermal ellipsoids drawn at the 50% probability level.

Acquisition data. A suitable crystal with dimensions 0.23×0.08×0.05 mm^3 was selected and mounted on a suitable support on an Rigaku Saturn724+ (2x2 bin mode) diffractometer. The crystal was kept at a steady T = 100(2) K during data collection. Using Olex2,[1] the structure was solved with the ShelXT structure solution program,[2] using the Direct Methods solution method. The model was refined with version of ShelXL using Least Squares minimisation.[3]

Crystal data. $C_{12}H_{15}NO_7S$, M_r = 317.3130, triclinic, $P1$ (No. 1), a = 7.6274(4) Å, b = 9.1304(5) Å, c = 10.6185(7) Å, α = 92.663(7)°, β = 99.327(7)°, γ = 90.796(6)°, V = 728.75(7) $Å^3$, T = 100(2) K, Z = 2, Z' = 2, μ(MoK_α) = 0.254, 12109 reflections measured, 5042 unique (R_{int} = 0.0462) which were used in all calculations. The final wR_2 was 0.0905 (all data) and R_1 was 0.0349 (I > 2(I)).

Compound 6	Summary
Formula	$C_{12}H_{15}NO_7S$
$D_{calc.}$/ g cm^{-3}	1.446
μ/mm^{-1}	0.254
Formula Weight	317.3130
Colour	colourless
Shape	chunk
Size/mm^3	0.23×0.08×0.05
T/K	100(2)
Crystal System	triclinic
Flack Parameter	0.03(5)
Space Group	$P\bar{1}$
a/Å	7.6274(4)
b/Å	9.1304(5)
c/Å	10.6185(7)
α/°	92.663(7)
β/°	99.327(7)
γ/°	90.796(6)
V/Å^3	728.75(7)
Z	2
Z'	2
Wavelength/Å	0.71075
Radiation type	MoK_α
Θ_{min}/°	3.035
Θ_{max}/°	27.485
Measured Refl.	12109
Independent Refl.	5042
Reflections with I > 2(I)	4803
R_{int}	0.0462
Parameters	385
Restraints	3
Largest Peak	0.255
Deepest Hole	-0.320
GooF	1.046
wR_2 (all data)	0.0905
wR_2	0.0886
R_1 (all data)	0.0368
R_1	0.0349

References

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339-341.

2. G. M. Sheldrick, *Acta Cryst.*, 2014, **A71**, 3-8.

3. G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112-122.

Relative stability and optimized geometries of skew-boat conformers of compounds 6 and 17

The relative stability of skew-boat conformers of **6** and **17** and their pyranose conformations ($^4C_1$) were obtained at the DFT level using the functional M06-2X and the basis set 6-311++G(d,p) as implemented in the Gaussian16 package[4] with solvent effects modeled with the SMD method (Table S1).

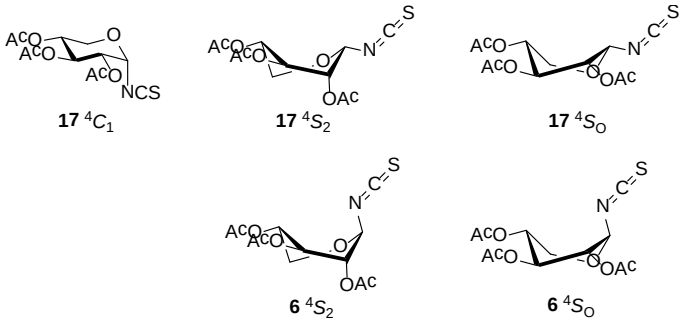


Table S1. Relative energies calculated for the conformers of **6** and **17**.[a,b]

	Conformer	Gas phase	Chloroform	Ethanol
17	$^4C_1$	0,00	0,00	0,00
17	$^4S_2$	7,54	6,38	7,56
17	^4S_O	6,29	5,14	5,45
6	$^4S_2$	5,14	5,66	6,21
6	^4S_O	4,46	3,58	3,33

[a]In kcal mol^{-1}, [b]at the M06-2X/6-311++G(d,p) level.

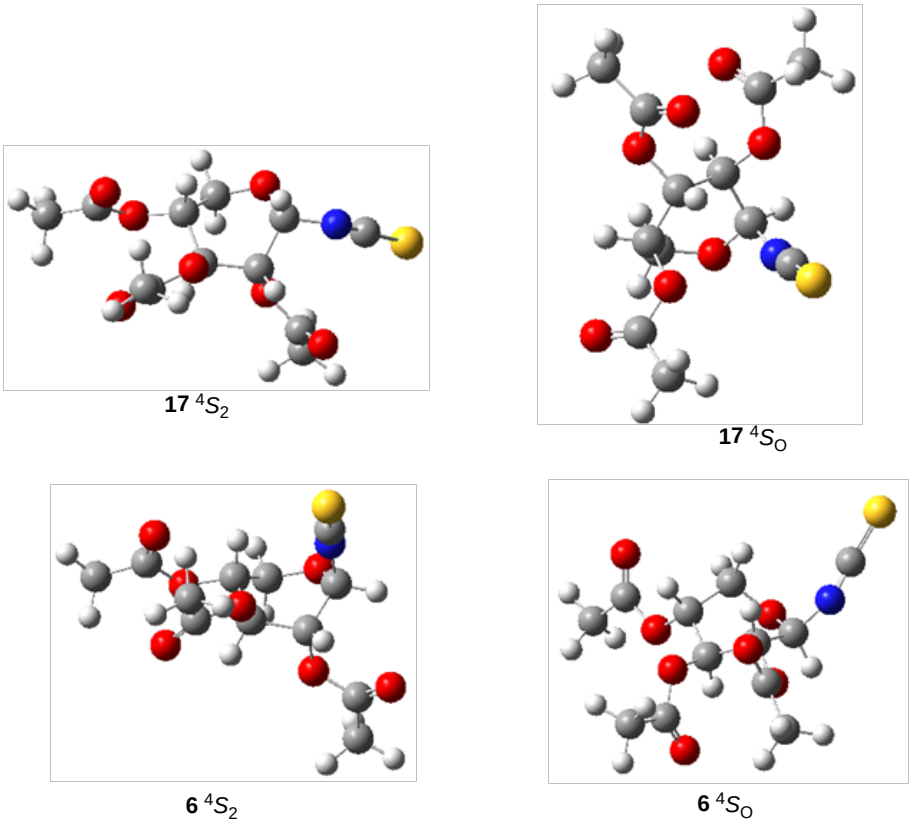


Figure S26. Optimized geometries for the skew-boat conformers of **6** and **17** (in chloroform).

Reference

4. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 16, Revision A.03*, Gaussian, Inc., Wallingford, CT, 2016.

Cartesian coordinates and calculated energies at the M06-2X/6-311G++G(d,p) level in the gas phase, EtOH and $CHCl_3$ (SMD Model) for chair and skew-boat structures

Structure 4 (M06-2X, Gas phase)

Energy (Hartrees): = -1622.3751846
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.553548	-0.661808	-0.070075
2	6	0	1.577100	0.471312	-0.087653
3	6	0	2.987540	-0.072934	-0.239690
4	6	0	3.253805	-1.173538	0.784958
5	6	0	2.115431	-2.189460	0.767039
6	1	0	3.138148	-0.471063	-1.247830
7	1	0	3.373539	-0.728395	1.775280
8	1	0	2.124288	-2.720772	-0.195341
9	1	0	1.496937	1.041383	0.841650
10	8	0	0.872339	-1.555312	0.979485
11	8	0	4.424972	-1.910253	0.433445
12	8	0	3.852654	1.042332	-0.032488
13	6	0	5.618184	-1.472819	0.897690
14	8	0	5.732806	-0.554178	1.659890
15	6	0	6.739254	-2.258085	0.288815
16	1	0	6.856746	-1.897993	-0.736242
17	1	0	7.653097	-2.081078	0.849715
18	1	0	6.494981	-3.318685	0.255219
19	6	0	5.037830	1.057472	-0.680704
20	8	0	5.366081	0.222580	-1.477687
21	6	0	5.875915	2.210322	-0.219325
22	1	0	5.268247	3.104388	-0.090190
23	1	0	6.287465	1.930096	0.753813
24	1	0	6.683083	2.378670	-0.927401
25	8	0	1.335734	1.319439	-1.203262
26	6	0	0.632529	2.459033	-0.972376
27	6	0	0.477861	3.243475	-2.241500
28	1	0	-0.016448	4.185752	-2.023000
29	1	0	1.455967	3.412566	-2.692177
30	1	0	-0.118110	2.661182	-2.946125
31	8	0	0.204225	2.760092	0.102465
32	1	0	2.249214	-2.916527	1.565873
33	1	0	0.586088	-1.198616	-1.030074
34	7	0	-0.763945	-0.150854	0.123766
35	1	0	-0.922868	0.662259	0.718587
36	6	0	-1.836279	-0.827294	-0.303280
37	6	0	-3.158312	-0.535972	-0.092249
38	6	0	-3.496519	0.630746	0.734466
39	8	0	-2.648830	1.355144	1.222930
40	8	0	-4.797181	0.850296	0.922749
41	6	0	-5.122395	1.985831	1.736886
42	1	0	-4.686279	2.881200	1.288902
43	1	0	-4.670406	1.856368	2.722651
44	6	0	-6.631193	2.055762	1.805058
45	1	0	-6.939492	2.904758	2.417689
46	1	0	-7.052407	2.173805	0.805753
47	1	0	-7.035012	1.142155	2.243262
48	1	0	-1.624230	-1.709803	-0.901168
49	6	0	-4.090422	-1.479805	-0.752178
50	8	0	-3.721778	-2.416604	-1.424124
51	8	0	-5.383010	-1.214270	-0.548770
52	6	0	-6.304846	-2.113360	-1.178064
53	1	0	-6.113219	-2.125352	-2.253121
54	1	0	-6.129882	-3.123129	-0.799835
55	6	0	-7.694068	-1.614370	-0.850281
56	1	0	-7.846083	-1.595504	0.229636
57	1	0	-7.835842	-0.603919	-1.236009
58	1	0	-8.443792	-2.268965	-1.298165

Structure 7 (M06-2X, Gas phase)
Energy (Hartrees): = -1622.3768024
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.740027	-1.392113	1.704638
2	6	0	-1.514533	-1.597100	0.386064
3	6	0	-2.328211	-0.370623	0.013419
4	6	0	-3.186295	0.057849	1.201765
5	6	0	-2.329187	0.187065	2.456759
6	1	0	-1.677177	0.455517	-0.290205
7	1	0	-3.992030	-0.666291	1.344027
8	1	0	-1.656469	1.047576	2.350032
9	1	0	-2.173379	-2.460867	0.508336
10	8	0	-1.615720	-1.006256	2.722979
11	8	0	-3.728952	1.359786	0.989524
12	8	0	-3.144334	-0.767736	-1.087732
13	6	0	-4.924174	1.462905	0.363801
14	8	0	-5.593481	0.515689	0.058792
15	6	0	-5.244462	2.898354	0.078841
16	1	0	-4.631581	3.195646	-0.775664
17	1	0	-6.298223	2.992988	-0.169742
18	1	0	-4.979542	3.528054	0.926710
19	6	0	-3.501550	0.172889	-1.988582
20	8	0	-3.121990	1.310286	-1.943982
21	6	0	-4.458321	-0.397459	-2.990859
22	1	0	-4.126124	-1.380270	-3.321805
23	1	0	-5.421094	-0.511471	-2.486953
24	1	0	-4.556334	0.287986	-3.828475
25	8	0	-0.607210	-1.827432	-0.685537
26	6	0	-0.005949	-3.043268	-0.720115
27	6	0	1.018295	-3.112876	-1.810425
28	1	0	1.154991	-4.150870	-2.104592
29	1	0	0.729281	-2.493985	-2.657375
30	1	0	1.963063	-2.738076	-1.401146
31	8	0	-0.251978	-3.905921	0.075869
32	1	0	-2.964739	0.367318	3.321850
33	1	0	-0.311187	-2.347635	2.004960
34	7	0	0.347414	-0.450370	1.528197
35	1	0	0.169966	0.547767	1.432325
36	6	0	1.539546	-0.850132	1.086136
37	6	0	2.551807	-0.059448	0.598028
38	6	0	2.314833	1.378552	0.456391
39	8	0	1.293610	1.925086	0.845247
40	8	0	3.273138	2.056757	-0.170304
41	6	0	3.042704	3.464329	-0.332068
42	1	0	2.890729	3.912582	0.651969
43	1	0	2.126789	3.609778	-0.908875
44	6	0	4.257817	4.026513	-1.033838
45	1	0	4.143366	5.102292	-1.177139
46	1	0	5.155573	3.844527	-0.441635
47	1	0	4.386225	3.556462	-2.009868
48	1	0	1.725675	-1.921895	1.127868
49	6	0	3.762522	-0.801543	0.191678
50	8	0	3.778114	-2.002307	0.018193
51	8	0	4.853812	-0.048031	0.056721
52	6	0	6.040627	-0.738202	-0.359999
53	1	0	6.294480	-1.490291	0.390235
54	1	0	5.835751	-1.260532	-1.296898
55	6	0	7.123697	0.305612	-0.513074
56	1	0	6.833097	1.047185	-1.258336
57	1	0	7.296581	0.816853	0.434776
58	1	0	8.055495	-0.164947	-0.831270

Structure 6 (M06-2X, Gas phase)
Energy (Hartrees): = -1445.7204377
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-4.891624	-1.420349	1.039514
2	8	0	1.316687	1.072666	0.493558
3	8	0	-1.132368	1.462633	-0.811676
4	8	0	-1.045382	-2.141478	-0.387354
5	8	0	2.520182	-1.574733	-0.426185
6	8	0	3.070919	1.355655	-0.882489
7	6	0	1.194104	-1.318144	0.035460
8	1	0	1.148271	-1.417192	1.122445
9	8	0	-2.540495	1.899716	0.891968
10	7	0	-2.884303	-0.797404	-0.754640
11	8	0	3.410669	-0.819958	1.494924
12	6	0	-1.476224	-0.918141	-0.928890
13	1	0	-1.257610	-0.875753	-2.004348
14	6	0	-0.757245	0.231448	-0.215327
15	1	0	-1.039800	0.220558	0.839980
16	6	0	0.324522	-2.366302	-0.653901
17	1	0	0.519806	-2.342432	-1.734734
18	1	0	0.564541	-3.358830	-0.277674
19	6	0	-3.714355	-1.089826	0.053893
20	6	0	0.748435	0.087511	-0.366286
21	1	0	1.051321	0.284788	-1.399412
22	6	0	-2.056184	2.216152	-0.152426
23	6	0	-2.359708	3.462021	-0.931433
24	1	0	-1.433223	3.982722	-1.173084
25	1	0	-3.019254	4.097161	-0.346664
26	1	0	-2.841904	3.183878	-1.869915
27	6	0	3.554020	-1.234714	0.379288
28	6	0	2.506236	1.610578	0.145253
29	6	0	3.018885	2.501965	1.234360
30	1	0	2.211397	3.093865	1.662079
31	1	0	3.810932	3.135415	0.843977
32	1	0	3.416724	1.848681	2.015057
33	6	0	4.857296	-1.402246	-0.339636
34	1	0	4.860275	-2.318355	-0.928066
35	1	0	5.673071	-1.391421	0.378293
36	1	0	4.951164	-0.553490	-1.021766

Structure 17 (M06-2X, Gas phase)
Energy (Hartrees): = -1445.7279771
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.626521	-1.007557	2.219246
2	8	0	-1.132169	1.337144	-0.313553
3	8	0	1.626760	1.041163	-0.235192
4	8	0	0.554619	-2.117383	-1.712929
5	8	0	-2.459545	-1.360899	0.129258
6	8	0	-2.076012	1.153921	1.718089
7	6	0	-1.399813	-1.040654	-0.771078
8	1	0	-1.809258	-0.706810	-1.727590
9	8	0	2.954568	1.257720	-2.029365
10	7	0	1.936963	-1.692998	0.136379
11	8	0	-3.821718	0.150921	-0.825494
12	6	0	1.449834	-1.220999	-1.144961
13	1	0	2.293306	-1.141516	-1.829843
14	6	0	0.788025	0.157816	-0.965094
15	1	0	0.602187	0.560665	-1.964416
16	6	0	-0.605021	-2.331596	-0.926375
17	1	0	-0.331713	-2.716423	0.062440
18	1	0	-1.200480	-3.079402	-1.445949
19	6	0	2.670986	-1.358785	1.012641
20	6	0	-0.513633	0.057508	-0.187319
21	1	0	-0.314782	-0.154173	0.867142
22	6	0	2.697561	1.548801	-0.896222
23	6	0	3.478167	2.469987	-0.008681
24	1	0	2.813430	3.221370	0.417409
25	1	0	4.273433	2.936145	-0.583487
26	1	0	3.897043	1.889839	0.816255
27	6	0	-3.612991	-0.659945	0.033170
28	6	0	-1.918436	1.765765	0.698478
29	6	0	-2.582815	3.058526	0.335398
30	1	0	-1.873226	3.735522	-0.137989
31	1	0	-3.018285	3.504440	1.225582
32	1	0	-3.368321	2.823207	-0.386745
33	6	0	-4.535237	-1.007968	1.160986
34	1	0	-4.524591	-2.079669	1.352585
35	1	0	-5.538047	-0.657500	0.931512
36	1	0	-4.155562	-0.495228	2.048342

Structure 17-$^1C_4$ (M06-2X, Gas phase)
Energy (Hartrees): = -1445.7189728
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.791854	-0.368624	-1.966385
2	6	0	-1.375460	-0.684630	-0.595384
3	6	0	-1.185131	0.495722	0.357296
4	6	0	0.237054	1.062573	0.307243
5	6	0	0.661771	1.267474	-1.149666
6	8	0	0.552845	0.069044	-1.872255
7	7	0	2.022465	1.700905	-1.203599
8	6	0	3.093398	1.213593	-1.001169
9	16	0	4.559940	0.690745	-0.762691
10	1	0	0.024417	2.040633	-1.594539
11	8	0	1.170077	0.151789	0.862473
12	6	0	1.227007	0.087333	2.212682
13	8	0	0.517745	0.738730	2.925037
14	6	0	2.279557	-0.888653	2.645477
15	1	0	3.247298	-0.570415	2.254487
16	1	0	2.301543	-0.939024	3.730446
17	1	0	2.055678	-1.867091	2.218370
18	1	0	0.259733	2.008994	0.851737
19	8	0	-2.017723	1.578014	-0.075127
20	6	0	-3.316893	1.533873	0.322281
21	8	0	-3.771669	0.624045	0.949633
22	6	0	-4.053779	2.758959	-0.134029
23	1	0	-5.092286	2.687387	0.176659
24	1	0	-3.587959	3.644127	0.300673
25	1	0	-3.986140	2.845595	-1.219195
26	8	0	-0.703771	-1.789215	0.015294
27	6	0	-1.041471	-3.014242	-0.443596
28	8	0	-1.846981	-3.187530	-1.313700
29	6	0	-0.271204	-4.084281	0.274578
30	1	0	-0.430220	-3.991984	1.349411
31	1	0	-0.597982	-5.058875	-0.076972
32	1	0	0.793548	-3.948807	0.078459
33	1	0	-1.411487	0.402887	-2.443421
34	1	0	-1.445463	0.206583	1.375442
35	1	0	-2.439055	-0.914830	-0.686632
36	1	0	-0.790084	-1.257039	-2.593484

Structure 17-$^4C_1$ (M06-2X, Gas phase)
Energy (Hartrees): = -1445.7233233
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.121174	1.672792	1.298255
2	6	0	0.826257	0.513633	0.971324
3	6	0	0.147524	-0.490939	0.041318
4	6	0	-1.210133	-0.876915	0.603039
5	6	0	-2.042649	0.348674	0.964259
6	1	0	0.336186	2.312427	2.054057
7	1	0	0.052749	-0.061940	-0.959858
8	1	0	-1.072662	-1.501898	1.488835
9	1	0	-2.335500	0.879090	0.050915
10	1	0	1.107469	0.015128	1.902193
11	8	0	-1.317328	1.202709	1.838370
12	8	0	-1.869586	-1.630078	-0.413555
13	8	0	0.898812	-1.702761	-0.017603
14	7	0	-0.337446	2.470836	0.118205
15	6	0	-1.069788	3.187432	-0.479178
16	16	0	-1.991887	4.127183	-1.352237
17	6	0	-2.847538	-2.470265	-0.000931
18	8	0	-3.198422	-2.552833	1.140977
19	6	0	-3.400374	-3.250222	-1.158274
20	1	0	-2.602019	-3.840831	-1.609100
21	1	0	-4.199121	-3.897000	-0.806519
22	1	0	-3.772025	-2.561681	-1.917802
23	6	0	1.863074	-1.812604	-0.957109
24	8	0	2.086273	-0.965691	-1.776933
25	6	0	2.622188	-3.092894	-0.783338
26	1	0	3.279468	-2.959238	0.079294
27	1	0	1.943234	-3.917416	-0.571896
28	1	0	3.214019	-3.287658	-1.673737
29	8	0	1.969536	1.096263	0.362966
30	6	0	3.161824	0.472341	0.517687
31	6	0	4.208514	1.129058	-0.327686
32	1	0	5.193503	0.799584	-0.008033
33	1	0	4.024928	0.815253	-1.358176
34	1	0	4.117601	2.212952	-0.279434
35	8	0	3.312498	-0.492938	1.212902
36	1	0	-2.936139	0.044536	1.504430

Structure 6-$^1C_4$ (M06-2X, Gas phase)
Energy (Hartrees): = -1445.721264
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.270326	-1.148034	-1.653874
2	6	0	0.778556	-1.140503	-0.221029
3	6	0	0.003505	-0.128379	0.622092
4	6	0	-0.139755	1.224058	-0.083960
5	6	0	-0.511795	1.070950	-1.567302
6	8	0	0.301582	0.155228	-2.221765
7	7	0	-1.904241	0.717464	-1.694635
8	6	0	-2.995191	0.641081	-1.244154
9	16	0	-4.482508	0.505843	-0.716995
10	1	0	-0.354840	2.026908	-2.068074
11	8	0	1.108464	1.907073	-0.106511
12	6	0	1.514899	2.457154	1.061370
13	8	0	0.851586	2.435185	2.057958
14	6	0	2.881711	3.057446	0.914237
15	1	0	2.909899	3.714540	0.045308
16	1	0	3.136793	3.600692	1.819869
17	1	0	3.596215	2.249616	0.745414
18	1	0	-0.889092	1.820586	0.441235
19	8	0	-1.331024	-0.600110	0.812140
20	6	0	-1.515979	-1.502616	1.812735
21	8	0	-0.612297	-1.932366	2.467423
22	6	0	-2.968313	-1.847532	1.950320
23	1	0	-3.084641	-2.608364	2.717208
24	1	0	-3.527266	-0.948464	2.214079
25	1	0	-3.356658	-2.197962	0.993297
26	8	0	2.147710	-0.727655	-0.154510
27	6	0	3.064164	-1.648293	-0.524501
28	8	0	2.773627	-2.749214	-0.896657
29	6	0	4.455341	-1.096138	-0.399708
30	1	0	4.658691	-0.863088	0.646672
31	1	0	5.167533	-1.830948	-0.764776
32	1	0	4.530660	-0.171435	-0.972862
33	1	0	-0.751933	-1.543657	-1.669303
34	1	0	0.491326	0.001963	1.588222
35	1	0	0.678587	-2.135398	0.217445
36	1	0	0.902566	-1.771018	-2.281351

Structure 6-$^4C_1$ (M06-2X, Gas phase)
Energy (Hartrees): = -1445.7189728
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.791854	-0.368624	-1.966385
2	6	0	-1.375460	-0.684630	-0.595384
3	6	0	-1.185131	0.495722	0.357296
4	6	0	0.237054	1.062573	0.307243
5	6	0	0.661771	1.267474	-1.149666
6	8	0	0.552845	0.069044	-1.872255
7	7	0	2.022465	1.700905	-1.203599
8	6	0	3.093398	1.213593	-1.001169
9	16	0	4.559940	0.690745	-0.762691
10	1	0	0.024417	2.040633	-1.594539
11	8	0	1.170077	0.151789	0.862473
12	6	0	1.227007	0.087333	2.212682
13	8	0	0.517745	0.738730	2.925037
14	6	0	2.279557	-0.888653	2.645477
15	1	0	3.247298	-0.570415	2.254487
16	1	0	2.301543	-0.939024	3.730446
17	1	0	2.055678	-1.867091	2.218370
18	1	0	0.259733	2.008994	0.851737
19	8	0	-2.017723	1.578014	-0.075127
20	6	0	-3.316893	1.533873	0.322281
21	8	0	-3.771669	0.624045	0.949633
22	6	0	-4.053779	2.758959	-0.134029
23	1	0	-5.092286	2.687387	0.176659
24	1	0	-3.587959	3.644127	0.300673
25	1	0	-3.986140	2.845595	-1.219195
26	8	0	-0.703771	-1.789215	0.015294
27	6	0	-1.041471	-3.014242	-0.443596
28	8	0	-1.846981	-3.187530	-1.313700
29	6	0	-0.271204	-4.084281	0.274578
30	1	0	-0.430220	-3.991984	1.349411
31	1	0	-0.597982	-5.058875	-0.076972
32	1	0	0.793548	-3.948807	0.078459
33	1	0	-1.411487	0.402887	-2.443421
34	1	0	-1.445463	0.206583	1.375442
35	1	0	-2.439055	-0.914830	-0.686632
36	1	0	-0.790084	-1.257039	-2.593484

Structure 17-$^1C_4$ (M06-2X, Chloroform)
Energy (Hartrees): = -1445.7404029
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.719755	0.249898	-1.985403
2	6	0	1.357721	0.629981	-0.658276
3	6	0	1.192413	-0.490413	0.369570
4	6	0	-0.237430	-1.041384	0.409793
5	6	0	-0.710031	-1.328781	-1.017229
6	8	0	-0.627119	-0.173797	-1.812406
7	7	0	-2.079060	-1.746321	-0.997866
8	6	0	-3.159672	-1.259358	-0.904038
9	16	0	-4.645491	-0.730503	-0.795819
10	1	0	-0.100036	-2.134644	-1.439139
11	8	0	-1.140983	-0.079814	0.934988
12	6	0	-1.138410	0.097602	2.273963
13	8	0	-0.414296	-0.517977	3.008117
14	6	0	-2.137654	1.136222	2.673765
15	1	0	-3.134653	0.818147	2.363419
16	1	0	-2.105430	1.280192	3.750695
17	1	0	-1.910086	2.070086	2.156621
18	1	0	-0.256371	-1.952928	1.010011
19	8	0	1.993722	-1.605448	-0.031782
20	6	0	3.307399	-1.568511	0.304675
21	8	0	3.801345	-0.635659	0.873158
22	6	0	4.003716	-2.820899	-0.125696
23	1	0	5.060687	-2.751574	0.118310
24	1	0	3.554316	-3.674685	0.384720
25	1	0	3.870581	-2.964576	-1.199239
26	8	0	0.721064	1.777597	-0.087528
27	6	0	1.081957	2.976633	-0.589118
28	8	0	1.890324	3.098398	-1.469992
29	6	0	0.341864	4.087926	0.088824
30	1	0	0.487259	4.021765	1.168103
31	1	0	0.699386	5.044612	-0.283738
32	1	0	-0.725413	3.981978	-0.116091
33	1	0	1.311100	-0.546509	-2.454486
34	1	0	1.496913	-0.144329	1.357106
35	1	0	2.419519	0.837677	-0.804304
36	1	0	0.691269	1.107190	-2.655259

Structure 17-$^4C_1$ (M06-2X, Chloroform)
Energy (Hartrees): = -1445.7464514
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.679183	1.656272	1.358556
2	6	0	0.635742	0.139893	1.113426
3	6	0	-0.442463	-0.213032	0.090092
4	6	0	-1.754308	0.437958	0.489724
5	6	0	-1.570253	1.929958	0.739088
6	1	0	1.365922	1.880623	2.175443
7	1	0	-0.135471	0.116457	-0.906349
8	1	0	-2.146964	-0.044311	1.388113
9	1	0	-1.300599	2.436446	-0.194648
10	1	0	0.422962	-0.356159	2.063551
11	8	0	-0.567944	2.140655	1.726599
12	8	0	-2.656595	0.237609	-0.598268
13	8	0	-0.680868	-1.621135	0.080549
14	7	0	1.166204	2.328666	0.168000
15	6	0	2.024865	2.302578	-0.650498
16	16	0	3.122396	2.359164	-1.790453
17	6	0	-3.975935	0.252066	-0.304963
18	8	0	-4.394572	0.455154	0.801914
19	6	0	-4.799315	-0.008565	-1.527901
20	1	0	-4.504202	-0.961515	-1.969685
21	1	0	-5.853014	-0.023729	-1.260839
22	1	0	-4.609601	0.774095	-2.264698
23	6	0	0.028897	-2.386756	-0.775047
24	8	0	0.832324	-1.938996	-1.548994
25	6	0	-0.307027	-3.833012	-0.593309
26	1	0	0.072689	-4.148760	0.381366
27	1	0	-1.388212	-3.973058	-0.596806
28	1	0	0.160702	-4.418389	-1.381066
29	8	0	1.930925	-0.217431	0.648141
30	6	0	2.408918	-1.452396	0.933310
31	6	0	3.730093	-1.668155	0.268293
32	1	0	4.168812	-2.598671	0.620180
33	1	0	3.559381	-1.717000	-0.809825
34	1	0	4.393904	-0.826073	0.466869
35	8	0	1.812882	-2.242204	1.612814
36	1	0	-2.487678	2.362668	1.132968

Structure 6-$^1C_4$ (M06-2X, Chloroform)
Energy (Hartrees): = -1445.7424779
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.254521	-1.099444	-1.685665
2	6	0	0.803493	-1.131502	-0.270246
3	6	0	0.036106	-0.164495	0.633440
4	6	0	-0.162268	1.208246	-0.017443
5	6	0	-0.568772	1.101041	-1.494959
6	8	0	0.241957	0.226891	-2.206949
7	7	0	-1.955042	0.709265	-1.586881
8	6	0	-3.067891	0.654728	-1.205659
9	16	0	-4.590597	0.539874	-0.760884
10	1	0	-0.463202	2.078884	-1.965822
11	8	0	1.072470	1.917050	-0.045948
12	6	0	1.480324	2.475237	1.116202
13	8	0	0.828691	2.423681	2.123214
14	6	0	2.819122	3.123732	0.957067
15	1	0	2.820268	3.773749	0.081622
16	1	0	3.060181	3.687164	1.855078
17	1	0	3.566306	2.342905	0.797165
18	1	0	-0.912036	1.771618	0.541765
19	8	0	-1.277130	-0.683449	0.855019
20	6	0	-1.399741	-1.616920	1.832248
21	8	0	-0.461449	-2.010899	2.467109
22	6	0	-2.823229	-2.050079	1.984792
23	1	0	-2.886472	-2.824322	2.745378
24	1	0	-3.432360	-1.190387	2.270022
25	1	0	-3.198316	-2.422908	1.030217
26	8	0	2.167109	-0.696250	-0.235876
27	6	0	3.095764	-1.592239	-0.628459
28	8	0	2.817645	-2.703931	-0.989779
29	6	0	4.473418	-1.011326	-0.543123
30	1	0	4.698254	-0.768896	0.497541
31	1	0	5.195324	-1.729856	-0.923174
32	1	0	4.515190	-0.087170	-1.121642
33	1	0	-0.757607	-1.520135	-1.691053
34	1	0	0.556082	-0.052800	1.585070
35	1	0	0.732511	-2.143832	0.132253
36	1	0	0.881307	-1.683470	-2.355618

Structure 6-$^4C_1$ (M06-2X, Chloroform)
Energy (Hartrees): = -1445.7430469
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.861070	-1.691099	-0.406825
2	6	0	-0.628243	-0.263928	0.104030
3	6	0	0.782385	0.200909	-0.254189
4	6	0	1.802872	-0.848539	0.148358
5	6	0	1.399195	-2.223265	-0.375393
6	1	0	-0.848348	-1.700635	-1.505756
7	1	0	0.842908	0.398998	-1.327929
8	1	0	1.897145	-0.879448	1.236154
9	1	0	1.416095	-2.223457	-1.473372
10	1	0	-0.772426	-0.236733	1.186871
11	8	0	0.107480	-2.559509	0.105601
12	8	0	3.044078	-0.448747	-0.433774
13	8	0	1.107836	1.384929	0.474185
14	7	0	-2.139605	-2.154035	0.031132
15	6	0	-3.281013	-1.838592	0.096997
16	16	0	-4.825634	-1.517883	0.230503
17	6	0	4.169088	-0.930999	0.140926
18	8	0	4.150224	-1.684562	1.075347
19	6	0	5.389880	-0.396648	-0.540736
20	1	0	5.414740	0.689347	-0.433569
21	1	0	6.278148	-0.837199	-0.095178
22	1	0	5.345235	-0.625930	-1.606451
23	6	0	0.831885	2.582432	-0.084988
24	8	0	0.365639	2.703676	-1.186265
25	6	0	1.153519	3.693181	0.863514
26	1	0	0.424502	3.659055	1.676970
27	1	0	2.145940	3.552228	1.292068
28	1	0	1.085886	4.647389	0.346827
29	8	0	-1.608464	0.534016	-0.550388
30	6	0	-2.103489	1.614956	0.102700
31	6	0	-3.063387	2.359610	-0.767474
32	1	0	-3.571419	3.122068	-0.182308
33	1	0	-2.492994	2.827659	-1.573617
34	1	0	-3.781509	1.671194	-1.213784
35	8	0	-1.770418	1.912137	1.216442
36	1	0	2.082735	-2.983795	-0.003599

Structure 17-$^4C_1$ (M06-2X, Ethanol)
Energy (Hartrees): = -1445.7525158
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.671214	1.682517	1.347305
2	6	0	0.633150	0.164680	1.114693
3	6	0	-0.437990	-0.201016	0.090651
4	6	0	-1.755547	0.432381	0.496090
5	6	0	-1.585189	1.930263	0.717538
6	1	0	1.351242	1.914862	2.166804
7	1	0	-0.142492	0.135980	-0.906667
8	1	0	-2.130430	-0.044986	1.404363
9	1	0	-1.318646	2.420503	-0.225354
10	1	0	0.418781	-0.318550	2.070559
11	8	0	-0.583384	2.166061	1.703041
12	8	0	-2.663964	0.203137	-0.582786
13	8	0	-0.655384	-1.614872	0.076031
14	7	0	1.163010	2.351083	0.155523
15	6	0	2.000946	2.285052	-0.681102
16	16	0	3.080539	2.294292	-1.841442
17	6	0	-3.981010	0.209733	-0.289874
18	8	0	-4.398740	0.419252	0.819903
19	6	0	-4.807168	-0.064240	-1.504658
20	1	0	-4.491481	-1.007176	-1.953911
21	1	0	-5.858337	-0.104938	-1.230083
22	1	0	-4.640363	0.728975	-2.236238
23	6	0	0.056953	-2.367935	-0.785813
24	8	0	0.863077	-1.904312	-1.552501
25	6	0	-0.275514	-3.815796	-0.631983
26	1	0	0.075101	-4.145632	0.349112
27	1	0	-1.356475	-3.955698	-0.669387
28	1	0	0.215057	-4.389253	-1.414669
29	8	0	1.932529	-0.195700	0.658052
30	6	0	2.420877	-1.415945	0.971925
31	6	0	3.768112	-1.619486	0.361851
32	1	0	4.201923	-2.545597	0.731033
33	1	0	3.645252	-1.669725	-0.723069
34	1	0	4.412926	-0.769874	0.590149
35	8	0	1.810915	-2.211222	1.638147
36	1	0	-2.505157	2.364854	1.102943

Structure 17-$^1C_4$ (M06-2X, Ethanol)
Energy (Hartrees): = -1445.7470627
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.730353	0.210489	-1.987154
2	6	0	1.349856	0.625154	-0.663180
3	6	0	1.197451	-0.480722	0.383384
4	6	0	-0.223973	-1.052764	0.426399
5	6	0	-0.686210	-1.371920	-0.996145
6	8	0	-0.616563	-0.223020	-1.807904
7	7	0	-2.052228	-1.803621	-0.976810
8	6	0	-3.132511	-1.315725	-0.881593
9	16	0	-4.617177	-0.783039	-0.773540
10	1	0	-0.064890	-2.173442	-1.406280
11	8	0	-1.138390	-0.082502	0.924131
12	6	0	-1.147840	0.134897	2.255068
13	8	0	-0.441884	-0.476588	3.014942
14	6	0	-2.120317	1.208961	2.615917
15	1	0	-3.122502	0.910904	2.301931
16	1	0	-2.096224	1.381942	3.688842
17	1	0	-1.855355	2.120254	2.075494
18	1	0	-0.240603	-1.951097	1.045424
19	8	0	2.020447	-1.586768	0.003101
20	6	0	3.329771	-1.523246	0.336096
21	8	0	3.801570	-0.581847	0.917330
22	6	0	4.063873	-2.740941	-0.120974
23	1	0	5.093734	-2.695552	0.224274
24	1	0	3.569817	-3.634406	0.263114
25	1	0	4.035616	-2.781907	-1.212045
26	8	0	0.677231	1.768985	-0.119060
27	6	0	1.017792	2.971118	-0.620112
28	8	0	1.850214	3.104943	-1.481356
29	6	0	0.233317	4.069568	0.022491
30	1	0	0.373169	4.032579	1.104126
31	1	0	0.561000	5.029741	-0.368431
32	1	0	-0.827454	3.919624	-0.188153
33	1	0	1.330581	-0.592059	-2.431733
34	1	0	1.490553	-0.112716	1.366327
35	1	0	2.407992	0.853429	-0.802226
36	1	0	0.694628	1.051827	-2.677019

Structure 6-$^1C_4$ (M06-2X, Ethanol)
Energy (Hartrees): = -1445.7486354
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.265271	-1.075808	-1.711929
2	6	0	0.799567	-1.128711	-0.292644
3	6	0	0.021665	-0.178199	0.620736
4	6	0	-0.173245	1.204316	-0.009576
5	6	0	-0.566680	1.125360	-1.491022
6	8	0	0.259298	0.262771	-2.209041
7	7	0	-1.949515	0.729014	-1.609677
8	6	0	-3.051282	0.679317	-1.193524
9	16	0	-4.563068	0.571248	-0.714023
10	1	0	-0.457721	2.111011	-1.943417
11	8	0	1.070895	1.901012	-0.020408
12	6	0	1.474085	2.458017	1.141449
13	8	0	0.803775	2.423720	2.140838
14	6	0	2.826746	3.074345	1.000584
15	1	0	2.848034	3.731068	0.130159
16	1	0	3.075720	3.624880	1.904480
17	1	0	3.553627	2.274576	0.837815
18	1	0	-0.922265	1.766639	0.550825
19	8	0	-1.292154	-0.705402	0.823947
20	6	0	-1.424445	-1.654932	1.778311
21	8	0	-0.489267	-2.058099	2.418979
22	6	0	-2.843936	-2.099218	1.910750
23	1	0	-2.908455	-2.888680	2.655643
24	1	0	-3.458862	-1.248056	2.209693
25	1	0	-3.206853	-2.456049	0.945340
26	8	0	2.162208	-0.684038	-0.244847
27	6	0	3.105786	-1.571160	-0.612782
28	8	0	2.841829	-2.692911	-0.965269
29	6	0	4.475210	-0.980211	-0.515159
30	1	0	4.685610	-0.736366	0.528379
31	1	0	5.207054	-1.692998	-0.887511
32	1	0	4.514074	-0.055557	-1.093270
33	1	0	-0.745978	-1.496644	-1.736041
34	1	0	0.534445	-0.079641	1.577964
35	1	0	0.731952	-2.146718	0.094140
36	1	0	0.900178	-1.645642	-2.386867

Structure 6-$^4C_1$ (M06-2X, Ethanol)
Energy (Hartrees): = -1445.7497131
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.854438	-1.696023	-0.439194
2	6	0	-0.629164	-0.273847	0.085406
3	6	0	0.779636	0.198813	-0.262415
4	6	0	1.800344	-0.845330	0.150512
5	6	0	1.413025	-2.216639	-0.393509
6	1	0	-0.836643	-1.702010	-1.536756
7	1	0	0.851967	0.394271	-1.335511
8	1	0	1.877970	-0.880395	1.239340
9	1	0	1.434820	-2.203371	-1.490147
10	1	0	-0.779236	-0.258837	1.167336
11	8	0	0.117163	-2.564228	0.076163
12	8	0	3.047276	-0.430622	-0.412260
13	8	0	1.091523	1.387259	0.470970
14	7	0	-2.132232	-2.169579	-0.004316
15	6	0	-3.266264	-1.835386	0.093523
16	16	0	-4.804187	-1.499543	0.266020
17	6	0	4.170063	-0.909289	0.162633
18	8	0	4.147763	-1.660755	1.103288
19	6	0	5.392607	-0.390917	-0.522947
20	1	0	5.373641	0.700124	-0.525745
21	1	0	6.280753	-0.754546	-0.012104
22	1	0	5.390205	-0.729340	-1.560970
23	6	0	0.829048	2.584251	-0.090707
24	8	0	0.361284	2.703807	-1.194840
25	6	0	1.164909	3.697636	0.846408
26	1	0	0.467197	3.655135	1.686637
27	1	0	2.174329	3.566772	1.237683
28	1	0	1.069444	4.651167	0.332772
29	8	0	-1.609540	0.531358	-0.565475
30	6	0	-2.124161	1.590240	0.101814
31	6	0	-3.098509	2.334698	-0.749336
32	1	0	-3.611959	3.081835	-0.149099
33	1	0	-2.542184	2.822638	-1.553990
34	1	0	-3.810251	1.642359	-1.200142
35	8	0	-1.793834	1.876061	1.222942
36	1	0	2.096913	-2.978348	-0.024829

Structure 17-$^4C_1$ (M06-2X, Gas phase, NBO)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.121174	1.672792	1.298255
2	6	0	0.826257	0.513633	0.971324
3	6	0	0.147524	-0.490939	0.041318
4	6	0	-1.210133	-0.876915	0.603039
5	6	0	-2.042649	0.348674	0.964259
6	1	0	0.336186	2.312427	2.054057
7	1	0	0.052749	-0.061940	-0.959858
8	1	0	-1.072662	-1.501898	1.488835
9	1	0	-2.335500	0.879090	0.050915
10	1	0	1.107469	0.015128	1.902193
11	8	0	-1.317328	1.202709	1.838370
12	8	0	-1.869586	-1.630078	-0.413555
13	8	0	0.898812	-1.702761	-0.017603
14	7	0	-0.337446	2.470836	0.118205
15	6	0	-1.069788	3.187432	-0.479178
16	16	0	-1.991888	4.127183	-1.352237
17	6	0	-2.847538	-2.470265	-0.000931
18	8	0	-3.198422	-2.552834	1.140977
19	6	0	-3.400373	-3.250223	-1.158274
20	1	0	-2.602018	-3.840831	-1.609100
21	1	0	-4.199120	-3.897001	-0.806519
22	1	0	-3.772025	-2.561682	-1.917802
23	6	0	1.863074	-1.812604	-0.957109
24	8	0	2.086273	-0.965691	-1.776933
25	6	0	2.622189	-3.092894	-0.783338
26	1	0	3.279469	-2.959237	0.079294
27	1	0	1.943235	-3.917416	-0.571896
28	1	0	3.214020	-3.287657	-1.673737
29	8	0	1.969536	1.096263	0.362966
30	6	0	3.161824	0.472342	0.517687
31	6	0	4.208514	1.129059	-0.327686
32	1	0	5.193503	0.799585	-0.008033
33	1	0	4.024928	0.815254	-1.358176
34	1	0	4.117601	2.212953	-0.279434
35	8	0	3.312498	-0.492937	1.212902
36	1	0	-2.936139	0.044536	1.504430

Structure 17-$^{1}C_{4}$ (M06-2X, Gas phase, NBO)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.791854	0.368624	-1.966385
2	6	0	1.375460	0.684630	-0.595384
3	6	0	1.185131	-0.495722	0.357296
4	6	0	-0.237054	-1.062573	0.307243
5	6	0	-0.661771	-1.267474	-1.149666
6	8	0	-0.552845	-0.069044	-1.872255
7	7	0	-2.022465	-1.700905	-1.203599
8	6	0	-3.093398	-1.213593	-1.001169
9	16	0	-4.559940	-0.690745	-0.762691
10	1	0	-0.024417	-2.040633	-1.594539
11	8	0	-1.170077	-0.151789	0.862473
12	6	0	-1.227007	-0.087333	2.212682
13	8	0	-0.517745	-0.738730	2.925037
14	6	0	-2.279557	0.888653	2.645477
15	1	0	-3.247298	0.570415	2.254487
16	1	0	-2.301543	0.939024	3.730446
17	1	0	-2.055678	1.867091	2.218370
18	1	0	-0.259733	-2.008994	0.851737
19	8	0	2.017723	-1.578014	-0.075127
20	6	0	3.316893	-1.533873	0.322281
21	8	0	3.771669	-0.624045	0.949633
22	6	0	4.053779	-2.758959	-0.134029
23	1	0	5.092286	-2.687387	0.176659
24	1	0	3.587959	-3.644127	0.300673
25	1	0	3.986140	-2.845595	-1.219195
26	8	0	0.703771	1.789215	0.015294
27	6	0	1.041471	3.014242	-0.443596
28	8	0	1.846981	3.187530	-1.313700
29	6	0	0.271204	4.084281	0.274578
30	1	0	0.430220	3.991984	1.349411
31	1	0	0.597981	5.058875	-0.076972
32	1	0	-0.793548	3.948807	0.078459
33	1	0	1.411487	-0.402887	-2.443421
34	1	0	1.445463	-0.206583	1.375442
35	1	0	2.439055	0.914830	-0.686632
36	1	0	0.790084	1.257039	-2.593484

Structure 6-$^4C_1$ (M06-2X, Gas phase, NBO)

Standard orientation:

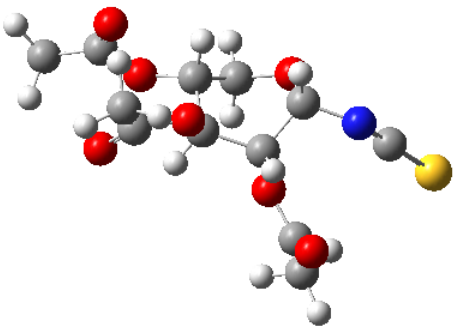
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.824985	-1.729157	-0.351799
2	6	0	-0.617692	-0.290096	0.134959
3	6	0	0.778894	0.202048	-0.244081
4	6	0	1.827598	-0.820245	0.154360
5	6	0	1.443524	-2.214904	-0.332085
6	1	0	-0.807753	-1.745986	-1.452624
7	1	0	0.819755	0.393157	-1.320727
8	1	0	1.944189	-0.831407	1.240591
9	1	0	1.455326	-2.236559	-1.431269
10	1	0	-0.750755	-0.245789	1.219020
11	8	0	0.167111	-2.567868	0.163952
12	8	0	3.048628	-0.404051	-0.455847
13	8	0	1.088546	1.398897	0.465661
14	7	0	-2.092655	-2.213364	0.087794
15	6	0	-3.232116	-1.866738	0.096768
16	16	0	-4.764289	-1.498127	0.154685
17	6	0	4.190609	-0.860130	0.111685
18	8	0	4.201419	-1.621846	1.035047
19	6	0	5.392835	-0.278057	-0.573320
20	1	0	5.386183	0.805641	-0.448798
21	1	0	6.294028	-0.702358	-0.139776
22	1	0	5.344782	-0.488874	-1.641962
23	6	0	0.747276	2.580110	-0.098768
24	8	0	0.271267	2.674739	-1.195528
25	6	0	1.004072	3.707676	0.853525
26	1	0	0.228438	3.659691	1.621658
27	1	0	1.972475	3.587878	1.337212
28	1	0	0.943241	4.653428	0.321822
29	8	0	-1.621162	0.473311	-0.520277
30	6	0	-2.125476	1.558039	0.123997
31	6	0	-3.107230	2.270417	-0.751899
32	1	0	-3.629995	3.024772	-0.170403
33	1	0	-2.541623	2.741807	-1.558997
34	1	0	-3.806915	1.558179	-1.188470
35	8	0	-1.779126	1.882484	1.223474
36	1	0	2.148502	-2.949108	0.051305

Structure 6-$^1C_4$ (M06-2X, Gas phase, NBO)

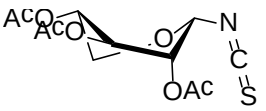
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.270326	-1.148034	-1.653874
2	6	0	0.778556	-1.140503	-0.221029
3	6	0	0.003505	-0.128379	0.622092
4	6	0	-0.139755	1.224058	-0.083960
5	6	0	-0.511795	1.070950	-1.567302
6	8	0	0.301582	0.155228	-2.221765
7	7	0	-1.904241	0.717464	-1.694635
8	6	0	-2.995191	0.641081	-1.244154
9	16	0	-4.482508	0.505843	-0.716995
10	1	0	-0.354840	2.026908	-2.068074
11	8	0	1.108464	1.907073	-0.106511
12	6	0	1.514899	2.457154	1.061370
13	8	0	0.851586	2.435185	2.057958
14	6	0	2.881711	3.057446	0.914237
15	1	0	2.909899	3.714540	0.045308
16	1	0	3.136793	3.600692	1.819869
17	1	0	3.596215	2.249616	0.745414
18	1	0	-0.889092	1.820586	0.441235
19	8	0	-1.331024	-0.600110	0.812140
20	6	0	-1.515979	-1.502616	1.812735
21	8	0	-0.612297	-1.932366	2.467423
22	6	0	-2.968313	-1.847532	1.950320
23	1	0	-3.084641	-2.608364	2.717208
24	1	0	-3.527266	-0.948464	2.214079
25	1	0	-3.356658	-2.197962	0.993297
26	8	0	2.147710	-0.727655	-0.154510
27	6	0	3.064164	-1.648293	-0.524501
28	8	0	2.773627	-2.749214	-0.896657
29	6	0	4.455341	-1.096138	-0.399708
30	1	0	4.658691	-0.863088	0.646672
31	1	0	5.167533	-1.830948	-0.764776
32	1	0	4.530660	-0.171435	-0.972862
33	1	0	-0.751933	-1.543657	-1.669303
34	1	0	0.491326	0.001963	1.588222
35	1	0	0.678587	-2.135398	0.217445
36	1	0	0.902566	-1.771018	-2.281351

17 $^4S_2$ (gas phase)



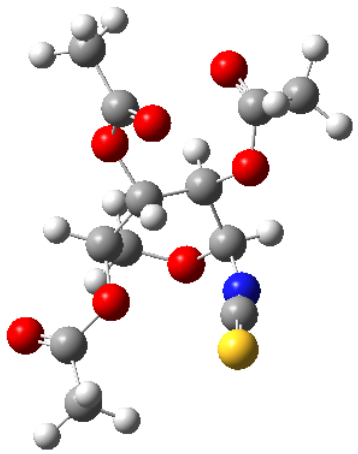
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.735612	Hartree
Zero-point Energy Correction	0.276682	Hartree
Thermal Correction to Energy	0.298511	Hartree
Thermal Correction to Enthalpy	0.299455	Hartree
Thermal Correction to Free Energy	0.222551	Hartree
EE + Zero-point Energy	-1445.458929	Hartree
EE + Thermal Energy Correction	-1445.437100	Hartree
EE + Thermal Enthalpy Correction	-1445.436156	Hartree
EE + Thermal Free Energy Correction	-1445.513061	Hartree
E (Thermal)	187.319	kcal/mol
Heat Capacity (Cv)	76.404	cal/mol-kelvin
Entropy (S)	161.859	cal/mol-kelvin



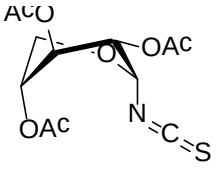
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.037219	-1.971763	-0.334890
2	6	0	-1.156520	-0.572494	1.219456
3	6	0	-0.649144	0.556476	0.314788
4	6	0	0.835473	0.364436	-0.017601
5	6	0	1.231833	-1.111657	0.045384
6	1	0	1.557736	-1.358263	1.059398
7	1	0	-0.347533	-1.682435	-1.317861
8	1	0	-0.793532	1.513621	0.815723
9	1	0	1.020228	0.744831	-1.023868
10	1	0	0.324595	-3.021739	-0.355397
11	1	0	-0.624565	-0.509233	2.174721
12	8	0	-0.978689	-1.852272	0.654463
13	7	0	-2.550764	-0.384840	1.483022
14	6	0	-3.597594	-0.616887	0.960544
15	16	0	-5.033496	-0.865345	0.362501
16	8	0	-1.393074	0.518836	-0.897990
17	6	0	-2.326092	1.496962	-1.099416
18	8	0	-2.490018	2.406933	-0.342429
19	6	0	-3.081543	1.239967	-2.367813
20	1	0	-3.735020	2.083599	-2.572272
21	1	0	-2.385961	1.078554	-3.191470
22	1	0	-3.674977	0.332463	-2.239415
23	8	0	1.586010	1.118998	0.934370
24	6	0	2.760631	1.649050	0.510146
25	8	0	3.121209	1.603546	-0.633550
26	6	0	3.526365	2.236190	1.653644
27	1	0	2.860266	2.739508	2.352404
28	1	0	4.009378	1.403220	2.171173
29	1	0	4.284900	2.914652	1.272089
30	8	0	2.282239	-1.389649	-0.875734
31	6	0	3.552801	-1.267460	-0.419763
32	8	0	3.817421	-1.048958	0.730559
33	6	0	4.537786	-1.395737	-1.539182
34	1	0	4.223008	-2.155589	-2.252440
35	1	0	4.562895	-0.429306	-2.049490
36	1	0	5.521803	-1.616451	-1.133768

17 ^4S_o (gas phase)



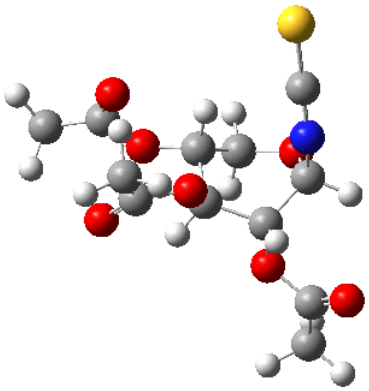
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.738404	Hartree
Zero-point Energy Correction	0.276704	Hartree
Thermal Correction to Energy	0.298471	Hartree
Thermal Correction to Enthalpy	0.299415	Hartree
Thermal Correction to Free Energy	0.223362	Hartree
EE + Zero-point Energy	-1445.461700	Hartree
EE + Thermal Energy Correction	-1445.439933	Hartree
EE + Thermal Enthalpy Correction	-1445.438989	Hartree
EE + Thermal Free Energy Correction	-1445.515042	Hartree
E (Thermal)	187.294	kcal/mol
Heat Capacity (Cv)	76.552	cal/mol-kelvin
Entropy (S)	160.067	cal/mol-kelvin



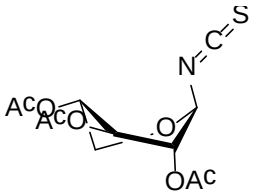
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.324501	0.692935	-0.083718
2	6	0	0.994122	1.380025	0.296215
3	6	0	1.178793	1.417738	1.803261
4	6	0	0.298607	-0.828826	1.838456
5	6	0	-0.848152	-0.169421	1.068764
6	1	0	2.142046	1.852254	2.061536
7	1	0	0.989274	2.401875	-0.087378
8	1	0	-1.402325	0.463397	1.767881
9	1	0	-0.178059	0.076268	-0.972924
10	1	0	-0.112347	-1.422417	2.655832
11	1	0	0.385473	2.043110	2.230205
12	8	0	1.152567	0.122293	2.402727
13	8	0	-1.686761	-1.210773	0.593923
14	8	0	-1.270574	1.729561	-0.357192
15	8	0	2.037083	0.633617	-0.331555
16	6	0	-3.018828	-0.960321	0.519126
17	6	0	-2.249438	1.463179	-1.256977
18	6	0	3.240005	1.239960	-0.455716
19	8	0	-3.517364	0.046541	0.941136
20	8	0	3.439699	2.365683	-0.091303
21	8	0	-2.296628	0.444416	-1.888819
22	6	0	-3.726665	-2.073259	-0.185452
23	1	0	-3.323707	-3.040110	0.111756
24	1	0	-4.793338	-2.009733	0.012834
25	1	0	-3.541378	-1.936630	-1.254124
26	6	0	-3.248583	2.576802	-1.302081
27	1	0	-2.757164	3.545721	-1.230794
28	1	0	-3.837141	2.498764	-2.212470
29	1	0	-3.900499	2.452784	-0.433411
30	6	0	4.233177	0.314133	-1.090747
31	1	0	3.841469	-0.048260	-2.041880
32	1	0	5.175506	0.836387	-1.231861
33	1	0	4.371131	-0.556605	-0.446977
34	7	0	1.024907	-1.734729	0.988917
35	6	0	1.353991	-2.179736	-0.054865
36	16	0	1.850461	-2.831479	-1.411223

6 $^4S_2$ (gas phase)



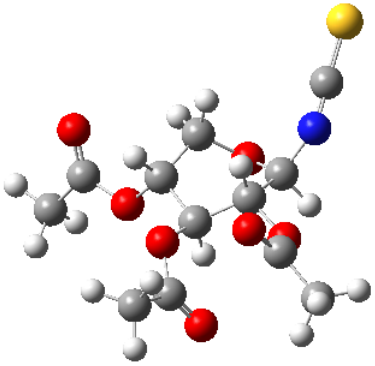
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.737842	Hartree
Zero-point Energy Correction	0.276809	Hartree
Thermal Correction to Energy	0.298678	Hartree
Thermal Correction to Enthalpy	0.299622	Hartree
Thermal Correction to Free Energy	0.220961	Hartree
EE + Zero-point Energy	-1445.461033	Hartree
EE + Thermal Energy Correction	-1445.439164	Hartree
EE + Thermal Enthalpy Correction	-1445.438220	Hartree
EE + Thermal Free Energy Correction	-1445.516882	Hartree
E (Thermal)	187.423	kcal/mol
Heat Capacity (Cv)	76.474	cal/mol-kelvin
Entropy (S)	165.558	cal/mol-kelvin



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.542557	0.094316	-2.044588
2	6	0	1.678808	1.257371	-0.262688
3	6	0	1.518569	-0.068054	0.490274
4	6	0	0.122112	-0.669394	0.296044
5	6	0	-0.529787	-0.178374	-0.999706
6	1	0	-1.122782	0.716881	-0.802331
7	1	0	1.104078	-0.824631	-2.241437
8	1	0	1.713464	0.095265	1.550288
9	1	0	0.222520	-1.755728	0.249660
10	1	0	0.079435	0.434987	-2.969440
11	8	0	1.438768	1.126325	-1.633344
12	8	0	2.446264	-1.013002	-0.047780
13	6	0	3.735283	-0.899434	0.358906
14	8	0	4.099559	-0.057906	1.129980
15	6	0	4.592477	-1.948465	-0.284647
16	1	0	5.607400	-1.863922	0.093723
17	1	0	4.185905	-2.937655	-0.072427
18	1	0	4.580705	-1.807798	-1.366597
19	8	0	-0.674660	-0.305267	1.421231
20	6	0	-1.620048	-1.192408	1.818776
21	8	0	-1.712973	-2.298443	1.360722
22	6	0	-2.521543	-0.581986	2.844673
23	1	0	-1.957868	0.038623	3.539333
24	1	0	-3.224589	0.056929	2.303500
25	1	0	-3.065984	-1.365970	3.364337
26	8	0	-1.374024	-1.192173	-1.542944
27	6	0	-2.674274	-1.188051	-1.156785
28	8	0	-3.153778	-0.323064	-0.478145
29	6	0	-3.380801	-2.412273	-1.649931
30	1	0	-3.048314	-2.680233	-2.651273
31	1	0	-3.118433	-3.224494	-0.966893
32	1	0	-4.454811	-2.247956	-1.620264
33	7	0	0.795181	2.215100	0.361040
34	6	0	-0.139751	2.925107	0.169682
35	16	0	-1.391110	3.869178	0.003388
36	1	0	2.695919	1.631270	-0.149475

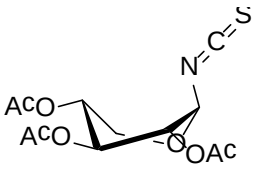
6 ^4S_o (gas phase)



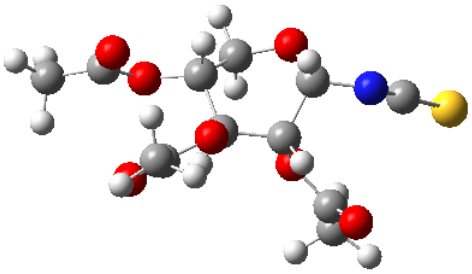
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.738421	Hartree
Zero-point Energy Correction	0.276764	Hartree
Thermal Correction to Energy	0.298641	Hartree
Thermal Correction to Enthalpy	0.299585	Hartree
Thermal Correction to Free Energy	0.220449	Hartree
EE + Zero-point Energy	-1445.461656	Hartree
EE + Thermal Energy Correction	-1445.439779	Hartree
EE + Thermal Enthalpy Correction	-1445.438835	Hartree
EE + Thermal Free Energy Correction	-1445.517971	Hartree
E (Thermal)	187.400	kcal/mol
Heat Capacity (Cv)	76.363	cal/mol-kelvin
Entropy (S)	166.555	cal/mol-kelvin

Standard orientation:

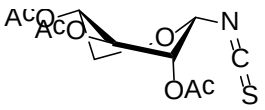
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.831563	0.126337	-0.218722
2	6	0	-0.399295	1.500144	0.288579
3	6	0	1.092356	1.729581	0.052132
4	6	0	1.529353	-0.360902	-0.906945
5	6	0	0.326108	-0.862501	-0.077478
6	1	0	1.299854	2.782104	-0.124108
7	1	0	-0.621260	1.577152	1.354750
8	1	0	0.589512	-0.975597	0.977478
9	1	0	-1.136954	0.189159	-1.265934
10	1	0	1.668108	1.410081	0.929027
11	8	0	1.517401	1.018861	-1.101890
12	8	0	0.020559	-2.134820	-0.632705
13	8	0	-1.943531	-0.251627	0.589554
14	8	0	-1.205532	2.446203	-0.420885
15	6	0	-0.579448	-3.062949	0.149943
16	6	0	-2.863205	-1.101474	0.081266
17	6	0	-1.273155	3.685170	0.112138
18	8	0	-0.826809	-2.883404	1.309864
19	8	0	-0.670331	4.000425	1.101281
20	8	0	-2.822560	-1.524613	-1.041426
21	6	0	-0.905984	-4.286129	-0.650540
22	1	0	-0.042574	-4.596754	-1.238007
23	1	0	-1.228598	-5.080599	0.016979
24	1	0	-1.711312	-4.022144	-1.340009
25	6	0	-3.883393	-1.450752	1.122192
26	1	0	-4.228779	-0.552999	1.633700
27	1	0	-4.711961	-1.977508	0.656344
28	1	0	-3.394298	-2.094273	1.857350
29	6	0	-2.178308	4.570678	-0.693009
30	1	0	-3.182290	4.144733	-0.710049
31	1	0	-2.196064	5.563321	-0.251625
32	1	0	-1.820504	4.617783	-1.722261
33	7	0	2.749974	-0.812213	-0.277148
34	6	0	3.827530	-0.427522	0.056060
35	16	0	5.266887	-0.012912	0.546103
36	1	0	1.477556	-0.818660	-1.895278



17 $^4S_2$ (chloroform)



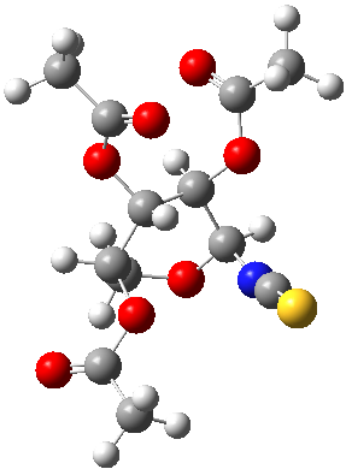
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.756587	Hartree
Zero-point Energy Correction	0.275800	Hartree
Thermal Correction to Energy	0.297898	Hartree
Thermal Correction to Enthalpy	0.298843	Hartree
Thermal Correction to Free Energy	0.220416	Hartree
EE + Zero-point Energy	-1445.480787	Hartree
EE + Thermal Energy Correction	-1445.458689	Hartree
EE + Thermal Enthalpy Correction	-1445.457745	Hartree
EE + Thermal Free Energy Correction	-1445.536171	Hartree
E (Thermal)	186.934	kcal/mol
Heat Capacity (Cv)	76.657	cal/mol-kelvin
Entropy (S)	165.062	cal/mol-kelvin



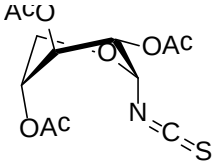
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.093351	-1.999874	0.269776
2	6	0	1.144772	-0.571808	-1.226583
3	6	0	0.646203	0.539798	-0.296992
4	6	0	-0.844142	0.361341	0.023499
5	6	0	-1.265770	-1.103294	-0.094665
6	1	0	-1.586016	-1.313215	-1.118128
7	1	0	0.282474	-1.758526	1.269033
8	1	0	0.807240	1.505489	-0.775283
9	1	0	-1.019070	0.709120	1.043057
10	1	0	-0.401750	-3.043980	0.244391
11	1	0	0.634857	-0.471996	-2.189434
12	8	0	0.944637	-1.864449	-0.700120
13	7	0	2.550053	-0.406575	-1.454700
14	6	0	3.614553	-0.592291	-0.963062
15	16	0	5.080698	-0.785240	-0.402033
16	8	0	1.376000	0.460920	0.924710
17	6	0	2.351692	1.382348	1.151046
18	8	0	2.608289	2.262162	0.376982
19	6	0	3.008122	1.140963	2.472694
20	1	0	3.902995	1.753811	2.549717
21	1	0	2.305922	1.410242	3.265574
22	1	0	3.253581	0.084322	2.582737
23	8	0	-1.575493	1.169912	-0.900281
24	6	0	-2.729044	1.727786	-0.464286
25	8	0	-3.116832	1.619449	0.669070
26	6	0	-3.422000	2.456539	-1.569595
27	1	0	-2.723100	3.118913	-2.081500
28	1	0	-3.782852	1.719853	-2.291414
29	1	0	-4.260845	3.019053	-1.167190
30	8	0	-2.324252	-1.399453	0.814011
31	6	0	-3.593615	-1.274708	0.364695
32	8	0	-3.858871	-0.985226	-0.772518
33	6	0	-4.577053	-1.521740	1.462678
34	1	0	-4.308320	-2.418582	2.021183
35	1	0	-4.539537	-0.670327	2.147130
36	1	0	-5.577137	-1.611181	1.045474

17 ^4S_o (chloroform)



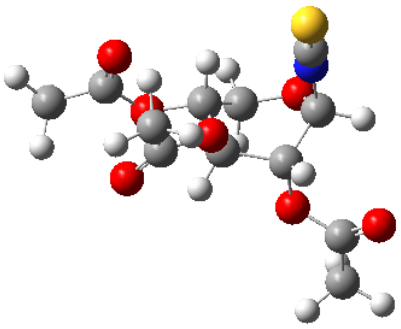
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.760020	Hartree
Zero-point Energy Correction	0.275930	Hartree
Thermal Correction to Energy	0.297864	Hartree
Thermal Correction to Enthalpy	0.298808	Hartree
Thermal Correction to Free Energy	0.221880	Hartree
EE + Zero-point Energy	-1445.484090	Hartree
EE + Thermal Energy Correction	-1445.462156	Hartree
EE + Thermal Enthalpy Correction	-1445.461212	Hartree
EE + Thermal Free Energy Correction	-1445.538140	Hartree
E (Thermal)	186.913	kcal/mol
Heat Capacity (Cv)	76.709	cal/mol-kelvin
Entropy (S)	161.908	cal/mol-kelvin



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.276436	-0.738339	-0.071559
2	6	0	-1.060398	-1.391245	0.308881
3	6	0	-1.259227	-1.402308	1.812992
4	6	0	-0.321631	0.820101	1.825462
5	6	0	0.814200	0.120140	1.076303
6	1	0	-2.233562	-1.809951	2.075250
7	1	0	-1.076614	-2.417015	-0.062500
8	1	0	1.340673	-0.514576	1.793725
9	1	0	0.144436	-0.126240	-0.965713
10	1	0	0.091660	1.426502	2.632214
11	1	0	-0.482531	-2.032255	2.260809
12	8	0	-1.213600	-0.091594	2.387957
13	8	0	1.679394	1.140157	0.597383
14	8	0	1.199642	-1.797233	-0.340484
15	8	0	-2.083751	-0.624153	-0.334622
16	6	0	3.008534	0.878463	0.552869
17	6	0	2.171962	-1.572926	-1.254391
18	6	0	-3.291918	-1.203679	-0.488833
19	8	0	3.482808	-0.147072	0.963980
20	8	0	-3.519144	-2.335345	-0.147367
21	8	0	2.258492	-0.546921	-1.875816
22	6	0	3.750529	2.008143	-0.081840
23	1	0	3.432958	2.959615	0.345469
24	1	0	4.820164	1.862565	0.047648
25	1	0	3.503243	2.015655	-1.146479
26	6	0	3.094408	-2.744901	-1.350707
27	1	0	2.524827	-3.669803	-1.445280
28	1	0	3.762767	-2.615480	-2.198456
29	1	0	3.675871	-2.796042	-0.426830
30	6	0	-4.260287	-0.254937	-1.121505
31	1	0	-3.856781	0.103645	-2.069955
32	1	0	-5.213818	-0.753399	-1.277662
33	1	0	-4.389399	0.609950	-0.467029
34	7	0	-1.014733	1.724497	0.937043
35	6	0	-1.184238	2.306190	-0.072760
36	16	0	-1.487607	3.122152	-1.404514

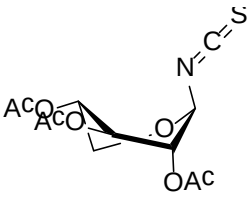
6 $^4S_2$ (chloroform)



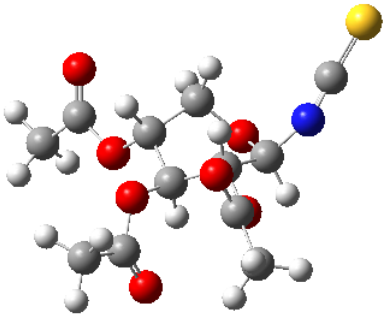
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.759296	Hartree
Zero-point Energy Correction	0.276022	Hartree
Thermal Correction to Energy	0.297965	Hartree
Thermal Correction to Enthalpy	0.298909	Hartree
Thermal Correction to Free Energy	0.221981	Hartree
EE + Zero-point Energy	-1445.483274	Hartree
EE + Thermal Energy Correction	-1445.461331	Hartree
EE + Thermal Enthalpy Correction	-1445.460387	Hartree
EE + Thermal Free Energy Correction	-1445.537315	Hartree
E (Thermal)	186.976	kcal/mol
Heat Capacity (Cv)	76.718	cal/mol-kelvin
Entropy (S)	161.908	cal/mol-kelvin

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.458000	-1.364919	-1.880117
2	6	0	1.726510	0.522865	-1.092866
3	6	0	1.413237	-0.041382	0.299375
4	6	0	-0.051134	-0.486854	0.402950
5	6	0	-0.633365	-0.812211	-0.974811
6	1	0	-1.076170	0.084390	-1.411380
7	1	0	0.887238	-2.269758	-1.438655
8	1	0	1.630270	0.712914	1.056632
9	1	0	-0.094580	-1.377285	1.032808
10	1	0	0.040291	-1.606661	-2.856409
11	8	0	1.495537	-0.404685	-2.104897
12	8	0	2.214217	-1.203471	0.507431
13	6	0	3.505634	-1.004122	0.868320
14	8	0	3.971385	0.094596	1.009597
15	6	0	4.216917	-2.305343	1.055330
16	1	0	5.248055	-2.118618	1.344328
17	1	0	3.708005	-2.889893	1.823853
18	1	0	4.182078	-2.872570	0.123299
19	8	0	-0.777931	0.580176	1.013669
20	6	0	-1.824170	0.252971	1.807174
21	8	0	-2.106640	-0.885015	2.076569
22	6	0	-2.549389	1.477238	2.262443
23	1	0	-1.843952	2.211519	2.653145
24	1	0	-3.047980	1.918122	1.395570
25	1	0	-3.285580	1.208449	3.015996
26	8	0	-1.624219	-1.834979	-0.873036
27	6	0	-2.911868	-1.450808	-0.717120
28	8	0	-3.254143	-0.297885	-0.708224
29	6	0	-3.806577	-2.636380	-0.547038
30	1	0	-3.606763	-3.375901	-1.323106
31	1	0	-3.589434	-3.093192	0.421583
32	1	0	-4.845452	-2.317306	-0.578091
33	7	0	0.911752	1.705466	-1.279159
34	6	0	0.466089	2.717479	-0.859343
35	16	0	-0.178993	4.088705	-0.390818
36	1	0	2.770662	0.827142	-1.167020



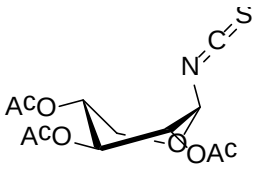
6 ^4S_o (chloroform)



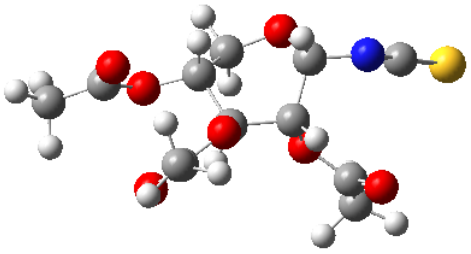
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.760657	Hartree
Zero-point Energy Correction	0.276004	Hartree
Thermal Correction to Energy	0.298166	Hartree
Thermal Correction to Enthalpy	0.299110	Hartree
Thermal Correction to Free Energy	0.220027	Hartree
EE + Zero-point Energy	-1445.484653	Hartree
EE + Thermal Energy Correction	-1445.462491	Hartree
EE + Thermal Enthalpy Correction	-1445.461546	Hartree
EE + Thermal Free Energy Correction	-1445.540630	Hartree
E (Thermal)	187.102	kcal/mol
Heat Capacity (Cv)	76.574	cal/mol-kelvin
Entropy (S)	166.446	cal/mol-kelvin

Standard orientation:

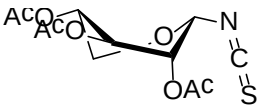
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.845811	-0.111311	-0.244531
2	6	0	-0.847148	1.302534	0.318502
3	6	0	0.493004	1.982209	0.021764
4	6	0	1.502470	0.117434	-1.009263
5	6	0	0.558514	-0.689909	-0.101281
6	1	0	0.359783	3.046224	-0.160664
7	1	0	-1.015189	1.270241	1.396848
8	1	0	0.878819	-0.640202	0.941698
9	1	0	-1.139234	-0.099226	-1.296065
10	1	0	1.174489	1.860226	0.870721
11	8	0	1.075661	1.436383	-1.161574
12	8	0	0.593943	-2.033933	-0.552017
13	8	0	-1.766504	-0.895796	0.505640
14	8	0	-1.945733	1.974923	-0.307803
15	6	0	0.549570	-3.028517	0.371001
16	6	0	-2.497985	-1.833502	-0.142670
17	6	0	-2.362685	3.116505	0.275601
18	8	0	0.540845	-2.825860	1.554172
19	8	0	-1.831151	3.573355	1.254994
20	8	0	-2.452251	-2.001095	-1.331458
21	6	0	0.503430	-4.363010	-0.303157
22	1	0	1.347891	-4.459129	-0.987377
23	1	0	0.528290	-5.151616	0.444771
24	1	0	-0.413466	-4.429569	-0.893489
25	6	0	-3.335917	-2.606036	0.827783
26	1	0	-3.962701	-1.919943	1.399740
27	1	0	-3.951201	-3.323399	0.290309
28	1	0	-2.679768	-3.122667	1.531960
29	6	0	-3.533056	3.702992	-0.448841
30	1	0	-4.357257	2.987275	-0.445685
31	1	0	-3.836384	4.627744	0.035628
32	1	0	-3.258765	3.892569	-1.488187
33	7	0	2.845495	0.046190	-0.476555
34	6	0	3.784258	0.657124	-0.090575
35	16	0	5.084799	1.385499	0.447280
36	1	0	1.519109	-0.332748	-2.002429



17 $^{4}S_{2}$ (Ethanol)



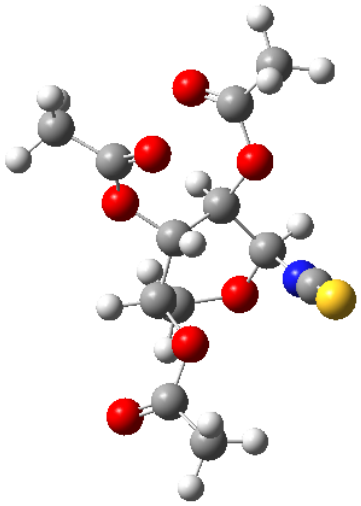
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.762960	Hartree
Zero-point Energy Correction	0.275429	Hartree
Thermal Correction to Energy	0.297459	Hartree
Thermal Correction to Enthalpy	0.298403	Hartree
Thermal Correction to Free Energy	0.220676	Hartree
EE + Zero-point Energy	-1445.487531	Hartree
EE + Thermal Energy Correction	-1445.465501	Hartree
EE + Thermal Enthalpy Correction	-1445.464557	Hartree
EE + Thermal Free Energy Correction	-1445.542284	Hartree
E (Thermal)	186.658	kcal/mol
Heat Capacity (Cv)	76.702	cal/mol-kelvin
Entropy (S)	163.591	cal/mol-kelvin



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.124677	-2.005286	0.348113
2	6	0	1.134851	-0.631184	-1.183300
3	6	0	0.648177	0.519384	-0.298516
4	6	0	-0.840909	0.356200	0.038777
5	6	0	-1.273020	-1.103937	-0.076847
6	1	0	-1.559664	-1.328952	-1.106677
7	1	0	0.212868	-1.746928	1.356869
8	1	0	0.805711	1.465443	-0.815069
9	1	0	-0.999458	0.707786	1.059410
10	1	0	-0.444048	-3.046140	0.329634
11	1	0	0.600106	-0.586647	-2.135776
12	8	0	0.960372	-1.895700	-0.577554
13	7	0	2.534524	-0.476857	-1.451312
14	6	0	3.606001	-0.624368	-0.961476
15	16	0	5.082142	-0.773553	-0.412667
16	8	0	1.384726	0.483677	0.923293
17	6	0	2.381376	1.383055	1.108065
18	8	0	2.673208	2.211394	0.284243
19	6	0	3.023800	1.201642	2.443527
20	1	0	3.936457	1.791084	2.491819
21	1	0	2.323922	1.539467	3.212246
22	1	0	3.234484	0.145790	2.617394
23	8	0	-1.574742	1.170393	-0.880983
24	6	0	-2.714939	1.745249	-0.444988
25	8	0	-3.109633	1.632014	0.689660
26	6	0	-3.396052	2.494742	-1.541189
27	1	0	-2.685404	3.151332	-2.044579
28	1	0	-3.765952	1.770471	-2.271635
29	1	0	-4.227071	3.065927	-1.134432
30	8	0	-2.363211	-1.381689	0.803388
31	6	0	-3.617474	-1.256398	0.324070
32	8	0	-3.852250	-0.946129	-0.818309
33	6	0	-4.631655	-1.524698	1.385773
34	1	0	-4.389133	-2.447200	1.914333
35	1	0	-4.596957	-0.701749	2.104769
36	1	0	-5.622454	-1.582925	0.941583

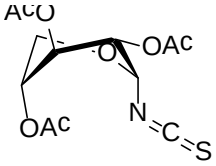
17 ^4S_o (Ethanol)



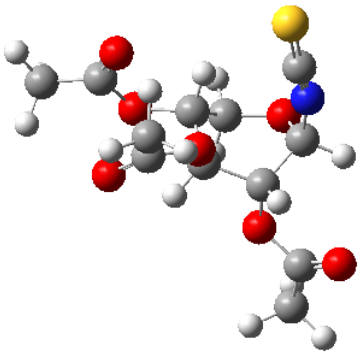
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.766568	Hartree
Zero-point Energy Correction	0.275388	Hartree
Thermal Correction to Energy	0.297399	Hartree
Thermal Correction to Enthalpy	0.298344	Hartree
Thermal Correction to Free Energy	0.220917	Hartree
EE + Zero-point Energy	-1445.491180	Hartree
EE + Thermal Energy Correction	-1445.469168	Hartree
EE + Thermal Enthalpy Correction	-1445.468224	Hartree
EE + Thermal Free Energy Correction	-1445.545651	Hartree
E (Thermal)	186.621	kcal/mol
Heat Capacity (Cv)	76.797	cal/mol-kelvin
Entropy (S)	162.959	cal/mol-kelvin

Standard orientation:

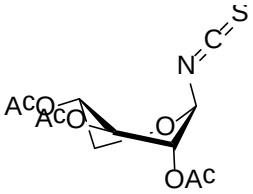
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.255723	-0.730832	-0.048614
2	6	0	-1.083059	-1.363672	0.357852
3	6	0	-1.275945	-1.335761	1.861306
4	6	0	-0.291470	0.870678	1.823285
5	6	0	0.821180	0.125919	1.084658
6	1	0	-2.255064	-1.721298	2.138734
7	1	0	-1.110511	-2.396559	0.008963
8	1	0	1.328332	-0.510003	1.814127
9	1	0	0.114262	-0.126698	-0.946148
10	1	0	0.139994	1.480102	2.617312
11	1	0	-0.503984	-1.960272	2.322405
12	8	0	-1.212643	-0.007318	2.400135
13	8	0	1.714426	1.116625	0.589101
14	8	0	1.163815	-1.802032	-0.328238
15	8	0	-2.105458	-0.600545	-0.298416
16	6	0	3.035013	0.828475	0.552807
17	6	0	2.114124	-1.603776	-1.265602
18	6	0	-3.310647	-1.174210	-0.460065
19	8	0	3.481640	-0.220578	0.944349
20	8	0	-3.547939	-2.303571	-0.104587
21	8	0	2.213305	-0.573893	-1.886194
22	6	0	3.813003	1.954635	-0.039917
23	1	0	3.569296	2.885268	0.474762
24	1	0	4.877102	1.743240	0.031445
25	1	0	3.521513	2.060606	-1.087922
26	6	0	2.996671	-2.799944	-1.399540
27	1	0	2.390204	-3.691596	-1.565417
28	1	0	3.693206	-2.652197	-2.221212
29	1	0	3.544976	-2.932261	-0.463579
30	6	0	-4.268523	-0.236434	-1.119636
31	1	0	-3.861024	0.080110	-2.081787
32	1	0	-5.229282	-0.726525	-1.257645
33	1	0	-4.382698	0.652381	-0.494981
34	7	0	-0.966174	1.775311	0.917315
35	6	0	-1.129646	2.315432	-0.116224
36	16	0	-1.424302	3.088497	-1.476332



6 $^4S_2$ (Ethanol)



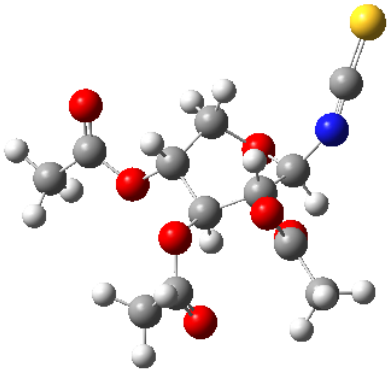
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.764917	Hartree
Zero-point Energy Correction	0.275546	Hartree
Thermal Correction to Energy	0.297647	Hartree
Thermal Correction to Enthalpy	0.298591	Hartree
Thermal Correction to Free Energy	0.220484	Hartree
EE + Zero-point Energy	-1445.489371	Hartree
EE + Thermal Energy Correction	-1445.467270	Hartree
EE + Thermal Enthalpy Correction	-1445.466326	Hartree
EE + Thermal Free Energy Correction	-1445.544433	Hartree
E (Thermal)	186.776	kcal/mol
Heat Capacity (Cv)	76.956	cal/mol-kelvin
Entropy (S)	164.390	cal/mol-kelvin



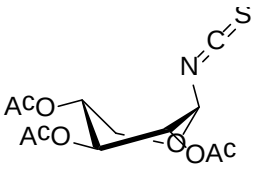
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.626167	-0.808687	-2.041763
2	6	0	1.683731	1.028574	-0.876710
3	6	0	1.508589	0.136274	0.358460
4	6	0	0.125332	-0.527200	0.387855
5	6	0	-0.479619	-0.630469	-1.013274
6	1	0	-1.068367	0.259701	-1.239669
7	1	0	1.207646	-1.707974	-1.818232
8	1	0	1.656624	0.726493	1.262711
9	1	0	0.240767	-1.527497	0.808403
10	1	0	0.194231	-0.896009	-3.037375
11	8	0	1.497095	0.330372	-2.074946
12	8	0	2.470768	-0.914619	0.283456
13	6	0	3.728927	-0.635248	0.695567
14	8	0	4.042560	0.451664	1.110705
15	6	0	4.620173	-1.823744	0.555363
16	1	0	5.608031	-1.588008	0.943375
17	1	0	4.189145	-2.669217	1.094080
18	1	0	4.685249	-2.093868	-0.500973
19	8	0	-0.709276	0.267188	1.236182
20	6	0	-1.658185	-0.365088	1.957602
21	8	0	-1.789650	-1.564556	1.952067
22	6	0	-2.502378	0.607605	2.711047
23	1	0	-1.877296	1.358159	3.195532
24	1	0	-3.149826	1.117286	1.991766
25	1	0	-3.110897	0.078495	3.440710
26	8	0	-1.314367	-1.785988	-1.115242
27	6	0	-2.634367	-1.637430	-0.875936
28	8	0	-3.133763	-0.572504	-0.607354
29	6	0	-3.350426	-2.944000	-0.965450
30	1	0	-3.063457	-3.470101	-1.876493
31	1	0	-3.049817	-3.555349	-0.110277
32	1	0	-4.424493	-2.776618	-0.938032
33	7	0	0.748735	2.116787	-0.767018
34	6	0	-0.197315	2.781841	-0.563846
35	16	0	-1.455878	3.730202	-0.324502
36	1	0	2.684652	1.456758	-0.906801

6 ^4S_o (Ethanol)



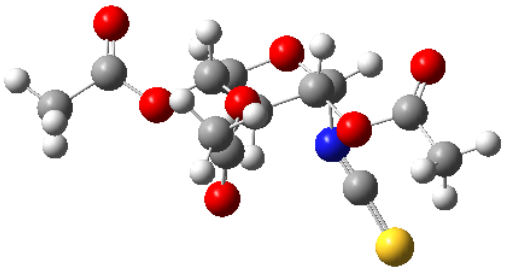
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.767622	Hartree
Zero-point Energy Correction	0.275355	Hartree
Thermal Correction to Energy	0.297636	Hartree
Thermal Correction to Enthalpy	0.298580	Hartree
Thermal Correction to Free Energy	0.218602	Hartree
EE + Zero-point Energy	-1445.492267	Hartree
EE + Thermal Energy Correction	-1445.469986	Hartree
EE + Thermal Enthalpy Correction	-1445.469042	Hartree
EE + Thermal Free Energy Correction	-1445.549021	Hartree
E (Thermal)	186.769	kcal/mol
Heat Capacity (Cv)	76.665	cal/mol-kelvin
Entropy (S)	168.329	cal/mol-kelvin



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.831235	-0.061665	-0.263229
2	6	0	-0.736026	1.347832	0.299538
3	6	0	0.640469	1.939732	-0.016424
4	6	0	1.525979	-0.009022	-1.018252
5	6	0	0.527998	-0.734582	-0.100683
6	1	0	0.570352	3.005495	-0.223526
7	1	0	-0.891490	1.323182	1.379598
8	1	0	0.847374	-0.687774	0.942272
9	1	0	-1.111089	-0.030229	-1.317923
10	1	0	1.316914	1.790343	0.831363
11	8	0	1.183732	1.334921	-1.192571
12	8	0	0.471087	-2.088048	-0.529047
13	8	0	-1.816106	-0.776200	0.479483
14	8	0	-1.800668	2.089823	-0.311241
15	6	0	0.322936	-3.059568	0.403455
16	6	0	-2.594328	-1.672939	-0.166236
17	6	0	-2.154634	3.243035	0.284355
18	8	0	0.280729	-2.831080	1.585214
19	8	0	-1.589869	3.661897	1.266889
20	8	0	-2.522791	-1.871470	-1.353064
21	6	0	0.205940	-4.400209	-0.242973
22	1	0	1.048063	-4.558721	-0.918337
23	1	0	0.175416	-5.173904	0.520315
24	1	0	-0.711331	-4.421686	-0.837017
25	6	0	-3.509907	-2.366710	0.788763
26	1	0	-4.070333	-1.628824	1.364863
27	1	0	-4.185865	-3.019319	0.241630
28	1	0	-2.906572	-2.952060	1.487452
29	6	0	-3.297951	3.898205	-0.418685
30	1	0	-4.158586	3.226369	-0.408241
31	1	0	-3.545267	4.834413	0.075832
32	1	0	-3.025186	4.079960	-1.459977
33	7	0	2.862153	-0.152502	-0.479935
34	6	0	3.810323	0.438803	-0.085643
35	16	0	5.124393	1.138562	0.458547
36	1	0	1.515962	-0.472942	-2.004733

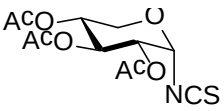
17 $^4C_1$ (gas phase)



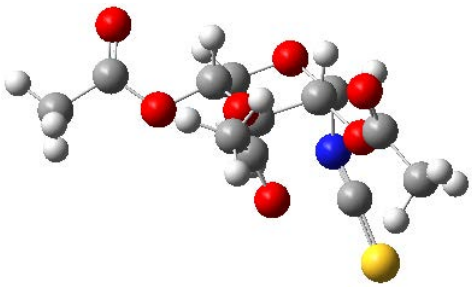
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.745612	Hartree
Zero-point Energy Correction	0.276599	Hartree
Thermal Correction to Energy	0.298746	Hartree
Thermal Correction to Enthalpy	0.299691	Hartree
Thermal Correction to Free Energy	0.220541	Hartree
EE + Zero-point Energy	-1445.469013	Hartree
EE + Thermal Energy Correction	-1445.446866	Hartree
EE + Thermal Enthalpy Correction	-1445.445922	Hartree
EE + Thermal Free Energy Correction	-1445.525072	Hartree
E (Thermal)	187.466	kcal/mol
Heat Capacity (Cv)	76.442	cal/mol-kelvin
Entropy (S)	166.585	cal/mol-kelvin

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.543052	0.304566	-0.153980
2	6	0	0.689159	0.002467	-0.990199
3	6	0	1.033845	-1.501338	-0.943229
4	6	0	-1.196575	-2.083682	-0.453268
5	6	0	-1.674337	-0.635965	-0.525397
6	1	0	1.815587	-1.727467	-1.667642
7	1	0	0.518796	0.265133	-2.037845
8	1	0	-0.307806	0.205353	0.908746
9	1	0	-1.969145	-2.757054	-0.818049
10	1	0	-0.940459	-2.340016	0.581325
11	1	0	-2.039586	-0.413347	-1.531307
12	7	0	1.512082	-1.848945	0.379956
13	6	0	2.395542	-1.570531	1.130577
14	16	0	3.527205	-1.280154	2.190244
15	8	0	1.737564	0.796948	-0.454034
16	6	0	2.858336	0.928241	-1.206338
17	8	0	2.982646	0.398669	-2.275202
18	6	0	3.870775	1.782037	-0.506184
19	1	0	4.163673	1.287316	0.422257
20	1	0	4.734525	1.919092	-1.150792
21	1	0	3.426670	2.742705	-0.244180
22	8	0	-0.072022	-2.263965	-1.300359
23	8	0	-0.943340	1.643068	-0.429138
24	8	0	-2.714018	-0.404012	0.423621
25	6	0	-1.039946	2.509605	0.612056
26	6	0	-3.962597	-0.783480	0.066038
27	8	0	-0.808138	2.215083	1.747661
28	8	0	-4.207929	-1.319467	-0.978086
29	6	0	-1.471754	3.861498	0.120586
30	1	0	-2.427979	3.773992	-0.396621
31	1	0	-1.557239	4.540374	0.964580
32	1	0	-0.740741	4.237756	-0.596245
33	6	0	-4.951404	-0.442101	1.142169
34	1	0	-4.923751	0.630692	1.336672
35	1	0	-5.945533	-0.746759	0.827030
36	1	0	-4.672908	-0.951192	2.065770



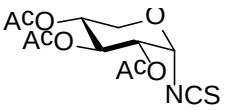
17 $^{4}C_{1}$ (chloroform)



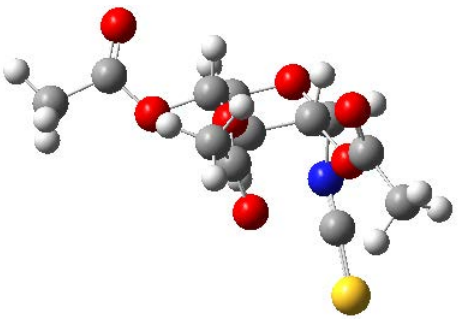
Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.768621	Hartree
Zero-point Energy Correction	0.276293	Hartree
Thermal Correction to Energy	0.298107	Hartree
Thermal Correction to Enthalpy	0.299051	Hartree
Thermal Correction to Free Energy	0.222282	Hartree
EE + Zero-point Energy	-1445.492328	Hartree
EE + Thermal Energy Correction	-1445.470514	Hartree
EE + Thermal Enthalpy Correction	-1445.469570	Hartree
EE + Thermal Free Energy Correction	-1445.546339	Hartree
E (Thermal)	187.065	kcal/mol
Heat Capacity (Cv)	76.463	cal/mol-kelvin
Entropy (S)	161.573	cal/mol-kelvin

Standard orientation:

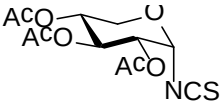
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.452561	0.217490	-0.094608
2	6	0	0.640890	-0.121076	-1.107237
3	6	0	0.715078	-1.637690	-1.347896
4	6	0	-1.534219	-1.952323	-0.737872
5	6	0	-1.750807	-0.462577	-0.497160
6	1	0	1.407282	-1.847974	-2.164036
7	1	0	0.427759	0.363727	-2.063230
8	1	0	-0.148155	-0.102186	0.905926
9	1	0	-2.438705	-2.410055	-1.133393
10	1	0	-1.255420	-2.448416	0.198634
11	1	0	-2.150745	0.009457	-1.397868
12	7	0	1.208741	-2.303986	-0.158479
13	6	0	2.086720	-2.288272	0.641363
14	16	0	3.203529	-2.365019	1.758902
15	8	0	1.926374	0.258162	-0.633029
16	6	0	2.390921	1.499847	-0.905790
17	8	0	1.784529	2.289753	-1.579182
18	6	0	3.713564	1.721043	-0.246384
19	1	0	4.395502	0.905829	-0.492153
20	1	0	4.126161	2.676014	-0.562416
21	1	0	3.560115	1.716761	0.835368
22	8	0	-0.523289	-2.145122	-1.720285
23	8	0	-0.721161	1.620003	-0.094104
24	8	0	-2.658036	-0.275023	0.589779
25	6	0	-0.037097	2.412636	0.756714
26	6	0	-3.978263	-0.329513	0.311060
27	8	0	0.788665	1.993458	1.525588
28	8	0	-4.401967	-0.562219	-0.790380
29	6	0	-0.436672	3.843825	0.586565
30	1	0	-1.520900	3.940124	0.658155
31	1	0	0.052303	4.452858	1.342918
32	1	0	-0.132901	4.170634	-0.410570
33	6	0	-4.797626	-0.058491	1.533614
34	1	0	-4.598638	0.957999	1.879252
35	1	0	-5.852881	-0.172648	1.298498
36	1	0	-4.508898	-0.745402	2.330539



17 $^{4}C_{1}$ (ethanol)



Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1445.775088	Hartree
Zero-point Energy Correction	0.275583	Hartree
Thermal Correction to Energy	0.297567	Hartree
Thermal Correction to Enthalpy	0.298511	Hartree
Thermal Correction to Free Energy	0.220756	Hartree
EE + Zero-point Energy	-1445.499505	Hartree
EE + Thermal Energy Correction	-1445.477521	Hartree
EE + Thermal Enthalpy Correction	-1445.476576	Hartree
EE + Thermal Free Energy Correction	-1445.554332	Hartree
E (Thermal)	186.726	kcal/mol
Heat Capacity (Cv)	76.601	cal/mol-kelvin
Entropy (S)	163.649	cal/mol-kelvin



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.432807	0.205991	-0.096615
2	6	0	0.644958	-0.143290	-1.120189
3	6	0	0.696717	-1.658617	-1.367512
4	6	0	-1.564267	-1.927774	-0.752230
5	6	0	-1.746158	-0.433020	-0.513740
6	1	0	1.380634	-1.874880	-2.188380
7	1	0	0.429032	0.342897	-2.074284
8	1	0	-0.141033	-0.141124	0.898404
9	1	0	-2.477964	-2.367272	-1.147338
10	1	0	-1.297492	-2.426987	0.185668
11	1	0	-2.122985	0.055105	-1.415284
12	7	0	1.184702	-2.342090	-0.186160
13	6	0	2.000475	-2.298583	0.674093
14	16	0	3.042204	-2.347898	1.866036
15	8	0	1.941079	0.221572	-0.658011
16	6	0	2.426200	1.446023	-0.955480
17	8	0	1.807853	2.251542	-1.605128
18	6	0	3.782528	1.639228	-0.363400
19	1	0	4.439510	0.826044	-0.676596
20	1	0	4.186162	2.599545	-0.674833
21	1	0	3.694708	1.602174	0.725152
22	8	0	-0.555520	-2.145325	-1.735341
23	8	0	-0.661547	1.617812	-0.067739
24	8	0	-2.657374	-0.226585	0.568065
25	6	0	0.040620	2.375598	0.797036
26	6	0	-3.975366	-0.231538	0.286509
27	8	0	0.867737	1.917989	1.547607
28	8	0	-4.401518	-0.421330	-0.826255
29	6	0	-0.336962	3.815567	0.679420
30	1	0	-1.411270	3.925551	0.838140
31	1	0	0.217000	4.401223	1.409045
32	1	0	-0.107665	4.157928	-0.332191
33	6	0	-4.792874	0.023456	1.510399
34	1	0	-4.513008	0.988942	1.936256
35	1	0	-5.849474	0.015563	1.254292
36	1	0	-4.578400	-0.747355	2.253188