Supporting information

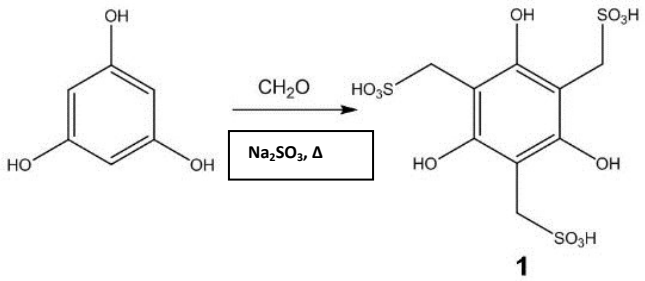
Supporting Information comprises:

- Experimental Details
- Crystallographic details
- NMR data for a water-soluble 1,3,5-trihydroxy-2,4,6-trimethylsulfonic acid
- TGA data for a water-soluble 1,3,5-trihydroxy-2,4,6-trimethylsulfonic acid
- IR data for a water-soluble 1,3,5-trihydroxy-2,4,6-trimethylsulfonic acid
- Computational Details
- Thermochemical Data
- XYZ Coordinates

Experimental Section

All chemicals used were purchased from Alfa-Aesar and Aldrich. ^{1}H NMR and ^{13}C NMR spectra were collected on a Bruker AC200 or a Bruker Advance 300. Thermal Gravimetric Analysis (TGA) was studied by TGA Q50-1316 at a heating rate of 10 °C min^{-1} under N_2, and single-crystal X-ray data were collected on a Bruker Apex II operating synchrotron radiation.

1,3,5-Trihydroxy-2,4,6- trimethylsulfonate, compound **1,** was synthesized using the procedure of Kazakova et al. involving refluxing 5.44 g (0.043 mol) 1,3,5-trihydroxybenzene, 4.1 g (0.05 mol) of a solution of 37% formaldehyde, and 6.3 g (0.05 mol) of sodium sulfite in 30 mL of DI water and stirring at 90-95 °C for 4 hours. The product was neutralized using dilute HCl, followed by adding 50 mL acetone, washing with 20 mL acetone, and drying the product on a vacuum filtration aspirator. The compound is a reddish-brown powder produced in 28. 5% yield.



1

Scheme 1. *Schematic representation of the synthesis of the water-soluble 1,3,5-trihydroxy-2,4,6-trimethylsulfonic acid benzene, compound **1**.*

Crystallization of **1·Eu** was achieved by reacting compound **1** and Eu(III)nitrate in methanol. Dissolve 50 mg (0.122 mmol) of compound **1** in 2 mL of methanol (mixture 1). Dissolve 35 mg

(0.103 mmol) of Eu(III)nitrate·xH_2O in 1 mL of methanol (mixture 2). Sonicate the mixtures separately for 30 minutes, combine and sonicate again for 30 minutes. Add 1 M HCl drop-wise until the pH of the combined mixture is ~1 and filter. After a few days, the formation of orange or yellow plate-shaped crystals was observed.

Crystal data for a water-soluble 1,3,5-trihydroxy-2,4,6-trimethylsulfonic acid (1) and Eu: Non-hydrogen atoms for fully ordered parts of the structure were located from the difference map and refined anisotropically by full matrix least squares refinement against F^2. Disordered atoms belonging to the outer sphere methanol and water molecules were refined isotropically. Hydrogen atoms bonded to carbon were placed in idealized positions, and their coordinates and thermal parameters were allowed to ride on the carrier atom. Hydrogen atoms bonded to the coordinated water molecules were located from the difference map and refined with the O-H bond distances restrained to 0.9 Å. Hydrogen atoms bonded to the phenolic – OH groups had their coordinates refined with restraints ensuring tetrahedral C-O-H bond angles. For the disordered methanol/water ligand, one H atom was refined at full occupancy with a distance restraint, while the other H atom (associated with the partial water molecule) was placed in an idealized position. H atoms for the disordered outer sphere water molecules were not included in the model, although they are included in the formula.

A-level PLAT375 and PLAT415 alerts are generated due to unusual geometry and unrealistic H···H contacts for the disordered methanol molecule; the exact identity and geometry of this disordered outer sphere molecule is not relevant to the interpretation of the main moiety of the structure. A B-level PLAT230 alert is generated for one of the phenolic oxygen atoms, which has an exceptionally large thermal ellispoid. Based on the longer C-O bond for this group compared to the other two and the difference in the arrangement of the surrounding H bond donors and acceptors, this –OH group is believed to be disordered between its phenol and phenolate forms. Because the H atom is likely disordered over a number of other possible positions, it was refined at full occupancy as part of the –OH group. This also leads to B-level PLAT417 alerts where this H atom is unrealistically close to other H atoms on H-bond donors.

Crystal data for **1·Eu**: $C_{9.60}H_{19.5}EuO_{17}S_3$, M = 672.72, 0.30 x 0.16 x 0.12 mm, monoclinic, space group $P2_1/n$ (No. 14), a = 8.9194(17), b = 8.8509(17), c = 25.242(5) Å,□□□ = 90.154(2)°, V = 1992.7(7) Å^3, Z = 4, D_c = 2.242 g/cm^3, F_{000} = 1335, MoK□ radiation,□□□ = 0.71073 Å, T = 296(2)K, 2□$_{max}$ = 55.2º, 22633 reflections collected, 4603 unique (R_{int} = 0.0358). Final *GooF* = 1.105, *R1* = 0.0293, *wR2* = 0.737, *R* indices based on 4281 reflections with I >2sigma(I)

(refinement on F^2), 274 parameters, 0 restraints. Lp and absorption corrections applied,□□□ = 3.554 mm^{-1}. CCDC number: 2004590.

Crystal data for a water-soluble 1,3,5-trihydroxy-2,4,6-trimethylsulfonic acid (1) and *Sm:* The structure of **Sm-1** was determined by refining the model of the isomorphous structure **Eu-1** against data collected from a crystal of Sm-1 until convergence. For **Sm-1**, the second hydrogen atom bonded to the disordered, coordinated water molecule could not be located.

Crystal data for **1·Sm**: $C_{9.60}H_{19.5}SmO_{17}S_3$; M = 669.48, 0.30 x 0.16 x 0.12 mm, , monoclinic, space group $P2_1/n$ (No. 14), a = 8.9342(15), b = 8.8762(15), c = 25.291(4) Å,□□□ = 90.340(2)°, V = 2005.5 (6), F_{000} = 1324, MoK□ radiation,□□□ = 0.71073 Å, T = 100.15 K, 2□$_{max}$ = 57.41°, 23152 reflections collected, 4866 unique (R_{int} = 0.0300). Final *GooF* = 1.254, *R1* = 0.0355, *wR2* = 0.0879, R indices based on 4729 reflections with I >2sigma(I) (refinement on F^2), 274 parameters, 0 restraints. Lp and absorption corrections applied, □ = 3.331 mm^{-1}. CCDC number: 2004591

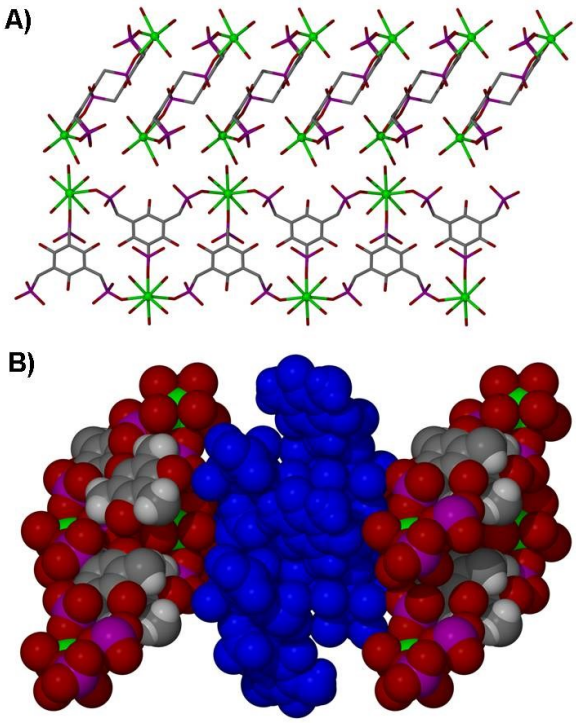


*Figure S1. A) Representation of the two different layer orientations observed in the extended structure of **1·Eu**. B) Space-filling representation of the extended structure of **1·Eu**. One orientation is colored blue so that it is possible to distinguish between the two differing layer orientations. Color codes: C: gray, O: red, Eu: green, S: magenta/dark pink.*

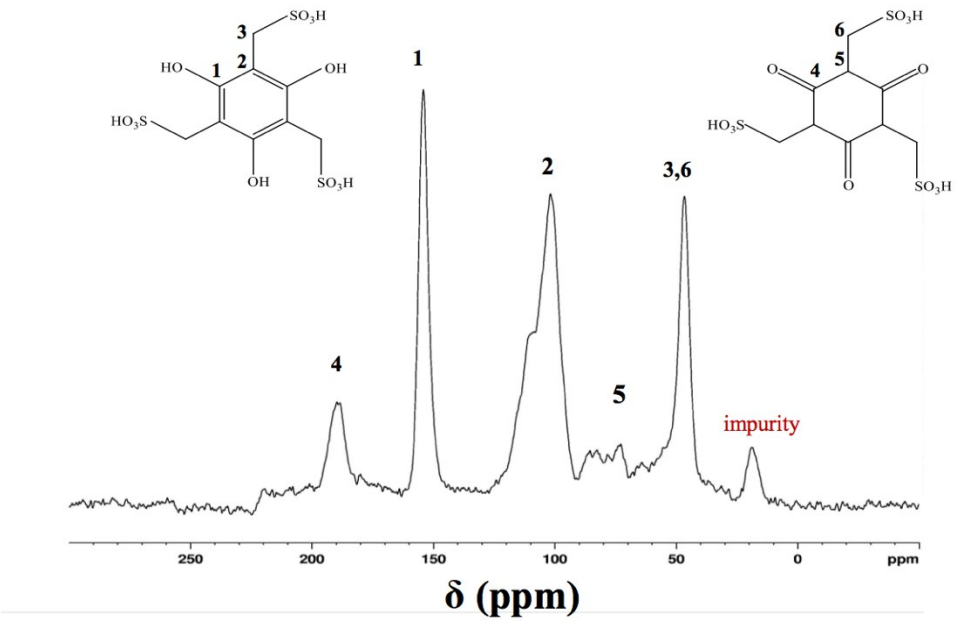


Figure S2. Zoomed in view of ^{13}C NMR spectrum of 1,3,5-trihydroxy-2,4,6-trimethylsulfonic acid, 1

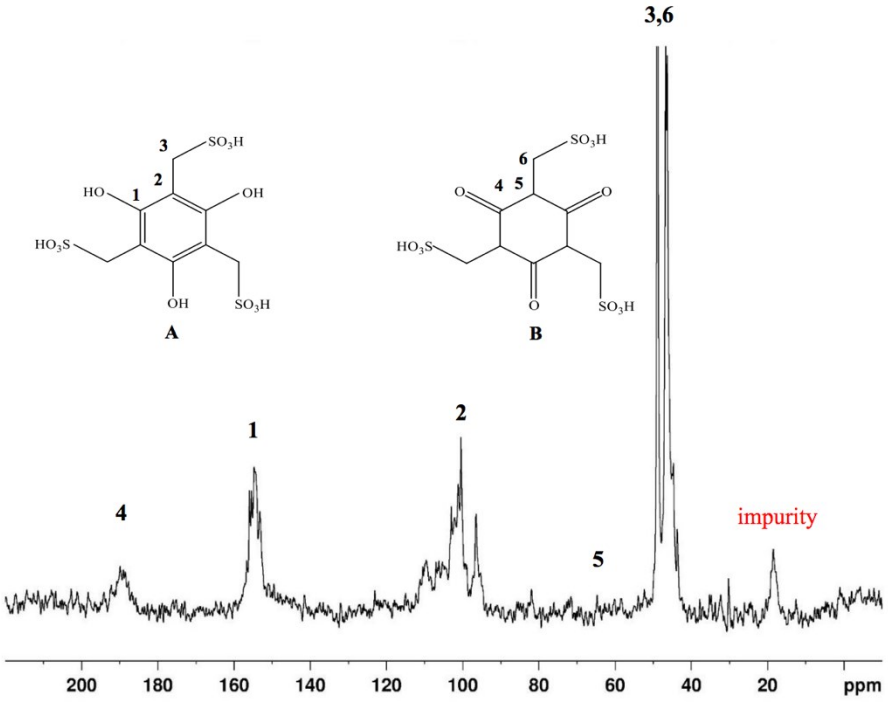


Figure S3. Zoomed out view of ^{13}C NMR spectrum of 1,3,5-trihydroxy-2,4,6-trimethylsulfonic acid, 1

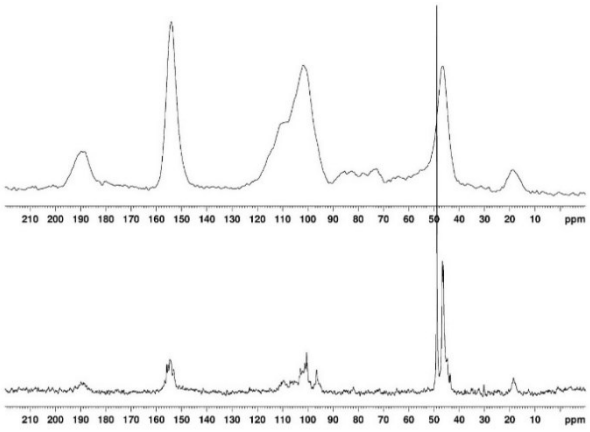


Figure S4. The comparison of the ^{13}C NMR spectrum of 1 (pH ~7) in D_2O (A) and the solid-state ^{13}C NMR spectrum of 1 (B).

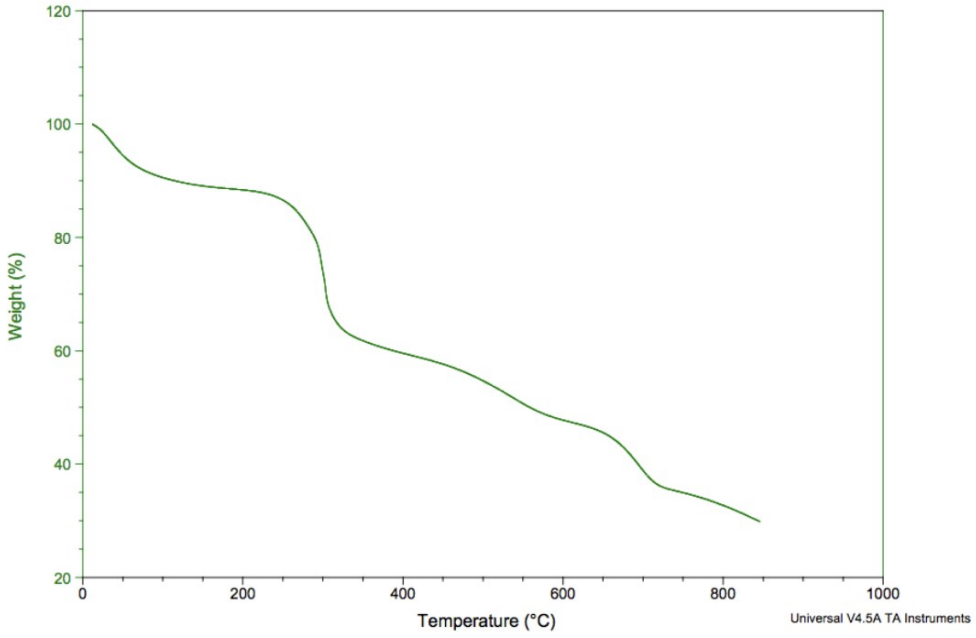


Figure S5. Thermogravimetric spectra of a water soluble 1,3,5-trihydroxy-2,4,6-trimethylsulfonic acid, 1

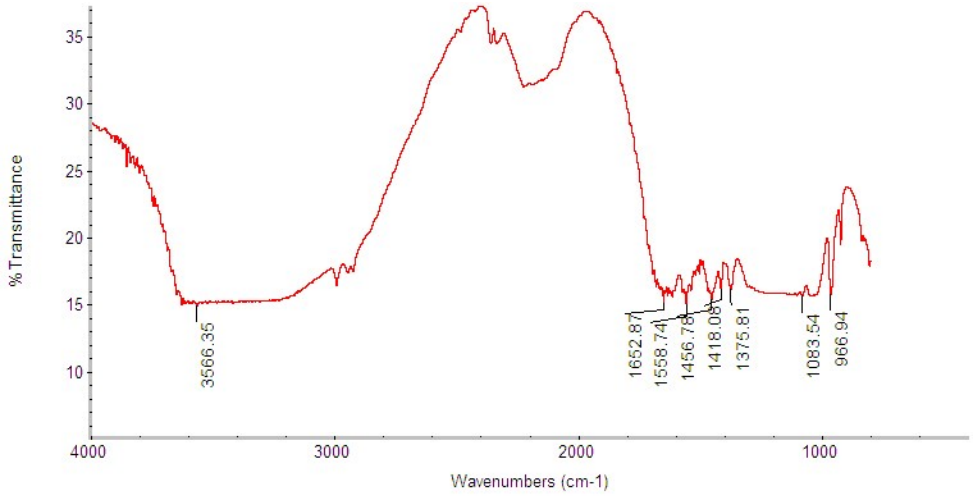


Figure S6. IR spectra of a water soluble 1,3,5-trihydroxy-2,4,6-trimethylsulfonic acid, 1

Computational Details

All quantum chemical calculations were carried out with use of the Gaussian 16[1] suite of programs, and structures were visualized with GaussView6.[2] Structures A, B and their building blocks, 1,3,5-trihydroxybenzene and 1,3,5-cyclohexanetrione, were optimized using the tight convergence criteria with the ultrafine pruned grid at the PBE0/cc-pVDZ level of theory, and vibrational frequencies were calculated to determine the nature of the stationary points. Starting structures for the hydroxyl compounds had a planar aromatic ring, and the CH_2S groups were rotated so the sulfurs were above, below or in the plane. Starting structures for the ketone compounds were nonplanar (chair or boat conformation) and, again, rotation of the CH_2S groups was explored. In addition, rotation of the oxygens of the sulfonato group and rotation of the hydroxyl hydrogen of the sulfonato group and on the benzene ring were explored. To investigate the effect of solvation on structures and energetics, the solvation model density (SMD) model[3] was implemented; gas-phase equilibrium structures were reoptimized and vibrational frequencies were recalculated in the presence of implicit MeOH solvent. To improve energetics, single-point energies (SPEs), with and without accounting for implicit solvent effects, were calculated at the ωB97X-D/aug-cc-pVTZ level of theory to include empirical dispersion corrections; all ΔH and ΔG values discussed were evaluated at this level. Because our thermochemical values are likely accurate to within ±10 kJ/mol, we believe the reported trends in these values are reliable. AIM analyses[4] were performed for the most stable structures identified, and those structures are discussed in the text. The AIM analysis was used to locate X···H-Y H-bonds. The presence of a bond critical point between the X and H atoms or a ring critical point involving these atoms

indicates the presence of an interaction. Structural criteria used to locate H-bonds are an X···Y distance <3.6 Å and an X···H-Y angle >90°.[5]

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

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(4) R.F.W. Bader, O. U. P., Oxford, UK, 1994. .

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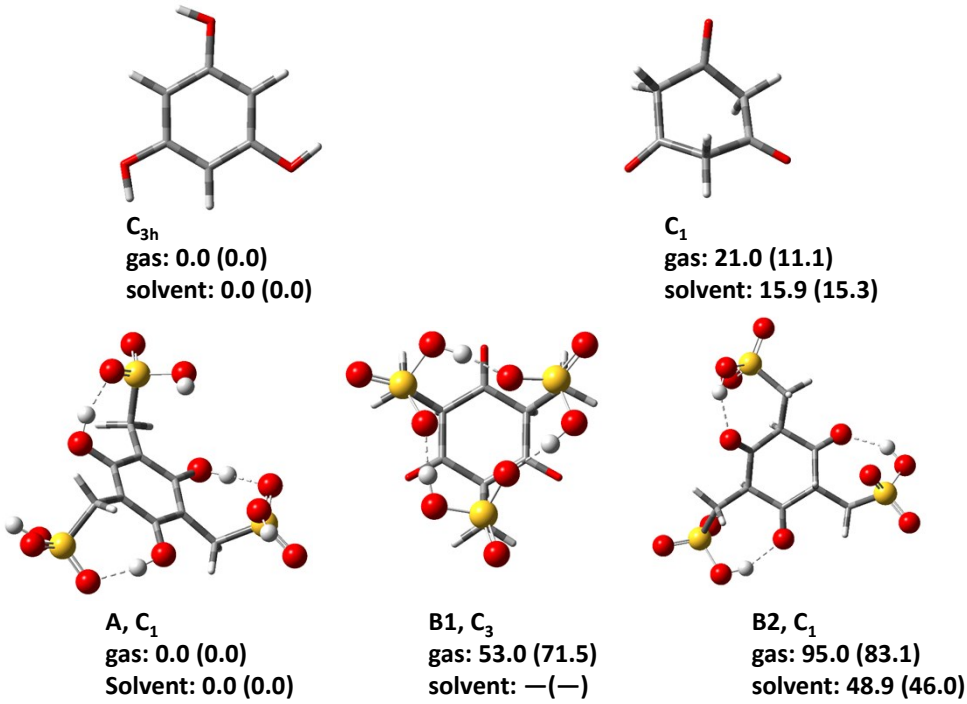

*Figure S7. PBE0/aug-cc-pVDZ fully optimized structures of the enol (left) and keto (right) tautomers of 1,3,5-trihydroxy-benzene (top) and compound **1** (bottom). Intramolecular H-bonding interactions are designated with dashed lines. Molecular point groups and ωB97X-D/aug-cc-pVTZ//PBE0/aug-cc-pVDZ relative enthalpies and free energies (in parentheses) in kJ/mol are given.*

Table S1: Thermochemical Data

compound (structure)	**calculation**	**Method**	**Basis**	**E (au)**	**E+ZPE (au)**	**H (au)**	**G (au)**	**S_{298} (cal $mol^{-1}K^{-1}$)**
1,3,5-trihydroxybenzene								
1	opt/freq	pbe0	cc-pVDZ	-457.447058	-457.3328249	-457.3241429	-457.3635639	82.97
	SPE	wb97xd	aVTZ	-457.942415	-457.8281822	-457.8195002	-457.8589212	
	SPE (solvent)	wb97xd	aVTZ	-457.965394	-457.8511606	-457.8424786	-457.8818996	
	opt/freq (solvent)	pbe0	cc-pVDZ	-457.4698774	-457.3558704	-457.3473484	-457.3875104	84.53
	SPE (solvent)	wb97xd	aVTZ	-457.965 4953	-457.851 4883	-457.842 9663	-457.883 1283	
2	opt/freq	pbe0	cc-pVDZ	-457.445738	-457.3316637	-457.3229197	-457.3634897	85.39
	SPE	wb97xd	aVTZ	-457.941254	-457.8271803	-457.8	-457.8590063	
1,3,5-cyclohexanetrione								
1	opt/freq	pbe0	cc-pVDZ	-457.4352432	-457.3239872	-457.3149442	-457.3581632	90.96
	SPE	wb97xd	aVTZ	-457.931787	-457.820531	-457.811488	-457.854707	
	SPE (solvent)	wb97xd	aVTZ	-457.955 3625	-457.844 1065	-457.835 0635	-457.878 2825	
	opt/freq (solvent)	pbe0	cc-pVDZ	-457.455 1303	-457.344 0763	-457.335 9633	-457.376 3223	84.94
	SPE (solvent)	wb97xd	aVTZ	-457.956 0938	-457.845 0398	-457.836 9268	-457.877 2858	
2	opt/freq	pbe0	cc-pVDZ	-457.437 4243	-457.325 4843	-457.316 6783	-457.357 6393	86.21

	SPE	wb97xd	aVTZ	-457.9335746	-457.8216346	-457.8128286	-457.8537896	
	SPE (solvent)	wb97xd	aVTZ	-457.9577442	-457.8458042	-457.8369982	-457.8779592	
A								
1	opt/freq	pbe0	cc-pVDZ	-2445.620171	-2445.376485	-2445.351306	-2445.431119	167.98
	SPE	wb97xd	aVTZ	-2447.532113	-2447.288427	-2447.263248	-2447.343061	
	SPE (solvent)	wb97xd	aVTZ	-2447.57193	-2447.328244	-2447.303065	-2447.382878	
	opt/freq (solvent)	pbe0	cc-pVDZ	-2445.661374	-2445.419367	-2445.394177	-2445.473241	166.40
	SPE (solvent)	wb97xd	aVTZ	-2447.576159	-2447.334152	-2447.308962	-2447.388026	
2	opt/freq	pbe0	cc-pVDZ	-2445.620213	-2445.376442	-2445.351256	-2445.431109	168.03
	SPE	wb97xd	aVTZ	-2447.532482	-2447.288711	-2447.263525	-2447.343359	
	SPE (solvent)	wb97xd	aVTZ	-2447.571696	-2447.327925	-2447.302739	-2447.382573	
3	opt/freq	pbe0	cc-pVDZ	-2445.61804	-2445.374807	-2445.349405	-2445.430017	169.66
	SPE	wb97xd	aVTZ	-2447.530304	-2447.287071	-2447.261669	-2447.342281	
4	opt/freq	pbe0	cc-pVDZ	-2445.618699	-2445.375378	-2445.349942	-2445.430622	169.80
	SPE	wb97xd	aVTZ	-2447.530198	-2447.286877	-2447.261441	-2447.342121	
5	opt/freq	pbe0	cc-pVDZ	-2445.617571	-2445.374514	-2445.34904	-2445.429953	170.29
	SPE	wb97xd	aVTZ	-2447.529276	-2447.286219	-2447.260745	-2447.341658	
6	opt/freq	pbe0	cc-pVDZ	-2445.617467	-2445.374231	-2445.348888	-2445.429388	169.43
	SPE	wb97xd	aVTZ	-2447.528672	-2447.285436	-2447.260093	-2447.340593	

7	opt/freq	pbe0	cc-pVDZ	-2445.615724	-2445.373259	-2445.347311	-2445.429101	172.14
	SPE	wb97xd	aVTZ	-2447.526999	-2447.284534	-2447.258586	-2447.340376	
8	opt/freq	pbe0	cc-pVDZ	-2445.615305	-2445.372174	-2445.34675	-2445.42648	167.81
	SPE	wb97xd	aVTZ	-2447.525601	-2447.28247	-2447.257046	-2447.336776	
9	opt/freq	pbe0	cc-pVDZ	-2445.616777	-2445.373769	-2445.348181	-2445.429306	170.74
10	opt/freq	pbe0	cc-pVDZ	-2445.61532	-2445.372269	-2445.346747	-2445.427671	170.32
11	opt/freq	pbe0	cc-pVDZ	-2445.614259	-2445.370672	-2445.345404	-2445.42545	168.47
12	opt/freq	pbe0	cc-pVDZ	-2445.613686	-2445.370366	-2445.344859	-2445.425797	170.35
13	opt/freq	pbe0	cc-pVDZ	-2445.609028	-2445.365275	-2445.340596	-2445.418311	163.57
14	opt/freq	pbe0	cc-pVDZ	-2445.60594	-2445.362909	-2445.337688	-2445.417002	166.93
15	opt/freq	pbe0	cc-pVDZ	-2445.605428	-2445.361733	-2445.336736	-2445.41513	165.00
16	opt/freq	pbe0	cc-pVDZ	-2445.605068	-2445.362211	-2445.336451	-2445.418157	171.96
17	opt/freq	pbe0	cc-pVDZ	-2445.603431	-2445.360843	-2445.334862	-2445.417211	173.32
B								
1	opt/freq	pbe0	cc-pVDZ	-2445.595218	-2445.352059	-2445.32855	-2445.401307	153.13
	SPE	wb97xd	aVTZ	-2447.510017	-2447.266858	-2447.243349	-2447.316106	
	SPE (solvent)	wb97xd	aVTZ	-2447.558232	-2447.315073	-2447.291564	-2447.364321	
2	opt/freq	pbe0	cc-pVDZ	-2445.578884	-2445.33593	-2445.31145	-2445.391372	168.21
	SPE	wb97xd	aVTZ	-2447.494648	-2447.253066	-2447.227359	-2447.311695	

	SPE (solvent)	wb97xd	aVTZ	-2447.550017	-2447.308435	-2447.282728	-2447.367064	
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3	opt/freq	pbe0	cc-pVDZ	-2445.575971	-2445.333442	-2445.308508	-2445.389909	171.32
	SPE	wb97xd	aVTZ	-2447.493468	-2447.250939	-2447.226005	-2447.307406	
4	opt/freq	pbe0	cc-pVDZ	-2445.572369	-2445.330522	-2445.305033	-2445.388054	174.73
	SPE	wb97xd	aVTZ	-2447.490885	-2447.249038	-2447.223549	-2447.30657	
5	opt/freq	pbe0	cc-pVDZ	-2445.569986	-2445.328404	-2445.302697	-2445.387033	177.50
	SPE	wb97xd	aVTZ	-2447.488054	-2447.246472	-2447.220765	-2447.305101	
6	opt/freq	pbe0	cc-pVDZ	-2445.562973	-2445.321143	-2445.295496	-2445.377576	172.75
	SPE	wb97xd	aVTZ	-2447.483994	-2447.242164	-2447.216517	-2447.298597	
7	opt/freq	pbe0	cc-pVDZ	-2445.564921	-2445.323781	-2445.297958	-2445.383087	179.17
	SPE	wb97xd	aVTZ	-2447.482214	-2447.241074	-2447.215251	-2447.30038	
8	opt/freq	pbe0	cc-pVDZ	-2445.562869	-2445.322113	-2445.295738	-2445.38227	182.12
	SPE	wb97xd	aVTZ	-2447.48167	-2447.240914	-2447.214539	-2447.301071	
9	opt/freq	pbe0	cc-pVDZ	-2445.560241	-2445.319654	-2445.293134	-2445.38067	184.23
	SPE	wb97xd	aVTZ	-2447.479628	-2447.239041	-2447.212521	-2447.300057	

Table S2: XYZ coordinates
compound
structure
charge multiplicity
atom XYZ coordinates

1,3,5-trihydroxybenzene
1

gas

0 1

C	-1.21336400	0.70325800	0.00000000
C	0.00000000	1.38829100	0.00000000
C	1.21572200	0.69917500	0.00000000
C	1.20229600	-0.69414600	0.00000000
C	-0.00235800	-1.40243400	0.00000000
C	-1.20229600	-0.69414600	0.00000000
H	-2.17063800	1.22817300	0.00000000
H	2.14894800	1.26574100	0.00000000
H	0.02169000	-2.49391400	0.00000000
O	2.34323400	-1.42582000	0.00000000
H	3.09219200	-0.81694600	0.00000000
O	0.06318000	2.74221000	0.00000000
H	-0.83860000	3.08639000	0.00000000
O	-2.40641300	-1.31639000	0.00000000
H	-2.25359200	-2.26944400	0.00000000

solvent

0 1

C	-0.00145300	-1.40493700	0.00000000
C	-1.20246100	-0.69492200	0.00000000
C	-1.21549300	0.70364100	0.00000000
C	0.00000000	1.38861900	0.00000000
C	1.21812800	0.70123600	0.00000000
C	1.20294500	-0.69391000	0.00000000
H	0.00880400	-2.49709700	0.00000000
H	-2.16574900	1.24191200	0.00000000
H	2.15911700	1.25566100	0.00000000
O	0.06071200	2.74359500	0.00000000
H	-0.84035200	3.10116900	0.00000000
O	-2.40703200	-1.31841800	0.00000000
H	-2.26885500	-2.27797600	0.00000000
O	2.34525800	-1.42497300	0.00000000
H	3.10552900	-0.82365700	0.00000000

2

0 1

C	0.01197800	-1.41565500	0.00000000
C	-1.19084400	-0.71496100	0.00000000
C	-1.21033200	0.68442500	0.00000000
C	0.00000000	1.38055600	0.00000000
C	1.21564500	0.69777600	0.00000000
C	1.20859400	-0.69863900	0.00000000
H	0.01832000	-2.50450200	0.00000000
H	-2.16140400	1.22616800	0.00000000
H	2.14609800	1.26890700	0.00000000
O	0.05350600	2.73555300	0.00000000
H	-0.84914000	3.07652200	0.00000000
O	-2.33262800	-1.44567200	0.00000000
H	-3.08352200	-0.83989500	0.00000000
O	2.35658300	-1.41811900	0.00000000
H	3.09970600	-0.80230600	0.00000000

1,3,5-cyclohexanetrione

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gas

0 1

C	1.13782900	-0.65260400	-0.60638600
C	0.00013300	-1.45803100	0.00000000
C	-1.13771700	-0.65281600	0.60637500
C	-1.27872500	0.73707300	0.02826000
C	-0.00014100	1.55600200	0.00000800
C	1.27859000	0.73730500	-0.02826000
H	2.08023800	-1.21019300	-0.54701800
H	-2.08002500	-1.21057600	0.54699000
H	-0.03023100	2.21853000	-0.88074500
O	-2.33134200	1.17224900	-0.37181400
O	0.00024800	-2.66293700	0.00000500
O	2.33113100	1.17266800	0.37181000
H	0.02982800	2.21851600	0.88077500
H	0.87470600	-0.53675700	-1.67664600
H	-0.87463300	-0.53693200	1.67664100

solvent

0 1

C	1.16734100	0.67087200	0.54268100
C	-0.00001900	1.45828700	0.00000000
C	-1.16736000	0.67084200	-0.54268100
C	-1.27564700	-0.73311700	-0.01519700
C	0.00002000	-1.53974300	-0.00000300
C	1.27566600	-0.73308400	0.01519700
H	2.10641900	1.22530100	0.42363200
H	-2.10645200	1.22524700	-0.42362900
H	-0.00793300	-2.20029800	0.88343800
O	-2.33559200	-1.20857600	0.34072200
O	-0.00003400	2.67188000	-0.00000100
O	2.33562400	-1.20851500	-0.34071900
H	0.00799000	-2.20029200	-0.88344800
H	0.96008100	0.57370800	1.62868600
H	-0.96009900	0.57368500	-1.62868600

2

0 1

C	-1.28288900	0.74067600	0.40058100
C	0.00000000	1.46287300	0.03441700
C	1.28288900	0.74067600	0.40058100
C	1.26688500	-0.73143700	0.03441700
C	0.00000000	-1.48135300	0.40058100
C	-1.26688500	-0.73143700	0.03441700
H	-2.14699300	1.23956700	-0.05287300
H	2.14699300	1.23956700	-0.05287300
H	0.00000000	-2.47913400	-0.05287300
O	2.19980900	-1.27006100	-0.50739600
O	0.00000000	2.54012100	-0.50739600
O	-2.19980900	-1.27006100	-0.50739600
H	0.00000000	-1.59287100	1.50205100
H	-1.37946700	0.79643600	1.50205100
H	1.37946700	0.79643600	1.50205100

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gas

0 1

C	-0.79985000	-1.18052900	0.00205700
C	-1.39068500	0.06484900	0.27199300
C	-0.70397400	1.23734400	-0.08229800
C	0.58618500	1.18067400	-0.63945900
C	1.19330600	-0.07526100	-0.81539700
C	0.49134800	-1.26131400	-0.54112600
O	2.43415800	-0.09773400	-1.33339200
H	2.93649400	-0.84057400	-0.92261100
O	-1.32232900	2.41107000	0.15108000
O	-1.43688100	-2.33610300	0.26983100
H	-2.39903300	-2.21943000	0.07918900
C	1.29357700	2.40363800	-1.12352300
H	2.16137300	2.15311100	-1.74538900
H	0.62889800	3.08898800	-1.67358600
S	1.93401800	3.43482800	0.20755000
O	2.91949700	2.42493600	1.02284000
H	2.35701700	1.88161000	1.60156100
O	2.77632000	4.50254200	-0.31273700
O	0.78149800	3.74158900	1.09832400
C	1.03146500	-2.59334500	-0.93276000
H	0.25079800	-3.36406000	-0.91667400
H	1.51960400	-2.58191700	-1.92105700
S	2.34509600	-3.17993500	0.14973300
O	3.40742900	-2.15186700	0.11838200
O	2.65056300	-4.58868200	-0.10961300
O	1.68254300	-3.05973500	1.63875600
H	1.35002300	-3.94740500	1.85731600
C	-2.67662500	0.17657000	1.01562200
S	-4.12413600	-0.23618700	0.02572000
O	-3.94750600	0.69318500	-1.30448400
H	-4.46914900	1.49855900	-1.14434900
O	-5.35635500	0.15828000	0.71219900
O	-3.92973100	-1.62365200	-0.44841600
H	-0.64984700	3.06361100	0.46648800
H	-2.74834800	-0.53525100	1.85412500
H	-2.83960300	1.19707200	1.38412700

solvent

0 1

C	-0.79188500	-1.18794900	-0.01662100
C	-1.39270200	0.04749000	0.27596800
C	-0.72015400	1.22780300	-0.07774300
C	0.56300000	1.19031700	-0.64907500
C	1.18703800	-0.05607300	-0.82104400
C	0.49768800	-1.25349700	-0.56578600
O	2.44008100	-0.05737700	-1.31840100
H	2.93775700	-0.81240900	-0.93468800
O	-1.35247900	2.39479500	0.16611100
O	-1.41677000	-2.35488200	0.24125700
H	-2.38177100	-2.24700700	0.08835500
C	1.24895300	2.42757600	-1.12451200
H	2.08135300	2.21312800	-1.80636000
H	0.55733600	3.13567100	-1.61016800
S	1.95511500	3.39264200	0.21384500
O	2.97367200	2.37393100	0.95520400
H	2.46648200	1.76939100	1.53370100
O	2.80236800	4.47340400	-0.30011900
O	0.84807700	3.71980400	1.15124700
C	1.05994800	-2.57198400	-0.97375900
H	0.29107600	-3.35414100	-1.02830600
H	1.59748200	-2.52764900	-1.93552000
S	2.31107700	-3.17702000	0.16172200
O	3.35437900	-2.12927300	0.26564900
O	2.70290000	-4.55440100	-0.17135400
O	1.58321800	-3.15496600	1.61075300
H	1.06225000	-3.97703800	1.71606900
C	-2.67024700	0.13192100	1.03848500
S	-4.11379100	-0.20051600	0.02303700
O	-3.94598700	0.79116500	-1.24843300
H	-4.21742200	1.69537600	-0.99056000
O	-5.35276300	0.12147800	0.74578100
O	-3.94380500	-1.55350900	-0.55874800
H	-0.69586800	3.06787600	0.45203200
H	-2.74294200	-0.62692100	1.83540800
H	-2.82710500	1.12706000	1.47529100

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0 1

C	-0.80720300	-1.17852700	-0.00063900
C	-1.40041200	0.06610400	0.26523300
C	-0.71399100	1.23820500	-0.09000400
C	0.57222200	1.17942400	-0.64996500
C	1.18879600	-0.07210100	-0.80422900
C	0.48711100	-1.25936300	-0.53700000
O	2.44192400	-0.09010000	-1.29697300
H	2.92895700	-0.84854600	-0.89431200
O	-1.32945000	2.41399300	0.14590500
O	-1.44484900	-2.33491600	0.26597400
H	-2.40640500	-2.21762900	0.07472100
C	1.28694100	2.39899000	-1.12260900
H	2.14859800	2.14745600	-1.75270400
H	0.62872300	3.09498100	-1.66732000
S	1.93347800	3.42555400	0.21071100
O	2.76312900	2.36573000	1.13342100
H	3.68837800	2.40921200	0.83633800
O	2.86747800	4.42699000	-0.30947100
O	0.77536700	3.82632500	1.03887000
C	1.02787900	-2.59193500	-0.92568700
H	0.24641400	-3.36185600	-0.90485400
H	1.51155600	-2.58495800	-1.91637600
S	2.34669500	-3.18511300	0.14754900
O	3.42135000	-2.16954700	0.09731800
O	2.63726400	-4.59752600	-0.11102400
O	1.70585400	-3.05253600	1.64303500
H	1.35776600	-3.93316700	1.86575500
C	-2.68246700	0.17757800	1.01482400
S	-4.13407900	-0.23402300	0.03107300
O	-3.96534400	0.69911900	-1.29833800
H	-4.47735300	1.50847400	-1.12799300
O	-5.36426500	0.15738200	0.72345300
O	-3.94176500	-1.61973800	-0.44918000
H	-0.65783700	3.06846600	0.45515200
H	-2.74996900	-0.53451700	1.85341300
H	-2.84314300	1.19773900	1.38538300

3

0 1

C	-0.91642900	-1.06952500	0.95583400
C	0.46499400	-1.31490600	0.99263700
C	1.35611800	-0.22949000	0.96222600
C	0.88149500	1.09342900	0.95158800
C	-0.50744500	1.31742300	0.92359200
C	-1.41571400	0.24473600	0.95422800
O	-0.92932600	2.59463500	0.91634400
H	-1.71609300	2.66078400	0.32336700
O	2.67140200	-0.51365200	0.98802500
O	-1.81151000	-2.07511600	0.96785800
H	-1.48015600	-2.79789600	0.38556200
C	1.79830700	2.26566200	1.07662900
H	1.24338100	3.19098500	1.27330400
H	2.56776800	2.12574600	1.85336000
S	2.77512900	2.59700300	-0.39894000
O	1.64633800	2.78132100	-1.56262800
H	1.52284700	1.90463400	-1.96457900
O	3.47946300	3.86543300	-0.27811300
O	3.51401600	1.34404400	-0.72054200
C	-2.88656300	0.46629400	1.08892500
H	-3.41521100	-0.45688300	1.35507200
H	-3.12920000	1.25630300	1.81787900
S	-3.66761800	1.05361600	-0.42302200
O	-2.89925000	2.24970800	-0.86206700
O	-5.11511400	1.10696700	-0.27548500
O	-3.35524600	-0.13809600	-1.49173000
H	-2.45998000	0.01750500	-1.83758200
C	1.01108800	-2.69630700	1.11712500
H	0.44339700	-3.31755700	1.82850900
H	2.07087400	-2.69383900	1.39856000
S	0.90226800	-3.63757700	-0.41488400
O	1.61465600	-2.64683100	-1.50501300
H	2.52704600	-2.96984800	-1.60345500
O	-0.52602700	-3.66414100	-0.79561000
O	1.68574800	-4.87205900	-0.33273300
H	3.15254300	0.14978200	0.43638700

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0 1

C	0.72817800	1.24795200	0.04503700
C	1.39345400	0.03869700	0.31020600
C	0.77973100	-1.17244400	-0.04797900
C	-0.51525200	-1.19343700	-0.59552800
C	-1.20091300	0.02359900	-0.76012200
C	-0.57679300	1.25298700	-0.47662400
O	-2.43620900	-0.03020900	-1.28569700
H	-2.98508200	0.68571600	-0.88397900
O	1.47818500	-2.30331600	0.16724700
O	1.30462300	2.43623000	0.29397500
H	2.26866700	2.37238700	0.08981900
C	-1.13848300	-2.44792800	-1.11217800
H	-2.03158300	-2.23842300	-1.71335500
H	-0.43642900	-3.06082600	-1.70065900
S	-1.68269600	-3.58794100	0.17042800
O	-2.72832900	-2.69198200	1.04754900
H	-2.21950500	-2.34282500	1.79856100
O	-2.43491500	-4.69231300	-0.40826500
O	-0.51003500	-3.84498500	1.05264300
C	-1.18623200	2.54921100	-0.89671200
H	-0.45565700	3.36679700	-0.85813500
H	-1.63704600	2.49942900	-1.90156100
S	-2.56585300	3.07320100	0.13203100
O	-3.53046200	1.93959600	0.16053600
O	-3.00047900	4.41636700	-0.22408400
O	-1.91013500	3.16775500	1.62369300
H	-2.00362800	2.28553800	2.02079500
C	2.69644900	0.00478400	1.03163900
S	4.10120200	0.48555800	0.01005300
O	3.94771600	-0.46379200	-1.30899300
H	4.51422400	-1.23911800	-1.15316300
O	5.36498200	0.16133300	0.67544600
O	3.82251800	1.85597600	-0.46973600
H	0.85570300	-3.01552100	0.45247300
H	2.74476700	0.72901800	1.86108300
H	2.92258900	-1.00103600	1.40700600

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0 1

C	1.37644600	-0.08442300	-0.92832200
C	0.58233500	-1.24316900	-0.94691400
C	-0.81829200	-1.11759500	-0.92941500
C	-1.42881300	0.14810700	-0.92349700
C	-0.61521000	1.29567500	-0.89785000
C	0.78630200	1.19219000	-0.93248000
O	-1.23062100	2.49133000	-0.89752200
H	-0.72070600	3.10857400	-0.31940000
O	-1.53687800	-2.25300500	-0.97240100
O	2.71955300	-0.14134900	-0.96285600
H	3.03117400	-0.90418300	-0.42120200
C	-2.90608500	0.31804800	-1.05752900
H	-3.17382800	1.36512900	-1.24378000
H	-3.33981400	-0.31781800	-1.84661000
S	-3.84734000	-0.16420500	0.39933900
O	-3.17572500	0.72874800	1.58952700
H	-2.54975600	0.14006500	2.04504800
O	-5.23737300	0.25032200	0.26915000
O	-3.50204100	-1.58221200	0.69554200
C	1.65735000	2.39543200	-1.08653900
H	2.68536700	2.12215600	-1.35287100
H	1.26131600	3.11206000	-1.82418700
S	1.79258200	3.38794600	0.40924700
O	0.40349900	3.70383900	0.83915700
O	2.78275800	4.44296200	0.24533600
O	2.40387400	2.34036500	1.49974400
H	1.65086000	1.85360700	1.87583100
C	1.18259600	-2.60650300	-1.05361400
H	2.00264100	-2.66240500	-1.78591500
H	0.41713700	-3.35874400	-1.27753500
S	1.94122300	-3.10368500	0.50063500
O	2.55183900	-4.57302900	0.10852500
H	2.06174700	-5.21195300	0.65488600
O	0.95856800	-3.29597200	1.56986800
O	3.10528900	-2.21318400	0.70450500
H	-2.35127900	-2.14446300	-0.42343800

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0 1

C	1.28848000	0.55974200	-0.91540500
C	1.11451300	-0.83433900	-0.92289600
C	-0.18807500	-1.36290800	-0.90066600
C	-1.30784700	-0.51561100	-0.92832600
C	-1.11385400	0.87679700	-0.92094100
C	0.17960500	1.42555300	-0.93818800
O	-2.21136100	1.65380600	-0.95364800
H	-2.05674400	2.44856900	-0.38638100
O	-0.30962700	-2.70210800	-0.91452600
O	2.50863700	1.12331400	-0.94494200
H	3.13336600	0.58862500	-0.39940300
C	-2.69871000	-1.04850600	-1.03634600
H	-3.41091000	-0.24489800	-1.25782100
H	-2.79353700	-1.85982600	-1.77442500
S	-3.24882000	-1.79476200	0.50664400
O	-4.74340800	-2.32547200	0.08762100
H	-5.36236300	-1.80474800	0.62844100
O	-2.42530800	-3.00774100	0.70585700
O	-3.40816100	-0.81486800	1.58275900
C	0.41108200	2.89434700	-1.07420200
H	1.46075500	3.11918100	-1.29745500
H	-0.23813900	3.36023000	-1.83307700
S	0.02382100	3.82702100	0.41738600
O	-1.39745200	3.53465000	0.74763500
O	0.49423600	5.20106300	0.30768400
O	0.93874600	3.10809700	1.55832400
H	0.43008100	2.34881700	1.89279100
C	2.27197000	-1.77197900	-1.03071200
H	3.01632800	-1.45147400	-1.77597100
H	1.93408200	-2.79309600	-1.24320900
S	3.20583700	-1.86360900	0.50565400
O	4.42620200	-2.86979500	0.07017800
H	4.31603800	-3.66198300	0.62431200
O	2.46001100	-2.50835300	1.58779600
O	3.82025400	-0.53221900	0.70550500
H	-1.08750600	-2.96937600	-0.36859800

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0 1

C	-0.06624400	-1.39746800	-0.88496500
C	-1.25528800	-0.64841300	-0.89901900
C	-1.17712100	0.75610300	-0.88496500
C	0.06610200	1.41131700	-0.89901900
C	1.24336500	0.64136500	-0.88496500
C	1.18918600	-0.76290500	-0.89901900
O	2.41319400	1.30384800	-0.91965000
H	3.07415900	0.82089500	-0.36901800
O	-2.33576300	1.43796300	-0.91965000
O	-0.07743100	-2.74181100	-0.91965000
H	-0.82616400	-3.07274700	-0.36901800
C	0.17630500	2.89026700	-1.06839300
H	1.20603700	3.19495700	-1.29162400
H	-0.49776800	3.28119600	-1.84820600
S	-0.30298000	3.84823600	0.37661300
O	0.69391200	3.27574500	1.53937700
H	0.13227100	2.73109200	2.11613000
O	0.00000000	5.25876800	0.17541500
O	-1.67383000	3.41392900	0.76500600
C	2.41489200	-1.59781800	-1.06839300
H	2.16389500	-2.64193700	-1.29162400
H	3.09048300	-1.20951900	-1.84820600
S	3.48416000	-1.66173000	0.37661300
O	3.79346400	-0.25738500	0.76500600
O	4.55422700	-2.62938400	0.17541500
O	2.48992200	-2.23881800	1.53937700
H	2.29905900	-1.48009600	2.11613000
C	-2.59119700	-1.29244900	-1.06839300
H	-2.59271600	-2.07167700	-1.84820600
H	-3.36993200	-0.55301900	-1.29162400
S	-3.18118000	-2.18650600	0.37661300
O	-3.18383500	-1.03692700	1.53937700
H	-2.43133100	-1.25099600	2.11613000
O	-2.11963400	-3.15654400	0.76500600
O	-4.55422700	-2.62938400	0.17541500
H	-2.24799500	2.25185200	-0.36901800

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C	-0.10808300	-1.39480800	-0.86359900
C	-1.27238500	-0.60971100	-0.88265900
C	-1.15389800	0.79100700	-0.86359900
C	0.10816700	1.40677300	-0.88265900
C	1.26198100	0.60380100	-0.86359900
C	1.16421800	-0.79706200	-0.88265900
O	2.45052100	1.23259100	-0.89537100
H	3.10590100	0.72842000	-0.35558800
O	-2.29271600	1.50591800	-0.89537100
O	-0.15780600	-2.73850900	-0.89537100
H	-0.92212000	-3.05399900	-0.35558800
C	0.26168900	2.88645400	-1.01216400
H	1.30313300	3.15619500	-1.22354300
H	-0.40789400	3.32209400	-1.76999100
S	-0.17967900	3.75768300	0.50080800
O	0.00000000	5.31771100	0.01969000
H	0.72610800	5.66966100	0.56321500
O	-1.63246700	3.55599500	0.69674400
O	0.76319500	3.51984400	1.59437700
C	2.36889800	-1.66985700	-1.01216400
H	2.08177900	-2.70664400	-1.22354300
H	3.08096500	-1.30780100	-1.76999100
S	3.34408800	-1.72323500	0.50080800
O	2.66667700	-2.42086900	1.59437700
O	3.89581500	-0.36424000	0.69674400
O	4.60527300	-2.65885500	0.01969000
H	4.54701600	-3.46365900	0.56321500
C	-2.63058800	-1.21659800	-1.01216400
H	-2.67307100	-2.01429300	-1.76999100
H	-3.38491100	-0.44955100	-1.22354300
S	-3.16441000	-2.03444800	0.50080800
O	-4.60527300	-2.65885500	0.01969000
H	-5.27312400	-2.20600200	0.56321500
O	-3.42987200	-1.09897600	1.59437700
O	-2.26334800	-3.19175500	0.69674400
H	-2.18378100	2.32557900	-0.35558800

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C	-0.54519200	1.32566000	-0.08170600
C	0.74037300	1.11767600	-0.61281800
C	1.20267700	-0.20024200	-0.77440400
C	0.37101800	-1.30141300	-0.49794600
C	-0.92143900	-1.06853700	0.00386800
C	-1.37465400	0.23967800	0.24926800
O	-1.68573700	-2.14450200	0.25883300
H	-2.63289000	-1.93350700	0.07651200
O	2.43446400	-0.36396900	-1.28503400
O	-1.02630300	2.55811600	0.14829300
H	-0.28708200	3.14599900	0.43540300
C	0.75402300	-2.68543400	-0.90502300
H	-0.10648400	-3.36520000	-0.87672500
H	1.22287600	-2.71881000	-1.90229000
S	2.00616400	-3.43410600	0.14786100
O	1.32454800	-3.39652900	1.63087700
H	1.55139500	-2.53295200	2.01496800
O	2.20125800	-4.83719100	-0.18907900
O	3.15516500	-2.48845000	0.18048900
C	-2.67365600	0.50168200	0.93579500
H	-2.85819200	-0.17795900	1.78160700
H	-2.74486800	1.54848100	1.25730000
S	-4.06976700	0.21772500	-0.16444200
O	-4.13513300	-1.25076200	-0.41346600
O	-4.09288700	1.15412800	-1.27885000
O	-5.32325400	0.54777000	0.84121500
H	-5.84953300	-0.27024000	0.87142900
C	1.58176200	2.24422200	-1.11478100
H	1.00323600	2.97844000	-1.69885200
H	2.42495100	1.88313500	-1.71606400
S	2.31670300	3.25537000	0.18032500
O	3.17559400	2.17450800	1.05365100
H	2.61683900	1.94231800	1.81428700
O	1.20594700	3.71241400	1.06118300
O	3.26062300	4.20932200	-0.38507800
H	2.84641400	-1.16212900	-0.87527300

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C	1.21982700	0.06161400	-0.73979700
C	0.54837500	1.26575700	-0.46774100
C	-0.77000200	1.21929300	0.01512900
C	-1.41136300	-0.01122300	0.23964600
C	-0.74006300	-1.20178100	-0.08635100
C	0.56706800	-1.17494700	-0.60174100
O	-1.39809300	-2.35570100	0.12607300
H	-0.76365000	-3.05602800	0.40911100
O	-1.37638100	2.39096100	0.26512800
O	2.47022500	0.04475300	-1.23343500
H	2.99921700	0.77294800	-0.82860900
C	-2.73196700	-0.08966700	0.92927200
H	-2.94228600	-1.11498300	1.25737200
H	-2.81520800	0.61146600	1.77431000
S	-4.08861600	0.38139900	-0.15628200
O	-5.36137100	0.30479000	0.87741500
H	-5.92594900	-0.40987500	0.53556700
O	-3.89853800	1.81580000	-0.46735700
O	-4.32864100	-0.58643800	-1.22866700
C	1.25690300	-2.41498300	-1.06577500
H	0.59874600	-3.07740500	-1.64812400
H	2.16159600	-2.17623400	-1.63805400
S	1.80204200	-3.43558200	0.31355800
O	0.57758000	-3.98203500	0.96576300
O	2.83259300	-2.78339700	1.10836400
O	2.47253000	-4.70431700	-0.48477500
H	1.94131600	-5.47704100	-0.22550200
C	1.14924900	2.58692400	-0.81387500
H	0.39964400	3.38625000	-0.75786100
H	1.64307600	2.58701100	-1.79770900
S	2.46013300	3.04341700	0.33059900
O	2.93534600	4.48146000	-0.30442900
H	3.86819700	4.35389600	-0.54958800
O	3.59611100	2.10990200	0.08703500
O	1.96263100	3.26626600	1.68050400
H	-2.34174400	2.30998600	0.07755300

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C	-0.73029800	1.22369700	-0.09002800
C	0.55264800	1.15580500	-0.65225400
C	1.15799600	-0.10325500	-0.81497500
C	0.46208700	-1.28571000	-0.50693100
C	-0.83449600	-1.19081100	0.02782800
C	-1.42337800	0.06035500	0.27837400
O	-1.47937400	-2.33721700	0.30532100
H	-2.43957800	-2.21973800	0.11118500
O	2.38568700	-0.12368400	-1.35643900
O	-1.34736500	2.40478200	0.13553200
H	-0.67959200	3.07200000	0.39263800
C	0.99523900	-2.62999300	-0.87559400
H	0.22362100	-3.40397000	-0.78199500
H	1.42778000	-2.65476800	-1.88924500
S	2.36670400	-3.17546700	0.15570600
O	1.77686400	-3.04269600	1.67045300
H	1.98091600	-2.13859100	1.96685500
O	2.65479800	-4.58545400	-0.06682200
O	3.43594900	-2.14932100	0.02010800
C	-2.71100500	0.18257600	1.01751200
H	-2.78721100	-0.52554100	1.85882000
H	-2.87284000	1.20448800	1.38180700
S	-4.15945100	-0.22926600	0.02771400
O	-5.39194100	0.17870100	0.70724800
O	-3.97183300	-1.62015600	-0.43635800
O	-3.97647600	0.69965900	-1.30377400
H	-4.55677000	1.46901200	-1.17214700
C	1.28507600	2.36642400	-1.11484500
H	0.64227100	3.13063100	-1.57467500
H	2.08852300	2.09693000	-1.81360400
S	2.16646400	3.24024500	0.20121600
O	0.81496500	3.84970700	1.01497500
H	0.97020200	4.80883700	1.07215200
O	2.84946300	4.42221800	-0.33758300
O	2.82382000	2.30201300	1.10310200
H	2.90354200	-0.87043700	-0.96658700

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C	-0.77209200	1.17097900	-0.04429500
C	0.51786000	1.18475000	-0.60379600
C	1.19491100	-0.03496800	-0.77717000
C	0.56938400	-1.26136400	-0.48503700
C	-0.73168500	-1.24809100	0.04594300
C	-1.39963300	-0.03987500	0.30086400
O	-1.29792900	-2.44131200	0.31443400
H	-2.26623500	-2.37089500	0.18850000
O	2.42630000	0.01163200	-1.31347800
O	-1.45298400	2.30082900	0.20219400
H	-0.82110200	3.01123300	0.46742600
C	1.18091100	-2.56046400	-0.89183600
H	0.45477600	-3.38140100	-0.84828800
H	1.63526100	-2.51816900	-1.89546100
S	2.55956700	-3.07380600	0.14542900
O	1.90206500	-3.14254600	1.63766300
H	2.00477800	-2.25645000	2.02399700
O	2.98642800	-4.42471700	-0.19089400
O	3.52834900	-1.94432600	0.15564400
C	-2.70551100	0.00399500	1.01162200
H	-2.82009700	-0.77260900	1.78299700
H	-2.87614200	0.99122300	1.46249600
S	-4.15248800	-0.21851500	-0.04837900
O	-4.03385700	0.49449800	-1.32261200
O	-5.35919100	-0.15021600	0.77047700
O	-3.88042600	-1.84479500	-0.41785900
H	-4.02997200	-1.91770900	-1.37729100
C	1.14615600	2.43720600	-1.11915100
H	0.44148000	3.06043500	-1.69359000
H	2.02813200	2.22344700	-1.73504300
S	1.71992600	3.56447000	0.16110400
O	2.75908100	2.64393700	1.02276600
H	2.27690100	2.38186300	1.82510000
O	0.56365400	3.83346000	1.06062300
O	2.47837900	4.66074600	-0.42522200
H	2.97941300	-0.69589600	-0.90406500

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C	0.32459400	-1.09511000	1.38288500
C	1.23982200	-0.03052300	1.41790600
C	0.82378900	1.28831800	1.15255700
C	-0.55198700	1.52838700	1.00495800
C	-1.49765400	0.49502100	1.07112200
C	-1.02413700	-0.82611500	1.14521300
O	-1.05594300	2.76979800	0.80746500
H	-0.36921700	3.42952600	0.96207800
O	2.51931700	-0.35659300	1.64838200
H	3.14357900	0.14793500	1.06612000
O	-1.83668000	-1.89304200	0.95050000
H	-2.62422400	-1.62020400	0.41322600
C	0.87628500	-2.47091300	1.25860000
S	1.24133200	-2.78858500	-0.50472200
H	1.84784800	-2.57581400	1.75504200
O	-0.21915300	-3.26655400	-1.04814600
O	1.58872400	-1.50559700	-1.15902600
O	2.13135100	-3.93265900	-0.66364400
H	-0.90337600	-2.74219300	-0.58081900
C	-2.95009600	0.83258100	1.06427900
S	-3.77756200	0.50440900	-0.50561000
H	-3.53436100	0.22387100	1.77347400
O	-2.81261500	1.23051000	-1.59879700
O	-3.62210800	-0.94727700	-0.75402600
O	-5.09781000	1.13524500	-0.54756200
H	-3.23993800	2.07507500	-1.82398700
C	1.83755100	2.34464600	0.87070100
S	2.82654400	1.96391500	-0.62716700
H	1.42163800	3.33839800	0.65714300
O	1.79215800	1.20793600	-1.59565800
O	3.21543100	3.20933200	-1.27744900
O	3.85826400	0.99202200	-0.17870700
H	1.77941100	0.23076000	-1.40453200
H	2.60234300	2.45432800	1.65523400
H	-3.12306400	1.89384400	1.28048600
H	0.19785100	-3.27406300	1.57054700

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C	0.24226700	-1.06155500	1.35484500
C	1.16969800	-0.00881500	1.38812100
C	0.77896200	1.30680000	1.07209900
C	-0.59134900	1.55745400	0.87523300
C	-1.55162500	0.54105800	0.99081100
C	-1.11412500	-0.78588600	1.14800300
O	-1.07962000	2.78987400	0.62183500
H	-0.36761100	3.43986600	0.63094300
O	2.43394400	-0.34406100	1.68844200
H	3.09657500	0.15906000	1.15139500
O	-1.96415000	-1.82480200	1.13537500
H	-2.67713500	-1.66492200	0.47322000
C	0.77030100	-2.44708700	1.22726900
S	1.19060000	-2.65769800	-0.53442900
H	1.70178800	-2.60892600	1.78031500
O	2.17678100	-3.96740300	-0.48697700
O	-0.00496800	-2.99941300	-1.29628400
O	2.06586300	-1.54233200	-0.99053800
H	3.05092000	-3.63730600	-0.75876500
C	-3.00415500	0.88169800	0.96279000
S	-3.75178200	0.46830500	-0.62407600
H	-3.58365900	0.29690000	1.69266400
O	-5.31286600	0.89671400	-0.34444100
O	-3.22590800	1.28978400	-1.70483200
O	-3.75896100	-1.01623100	-0.72961400
H	-5.82444400	0.07603900	-0.45205100
C	1.81483600	2.35271500	0.83625100
S	2.92644800	1.95165500	-0.56694400
H	1.42127900	3.34405100	0.57358700
O	1.99259800	1.14572400	-1.59542200
O	3.34980700	3.18641700	-1.21668700
O	3.93742800	1.01044100	-0.01319500
H	2.00349300	0.17324900	-1.37758800
H	2.51713800	2.48144500	1.67504400
H	-3.17870700	1.95442500	1.10989500
H	0.02766900	-3.22603900	1.43471100

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C	0.26521400	-1.12956000	1.34762200
C	1.17349300	-0.06580800	1.41326800
C	0.76401900	1.25533200	1.14584400
C	-0.61015200	1.49184400	0.95736900
C	-1.55398200	0.46030700	1.04200300
C	-1.09647500	-0.86487400	1.15679500
O	-1.11177000	2.72865200	0.72931800
H	-0.42637300	3.39327600	0.86425400
O	2.45296400	-0.38866800	1.68359100
H	3.08026000	0.15791400	1.15465400
O	-1.93413100	-1.90994200	1.11570100
H	-2.64004400	-1.73704600	0.44800100
C	0.79857600	-2.50848800	1.20446000
S	1.20115200	-2.82954000	-0.54707200
H	1.72845300	-2.68757200	1.75536700
O	2.06330900	-1.45201500	-0.99087900
O	2.14988900	-3.94428200	-0.62573200
O	-0.01135400	-2.75389400	-1.35412900
H	2.99758100	-1.61540400	-0.77218200
C	-3.00827900	0.78619600	1.03532100
S	-3.83753900	0.41497600	-0.52335400
H	-3.57419600	0.17574800	1.75742600
O	-2.88943400	1.15672700	-1.62671300
O	-3.67149800	-1.03329200	-0.75629800
O	-5.16306900	1.03940000	-0.56603600
H	-3.36709600	1.96361700	-1.88480300
C	1.78405400	2.31944700	0.92434600
S	2.80880200	1.99994500	-0.56130800
H	1.37920800	3.32428500	0.74295300
O	1.78542500	1.32031100	-1.60403800
O	3.25873300	3.26174000	-1.13446100
O	3.79715000	0.96078200	-0.15440400
H	1.76680800	0.34400500	-1.43809900
H	2.53083700	2.39983300	1.73025000
H	-3.19744000	1.84857100	1.23036600
H	0.05483200	-3.28383200	1.43004100

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C	-0.07554300	-1.26947100	1.16848500
C	1.19705000	-0.69927500	1.07359700
C	1.36168800	0.69500200	1.01567800
C	0.22522000	1.50665200	0.90563000
C	-1.05950200	0.96582300	1.02906400
C	-1.20085200	-0.42998600	1.14641600
O	0.34128800	2.85016700	0.74635900
H	1.02546700	3.01122600	0.07421900
O	2.27350100	-1.51692300	1.07092000
H	2.85330300	-1.24475500	0.33043800
O	-2.41113000	-1.00905100	1.24478300
H	-3.01710400	-0.61554700	0.57646700
C	-0.23849200	-2.75218200	1.15194300
S	-0.34779100	-3.32458600	-0.56087400
H	0.62697900	-3.27187200	1.57923800
O	-0.51779800	-4.94430800	-0.29280100
O	-1.58938800	-2.83890100	-1.15930400
O	0.94630700	-3.14613700	-1.23820200
H	0.27992000	-5.34069800	-0.68233700
C	-2.24620800	1.87133500	1.03225400
S	-3.09355400	1.79402500	-0.55342200
H	-3.00346500	1.57261700	1.77171400
O	-4.31253800	2.86673300	-0.31478300
O	-2.24206600	2.29041700	-1.62763700
O	-3.74141100	0.46001100	-0.64653400
H	-5.12995000	2.34436400	-0.39150300
C	2.71753000	1.29938600	1.12595300
S	3.54523100	1.35071700	-0.47062500
H	2.70106400	2.33350100	1.49740000
O	2.41320000	2.20805900	-1.33034900
O	4.75525900	2.16126200	-0.42901500
O	3.54638100	-0.02419900	-1.01499300
H	1.96644200	1.56750400	-1.91377800
H	3.38923700	0.69628000	1.75577600
H	-1.95941800	2.92023000	1.17378600
H	-1.17284400	-3.07608300	1.62565400

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C	-0.22780300	-1.28007500	1.12445700
C	1.10291400	-0.86960900	1.02509500
C	1.43405700	0.49276300	0.98080100
C	0.41105300	1.43929100	0.84004100
C	-0.93096800	1.06119600	0.96747600
C	-1.24119200	-0.30616800	1.10306700
O	0.70481700	2.74969400	0.65797300
H	1.40857300	2.80455500	-0.01902800
O	2.07873700	-1.81000500	1.01606800
H	2.67049100	-1.61790500	0.26427000
O	-2.50964900	-0.73377700	1.22314200
H	-3.08373900	-0.25297600	0.58267400
C	-0.57357900	-2.73092600	1.13259400
S	-0.75177600	-3.33044300	-0.56477500
H	0.21784100	-3.34690200	1.57553800
O	-1.16392400	-4.89830900	-0.24531900
O	-1.90210000	-2.68500700	-1.19276000
O	0.56059100	-3.37419900	-1.22840800
H	-0.44158000	-5.42123000	-0.63236700
C	-1.99279000	2.11062600	0.99403900
S	-2.94074700	2.13507900	-0.53661900
H	-2.74262400	1.92810200	1.77805400
O	-4.02116800	3.32758200	-0.20326900
O	-2.12272500	2.55122900	-1.66691100
O	-3.73691300	0.88022700	-0.58715200
H	-4.89214600	2.89518700	-0.23633200
C	2.85425000	0.92623400	1.11936500
S	3.55099600	1.05716300	-0.52247000
H	2.94720600	1.91985800	1.57974800
O	5.09588700	1.52835700	-0.24849600
O	3.59040400	-0.28773500	-1.10783100
O	2.87998000	2.18433600	-1.20916700
H	5.17885500	2.40406000	-0.66493200
H	3.46085600	0.18857200	1.66283500
H	-1.56449900	3.11499700	1.09747700
H	-1.54194700	-2.92424500	1.60932600

B

I

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C	-0.05456600	1.51452100	1.73257400
C	-1.33322800	0.70757000	1.55166900
C	-1.28433100	-0.80451600	1.73257400
C	0.05384000	-1.50839400	1.55166900
C	1.33889700	-0.71000500	1.73257400
C	1.27938800	0.80082400	1.55166900
O	0.09272800	-2.70409300	1.39780400
O	-2.38817700	1.27174200	1.39780400
O	2.29544900	1.43235100	1.39780400
H	-0.06526300	1.74007700	2.82143800
C	-0.08489000	2.86615600	1.03414100
S	0.00000000	2.77415600	-0.77233900
H	-1.00180400	3.42286800	1.26349600
O	-1.51193500	2.52302900	-1.22862300
O	0.39619700	4.09036300	-1.25451700
O	0.77435500	1.55887900	-1.12620000
H	-1.68339500	1.53993100	-1.24868500
H	0.80121900	3.45497000	1.30314900
H	1.53958200	-0.81351900	2.82143800
C	2.52460900	-1.35956100	1.03414100
S	2.40249000	-1.38707800	-0.77233900
H	3.46519300	-0.84384600	1.26349600
O	2.94097500	0.04786000	-1.22862300
O	3.34426000	-2.38829800	-1.25451700
O	0.96285100	-1.45005100	-1.12620000
H	2.17531700	0.68789700	-1.24868500
H	2.59148200	-2.42136100	1.30314900
H	-1.47431900	-0.92655800	2.82143800
C	-2.43971900	-1.50659500	1.03414100
S	-2.40249000	-1.38707800	-0.77233900
H	-2.46338900	-2.57902200	1.26349600
O	-1.42904000	-2.57088900	-1.22862300
O	-3.74045700	-1.70206500	-1.25451700
O	-1.73720600	-0.10882800	-1.12620000
H	-0.49192200	-2.22782800	-1.24868500
H	-3.39270100	-1.03360900	1.30314900

2

gas

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C	-1.37538000	-0.55546700	0.04631100
C	-0.92311800	0.83076500	0.45391800
C	0.22395000	1.39265000	-0.35720800
C	1.35002300	0.38973900	-0.58003800
C	1.18579700	-1.00271700	-0.01210000
C	-0.22969900	-1.54679700	-0.04574600
O	2.36577500	0.73575000	-1.14265000
O	-1.49261600	1.45863900	1.32084600
O	-0.42921200	-2.74047700	-0.11235300
H	-1.70833300	-0.45710100	-1.01393800
C	-2.57725000	-1.05942700	0.82850800
S	-3.62255700	-2.15935300	-0.16742800
H	-2.32039500	-1.59333400	1.75307200
O	-3.02415300	-3.62308000	0.18288000
O	-4.97412300	-2.13775900	0.37694600
O	-3.33824900	-1.83696300	-1.57659700
H	-2.07871900	-3.59296200	-0.08530500
H	-3.22949400	-0.21428300	1.08745100
H	-0.21620700	1.56256500	-1.36271600
C	0.77283200	2.72855900	0.12077600
S	-0.40432800	4.08624300	-0.14403600
H	1.05112500	2.73354400	1.18346200
O	-1.11962800	4.20675400	1.30562000
O	0.34175900	5.32517400	-0.32374600
O	-1.37734600	3.60468600	-1.13823500
H	-1.52021600	3.32643400	1.47676800
H	1.65125800	2.99838800	-0.48062500
H	1.36652900	-0.81778500	1.07609200
C	2.22327400	-2.00995800	-0.46677500
S	3.84148400	-1.70454500	0.29756600
H	1.93651500	-3.01598400	-0.13320900
O	4.61381400	-0.86066200	-0.84976300
O	3.58960700	-0.83816300	1.46337900
O	4.55829900	-2.96764200	0.41536500
H	4.05272000	-0.07325500	-1.02280100
H	2.36764100	-2.02789300	-1.55529800

solvent

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C	1.41291100	-0.50524700	0.01559500
C	0.95012100	0.88142400	-0.37042500
C	-0.26334800	1.38782800	0.36766600
C	-1.37016500	0.34960000	0.50130800
C	-1.13742200	-1.02935800	-0.06523500
C	0.29077300	-1.52263100	0.03925400
O	-2.42871000	0.66895400	1.00190500
O	1.57632500	1.56230000	-1.15862800
O	0.52393700	-2.71265100	0.11452900
H	1.68796800	-0.40134000	1.08919200
C	2.64154900	-0.94127600	-0.76623700
S	3.71946100	-2.05843500	0.13659000
H	2.40641100	-1.42179300	-1.72634900
O	3.05845400	-3.50836100	-0.09968100
O	5.02486300	-2.11260500	-0.53522800
O	3.65791000	-1.71030100	1.56966200
H	2.08106200	-3.40578400	0.07433800
H	3.27889600	-0.06669800	-0.96229200
H	0.08907400	1.52950700	1.41088500
C	-0.85118300	2.69519700	-0.14222400
S	0.19966200	4.13082100	0.12052100
H	-1.09629200	2.66907000	-1.21363000
O	1.09200900	4.19820000	-1.22135500
O	-0.62824000	5.34425000	0.08976600
O	1.06726200	3.87285600	1.28544800
H	1.45708000	3.28244500	-1.35432400
H	-1.76372200	2.92761300	0.42525600
H	-1.24410500	-0.85135000	-1.16279400
C	-2.12384500	-2.09658100	0.37026500
S	-3.79164300	-1.87267100	-0.26078600
H	-1.81800300	-3.06848200	-0.04136400
O	-4.52402100	-0.99971600	0.88107000
O	-3.72056800	-1.09651700	-1.51366000
O	-4.48425600	-3.16803600	-0.24971700
H	-3.93165500	-0.21936700	1.04445700
H	-2.20248200	-2.18996700	1.46273900

3

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C 1.00316300 -1.18283300 0.15360400
C -0.49643400 -1.41323000 0.21347500
C -1.20042400 -0.31106600 0.99148400
C -0.87871700 1.12057300 0.56292700
C 0.32802000 1.19350000 -0.34745000
C 1.46402100 0.25979500 0.02646200
H -0.79956100 -1.25702000 -0.84805600
H -0.57067500 1.65463600 1.48398200
H 1.74334000 0.52661900 1.07245000
O 0.42643200 1.96958400 -1.27476900
O -1.99030600 -0.54301600 1.86946700
O 1.78581300 -2.10665500 0.18820900
C -2.13969800 1.80533700 0.05155100
S -1.99576400 3.61666500 0.03762700
H -2.43932100 1.49113300 -0.95795200
O -1.51596600 3.91073900 -1.48173100
O -3.33342200 4.18575200 0.15092700
O -0.91461600 3.95895200 0.97450000
H -0.66806600 3.42335400 -1.58649400
C 2.71080400 0.44832700 -0.82161500
S 4.22405900 0.04611300 0.09516400
H 2.71713600 -0.14193100 -1.74763100
O 4.44044600 -1.52013800 -0.25646600
O 5.34238500 0.75255400 -0.51686600
O 3.89468100 0.18808700 1.52398700
H 3.62684700 -1.97646300 0.05532200
C -0.88646300 -2.81009900 0.64100000
S -2.21573600 -3.44317500 -0.38794200
H -0.05405400 -3.51305200 0.49498900
O -3.39307300 -2.32768300 -0.13528700
O -1.82302200 -3.24727300 -1.78381200
O -2.65979600 -4.72725100 0.15270000
H -3.88660900 -2.60242900 0.65683000
H 2.82100400 1.50814800 -1.08882600
H -2.96605500 1.60520300 0.74775500
H -1.22702500 -2.84288300 1.68456700

4

0 1

C	-0.85462800	-1.27697500	-0.22219700
C	-0.94849600	0.16928100	-0.66864200
C	-0.00058400	1.13598600	0.02273000
C	1.12414900	0.40115400	0.73109500
C	1.67211600	-0.77825400	-0.06188200
C	0.57308400	-1.81410600	-0.30234000
O	1.55230100	0.71931500	1.81259300
O	-1.75168500	0.53427400	-1.49799500
O	0.81102400	-2.97410300	-0.51236700
H	0.48554100	1.72618200	-0.78236600
C	-0.73578400	2.12830200	0.91630600
S	-1.31195100	3.56746400	-0.01745600
H	-1.60785200	1.70724100	1.43694100
O	-2.68264200	3.02146600	-0.69007300
O	-1.71516700	4.59933500	0.93015900
O	-0.31742200	3.81490500	-1.07355400
H	-2.43223600	2.29468500	-1.30318500
H	-0.03551300	2.53091400	1.66269800
H	1.88982600	-0.40640600	-1.08611100
H	-1.01189900	-1.22258200	0.87785900
C	2.92804500	-1.38768400	0.52180000
S	4.40059000	-0.62597300	-0.16800700
H	2.97341300	-1.26941900	1.61298100
O	4.15738000	0.95553800	0.19936400
O	5.56773800	-1.10350000	0.57476200
O	4.29375900	-0.68809500	-1.62504300
H	4.53269200	1.10563000	1.08412000
C	-1.89017000	-2.18097200	-0.85218900
S	-3.37589400	-2.22392000	0.15498800
H	-2.21688100	-1.79173400	-1.82734300
O	-2.82885400	-3.09368200	1.44233600
O	-3.61853600	-0.87518000	0.66796000
O	-4.40062100	-3.02174700	-0.52049000
H	-3.20933000	-3.98361900	1.34652800
H	-1.52339800	-3.21039300	-0.95404400
H	3.00711500	-2.45023000	0.25020900

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C	-0.80499400	-1.28292200	-0.22428700
C	-0.98345900	0.15831500	-0.66319000
C	-0.08669300	1.17536100	0.02504700
C	1.07124900	0.49616100	0.73764400
C	1.68864100	-0.64278200	-0.06494000
C	0.65048700	-1.73831700	-0.31085300
O	1.46678200	0.81636300	1.82918500
O	-1.81193200	0.47857200	-1.48616500
O	0.95321900	-2.88165000	-0.52934700
H	0.36465200	1.78745400	-0.78357700
C	-0.86914300	2.13093800	0.91852600
S	-1.53380800	3.52964600	-0.01761300
H	-1.71148900	1.66526800	1.44987200
O	-2.88065300	2.90443300	-0.67048900
O	-1.98308300	4.54441800	0.92773600
O	-0.56796800	3.82375500	-1.08819300
H	-2.59596800	2.19221900	-1.28550900
H	-0.18592700	2.57620100	1.65663300
H	1.88440300	-0.25522100	-1.08790200
H	-0.96212900	-1.24287600	0.87639700
C	2.97847600	-1.19057700	0.51098500
S	4.37829100	-0.29417600	-0.16980700
H	3.01752300	-1.07832800	1.60273500
O	5.57742400	-1.32172600	0.27347500
O	4.24969800	-0.33170000	-1.62878000
O	4.59812700	0.96906000	0.54279200
H	6.19237900	-0.78153200	0.79993800
C	-1.78826300	-2.24182600	-0.85713600
S	-3.26357500	-2.38432600	0.15552100
H	-2.14301600	-1.86394700	-1.82695400
O	-2.65644500	-3.22409900	1.43614500
O	-3.59070900	-1.05668700	0.67599300
O	-4.23755400	-3.24369400	-0.51993500
H	-2.98215000	-4.13518600	1.33779500
H	-1.36093500	-3.24640300	-0.97029300
H	3.11507100	-2.23841500	0.21111900

6

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C	-0.41787900	-1.60831200	0.50194900
C	-0.57364800	-0.17805500	1.02698900
C	-0.08504100	0.94994300	0.11671000
C	1.15090100	0.50388200	-0.65486500
C	1.92845200	-0.63850400	-0.00196700
C	1.01525400	-1.86026900	0.01406900
H	-0.59317800	-2.27122700	1.36346000
O	1.48297900	0.98578800	-1.70914000
O	-0.95651500	0.01515100	2.15067700
O	1.37108400	-2.95202200	-0.34868200
H	2.06301000	-0.37390700	1.06805900
H	0.25441200	1.76039400	0.79126900
C	3.26356000	-0.91313000	-0.65368800
H	3.54045600	-1.97295900	-0.56295300
S	4.57529900	-0.00288000	0.16258100
O	4.02518900	1.54010900	0.03489000
O	4.50999600	-0.30711300	1.59136400
O	5.80063700	-0.12440000	-0.62904100
H	4.37653700	1.89885000	-0.79814000
C	-1.34420100	-2.04199900	-0.63447600
H	-1.22918100	-1.44334700	-1.55220600
S	-3.10021400	-1.94008500	-0.26896600
O	-3.15966800	-2.69586100	1.17800900
O	-3.44046500	-0.52814700	-0.04058000
O	-3.84549000	-2.74438800	-1.23756500
H	-3.73222600	-3.47284700	1.04791600
C	-1.12972900	1.53877900	-0.82470700
H	-0.61715700	2.06478700	-1.64412200
S	-2.17015800	2.80264500	-0.07269400
O	-2.92844100	1.99198100	1.11184600
O	-1.30826700	3.76238100	0.61714900
O	-3.13288100	3.20669000	-1.09962400
H	-3.43158200	1.25235900	0.71380400
H	-1.14828300	-3.09352300	-0.88897100
H	-1.81994500	0.80191200	-1.25486500
H	3.26701900	-0.62072800	-1.71248700

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C	1.56038400	-0.10894600	0.18887500
C	0.63924500	-1.30074000	0.35180300
C	-0.81404100	-1.12504900	-0.08209600
C	-1.04614800	0.23323800	-0.72737700
C	-0.56030800	1.39279900	0.12164800
C	0.92988200	1.25001400	0.44187300
O	-1.56192300	0.37118800	-1.80835000
O	1.05644900	-2.37683300	0.72212800
O	1.58394100	2.17433600	0.84747500
H	-1.03893900	1.28825000	1.11808700
H	-1.39679900	-1.10162000	0.86183300
C	-0.89802200	2.75990700	-0.43701100
H	-0.17005000	3.50800500	-0.09100500
S	-2.47825100	3.34786400	0.18415600
O	-3.48837100	2.13653800	-0.26750600
O	-2.44042400	3.26883700	1.64379000
O	-2.84415000	4.56147300	-0.54743600
H	-3.77941200	2.32612400	-1.17604700
C	-1.28220700	-2.29786500	-0.93130300
H	-1.98354000	-1.94970000	-1.70341700
S	-2.20514800	-3.52652800	0.01685400
O	-1.31697300	-3.62668900	1.38593900
O	-3.47033500	-2.93359800	0.44730600
O	-2.13985200	-4.78643600	-0.72361700
H	-0.36915800	-3.66801400	1.13833900
H	-0.45675600	-2.83468200	-1.41776600
H	-0.95175200	2.75837800	-1.53409500
H	1.72449400	-0.09791100	-0.91813600
C	2.91541400	-0.28853500	0.84083900
S	4.24123300	0.28523500	-0.24735100
H	3.02076800	0.27852500	1.77440900
O	5.34037000	-0.89028200	0.08164900
O	3.77333700	0.10869600	-1.62883700
O	4.82360100	1.55184200	0.20181000
H	6.17603600	-0.41787800	0.24313000
H	3.10920900	-1.35611400	1.00784000

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C	-1.75978300	-0.57675000	0.05096300
C	-0.78144900	-1.74929400	0.19669800
C	0.68680400	-1.34113100	0.22884400
C	0.82193500	0.02012100	0.90669400
C	0.12299500	1.14286800	0.14940800
C	-1.06100300	0.58880900	-0.63772300
O	1.41055900	0.17928000	1.94208600
O	-1.14673500	-2.89349500	0.26453800
O	-1.39913600	1.00774100	-1.71546700
H	0.90539800	-1.16512000	-0.84504300
C	1.61419700	-2.39125800	0.79298100
H	1.91756000	-2.12787800	1.81765300
S	3.13607400	-2.43259400	-0.15619300
O	2.60325400	-3.14310500	-1.54468400
O	3.47892600	-1.05882700	-0.53093300
O	4.08785200	-3.34949300	0.47403400
H	2.91485800	-4.06355300	-1.50933600
H	1.17324300	-3.39610900	0.76796800
H	-1.94281600	-0.27842800	1.10562900
C	-3.06654600	-0.99461300	-0.58963100
S	-4.42605600	-0.08480500	0.14836400
H	-3.07676800	-0.78135500	-1.66688900
O	-5.67728900	-0.96785800	-0.44140700
O	-4.35619500	-0.29082500	1.59680300
O	-4.53412300	1.26165900	-0.42502600
H	-6.22488300	-0.33154300	-0.93343700
H	-3.26586200	-2.05651700	-0.39112600
H	-0.29176500	1.85006400	0.89261800
C	1.09384400	1.89588100	-0.75450400
S	1.89467700	3.24615600	0.12796100
H	1.89767800	1.26085500	-1.15662000
O	2.37017100	4.12886800	-1.17522700
O	0.85083600	3.99606700	0.82771500
O	3.11431100	2.79511500	0.80433400
H	3.33911700	4.17805600	-1.10263900
H	0.53371900	2.36259300	-1.57739700

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C	1.75758300	0.64875700	-0.01234800
C	1.10171700	-0.55127100	0.66126300
C	-0.06839400	-1.12755700	-0.13100500
C	-0.80493600	-0.00660400	-0.85590900
C	-0.71283300	1.33962600	-0.13797200
C	0.74185500	1.79562000	-0.10703900
O	-1.38122200	-0.15120000	-1.90004600
O	1.45228800	-0.97041000	1.73436900
O	1.07158500	2.95149600	-0.14448400
H	1.91352200	0.37882100	-1.07809600
C	3.06317600	1.08038200	0.62359600
S	4.41665300	0.22932600	-0.18420400
H	3.22974900	2.15671300	0.48651000
O	5.65996500	0.70965500	0.77082100
O	4.23125700	-1.21036600	-0.01679900
O	4.63137700	0.82096800	-1.51357200
H	6.25041500	1.21439100	0.18500400
H	3.09346100	0.80101400	1.68593100
H	0.36841100	-1.79913400	-0.89442200
C	-1.00313700	-1.93523700	0.76543300
S	-1.75068800	-3.29784100	-0.14666600
H	-0.41646400	-2.38433700	1.57886300
O	-2.24453000	-4.22956200	1.11352600
O	-2.94494600	-2.83799200	-0.84233500
O	-0.67357100	-4.03332400	-0.82898700
H	-1.64935300	-4.99890400	1.11046500
H	-1.83242100	-1.34217400	1.18014000
H	-0.91978300	1.12070300	0.93035600
C	-1.67800500	2.37342600	-0.67250600
S	-3.17443400	2.34464100	0.32329100
H	-1.27143200	3.39123400	-0.61824700
O	-4.25542100	2.82703300	-0.80903600
O	-3.44726700	0.94833900	0.68249600
O	-3.13388800	3.38547700	1.35909500
H	-4.76015100	3.54511000	-0.38849500
H	-1.97760500	2.11477300	-1.69820500