A synthetic, NMR and computational study of a set of arylacetic acid 1 β-O-acyl glucuronides: a first computational and mechanistic explanation of observed acyl migration rates

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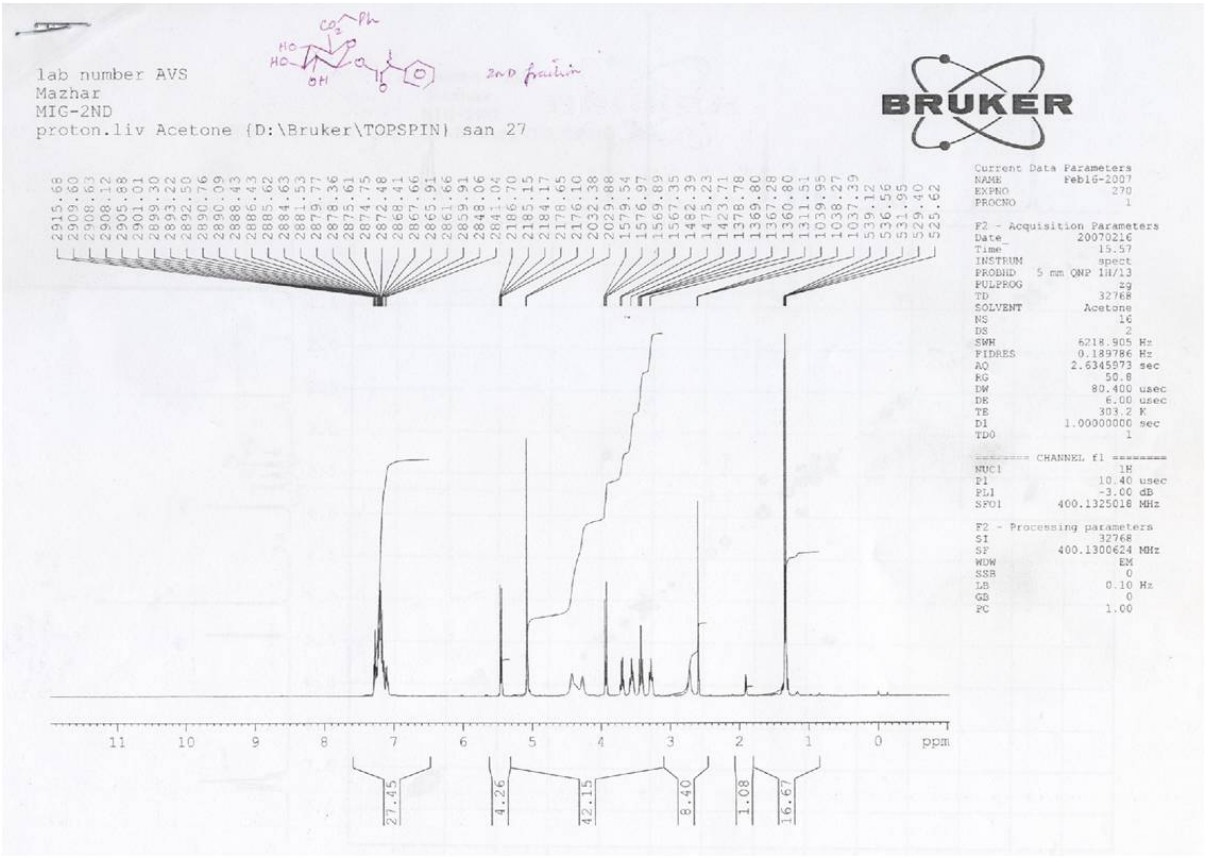
Contents: Synthesis of compound **7**; photocopy NMR spectra for compounds **10**, **11** and **14**; pulse sequences and parameters used in the NMR rate measurements. Tabulated data for some of the parameters used in the DFT study are appended as well as further computational data, including figures and detailed coordinates of transition states.

Chemical synthesis

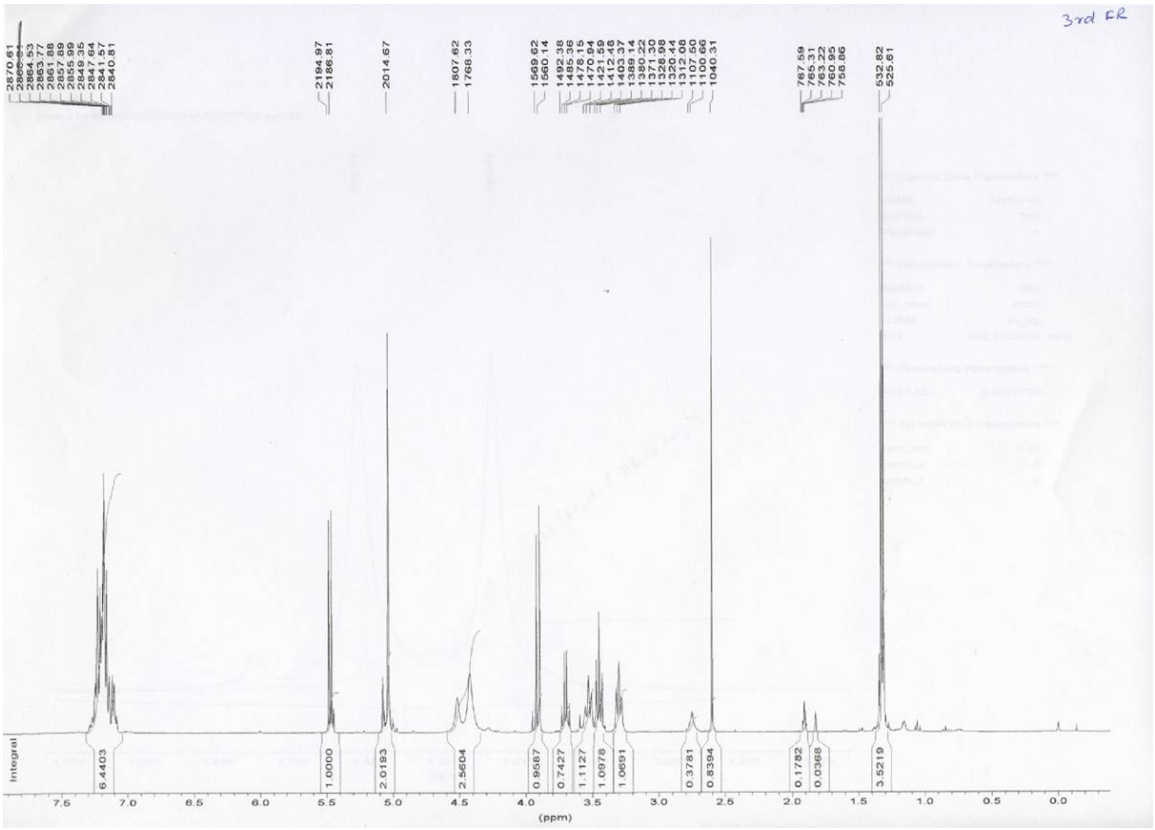
α,α-(Dimethyl)phenylacetic Acid, 7. This compound was prepared according to literature procedures [38, 39] by methylation of 2-phenylpropanal followed by sodium chlorite oxidation. The product was obtained as a white solid. Found: m/z, 182.119. $C_{10}H_{16}NO_2$ [MNH_4^+] requires m/z, 182.118; δ_H ($CDCl_3$) 1.52 [6 H, s, $(CH_3)_2C$], 7.18 (1 H, m, ArH), 7.25 (2 H, m, ArH) and 7.32 (2 H, m, ArH); δ_C ($CDCl_3$) 26.2, 45.3, 124.8, 125.9, 127.4, 142.9 and 181.9; m/z (CI, NH_3) 182 (MNH_4^+, 100%).

1H NMR Spectra of compounds 10, 11 and 14

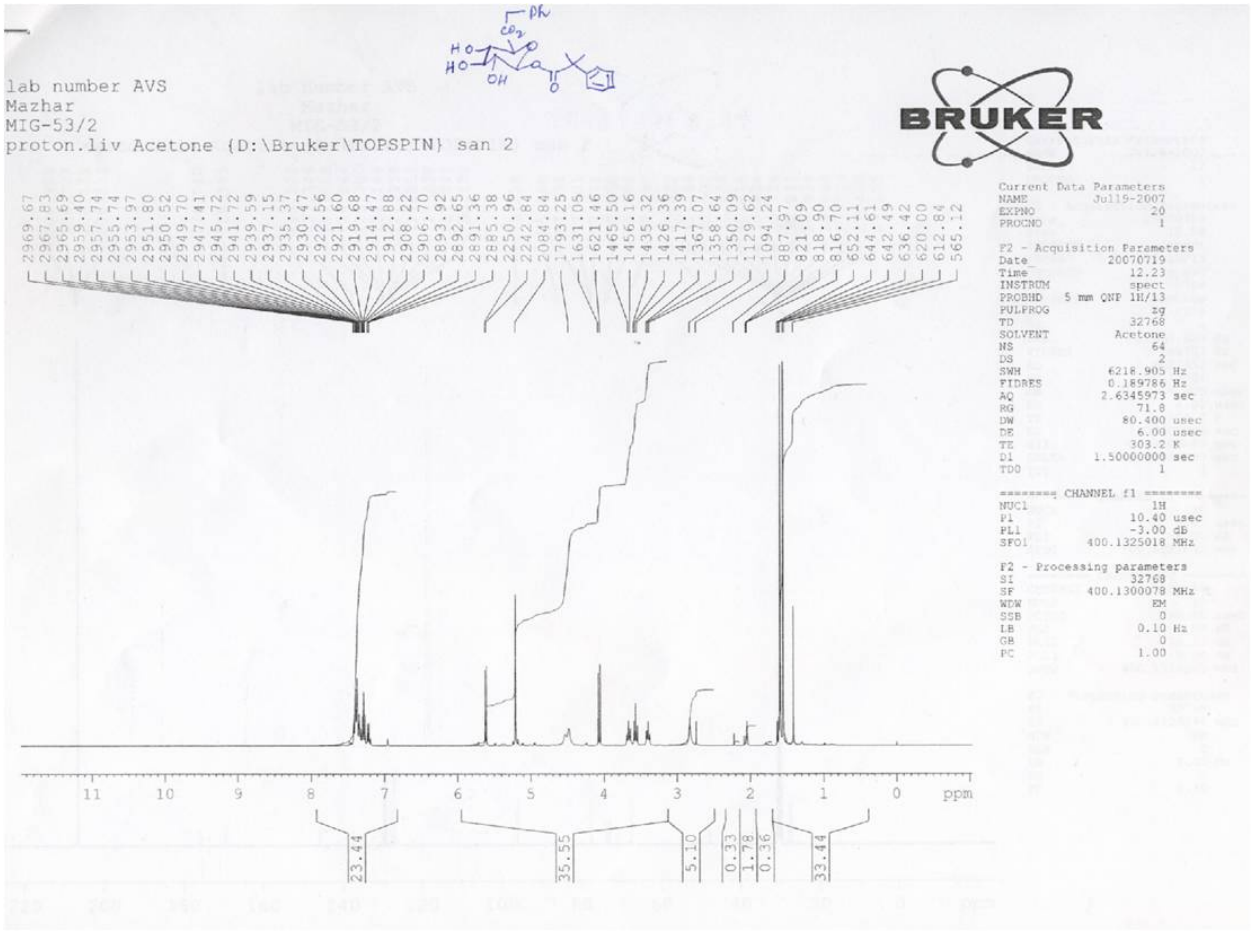
Compound **10**



Compound **11**



Compound **14**



NMR Measurements: Pulse sequences and parameters used

Degradation rate measurements

Once the acquisition parameters were optimized using a standard sample, 550 µL of 100mM sodium phosphate buffer (pH 7.4) was added quickly to one of the samples (e.g. 1.5 mg of synthesized sample). The sample was transferred to a 5 mm NMR tube containing 50 µL TSP (0.5 mg/mL in ^2H_2O) and 16 scans were acquired with a spectral width of 20.017 ppm. The spectrum was phased manually, and an automated program was run by which 158 spectra were acquired sequentially. The first 61 experiments were acquired with a time delay of 59.2 s between experiments; the subsequent 95 experiments were acquired with a time delay of 636.4 s between each experiment. The total reaction times for the two segments are 1.48 and 17.58 h respectively. An exponential apodization function corresponding to a line-broadening factor of 0.3 Hz was applied to the FIDs. Spectra were chosen at different time points, and manually phase- and baseline-

corrected. The β-anomeric proton doublet (at δ~ 5.6 ppm) of the AGs was chosen to monitor the degradation. Integration was used to measure the intensity of the doublet which was referenced to the TSP peak set at unity. The logarithms of the intensities were plotted against time, and the slope of the graph gave the degradation rate constant assuming first-order kinetics.

^{13}C NMR spectroscopy to determine the carbonyl carbon chemical shift: ^{1}H-decoupled ^{13}C NMR spectra were measured on the AGs. The samples were dissolved in 600 µl DMSO-d_6, and 550 µl were added to a 5 mm NMR tube containing 50 µl TSP (0.5 mg/ml in $^{2}H_2O$). Each sample was analysed using a Bruker AVANCE DRX800 NMR spectrometer, with a 5 mm z-gradient triple-resonance inverse (TXI) cryoprobe. A standard ^{1}H-decoupled ^{13}C pulse sequence was used with a waltz-16 ^{1}H-decoupling sequence. The ^{13}C transmitter pulse angle was set to 30 ^{o} and 5 k FIDs were collected into 64 k data points with a spectral width of 354.9 ppm and a relaxation delay of 2 s. A ^{1}H-^{13}C HMBC spectrum using the standard pulse sequence (Bruker Biospin) was also measured to confirm the assignment of the carbonyl ^{13}C chemical shift. 220 (F_1) x 2 k (F_2) data points were acquired which were zero-filled into a 2 k (F_1) x 16 k (F_2) matrix. The spectral width in the ^{1}H domain was 11.0 ppm, and in the ^{13}C domain was 250.0 ppm.

Computational Chemistry

Calculation of transition state energies

Comparing the bond lengths among the transition states for **9**, we infer that there is a decrease in the bond length (distance a of TS2) when the C=O and the phenyl ring have a dihedral angle above 170° (Figure S1). This may be due to the reduced steric interaction between the phenyl ring and the oxygen of the 2-hydroxyl group, when compared with the other conformers whose corresponding dihedral angles are below 100° (Table S1). Even though TS 4 of **9** has a dihedral angle of 174.41°, it has a somewhat longer distance a (2.11 Å) when compared to TS1 (1.91Å) (Figure S1). This is presumably due to the influence of the phenyl hydrogen on the alkoxide oxygen. This increase in distance for TS4 was reflected in the markedly higher activation energy for TS4 (9.74 kcal/mol cf. TS1 6.85 kcal/mol). This is similar to the carbon-fluorine (on

the phenyl ring) interaction observed by Nicholls *et al*[1], which influences the acyl group migration. While comparing the transition states whose dihedral angles are below 80, (i.e. TS1, TS3 and TS5 of 9) it is noted that as the distance a increases, the activation energy decreases (6.85, 6.34, 5.44 kcal/mol respectively).

From examination of Table S1, similarly to **9**, the distance a, becomes shorter and the bond b become longer from the ground state to the transition state. For TS4 of **12** distance **a** is longer (2.17 Å) compared with the other transition states (Figure S2). Even though the carbonyl group and the phenyl ring are away from each other [O=C-C-C (Ph) 173.0°, hence reduced hindrance], there is an unfavourable interaction between the phenyl proton and the oxygen, leading to the longer bond distance (similar to TS4 of 9). This may lead to the higher calculated activation energy (12.93 kcal/mol) when compared to the other four transition states (TS1 10.00 kcal/mol, TS2 9.30 kcal/mol, TS3 10.10kcal/mol and TS5 6.16 kcal/mol).

A similar trend was observed in the bond formation and cleavage as described above for **9** and **12**. Examination of the transition states TS1 and TS3 of **13** revealed that the C=O and phenyl group are disposed near anti-periplanar and hence have reduced hindrance with the hydroxyl oxygen (2.07 Å and 1.91 Å for TS1 and TS3 respectively, Figure S2). However, TS1 has distance a of 0.16 Å longer that TS3. This could be explained by the influence of the substituted methyl group, which is close to the alkoxide oxygen whereas in TS3 it is opposite to the oxygen. The interaction of the methyl group was also influenced by the formation of a longer bond (2.30 Å) in TS2 of **13**.

While comparing the distance a among the transition states, TS2 has the longest (2.27 Å) and TS4 has the smallest (1.89 Å) bond distance. In TS2 the hydroxyl oxygen was influenced by one of the methyl groups and the phenyl ring whereas in TS4 it is not. TS1 follows the lowest energy favourable energy pathway (Figure S3).

Figure S1

[1] Nicholls, A. W.; Akira, K.; Lindon, J. C.; Farrant, R. D.; Wilson, I. D.; Harding, J.; Killick, D. A.; Nicholson, J. K. NMR Spectroscopy and Theoretical Chemistry Studies on the Internal Acyl Migration Reactions of the 1-*O*-Acyl-β-D-glucopyranuronate Conjugates of 2-, 3-, and 4-(Trifluoromethyl)benzoic Acids. *Chem. Res. Toxicol.* **1996,** *9*, 1414-1424.

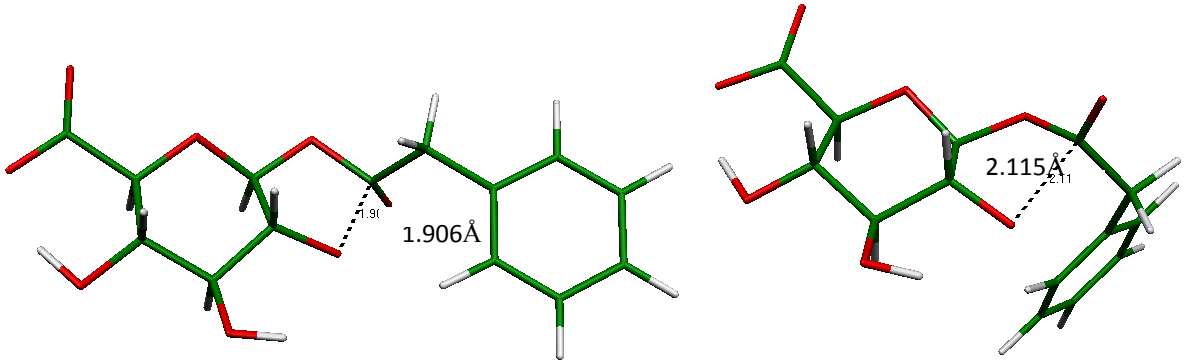

1.906Å
2.115Å

Figure S2

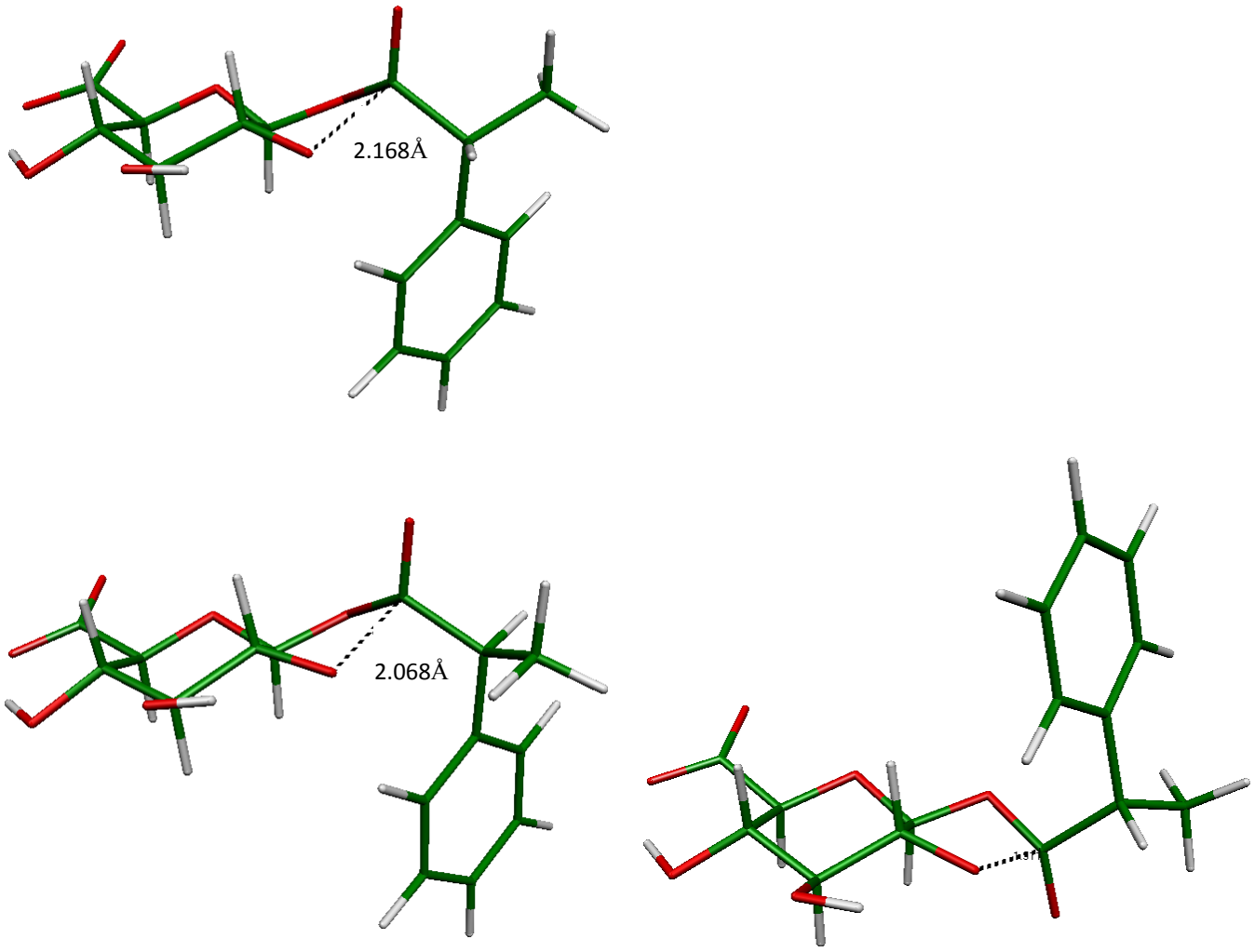


Figure S3

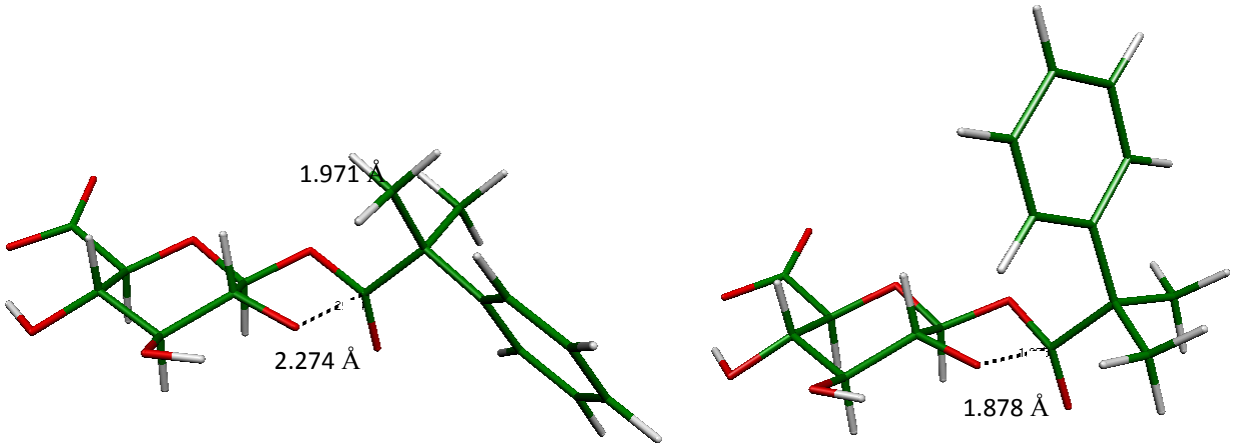


Table S1 The calculated intramolecular bond length using B3LYP/6-31G** level of theory. Distances: **a** (nucleophilic alkoxide – carbonyl carbon) and **b** (carbonyl oxygen – carbonyl carbon).

Bond length/Angle	Reactant							TS				
	GS1	GS2	GS3	GS4	GS5	GS6	GS7	TS1	TS2	TS3	TS4	TS5
Distance **a**	4.78	4.75	4.57	4.31	4.31	4.78	3.69	1.91	1.82	2.26	2.11	2.27
Distance **b**	1.33	1.33	1.32	1.32	1.32	1.33	1.34	1.46	1.46	1.40	1.42	1.38
Angle O=C-C-C(Ph)	23.66	126.70	100.23	23.96	23.96	124.58	62.83	41.95	179.16	86.22	174.41	64.64
12 (R)												
	GS1	GS2	GS3	GS4	GS5	GS6		TS1	TS2	TS3	TS4	TS5
Distance **a**	4.80	4.51	4.78	4.76	4.55	4.16		1.93	2.03	1.96	2.17	2.12
Distance **b**	1.33	1.31	1.32	1.32	1.32	1.34		1.46	1.43	1.45	1.41	1.40
Angle O=C-C-C(Ph)	106.07	90.12	119.73	62.85	85.51	58.83		44.26	65.02	42.64	173.00	71.92
13 (S)												
	GS1	GS2	GS3	GS4				TS1	TS2	TS3	TS4	
Distance **a**	4.81	4.17	4.23	4.54				2.07	2.30	1.91	1.91	
Distance **b**	1.33	1.34	1.33	1.32				1.42	1.38	1.43	1.46	
Angle O=C-C-C(Ph)	36.62	57.96	45.48	105.45				176.78	73.90	177.42	50.92	
15												
Distance **a**	GS1	GS2	GS3	GS4	GS5			TS1	TS2	TS3	TS4	TS5
Distance **b**	4.26	4.26	4.58	4.56	4.56			1.92	2.27	2.07	1.89	2.11
Angle O=C-C-C(Ph)	1.34	1.34	1.32	1.31	1.31			1.45	1.39	1.43	1.44	1.42
	172.77	172.78	95.75	101.36	101.29			66.33	35.92	44.52	179.28	178.34

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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Table S2. Partial charges on the atoms (from NPA analysis), frontier orbital energies, global hardness, softness, electronegativity and electrophilicity involved in the ground states using B3LYP/6-31G**.

Properties				**9**				
	GS1	GS2	GS3	GS4	GS5	GS6	GS7	Boltzmann Weighted
Acyl oxygen	-0.59	-0.59	-0.57	-0.59	-0.59	-0.58	-0.56	-0.588
Attacking oxygen	-0.98	-0.98	-0.98	-0.97	-0.97	-0.98	-0.99	-0.980
Carbonyl carbon	0.84	0.84	0.82	0.83	0.83	0.84	0.84	0.838
Carbonyl oxygen	-0.65	-0.66	-0.67	-0.67	-0.67	-0.66	-0.65	-0.655
HOMO	-0.203	-0.203	-0.203	-0.203	-0.203	-0.203	-0.206	-0.203
LUMO	-0.019	-0.019	-0.023	-0.019	-0.019	-0.021	-0.031	-0.019
Hardness	0.092	0.092	0.090	0.092	0.092	0.091	0.088	0.092
Softness	5.435	5.435	5.556	5.435	5.435	5.495	5.714	5.449
Electronegtivity	-0.111	-0.111	-0.113	-0.111	-0.111	-0.112	-0.119	-0.111
Electrophilicity	0.046	0.046	0.045	0.046	0.046	0.046	0.044	0.046
				12				
Acyl oxygen	-0.59	-0.57	-0.58	-0.58	-0.57	-0.55		-0.57
Attacking oxygen	-0.98	-0.98	-0.98	-0.98	-0.98	-0.99		-0.98
Carbonyl carbon	0.85	0.83	0.85	0.84	0.83	0.84		0.83
Carbonyl oxygen	-0.66	-0.68	-0.66	-0.67	-0.68	-0.65		-0.68
HOMO	-0.201	-0.203	-0.203	-0.202	-0.203	-0.205		-0.203
LUMO	-0.024	-0.022	-0.022	-0.022	-0.022	-0.030		-0.022
Hardness	0.089	0.091	0.091	0.090	0.091	0.088		0.090
Softness	5.650	5.525	5.525	5.556	5.525	5.714		5.537
Electronegtivity	-0.113	-0.113	-0.113	-0.112	-0.113	-0.118		-0.112
Electrophilicity	0.044	0.045	0.045	0.045	0.045	0.044		0.045
				13				
Acyl oxygen	-0.59							-0.59
Attacking oxygen	-0.98							-0.98
Carbonyl carbon	0.84							0.84
Carbonyl oxygen	-0.65							-0.65

HOMO	-0.202					-0.202
LUMO	-0.018					-0.018
Hardness	0.092					0.092
Softness	5.435					5.435
Electronegtivity	-0.110					-0.110
Electrophilicity	0.046					0.046
			15			
Acyl oxygen	-0.57	-0.57	-0.57	-0.57	-0.57	-0.570
Attacking oxygen	-0.99	-0.99	-0.98	-0.98	-0.98	-0.980
Carbonyl carbon	0.86	0.86	0.84	0.84	0.84	0.840
Carbonyl oxygen	-0.65	-0.65	-0.68	-0.68	-0.68	-0.680
HOMO	-0.203	-0.203	-0.202	-0.202	-0.202	-0.202
LUMO	-0.024	-0.024	-0.022	-0.021	-0.021	-0.021
Hardness	0.090	0.090	0.090	0.091	0.091	0.090
Softness	5.587	5.587	5.556	5.525	5.525	5.527
Electronegtivity	-0.114	-0.114	-0.112	-0.112	-0.112	-0.112
Electrophilicity	0.045	0.045	0.045	0.045	0.045	0.045

Table S3. The frontier orbital energies, global hardness, softness, electronegativity and electrophilicity involved in the transition state using B3LYP/6-31G**.

Properties			**9**			
	TS1	TS2	TS3	TS4	TS5	Boltzmann Weighted
HOMO (Hartree)	-0.225	-0.225	-0.212	-0.216	-0.212	-0.213
Hardness	0.106	0.105	0.095	0.100	0.094	0.095
Softness	4.739	4.746	5.291	5.000	5.348	5.294
Electronegtivity	-0.120	-0.120	-0.118	-0.116	-0.119	-0.118
Electrophilicity	0.053	0.053	0.047	0.050	0.047	0.047
			12			
HOMO (Hartree)	-0.222	-0.218	-0.225	-0.213	-0.223	-0.223
Hardness	0.105	0.101	0.107	0.099	0.102	0.102
Softness	4.785	4.950	4.695	5.051	4.902	4.902
Electronegtivity	-0.118	-0.117	-0.119	-0.114	-0.121	-0.121
Electrophilicity	0.052	0.051	0.053	0.050	0.051	0.051
			13			
HOMO (Hartree)	-0.217	-0.208	-0.22	-0.228		-0.210
Hardness	0.102	0.094	0.104	0.108		0.095
Softness	4.902	5.348	4.831	4.651		5.286
Electronegtivity	-0.115	-0.115	-0.117	-0.121		-0.115
Electrophilicity	0.051	0.047	0.052	0.054		0.047
			15			
HOMO	-0.220	-0.204	-0.218	-0.219	-0.214	-0.216
Hardness	0.103	0.096	0.104	0.105	0.102	0.101
Softness	4.854	5.236	4.808	4.785	4.926	4.935
Electronegtivity	-0.117	-0.109	-0.114	-0.115	-0.113	-0.115
Electrophilicity	0.052	0.048	0.052	0.052	0.051	0.051

Table S4. Normalised Fukui indices of the alkoxide oxygen and carbonyl carbon ground states using B3LYP/6-31G**.

Normalised Fukui indices			**9**					
	GS1	GS2	GS3	GS4	GS5	GS6	GS7	Boltzmann Weighted
f^+ (carbonyl C)	-18.406	-11.435	-25.531	-74.143	-74.143	-8.800	-8.836	-17.428
f^- (alkoxide O)	-1.462	-1.492	-1.428	-1.411	-1.411	-1.407	-1.726	-1.457
		12						
f^+ (carbonyl C)	-10.972	-11.284	-15.353	-8.448	-14.118	-23.137		-11.769
f^- (alkoxide O)	-1.462	-1.442	-1.401	-1.461	-1.439	-1.754		-1.446
		13						
f^+ (carbonyl C)	-115.019							-115.019
f^- (alkoxide O)	-1.456							-1.456
		15						
f^+ (carbonyl C)	-154.384	-154.264	-23.479	-9.919	-9.799			-10.779
f^- (alkoxide O)	-1.766	-1.766	-1.423	-1.404	-1.398			-1.402

Table S5. Normalised Fukui indices of the alkoxide oxygen and carbonyl carbon transition states states using B3LYP/6-31G**.

Normalised Fukui indices	**9**					
	TS1	TS2	TS3	TS4	TS5	Boltzmann Weighted
f^+ (carbonyl C)	-83.947	-9.797	-20.853	-8.144	-16.448	-21.962
f (alkoxide O)	-5.223	-0.741	-1.720	-0.070	-0.017	-0.672
		12				
f^+ (carbonyl C)	-95.382	-97.284	-83.687	-29.182	-95.382	-26.487
f (alkoxide O)	-0.886	-0.902	-1.422	-0.061	-0.886	-0.049
		13				
f^+ (carbonyl C)	-30.967	-14.687	-16.160	-29.249		-15.974
f (alkoxide O)	-1.652	-1.766	-1.063	-1.403		-1.734
		15				
f^+ (carbonyl C)	-228.199	-14.850	-174.404	-20.142	-13.135	-169.771
f (alkoxide O)	-1.125	-1.796	-0.018	-0.019	-0.011	-1.129

Coordinates in xyz format of the ground and transition states of molecules 9, 12, 13, & 15.

Molecule 9

36
gs1

C	-2.93113	-2.13433	-0.62249
C	-1.95891	-1.17813	-2.70445
O	-2.21547	0.24157	-0.68075
C	-1.49036	0.02505	-1.84206
C	-2.43727	-0.90955	0.18509
C	-2.01469	-2.47068	-1.82669
H	-1.14467	-1.32864	-3.46378
H	-1.55244	0.95191	-2.41714
H	-3.27964	-0.58467	0.80438
H	-2.56679	-3.19829	-2.44113
H	-2.95202	-2.99223	0.07291
O	-0.05360	-0.18314	-1.46947
C	0.64274	0.81447	-0.92972
O	-3.19182	-0.89464	-3.22082
O	-0.77441	-3.05967	-1.47091
H	-0.52737	-2.68498	-0.58560
O	-4.23964	-1.88627	-1.11515
H	-4.02552	-1.40499	-2.01122
C	-1.21439	-1.07325	1.15632
O	-1.13468	-0.20366	2.06061
O	-0.39397	-2.02697	0.96134
C	1.80778	0.22278	-0.11359
H	2.59710	-0.05138	-0.82749
H	1.42609	-0.70377	0.33303
C	2.34961	1.14841	0.94723
C	3.35265	2.83667	2.96756
C	3.52063	1.89082	0.74979
C	1.67598	1.26182	2.17710
C	2.17993	2.10145	3.17158
C	4.02352	2.72929	1.74848
H	4.04578	1.80916	-0.20066
H	0.75505	0.68759	2.32987
H	1.64910	2.18221	4.11854
H	4.93708	3.29611	1.57321
H	3.73875	3.48741	3.75110
O	0.43560	2.00650	-1.06958

36
gs2

C	-0.86171	-1.34255	2.67453
C	-0.40130	-1.24954	0.23133
O	-1.78875	0.50530	1.32707
C	-0.95628	0.20127	0.26226
C	-1.30117	0.14019	2.64389
C	0.22826	-1.62379	1.61114
H	0.42891	-1.23227	-0.52429
H	-1.53014	0.39436	-0.64582
H	-2.20329	0.21360	3.26560
H	0.36146	-2.71663	1.56852
H	-0.45739	-1.53349	3.68172
O	0.19018	1.16825	0.27893
C	-0.02049	2.43986	-0.04698
O	-1.43188	-2.09937	-0.05959
O	1.48900	-1.02648	1.91564
H	1.32931	-0.39055	2.66399
O	-1.96498	-2.19911	2.43143
H	-1.95798	-2.25107	1.39395
C	-0.28844	1.20683	3.20673
O	-0.64170	2.40650	3.12197
O	0.78157	0.76477	3.73754
C	1.03235	3.34645	0.59962
H	0.80524	3.26825	1.67716
H	0.82248	4.36841	0.26973
C	2.48148	3.00104	0.32568
C	5.20617	2.44199	-0.17467
C	3.31957	3.94772	-0.28349
C	3.03388	1.75587	0.68223
C	4.37942	1.48832	0.42826
C	4.66840	3.67863	-0.53184
H	2.90436	4.91403	-0.56623
H	2.40662	0.98997	1.13157
H	4.78026	0.51659	0.70772
H	5.29375	4.43475	-1.00527
H	6.25553	2.22179	-0.36545
O	-0.92938	2.87049	-0.73669

36
gs3

C	-1.75144	-1.16367	0.70908
C	-0.87114	-0.08255	-1.34833
O	-1.04553	1.24238	0.76284
C	-0.43929	1.12263	-0.46937
C	-1.32381	0.05143	1.56803
C	-0.81974	-1.39484	-0.50945
H	-0.08044	-0.16404	-2.14038
H	-0.62554	2.05050	-1.01107
H	-2.20504	0.35217	2.14176
H	-1.31334	-2.15548	-1.13399
H	-1.71284	-2.04614	1.37263
O	1.06669	1.09056	-0.22745
C	1.83918	2.08100	-0.62649
O	-2.13353	0.15662	-1.81569
O	0.47458	-1.86941	-0.18278
H	0.70177	-1.49126	0.71128
O	-3.07570	-0.98996	0.23230
H	-2.90078	-0.45646	-0.64765
C	-0.17131	-0.16750	2.60534
O	0.81693	-0.89594	2.24784
O	-0.29293	0.41326	3.70743
C	3.27117	1.89126	-0.08679
H	3.94349	2.48260	-0.71649
H	3.52645	0.83049	-0.18551
C	3.39049	2.31918	1.36585
C	3.50211	3.15984	4.04790
C	2.71008	1.60668	2.36483
C	4.13818	3.44767	1.72982
C	4.20429	3.86086	3.06373

C	2.75166	2.03532	3.69199
H	2.12878	0.71753	2.12049
H	4.66586	4.01133	0.96144
H	4.79274	4.73857	3.32917
H	2.14947	1.48643	4.41124
H	3.53410	3.49585	5.08346
O	1.52902	3.04313	-1.31588

36
gs4.out

C	-1.08610	-0.90092	3.60770
C	0.33788	-1.59793	1.69402
O	-1.85894	-0.50915	1.26163
C	-0.59610	-0.75139	0.77793
C	-2.00606	-0.09322	2.66109
C	0.38198	-0.94988	3.11184
H	1.36257	-1.49602	1.25348
H	-0.70381	-1.24314	-0.19313
H	-3.03179	-0.39814	2.88655
H	0.90264	-1.68137	3.74978
H	-1.12713	-0.39804	4.58981
O	-0.00333	0.61899	0.52213
C	1.12894	0.80163	-0.11800
O	-0.13859	-2.87517	1.73619
O	1.07173	0.28989	3.20407
H	0.37027	1.01243	3.14536
O	-1.55442	-2.23399	3.74493
H	-1.10062	-2.68931	2.92959
C	-1.97776	1.47503	2.80174
O	-0.86113	2.02953	3.08171
O	-3.07595	2.05251	2.65282
C	1.81774	2.03909	0.47381
H	2.25860	1.63589	1.40007
H	1.04151	2.72462	0.82497
C	2.84579	2.73600	-0.37740
C	4.80280	4.09568	-1.90385
C	3.84738	2.02802	-1.06568
C	2.84688	4.13578	-0.47973
C	3.81228	4.81161	-1.22953
C	4.81045	2.70043	-1.81858
H	3.83163	0.94514	-1.02223
H	2.07572	4.69860	0.04151
H	3.78753	5.89843	-1.28782
H	5.57372	2.12965	-2.34476
H	5.55741	4.61691	-2.49017
O	1.60447	0.09598	-1.00105

36
gs5.out

C	-1.08610	-0.90092	3.60770
C	0.33788	-1.59793	1.69402
O	-1.85894	-0.50915	1.26163
C	-0.59610	-0.75139	0.77793
C	-2.00606	-0.09322	2.66109
C	0.38198	-0.94988	3.11184
H	1.36257	-1.49602	1.25348
H	-0.70381	-1.24314	-0.19313
H	-3.03179	-0.39814	2.88655
H	0.90264	-1.68137	3.74978
H	-1.12713	-0.39804	4.58981
O	-0.00333	0.61899	0.52213
C	1.12894	0.80163	-0.11800
O	-0.13859	-2.87517	1.73619
O	1.07173	0.28989	3.20407
H	0.37027	1.01243	3.14536
O	-1.55442	-2.23399	3.74493
H	-1.10062	-2.68931	2.92959
C	-1.97776	1.47503	2.80174
O	-0.86113	2.02953	3.08171
O	-3.07595	2.05251	2.65282
C	1.81774	2.03909	0.47381
H	2.25860	1.63589	1.40007
H	1.04151	2.72462	0.82497
C	2.84579	2.73600	-0.37740
C	4.80280	4.09568	-1.90385
C	3.84738	2.02802	-1.06568
C	2.84688	4.13578	-0.47973
C	3.81228	4.81161	-1.22953
C	4.81045	2.70043	-1.81858
H	3.83163	0.94514	-1.02223
H	2.07572	4.69860	0.04151
H	3.78753	5.89843	-1.28782
H	5.57372	2.12965	-2.34476
H	5.55741	4.61691	-2.49017
O	1.60447	0.09598	-1.00105

36
gs6.out

C	-1.54201	-1.09226	2.17086
C	0.84788	-0.90124	2.83998
O	0.26767	-1.68968	0.54057
C	1.23350	-1.13097	1.35570
C	-1.14107	-1.32447	0.69009
C	-0.53236	-0.17277	2.90235
H	1.61842	-0.18530	3.22970
H	2.10800	-1.78382	1.29080
H	-1.66315	-2.22888	0.36820
H	-0.81395	-0.17243	3.96546
H	-2.53458	-0.60652	2.15426
O	1.64800	0.20255	0.80345
C	2.19438	0.30213	-0.39806
O	0.80019	-2.10037	3.49397

O	-0.56569	1.17820	2.45105
H	-0.70869	1.15639	1.46003
O	-1.63037	-2.31892	2.87085
H	-0.64138	-2.44012	3.19083
C	-1.55768	-0.19779	-0.31886
O	-1.05863	0.96870	-0.13853
O	-2.36315	-0.52939	-1.21251
C	1.93985	1.70400	-0.97058
H	0.84130	1.74753	-1.04917
H	2.38538	1.73819	-1.96922
C	2.44296	2.86023	-0.13239
C	3.38790	5.05601	1.37316
C	3.43342	3.71614	-0.63732
C	1.92755	3.12150	1.15215
C	2.40222	4.20754	1.88832
C	3.90426	4.80486	0.10190
H	3.83999	3.52423	-1.62908
H	1.17104	2.46400	1.57732
H	1.99219	4.38988	2.87938
H	4.67349	5.45251	-0.31687
H	3.74903	5.90140	1.95684
O	2.78278	-0.57175	-1.01334

36
gs7.out

C	0.39094	3.54147	2.74127
C	2.17243	1.78032	3.31417
O	0.20215	1.16354	1.98330
C	1.08935	0.72335	2.99608
C	-0.53078	2.35127	2.32384
C	1.35406	3.03225	3.80161
H	2.57182	2.07632	2.29495
H	0.53558	0.47438	3.91548
H	-1.16299	2.13568	3.20476
H	0.73226	2.70947	4.66430
H	0.97040	3.86352	1.85588
O	1.60396	-0.58013	2.61313
C	2.28963	-0.88130	1.50509
O	3.11375	1.48137	4.21740
O	2.34184	3.94597	4.24053
H	3.02465	3.24696	4.48223
O	-0.42058	4.60346	3.22488
H	-1.20658	4.55940	2.61844
C	-1.49480	2.74920	1.15910
O	-1.55330	2.04147	0.13195
O	-2.16114	3.80648	1.40345
C	2.31489	0.07749	0.30600
H	3.37553	0.22284	0.07057
H	1.86874	1.03592	0.55465
C	1.60202	-0.53538	-0.88775
C	0.28552	-1.66180	-3.10361
C	0.29711	-0.13210	-1.21207
C	2.22908	-1.51561	-1.67154
C	1.57934	-2.07459	-2.77314
C	-0.34730	-0.69567	-2.31785
H	-0.22257	0.61463	-0.60377
H	3.22588	-1.84933	-1.39587
H	2.08222	-2.83295	-3.37195
H	-1.35620	-0.36743	-2.55814
H	-0.22343	-2.09226	-3.96520
O	2.84441	-1.96633	1.43153

36
ts1.out

C	2.18056	3.76453	-0.69361
C	2.06431	1.82443	0.84421
O	1.92096	1.40188	-1.52837
C	1.37890	1.06041	-0.27399
C	1.64643	2.78474	-1.80125
C	1.72842	3.30490	0.69713
H	3.15753	1.72569	0.64584
H	0.28842	1.26758	-0.27202
H	0.54917	2.93413	-1.81771
H	0.63390	3.43688	0.76005
H	3.28641	3.72599	-0.71020
O	1.60407	-0.29627	0.02742
C	1.37643	-0.55235	1.44620
O	1.68136	1.23528	2.03173
O	2.35611	4.05058	1.75243
H	2.29040	3.42694	2.49509
O	1.71267	5.07142	-0.96647
H	1.80660	5.10267	-1.96589
C	2.17047	3.19103	-3.22472
O	2.08302	4.44992	-3.44897
O	2.57547	2.31063	-3.99816
C	2.67945	-1.19378	1.98673
H	3.51977	-0.54568	1.72084
H	2.81876	-2.13876	1.44186
C	2.68094	-1.46749	3.47193
C	2.76261	-1.95266	6.25629
C	2.94001	-2.74802	3.97887
C	2.45288	-0.42705	4.39136
C	2.49507	-0.67017	5.76316
C	2.98285	-2.99408	5.35500
H	3.11038	-3.56649	3.28134
H	2.23303	0.55533	3.97867
H	2.31388	0.14821	6.45839
H	3.18670	-4.00008	5.71985
H	2.79362	-2.13667	7.32920
O	0.27382	-0.93426	1.82652

36

ts2.out

C	1.68174	4.13736	-0.67061
C	2.15090	2.24272	0.83779
O	2.29091	1.84457	-1.53625
C	1.81113	1.32159	-0.32229
C	1.58244	3.06327	-1.81776
C	1.33485	3.51931	0.69081
H	3.21755	2.51874	0.69515
H	0.71679	1.16373	-0.39229
H	0.50262	2.83324	-1.90444
H	0.25917	3.27215	0.69013
H	2.73230	4.48033	-0.61639
O	2.43171	0.10974	0.04215
C	1.95309	-0.19478	1.38576
O	1.95924	1.51258	2.00523
O	1.61246	4.41427	1.78222
H	1.70489	3.79443	2.52417
O	0.81065	5.21144	-0.96839
H	0.95392	5.30250	-1.95871
C	2.01832	3.66238	-3.20233
O	1.53113	4.82825	-3.41915
O	2.72967	2.98711	-3.96039
C	3.10727	-0.82710	2.21770
H	3.09867	-1.89708	1.96919
H	2.76371	-0.74367	3.25475
C	4.51813	-0.30524	2.10521
C	7.19215	0.61545	2.01493
C	4.84938	0.99643	2.52123
C	5.55513	-1.12476	1.63624
C	6.87738	-0.67538	1.58920
C	6.16721	1.44843	2.47600
H	4.02859	1.63455	2.83800
H	5.31810	-2.13273	1.30016
H	7.66025	-1.33415	1.21575
H	6.39664	2.46402	2.79361
H	8.21944	0.97370	1.97603
O	0.83060	-0.69518	1.52759

36

ts3.out

C	2.96417	4.25334	-0.65927
C	1.92614	2.74271	1.04252
O	2.51340	1.81634	-1.12411
C	1.53693	1.83483	-0.11823
C	2.64538	3.12549	-1.70601
C	1.96636	4.17913	0.49718
H	2.99475	2.46899	1.25277
H	0.55027	2.11432	-0.53250
H	1.67540	3.41153	-2.15710
H	0.96882	4.43705	0.09429
H	3.97428	4.06540	-0.24916
O	1.43364	0.52401	0.45362
C	0.49608	0.48627	1.48870
O	1.09783	2.57109	2.11019
O	2.27069	5.04908	1.59361
H	1.84072	4.54629	2.31591
O	2.90618	5.51151	-1.30892
H	3.33700	5.29603	-2.18750
C	3.69347	3.10500	-2.87518
O	3.95143	4.27213	-3.33582
O	4.14541	2.01851	-3.26804
C	1.11713	-0.11282	2.76207
H	0.42609	0.10245	3.58093
H	2.04450	0.42944	2.95345
C	1.36937	-1.60415	2.67402
C	1.87544	-4.38447	2.53260
C	2.28500	-2.12751	1.74223
C	0.71175	-2.50745	3.52204
C	0.95949	-3.88143	3.45710
C	2.53297	-3.49750	1.67343
H	2.77424	-1.43955	1.05926
H	-0.00562	-2.12213	4.24379
H	0.43399	-4.55825	4.12928
H	3.24289	-3.87649	0.94102
H	2.07211	-5.45354	2.47716
O	-0.70729	0.50041	1.28809

36

ts4.out

C	2.61287	3.93845	-0.57736
C	2.28698	1.90693	0.82994
O	1.43448	1.88904	-1.43085
C	1.14157	1.53319	-0.09623
C	1.53122	3.31799	-1.53244
C	2.39955	3.43181	0.85171
H	3.20488	1.53141	0.32416
H	0.20426	2.03943	0.21068
H	0.56904	3.76505	-1.21249
H	1.44964	3.86470	1.21809
H	3.60688	3.58725	-0.91263
O	0.94286	0.13341	0.02218
C	1.55683	-0.50487	1.12722
O	2.55649	-1.18684	0.96068
C	0.57456	-0.92031	2.24854
H	0.37178	-1.98861	2.08255
H	1.16550	-0.84997	3.16667
C	-0.73945	-0.19601	2.42424
C	-3.20703	1.10489	2.87248
C	-1.95627	-0.87643	2.27478
C	-0.77903	1.15902	2.79979
C	-2.00014	1.79718	3.01793
C	-3.18014	-0.23824	2.49520

H	-1.94325	-1.92469	1.97979
H	0.18056	1.67473	2.86056
H	-2.01072	2.84901	3.29811
H	-4.11038	-0.79047	2.36870
H	-4.15681	1.60943	3.04276
O	2.09809	1.31587	2.05623
O	3.45800	3.79241	1.75027
H	3.40029	3.06217	2.39422
O	2.52597	5.35070	-0.63041
H	2.36044	5.49432	-1.61019
C	1.74508	3.76237	-3.02391
O	2.01255	5.01042	-3.14186
O	1.60707	2.92976	-3.93222

36
ts5.out

C	-0.52375	3.39131	-1.42002
C	0.87232	1.73755	-0.15279
O	-0.43217	0.95784	-2.05233
C	-0.02934	0.65772	-0.74193
C	-1.24016	2.14778	-2.05621
C	0.02513	3.01561	-0.04351
H	1.62821	1.93589	-0.95511
H	-0.92808	0.51159	-0.10675
H	-2.13446	1.97062	-1.42621
H	-0.84206	2.81126	0.61402
H	0.33204	3.66190	-2.06645
O	0.73742	-0.54330	-0.76488
C	1.41599	-0.85262	0.39954
O	2.52633	-1.36457	0.31257
C	0.56266	-1.09271	1.66009
H	1.19878	-0.78116	2.49260
H	-0.31170	-0.44406	1.67978
C	0.15713	-2.54516	1.83378
C	-0.59959	-5.24271	2.22961
C	1.11815	-3.57233	1.85128
C	-1.18713	-2.90490	2.00787
C	-1.56534	-4.23559	2.20561
C	0.74428	-4.90149	2.04542
H	2.15303	-3.29608	1.67464
H	-1.94652	-2.12652	1.98374
H	-2.61710	-4.48425	2.33635
H	1.50619	-5.67949	2.05020
H	-0.88938	-6.28071	2.38265
O	1.42057	1.33171	1.02474
O	0.84208	4.02598	0.55779
H	1.40436	3.46076	1.12574
O	-1.44958	4.45992	-1.32693
H	-1.94119	4.36554	-2.19545
C	-1.77353	2.45074	-3.50215
O	-2.35953	3.58630	-3.59156
O	-1.63145	1.59901	-4.39226

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gs1.out

C	-3.31266	-1.54051	0.18891
C	-1.91023	-0.83733	2.12133
O	-1.13055	-2.63585	0.59674
C	-0.74564	-1.61321	1.44755
C	-2.10046	-2.27960	-0.42748
C	-2.88886	-0.30338	1.02281
H	-1.42877	0.05703	2.60108
H	-0.09465	-2.06551	2.19998
H	-2.46768	-3.25606	-0.76380
H	-3.78148	0.01987	1.58019
H	-3.95362	-1.21897	-0.65016
O	0.06093	-0.62639	0.66867
C	1.24255	-0.94346	0.14963
O	-2.56582	-1.67345	2.97878
O	-2.44185	0.79731	0.23575
H	-2.13626	0.41543	-0.63338
O	-4.03926	-2.41863	1.03454
H	-3.52961	-2.29889	1.93242
C	-1.36268	-1.63323	-1.65680
O	-1.65515	-0.42911	-1.97013
O	-0.52424	-2.36248	-2.23101
C	1.54329	-0.00062	-1.04048
H	0.58965	0.07130	-1.58088
C	1.88253	1.39454	-0.52584
C	2.44728	3.99233	0.43462
C	3.17861	1.92552	-0.59073
C	0.86517	2.19065	0.03880
C	1.15089	3.47111	0.51054
C	3.46151	3.21107	-0.11775
H	3.97884	1.32851	-1.01904
H	-0.14369	1.78849	0.12215
H	0.34971	4.06676	0.94309
H	4.47788	3.59807	-0.18160
H	2.66213	4.99410	0.80358
O	1.99978	-1.81356	0.54096
C	2.57721	-0.64276	-1.96565
H	2.85849	0.03957	-2.77770
H	2.11875	-1.53480	-2.40018
H	3.47869	-0.94502	-1.42162

39
gs2.out

C	-2.30600	-0.46672	0.09498
C	-0.98943	-1.36694	2.00216
O	0.09476	-1.01954	-0.20870
C	0.28391	-1.07333	1.15707
C	-1.00013	-0.18255	-0.68452
C	-2.11528	-0.35339	1.62947
H	-0.69125	-1.16056	3.06461
H	1.04062	-1.83472	1.35488
H	-1.15817	-0.55353	-1.70365
H	-3.02858	-0.76428	2.08841
H	-3.04583	0.27939	-0.24183
O	0.89106	0.25564	1.53632
C	1.92308	0.36249	2.34403
O	-1.38532	-2.64822	1.74861
O	-1.93990	0.97581	2.10026
H	-1.62317	1.51163	1.32448
O	-2.77694	-1.77265	-0.20167
H	-2.25598	-2.33561	0.49764
C	-0.51932	1.30744	-0.82441
O	-1.08637	2.19045	-0.10128
O	0.39348	1.50547	-1.66136
C	2.30901	1.84655	2.53876
H	2.82424	1.87261	3.50708
C	3.31147	2.28724	1.47624
C	5.17574	3.16613	-0.44942
C	2.97941	2.28182	0.10906
C	4.58639	2.73284	1.85368
C	5.51385	3.17106	0.90475
C	3.90903	2.71865	-0.83603
H	2.00639	1.93831	-0.24541
H	4.85393	2.73522	2.90922
H	6.49720	3.51300	1.22517
H	3.62314	2.70326	-1.88485
H	5.89290	3.50559	-1.19544
O	2.54053	-0.54669	2.88293
C	1.07360	2.76853	2.57836
H	1.37636	3.78539	2.86249
H	0.33704	2.39631	3.29679
H	0.56820	2.79973	1.60886

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gs3.out

C	-1.70943	-0.38991	-1.10541
C	-1.63379	-0.07906	1.36240
O	0.02215	-1.58731	0.25531
C	-0.26996	-0.81640	1.36377
C	-0.34589	-1.12932	-1.08516
C	-1.80327	0.68255	0.00884
H	-1.54358	0.69488	2.16926
H	-0.19990	-1.47968	2.22966
H	-0.49529	-2.06509	-1.62929
H	-2.84042	1.04871	0.01070
H	-1.78548	0.10021	-2.09309
O	0.79345	0.23252	1.53325
C	2.04826	-0.09754	1.78180
O	-2.64231	-0.98282	1.54682

O	-0.95284	1.80393	-0.20651
H	-0.10534	1.45706	-0.61351
O	-2.78020	-1.30212	-0.94871
H	-2.85654	-1.34654	0.09382
C	0.85117	-0.40216	-1.79306
O	1.17448	0.76128	-1.36337
O	1.38787	-1.01694	-2.73713
C	2.99105	1.03251	1.30120
H	2.67398	1.16945	0.25501
C	2.73340	2.34540	2.03778
C	2.23698	4.79460	3.36558
C	3.67561	2.90188	2.91602
C	1.52417	3.04226	1.83753
C	1.28712	4.24818	2.49612
C	3.43455	4.11262	3.57371
H	4.61622	2.38787	3.09140
H	0.76001	2.62522	1.18426
H	0.34435	4.76335	2.32550
H	4.18706	4.51793	4.24912
H	2.04362	5.73792	3.87402
O	2.44937	-1.13699	2.28110
C	4.44315	0.55119	1.33207
H	5.12420	1.32752	0.96296
H	4.54526	-0.33058	0.69484
H	4.75369	0.25580	2.34021

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gs4.out

C	-0.89201	4.43924	-0.12787
C	-1.18470	2.20027	-1.17162
O	1.09270	3.16696	-0.90664
C	0.34623	2.00913	-1.00537
C	0.62508	4.18348	0.03176
C	-1.73047	3.13824	-0.04785
H	-1.62986	1.18387	-0.99882
H	0.75033	1.44682	-1.84928
H	1.13348	5.08587	-0.32329
H	-2.74691	3.40418	-0.37775
H	-1.19008	5.11826	0.69039
O	0.60722	1.18825	0.23973
C	1.75495	0.55341	0.38742
O	-1.41704	2.73608	-2.40726
O	-1.82608	2.58204	1.25223
H	-0.99060	2.83348	1.73203
O	-1.14900	5.06010	-1.37952
H	-1.24735	4.23189	-1.99651
C	1.20583	3.88582	1.46158
O	2.43663	4.10089	1.58933
O	0.42041	3.44783	2.36185
C	2.02580	0.26511	1.87748
H	1.19955	0.71052	2.43715
C	2.10585	-1.22018	2.18490
C	2.30622	-3.95909	2.86085
C	1.40379	-1.75182	3.27706
C	2.90745	-2.09438	1.42993
C	3.00325	-3.44567	1.76320
C	1.50216	-3.10335	3.61568
H	0.76960	-1.09119	3.86346
H	3.42394	-1.69332	0.56381
H	3.62491	-4.10473	1.15932
H	0.94442	-3.48804	4.46774
H	2.38365	-5.01360	3.11935
O	2.53478	0.22987	-0.50065
C	3.32433	1.00207	2.28795
H	3.56202	0.78138	3.33649
H	3.18729	2.08522	2.16988
H	4.16075	0.66755	1.66433

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gs5.out

C	-2.30778	0.14833	-0.55428
C	-2.14137	0.49872	1.90114
O	-0.50774	-0.97200	0.73933
C	-0.72445	-0.13719	1.81692
C	-0.88618	-0.46180	-0.57309
C	-2.47942	1.21588	0.55722
H	-2.06216	1.29104	2.69286
H	-0.52112	-0.71114	2.72243
H	-0.94604	-1.37506	-1.17582
H	-3.55794	1.43192	0.61682
H	-2.46584	0.61528	-1.54161
O	0.33720	0.93254	1.73214
C	1.13219	1.22469	2.73850
O	-3.04189	-0.49368	2.16211
O	-1.79582	2.43607	0.30945
H	-1.06132	2.22538	-0.32703
O	-3.27411	-0.87063	-0.34817
H	-3.29582	-0.91614	0.68949
C	0.28774	0.38985	-1.17804
O	1.34341	-0.24233	-1.42321
O	0.08804	1.63198	-1.38004
C	2.15567	2.30915	2.33001
H	2.37954	2.84271	3.26252
C	3.45249	1.66036	1.85519
C	5.88028	0.52472	0.97710
C	3.48291	0.84011	0.71283
C	4.65093	1.89225	2.54516
C	5.85721	1.33380	2.11426
C	4.68941	0.28272	0.28628
H	2.58130	0.61408	0.14105
H	4.63537	2.51962	3.43498
H	6.77414	1.53008	2.66860

H	4.68028	-0.34699	-0.59992
H	6.81624	0.08552	0.63478
O	1.12211	0.73294	3.85934
C	1.58937	3.29411	1.28855
H	2.30278	4.11288	1.12422
H	0.63678	3.71020	1.63045
H	1.38429	2.79612	0.33648

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gs6.out

C	-0.94009	3.69491	-0.47936
C	1.03374	4.22027	1.08549
O	0.62935	1.92969	0.28595
C	1.08465	2.70849	1.37721
C	-0.73153	2.20022	-0.09824
C	-0.46121	4.51917	0.70437
H	1.61378	4.30168	0.11774
H	0.51631	2.48007	2.29797
H	-1.39164	2.01650	0.77243
H	-1.09041	4.21864	1.57049
H	-0.31447	3.92233	-1.36166
O	2.46783	2.32189	1.59895
C	2.81692	1.14573	2.12649
O	1.41575	5.06550	2.05464
O	-0.50506	5.92678	0.55646
H	0.24206	6.11548	1.20462
O	-2.31539	3.91821	-0.76148
H	-2.53423	3.11672	-1.30636
C	-1.18081	1.18127	-1.20181
O	-0.57060	0.09454	-1.29903
O	-2.19625	1.54518	-1.87487
C	1.75729	0.03829	2.32541
H	0.80921	0.36455	1.90240
C	2.17523	-1.21095	1.55469
C	2.88560	-3.51429	0.10161
C	3.15268	-2.09206	2.04139
C	1.57179	-1.48043	0.31593
C	1.92799	-2.62868	-0.39726
C	3.50264	-3.23763	1.32421
H	3.65558	-1.87065	2.97747
H	0.83402	-0.79096	-0.10884
H	1.44588	-2.81956	-1.35324
H	4.26195	-3.91128	1.71908
H	3.15581	-4.40866	-0.45826
O	3.97547	0.94942	2.45625
C	1.58628	-0.20241	3.83823
H	0.90731	-1.04319	4.01976
H	1.16816	0.68847	4.31987
H	2.54780	-0.41671	4.31403

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ts1.out

C	2.10236	3.78691	-0.66554
C	2.09059	1.82705	0.85269
O	2.01141	1.42201	-1.52720
C	1.47700	1.03298	-0.28493
C	1.65002	2.78711	-1.79102
C	1.65863	3.28348	0.71290
H	3.19095	1.80325	0.67234
H	0.37472	1.15888	-0.29518
H	0.54576	2.86365	-1.82296
H	0.55677	3.34122	0.75762
H	3.20857	3.81965	-0.66454
O	1.79615	-0.30818	0.00510
C	1.53310	-0.61355	1.40564
O	1.72727	1.20072	2.02692
O	2.21646	4.05949	1.78503
H	2.17396	3.42856	2.52314
O	1.55534	5.06353	-0.93343
H	1.66375	5.11186	-1.93074
C	2.16767	3.24085	-3.20251
O	2.00467	4.49402	-3.41538
O	2.63758	2.39541	-3.97815
C	2.84857	-1.21976	1.99059
H	3.63493	-0.47711	1.82043
C	2.75622	-1.45914	3.49287
C	2.66126	-1.80929	6.30404
C	2.88345	-2.72857	4.07446
C	2.56827	-0.36234	4.35645
C	2.52347	-0.53676	5.73774
C	2.83730	-2.90552	5.46210
H	3.02231	-3.59966	3.44147
H	2.43018	0.61128	3.89033
H	2.37471	0.32876	6.38174
H	2.93995	-3.90610	5.88075
H	2.62611	-1.94200	7.38444
O	0.43624	-1.05473	1.73401
C	3.19943	-2.48003	1.18199
H	4.13874	-2.93881	1.51951
H	3.29965	-2.20632	0.12998
H	2.40058	-3.22706	1.26083

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ts2.out

C	2.76098	4.44258	-0.73026
C	1.96074	2.79259	0.94274
O	2.92193	1.95022	-1.11034
C	1.86629	1.79172	-0.19942
C	2.80773	3.23812	-1.74226
C	1.71646	4.18471	0.36071
H	3.03459	2.76832	1.24990
H	0.89393	1.87058	-0.72097

H	1.84491	3.27963	-2.28758
H	0.71837	4.21324	-0.11213
H	3.74831	4.51177	-0.23591
O	1.93397	0.52934	0.45181
C	0.89701	0.46426	1.43602
O	1.10932	2.41363	1.95262
O	1.76175	5.14616	1.42582
H	1.38756	4.61922	2.15533
O	2.46700	5.62884	-1.44485
H	3.01942	5.49630	-2.27162
C	3.93575	3.43251	-2.81703
O	3.96535	4.61813	-3.30179
O	4.65265	2.46909	-3.12679
C	1.43074	-0.16004	2.74895
H	0.69222	0.13800	3.50134
C	1.42537	-1.68243	2.67659
C	1.50761	-4.51127	2.61655
C	1.97287	-2.36785	1.57743
C	0.91676	-2.44933	3.73510
C	0.95564	-3.84592	3.71196
C	2.01209	-3.76177	1.54916
H	2.34604	-1.78575	0.73964
H	0.47993	-1.93724	4.59056
H	0.54988	-4.41325	4.54852
H	2.43585	-4.26759	0.68362
H	1.53843	-5.59907	2.59021
O	-0.27102	0.28544	1.10512
C	2.80870	0.36073	3.18729
H	3.56702	0.12417	2.43610
H	3.11238	-0.08351	4.14593
H	2.73328	1.44631	3.27639

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ts3.out

C	2.19867	3.72958	-0.67450
C	1.89827	1.74623	0.78989
O	1.58884	1.47057	-1.59091
C	1.06686	1.13704	-0.32247
C	1.47292	2.88834	-1.78492
C	1.76395	3.26302	0.72002
H	2.95464	1.50100	0.54949
H	0.02089	1.50876	-0.26557
H	0.40389	3.17257	-1.71395
H	0.70271	3.54223	0.85167
H	3.28560	3.54343	-0.76221
O	1.07711	-0.25538	-0.10567
C	1.40780	-0.65605	1.25023
O	2.46744	-1.24436	1.43590
C	0.13162	-1.14491	1.98931
H	-0.12005	-2.08947	1.48032
C	0.41143	-1.49097	3.44464
C	0.79998	-2.10882	6.17620
C	1.23413	-0.68554	4.25238
C	-0.19951	-2.60727	4.03302
C	-0.01331	-2.91847	5.38331
C	1.42093	-0.99540	5.59966
H	1.71590	0.17063	3.78566
H	-0.83141	-3.24733	3.41844
H	-0.49941	-3.79461	5.81084
H	2.06407	-0.36184	6.20852
H	0.95401	-2.34435	7.22825
O	1.48701	1.16205	1.97148
O	2.54173	3.85935	1.76934
H	2.45834	3.19517	2.47442
O	1.89872	5.10022	-0.85720
H	1.94076	5.17159	-1.85831
C	1.93696	3.30032	-3.22799
O	2.03021	4.56925	-3.38212
O	2.12559	2.41881	-4.07891
C	-1.08769	-0.21533	1.86949
H	-0.83843	0.75928	2.29283
H	-1.96040	-0.63917	2.38569
H	-1.34028	-0.07340	0.81477

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ts4.out

C	2.52453	3.92248	-0.52942
C	2.07720	1.87606	0.82753
O	1.33436	1.91983	-1.47176
C	0.96555	1.55500	-0.15980
C	1.47561	3.34755	-1.54678
C	2.22650	3.39877	0.87795
H	3.00721	1.48671	0.35521
H	0.03088	2.08486	0.11037
H	0.51084	3.81650	-1.26846
H	1.26984	3.84931	1.20364
H	3.52387	3.54918	-0.82192
O	0.69547	0.16051	-0.07256
C	1.30362	-0.54478	0.98035
O	2.33690	-1.16932	0.79533
C	0.31608	-1.04383	2.08212
H	0.85688	-0.81782	3.00702
C	-1.02961	-0.33637	2.16737
C	-3.50154	1.01140	2.46299
C	-2.24643	-0.98356	1.90759
C	-1.07556	1.01065	2.57654
C	-2.29493	1.67107	2.71941
C	-3.46951	-0.32005	2.05117
H	-2.25087	-2.02187	1.58902
H	-0.11456	1.51108	2.71604
H	-2.30308	2.71517	3.02731
H	-4.39729	-0.84971	1.83841

H	-4.45171	1.53119	2.57544
O	1.82460	1.27633	2.03590
O	3.24540	3.71451	1.83576
H	3.13350	2.97271	2.46020
O	2.47818	5.33736	-0.56287
H	2.36833	5.50090	-1.54695
C	1.77639	3.80577	-3.01888
O	2.08586	5.04656	-3.10400
O	1.65927	2.99000	-3.94526
C	0.21157	-2.57579	1.97077
H	-0.27501	-2.88443	1.03740
H	-0.35330	-3.00753	2.80746
H	1.22263	-2.98762	1.96277

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ts5.out

C	2.62347	5.04611	-0.98099
C	1.90596	3.22159	0.56236
O	2.63679	2.62429	-1.67311
C	1.67765	2.37130	-0.67895
C	2.50541	3.98161	-2.13065
C	1.67755	4.68336	0.16601
H	2.99603	3.12186	0.78287
H	0.66516	2.56002	-1.09567
H	1.48912	4.11731	-2.55052
H	0.64189	4.79615	-0.20647
H	3.65722	5.01232	-0.58886
O	1.77416	1.02463	-0.24519
C	1.09306	0.74936	0.95154
O	1.62785	-0.00873	1.75814
C	-0.45253	0.77386	0.83215
H	-0.74570	1.63322	0.22610
C	-0.97612	-0.48963	0.15902
C	-2.04913	-2.82052	-1.03566
C	-0.55602	-1.76983	0.56228
C	-1.93558	-0.40933	-0.86131
C	-2.46964	-1.55687	-1.45283
C	-1.08446	-2.91746	-0.02797
H	0.21531	-1.83119	1.32398
H	-2.26345	0.57194	-1.19789
H	-3.21014	-1.46157	-2.24526
H	-0.73656	-3.89708	0.29620
H	-2.45956	-3.71777	-1.49545
O	1.11053	2.76975	1.57884
O	1.84975	5.50125	1.33104
H	1.53409	4.88960	2.02234
O	2.31808	6.32591	-1.50406
H	2.76984	6.28008	-2.39889
C	3.50842	4.27472	-3.30325
O	3.54258	5.51220	-3.63389
O	4.12938	3.33461	-3.82036
C	-1.06892	0.95002	2.22994
H	-0.71920	0.15626	2.89728
H	-2.16616	0.92166	2.18805
H	-0.72935	1.91248	2.61713

Molecule 13

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gs1.out

C	3.09990	-2.14390	0.69280
C	3.35070	0.27230	1.23430
O	2.34530	-0.42280	-0.93010
C	2.38980	0.55800	0.04850
C	2.15160	-1.79480	-0.47950
C	3.01750	-1.12330	1.85690
H	3.09980	1.04680	2.00870
H	2.67360	1.48250	-0.46040
H	2.49150	-2.38050	-1.33990
H	3.86840	-1.34130	2.52020
H	2.80550	-3.14370	1.05830
O	1.01100	0.74170	0.59900
C	0.03030	1.21470	-0.16860
O	4.63760	0.30200	0.77770
O	1.83120	-1.21330	2.63150
H	1.11950	-1.53780	2.02030
O	4.44130	-2.18140	0.22920
H	4.71260	-1.18270	0.32660
C	0.61450	-2.07910	-0.33240
O	-0.02250	-2.13760	-1.41350
O	0.12040	-2.20200	0.83520
C	-1.31970	0.74350	0.41880
H	-1.15850	-0.31880	0.64930
C	-2.44610	0.83970	-0.59310
C	-4.52430	0.90170	-2.50050
C	-3.37510	1.88780	-0.61320
C	-2.56940	-0.18510	-1.55040
C	-3.59890	-0.14760	-2.49090
C	-4.40670	1.92200	-1.55660
H	-3.29790	2.68960	0.11670
H	-1.84000	-1.00210	-1.54250
H	-3.67950	-0.94830	-3.22390
H	-5.11730	2.74770	-1.55170
H	-5.32720	0.92360	-3.23620
O	0.15440	1.92770	-1.14800
C	-1.56280	1.46840	1.75580
H	-1.59400	2.55950	1.63840
H	-0.74610	1.22280	2.43890
H	-2.50980	1.14870	2.20770

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ts1.out

C	2.90450	1.51828	-0.08301
C	0.72391	0.86853	-0.53850
C	2.35987	-0.95966	-0.27560
C	1.13923	-0.49321	-1.06605
C	3.46921	0.08916	-0.40954
O	1.71168	1.83878	-0.81494
H	0.55759	0.83266	0.55731
H	2.09844	-1.03060	0.79668
H	3.80356	0.08748	-1.46405
H	2.66526	1.49808	0.99887
O	4.54185	-0.20033	0.46730
H	5.00287	0.69112	0.50457
O	2.74706	-2.25631	-0.75273
H	1.88202	-2.62261	-1.01079
C	3.99642	2.63215	-0.26816
O	5.13477	2.30365	0.22106
O	3.68577	3.70460	-0.80698
O	-0.50785	1.19439	-1.15762
C	-1.17332	0.12547	-1.82064
H	1.48470	-0.31380	-2.10757
O	0.05273	-1.33933	-1.02804
C	-2.49011	-0.29715	-1.10910
O	-1.13105	0.05195	-3.04220
C	-2.86115	-1.71990	-1.56429
H	-2.11766	-2.42643	-1.18904
H	-2.83753	-1.75462	-2.65692
H	-3.85923	-2.00844	-1.20775
C	-2.58774	-0.14316	0.39795
C	-2.92386	0.05421	3.19976
C	-1.71921	-0.81612	1.27642
C	-3.61907	0.62695	0.95619
C	-3.79060	0.72896	2.33926
C	-1.88743	-0.71233	2.65762
H	-0.89618	-1.36991	0.82390
H	-4.29930	1.15875	0.29235
H	-4.59820	1.33892	2.74188
H	-1.19496	-1.22996	3.31913
H	-3.04733	0.13237	4.27879
H	-3.23668	0.38899	-1.54135

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ts2.out

C	0.83620	-2.69582	2.48268
C	0.31294	-0.74521	1.32814
C	-1.59500	-2.07959	2.12432
C	-1.09144	-1.21520	0.95719
C	-0.62997	-3.24402	2.34916
O	1.21968	-1.80898	1.41577
H	0.30386	-0.15612	2.26325
H	-1.59941	-1.46698	3.04545
H	-0.67170	-3.89792	1.45774
H	0.85221	-2.13140	3.43524
O	-0.95964	-3.96507	3.52351
H	-0.09843	-4.44477	3.70404
O	-2.93583	-2.47909	1.81792

H	-3.22010	-1.69312	1.30751
C	1.88094	-3.85830	2.63613
O	1.51079	-4.75542	3.47226
O	2.94385	-3.80888	1.99869
O	0.70737	0.11758	0.24935
C	-0.13266	1.20744	0.13575
H	-0.92554	-1.92288	0.10278
O	-1.90640	-0.16795	0.65233
C	-0.60446	1.40535	-1.31670
O	-0.16914	2.11642	0.95811
C	0.39501	2.22610	-2.12155
C	2.16849	3.78910	-3.67580
C	0.89962	3.44604	-1.63725
C	0.80994	1.80590	-3.39359
C	1.68353	2.57544	-4.16562
C	1.77440	4.21540	-2.40377
H	0.61168	3.75494	-0.63679
H	0.44276	0.85691	-3.77817
H	1.99030	2.22177	-5.14848
H	2.15750	5.15263	-2.00348
H	2.85180	4.39068	-4.27228
C	-1.99560	2.06222	-1.32036
H	-1.96471	3.01600	-0.78388
H	-2.66805	1.38053	-0.79505
H	-2.34433	2.24477	-2.34585
H	-0.68365	0.41255	-1.76491

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ts3.out

C	1.52343	-1.77523	3.12867
C	1.07781	-0.66919	1.15362
C	2.01434	0.72858	2.95321
C	0.98983	0.69438	1.82447
C	1.69435	-0.42285	3.91484
O	0.62526	-1.68671	2.00819
H	2.11296	-0.88447	0.82710
H	3.02397	0.55781	2.54009
H	0.72884	-0.18739	4.40091
H	2.53539	-2.02054	2.75165
O	2.72300	-0.57594	4.87431
H	2.53253	-1.50286	5.21076
O	1.98075	2.01216	3.59946
H	1.81002	2.59965	2.84396
C	1.11247	-2.95045	4.08603
O	1.78346	-2.96452	5.17798
O	0.24586	-3.75761	3.71970
O	0.25803	-0.51843	0.00799
C	0.76453	0.61215	-0.71250
H	-0.01512	0.71989	2.30156
O	1.12403	1.66146	0.84324
C	-0.39945	1.44334	-1.35242
O	1.81226	0.51368	-1.35983
C	-1.71113	1.51708	-0.58706
C	-4.14612	1.81245	0.83177
C	-2.90522	0.95619	-1.06359
C	-1.76472	2.22629	0.62755
C	-2.96215	2.37129	1.32437
C	-4.10813	1.09840	-0.36468
H	-2.90465	0.39698	-1.99428
H	-0.82148	2.60916	1.01106
H	-2.97050	2.91631	2.26652
H	-5.01653	0.64579	-0.76011
H	-5.08021	1.92251	1.38006
H	0.01623	2.45787	-1.37010
C	-0.55392	0.98562	-2.81295
H	0.43124	1.02012	-3.28228
H	-1.25377	1.62032	-3.37364
H	-0.90910	-0.05011	-2.87290

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ts4.out

C	2.09966	1.62773	-0.20063
C	0.58993	0.53595	-1.57399
C	1.46046	-0.78992	0.31958
C	1.04616	-0.84544	-1.14614
C	2.54601	0.28237	0.47700
O	1.64709	1.46432	-1.55446
H	-0.21445	0.89850	-0.89416
H	0.59263	-0.48431	0.93195
H	3.44777	-0.08083	-0.05109
H	1.25607	1.99904	0.41435
O	2.81600	0.51922	1.84533
H	3.27970	1.40895	1.79782
O	1.90615	-2.08679	0.74575
H	1.33546	-2.67445	0.22288
C	3.22246	2.72228	-0.11187
O	3.77453	2.78075	1.04297
O	3.45119	3.43724	-1.09831
O	0.08583	0.35815	-2.87396
C	-0.68629	-0.86873	-3.00756
H	1.96644	-1.05481	-1.73401
O	0.02182	-1.71987	-1.45207
C	-2.14257	-0.62867	-2.47636
O	-0.52758	-1.51585	-4.03795
H	-2.06458	-0.22089	-1.46393
C	-2.94104	-1.92072	-2.37960
C	-4.43620	-4.31149	-2.08848
C	-4.00262	-2.22698	-3.24340
C	-2.63552	-2.85195	-1.36864
C	-3.37235	-4.02574	-1.22568
C	-4.74270	-3.40579	-3.10273
H	-4.26212	-1.53695	-4.04001

H	-1.77453	-2.63613	-0.74222
H	-3.11139	-4.72839	-0.43577
H	-5.56142	-3.61248	-3.79112
H	-5.01146	-5.22912	-1.97426
C	-2.79445	0.43189	-3.37931
H	-2.20955	1.35295	-3.32656
H	-3.83016	0.64920	-3.08455
H	-2.78912	0.09917	-4.42337

Molecule 15

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gs1.out

C	1.83133	-0.40046	2.01212
C	-0.59296	-0.20154	1.72920
C	0.32397	-2.08670	3.02840
C	-0.81657	-1.69025	2.01123
C	1.70264	-1.89873	2.41732
O	0.71563	0.08844	1.26735
H	-0.87745	0.42649	2.58522
H	0.26121	-1.39797	3.89947
H	1.77497	-2.52259	1.50778
H	1.91477	0.15953	2.96135
O	2.75874	-2.20850	3.32021
H	3.52172	-1.72535	2.90911
O	-0.01886	-3.39819	3.42959
H	-1.01098	-3.29383	3.26173
C	3.13420	-0.13240	1.19094
O	3.05381	0.47450	0.10013
O	4.18529	-0.58118	1.75265
O	-1.37736	0.23064	0.57037
C	-1.40810	1.54786	0.34793
O	-1.63905	2.39623	1.19224
C	-1.06373	1.96917	-1.11148
C	0.33686	2.64687	-0.99120
H	1.09226	1.97189	-0.57435
H	0.25741	3.51774	-0.33303
H	0.66654	2.98008	-1.98318
H	-0.52914	-2.18458	1.03607
O	-2.00471	-2.06643	2.51272
C	-0.97086	0.79501	-2.09495
C	-0.71167	-1.32971	-3.94538
C	-1.85933	0.65267	-3.17006
C	0.06030	-0.15707	-1.96264
C	0.18153	-1.20103	-2.87765
C	-1.73567	-0.39660	-4.08709
H	-2.66611	1.36572	-3.30849
H	0.76767	-0.09166	-1.13902
H	0.98263	-1.92351	-2.74468
H	-2.44500	-0.47802	-4.90946
H	-0.61084	-2.15010	-4.65375
C	-2.08715	3.04048	-1.53685
H	-2.09853	3.83067	-0.78344
H	-3.10379	2.63663	-1.60575
H	-1.82239	3.47474	-2.50818

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gs2.out

C	1.83252	-0.41930	2.00662
C	-0.59159	-0.20925	1.72913
C	0.32038	-2.10549	3.01564
C	-0.82044	-1.69871	2.00290
C	1.69863	-1.91945	2.40303
O	0.71739	0.07855	1.26696
H	-0.87243	0.41481	2.58924
H	0.26202	-1.42153	3.89078
H	1.76670	-2.53814	1.48966
H	1.92001	0.13458	2.95907
O	2.75522	-2.23881	3.30198
H	3.51931	-1.75616	2.89235
O	-0.02688	-3.41789	3.40997
H	-1.01890	-3.30868	3.24457
C	3.13490	-0.15148	1.18458
O	4.18527	-0.60765	1.74166
O	3.05487	0.46211	0.09749
O	-1.37612	0.23265	0.57405
C	-1.40193	1.55127	0.35922
O	-1.62853	2.39561	1.20872
C	-1.05770	1.97973	-1.09816
C	0.34565	2.65131	-0.97569
H	1.09912	1.97082	-0.56432
H	0.27052	3.51826	-0.31187
H	0.67511	2.98959	-1.96604
H	-0.53677	-2.18851	1.02437
O	-2.00912	-2.07315	2.50443
C	-0.97057	0.81100	-2.08857
C	-0.72130	-1.30416	-3.95132
C	-1.86080	0.67803	-3.16343
C	0.05722	-0.14561	-1.96291
C	0.17359	-1.18481	-2.88393
C	-1.74202	-0.36649	-4.08654
H	-2.66513	1.39478	-3.29696
H	0.76585	-0.08743	-1.13983
H	0.97220	-1.91095	-2.75598
H	-2.45259	-0.44063	-4.90853
H	-0.62431	-2.12085	-4.66447
C	-2.07749	3.05744	-1.51604
H	-2.08486	3.84324	-0.75800
H	-3.09575	2.65791	-1.58608
H	-1.81217	3.49629	-2.48515

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gs3.out

C	1.45624	-1.81228	1.77944
C	-0.54379	-0.40884	2.08993
C	-0.86700	-2.92809	1.88720
C	-1.38458	-1.62434	2.56684
C	0.63581	-3.03719	2.25337
O	0.82687	-0.54097	2.14007
H	-0.80387	0.46855	2.68249
H	-1.37394	-3.74774	2.41937

H	1.07165	-3.92025	1.75212
H	2.37270	-1.80337	2.37599
O	0.74575	-3.18954	3.65832
H	-0.03250	-2.57658	3.98673
O	-1.14577	-3.06396	0.50361
H	-0.34865	-2.71488	0.01497
C	1.90303	-1.77010	0.27943
O	1.06539	-2.16659	-0.60305
O	3.04743	-1.31856	0.05138
O	-0.91560	-0.05462	0.65435
C	-1.38784	1.13295	0.34053
O	-1.66223	2.04548	1.10967
C	-1.56749	1.28078	-1.20672
C	-2.65291	2.34207	-1.45062
H	-2.40713	3.28288	-0.95332
H	-3.60574	1.99606	-1.03675
H	-2.79220	2.52145	-2.52387
H	-2.41910	-1.43483	2.17570
O	-1.28718	-1.70786	3.92763
C	-0.19679	1.69205	-1.78423
C	2.36584	2.39289	-2.74815
C	0.87997	0.79278	-1.70177
C	0.03672	2.94713	-2.36808
C	1.30199	3.29069	-2.85497
C	2.14881	1.14284	-2.16327
H	0.75236	-0.19606	-1.26789
H	-0.76648	3.67378	-2.44403
H	1.45448	4.27073	-3.30628
H	2.94765	0.42129	-2.01257
H	3.35516	2.67101	-3.10893
C	-2.02263	-0.06423	-1.82095
H	-3.00604	-0.34471	-1.42598
H	-1.33674	-0.87425	-1.57379
H	-2.10123	0.03014	-2.91183

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gs4.out

C	2.33166	-1.04697	2.20516
C	0.01335	-0.23088	2.14680
C	0.45834	-2.62490	1.40900
C	-0.55240	-1.67788	2.12351
C	1.79276	-2.49833	2.18742
O	1.30578	-0.07684	2.59448
H	-0.62398	0.39982	2.76758
H	0.08340	-3.64302	1.59428
H	2.56521	-3.11413	1.69291
H	3.03987	-0.98883	3.03606
O	1.58906	-2.97240	3.50746
H	0.61847	-2.64062	3.69123
O	0.59268	-2.45254	0.00389
H	1.38462	-1.84298	-0.14137
C	3.11075	-0.55689	0.93330
O	4.14150	0.11375	1.14481
O	2.64493	-0.88755	-0.21355
O	-0.04353	0.37173	0.75082
C	-0.79790	1.41067	0.46827
O	-1.55508	2.00117	1.22873
C	-0.62288	1.83953	-1.02372
C	0.87313	1.75737	-1.42307
H	1.30961	0.77369	-1.23157
H	1.45539	2.47839	-0.83694
H	0.98511	2.01185	-2.48543
H	-1.47123	-1.62268	1.48176
O	-0.77466	-2.07667	3.41038
C	-1.44378	0.88253	-1.91486
C	-2.88002	-0.89508	-3.58822
C	-2.39586	1.35312	-2.83324
C	-1.22968	-0.50828	-1.84601
C	-1.94229	-1.37765	-2.67171
C	-3.10461	0.47874	-3.66317
H	-2.59713	2.41665	-2.91104
H	-0.52785	-0.93677	-1.13181
H	-1.75357	-2.44435	-2.58001
H	-3.83521	0.87875	-4.36521
H	-3.43313	-1.58000	-4.22903
C	-1.09570	3.29915	-1.13874
H	-0.50442	3.92544	-0.46446
H	-2.14366	3.40860	-0.84835
H	-0.95902	3.67801	-2.15880

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gs5.out

C	2.26171	-1.13207	2.28287
C	-0.01788	-0.22325	2.14082
C	0.35172	-2.64320	1.44617
C	-0.64147	-1.64636	2.11662
C	1.66441	-2.56073	2.26637
O	1.26479	-0.11649	2.62914
H	-0.64817	0.44127	2.73283
H	-0.07154	-3.64251	1.62981
H	2.42680	-3.21392	1.80515
H	2.94673	-1.09150	3.13400
O	1.39939	-3.00773	3.58473
H	0.43754	-2.63308	3.73250
O	0.53787	-2.49308	0.04444
H	1.35747	-1.91640	-0.08247
C	3.10001	-0.69144	1.03060
O	2.65611	-1.01521	-0.12683
O	4.15284	-0.06495	1.26726
O	-0.00589	0.36263	0.73692
C	-0.70746	1.42767	0.41774
O	-1.45919	2.06194	1.14776

C	-0.47261	1.82494	-1.07483
C	1.02901	1.67142	-1.42935
H	1.41654	0.67349	-1.20839
H	1.62531	2.37664	-0.83811
H	1.18247	1.90171	-2.49196
H	-1.53680	-1.56252	1.44566
O	-0.91932	-2.01804	3.40098
C	-1.31032	0.89124	-1.97443
C	-2.78018	-0.84713	-3.65986
C	-2.21899	1.38877	-2.92208
C	-1.15778	-0.50624	-1.88184
C	-1.88659	-1.35602	-2.71402
C	-2.94364	0.53382	-3.75849
H	-2.37337	2.45869	-3.01772
H	-0.49155	-0.95463	-1.14593
H	-1.74683	-2.42844	-2.60301
H	-3.63939	0.95502	-4.48316
H	-3.34556	-1.51707	-4.30576
C	-0.87655	3.30210	-1.22380
H	-0.28297	3.91062	-0.53550
H	-1.92827	3.46142	-0.97276
H	-0.68666	3.66086	-2.24270

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ts1.out

C	2.24141	-2.38561	1.96053
C	0.60068	-1.34512	0.70691
C	2.55626	-2.13912	-0.56517
C	1.55359	-0.99892	-0.42412
C	3.27695	-2.30217	0.77870
O	1.25746	-1.33586	1.94825
H	0.12429	-2.32994	0.53683
H	2.01795	-3.07883	-0.78033
H	3.89647	-1.39836	0.93220
H	1.72501	-3.35566	1.82632
O	4.07379	-3.47122	0.78389
H	4.22219	-3.59688	1.76873
O	3.45823	-1.85277	-1.64614
H	2.86666	-1.39801	-2.26991
C	2.96643	-2.45494	3.35159
O	3.95123	-3.27457	3.36126
O	2.53605	-1.77560	4.29529
O	-0.38821	-0.33594	0.62823
C	-0.89272	-0.29868	-0.73194
O	-1.72208	-1.13268	-1.09383
C	-1.05477	1.19213	-1.20826
C	0.14568	2.07488	-0.80870
H	1.04417	1.66021	-1.27058
H	0.29116	2.07959	0.27328
H	-0.00291	3.10961	-1.14982
H	2.12944	-0.11674	-0.06065
O	0.79744	-0.71170	-1.54223
C	-2.32903	1.77937	-0.57016
C	-4.60721	2.94450	0.66666
C	-2.49680	1.75823	0.82905
C	-3.34165	2.39261	-1.32404
C	-4.46381	2.96858	-0.71926
C	-3.61451	2.32869	1.43519
H	-1.74742	1.25541	1.43154
H	-3.26075	2.42024	-2.40551
H	-5.22848	3.43429	-1.33996
H	-3.71320	2.28588	2.51828
H	-5.47993	3.38959	1.14156
C	-1.14463	1.13506	-2.74276
H	-0.23239	0.65772	-3.10497
H	-1.23058	2.13614	-3.18815
H	-1.99480	0.52193	-3.05407

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ts2.out

C	1.45516	-2.20944	3.07205
C	0.12834	-0.98427	1.61127
C	1.93319	-2.30085	0.58091
C	1.17939	-0.96450	0.50538
C	2.55115	-2.44986	1.97266
O	0.70726	-0.99323	2.88680
H	-0.57060	-1.83092	1.49039
H	1.21366	-3.12939	0.44297
H	3.32599	-1.66833	2.08416
H	0.76084	-3.06772	2.98578
O	3.10429	-3.74194	2.15246
H	3.16573	-3.78949	3.15123
O	2.88849	-2.32302	-0.48590
H	2.39952	-1.79646	-1.15015
C	2.05825	-2.26857	4.52080
O	2.85687	-3.25521	4.69036
O	1.70905	-1.42290	5.35869
O	-0.60698	0.23561	1.43313
C	-1.23219	0.25969	0.19487
O	-2.15183	-0.50002	-0.08055
C	-1.09287	1.67269	-0.46121
C	0.33937	2.20745	-0.31226
H	1.02276	1.50470	-0.79612
H	0.59985	2.24403	0.74663
H	0.43328	3.21964	-0.73087
H	1.91064	-0.18461	0.84340
O	0.62321	-0.69437	-0.71066
C	-1.55241	1.62770	-1.92530
C	-2.47525	1.65884	-4.61216
C	-2.86205	1.23089	-2.25734
C	-0.71815	2.01816	-2.98277
C	-1.16955	2.03774	-4.30575

C	-3.31621	1.24676	-3.57521
H	-3.50772	0.86495	-1.46935
H	0.30735	2.29999	-2.77689
H	-0.48930	2.34521	-5.09827
H	-4.33352	0.92632	-3.79433
H	-2.82961	1.67240	-5.64146
C	-2.05177	2.60393	0.33689
H	-1.74522	2.62806	1.38702
H	-3.08745	2.25337	0.29494
H	-2.01854	3.62638	-0.06195

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ts3.out

C	3.18665	1.47197	1.46732
C	1.34037	0.54060	0.41657
C	3.08250	-1.04705	1.13682
C	2.07071	-0.73229	0.03552
C	4.02119	0.15133	1.31154
O	2.20996	1.64977	0.42966
H	0.88384	0.43400	1.42297
H	2.54382	-1.19114	2.09156
H	4.62751	0.23787	0.39030
H	2.66195	1.37367	2.43857
O	4.84303	-0.01806	2.45100
H	5.14181	0.92685	2.61268
O	3.77566	-2.25663	0.79934
H	3.07662	-2.75033	0.33544
C	4.10814	2.73739	1.59554
O	5.10614	2.55294	2.37781
O	3.79598	3.77783	0.99809
O	0.31023	0.72350	-0.53604
C	-0.09881	-0.44318	-1.26361
H	2.65401	-0.48254	-0.87783
O	1.13300	-1.71312	-0.19298
C	-1.49001	-0.95937	-0.76424
O	0.17606	-0.51803	-2.45316
C	-1.56644	-1.10081	0.76959
H	-1.40820	-0.12562	1.24109
H	-0.77805	-1.77383	1.10962
H	-2.55288	-1.47839	1.07335
C	-2.48744	0.13734	-1.21843
H	-2.14249	1.10222	-0.83771
H	-3.49992	-0.03596	-0.83142
H	-2.52968	0.19280	-2.31057
C	-1.82262	-2.31813	-1.40572
C	-2.45393	-4.86889	-2.47269
C	-3.14373	-2.67797	-1.71360
C	-0.81558	-3.27358	-1.64290
C	-1.13284	-4.52612	-2.16816
C	-3.46135	-3.93461	-2.23993
H	-3.94973	-1.96962	-1.54477
H	0.20870	-3.00420	-1.39292
H	-0.33427	-5.24515	-2.34402
H	-4.49873	-4.17655	-2.46859
H	-2.69238	-5.84840	-2.88496

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ts4.out

C	2.34083	-2.71280	1.83083
C	0.75850	-1.46394	0.71230
C	2.58750	-2.33546	-0.68972
C	1.69794	-1.12524	-0.43557
C	3.33576	-2.64657	0.61356
O	1.45974	-1.57893	1.92278
H	0.20428	-2.39942	0.50834
H	1.96026	-3.20846	-0.94079
H	4.03970	-1.81254	0.79489
H	1.73099	-3.62065	1.65773
O	4.02243	-3.87929	0.51356
H	4.19602	-4.07916	1.48250
O	3.48190	-2.06642	-1.78232
H	2.91455	-1.54366	-2.37291
C	3.10274	-2.94413	3.18444
O	4.01624	-3.83888	3.09743
O	2.75785	-2.30905	4.19145
O	-0.15270	-0.38102	0.70777
C	-0.69467	-0.31831	-0.62345
O	-1.52136	-1.16571	-0.98675
C	-0.99729	1.18656	-1.00567
H	2.35484	-0.31629	-0.04788
O	0.92239	-0.69373	-1.50208
C	-1.13595	1.23015	-2.54454
H	-0.18055	1.00341	-3.02141
H	-1.48561	2.21567	-2.88271
H	-1.85144	0.46109	-2.84896
C	0.04535	2.22012	-0.56290
C	1.96784	4.21052	0.08553
C	-0.27932	3.32117	0.24610
C	1.37137	2.14053	-1.03249
C	2.31321	3.11598	-0.71300
C	0.66426	4.30228	0.56798
H	-1.28390	3.42495	0.64189
H	1.63536	1.26059	-1.61374
H	3.33214	3.01314	-1.08172
H	0.37278	5.13831	1.20255
H	2.70694	4.96914	0.33769
C	-2.38759	1.47138	-0.39349
H	-2.35199	1.44737	0.70088
H	-3.06632	0.68174	-0.72202
H	-2.78603	2.44497	-0.71119

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ts5.out

C	3.15803	0.00033	1.53088
C	0.98031	0.36161	0.81820
C	2.67606	0.17388	-0.96120
C	1.41052	0.91425	-0.53009
C	3.74900	0.35189	0.11839
O	1.92508	0.67978	1.81635
H	0.86262	-0.73963	0.77553
H	2.46052	-0.90803	-1.04032
H	4.03936	1.41927	0.12616
H	2.96584	-1.09071	1.50413
O	4.86484	-0.47970	-0.13935
H	5.30228	-0.49584	0.76436
O	3.07758	0.66963	-2.24583
H	2.21188	0.89419	-2.63301
C	4.20757	0.23192	2.67626
O	5.37566	-0.20488	2.38059
O	3.84127	0.75374	3.73947
O	-0.29637	0.90912	1.11232
C	-0.92911	1.61898	0.06393
H	1.71082	1.96650	-0.33520
O	0.35758	0.84113	-1.41368
C	-2.28784	0.95751	-0.37785
O	-0.82924	2.83672	-0.00648
C	-2.52302	1.34050	-1.85678
H	-1.74212	0.90923	-2.48386
H	-2.46312	2.42883	-1.95240
H	-3.51023	0.99858	-2.19765
C	-2.36250	-0.56873	-0.22802
C	-2.56325	-3.39898	-0.11167
C	-1.44034	-1.39435	-0.90247
C	-3.37783	-1.20357	0.50565
C	-3.47988	-2.59749	0.56555
C	-1.54040	-2.78352	-0.83955
H	-0.61822	-0.89623	-1.42065
H	-4.10798	-0.61282	1.04868
H	-4.27994	-3.05198	1.14871
H	-0.80287	-3.39261	-1.35934
H	-2.63671	-4.48443	-0.06527
C	-3.36223	1.67196	0.47746
H	-3.24952	1.43703	1.54177
H	-4.37943	1.39977	0.16581
H	-3.23185	2.74924	0.35662