Supplementary Information

A Theoretical Study of Selective Radical Relay and Coupling Reactions for Alkene Difunctionalization

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1. Complete reference for Gaussian 16

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

2. Computational Methods

The density functional theory (DFT)[1] calculations were performed by using the *Gaussian 16* program. The geometric structures of all involved transition states were optimized by using the M06-2X density functional, combined with the def2-SVP. The solvent effects of EtOAc were simulated by the IEF-PCM[2, 3] model. The harmonic frequency calculations were conducted at the same level to corroborate each transition state has one and only one imaginary frequency and other structures have no imaginary frequency. Based on the optimized structures, all energies were refined by conducting single point energy calculations at the M06-2X/def2-TZVP/ IEF-PCM$_{EtOAc}$ level of theory.

The analysis for the electrophilicity and nucleophilicity

The electronic chemical potential μ and chemical hardness η can be obtained by the frontier HOMO and LUMO energies[4-6]:

$$\mu = (E_{LUMO} + E_{HOMO}) / 2 \qquad (1)$$

$$\eta = (E_{LUMO} - E_{HOMO}) \qquad (2)$$

In 1999, Parr defined the electrophilicity ω index[7]:

$$\omega = \mu^2 / 2\eta \qquad (3)$$

In 2008, Domingo et al. proposed an empirical (relative) nucleophilicity N index for closed-shell organic molecules based on the HOMO energies. The nucleophilicity N index is referred to tetracyanoethylene (TCE), which is the most electrophilic neutral species[8]:

$$N = E_H - E_H(TCE) \qquad (4)$$

The Fukui function [9](FF), one of the fundamental quantities in conceptual density functional theory[10] (CDFT), has been extensively explored to describe reactivity and regioselectivity of many chemical reactions. In practice, the condensed-to-atom Fukui functions (f_k) at the atom k are usually evaluated from differences in atomic charges.

$$f_k^+ = q_k(N+1) - q_k(N) \qquad (5)$$

$$f_k^- = q_k(N) - q_k(N-1) \qquad (6)$$

where q_k is the electronic charge of atom k and N is the number of electrons. The three condensed Fukui functions f_k^+ f_k^- and characterize the reactivity preferences for nucleophilic, electrophilic, and radical attacks, respectively. In general, the larger the value of a condensed-to-atom Fukui function, the greater the reactivity of the corresponding atom.

In addition, according to Domingo's definition, the local electrophilicity (ω_k) and local nucleophilicity (N_k) index can be expressed by the following equations[11]:

$$N_k = N \times f_k^- \qquad (7)$$

$$\omega_k = \omega \times f_k^+ \qquad (8)$$

The calculation for the rate of EET

Excitation energy transfer (EET) is a process which an excited-state donor molecule transfers energy to a nearby ground state receptor molecule. The calculation of the rate constant of the energy switch theory uses Dexter theory[12] .Within Fermi's Golden

Rule[13], the rate of EET (k_{EET}) can be expressed as:

$$k_{EET} = \frac{2\pi}{\hbar} |V|^2 J_D$$

where $\hbar$ is the reduced Planck's constant, V is the electronic coupling factor, and J_D is known as the spectral overlap term. Each of the terms can be computed for a system of interest using quantum chemical calculations where the J_D is considered to be 1[14, 15].

Conformations searching

In order to investigate the multistructural and torsional effect, by using CREST (version 2.12)[16] in combination with the xTB package (version 6.4.0)[17], the conformations of transition states and intermediates have been carried out at the GFN2-xTB level[18].

3. Possible Pathways for intermediate ^{T}2 direct radical addition to styrene

All of four possible pathway for the triplet intermediate ^{T}2 radical addition to the styrene 6 have been investigated as shown in the Scheme. S1.
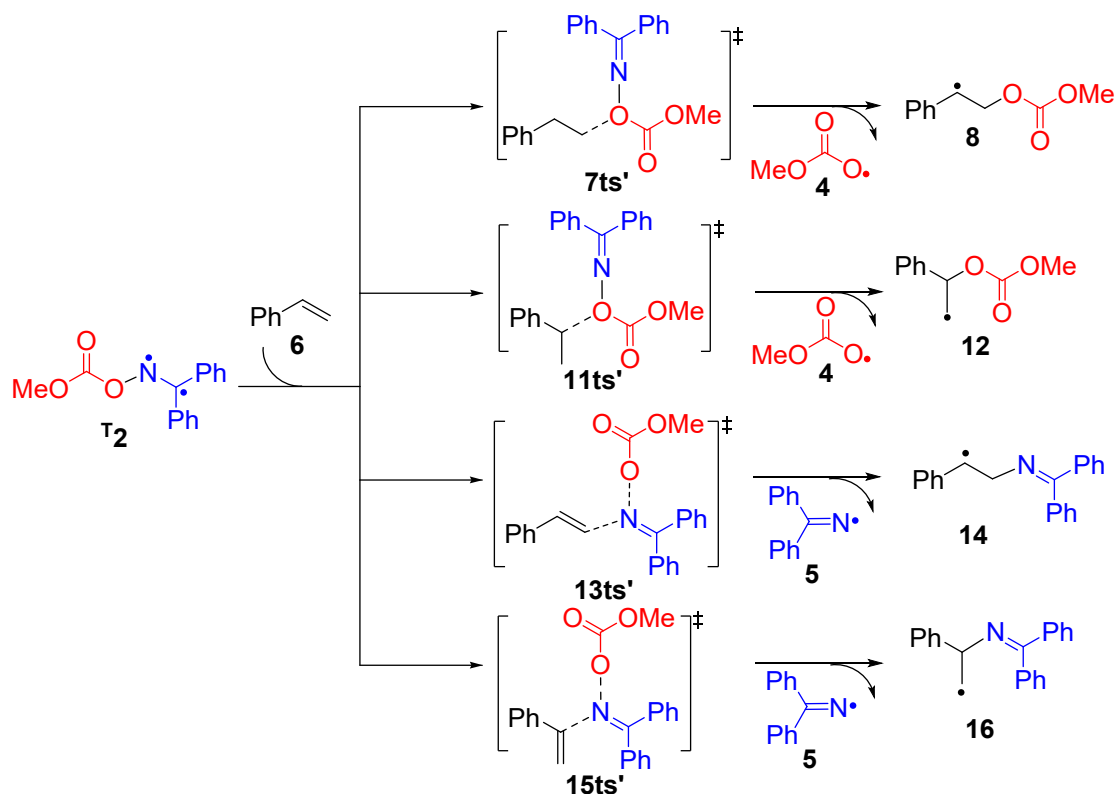
Scheme. S1 Four possible pathways for the triplet intermediate ^{T}2 radical addition to the styrene **6**

The calculated results (Fig. S1) clearly show that the radical addition process would overcome the free energy barrier of at least 22.0 kcal/mol (**13ts'**), which would be much higher than that of homolysis of intermediate $^T2$ (7.1 kcal/mol). Hence, we can exclude that intermediate $^T2$ directly reacts with styrene **6** without the process of hemolysis.
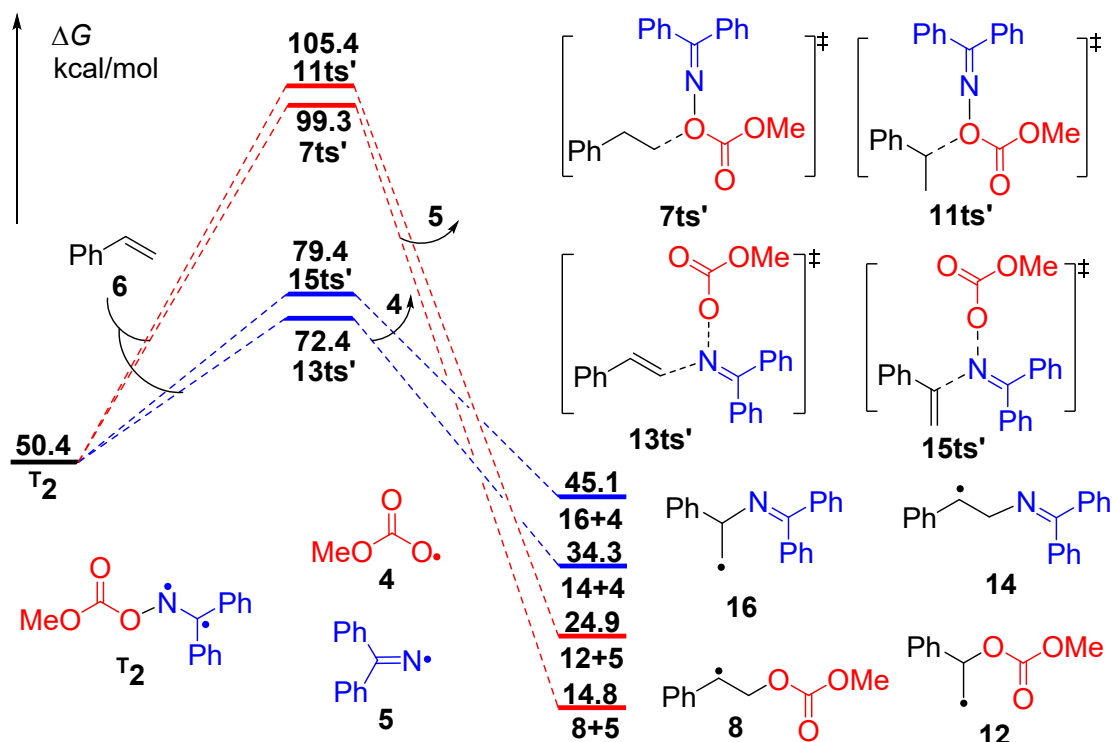
Fig. S1 The energy profile for the intermediate $^T2$ direct radical addition to styrene

4. The SET process between the radical 4, 5, 8 and radical 8

The SET process for the radical species could occur leading to the formation of anions and cations. We have calculated the possible transformation of intermediate 8 as shown in the Fig. S2. It should be noticed that the thermodynamic for the most of SET would be endothermic (at least 55 kcal/mol), implying the process would be impossible to happen. The SET of 8 and 4 is exothermic. Furthermore, the calculated barrier would be only 1.9 kcal/mol, which would be lower than the radical coupling process.
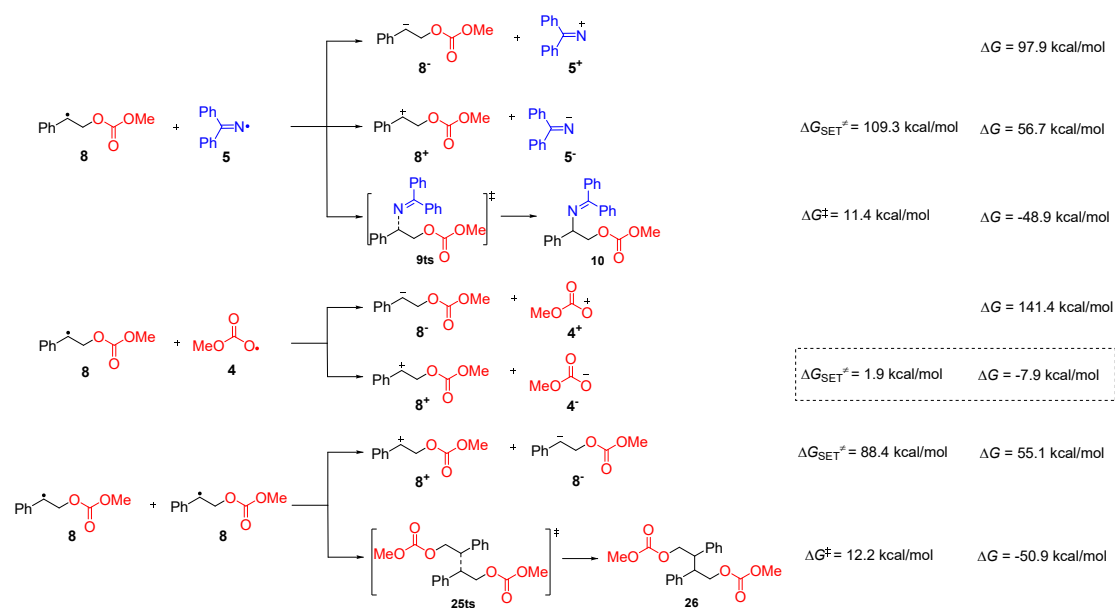
Fig. S2 The SET process between the radical **4**, **5**, **8** and radical **8** (kcal/mol)

5. The local electrophilicity and nucleophilicity, free energy barrier for radical addition and thermodynamic results for other radical species

We have calculated local electrophilicity and nucleophilicity of the extra three radical as shown in the Table S1. The results shows the index for local electrophilicity are bigger than that of nucleophilicity. Furthermore, free energy barrier for the radical addition process have been also calculated. Based on the general model, the stronger electrophilicity, the faster the reaction undergoes.

Table S1 The local electrophilicity and nucleophilicity, free energy barrier for radical addition and thermodynamic results for five radical species

Radicals	Local electrophilicity	Local nucleophilicity	Transition state of radicals adding to styrene	Energy barrier of transition state $\Delta G^{\ddagger}$ (kcal/mol)
	0.470	0.292		23.1
Me–O•	0.918	-0.008		14.2
	1.365	-0.376		10.2

MeO–C(=O)–O•	1.624	0.245	[Ph $\diagup$ S $\diagdown$ Me]‡ (O)	9.7
Br•	3.135	-0.659	[Ph $\diagup$ --Br]‡	6.0
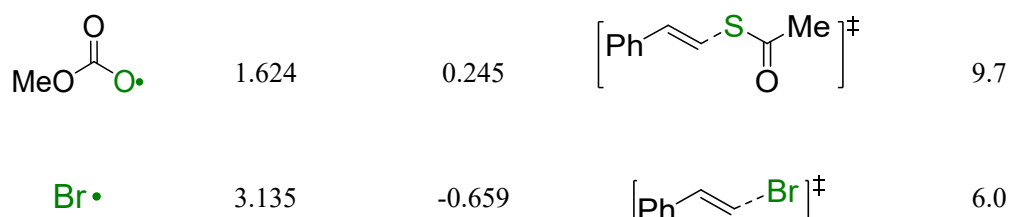
6. Main conformations of transition states and intermediates

In order to find out the favorable structures in the calculations, we have used the CREST program to perform a conformational search for key transition states **7ts** and **9ts**, and intermediate **8** in the revised manuscript. After locating the transition state conformation with the lowest energy, we have computed intrinsic reaction coordinate (IRC) to ensure that the transition state connects the two expected intermediates. The calculated results show the difference for the conformers would be quite close.
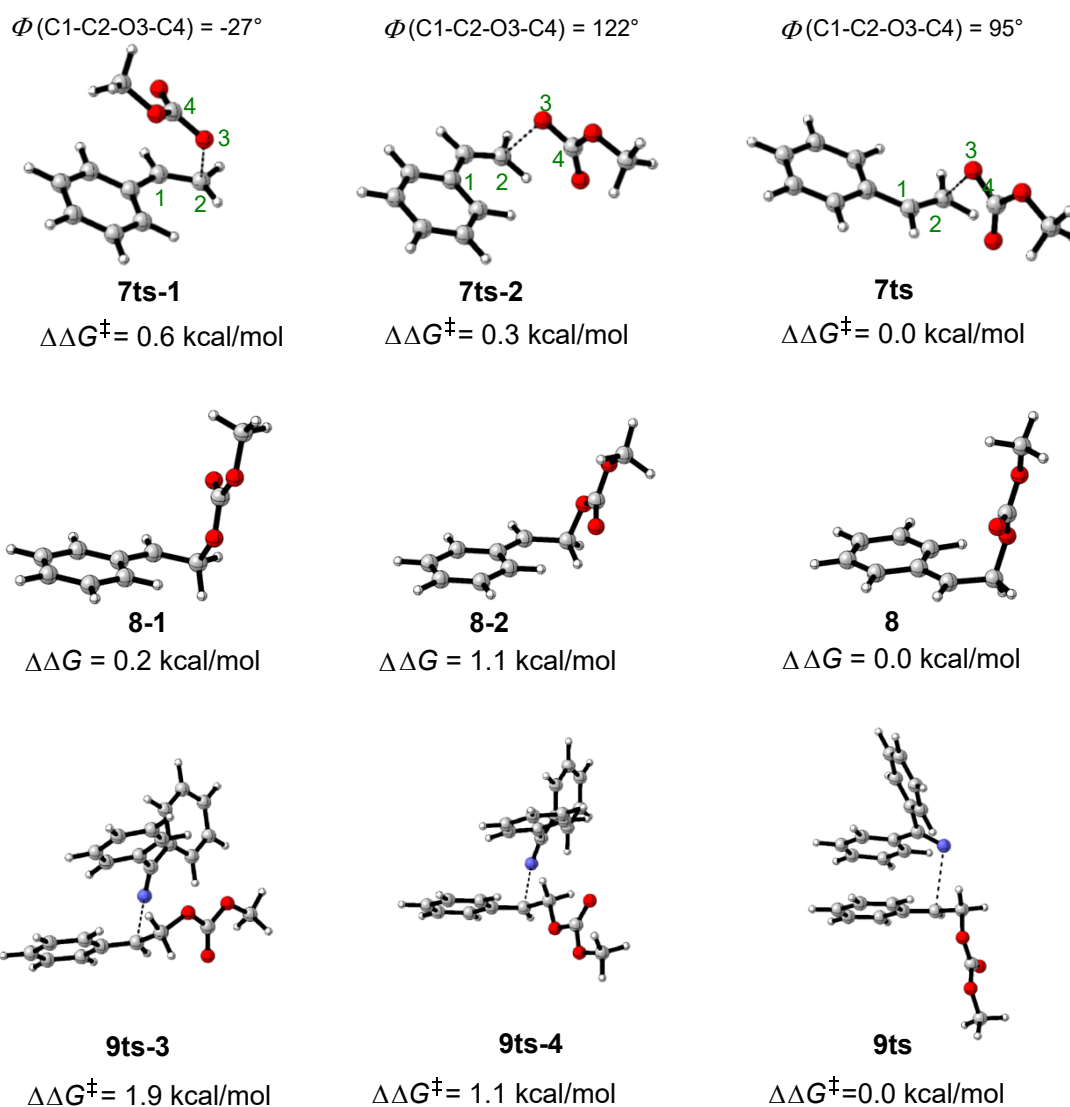
Φ(C1-C2-O3-C4) = -27° Φ(C1-C2-O3-C4) = 122° Φ(C1-C2-O3-C4) = 95°

7ts-1
$\Delta\Delta G^{\ddagger}$ = 0.6 kcal/mol

7ts-2
$\Delta\Delta G^{\ddagger}$ = 0.3 kcal/mol

7ts
$\Delta\Delta G^{\ddagger}$ = 0.0 kcal/mol

8-1
$\Delta\Delta G$ = 0.2 kcal/mol

8-2
$\Delta\Delta G$ = 1.1 kcal/mol

8
$\Delta\Delta G$ = 0.0 kcal/mol

9ts-3
$\Delta\Delta G^{\ddagger}$ = 1.9 kcal/mol

9ts-4
$\Delta\Delta G^{\ddagger}$ = 1.1 kcal/mol

9ts
$\Delta\Delta G^{\ddagger}$ = 0.0 kcal/mol

7. The multistrutureral and torsional effect

The multistrutureral and torsional effect would be very important in the organic chemistry. The most stable intermediate and transition state would majorly affect the kinetic rate. As shown in the Table S2, S3, S4 and S5, the Boltzmann distribution, average Gibbs free energy and $\Delta\Delta G$ for the species have been calculated based on the free energy. The calculated results clearly show the free energy barrier based on the multistructural and torsional effect would be quite close to the most stable one.

Table S2 The free energy, proportion and the relative free energy (ΔG) for the conformations of transition state **7ts** ($\Delta\Delta G$ = Average ΔG-Minimum ΔG)

Conformations	Gibbs free energy corrections G (Hartree)	Proportion (%)	(kca $\Delta G^{\ddagger}$ l/mol)
7ts-1	-613.109262	17.97	48.9
7ts-2	-613.109769	30.85	48.6
7ts	**-613.110251**	**51.18**	**48.3**
Average $\Delta G^{\ddagger}$		48.5 kcal/mol	
$\Delta\Delta G$		0.2 kcal/mol	

Table S3 The free energy, proportion and the relative free energy (ΔG) for the conformations of intermediate **8** ($\Delta\Delta G$ = Average ΔG-Minimum ΔG)

Conformations	Gibbs free energy corrections G (Hartree)	Proportion (%)	ΔG (kcal/mol)
8-1	-613.163263	36.07	15.0
8-2	-613.161735	7.63	15.9
8-3	-613.161473	5.45	16.1
8-4	-613.15933	0.61	17.4
8-5	-613.159675	0.85	17.2
8	**-613.163551**	**48.88**	**14.8**
8-6	-613.15921	0.51	17.5
Average ΔG		15.1 kcal/mol	
$\Delta\Delta G$		0.3 kcal/mol	

Table S4 The free energy, proportion and the relative free energy (ΔG) for the conformations of transition state **9ts** ($\Delta\Delta G$ = Average ΔG-Minimum ΔG)

Conformations	Gibbs free energy	Proportion	(kca $\Delta G^{\ddagger}$

	corrections G (Hartree)	(%)	l/mol)
9ts-1	-1169.058719	4.49	24.4
9ts-2	-1169.0572	0.83	25.4
9ts	**-1169.06142**	**79.12**	**22.7**
9ts-3	-1169.058334	3.20	24.6
9ts-4	-1169.05967	12.36	23.8
Average $\Delta G^{\ddagger}$		23.0 kcal/mol	
$\Delta\Delta G$		0.3 kcal/mol	

Table S5 The free energy, proportion and f the relative free energy (ΔG) for the conformations of intermediate **10** ($\Delta\Delta G$ = Average ΔG-Minimum ΔG)

Conformations	Gibbs free energy corrections G (Hartree)	Proportion (%)	ΔG (kcal/mol)
10-1	-1169.150055	0.13	40.2
10	**-1169.155813**	**58.71**	**36.6**
10-2	-1169.147627	0.01	41.7
10-3	-1169.150087	0.13	40.2
10-4	-1169.149857	0.11	40.3
10-5	-1169.154069	9.17	37.7
10-6	-1169.155158	29.89	37.0
10-7	-1169.14139	0.00	45.7
10-8	-1169.1501	0.13	40.2
10-9	-1169.152468	1.70	38.7
10-10	-1169.1433	0.00	44.7
10-11	-1169.1425	0.00	45.0
10-12	-1169.144829	0.00	43.5
Average ΔG		6.9 kcal/mol	
$\Delta\Delta G$		0.3 kcal/mol	

8. The energies of all the optimized structures

Table S6. The single-point energies (E) at M06-2X/def2-TZVP/IEF-PCM, Gibbs free energy corrections (GFEC) at M06-2X/def2-SVP/IEF-PCM, Zero-point Energy Correction (ZPE) at M06-2X/def2-SVP/IEF-PCM and GFE (=E+GFEC) energies of the stationary points (SPs) involved in the reaction (unit: a.u.)

SP	GFEC	ZPE	E	GFE	Imaginary Frequency	Rotational Constants (GHZ)	Point Group
1	0.136367	0.173820	-973.612450	-973.476083		1.22662 0.42501	CS

						0.31564	
*1	0.132197	0.170665	-973.477007	-973.34481		1.23113 0.42171 0.31411	CS
ᵀ1	0.130899	0.169412	-973.502555	-973.371656		1.22502 0.42554 0.31583	CS
1⁻	0.133373	0.169975	-973.696498	-973.563125		1.21450 0.42222 0.31330	CS
1⁺	0.135604	0.173340	-973.371645	-973.236041		1.23506 0.42637 0.31695	CS
2	0.207313	0.253356	-859.788764	-859.581451		0.40857 0.30187 0.18264	C1
ᵀ2	0.202569	0.250612	-859.703718	-859.501149		0.38765 0.30998 0.18484	C1
2⁻	0.203388	0.249818	-859.862957	-859.659569		0.41134 0.29693 0.17935	C1
2⁺	0.206643	0.251997	-859.527346	-859.320703		0.40530 0.30873 0.18234	C1
ᵀ3ts	0.200177	0.248794	-859.689956	-859.489779	531.38*i*	0.42588 0.29669 0.18735	C1
4	0.024361	0.053924	-303.634779	-303.610418		12.03310 4.54543 3.37061	C1
5	0.153932	0.192388	-556.064275	-555.910343		1.72028 0.41184 0.35911	C1
6	0.103074	0.134473	-309.619158	-309.516084		5.17097 1.54248 1.18808	C1
7ts	0.146979	0.190340	-613.257230	-613.110251	62.21*i*	0.99820 0.78834 0.57543	C1
8	0.153826	0.194357	-613.317097	-613.163271		1.61194 0.40105 0.38149	C1
9ts	0.330697	0.38759	-	-1169.06142	16.78*i*	0.26661	C1

		8	1169.392121		0.12562 0.10411	
10	0.336845	0.394102	-1169.492658	-1169.155813	0.20442 0.17201 0.11805	C1
11ts	0.150291	0.190201	-613.255257	-613.104966	126.22*i* 1.13103 0.68649 0.63002	C1
12	0.149357	0.191749	-613.296876	-613.147519	1.4015679 0.5015610 0.4388015	C1
13ts	0.279029	0.327624	-865.668549	-865.38952	564.31*i* 0.54717 0.18917 0.17027	C1
14	0.280785	0.330491	-865.713296	-865.432511	0.33862 0.20805 0.15900	C1
15ts	0.277689	0.327306	-865.658348	-865.380659	635.08*i* 0.35671 0.19423 0.13742	C1
16	0.279390	0.329114	-865.694644	-865.415254	0.38625 0.21301 0.16508	C1
17ts	0.072971	0.111553	-607.268380	-607.195409	161.14*i* 3.64827 0.61141 0.57933	C1
18	0.078729	0.115877	-607.336874	-607.258145	4.13165 0.67156 0.64805	C1
19ts	0.331424	0.386122	-1112.131126	-1111.799702	155.32*i* 0.35054 0.11652 0.11241	C1
20	0.336218	0.390432	-1112.220296	-1111.884078	0.29314 0.12835 0.12198	C1
21ts	0.201995	0.248436	-859.704732	-859.502737	48.70*i* 0.72820 0.23907 0.20552	C1
22ts	0.021799	0.051441	-303.611430	-303.589631	716.12*i* 9.84256 4.41955 3.44924	C1
23	0.013292	0.036365	-115.044003	-115.030711	156.46938 28.08320 27.85303	C3V

24	0.209046	0.256815	-917.089591	-916.880545		0.36048 0.34132 0.20711	C1
25ts	0.332345	0.389054	-1226.640378	-1226.308033	32.27i	0.33270 0.14850 0.12375	C1
26	0.338245	0.396599	-1226.746466	-1,226.408221		0.29473 0.15177 0.10991	C1
CO$_2$	-0.004650	0.010519	-188.598845	-188.603495		11.81900 11.81900	CS

9. Reference

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10. Geometrical Coordinates of the Listed Compounds

1
0 1

C	0.000008	-0.624433	3.791538
C	0.000015	-1.391240	2.637620
C	-0.000032	-0.771049	1.375477
C	-0.000022	0.630016	1.284154
C	-0.000032	1.386144	2.470702
C	-0.000032	0.775453	3.712444
C	0.000022	1.382837	-0.000000
C	-0.000022	0.630016	-1.284154
C	-0.000032	-0.771049	-1.375477
C	0.000015	-1.391240	-2.637620
H	0.000025	-2.481039	-2.700592
C	0.000008	-0.624433	-3.791538
C	-0.000032	0.775453	-3.712444
C	-0.000032	1.386144	-2.470702
H	0.000025	-1.119226	4.763754
H	0.000025	-2.481039	2.700592
H	-0.000038	2.471679	2.371218
H	-0.000026	1.377014	4.621598
H	0.000025	-1.119226	-4.763754
H	-0.000026	1.377014	-4.621598
H	-0.000038	2.471679	-2.371218
S	0.000030	-1.853348	0.000000
O	0.000071	2.600125	-0.000000

*1
0 1

C	-0.614093	0.000307	3.810199

C	-1.380782	0.000149	2.646631
C	-0.773785	-0.000128	1.388731
C	0.634711	-0.000162	1.289847
C	1.395626	0.000016	2.478281
C	0.778809	0.000206	3.722307
C	1.307387	-0.000313	0.000000
C	0.634711	-0.000162	-1.289847
C	-0.773785	-0.000128	-1.388731
C	-1.380782	0.000149	-2.646631
H	-2.470953	0.000232	-2.709345
C	-0.614093	0.000307	-3.810199
C	0.778809	0.000206	-3.722307
C	1.395626	0.000016	-2.478281
H	-1.108514	0.000507	4.781868
H	-2.470953	0.000232	2.709345
H	2.484151	0.000012	2.408061
H	1.388321	0.000350	4.626540
H	-1.108514	0.000507	-4.781868
H	1.388321	0.000350	-4.626540
H	2.484151	0.000012	-2.408061
S	-1.858392	-0.000270	-0.000000
O	2.602264	-0.000084	0.000000

$^T1$

0 3

C	0.663178	0.000083	3.800162
C	1.412773	0.000038	2.631466
C	0.767703	-0.000039	1.385140
C	-0.657090	-0.000090	1.262283
C	-1.381939	-0.000046	2.472280
C	-0.738935	0.000044	3.702811
C	-1.373573	-0.000205	0.000000
C	-0.657090	-0.000090	-1.262283
C	0.767703	-0.000039	-1.385140
C	1.412773	0.000038	-2.631466
H	2.504189	0.000069	-2.670224
C	0.663178	0.000083	-3.800162
C	-0.738935	0.000044	-3.702811
C	-1.381939	-0.000046	-2.472280
H	1.156470	0.000145	4.771148
H	2.504189	0.000069	2.670224
H	-2.468492	-0.000094	2.400793
H	-1.339405	0.000072	4.614586
H	1.156470	0.000145	-4.771148
H	-1.339405	0.000072	-4.614586

H	-2.468492	-0.000094	-2.400793
S	1.808492	-0.000029	0.000000
O	-2.648528	0.000181	0.000000

1⁻

-1 2

C	0.619357	-0.000181	3.821814
C	1.386090	-0.000069	2.648877
C	0.778610	0.000078	1.395715
C	-0.634252	0.000167	1.263222
C	-1.382241	0.000047	2.467510
C	-0.773802	-0.000131	3.716169
C	-1.368973	0.000391	0.000000
C	-0.634252	0.000167	-1.263222
C	0.778610	0.000078	-1.395715
C	1.386090	-0.000069	-2.648877
H	2.477634	-0.000116	-2.710185
C	0.619357	-0.000181	-3.821814
C	-0.773802	-0.000131	-3.716169
C	-1.382241	0.000047	-2.467510
H	1.110576	-0.000309	4.795706
H	2.477634	-0.000116	2.710185
H	-2.466576	0.000126	2.361459
H	-1.390064	-0.000212	4.618294
H	1.110576	-0.000309	-4.795706
H	-1.390064	-0.000212	-4.618294
H	-2.466576	0.000126	-2.361459
S	1.869515	0.000089	0.000000
O	-2.635834	-0.000211	0.000000

1⁺

1 2

C	0.000040	0.666678	3.783397
C	0.000040	1.417097	2.617229
C	0.000010	0.757749	1.369005
C	-0.000024	-0.654118	1.289459
C	-0.000022	-1.380118	2.474305
C	0.000010	-0.729597	3.713342
C	-0.000075	-1.411123	0.000000
C	-0.000024	-0.654118	-1.289459
C	0.000010	0.757749	-1.369005
C	0.000040	1.417097	-2.617229
H	0.000063	2.507884	-2.656006
C	0.000040	0.666678	-3.783397
C	0.000010	-0.729597	-3.713342
C	-0.000022	-1.380118	-2.474305

H	0.000064	1.170155	4.749836
H	0.000063	2.507884	2.656006
H	-0.000050	-2.468433	2.410065
H	0.000012	-1.320107	4.629837
H	0.000064	1.170155	-4.749836
H	0.000012	-1.320107	-4.629837
H	-0.000050	-2.468433	-2.410065
S	0.000024	1.794316	0.000000
O	-0.000097	-2.619200	0.000000

2

0 1

C	-3.159314	-0.191145	-0.021886
O	-4.079836	0.572534	-0.039938
O	-3.235443	-1.505975	-0.028624
C	-4.556800	-2.040838	-0.054260
H	-4.440883	-3.127874	-0.059593
H	-5.115630	-1.719077	0.833630
H	-5.085535	-1.706508	-0.955813
O	-1.895895	0.282766	0.003355
N	-0.883393	-0.659269	0.068232
C	0.279987	-0.122732	0.036123
C	0.554542	1.341520	-0.025088
C	-0.025896	2.227560	0.890698
C	1.427193	1.833138	-1.003901
C	0.267122	3.587698	0.826898
H	-0.707319	1.846466	1.651736
C	1.703487	3.197050	-1.076446
H	1.887823	1.141329	-1.712193
C	1.126536	4.074984	-0.158832
H	-0.181339	4.272275	1.548169
H	2.376098	3.573778	-1.848175
H	1.348424	5.142011	-0.210056
C	1.424375	-1.077194	0.055783
C	1.255076	-2.394857	-0.394716
C	2.672175	-0.678372	0.552326
C	2.315839	-3.293672	-0.347919
H	0.283404	-2.700553	-0.783498
C	3.731305	-1.583641	0.602227
H	2.812274	0.342447	0.911035
C	3.556791	-2.891057	0.151249
H	2.176651	-4.314213	-0.707542
H	4.696707	-1.263479	0.996707
H	4.387951	-3.596967	0.186068

T2

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0 3
C        2.883995      -0.863764       0.548337
O        3.481313      -1.206472       1.521218
O        3.360511      -0.679756      -0.659059
C        4.755951      -0.946468      -0.812650
H        4.986098      -0.740189      -1.860948
H        5.339416      -0.292967      -0.152560
H        4.967039      -1.995440      -0.570649
O        1.544977      -0.589869       0.642843
N        0.878121      -0.378761      -0.530500
C       -0.431764       0.044457      -0.231439
C       -0.616407       1.477337      -0.102830
C        0.370634       2.358575      -0.605072
C       -1.724368       2.037134       0.572666
C        0.234957       3.733322      -0.464302
H        1.240597       1.945498      -1.117838
C       -1.848981       3.414607       0.710518
H       -2.468725       1.382487       1.025682
C       -0.877468       4.271426       0.187850
H        1.003116       4.394549      -0.868224
H       -2.708165       3.824649       1.243611
H       -0.981188       5.351666       0.297903
C       -1.453402      -0.984002      -0.160446
C       -1.091683      -2.312379       0.160489
C       -2.807043      -0.720361      -0.468695
C       -2.048216      -3.318742       0.208461
H       -0.051787      -2.544891       0.392241
C       -3.756609      -1.734126      -0.419629
H       -3.105151       0.279541      -0.784106
C       -3.386890      -3.035945      -0.073551
H       -1.747752      -4.334234       0.470944
H       -4.795244      -1.508960      -0.667053
H       -4.135750      -3.828035      -0.033767
2⁻
-1 2
C        3.072680      -0.497635       0.259068
O        4.046276       0.122630       0.615999
O        3.124525      -1.735036      -0.234294
C        4.422529      -2.300336      -0.301409
H        4.298107      -3.302266      -0.724427
H        5.078230      -1.697288      -0.943870
H        4.872706      -2.364316       0.698466
O        1.863682       0.014800       0.331356
N        0.770765      -0.813297      -0.089426
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C	-0.376673	-0.105581	-0.001819
C	-0.436746	1.362926	-0.017810
C	0.447402	2.123466	-0.819161
C	-1.360003	2.083128	0.772633
C	0.396718	3.512417	-0.838099
H	1.171734	1.598822	-1.442767
C	-1.410870	3.473759	0.749598
H	-2.036473	1.530339	1.427568
C	-0.533508	4.204756	-0.056415
H	1.088891	4.066023	-1.476786
H	-2.136445	3.994918	1.378250
H	-0.570364	5.295165	-0.071772
C	-1.584382	-0.913794	-0.002411
C	-1.508612	-2.315605	0.241498
C	-2.874142	-0.404559	-0.322111
C	-2.635212	-3.125584	0.199241
H	-0.532439	-2.740458	0.471794
C	-3.994438	-1.224078	-0.355566
H	-2.987764	0.652404	-0.566378
C	-3.898491	-2.597217	-0.091930
H	-2.528700	-4.194346	0.403436
H	-4.963962	-0.785099	-0.604697
H	-4.782251	-3.236341	-0.119168

2⁺

1 2

C	3.187266	0.037798	0.011034
O	3.997622	0.899092	-0.016927
O	3.322057	-1.249248	0.083177
C	4.676392	-1.731020	0.135074
H	4.599469	-2.817504	0.211612
H	5.204939	-1.439304	-0.779950
H	5.181590	-1.310370	1.012151
O	1.829966	0.424445	-0.034746
N	0.942178	-0.534366	-0.052730
C	-0.322657	-0.088265	-0.053227
C	-0.710401	1.321434	0.006085
C	-0.081389	2.304625	-0.784835
C	-1.752658	1.691315	0.882363
C	-0.509127	3.622039	-0.711023
H	0.715291	2.030004	-1.474137
C	-2.152893	3.018504	0.968229
H	-2.215560	0.937731	1.521994
C	-1.536621	3.981694	0.167689
H	-0.039583	4.377894	-1.340620

H	-2.943477	3.303849	1.662169
H	-1.855751	5.023017	0.229548
C	-1.292905	-1.154376	-0.078755
C	-0.911360	-2.480435	0.285994
C	-2.630321	-0.900310	-0.496166
C	-1.846934	-3.493398	0.270547
H	0.115029	-2.670236	0.596592
C	-3.551990	-1.927533	-0.517333
H	-2.909447	0.096260	-0.838697
C	-3.165893	-3.220527	-0.127173
H	-1.565215	-4.503627	0.566330
H	-4.571828	-1.742190	-0.853225
H	-3.898918	-4.028556	-0.147697

3ts

0 3

C	2.495792	-1.748357	0.476146
O	3.072685	-2.529824	1.189665
O	3.091059	-1.044801	-0.489645
C	4.478973	-1.298076	-0.660277
H	4.802338	-0.672482	-1.497727
H	5.034388	-1.033899	0.249198
H	4.653484	-2.357692	-0.888321
O	1.210560	-1.487041	0.610433
N	0.529722	-0.752212	-0.798877
C	-0.449069	0.036972	-0.402755
C	-0.116953	1.445845	-0.143331
C	1.078537	1.978524	-0.665239
C	-0.929131	2.252298	0.673681
C	1.435576	3.293183	-0.394183
H	1.717807	1.346725	-1.284199
C	-0.562127	3.567657	0.941894
H	-1.832275	1.838398	1.122688
C	0.614012	4.092961	0.405060
H	2.358935	3.699936	-0.808408
H	-1.194385	4.183970	1.582279
H	0.895247	5.125779	0.615962
C	-1.789222	-0.550660	-0.245587
C	-1.906638	-1.890480	0.165573
C	-2.947713	0.181588	-0.559580
C	-3.163538	-2.473634	0.287488
H	-1.003522	-2.452929	0.407096
C	-4.199771	-0.413147	-0.443557
H	-2.862559	1.207573	-0.920270
C	-4.310959	-1.737478	-0.014323

H	-3.249113	-3.508580	0.620808
H	-5.094220	0.157529	-0.696436
H	-5.295218	-2.198697	0.079786

4

0 2

C	0.538616	0.030440	-0.000022
O	0.627363	1.236087	-0.000035
O	-0.549144	-0.695702	-0.000136
C	-1.789745	0.023683	0.000090
H	-2.573767	-0.737233	0.001374
H	-1.859753	0.651198	0.896780
H	-1.860950	0.649285	-0.897851
O	1.646936	-0.651383	0.000082

5

0 2

N	-0.000003	2.431762	0.000077
C	-0.000002	1.172933	0.000047
C	-1.301396	0.428735	0.035166
C	-2.424440	0.971381	-0.601728
C	-1.417691	-0.774973	0.740265
C	-3.649579	0.312291	-0.538736
H	-2.324335	1.908806	-1.150971
C	-2.647287	-1.428199	0.805084
H	-0.546522	-1.197265	1.244307
C	-3.762788	-0.887845	0.164726
H	-4.519390	0.735773	-1.042855
H	-2.733381	-2.364132	1.358886
H	-4.722555	-1.404515	0.212803
C	1.301394	0.428743	-0.035106
C	2.424440	0.971370	0.601799
C	1.417689	-0.774937	-0.740253
C	3.649581	0.312287	0.538773
H	2.324336	1.908774	1.151076
C	2.647287	-1.428156	-0.805106
H	0.546518	-1.197214	-1.244304
C	3.762790	-0.887821	-0.164736
H	4.519394	0.735754	1.042902
H	2.733381	-2.364067	-1.358945
H	4.722559	-1.404485	-0.212841

6

0 1

C	2.259819	0.267145	0.000000
C	1.782003	-1.042183	0.000000
C	0.408672	-1.283560	0.000000

C	-0.512196	-0.226094	0.000000
C	-0.016227	1.087845	0.000000
C	1.353807	1.330856	0.000000
H	3.333514	0.460830	0.000000
H	2.479981	-1.880843	0.000000
H	0.037468	-2.311024	0.000000
H	-0.707509	1.932074	0.000000
H	1.719816	2.358919	0.000000
C	-1.956082	-0.536569	0.000000
H	-2.193479	-1.605399	0.000000
C	-2.964472	0.340562	0.000000
H	-3.999913	-0.003267	0.000000
H	-2.801818	1.420697	0.000000

7ts

0 2

C	4.336940	-0.742335	-0.398461
C	3.437574	-1.592300	0.243438
C	2.175983	-1.125159	0.607581
C	1.788452	0.195927	0.336592
C	2.706201	1.041517	-0.309592
C	3.965693	0.577085	-0.672264
H	5.325689	-1.103306	-0.685653
H	3.718167	-2.623905	0.461870
H	1.472012	-1.792507	1.109611
H	2.435425	2.075521	-0.529029
H	4.665993	1.248509	-1.171607
C	0.443288	0.639470	0.738334
H	-0.160929	-0.103471	1.268577
C	-0.106375	1.844186	0.511074
C	-2.784971	-0.009357	-0.167156
O	-1.782731	0.216761	-0.996980
O	-3.817229	-0.489874	-0.836519
C	-4.998709	-0.737287	-0.070091
H	-5.724233	-1.160996	-0.769441
H	-5.377662	0.201682	0.352549
H	-4.786923	-1.445390	0.740381
O	-2.732575	0.205331	1.015478
H	-1.113856	2.055878	0.869312
H	0.422137	2.639760	-0.019133

7ts-1

0 2

C	-2.709516	-0.871926	-0.252508
C	-2.120494	-0.898739	1.012215
C	-1.162599	0.052509	1.352283

C	-0.773650	1.041943	0.433802
C	-1.377325	1.058467	-0.836218
C	-2.338280	0.112094	-1.172605
H	-3.461131	-1.615657	-0.521680
H	-2.407508	-1.664852	1.734123
H	-0.688466	0.025262	2.335773
H	-1.094656	1.820453	-1.563802
H	-2.800751	0.137844	-2.160216
C	0.310965	1.951723	0.804983
H	0.628283	1.903831	1.850440
C	1.007873	2.741117	-0.042059
C	1.753474	-0.423306	-0.223365
O	2.155488	-0.386232	0.912151
O	1.218857	-1.492737	-0.810967
C	1.183650	-2.676581	-0.019923
H	0.762013	-3.455717	-0.661728
H	0.546397	-2.521727	0.861243
H	2.194299	-2.954650	0.306524
O	1.762021	0.581242	-1.069839
H	0.750292	2.834022	-1.096893
H	1.835710	3.349205	0.325831

7ts-2

0 2

C	2.724126	-1.965854	0.101579
C	3.359236	-1.001840	-0.679267
C	2.870330	0.303638	-0.708152
C	1.742868	0.670625	0.041108
C	1.110781	-0.311414	0.823093
C	1.597570	-1.614380	0.851142
H	3.102752	-2.988855	0.127821
H	4.238429	-1.265876	-1.269277
H	3.368763	1.057607	-1.321722
H	0.224309	-0.056261	1.406424
H	1.095154	-2.365353	1.463263
C	1.265487	2.063626	-0.023759
H	1.840953	2.715282	-0.689396
C	0.219960	2.582628	0.635092
C	-2.253860	0.217012	-0.170966
O	-1.532470	0.972155	-0.975729
O	-3.029738	-0.591468	-0.858699
C	-3.863738	-1.466581	-0.091444
H	-4.430936	-2.050762	-0.820229
H	-4.539608	-0.881314	0.543890
H	-3.246180	-2.123742	0.532901

O	-2.168173	0.303272	1.026973
H	-0.399522	1.990284	1.311345
H	-0.047635	3.632570	0.504073

8

0 2

C	3.658497	-1.132394	0.091434
C	3.496444	-0.182435	1.106801
C	2.408606	0.677198	1.092241
C	1.440946	0.617250	0.055924
C	1.620401	-0.357661	-0.960857
C	2.714005	-1.212881	-0.937349
H	4.514949	-1.807761	0.103149
H	4.228830	-0.116142	1.912970
H	2.284446	1.418261	1.884708
H	0.881585	-0.446926	-1.758814
H	2.833810	-1.955741	-1.727779
C	0.342033	1.521174	0.061013
H	0.256788	2.230908	0.884640
C	-0.707757	1.537297	-0.998167
C	-2.282757	0.093978	-0.042807
O	-1.455077	0.307101	-1.059813
O	-2.880333	-1.076437	-0.213746
C	-3.815345	-1.441735	0.794529
H	-4.235899	-2.402442	0.484059
H	-4.607730	-0.686635	0.876236
H	-3.313044	-1.542070	1.765452
O	-2.466829	0.843950	0.878433
H	-1.406745	2.367381	-0.838086
H	-0.269518	1.625514	-2.002082

8-1

0 2

C	3.810912	-1.300842	0.090692
C	4.050477	-0.052872	-0.496128
C	3.039922	0.894507	-0.559800
C	1.749247	0.624471	-0.035571
C	1.525834	-0.649279	0.549535
C	2.544541	-1.590115	0.609738
H	4.606760	-2.045083	0.141827
H	5.035935	0.176846	-0.904642
H	3.228532	1.868202	-1.017215
H	0.538598	-0.895204	0.943388
H	2.353466	-2.563841	1.063876
C	0.731984	1.616462	-0.103055
H	0.967442	2.568957	-0.579903

C	-0.637645	1.417186	0.443014
C	-2.554754	0.136275	0.047551
O	-3.133997	0.657267	0.963522
O	-3.051766	-0.803557	-0.743685
C	-4.384443	-1.209629	-0.454645
H	-4.636286	-1.972823	-1.196418
H	-5.072262	-0.357965	-0.534976
H	-4.447434	-1.627861	0.558414
O	-1.313216	0.410068	-0.335008
H	-0.615218	1.077295	1.491876
H	-1.224153	2.344272	0.407153

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0 2

C	3.547199	-1.325016	-0.094662
C	3.715189	-0.122813	-0.791854
C	2.729016	0.850090	-0.751965
C	1.534771	0.658535	-0.006136
C	1.381625	-0.570974	0.688843
C	2.375456	-1.539321	0.638569
H	4.322505	-2.091636	-0.128183
H	4.624991	0.051233	-1.368699
H	2.863663	1.788167	-1.294837
H	0.460658	-0.770289	1.238200
H	2.235049	-2.479994	1.173747
C	0.562958	1.697599	0.020595
H	0.749677	2.575180	-0.602302
C	-0.704939	1.682209	0.803834
C	-2.272709	0.042844	0.113879
O	-1.825674	1.284233	-0.015810
O	-3.259501	-0.145206	-0.750316
C	-3.862489	-1.434037	-0.726711
H	-4.629285	-1.423815	-1.506456
H	-4.318779	-1.625878	0.253246
H	-3.115694	-2.210963	-0.934546
O	-1.867635	-0.784156	0.889589
H	-0.651944	1.018755	1.675130
H	-0.954831	2.695582	1.140640

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0 2

C	-3.485897	-1.378201	-0.083267
C	-3.708466	-0.171925	-0.757699
C	-2.755768	0.833965	-0.721121
C	-1.541093	0.671492	-0.002136
C	-1.333126	-0.561973	0.670972

C	-2.294056	-1.563118	0.624884
H	-4.235119	-2.170463	-0.114144
H	-4.635054	-0.020986	-1.314012
H	-2.932916	1.774851	-1.246719
H	-0.398889	-0.736334	1.206627
H	-2.112368	-2.505385	1.144618
C	-0.601092	1.739456	0.023859
H	-0.831791	2.627870	-0.567833
C	0.695708	1.726039	0.758959
C	2.261662	0.060464	0.114663
O	1.926175	-0.707535	0.979264
O	3.199068	-0.178970	-0.790979
C	3.822111	-1.455906	-0.710835
H	4.314718	-1.583080	0.261875
H	4.560046	-1.483658	-1.517475
H	3.079586	-2.253015	-0.845662
O	1.773767	1.275854	-0.091286
H	0.976005	2.743905	1.055291
H	0.663796	1.089743	1.651770

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0 2

C	-3.707973	-0.218465	-0.833618
C	-3.366009	1.103853	-0.527257
C	-2.182399	1.383748	0.138743
C	-1.295680	0.345029	0.524802
C	-1.658868	-0.988738	0.199790
C	-2.846730	-1.257607	-0.466153
H	-4.638558	-0.437065	-1.358695
H	-4.032350	1.919372	-0.812594
H	-1.919507	2.416575	0.377217
H	-0.988711	-1.808753	0.460493
H	-3.106076	-2.289751	-0.707403
C	-0.092437	0.657782	1.217219
H	0.127773	1.704902	1.428424
C	0.882335	-0.376052	1.671650
C	2.246322	-0.591788	-0.293599
O	2.661406	-1.177005	-1.253436
O	2.551708	0.664679	0.023758
C	3.425924	1.334743	-0.878638
H	4.385233	0.805883	-0.942822
H	3.569600	2.339749	-0.472161
H	2.974328	1.385358	-1.877282
O	1.424171	-1.155302	0.585604
H	1.704967	0.081830	2.233411

H	0.398114	-1.132119	2.306366

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0 2

C	3.526335	0.828717	-0.010354
C	3.361012	-0.190537	-0.954979
C	2.214762	-0.970962	-0.948211
C	1.184677	-0.760930	0.007544
C	1.373212	0.281222	0.954456
C	2.524509	1.055704	0.940009
H	4.427977	1.442575	-0.015216
H	4.135846	-0.372941	-1.701423
H	2.090062	-1.765089	-1.687433
H	0.600662	0.488761	1.694838
H	2.646271	1.850622	1.677788
C	0.028800	-1.588371	-0.023730
H	-0.039230	-2.339610	-0.814745
C	-1.119308	-1.531524	0.922463
C	-2.552195	0.039678	-0.192101
O	-3.522351	0.348330	-0.824934
O	-1.571096	0.869255	0.153982
C	-1.690793	2.211106	-0.304148
H	-2.576690	2.686712	0.135869
H	-1.773989	2.233010	-1.397926
H	-0.779362	2.722630	0.019620
O	-2.351736	-1.196627	0.252252
H	-1.322412	-2.525812	1.341918
H	-0.953732	-0.833149	1.750623

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0 2

C	3.926232	-1.113591	-0.131770
C	4.097381	0.223318	0.245886
C	3.009950	1.082768	0.286144
C	1.708084	0.632285	-0.052776
C	1.555478	-0.728124	-0.427107
C	2.650621	-1.580204	-0.466245
H	4.782631	-1.788833	-0.161378
H	5.089908	0.592072	0.510674
H	3.145740	2.125902	0.580784
H	0.563953	-1.111633	-0.673206
H	2.511764	-2.623288	-0.755874
C	0.609511	1.536021	-0.014575
H	0.797156	2.567361	0.288545
C	-0.782240	1.145403	-0.368305
C	-2.496433	-0.283698	0.512454

O	-2.944670	-1.074792	1.293662
O	-3.152853	0.210495	-0.535558
C	-4.488005	-0.254033	-0.705067
H	-5.097638	0.014331	0.167221
H	-4.498577	-1.344150	-0.830520
H	-4.869980	0.238298	-1.604026
O	-1.263595	0.199789	0.610300
H	-1.447723	2.017464	-0.380757
H	-0.831760	0.667673	-1.360522

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C	-0.067323	1.785798	2.816561
C	-0.263116	0.408421	2.676052
C	-0.814046	-0.110898	1.510813
C	-1.173325	0.742061	0.438154
C	-0.967180	2.133954	0.602043
C	-0.427852	2.644930	1.773033
H	0.361532	2.187451	3.735914
H	0.012594	-0.265680	3.488917
H	-0.975650	-1.187013	1.425944
H	-1.236657	2.805635	-0.215874
H	-0.275169	3.720880	1.873980
C	-1.698821	0.238234	-0.789925
C	-2.143360	-1.175791	-0.956181
C	-4.419425	-0.943202	-0.447794
O	-4.607067	-0.241981	-1.406746
O	-5.344324	-1.295963	0.435530
C	-6.650875	-0.792037	0.186139
H	-6.644677	0.305508	0.179587
H	-7.280955	-1.163203	0.999445
H	-7.024351	-1.154675	-0.780450
O	-3.263069	-1.494033	-0.104569
H	-2.415824	-1.379162	-1.999226
H	-1.363127	-1.882506	-0.651042
H	-1.906655	0.946976	-1.592493
N	0.681798	-0.989189	-1.632327
C	1.668283	-0.499075	-1.019796
C	2.679583	-1.438512	-0.431019
C	2.247412	-2.626051	0.170896
C	4.049780	-1.163676	-0.518504
C	3.176694	-3.528125	0.685004
H	1.177565	-2.829952	0.239372
C	4.975989	-2.071667	-0.008883
H	4.389999	-0.240906	-0.992304

C	4.541451	-3.252767	0.594622
H	2.833511	-4.448511	1.159674
H	6.042760	-1.856189	-0.084194
H	5.268801	-3.959506	0.997153
C	1.850067	0.979857	-0.889475
C	1.342671	1.824392	-1.885463
C	2.490272	1.528806	0.226277
C	1.483462	3.204008	-1.768772
H	0.845742	1.384946	-2.752069
C	2.627048	2.911452	0.340276
H	2.867992	0.874033	1.013741
C	2.127861	3.749335	-0.656213
H	1.094663	3.858278	-2.550546
H	3.118404	3.335995	1.217124
H	2.241087	4.831056	-0.567149

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C	-5.496548	-1.726982	0.279322
C	-4.808849	-2.020194	-0.901743
C	-3.618420	-1.371463	-1.205323
C	-3.075892	-0.402435	-0.325841
C	-3.790677	-0.115865	0.863981
C	-4.978895	-0.768668	1.158735
H	-6.430176	-2.240392	0.512731
H	-5.207580	-2.764396	-1.593382
H	-3.098955	-1.617324	-2.133061
H	-3.389123	0.632377	1.551608
H	-5.512207	-0.532158	2.081057
C	-1.847279	0.267052	-0.598607
C	-1.115100	0.120713	-1.887259
C	0.284173	1.995089	-1.819152
O	-0.646211	2.755441	-1.850118
O	1.562586	2.345176	-1.784507
C	1.811804	3.745778	-1.747413
H	2.898403	3.859946	-1.696538
H	1.336804	4.195196	-0.865160
H	1.419529	4.228712	-2.651697
O	0.202088	0.668920	-1.821300
H	-0.965987	-0.939323	-2.135324
H	-1.662403	0.603913	-2.716036
H	-1.512801	1.047429	0.086979
N	-0.159643	-1.686977	0.191108
C	0.871922	-1.095121	0.609637
C	0.760597	0.166239	1.407067

C	1.614338	1.241935	1.140428
C	-0.250206	0.298124	2.366609
C	1.440905	2.450154	1.815282
H	2.394463	1.138015	0.384425
C	-0.411003	1.502690	3.048038
H	-0.911730	-0.547511	2.564915
C	0.429993	2.581925	2.768432
H	2.102504	3.291042	1.600051
H	-1.195998	1.602108	3.799356
H	0.300502	3.526585	3.298719
C	2.225127	-1.650073	0.282410
C	2.428818	-2.290760	-0.945659
C	3.278555	-1.556127	1.199528
C	3.673794	-2.834671	-1.251574
H	1.605838	-2.343940	-1.660042
C	4.521125	-2.107488	0.892028
H	3.121563	-1.055628	2.156989
C	4.720627	-2.746314	-0.332509
H	3.829879	-3.325017	-2.213587
H	5.337611	-2.036618	1.612133
H	5.696212	-3.171707	-0.572990

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C	-5.201460	0.127142	-0.222449
C	-4.409621	-0.046048	0.914922
C	-3.195918	-0.717958	0.836149
C	-2.741696	-1.249861	-0.396074
C	-3.561772	-1.067581	-1.538150
C	-4.766666	-0.387189	-1.450969
H	-6.151854	0.658572	-0.155052
H	-4.740507	0.355468	1.874674
H	-2.589945	-0.829722	1.737497
H	-3.222696	-1.465751	-2.497051
H	-5.379470	-0.255263	-2.344435
C	-1.499272	-1.936484	-0.511675
C	-0.606976	-2.149908	0.660040
C	1.804221	-2.319574	0.624425
O	2.822231	-2.831356	0.250561
O	1.741964	-1.295336	1.476227
C	2.988912	-0.849832	2.005692
H	2.748435	-0.059039	2.723312
H	3.627674	-0.457228	1.203869
H	3.501111	-1.678946	2.510206
O	0.613882	-2.745963	0.223825

H	-0.411072	-1.202294	1.181394
H	-1.066088	-2.838830	1.393195
H	-1.248366	-2.452745	-1.436590
N	0.376083	-0.463196	-1.711730
C	0.733479	0.477392	-0.950735
C	2.187402	0.838290	-0.853253
C	2.608260	2.025939	-0.245041
C	3.143827	-0.034654	-1.394750
C	3.968715	2.325750	-0.160525
H	1.874258	2.723560	0.159657
C	4.498236	0.271453	-1.314796
H	2.815263	-0.964587	-1.860880
C	4.915014	1.450485	-0.691216
H	4.287940	3.251888	0.319723
H	5.233361	-0.419079	-1.730503
H	5.978084	1.685846	-0.621321
C	-0.300781	1.247282	-0.182334
C	-1.415014	1.748682	-0.865118
C	-0.181677	1.454430	1.197088
C	-2.389911	2.468647	-0.178901
H	-1.505262	1.574553	-1.938476
C	-1.166442	2.165524	1.882382
H	0.681821	1.052048	1.730563
C	-2.265917	2.679229	1.194351
H	-3.255226	2.858377	-0.717306
H	-1.071477	2.320760	2.958144
H	-3.032837	3.239090	1.732211

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C	5.198005	-0.320192	-1.641031
C	4.897411	-0.497698	-0.288178
C	3.766605	0.089400	0.268507
C	2.897235	0.881011	-0.520135
C	3.228846	1.060144	-1.886239
C	4.354797	0.465385	-2.435957
H	6.084594	-0.785714	-2.073534
H	5.553325	-1.102535	0.340689
H	3.556623	-0.068504	1.327358
H	2.568312	1.666761	-2.509403
H	4.582361	0.612181	-3.493118
C	1.702881	1.485408	-0.013762
C	1.277923	1.412586	1.415544
C	-0.835180	2.421470	1.144208
O	-0.379606	3.472136	0.777519

O	-2.125687	2.115031	1.187589
C	-3.019411	3.145797	0.785449
H	-2.766326	3.502802	-0.221700
H	-2.972126	3.989480	1.486819
H	-4.018995	2.700751	0.793633
O	-0.142104	1.378419	1.576530
H	1.622331	0.488047	1.896689
H	1.674653	2.274889	1.981474
H	1.226367	2.245925	-0.627603
N	-0.301793	0.414520	-1.257071
C	-0.873546	-0.530139	-0.646164
C	-2.323966	-0.798908	-0.925754
C	-3.153680	0.254416	-1.331988
C	-2.852753	-2.089774	-0.812036
C	-4.495490	0.019814	-1.617742
H	-2.732238	1.257375	-1.411547
C	-4.196650	-2.322213	-1.103771
H	-2.209888	-2.914689	-0.499810
C	-5.019692	-1.269809	-1.504092
H	-5.137176	0.846618	-1.926359
H	-4.602189	-3.331285	-1.016439
H	-6.072385	-1.453617	-1.724653
C	-0.150982	-1.386309	0.347265
C	1.119199	-1.885275	0.047757
C	-0.726477	-1.646943	1.597547
C	1.812990	-2.639758	0.994992
H	1.563625	-1.674963	-0.926901
C	-0.025760	-2.387935	2.544607
H	-1.713425	-1.241943	1.829574
C	1.244473	-2.887513	2.243789
H	2.804582	-3.027244	0.755231
H	-0.470490	-2.575501	3.523126
H	1.789505	-3.472955	2.985979

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C	-2.462836	4.314297	0.526792
C	-1.700606	4.377606	-0.645241
C	-1.285910	3.211444	-1.272819
C	-1.614024	1.941738	-0.741717
C	-2.395186	1.897190	0.436800
C	-2.811024	3.069337	1.057680
H	-2.788982	5.231253	1.019679
H	-1.429211	5.346687	-1.067257
H	-0.681189	3.259345	-2.180828

H	-2.686241	0.933499	0.858459
H	-3.417006	3.015103	1.963867
C	-1.133513	0.757491	-1.389445
C	-1.384260	-0.611012	-0.860142
C	-3.115937	-2.178361	-0.740475
O	-2.466243	-2.895530	-0.026144
O	-4.347788	-2.427471	-1.164547
C	-4.916549	-3.650404	-0.713058
H	-5.913381	-3.705814	-1.159781
H	-4.989677	-3.658843	0.382279
H	-4.305423	-4.502315	-1.038385
O	-2.718820	-1.012206	-1.232695
H	-0.667680	-1.335305	-1.274485
H	-1.305655	-0.651913	0.235786
H	-0.743035	0.852436	-2.400471
N	1.477353	0.878735	-1.260800
C	2.033140	0.241352	-0.325129
C	3.484623	-0.123834	-0.435769
C	4.252715	-0.355695	0.710918
C	4.086119	-0.200717	-1.699327
C	5.609426	-0.657167	0.593356
H	3.790032	-0.291759	1.697298
C	5.439276	-0.504598	-1.812078
H	3.479402	-0.024933	-2.588770
C	6.203713	-0.732597	-0.665629
H	6.203393	-0.833845	1.491186
H	5.900256	-0.569550	-2.798739
H	7.264304	-0.972465	-0.755097
C	1.266577	-0.151868	0.900782
C	0.540540	0.813069	1.604808
C	1.219954	-1.493117	1.299921
C	-0.238081	0.435026	2.698603
H	0.574800	1.855254	1.281202
C	0.425861	-1.868577	2.381191
H	1.790102	-2.243636	0.748179
C	-0.303579	-0.904910	3.081475
H	-0.805241	1.191015	3.244132
H	0.371375	-2.917539	2.675236
H	-0.922242	-1.200326	3.930209
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C	5.230130	1.845138	0.718184
C	4.206254	2.659551	0.236240
C	2.961991	2.113645	-0.084312

C	2.731878	0.745341	0.078359
C	3.763129	-0.067569	0.564760
C	5.005621	0.476876	0.881813
H	6.200803	2.275256	0.970294
H	4.374876	3.730568	0.110811
H	2.153550	2.746038	-0.451440
H	3.583094	-1.137924	0.699837
H	5.799098	-0.167572	1.263659
C	1.406311	0.101204	-0.283272
C	1.532468	-0.580927	-1.649977
C	0.283607	-2.538826	-1.374239
O	1.081372	-3.000234	-0.600820
O	-0.813795	-3.145439	-1.799333
C	-1.020438	-4.460285	-1.295516
H	-1.990690	-4.785173	-1.682770
H	-1.027220	-4.453248	-0.197953
H	-0.226420	-5.131799	-1.648185
O	0.367704	-1.344442	-1.954801
H	1.610930	0.174806	-2.440939
H	2.415538	-1.233464	-1.661917
H	1.209983	-0.698967	0.447558
N	0.341913	1.074190	-0.371800
C	-0.815821	0.847602	0.108541
C	-1.192706	-0.379253	0.887803
C	-2.123222	-1.281898	0.361484
C	-0.623324	-0.627415	2.141858
C	-2.467256	-2.428515	1.077380
H	-2.570824	-1.088827	-0.615936
C	-0.968921	-1.774026	2.855266
H	0.097524	0.081714	2.555659
C	-1.889926	-2.677133	2.323168
H	-3.192486	-3.129731	0.660435
H	-0.518284	-1.961152	3.831048
H	-2.160903	-3.573830	2.882730
C	-1.886847	1.870803	-0.104730
C	-1.720604	2.856910	-1.088363
C	-3.047398	1.881224	0.679656
C	-2.693393	3.832279	-1.280447
H	-0.815720	2.838519	-1.696499
C	-4.018268	2.865594	0.491734
H	-3.190657	1.122553	1.450750
C	-3.845054	3.840883	-0.488554
H	-2.556486	4.590961	-2.052693
H	-4.913506	2.868226	1.115355

H	-4.607104	4.607412	-0.638583

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C	-2.471982	1.576694	2.286062
C	-1.620599	0.522104	2.623078
C	-0.984499	-0.210868	1.624286
C	-1.185214	0.107515	0.277234
C	-2.039155	1.161748	-0.055096
C	-2.681785	1.894142	0.944750
H	-2.969869	2.150088	3.069739
H	-1.455926	0.267921	3.671539
H	-0.322529	-1.038502	1.889262
H	-2.200938	1.411894	-1.106440
H	-3.341418	2.720140	0.673302
C	-0.553639	-0.726536	-0.823609
C	-1.405259	-1.967880	-1.108492
C	-3.644023	-1.527661	-0.524462
O	-3.557858	-2.021138	0.566483
O	-4.696083	-0.864883	-0.985682
C	-5.767210	-0.705745	-0.062995
H	-6.550301	-0.159305	-0.596349
H	-5.429504	-0.133761	0.812054
H	-6.141282	-1.683161	0.267909
O	-2.717433	-1.562230	-1.481013
H	-0.987406	-2.519467	-1.959532
H	-1.440197	-2.621040	-0.226608
H	-0.552319	-0.116666	-1.742297
N	0.787742	-1.195563	-0.513447
C	1.744594	-0.363872	-0.374332
C	3.104989	-0.880405	-0.032642
C	4.217758	-0.030450	-0.001629
C	3.280263	-2.244294	0.247274
C	5.482593	-0.534551	0.304111
H	4.098228	1.031310	-0.222277
C	4.540473	-2.744110	0.553927
H	2.407053	-2.896135	0.216951
C	5.646722	-1.889706	0.583124
H	6.342505	0.136487	0.322370
H	4.665234	-3.805911	0.772163
H	6.635823	-2.283036	0.823548
C	1.576742	1.120582	-0.520934
C	1.409315	1.694871	-1.784110
C	1.542959	1.933433	0.618262
C	1.191613	3.067787	-1.905939

H	1.448608	1.064931	-2.675741
C	1.319433	3.302835	0.494960
H	1.676738	1.483829	1.604794
C	1.139725	3.871335	-0.767448
H	1.062208	3.510496	-2.894846
H	1.284854	3.929154	1.387683
H	0.964333	4.943872	-0.863676

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0 1

C	-2.225277	1.825873	2.412286
C	-2.444367	2.127054	1.069119
C	-1.929186	1.294209	0.074389
C	-1.192990	0.157183	0.413541
C	-0.986780	-0.145902	1.763287
C	-1.496862	0.684933	2.757133
H	-2.623927	2.477516	3.191385
H	-3.012079	3.017206	0.792783
H	-2.081235	1.541732	-0.979500
H	-0.414212	-1.036240	2.034099
H	-1.328334	0.442220	3.807627
C	-0.656621	-0.760643	-0.670120
C	-1.519448	-2.018779	-0.783443
C	-3.740245	-1.666687	-0.037603
O	-3.532700	-2.101612	1.058827
O	-4.913524	-1.155662	-0.386677
C	-5.107628	-0.630349	-1.695471
H	-4.409132	0.193136	-1.890418
H	-6.137746	-0.262377	-1.718892
H	-4.969689	-1.411284	-2.453687
O	-2.867817	-1.646361	-1.050568
H	-1.181621	-2.632567	-1.627740
H	-1.467613	-2.605453	0.142788
H	-0.725331	-0.221859	-1.630133
N	0.707347	-1.216518	-0.438284
C	1.671856	-0.383995	-0.380734
C	3.049613	-0.896665	-0.109493
C	4.164549	-0.051141	-0.169038
C	3.237747	-2.253126	0.197044
C	5.444244	-0.552233	0.074196
H	4.034884	1.004695	-0.411236
C	4.512750	-2.749915	0.440891
H	2.362597	-2.901867	0.236245
C	5.621119	-1.899912	0.380094
H	6.305365	0.115661	0.023746

H	4.647605	-3.805920	0.680158
H	6.621704	-2.291221	0.571368
C	1.497334	1.096214	-0.556660
C	1.236042	1.632764	-1.820379
C	1.542952	1.941101	0.558206
C	1.002080	3.000987	-1.965045
H	1.216160	0.977665	-2.694367
C	1.298502	3.304586	0.413299
H	1.747452	1.520110	1.545320
C	1.024205	3.835907	-0.848357
H	0.802040	3.415476	-2.954468
H	1.318937	3.955076	1.288986
H	0.833538	4.904218	-0.961577

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C	5.344996	-0.789272	-1.376586
C	4.289456	-1.694793	-1.495844
C	3.051962	-1.410082	-0.920574
C	2.857352	-0.215068	-0.219407
C	3.917653	0.688808	-0.105152
C	5.156476	0.404021	-0.679820
H	6.312105	-1.011296	-1.830571
H	4.430516	-2.628399	-2.043090
H	2.219626	-2.108294	-1.020840
H	3.768496	1.628282	0.432913
H	5.974584	1.120139	-0.587057
C	1.534294	0.084342	0.456225
C	1.486517	-0.620417	1.820586
C	-0.815701	-1.091979	2.369780
O	-1.913172	-0.704286	2.667555
O	-0.537016	-2.321172	1.954782
C	-1.647414	-3.210540	1.870945
H	-2.082520	-3.367802	2.866209
H	-1.253183	-4.150309	1.473242
H	-2.412141	-2.799482	1.199656
O	0.254410	-0.307466	2.466502
H	1.599645	-1.704125	1.697842
H	2.282624	-0.234054	2.468737
H	1.470168	1.168512	0.648321
N	0.416339	-0.422341	-0.305420
C	-0.614955	0.295005	-0.522543
C	-1.800761	-0.345412	-1.171441
C	-2.904031	0.412551	-1.582427
C	-1.814601	-1.734375	-1.370782

C	-4.001904	-0.206425	-2.181441
H	-2.906393	1.493618	-1.436317
C	-2.911488	-2.350005	-1.963925
H	-0.949454	-2.313719	-1.044916
C	-4.009383	-1.586672	-2.371825
H	-4.855071	0.395347	-2.497926
H	-2.914096	-3.431381	-2.110718
H	-4.869542	-2.070476	-2.837391
C	-0.725531	1.751032	-0.169601
C	-1.464479	2.156307	0.947279
C	-0.084488	2.706985	-0.964408
C	-1.556675	3.511524	1.263508
H	-1.950919	1.404736	1.573605
C	-0.183672	4.061362	-0.646277
H	0.495846	2.386727	-1.832928
C	-0.920132	4.464932	0.467682
H	-2.129318	3.823004	2.138601
H	0.316867	4.803247	-1.270366
H	-0.996945	5.524539	0.716496

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C	-3.118223	0.584952	2.720153
C	-3.127204	1.453842	1.629567
C	-2.292392	1.212769	0.537371
C	-1.446980	0.099273	0.521903
C	-1.439870	-0.767850	1.619778
C	-2.269928	-0.524657	2.712984
H	-3.767631	0.773785	3.576529
H	-3.782655	2.326264	1.627982
H	-2.297781	1.896781	-0.314790
H	-0.777206	-1.635237	1.610947
H	-2.255975	-1.205360	3.566025
C	-0.613046	-0.185700	-0.713387
C	-1.378753	-1.088591	-1.691688
C	-3.729603	-0.592183	-1.489574
O	-4.680623	0.095307	-1.735187
O	-3.707099	-1.569392	-0.590657
C	-4.862998	-1.680812	0.231060
H	-4.652898	-2.484075	0.943436
H	-5.743793	-1.924175	-0.376921
H	-5.032254	-0.734674	0.762682
O	-2.572739	-0.450273	-2.134358
H	-0.770517	-1.242689	-2.591695
H	-1.592982	-2.058197	-1.226723

H	-0.428553	0.775342	-1.224783
N	0.616557	-0.886575	-0.398824
C	1.707063	-0.246276	-0.235414
C	2.964019	-1.017286	0.012348
C	4.121355	-0.386734	0.486677
C	2.989398	-2.399577	-0.226033
C	5.281047	-1.125685	0.722463
H	4.116189	0.686920	0.680674
C	4.147921	-3.133322	0.003224
H	2.083462	-2.878998	-0.597553
C	5.298045	-2.497826	0.479852
H	6.174553	-0.624689	1.097811
H	4.158377	-4.206793	-0.191978
H	6.207210	-3.073612	0.660436
C	1.814731	1.250185	-0.278179
C	1.238858	2.028329	0.732093
C	2.490100	1.875919	-1.332646
C	1.332368	3.419153	0.683217
H	0.718225	1.540976	1.559136
C	2.571244	3.266603	-1.385179
H	2.951308	1.268736	-2.114823
C	1.993656	4.039469	-0.376952
H	0.884396	4.019651	1.476393
H	3.089785	3.749267	-2.214983
H	2.061695	5.127684	-0.416254

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C	2.966556	3.539172	1.683501
C	3.246487	2.189919	1.898074
C	2.478114	1.210336	1.268924
C	1.429616	1.567412	0.415774
C	1.152296	2.922043	0.206174
C	1.916955	3.902028	0.837811
H	3.562854	4.307993	2.177474
H	4.062288	1.897981	2.561340
H	2.687000	0.151674	1.448351
H	0.324222	3.198946	-0.448240
H	1.691729	4.956843	0.670835
C	0.653027	0.480689	-0.300867
C	1.207611	0.255516	-1.718668
C	3.129040	-0.993535	-1.237177
O	2.493815	-1.915703	-0.797952
O	4.449799	-0.930324	-1.299413
C	5.143668	-2.062604	-0.787874

H	6.208382	-1.851924	-0.921341
H	4.861940	-2.967791	-1.341160
H	4.914011	-2.204204	0.276275
O	2.623356	0.128431	-1.737926
H	0.745859	-0.642966	-2.154854
H	0.981454	1.127826	-2.343601
H	0.780204	-0.460091	0.256646
N	-0.736508	0.855303	-0.469362
C	-1.671020	0.056103	-0.135219
C	-3.092118	0.477815	-0.332024
C	-3.377767	1.747020	-0.857808
C	-4.152189	-0.375781	-0.001625
C	-4.694213	2.151421	-1.047043
H	-2.545049	2.403050	-1.112241
C	-5.473122	0.032014	-0.192034
H	-3.947502	-1.366422	0.407084
C	-5.747257	1.294129	-0.713826
H	-4.903936	3.140826	-1.456739
H	-6.290175	-0.641951	0.069269
H	-6.780283	1.612800	-0.862162
C	-1.433757	-1.302809	0.460411
C	-1.232131	-2.411907	-0.366294
C	-1.397247	-1.458903	1.850125
C	-0.987741	-3.666241	0.192967
H	-1.267299	-2.292812	-1.451477
C	-1.152065	-2.713600	2.406139
H	-1.557625	-0.592601	2.495865
C	-0.946934	-3.818238	1.578577
H	-0.826745	-4.526977	-0.457766
H	-1.120662	-2.829008	3.490612
H	-0.755722	-4.799527	2.015591

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C	5.241816	1.819605	0.714784
C	4.222354	2.639760	0.233165
C	2.975083	2.100762	-0.087399
C	2.737452	0.733742	0.074949
C	3.764325	-0.084917	0.561022
C	5.009812	0.452536	0.878045
H	6.214846	2.244219	0.967103
H	4.396765	3.709876	0.108096
H	2.169852	2.737496	-0.454095
H	3.578549	-1.154269	0.696119
H	5.799779	-0.196331	1.259665

C	1.408127	0.096741	-0.285225
C	1.527614	-0.585980	-1.651981
C	0.262265	-2.532969	-1.369923
O	1.051223	-2.994690	-0.587683
O	-0.834753	-3.136174	-1.801046
C	-1.049698	-4.449425	-1.296613
H	-1.068136	-4.440219	-0.199218
H	-0.253589	-5.123412	-1.639690
H	-2.016633	-4.772876	-1.693301
O	0.357457	-1.342098	-1.955840
H	1.610263	0.168467	-2.443715
H	2.406337	-1.244414	-1.664611
H	1.210233	-0.703048	0.445152
N	0.347980	1.074652	-0.370442
C	-0.810615	0.850923	0.109506
C	-1.877411	1.879109	-0.100374
C	-3.033099	1.897290	0.691044
C	-1.711661	2.862384	-1.086844
C	-3.999595	2.886698	0.507361
H	-3.175960	1.140583	1.464084
C	-2.680311	3.842776	-1.274768
H	-0.810518	2.838072	-1.700305
C	-3.826919	3.859236	-0.475769
H	-4.891097	2.895206	1.136222
H	-2.544089	4.599300	-2.049233
H	-4.585669	4.629620	-0.622666
C	-1.192141	-0.377019	0.884923
C	-2.136883	-1.267287	0.362764
C	-0.611595	-0.639520	2.130902
C	-2.483329	-2.415937	1.074166
H	-2.593323	-1.063388	-0.608295
C	-0.959407	-1.788194	2.839787
H	0.119389	0.060559	2.542295
C	-1.894251	-2.679094	2.311379
H	-3.219154	-3.107727	0.660130
H	-0.499884	-1.986337	3.809177
H	-2.166841	-3.577552	2.867320

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C	4.694647	-0.156061	-1.012247
C	4.274175	0.461425	0.164267
C	3.015314	1.060008	0.234173
C	2.160138	1.044485	-0.871218
C	2.600023	0.439345	-2.054988

C	3.853455	-0.162094	-2.126565
H	5.677704	-0.626850	-1.064619
H	4.925629	0.473122	1.039831
H	2.701685	1.519268	1.173343
H	1.939721	0.430888	-2.926021
H	4.178162	-0.634198	-3.055500
C	0.769225	1.657821	-0.867726
C	0.489043	2.547147	0.345488
C	-1.912029	2.652267	0.509045
O	-2.962031	3.037059	0.079792
O	-1.775715	1.677633	1.408611
C	-2.982762	1.031656	1.806590
H	-2.685645	0.225257	2.484869
H	-3.499505	0.618447	0.930342
H	-3.641345	1.743073	2.321161
O	-0.756351	3.215537	0.163708
H	0.485526	1.973689	1.280501
H	1.246297	3.338255	0.410479
H	0.725999	2.333321	-1.737492
N	-0.360374	0.750758	-1.045268
C	-0.484281	-0.381480	-0.477210
C	-1.776367	-1.114835	-0.677957
C	-2.046060	-2.313832	-0.006233
C	-2.758432	-0.571157	-1.521532
C	-3.275819	-2.954543	-0.169097
H	-1.295937	-2.748772	0.655948
C	-3.981845	-1.211080	-1.682676
H	-2.542987	0.367214	-2.033236
C	-4.245566	-2.405762	-1.005104
H	-3.474672	-3.886065	0.362928
H	-4.737797	-0.777951	-2.339674
H	-5.207320	-2.905660	-1.131653
C	0.521294	-1.029847	0.432687
C	1.415267	-1.985432	-0.062977
C	0.549063	-0.696915	1.790263
C	2.357348	-2.566430	0.782545
H	1.384326	-2.256524	-1.120467
C	1.489052	-1.286244	2.636741
H	-0.166778	0.029808	2.180569
C	2.399942	-2.213710	2.132989
H	3.065074	-3.295566	0.384459
H	1.508723	-1.018283	3.694468
H	3.139586	-2.668019	2.794198

10-8

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0 1
C        1.885335        4.101595        1.846398
C        2.596687        3.794945        0.688999
C        2.270772        2.663119       -0.062458
C        1.226919        1.823802        0.337016
C        0.519993        2.138903        1.505232
C        0.843481        3.266479        2.255038
H        2.141841        4.986489        2.431013
H        3.415799        4.438517        0.363900
H        2.856322        2.434054       -0.953140
H       -0.296756        1.488165        1.828942
H        0.280906        3.495645        3.161572
C        0.821447        0.569697       -0.428369
C        1.563509        0.371405       -1.748474
C        3.271574       -1.147674       -1.237581
O        2.499570       -2.063694       -1.125171
O        4.582051       -1.223821       -1.077872
C        5.089316       -2.512137       -0.746343
H        4.654379       -2.863947        0.198029
H        6.171827       -2.394414       -0.646067
H        4.855929       -3.231389       -1.541881
O        2.949066        0.103682       -1.550600
H        1.102533       -0.460278       -2.297602
H        1.513298        1.279290       -2.360894
H        1.043248       -0.299480        0.214741
N       -0.582633        0.670207       -0.780556
C       -1.472890       -0.098834       -0.287883
C       -2.896757        0.136963       -0.688171
C       -3.264084        1.372141       -1.241177
C       -3.869259       -0.861223       -0.544651
C       -4.577129        1.604727       -1.636875
H       -2.497904        2.140130       -1.350600
C       -5.183432       -0.629822       -0.951444
H       -3.596802       -1.829473       -0.121433
C       -5.540993        0.602980       -1.494414
H       -4.854137        2.572752       -2.057511
H       -5.930268       -1.417493       -0.841522
H       -6.570904        0.785832       -1.805343
C       -1.218095       -1.211376        0.686775
C       -0.385836       -2.287396        0.357838
C       -1.825241       -1.172236        1.948525
C       -0.159728       -3.306223        1.283291
H        0.107744       -2.321439       -0.615474
C       -1.590884       -2.186872        2.874461
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H	-2.486603	-0.340394	2.202922
C	-0.759551	-3.257489	2.541446
H	0.493453	-4.138829	1.017658
H	-2.061472	-2.142962	3.857743
H	-0.580405	-4.054404	3.264893

10-9

0 1

C	-3.142603	1.670068	2.228268
C	-2.796354	2.530469	1.185213
C	-1.945679	2.092440	0.172425
C	-1.430323	0.793686	0.191069
C	-1.768700	-0.062070	1.244970
C	-2.624673	0.374929	2.256743
H	-3.810853	2.011177	3.020535
H	-3.191945	3.547134	1.159903
H	-1.677043	2.765799	-0.645342
H	-1.363617	-1.075105	1.258518
H	-2.887612	-0.300616	3.072807
C	-0.581278	0.299906	-0.966494
C	-1.469284	-0.380820	-2.015939
C	-3.471830	-1.111350	-1.023923
O	-4.079584	-0.112447	-1.299640
O	-3.932621	-2.106301	-0.278106
C	-5.231302	-1.906575	0.266159
H	-5.234631	-1.025778	0.922893
H	-5.464114	-2.808994	0.838729
H	-5.968422	-1.762181	-0.534113
O	-2.239128	-1.418999	-1.421510
H	-2.135369	0.353231	-2.487161
H	-0.840047	-0.859466	-2.776299
H	-0.125464	1.176578	-1.460608
N	0.416107	-0.657152	-0.523875
C	1.606658	-0.284812	-0.262762
C	2.610116	-1.320258	0.134735
C	2.296172	-2.679622	-0.012829
C	3.856372	-0.962946	0.664465
C	3.210971	-3.658219	0.358812
H	1.321864	-2.944285	-0.424526
C	4.771884	-1.946731	1.040574
H	4.111780	0.090087	0.792136
C	4.453011	-3.294292	0.887093
H	2.958556	-4.712580	0.235499
H	5.737829	-1.655504	1.455902
H	5.170395	-4.063330	1.178127

C	2.069106	1.142520	-0.322968
C	2.960100	1.557624	-1.319268
C	1.599007	2.070866	0.612812
C	3.360681	2.891267	-1.389810
H	3.338549	0.831661	-2.042559
C	2.008977	3.402265	0.546002
H	0.908960	1.746697	1.394529
C	2.885641	3.814938	-0.457275
H	4.047738	3.210624	-2.174858
H	1.639080	4.119526	1.280363
H	3.202273	4.857671	-0.511738

10-10

0 1

C	-1.451638	3.725883	-2.149006
C	-2.190045	3.293850	-1.049122
C	-2.045108	1.991273	-0.567356
C	-1.151444	1.104202	-1.176150
C	-0.427539	1.540598	-2.294047
C	-0.573262	2.839950	-2.774803
H	-1.562438	4.745782	-2.520487
H	-2.885999	3.974546	-0.555843
H	-2.640962	1.674207	0.289047
H	0.273218	0.856869	-2.775814
H	0.006673	3.162726	-3.641218
C	-0.941782	-0.317623	-0.660323
C	-1.489001	-0.558170	0.755561
C	-3.424685	-1.827461	0.355217
O	-2.791825	-2.808171	0.067943
O	-4.745171	-1.737128	0.361859
C	-5.441244	-2.920885	-0.014476
H	-5.212936	-3.737271	0.682752
H	-5.158016	-3.224574	-1.030475
H	-6.505567	-2.673065	0.025896
O	-2.913455	-0.655738	0.724779
H	-1.066111	-1.490124	1.155086
H	-1.275867	0.267928	1.441888
H	-1.538982	-0.983107	-1.306329
N	0.437039	-0.750609	-0.860258
C	1.399979	-0.424253	-0.092592
C	2.769841	-0.929849	-0.428841
C	3.907653	-0.428211	0.215519
C	2.925593	-1.905602	-1.425165
C	5.178137	-0.887980	-0.134246
H	3.803536	0.333587	0.989551

C	4.191525	-2.366467	-1.768514
H	2.032145	-2.288654	-1.918354
C	5.322987	-1.857201	-1.124610
H	6.057172	-0.483902	0.369967
H	4.301244	-3.128293	-2.542012
H	6.316308	-2.218047	-1.396455
C	1.281877	0.439956	1.130481
C	1.064537	1.817160	1.016565
C	1.376322	-0.142555	2.400388
C	0.906252	2.596027	2.163395
H	1.005757	2.278477	0.029134
C	1.209106	0.636292	3.543299
H	1.567149	-1.214682	2.489609
C	0.967247	2.006445	3.425741
H	0.731120	3.668640	2.067331
H	1.269384	0.173224	4.529360
H	0.835655	2.616017	4.321044

10-11

0 1

C	4.714925	-0.781419	-1.613021
C	4.618485	0.189482	-0.619074
C	3.398574	0.819334	-0.364011
C	2.255760	0.481844	-1.096305
C	2.366574	-0.482935	-2.107125
C	3.583128	-1.111138	-2.361703
H	5.667082	-1.277617	-1.806772
H	5.496508	0.459898	-0.030055
H	3.354462	1.571414	0.424508
H	1.480548	-0.753198	-2.684102
H	3.648875	-1.865583	-3.147528
C	0.904687	1.137305	-0.840384
C	0.860968	1.892945	0.499351
C	-1.123744	3.097053	0.173808
O	-0.653323	3.749840	-0.719321
O	-2.372127	3.171791	0.607858
C	-3.201414	4.110366	-0.068885
H	-3.261988	3.865964	-1.137212
H	-2.803156	5.126760	0.046336
H	-4.188417	4.033091	0.395691
O	-0.475399	2.186327	0.892605
H	1.275532	1.305471	1.325652
H	1.426040	2.830681	0.399433
H	0.779187	1.907520	-1.617002
N	-0.204103	0.211482	-1.059128

C	-0.573135	-0.666267	-0.212277
C	-1.761259	-1.512566	-0.557246
C	-2.560249	-1.164801	-1.656979
C	-2.089362	-2.653576	0.186179
C	-3.661075	-1.939748	-2.003790
H	-2.294830	-0.274580	-2.227208
C	-3.192467	-3.433225	-0.165912
H	-1.477946	-2.942209	1.042535
C	-3.980826	-3.078384	-1.258522
H	-4.277136	-1.656007	-2.858634
H	-3.435147	-4.321797	0.418807
H	-4.845556	-3.685988	-1.530447
C	0.082801	-0.934859	1.111606
C	1.332209	-1.560829	1.173431
C	-0.562542	-0.558050	2.295924
C	1.943558	-1.780033	2.408805
H	1.832347	-1.867950	0.253212
C	0.055090	-0.769593	3.526665
H	-1.539923	-0.074447	2.243544
C	1.311208	-1.377279	3.584376
H	2.919752	-2.265693	2.450343
H	-0.445746	-0.459351	4.445023
H	1.793667	-1.542186	4.549160

10-12

0 1

C	-1.197023	4.385674	0.498498
C	-0.108385	4.135345	-0.338331
C	0.070809	2.870986	-0.895445
C	-0.831187	1.833963	-0.622967
C	-1.930488	2.098579	0.199443
C	-2.108570	3.364646	0.760020
H	-1.334839	5.373213	0.941753
H	0.609474	4.928460	-0.554446
H	0.932151	2.673656	-1.535750
H	-2.660835	1.317228	0.411668
H	-2.966878	3.550557	1.407882
C	-0.587719	0.455067	-1.230091
C	-1.410908	-0.666458	-0.592805
C	-3.576048	-1.521686	-0.768244
O	-3.318511	-2.432899	-0.028665
O	-4.749491	-1.297708	-1.339884
C	-5.771711	-2.237883	-1.028464
H	-6.660446	-1.912953	-1.576695
H	-5.970203	-2.244471	0.050995

H	-5.475643	-3.245879	-1.346461
O	-2.725131	-0.572566	-1.145778
H	-0.977927	-1.644814	-0.848759
H	-1.477427	-0.596036	0.501280
H	-0.952303	0.501014	-2.270108
N	0.840669	0.171402	-1.337613
C	1.551729	-0.243350	-0.365117
C	3.005338	-0.505526	-0.616418
C	3.897479	-0.721435	0.441432
C	3.491768	-0.523838	-1.932316
C	5.251650	-0.945564	0.188818
H	3.535699	-0.708174	1.470696
C	4.840000	-0.753615	-2.182576
H	2.786899	-0.355783	-2.746694
C	5.725191	-0.964356	-1.121423
H	5.938055	-1.107050	1.021267
H	5.206211	-0.770814	-3.210375
H	6.783253	-1.144600	-1.318579
C	1.050654	-0.501897	1.026807
C	0.718473	0.556213	1.879314
C	0.894942	-1.821698	1.467729
C	0.200875	0.292848	3.148082
H	0.854399	1.586400	1.544776
C	0.367394	-2.081304	2.730452
H	1.173053	-2.647811	0.808942
C	0.013961	-1.023252	3.570341
H	-0.061517	1.122319	3.806592
H	0.230765	-3.112084	3.060447
H	-0.400904	-1.225569	4.559029

11ts

0 2

C	2.947102	-0.530826	0.401617
C	2.329373	-1.054858	-0.732264
C	1.198087	-0.434368	-1.254668
C	0.665989	0.712114	-0.635799
C	1.307555	1.237347	0.504200
C	2.438797	0.620290	1.015303
H	3.834024	-1.016457	0.811499
H	2.728748	-1.949413	-1.210834
H	0.700916	-0.845506	-2.134243
H	0.928018	2.138705	0.987461
H	2.932731	1.033221	1.895354
C	-0.556813	1.282765	-1.175341
H	-0.877774	0.910487	-2.149128

C	-1.256173	2.340143	-0.626078
H	-0.966968	2.803504	0.317433
H	-2.149255	2.716370	-1.122740
O	-2.264484	0.020721	-0.439372
C	-1.606345	-1.038590	-0.114866
O	-1.116815	-1.094623	1.149393
O	-1.376800	-1.983439	-0.847474
C	-1.510101	-0.099801	2.072117
H	-1.117435	-0.409298	3.047430
H	-1.089223	0.881854	1.810632
H	-2.603820	-0.010036	2.121434

12

0 2

C	-3.245509	-1.317144	-0.195214
C	-3.156553	-0.501169	0.933801
C	-2.074245	0.363372	1.087045
C	-1.073011	0.420762	0.113399
C	-1.166431	-0.394402	-1.017835
C	-2.248263	-1.262480	-1.168660
H	-4.090180	-1.997386	-0.313730
H	-3.930503	-0.542925	1.701748
H	-2.001983	0.998052	1.973538
H	-0.384701	-0.352621	-1.778660
H	-2.311628	-1.899532	-2.052299
C	0.061333	1.415611	0.267539
H	0.316848	1.504390	1.332739
C	-0.298689	2.746041	-0.296488
C	1.922123	-0.023307	0.169214
O	1.690586	-0.479538	1.256125
O	2.908237	-0.402691	-0.631084
C	3.746926	-1.434789	-0.123848
H	4.496500	-1.624304	-0.897150
H	3.161746	-2.342589	0.071163
H	4.231912	-1.112503	0.806516
O	1.236227	0.947099	-0.430606
H	-0.787852	2.795189	-1.269832
H	0.060046	3.662710	0.170454

13ts

0 2

C	-4.249051	0.443901	-1.211157
C	-3.664662	-0.537747	-2.013207
C	-2.777468	-1.455491	-1.458044
C	-2.438705	-1.403548	-0.092309
C	-3.042915	-0.412267	0.703341

C	-3.937033	0.496398	0.149481
H	-4.951570	1.159673	-1.641251
H	-3.906209	-0.591568	-3.076187
H	-2.325675	-2.226233	-2.086776
H	-2.820799	-0.365174	1.770858
H	-4.394251	1.257097	0.784965
C	-1.510043	-2.384807	0.455654
C	-0.807425	-2.274078	1.630527
H	-1.006445	-1.452042	2.321736
H	-0.349272	-3.161257	2.061310
H	-1.323236	-3.264095	-0.168596
N	1.142707	-1.718318	1.106052
C	1.317937	-0.576445	0.595182
C	0.297011	0.521295	0.519582
C	-0.162561	0.974357	-0.722471
C	-0.131487	1.152850	1.689698
C	-1.047036	2.047583	-0.789219
H	0.180102	0.485056	-1.636938
C	-1.004004	2.240365	1.618195
H	0.240053	0.805029	2.656268
C	-1.459183	2.689402	0.380268
H	-1.414393	2.388213	-1.758703
H	-1.323767	2.739761	2.534319
H	-2.143557	3.537627	0.324780
C	2.688052	-0.255998	0.051911
C	3.559496	-1.297594	-0.296906
C	3.114791	1.070029	-0.089017
C	4.834586	-1.016166	-0.777257
H	3.217028	-2.327432	-0.188997
C	4.395801	1.348593	-0.566193
H	2.445463	1.888954	0.179553
C	5.256926	0.308575	-0.912510
H	5.502533	-1.833932	-1.052368
H	4.720432	2.385195	-0.668402
H	6.256461	0.528104	-1.291221

14

0 2

C	-4.406381	-0.610835	-1.793402
C	-4.943236	-1.115357	-0.602718
C	-4.262104	-0.957055	0.594638
C	-3.011984	-0.285577	0.646689
C	-2.486444	0.219004	-0.572904
C	-3.176915	0.055831	-1.766437
H	-4.942045	-0.736605	-2.735253

H	-5.901397	-1.637679	-0.615602
H	-4.683634	-1.353886	1.520933
H	-1.528903	0.743468	-0.574752
H	-2.753356	0.452463	-2.691044
C	-2.333153	-0.135649	1.886850
C	-0.975685	0.489683	2.005594
H	-0.953614	1.457068	1.472463
H	-0.768840	0.699257	3.066467
H	-2.794384	-0.565567	2.778023
N	0.036003	-0.445145	1.532799
C	0.956950	-0.097943	0.723422
C	1.180662	1.302013	0.229766
C	1.087963	1.593427	-1.137149
C	1.483565	2.329502	1.130129
C	1.275889	2.897678	-1.592270
H	0.867136	0.790999	-1.845433
C	1.685596	3.630928	0.672520
H	1.564467	2.104196	2.195769
C	1.577036	3.917437	-0.688444
H	1.192344	3.117405	-2.657639
H	1.925746	4.424400	1.381711
H	1.729549	4.936688	-1.046546
C	1.893144	-1.155965	0.225836
C	1.536399	-2.506204	0.354377
C	3.130172	-0.831073	-0.344878
C	2.397539	-3.508199	-0.079629
H	0.571222	-2.744194	0.802397
C	3.996207	-1.837763	-0.773942
H	3.425840	0.214469	-0.445782
C	3.632018	-3.176591	-0.644704
H	2.106423	-4.555135	0.019847
H	4.960255	-1.572060	-1.210388
H	4.307743	-3.963035	-0.984839

15ts

0 2

C	5.334667	-1.140831	-0.136347
C	5.095870	-0.242557	0.902216
C	3.916882	0.503459	0.930387
C	2.953284	0.355991	-0.073881
C	3.207925	-0.546423	-1.115930
C	4.385862	-1.287047	-1.150629
H	6.257957	-1.721961	-0.159292
H	5.835720	-0.112573	1.693851
H	3.760482	1.221255	1.736613

H	2.456294	-0.675235	-1.897315
H	4.564105	-1.986144	-1.969444
C	1.686649	1.143704	-0.086085
C	1.309425	1.963590	0.958859
H	0.518073	2.702184	0.831901
H	1.724655	1.836668	1.959850
H	1.350128	1.431404	-1.086197
N	0.417932	-0.428752	-0.100442
C	-0.827356	-0.207666	-0.067669
C	-1.751595	-1.393949	0.011833
C	-3.084723	-1.293320	-0.403156
C	-1.269868	-2.622954	0.484358
C	-3.922557	-2.407701	-0.351600
H	-3.468248	-0.341075	-0.773772
C	-2.109931	-3.730702	0.540530
H	-0.230879	-2.690374	0.809190
C	-3.438417	-3.626486	0.121091
H	-4.958645	-2.320786	-0.682181
H	-1.728800	-4.681338	0.917144
H	-4.096260	-4.495865	0.165757
C	-1.464114	1.150947	-0.102695
C	-2.188713	1.602401	1.005329
C	-1.319449	1.976640	-1.220574
C	-2.723811	2.888794	1.012412
H	-2.316272	0.946440	1.869271
C	-1.866611	3.259848	-1.215892
H	-0.776201	1.613036	-2.095292
C	-2.559172	3.721308	-0.096269
H	-3.272938	3.242880	1.886252
H	-1.751056	3.902261	-2.090165
H	-2.979123	4.728198	-0.090817

16

0 2

C	4.368634	-1.227007	-1.478024
C	3.320888	-2.139626	-1.344066
C	2.310771	-1.918411	-0.408447
C	2.336110	-0.776369	0.399816
C	3.387834	0.134388	0.261681
C	4.400173	-0.089229	-0.671308
H	5.156453	-1.400193	-2.212808
H	3.289849	-3.030227	-1.974333
H	1.486122	-2.626054	-0.306222
H	3.405174	1.034242	0.881960
H	5.212100	0.632707	-0.774251

C	1.252186	-0.533712	1.451130
C	1.588306	-1.283908	2.701423
H	2.391680	-0.921645	3.343443
H	1.247277	-2.315381	2.801023
H	1.259553	0.550209	1.668065
N	-0.044630	-0.982269	0.964709
C	-0.862004	-0.162686	0.433141
C	-2.206260	-0.661945	0.005149
C	-3.026752	0.096451	-0.839691
C	-2.657029	-1.914999	0.446791
C	-4.272041	-0.389770	-1.238928
H	-2.688475	1.070732	-1.195780
C	-3.901251	-2.395435	0.053093
H	-2.011842	-2.496870	1.105517
C	-4.712941	-1.634118	-0.792778
H	-4.899074	0.208821	-1.901393
H	-4.244840	-3.368237	0.408735
H	-5.689124	-2.011714	-1.101457
C	-0.567786	1.291118	0.196628
C	-1.232261	2.274438	0.938640
C	0.366784	1.671863	-0.772370
C	-0.950821	3.623168	0.726126
H	-1.972310	1.978250	1.685512
C	0.638825	3.022596	-0.990755
H	0.879388	0.906192	-1.358647
C	-0.015851	3.998735	-0.239545
H	-1.466561	4.384524	1.313276
H	1.364984	3.312434	-1.751857
H	0.198983	5.054840	-0.409969

17ts

0 1

C	1.591817	0.231707	0.148453
O	1.133136	-0.469543	0.999506
O	2.770859	0.140708	-0.430323
C	3.610098	-0.922604	0.034342
H	4.542473	-0.833402	-0.528604
H	3.795709	-0.812005	1.109669
H	3.131546	-1.890009	-0.160706
O	0.960544	1.288937	-0.389231
C	-1.591817	0.231706	-0.148453
O	-1.133134	-0.469547	-0.999502
O	-2.770860	0.140709	0.430320
C	-3.610098	-0.922604	-0.034342
H	-4.542475	-0.833399	0.528601

H	-3.795705	-0.812010	-1.109670
H	-3.131547	-1.890009	0.160713
O	-0.960545	1.288937	0.389229

18

0 1

C	-1.427866	-0.129697	-0.371772
O	-1.145998	-0.984878	0.405820
O	-2.546300	0.543808	-0.483540
C	-3.559491	0.218410	0.472028
H	-4.409581	0.863504	0.237572
H	-3.838940	-0.837938	0.377636
H	-3.193936	0.415036	1.487246
O	-0.599209	0.349065	-1.355011
C	1.427884	0.130175	-0.371583
O	1.145963	0.984521	0.406907
O	2.546341	-0.543177	-0.484030
C	3.559478	-0.218790	0.471935
H	4.409626	-0.863544	0.236759
H	3.838840	0.837689	0.378763
H	3.193913	-0.416615	1.486918
O	0.599275	-0.347570	-1.355352

19ts

0 1

N	-1.149044	-0.082230	-1.923503
C	-1.738580	0.426295	-0.928902
C	-1.074109	1.208504	0.159398
C	-0.094882	2.161967	-0.140557
C	-1.410496	0.953381	1.493797
C	0.558292	2.836569	0.888468
H	0.154897	2.358574	-1.183722
C	-0.750543	1.625624	2.520887
H	-2.176669	0.210339	1.725847
C	0.236152	2.564093	2.219950
H	1.320647	3.580635	0.652013
H	-1.003262	1.409824	3.560255
H	0.751761	3.091419	3.024384
C	-3.220748	0.186817	-0.830828
C	-3.760425	-1.024348	-1.281164
C	-4.070190	1.175596	-0.319663
C	-5.134842	-1.243260	-1.220355
H	-3.090323	-1.792022	-1.671048
C	-5.445374	0.955218	-0.267071
H	-3.652265	2.119877	0.034589
C	-5.979396	-0.253638	-0.715179

H	-5.548210	-2.191632	-1.567001
H	-6.103497	1.731303	0.126324
H	-7.055727	-0.425776	-0.667743
N	1.148894	0.082759	-1.923858
C	1.738572	-0.426009	-0.929466
C	1.074291	-1.209254	0.158175
C	0.095325	-2.162717	-0.142611
C	1.410513	-0.955131	1.492816
C	-0.557732	-2.838327	0.885828
H	-0.154331	-2.358632	-1.185930
C	0.750640	-1.628355	2.519314
H	2.176546	-0.212170	1.725579
C	-0.235776	-2.566844	2.217555
H	-1.319905	-3.582355	0.648686
H	1.003229	-1.413314	3.558866
H	-0.751370	-3.094867	3.021543
C	3.220602	-0.185809	-0.831047
C	3.759692	1.025876	-1.280647
C	4.070522	-1.174471	-0.320449
C	5.134007	1.245400	-1.219730
H	3.089274	1.793444	-1.670201
C	5.445597	-0.953459	-0.267693
H	3.653038	-2.119177	0.033153
C	5.979042	0.255885	-0.715154
H	5.546947	2.194178	-1.565752
H	6.104061	-1.729455	0.125316
H	7.055294	0.428499	-0.667658

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0 1

N	-1.354878	-1.923649	-1.016127
C	-2.135937	-1.113164	-1.632020
C	-1.686418	-0.232957	-2.753912
C	-0.992590	-0.757778	-3.850291
C	-1.909964	1.147382	-2.680044
C	-0.529520	0.085767	-4.858175
H	-0.810803	-1.832634	-3.906224
C	-1.439267	1.991018	-3.684599
H	-2.440733	1.561302	-1.819335
C	-0.748356	1.461927	-4.774982
H	0.006465	-0.333382	-5.711044
H	-1.609077	3.066401	-3.612672
H	-0.380234	2.122574	-5.561466
C	-3.544218	-1.021989	-1.153519
C	-3.877678	-1.466179	0.134665

C	-4.556293	-0.518405	-1.980794
C	-5.192585	-1.403149	0.584160
H	-3.088612	-1.862310	0.774876
C	-5.875187	-0.461074	-1.530216
H	-4.312788	-0.178313	-2.988559
C	-6.196617	-0.900312	-0.247221
H	-5.438164	-1.745712	1.590611
H	-6.653939	-0.073045	-2.188435
H	-7.227515	-0.851119	0.106958
N	-0.075978	-2.093499	-1.387932
C	0.839541	-1.250805	-1.075677
C	0.570338	0.020775	-0.337137
C	-0.153847	0.021868	0.860740
C	1.001251	1.237186	-0.880449
C	-0.439503	1.222913	1.507058
H	-0.499396	-0.924809	1.280606
C	0.706655	2.438326	-0.238193
H	1.557941	1.238857	-1.820563
C	-0.013225	2.432941	0.956980
H	-1.001458	1.214609	2.442167
H	1.038725	3.381823	-0.674269
H	-0.242349	3.372705	1.461881
C	2.226205	-1.546964	-1.533797
C	2.435889	-2.441371	-2.593999
C	3.335436	-0.959568	-0.911613
C	3.725557	-2.739237	-3.021724
H	1.570053	-2.898592	-3.074263
C	4.628130	-1.263517	-1.338547
H	3.187822	-0.265324	-0.082838
C	4.826885	-2.151071	-2.394756
H	3.874836	-3.433805	-3.849839
H	5.483158	-0.803390	-0.840987
H	5.838281	-2.384789	-2.731037

21ts

0 1

C	2.559318	-1.192234	0.771791
O	3.236077	-0.448353	1.441510
O	2.817173	-1.640876	-0.432812
C	4.032860	-1.172409	-1.022941
H	4.070019	-1.614795	-2.021843
H	4.021949	-0.076832	-1.085495
H	4.892977	-1.499231	-0.425473
O	1.450910	-1.644655	1.293620
N	-0.344382	-1.647567	-0.792824

C	-0.796792	-0.523882	-0.447251
C	0.158268	0.617976	-0.268973
C	1.137590	0.851912	-1.240358
C	0.117529	1.409481	0.885171
C	2.064587	1.878507	-1.061971
H	1.161210	0.227387	-2.135171
C	1.056355	2.423070	1.065377
H	-0.642922	1.221027	1.645740
C	2.028618	2.660320	0.092381
H	2.816631	2.069453	-1.829615
H	1.030807	3.029685	1.971657
H	2.759600	3.457490	0.234668
C	-2.264455	-0.332415	-0.223398
C	-3.061465	-1.439431	0.099614
C	-2.855920	0.927295	-0.374108
C	-4.433715	-1.286046	0.268970
H	-2.592356	-2.416751	0.223136
C	-4.232073	1.075473	-0.204829
H	-2.240033	1.790404	-0.632852
C	-5.021667	-0.028233	0.116584
H	-5.048147	-2.150157	0.525684
H	-4.688867	2.058609	-0.327047
H	-6.097706	0.091438	0.251497

22ts

0 2

C	-0.791631	0.029194	-0.014979
O	-1.388305	-0.975872	0.130738
O	0.694662	-0.115948	-0.630200
C	1.737888	-0.140339	0.302063
H	2.462463	-0.872133	-0.095383
H	2.243218	0.837183	0.324093
H	1.399022	-0.445427	1.301183
O	-0.779138	1.235227	0.092913

23

0 2

O	-0.790164	0.005095	0.000059
C	0.570708	0.012489	0.000109
H	1.029611	1.016549	0.001959
H	0.934217	-0.568266	0.872705
H	0.933235	-0.563980	-0.875789

24

0 1

C	3.323092	2.688857	-0.606266
C	2.538620	1.958544	-1.500636

C	1.352907	1.365392	-1.071737
C	0.939556	1.507891	0.256199
C	1.725259	2.241407	1.148352
C	2.916150	2.828028	0.720041
H	4.251352	3.151737	-0.945131
H	2.854128	1.848611	-2.539318
H	0.736829	0.789055	-1.762536
H	1.400450	2.360528	2.184911
H	3.521944	3.402495	1.422381
C	-0.320839	0.839759	0.750102
C	-0.098821	-0.600489	1.181156
C	0.670414	-2.604749	0.281427
O	0.539999	-3.171741	1.332624
O	1.106869	-3.148054	-0.843487
C	1.450389	-4.527165	-0.764180
H	1.804273	-4.809411	-1.759619
H	0.572160	-5.125030	-0.488106
H	2.240908	-4.682750	-0.018882
O	0.396735	-1.322547	0.062365
H	0.626019	-0.635042	2.007666
H	-1.042888	-1.045442	1.527557
H	-0.716039	1.378325	1.623398
O	-1.289304	0.884883	-0.301559
C	-2.566830	0.782223	0.056526
O	-2.969407	0.658560	1.182832
O	-3.318615	0.840930	-1.029294
C	-4.722438	0.736417	-0.812659
H	-5.187036	0.808842	-1.799871
H	-4.965896	-0.226149	-0.344749
H	-5.071186	1.551298	-0.165496

25ts

0 1

C	2.488904	3.096027	0.964894
C	3.047964	2.403381	-0.117638
C	2.243299	1.645306	-0.951400
C	0.838555	1.529094	-0.737180
C	0.293294	2.249524	0.363416
C	1.111298	3.014004	1.187352
H	3.120539	3.694979	1.622167
H	4.122408	2.453730	-0.302627
H	2.688460	1.100602	-1.787242
H	-0.772850	2.192024	0.566286
H	0.664578	3.552665	2.025377
C	0.111111	0.678216	-1.609347

H	0.697424	0.153527	-2.367952
C	-1.333639	0.332117	-1.673451
C	-3.421241	0.851326	-0.785697
O	-3.992206	0.158884	-1.583748
O	-3.992025	1.508184	0.215985
C	-5.408563	1.396875	0.293390
H	-5.714115	1.997238	1.154865
H	-5.705786	0.349386	0.434247
H	-5.873769	1.781092	-0.623590
O	-2.116339	1.090557	-0.760095
H	-1.716567	0.493544	-2.696017
H	-1.482485	-0.743012	-1.455662
C	-2.737345	-2.984747	0.003191
C	-3.072102	-1.884109	0.802321
C	-2.079089	-1.115902	1.388977
C	-0.701627	-1.416024	1.197850
C	-0.384691	-2.544620	0.393294
C	-1.390412	-3.308450	-0.186103
H	-3.519988	-3.583904	-0.463523
H	-4.121127	-1.626793	0.960359
H	-2.349779	-0.249023	1.996319
H	0.657587	-2.808532	0.226178
H	-1.120699	-4.170386	-0.799087
C	0.267730	-0.573830	1.807983
H	-0.100429	0.202477	2.480556
C	1.750066	-0.656836	1.700431
C	3.440388	-0.990603	0.127771
O	4.291162	-0.613642	0.888425
O	3.642085	-1.361225	-1.130965
C	4.989784	-1.283040	-1.580600
H	4.988246	-1.644800	-2.612669
H	5.640330	-1.909345	-0.956815
H	5.345929	-0.244638	-1.541825
O	2.149412	-1.108884	0.404303
H	2.194224	0.335562	1.878279
H	2.179043	-1.343635	2.454422

26

0 1

C	3.067758	3.493396	0.153232
C	3.410735	2.380719	-0.613604
C	2.457657	1.398373	-0.882626
C	1.152674	1.507975	-0.388485
C	0.818009	2.629991	0.382599
C	1.768091	3.615587	0.647407

H	3.810606	4.264043	0.364698
H	4.424010	2.275611	-1.005367
H	2.730343	0.525026	-1.482081
H	-0.196509	2.731136	0.773183
H	1.491997	4.484913	1.246819
C	0.151788	0.400374	-0.647037
H	0.611591	-0.297405	-1.364441
C	-1.138958	0.868104	-1.312526
C	-3.285225	1.356667	-0.474467
O	-3.846999	0.825193	-1.392891
O	-3.878593	1.887909	0.586725
C	-5.298586	1.789615	0.606054
H	-5.625825	2.299413	1.516530
H	-5.607158	0.735833	0.626129
H	-5.729893	2.273735	-0.279450
O	-1.971035	1.505216	-0.339705
H	-0.927369	1.582423	-2.121594
H	-1.685603	0.013185	-1.730968
C	-3.069158	-3.488498	-0.153066
C	-3.410372	-2.376899	0.616062
C	-2.456342	-1.395505	0.885202
C	-1.152225	-1.504876	0.388836
C	-0.819220	-2.625994	-0.384325
C	-1.770209	-3.610653	-0.649253
H	-3.812741	-4.258377	-0.364754
H	-4.423003	-2.271778	1.009512
H	-2.727740	-0.522910	1.486334
H	0.194668	-2.727151	-0.776577
H	-1.495433	-4.479210	-1.250380
C	-0.150637	-0.397900	0.647074
H	-0.609721	0.300046	1.364808
C	1.140337	-0.866187	1.311590
C	3.285364	-1.360620	0.474055
O	3.848164	-0.831780	1.393367
O	3.877835	-1.892973	-0.587067
C	5.298131	-1.798756	-0.605224
H	5.624255	-2.303771	-1.518763
H	5.727540	-2.289901	0.277336
H	5.609923	-0.745828	-0.618482
O	1.970780	-1.504507	0.338129
H	1.688027	-0.011228	1.728637
H	0.929149	-1.579760	2.121411

CO$_2$

0 1

C	0.000000	0.000060	0.000007
O	0.004970	-0.002450	-1.156134
O	-0.004970	0.002406	1.156129