# Calculation details

Restricted MPW1K/LACV3P**, with single point solvation from Poisson-Boltzmann continuum theory (DMSO solvent, ε=47.24, r_{probe}=2.41 Å) using Jaguar 6.0 (Schrödinger Inc). Thermochemical corrections (ΔG, ZPE) used calculated vibrational frequencies. Intermediates and transition states were stationary points with the correct number of positive eigenvalues; reactants and products were optimized from transition structures perturbed along a negative eigenvalue path.

# Comparison of geometries against known crystal structures

To validate our theoretical method, we calculated the structures of a variety of cationic and anionic iodine(V) and iodine (III) geometries for which crystal structures are available. In all cases, we determined the effect of crystal packing forces by computing and comparing the geometries of single molecule compounds to multiple molecule clusters.

We found excellent agreement between experiment and theory.
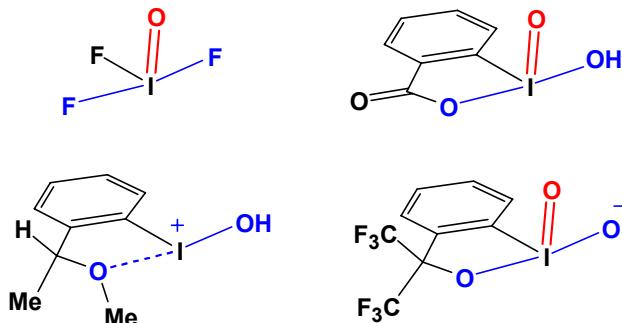
The simplest case, IOF$_3$

|		expt	theory	
			mono	4-mer
bonds (A)	1-4	**1.89**	**1.94**	
	1-3	**1.91**	**1.94**	
	1-5	1.84	1.89	
	1-2	1.67	1.75	
angles (^{O})	4-1-3	165.9	163.1	
	4-1-5	85.9	81.7	
	3-1-5	80.0	81.7	
	4-1-2	94.3	94.0	
	3-1-2	89.8	94.0	
	5-1-2	102.0	106.9	
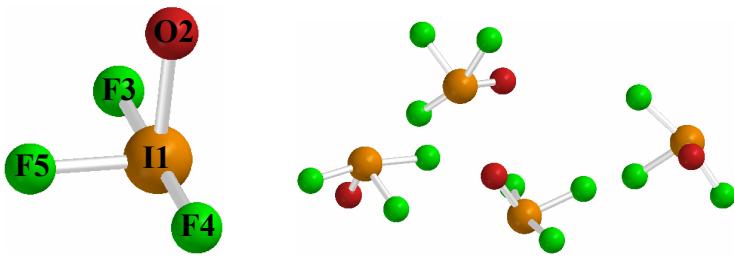
"Iodine oxide trifluoride (mol. wt. = 200) is orthorhombic, a = 5.70(1), b = 5.62(1), c = 10.49(2) Å ... U = 336 Å^3, Z = 4, calculated density = 3.95 g/cm-3, F(000)=352; space group P2$_1$2$_1$2$_1$ ... R = 0.060." from *J. Fluor. Chem, 4* **1974** 173-179.

Good agreement of all parameters, particularly key bond lengths **1-4** and **1-3**, with experiment. The *oxo* bond is slightly too long. There is a slight asymmetry in the crystal structure bonds (e.g. **1-4** and **1-3**, **4-1-5** and **3-1-5**) due to crystal packing effects.

Our key geometry, o-iodobenzoic acid (IBX)

|		expt	theory mono	4-mer
bonds (A)	**4-13**	1.78	1.82	1.81
	4-3	2.10	2.10	2.09
	4-5	1.93	2.01	2.03
	4-8	2.26	2.12	2.13
angles (°)	**5-4-3**	86.3	88.6	84.8
	3-4-8	77.2	78.2	78.4
	13-4-5	96.3	91.8	92.5
	13-4-8	88.1	93.5	95.1
	13-4-3	100.3	108.9	104.0
	5-4-8	163.4	166.7	162.8
	5-4-13-3	-87.4	-89.1	85.3
	5-4-13-8	-164.0	-167.8	164.5
	3-4-13-8	-76.6	-78.7	79.2
	3-4-8-6	0.4	3.5	0.1
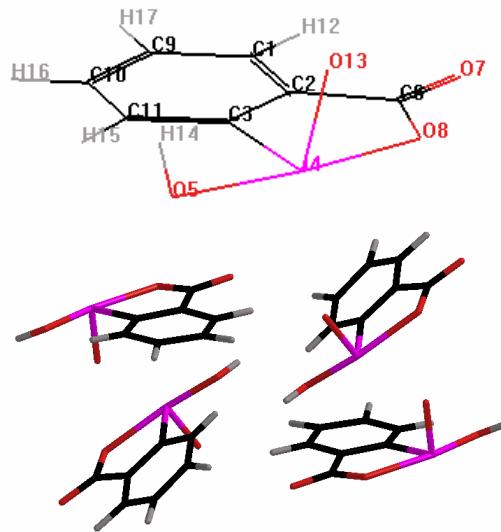
"The crystals were found to be racemic 1-hydroxy-1,2-benziodoxol-3(1*H*)-one 1-oxide, cell parameters *a* = 7.854(1), *b* = 11.584(2), *c* = 8.385(2), β = 101.29(1)°, space group P2₁/*c*, Z=4 ... Final parameters were *wR2* = 0.0385 and *R1* = 0.0160." from *J. Chem. Soc. Perkin Trans 2*, **1997** 589-591. The crystals are a true racemate, with alternating enantiomers stacked; single enantiomer crystals have also been observed.

Good agreement of most geometrical parameters, but the bond lengths in the hypervalent three-center four-electron O-I-O bonds are unbalanced, with bond **4-5** being too long by 0.08 Å, and bond **4-8** being too short by 0.14 Å. This difference persists even when using other "best of breed" functionals and basis sets (LACV3P** vs. LACVP**). We believe the discrepancy is not severe enough to affect the chemistry described in our paper, and that the conclusions remain valid.

		expt	mpw1k ζ^3	mpw1k ζ^2	b3lyp ζ^3	b3lyp ζ^2
bonds (A)	**4-5**	**1.93**	**2.01**	1.97	2.06	2.02
	4-8	**2.26**	**2.12**	2.09	2.18	2.15
angles (°)	**13-4-5**	**96.3**	**91.8**	92.0	92.8	92.8
	13-4-8	**88.1**	**93.5**	93.0	93.9	93.5
	13-4-3	**100.3**	**108.9**	109.5	109.3	109.7

.

Cationic iodine(III) compound

|		expt	theory mono	theory +counter
bonds (A)	**7-2**	2.12	2.13	2.12
	7-8	2.47	2.42	2.52
	7-12	1.93	1.97	1.97
angles (^{O})	**2-7-8**	72.2	73.9	73.2
	2-7-12	94.2	92.8	88.4
	8-7-2-12	178.5	177.5	178.4
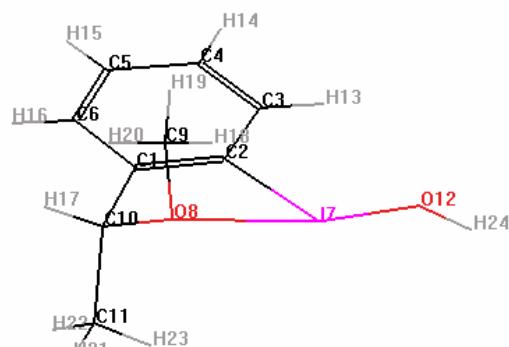
"Crystal data and parameters: formula $C_{16}H_{19}IO_5S$ [bound tosylate counterion]. Crystal system: orthorhombic. Space group: P212121. $a = 6.5239(7)$ Å, $b = 8.3071(20)$ Å, $c = 32.7576(43)$ Å. $\alpha = \beta = \gamma = 90^o$. Z = 4. Final R = 0.0683, final R_w = 0.0818." from *J. Org. Chem* **1998** *63* 7674-7679, supporting information. The cationic iodine compound packs loosely in the crystal with its tosylate counterion, producing a large unit cell with minimal packing effects.
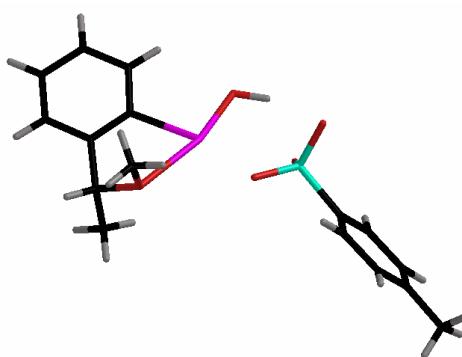
All key geometrical parameters show excellent agreement with experiment.

Anionic iodine(V) compound

		expt	theory mono	theory dimer
bonds (A)	**1-3**	2.30	2.36	2.45
	1-4	1.78	1.84	1.85
	1-5	2.14	2.12	2.14
	1-2	1.79	1.83	1.83
angles (^{O})	**3-1-5**	73.9	72.3	70.5
	4-1-5	91.9	91.7	89.7
	2-1-5	105.3	103.4	93.8
	3-1-4	165.3	158.8	152.3
	3-1-2-5	-72.4	-72.3	-70.8
	4-1-2-5	95.1	95.6	90.7
	3-1-5-4	-176.0	-165.8	-160.3
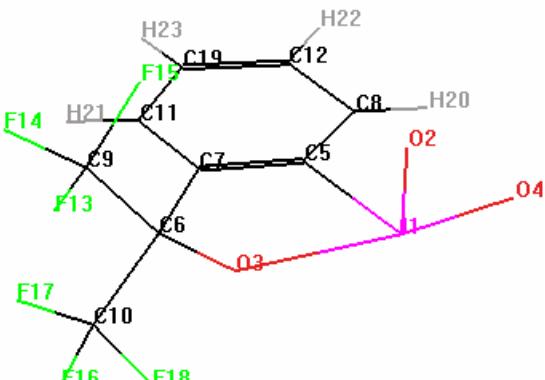
"Crystal data: $C_{19}H_8F_{15}O_5SI$, mol wt = 760.16, triclinic, a = 12.041(2) Å, b = 12.472(2) Å, c = 11.056(2) Å, V = 1294.1(4) Å^3 ... R and R_w of 0.0348 and 0.0467." from *J. Am. Chem. Soc.* **1993** *115* 2488-2495. The anionic iodine compound forms dimers with the lone pair of one oxo donating into the σ* orbital of the Ph-I covalent bond of another monomer. Each dimer is charge neutralized by two quaternary ammonium counterions (NBu4+) and two bridging waters.
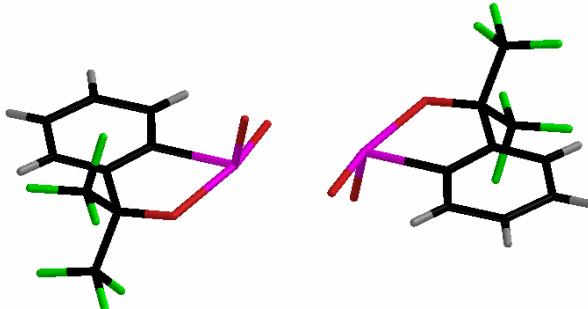
All key geometrical parameters show excellent agreement with experiment.

NMR shifts of IBX-alcoholate complex
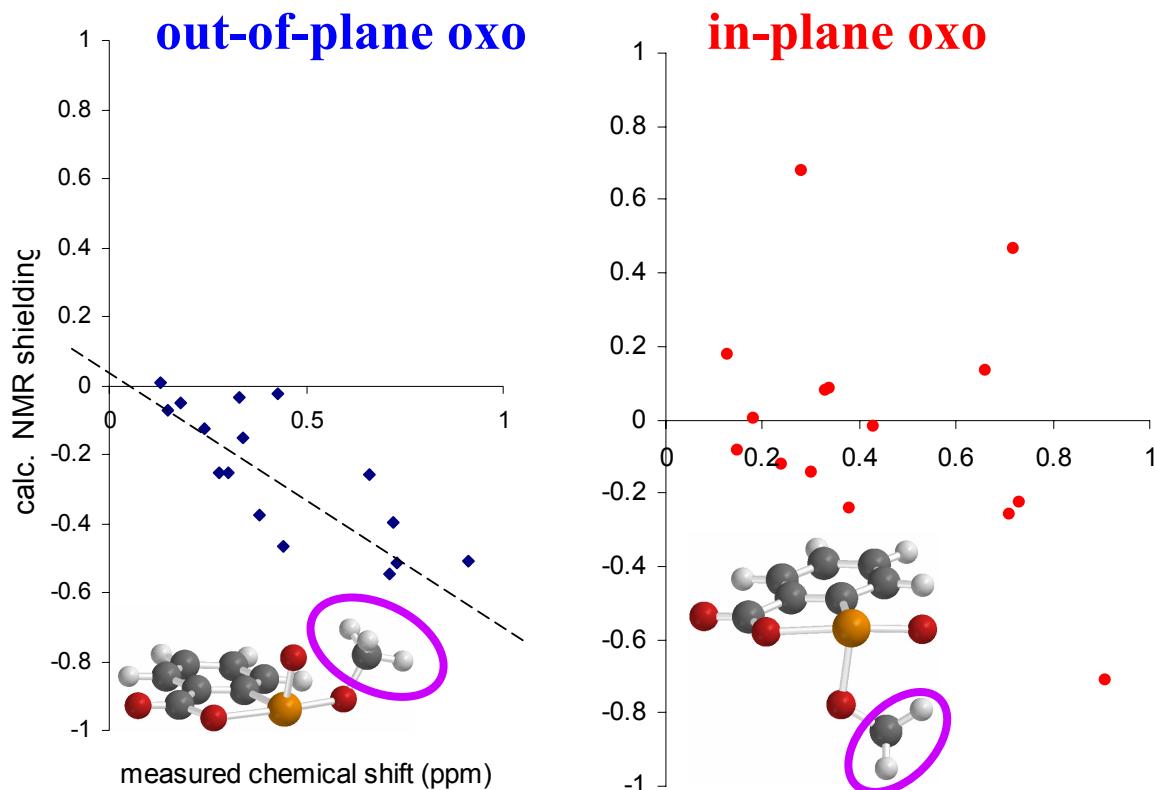
We have calculated the difference in NMR shielding constants between the alkyl hydrogens in nine free alcohols and their corresponding IBX-alcoholate complexes. The calculated shielding constants correlate well to the experimentally measured chemical shift differences (*J. Org. Chem.* **1995**, *60*, 7272-7276). The correlation is only present in the calculated geometry where the *oxo* group is out-of-plane, and not in the twisted geometry, supporting our contention that the IBX-alcoholate complex has the *oxo* group out-of-plane (termed "equatorial" in the experimental reference).

Reaction schemes

Twisting, different alcohols

Elimination, different alcohols

Constrained complexes, different n *(chain lengths)*
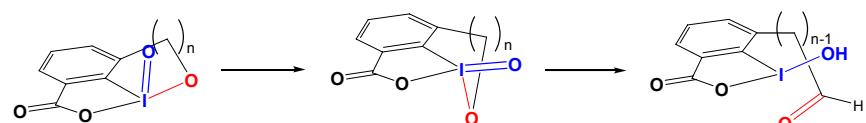
Potential energy curves
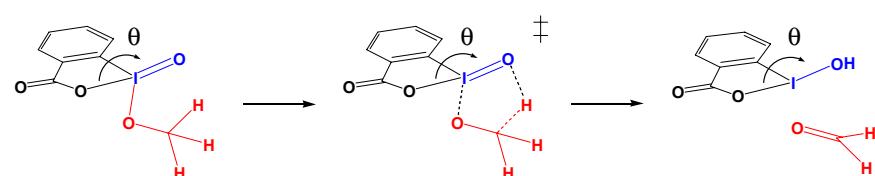
Ligand exchange steps

Reference structures

i1   i2   i3
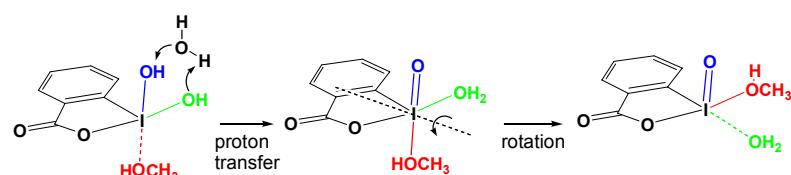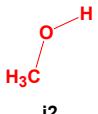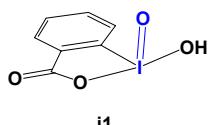
Key to structures in reaction schemes

Twisting, different alcohols	a1-9	IBX(OR)
	b1-9	o-Me-IBX(OR)
Elimination, different alcohols	c1-7	IBX(OR)
	d1-7	o-Me-IBX(OR)
Constrained complexes, diff. n	e4-5	twisting reaction
	f2-5	elimination reaction
Potential energy curves	g1-13	elim reaction vs. angle
Ligand exchange steps	h1	proton transfer
	h2	coordinated ligand motion
Reference structures	i1,2	IBX, water
	j1-9	alcohols

Key to numbers in figures

Figure 1. Ligand exchange barrier is h2(ts-sm), twisting barrier is a1(ts-sm), elimination barrier is c1(ts-sm).

Figure 2. Twisting barriers are a1-9(ts-sm) for the unmodified IBX, and b1-9(ts-sm) for the *o*-Me-IBX. Experimental k are from reference (5), reproduced below.

Figure S1. Twisting barriers are e4-5 (ts-sm), and elimination barriers are f2-5 (ts-sm).

Figure 4. Curves corresponding to g1-13(sm, ts, p) are plotted relative to IBX + MeOH – HOH.

Scheme 1. Proton transfer barrier is h1(ts-sm) and coordinated ligand motion barrier is h2(ts-sm).

Figure S2. Energy differences are a1(sm) + HOH (i2) – IBX (i1) – alcohol (j*), compared to experimental K_{eq} from reference (5), reproduced below.

Additional figures

Figure S1. Constrained alcohol-IBX complexes probe the conformational requirements for oxidation. Reaction barriers (kcal/mol) indicate that a minimum chain length of 4 carbons is required before twisting is allowed and the oxidation can proceed with low barrier.

n	$E_{twist}^{\ddagger}$	$E_{elim}^{\ddagger}$
2	-	**21.9**
3	-	**12.8**
4	**5.9**	4.8
5	**5.5**	3.8
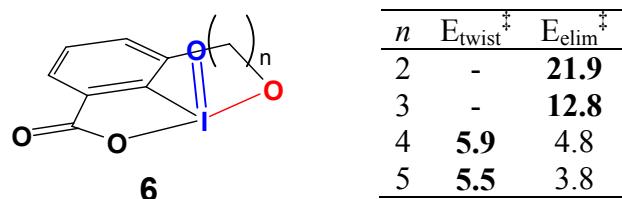
Figure S2. Correlation of measured equilibrium constants with computer energy differences suggests that a thermodynamic mixture of 1 and 2 is present.
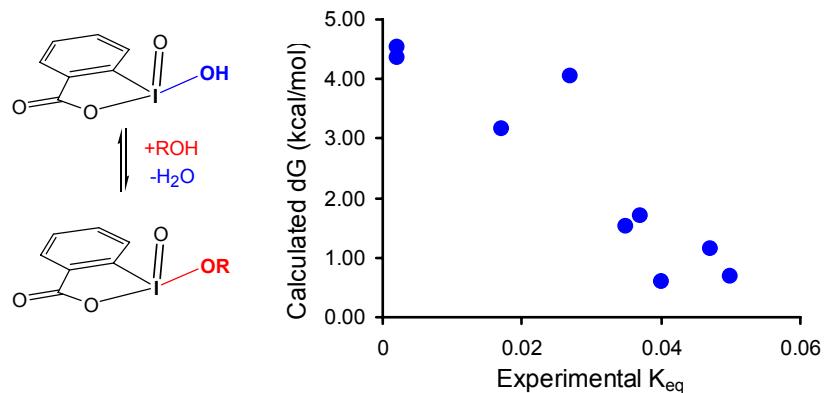
Figure S3. Rapid screening for optimal *ortho* substituent, evaluating twisting and ligand exchange thermodynamics (dE only, gas phase, B3LYP/LACVP**). Methyl, ethyl, and isopropyl provide the best balance of good twisting and ligand exchange thermodynamics.
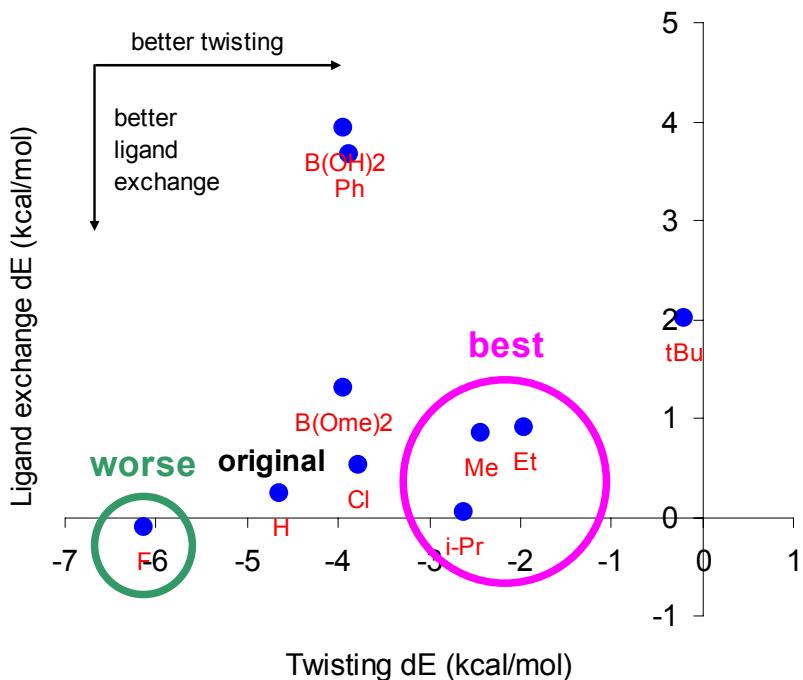
Referenced experimental results

Frigerio, M.; Santagostino, M.; Sputore, S.; Palmisano, G. *J. Org. Chem.* **1995**, *60*, 7272-7276

Table 1. Equilibrium Constants K_{eq} for Formation of the IBX−Alcoholate Complex in DMSO-d_6 Solutions and Rate Constant k_2 for Disproportionation Reaction

entry	alcohol	$K_{eq}{}^a$	$k_2{}^a$ (s^{-1})
1	methanol	0.040	0.006
2	ethanol	0.050	0.007
3	isopropyl alcohol	0.037	0.005
4	isobutyl alcohol	0.047	0.009
5	neopentyl alcohol	0.035	0.011
6	2,4-dimethyl-3-pentanol	0.017	0.022
7	benzyl alcohol	0.027	0.234
8	*tert*-butyl alcohol	0.002	
9	*tert*-pentyl alcohol	0.002	
10	pinacol	0.059	

^{a} Due to the low relative intensity of the adduct signals, the precision of the ^{1}H-NMR integrals of **5** is very low. Consequently, also K_{eq} and k_2 values are imprecise (ca. ±20%).

Scheme 1
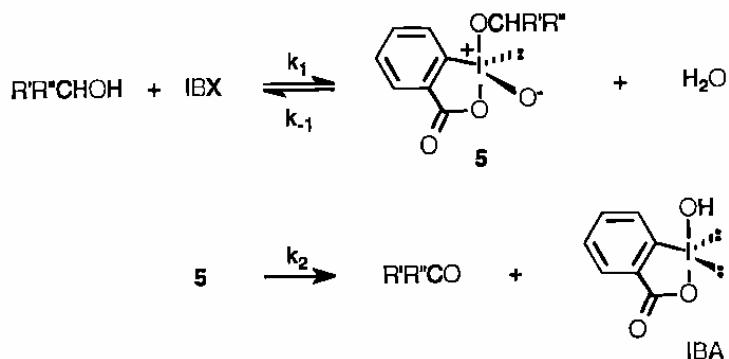
Measurement of equilibrium and rate constants for overall oxidation reaction.

	5ax		
R	α^b	β	γ
methyl	0.66		
ethyl	0.72	0.24	
propyl	0.71	0.27	0.12
isopropyl	0.91	0.28, 0.30^e	
sec-butyl	0.95, 0.97^f	0.29^g	0.10
		h,i	
neopentyl	0.71		0.18
isobutyl	0.73	0.33	0.15, 0.13^e
tert-butyl		0.38	
tert-pentyl		0.34^g	i
		0.43, 0.44^e	

NMR shifts of alkyl protons in IBX-alcoholate complex.

Relative energies of structures

dE, dG, and solvation in kcal/mol; *G* contains enthalpic, entropic, and zero point energy effects.

Twisting, different alcohols

IBX			dE	dG-dE	d(solv)	d(total)
methanol	1	ts-sm	16.41	-0.64	-3.62	12.14
ethanol	2	(a)	16.19	-0.57	-2.68	12.93
isopropanol	3		15.03	-0.48	-2.35	12.20
isobutyl alcohol	4		15.75	-0.56	-3.67	11.53
neopentyl alcohol	5		15.99	-0.50	-3.24	12.25
2,4-dimethyl-3-pentanol	6		13.80	-0.41	-1.65	11.74
benzyl alcohol	7		14.47	-0.56	-2.85	11.06
tert-butyl alcohol	8		13.58	-0.56	-3.00	10.02
tert-pentyl alcohol	9		13.54	-0.54	-3.46	9.54
	1	p-sm	6.68	-0.20	-2.49	3.99
	2	(a)	6.39	-0.13	-2.78	3.48
	3		5.72	-0.18	-2.84	2.69
	4		6.11	-0.04	-1.73	4.34
	5		6.00	-0.04	-1.75	4.21
	6		4.23	0.09	-1.82	2.49
	7		5.93	0.04	-2.44	3.52
	8		7.21	-0.03	-2.85	4.33
	9		7.00	0.02	-2.48	4.53

o-me-IBX			dE	dG-dE	d(solv)	d(total)
methanol	1	ts-sm	12.09	-0.39	-1.99	9.71
ethanol	2	(b)	11.74	-0.44	-1.71	9.60
isopropanol	3		9.17	-0.31	-1.44	7.42
isobutyl alcohol	4		11.62	-0.35	-2.18	9.08
neopentyl alcohol	5		11.75	-0.37	-2.62	8.76
2,4-dimethyl-3-pentanol	6		9.26	0.24	-1.76	7.74
benzyl alcohol	7		9.76	-0.20	-2.30	7.26
tert-butyl alcohol	8		7.04	0.18	-1.36	5.86
tert-pentyl alcohol	9		8.04	-1.81	-1.30	4.93
	1	p-sm	4.58	-0.03	-1.08	3.48
	2	(b)	4.75	-0.19	-1.32	3.24
	3		2.57	-0.12	-1.87	0.59
	4		4.13	-0.01	-0.97	3.15
	5		3.96	0.02	-0.80	3.17
	6		4.59	0.62	-1.51	3.70
	7		3.44	0.10	-1.81	1.73
	8		3.70	0.33	-1.10	2.93
	9		4.41	-0.03	-1.89	2.49

Elimination, different alcohols

IBX			dE	dG-dE	d(solv)	d(total)
methanol	1	ts-sm	4.21	-1.42	1.95	4.74
ethanol	2	(c)	4.10	-1.58	1.88	4.40
isopropanol	3		4.79	-1.61	2.41	5.60

isobutyl alcohol	4		4.13	-1.67	1.68	4.14
neopentyl alcohol	5		4.04	-1.70	1.69	4.03
2,4-dimethyl-3-pentanol	6		5.11	-1.73	2.53	5.91
benzyl alcohol	7		3.55	-1.34	0.86	3.07
	1	p-sm	-84.96	-2.64	2.79	-84.81
	2	(c)	-92.06	-2.43	2.01	-92.48
	3		-95.82	-2.74	2.71	-95.85
	4		-91.54	-2.31	2.19	-91.65
	5		-91.37	-2.10	1.37	-92.10
	6		-95.54	-2.12	1.50	-96.16
	7		-95.28	-1.35	2.14	-94.49

o-me-IBX			dE	dG-dE	d(solv)	d(total)
methanol	1	ts-sm	4.37	-1.54	1.42	4.25
ethanol	2	(d)	4.16	-1.70	1.29	3.75
isopropanol	3		4.78	-1.69	1.99	5.07
isobutyl alcohol	4		4.26	-1.78	0.96	3.45
neopentyl alcohol	5		4.18	-1.82	0.82	3.18
2,4-dimethyl-3-pentanol	6		4.89	-1.80	2.53	5.62
benzyl alcohol	7		3.36	-1.38	0.46	2.44
	1	p-sm	-82.95	-2.86	2.50	-83.32
	2	(d)	-91.51	-1.85	2.13	-91.22
	3		-94.38	-2.81	1.46	-95.73
	4		-89.50	-2.89	1.28	-91.10
	5		-90.17	-1.67	0.85	-90.99
	6		-94.42	-1.66	2.25	-93.83
	7		-93.63	-1.53	1.87	-93.29

Constrained complexes, different n (chain lengths)

				dE	dG-dE	d(solv)	d(total)
twist	n=4	e4	ts-sm	6.96	0.36	-1.39	5.93
	n=5	e5	(e, f)	8.29	0.33	-3.11	5.51
elim	n=2	f2		23.66	-2.24	0.47	21.89
	n=3	f3		13.88	-1.02	-0.11	12.75
	n=4	f4		3.71	-1.35	2.48	4.84
	n=5	f5		4.15	-1.56	1.25	3.84
			p-sm	3.92	0.54	-2.16	2.31
			(e, f)	5.19	0.45	-3.24	2.40
				-77.38	-0.97	2.31	-76.04
				-85.37	-0.84	0.23	-85.98
				-93.24	-1.38	2.62	-92.00
				-94.15	-1.70	2.55	-93.30

Potential energy curves

angle			dE	dG-dE	d(solv)	d(total)
0	g1	sm	-0.40	1.09	0.14	0.83
10	g2		0.71	0.95	0.27	1.93
20	g3		2.61	0.83	0.25	3.68

30	g4		5.15	0.53	0.01	5.69
40	g5		8.05	0.36	-0.25	8.16
50	g6		9.76	0.25	-0.45	9.56
60	g7		12.43	0.33	-3.13	9.63
70	g8		10.71	0.47	-3.00	8.17
80	g9		8.02	0.69	-2.76	5.95
90	g10		6.49	0.85	-2.53	4.81
100	g11		6.11	0.92	-2.33	4.70
110	g12		6.91	0.93	-2.62	5.22
120	g13		8.90	0.86	-3.03	6.73
		ts	24.27	-2.24	-1.65	20.39
			22.38	-1.84	-0.89	19.64
			20.97	-1.57	-0.50	18.91
			20.15	-1.35	-0.42	18.38
			19.72	-1.30	-0.95	17.47
			19.11	-1.07	-1.48	16.56
			17.31	-0.73	-1.25	15.33
			14.61	-0.59	-0.83	13.19
			12.30	-0.53	-0.52	11.25
			10.80	-0.50	-0.45	9.86
			10.29	-0.49	-0.45	9.34
			10.87	-0.54	-0.70	9.63
			12.52	-0.64	-1.35	10.53
		p	-42.87	-2.51	-2.65	-48.03
			-49.92	-2.33	-1.84	-54.08
			-56.23	-1.95	-1.90	-60.07
			-61.93	-1.91	-1.80	-65.64
			-66.74	-1.84	-1.38	-69.96
			-71.00	-1.51	-0.46	-72.97
			-74.24	-1.14	-0.03	-75.41
			-77.20	-1.12	0.46	-77.87
			-78.90	-1.00	0.74	-79.16
			-79.56	-0.96	1.08	-79.43
			-79.05	-0.99	1.11	-78.93
			-77.21	-1.33	1.68	-76.86
			-74.63	-1.84	-0.02	-76.49

Ligand exchange steps

			dE	dG-dE	d(solv)	d(total)
proton transfer	h1	ts-sm	7.08	-0.09	-1.03	5.96
		p-sm	1.37	0.49	2.86	4.72
rotation	h2	ts-sm	7.25	-1.01	2.84	9.07
		p-sm	-4.16	0.81	1.59	-1.76

Absolute energies of structures

E and *G* in hartrees, solvation in kcal/mol, and lowest calculated vibration frequency in cm^{-1}.
G contains enthalpic, entropic, and zero point energy effects.

Twisting, different alcohols

IBX			E	G	solv	freq
methanol	a1	sm	-621.2877411	-621.184191	-21.3199	112.1
ethanol	a2		-660.6270908	-660.496123	-21.4009	93.33
isopropanol	a3		-699.9656083	-699.807847	-21.3732	87.56
isobutyl alcohol	a4		-739.2963348	-739.110848	-20.6271	74.99
neopentyl alcohol	a5		-778.6318834	-778.419663	-20.4998	72.23
2,4-dimethyl-3-pentanol	a6		-857.2982014	-857.031265	-20.2098	71.5
benzyl alcohol	a7		-852.4296836	-852.248858	-21.2611	55.43
tert-butyl alcohol	a8		-739.3009076	-739.116529	-20.7011	83.34
tert-pentyl alcohol	a9		-778.6333838	-778.421476	-19.9054	79.58
		ts	-621.2615965	-621.159062	-24.9439	-42.8
			-660.6012893	-660.471236	-24.0834	-23
			-699.9416514	-699.784663	-23.7243	-15.37
			-739.27123	-739.086632	-24.294	-30.55
			-778.606403	-778.394979	-23.7416	-25.93
			-857.2762066	-857.009929	-21.8568	-19.42
			-852.4066212	-852.226687	-24.1146	-44.6
			-739.2792599	-739.09578	-23.7047	-21.77
			-778.6118039	-778.400753	-23.3703	-17.86
		p	-621.2770941	-621.173868	-23.808	94
			-660.6169058	-660.486153	-24.1796	73.62
			-699.9565003	-699.79903	-24.2167	68.98
			-739.2865971	-739.101175	-22.3615	69.26
			-778.6223275	-778.410177	-22.2449	66.68
			-857.2914632	-857.024387	-22.0333	60.23
			-852.4202414	-852.239352	-23.706	56.4
			-739.2894206	-739.105091	-23.5522	68.49
			-778.6222336	-778.410298	-22.3889	65.35

o-Me-IBX			E	G	solv	freq
methanol	b1	sm	-660.6164064	-660.486493	-21.5958	100.94
ethanol	b2		-699.9562448	-699.798791	-21.2406	85.22
isopropanol	b3		-739.292515	-739.108293	-21.2868	87.22
isobutyl alcohol	b4		-778.6250397	-778.413012	-20.2269	77.98
neopentyl alcohol	b5		-817.960504	-817.721771	-20.1108	75.11
2,4-dimethyl-3-pentanol	b6		-896.6257845	-896.33329	-18.5604	65.32
benzyl alcohol	b7		-891.7576401	-891.550593	-20.7718	52.09
tert-butyl alcohol	b8		-778.6266676	-778.416784	-21.1191	74.35
tert-pentyl alcohol	b9		-817.9606576	-817.72267	-19.9119	72.17
		ts	-660.5971369	-660.467853	-23.581	-42.72
			-699.9375355	-699.780775	-22.9481	-25.12
			-739.277898	-739.094176	-22.7276	-14.24
			-778.606527	-778.39506	-22.4093	-7.72

E	G	solv	freq
-817.9417869	-817.703642	-22.7285	-29.03
-896.6110225	-896.318144	-20.3215	-31.55
-891.7420864	-891.535357	-23.075	-30.37
-778.6154495	-778.405276	-22.4799	-2.7
-817.9478463	-817.712738	-21.2111	12.96

	E	G	solv	freq
p	-660.6091003	-660.479239	-22.6713	91.95
	-699.9486804	-699.79153	-22.5619	76.53
	-739.288418	-739.104384	-23.154	67.04
	-778.6184641	-778.406446	-21.1954	67.71
	-817.9541992	-817.715432	-20.915	65
	-896.6184695	-896.324985	-20.0697	61.51
	-891.7521588	-891.544946	-22.5846	50.78
	-778.6207675	-778.410355	-22.2203	74.23
	-817.9536245	-817.715678	-21.8063	67.76

Elimination, different alcohols

IBX			E	G	solv	freq
methanol	c1	sm	-621.2770826	-621.17386	-23.7334	93.8
ethanol	c2		-660.6168598	-660.486288	-23.6844	77.74
isopropanol	c3		-699.9565132	-699.799044	-24.2864	69.22
isobutyl alcohol	c4		-739.2866358	-739.101228	-22.4632	69.01
neopentyl alcohol	c5		-778.6222965	-778.410165	-22.4243	66.34
2,4-dimethyl-3-pentanol	c6		-857.2914735	-857.0244	-22.0795	60.13
benzyl alcohol	c7		-852.420246	-852.239576	-23.9454	52.06
		ts	-621.2703764	-621.169413	-21.7802	-542.7
			-660.610331	-660.482279	-21.8016	-483.3
			-699.9488799	-699.793969	-21.874	-413.5
			-739.2800515	-739.0973	-20.7855	-464.6
			-778.6158514	-778.406429	-20.7377	-456.5
			-857.2833329	-857.019011	-19.5463	-411.4
			-852.4145951	-852.236056	-23.0843	-430.2
		p	-621.4124702	-621.313458	-20.9396	32.59
			-660.7635634	-660.636866	-21.6793	31.27
			-700.109206	-699.956102	-21.5779	26.67
			-739.432508	-739.250776	-20.2731	30.34
			-778.7678964	-778.559106	-21.059	31.11
			-857.4437244	-857.180031	-20.5793	22.55
			-852.5720889	-852.393577	-21.8027	33.28

o-Me-IBX			E	G	solv	freq
methanol	d1	sm	-660.6091043	-660.479249	-22.6085	91.88
ethanol	d2		-699.9487347	-699.791543	-22.4372	76.24
isopropanol	d3		-739.2884264	-739.104392	-22.1365	67.15
isobutyl alcohol	d4		-778.6184857	-778.406488	-21.0558	67.58
neopentyl alcohol	d5		-817.9541624	-817.715432	-20.7611	64.95
2,4-dimethyl-3-pentanol	d6		-896.6232892	-896.32972	-20.9624	58.45
benzyl alcohol	d7		-891.7520804	-891.544867	-22.5047	50.65

ts	-660.6021367	-660.474743	-21.1842	-591.7
	-699.9421088	-699.787626	-21.1436	-518.8
	-739.2808146	-739.099475	-20.1504	-438.4
	-778.6116919	-778.402529	-20.0935	-502.5
	-817.9475005	-817.711666	-19.9414	-496.3
	-896.6154907	-896.324794	-18.4286	-429.1
	-891.7467239	-891.541705	-22.0495	-457.5
p	-660.7412969	-660.616004	-20.1098	26.42
	-700.0945573	-699.940308	-20.3105	45.02
	-739.4388362	-739.259285	-20.6732	23.82
	-778.7611072	-778.553708	-19.7776	14.44
	-818.0978534	-817.861786	-19.9106	40.74
	-896.7737556	-896.482831	-18.7124	30.16
	-891.9012957	-891.696521	-20.631	27.88

Constrained complexes, different n (chain lengths)

				E	G	solv	freq
twist	n=4	e4	sm	-738.0688819	-737.901469	-21.4022	100.1
	n=5	e5		-777.4042227	-777.208691	-19.964	97.51
elim	n=2	f2		-659.4225307	-659.309794	-23.3273	116.55
	n=3	f3		-698.7450803	-698.605273	-21.8645	104.61
	n=4	f4		-738.0626515	-737.894378	-23.5895	103.94
	n=5	f5		-777.3939045	-777.197473	-22.199	97.35
			ts	-738.0577953	-737.889816	-22.7894	-41.87
				-777.3910119	-777.19496	-23.075	-30.38
				-659.3848276	-659.275658	-22.8549	-668.42
				-698.722967	-698.584789	-21.9726	-445.84
				-738.0567451	-737.890619	-21.1133	-465.34
				-777.3872914	-777.193343	-20.9491	-452.55
			p	-738.0626283	-737.894356	-23.5583	103.68
				-777.3959571	-777.199704	-23.2082	95.73
				-659.5458493	-659.434661	-21.0162	94.61
				-698.8811242	-698.742652	-21.6337	83.67
				-738.2112462	-738.045166	-20.9658	75.85
				-777.5439402	-777.350224	-19.6455	67.84

Potential energy curves

angle			E	G	solv	freq
0	g1	sm	-621.2874219	-621.183934	-21.2194	110.91
10	g2		-621.2856563	-621.182387	-21.0911	107.85
20	g3		-621.2826379	-621.179555	-21.1168	104.78
30	g4		-621.2785828	-621.175983	-21.3561	100
40	g5		-621.2739673	-621.171631	-21.6164	91.13
50	g6		-621.2712318	-621.169082	-21.8159	87.11
60	g7		-621.2669776	-621.164693	-24.494	87.35
70	g8		-621.2697301	-621.16723	-24.3621	90.9
80	g9		-621.274004	-621.171144	-24.1251	92.95
90	g10		-621.2764486	-621.173342	-23.8945	93.95
100	g11		-621.2770593	-621.173829	-23.6913	93.71
110	g12		-621.2757732	-621.17254	-23.9828	92.17

		E	G	solv	freq
120	g13	-621.2726144	-621.169489	-24.393	90.31
	ts	-621.2481086	-621.149922	-23.0113	-1038.91
		-621.2511303	-621.152307	-22.2566	-940.13
		-621.2533723	-621.154112	-21.8617	-839.1
		-621.2546829	-621.15508	-21.7787	-729.52
		-621.2553682	-621.15568	-22.3107	-618.15
		-621.2563339	-621.15629	-22.8417	-471.63
		-621.2592057	-621.15862	-22.6097	-385.52
		-621.2635017	-621.162688	-22.1925	-428.85
		-621.2671926	-621.166284	-21.8796	-478.93
		-621.2695764	-621.168609	-21.8104	-516.85
		-621.2703932	-621.169424	-21.8166	-542.25
		-621.269466	-621.168577	-22.064	-556.66
		-621.2668354	-621.166101	-22.7116	-562.63
	p	-621.3551147	-621.257365	-24.0096	37.44
		-621.3663357	-621.26829	-23.2028	41.42
		-621.376397	-621.277742	-23.2616	44.24
		-621.3854759	-621.286771	-23.1603	45.59
		-621.3931551	-621.294329	-22.7402	43.13
		-621.3999314	-621.300587	-21.8197	46.45
		-621.4050923	-621.305156	-21.398	47.87
		-621.4098242	-621.309859	-20.9039	49.4
		-621.412526	-621.312361	-20.6202	50.57
		-621.4135767	-621.313344	-20.2792	51.05
		-621.4127711	-621.312589	-20.2553	50.94
		-621.4098263	-621.31019	-19.6851	46.93
		-621.4057218	-621.306899	-21.3861	25.08
IBX+MeOH-HOH		-621.2867906	-621.185034	-21.3636	

Ligand exchange steps

			E	G	solv	freq
proton transfer	h1	sm	-774.5899275	-774.429639	-66.1373	48.79
		ts	-774.5786479	-774.418506	-67.163	-192.74
		p	-774.5877382	-774.426675	-63.2738	52.12
rotation	h2	sm	-698.1055076	-697.970094	-66.5749	59.58
		ts	-698.0939565	-697.960158	-63.7363	36.04*
		p	-698.1121309	-697.975429	-64.9868	81.93

* numerical frequency calculation gives a lowest λ of -50 cm^{-1}; perturbing the stationary point along this eigenvector and optimizing led to the desired reactant and product structures.

Reference structures

		E	G	solv	freq
IBX	i1	-581.9711037	-581.894567	-24.307	126.76
water	i2	-76.44554562	-76.440931	-9.461	1634.9
methanol	j1	-115.7612328	-115.731399	-6.5492	394.36
ethanol	j2	-155.1007007	-155.044166	-6.185	314.84
isopropanol	j3	-194.4399507	-194.357057	-6.4347	279.72
isobutyl alcohol	j4	-233.7691532	-233.658848	-5.9077	185.71
neopentyl alcohol	j5	-273.1046289	-272.967863	-6.0326	191

2,4-dimethyl-3-pentanol	j6	-351.7733273	-351.581999	-5.7848	137.67
benzyl alcohol	j7	-346.9038395	-346.797903	-8.7727	159.5
tert-butyl alcohol	j8	-233.7779188	-233.668821	-6.4871	261.92
tert-pentyl alcohol	j9	-273.1103043	-272.973819	-5.8377	169.32

Plotted points in figures

Figure 1. Alcohol oxidation rates estimated from hypervalent twisting barriers show good correlation with experimentally measured rates. We predict that *ortho*-methyl IBX accelerates the twisting rate by a factor of 100, to the point that ligand exchange becomes the rate-limiting step of the overall oxidation.

| | log (k_{alc}/k_{MeOH}) | | |
| | IBX | | o-Me-IBX |
	measured	predicted	predicted
ethanol	0.07	-0.58	1.87
isopropanol	-0.08	-0.04	3.47
isobutyl alcohol	0.18	0.45	2.25
neopentyl alcohol	0.26	-0.08	2.48
2,4-dimethyl-3-pentanol	0.56	0.30	3.23
benzyl alcohol	1.59	0.80	3.58

Figure 5. The alcohol-IBX intermediate **2** (blue curve) twists so that a stable, planar form of IBA **4** can be eliminated to form the oxidation product **5** (red curve). Note that the intermediate must past through ‡(twist) to access ‡(elim), shown as a dotted blue line. Relative energies are in kcal/mol.

angle	sm	ts	p
0	0.83	20.39	-48.03
10	1.93	19.64	-54.08
20	3.68	18.91	-60.07
30	5.69	18.38	-65.64
40	8.16	17.47	-69.96
50	9.56	16.56	-72.97
60	9.63	15.33	-75.41
70	8.17	13.19	-77.87
80	5.95	11.25	-79.16
90	4.81	9.86	-79.43
100	4.70	9.34	-78.93
110	5.22	9.63	-76.86
120	6.73	10.53	-76.49

Figure S2. Correlation of measured equilibrium constants with computed free energy differences suggests that a thermodynamic mixture of **1** and **2** is present.

	expt(K_{eq})	dG (kcal/mol)
methanol	0.04	0.60
ethanol	0.05	0.68
isopropanol	0.037	1.69
isobutyl alcohol	0.047	1.15
neopentyl alcohol	0.035	1.53
2,4-dimethyl-3-pentanol	0.017	3.16
benzyl alcohol	0.027	4.04
tert-butyl alcohol	0.002	4.35
tert-pentyl alcohol	0.002	4.53

Figure S3. Rapid screening for optimal *ortho* substituent, evaluating twisting and ligand exchange thermodynamics (dE only, gas phase, B3LYP/LACVP**). Methyl, ethyl, and isopropyl provide the best balance of good twisting and ligand exchange thermodynamics.

	dE (kcal/mol)	
	twisting	ligand exchange
H	-4.64	0.25
Me	-2.42	0.85
F	-6.13	-0.11
Cl	-3.77	0.52
Ph	-3.89	3.67
Et	-1.95	0.91
i-Pr	-2.62	0.05
t-Bu	-0.20	2.02
B(OH)$_2$	-3.94	3.94
B(OMe)$_2$	-3.94	1.31

Coordinates of structures

a1-9(sm, ts, p)

a1_sm
```
C   0.000000   0.000000   0.000000
C   1.373040   0.000000   0.000000
I   2.182750   1.939070   0.000000
O   2.220010   2.585120  -1.699350
O   4.017720   1.119390  -0.084010
C   4.641110   0.945970  -1.338050
H   4.474210   1.796500  -1.992950
H   4.278480   0.050250  -1.843110
H   5.703760   0.839160  -1.140310
O   0.091240   2.323940   0.169990
C  -0.725470   1.310450   0.082540
O  -1.917090   1.371260   0.101370
C  -0.653640  -1.217410  -0.029640
C   0.086920  -2.384710  -0.056490
C   1.472860  -2.346710  -0.042660
C   2.145220  -1.136220  -0.013260
H  -1.731420  -1.219410  -0.026440
H  -0.418180  -3.336780  -0.081350
H   2.038400  -3.264320  -0.052620
H   3.219090  -1.074570   0.014360
```
a2_sm
```
I   0.000000   0.000000   0.000000
O   1.818190   0.000000   0.000000
O  -0.190870   1.999900   0.000000
C   0.921610   2.840170   0.265760
C   1.024010   3.875850  -0.822600
C  -0.685480  -0.020310   1.985340
C  -0.721140  -1.283780   2.521780
C  -1.124480  -1.424340   3.836100
C  -1.476670  -0.301260   4.561650
C  -1.036190   1.118700   2.668000
C  -1.438310   0.958420   3.983500
O  -0.069430  -2.089610   0.433590
C  -0.363270  -2.451950   1.651210
O  -0.392320  -3.573330   2.058520
H   1.834500   2.249850   0.325430
H   0.765320   3.316310   1.234930
H   1.832640   4.570620  -0.604900
H   0.098690   4.439230  -0.903580
H   1.225100   3.405420  -1.780910
H  -1.155050  -2.415570   4.258190
H  -1.790420  -0.405410   5.587770
H  -1.010130   2.080450   2.186430
H  -1.724590   1.824880   4.557300
```
a3_sm
```
I   0.000000   0.000000   0.000000
O   1.821490   0.000000   0.000000
O  -0.209250   1.994980   0.000000
C   0.923450   2.854190   0.134460
C   0.387840   4.169100   0.651430
C   1.629160   3.005360  -1.193550
C  -0.661280  -0.027990   1.995950
C  -0.679410  -1.293860   2.528500
C  -1.062970  -1.440840   3.848010
C  -1.413280  -0.322980   4.582590
C  -1.009070   1.105490   2.687810
C  -1.391290   0.938640   4.008560
O  -0.049210  -2.091260   0.431440
C  -0.323460  -2.457930   1.651790
O  -0.337310  -3.580030   2.058420
H   1.618990   2.423210   0.854990
H   1.195850   4.889940   0.750410
H  -0.082680   4.053750   1.623860
H  -0.349310   4.567760  -0.040630
H   2.449210   3.714620  -1.108530
H   0.933570   3.371790  -1.945460
H   2.043580   2.054890  -1.514730
```

H -1.079820 -2.433670   4.267090
H -1.712260 -0.433230   5.612460
H -0.992820   2.067880   2.207650
H -1.674800   1.801520   4.589040
a4_sm
```
I   0.000000   0.000000   0.000000
O   1.819190   0.000000   0.000000
O  -0.207530   1.999140   0.000000
C   0.927110   2.842240   0.114000
C   1.167520   3.599180  -1.178240
C   0.016040   4.539020  -1.490030
C   1.441280   2.647940  -2.330980
C  -0.655240  -0.007100   1.995120
C  -0.693980  -1.268970   2.535320
C  -1.077020  -1.401350   3.856530
C  -1.405610  -0.272570   4.584370
C  -0.979780   1.138020   2.680120
C  -1.361300   0.985180   4.002750
O  -0.071530  -2.088920   0.443380
C  -0.355230  -2.443430   1.665660
O  -0.387010  -3.562730   2.078710
H   1.808400   2.255600   0.370650
H   0.726420   3.541310   0.926970
H   2.066360   4.195590  -1.005230
H   0.194290   5.085090  -2.413540
H  -0.127490   5.267700  -0.694310
H  -0.909510   3.978930  -1.601320
H   2.219830   1.931040  -2.080750
H   1.749660   3.192560  -3.219930
H   0.539170   2.095270  -2.591440
H  -1.109790  -2.390900   4.282330
H  -1.704010  -0.370870   5.615600
H  -0.946230   2.097980   2.195420
H  -1.626790   1.856510   4.579110
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a5_sm
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I   0.000000   0.000000   0.000000
O   1.819330   0.000000   0.000000
O  -0.209260   1.999890   0.000000
C   0.924660   2.839750   0.110260
C   1.175780   3.608320  -1.180570
C   2.430870   4.445930  -0.972460
C  -0.012670   4.511090  -1.479840
C   1.391570   2.630300  -2.327850
C  -0.651900  -0.007790   1.996430
C  -0.691970  -1.270900   2.534920
C  -1.073130  -1.404320   3.856580
C  -1.397660  -0.275950   4.586830
C  -0.972190   1.136930   2.684090
C  -1.351340   0.982690   4.007260
O  -0.071940  -2.089860   0.441750
C  -0.355620  -2.445280   1.663930
O  -0.389040  -3.565040   2.075520
H   1.807460   2.252230   0.362370
H   0.730280   3.540750   0.924060
H   3.299680   3.816540  -0.788780
H   2.319180   5.122400  -0.126180
H   2.636710   5.050950  -1.852790
H   0.131560   5.042780  -2.418430
H  -0.147480   5.253140  -0.694060
H  -0.927500   3.929000  -1.553980
H   2.178350   1.915740  -2.094360
H   1.669480   3.160410  -3.236340
H   0.477960   2.078860  -2.543360
H  -1.107350  -2.394440   4.280900
H  -1.694200  -0.375240   5.618470
H  -0.937320   2.097850   2.201320
H  -1.613170   1.853710   4.585710
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a6_sm
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I   0.000000   0.000000   0.000000
O   1.819420   0.000000   0.000000
O  -0.184420   1.999220   0.000000
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C   0.798770   2.809450 -0.639650
C   0.227740   3.308370 -1.964830
C -0.987640   4.200830 -1.780610
C -0.099910   2.134470 -2.874200
C   1.233110   3.884750   0.351570
C   2.155410   4.907190 -0.295640
C   1.919820   3.252340   1.551450
C -0.768410   0.065010   1.956300
C -0.855700 -1.181590   2.527690
C -1.346290 -1.276140   3.816340
C -1.733310 -0.128640   4.482550
C -1.148840   1.228770   2.580960
C -1.639050   1.111580   3.870750
O -0.068370 -2.072630   0.523250
C -0.449680 -2.384740   1.729330
O -0.514900 -3.489090   2.177960
H   1.677860   2.195690 -0.852520
H   1.017530   3.882670 -2.449200
H -1.395870   4.498430 -2.743940
H -0.749620   5.107940 -1.230800
H -1.764790   3.671320 -1.234420
H   0.747300   1.456240 -2.973600
H -0.363250   2.475410 -3.872230
H -0.954220   1.575120 -2.495600
H   0.332250   4.396230   0.695080
H   3.024630   4.420960 -0.737520
H   2.519730   5.608330   0.451330
H   1.661520   5.484230 -1.072480
H   2.832100   2.742260   1.247890
H   1.286900   2.518910   2.039490
H   2.184720   4.009510   2.286180
H -1.414310 -2.253710   4.264920
H -2.115920 -0.198310   5.487990
H -1.064070   2.174900   2.076840
H -1.948170   1.999450   4.398050
a7_sm
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C   0.000000   0.000000   0.000000
C   1.374680   0.000000   0.000000
I   2.174580   1.944350   0.000000
O   2.297450   2.525270  -1.723000
O   3.986050   1.046570   0.034340
C   4.995250   1.628930  -0.773120
O   0.069410   2.332050   0.063830
C  -0.736350   1.307820   0.029890
O  -1.929390   1.357150   0.043930
C  -0.651330  -1.219810  -0.024330
C   0.089870  -2.387190  -0.049440
C   1.475890  -2.346900  -0.051620
C   2.148660  -1.135860  -0.026810
H  -1.729290  -1.221060  -0.025590
H  -0.414920  -3.340090  -0.070300
H   2.043190  -3.263760  -0.073910
H   3.222030  -1.067690  -0.029630
H   4.642780   1.738120  -1.795740
H   5.812400   0.911160  -0.757670
C   5.438340   2.955400  -0.230040
C   5.046230   4.135950  -0.845320
C   5.421530   5.360170  -0.315200
C   6.190360   5.412370   0.833370
C   6.583820   4.237900   1.454970
C   6.208930   3.018670   0.926260
H   6.513990   2.103400   1.411010
H   7.186900   4.276190   2.349460
H   6.484840   6.364920   1.245130
H   5.111780   6.271430  -0.801570
H   4.431570   4.089070  -1.732360
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a8_sm
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I   0.000000   0.000000   0.000000
O   1.821550   0.000000   0.000000
O  -0.305390   1.980600   0.000000
C   0.680820   3.009080  -0.188370
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C   1.666990   3.026150   0.965570
C  -0.150260   4.277920  -0.208550
C   1.389410   2.816600  -1.517630
C  -0.692460  -0.025170   1.987410
C  -0.713700  -1.291130   2.520160
C  -1.125460  -1.439430   3.831230
C  -1.501030  -0.324110   4.556450
C  -1.065340   1.106430   2.669690
C  -1.475550   0.937000   3.981500
O  -0.022330  -2.089550   0.443600
C  -0.326430  -2.454830   1.656610
O  -0.342220  -3.575830   2.066770
H   2.375470   3.841450   0.837860
H   2.221120   2.093820   1.009630
H   1.150150   3.179040   1.910230
H   0.490070   5.144700  -0.355960
H  -0.683430   4.398880   0.730540
H  -0.878300   4.238170  -1.013330
H   2.044090   3.660290  -1.721570
H   0.660130   2.753140  -2.322490
H   1.996410   1.915610  -1.505480
H  -1.143150  -2.432100   4.250620
H  -1.822030  -0.435780   5.579510
H  -1.043090   2.067710   2.188230
H  -1.778270   1.798430   4.554470
a9_sm
I   0.000000   0.000000   0.000000
O   1.821120   0.000000   0.000000
O  -0.309350   1.979870   0.000000
C   0.657060   3.007130  -0.268630
C   1.344050   2.754770  -1.600010
C   1.673620   3.077830   0.857030
C  -0.178000   4.285560  -0.293280
C  -1.257490   4.341580  -1.355070
C  -0.672880  -0.013110   1.993810
C  -0.701830  -1.278070   2.529030
C  -1.095040  -1.418810   3.846660
C  -1.443470  -0.297440   4.575940
C  -1.017520   1.124810   2.680550
C  -1.408270   0.962530   3.999180
O  -0.033440  -2.088120   0.449200
C  -0.334470  -2.447730   1.664770
O  -0.359860  -3.567760   2.077020
H   1.952870   3.612080  -1.877290
H   0.612180   2.592560  -2.387080
H   1.994980   1.887440  -1.533910
H   2.383610   3.880600   0.671210
H   2.222990   2.144690   0.933040
H   1.181370   3.279890   1.805780
H   0.510310   5.122920  -0.411370
H  -0.632240   4.394300   0.690910
H  -0.841530   4.351980  -2.359240
H  -1.853330   5.243820  -1.242340
H  -1.921850   3.486720  -1.270950
H  -1.118390  -2.410400   4.268240
H  -1.748930  -0.403280   5.604320
H  -0.986510   2.085300   2.198120
H  -1.687440   1.829050   4.576340
a1_ts
I   0.000000   0.000000   0.000000
O   1.813370   0.000000   0.000000
O  -0.399370   1.972210   0.000000
H  -0.339120   3.702250  -0.992740
C  -0.119210   2.659770  -1.199250
H   0.929450   2.572480  -1.478870
H  -0.753900   2.326970  -2.020340
C  -0.209400   0.095460   2.073920
O  -1.859470  -1.271810   0.466960
C  -2.257130  -1.279130   1.687630
C  -1.316840  -0.518580   2.597400
O  -3.233930  -1.804920   2.146310
C  -1.484130  -0.455390   3.969050
C  -0.546980   0.203140   4.743920
C   0.570680   0.792080   4.169470
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C   0.760290   0.743010   2.800340
H   1.625860   1.165080   2.317620
H   1.300560   1.288130   4.788150
H  -0.678470   0.249030   5.813120
H  -2.347630  -0.938550   4.396030
a2_ts
C   0.000000   0.000000   0.000000
C   1.370350   0.000000   0.000000
I   2.286350   1.875970   0.000000
O   3.683980   1.388150  -1.042090
O   2.935060   1.415910   1.846800
C   3.344630   2.504480   2.657080
O   0.039670   2.319040  -0.159300
C  -0.751930   1.309900  -0.073590
O  -1.951980   1.313060  -0.054470
C  -0.632790  -1.230120   0.006160
C   0.121990  -2.388720   0.005800
C   1.508450  -2.338630  -0.016410
C   2.164370  -1.120760  -0.024170
H  -1.710350  -1.244850  -0.001120
H  -0.373200  -3.346470   0.007990
H   2.083740  -3.249850  -0.033470
H   3.237570  -1.041350  -0.067970
H   3.951710   3.209870   2.085220
H   4.001660   2.056720   3.398520
C   2.173300   3.191180   3.310310
H   1.511530   3.642880   2.573040
H   1.593190   2.477370   3.887180
H   2.516040   3.979630   3.975850
a3_ts
C   0.000000   0.000000   0.000000
C   1.370440   0.000000   0.000000
I   2.289620   1.875440   0.000000
O   3.685510   1.390350  -1.046040
O   2.949580   1.416240   1.836370
C   3.345600   2.512710   2.660050
O   0.036040   2.318700  -0.164990
C  -0.753690   1.309490  -0.074820
O  -1.954050   1.309680  -0.052660
C  -0.632610  -1.230330   0.006610
C   0.121840  -2.389010   0.006070
C   1.508300  -2.339000  -0.016170
C   2.164100  -1.121100  -0.023680
H  -1.710210  -1.244730  -0.000770
H  -0.373510  -3.346700   0.007940
H   2.083600  -3.250230  -0.033340
H   3.237380  -1.041990  -0.067300
H   3.925880   3.224090   2.065280
C   4.247000   1.908090   3.708250
C   2.131320   3.198760   3.241030
H   5.097660   1.423290   3.241160
H   4.606450   2.679130   4.385360
H   3.698760   1.166900   4.283140
H   1.482580   3.599440   2.463860
H   2.426810   4.024880   3.882670
H   1.551450   2.490970   3.827400
a4_ts
I   0.000000   0.000000   0.000000
O   1.813020   0.000000   0.000000
O  -0.419970   1.962100   0.000000
C  -0.250040   2.639660  -1.232720
C  -0.520230   4.109900  -0.982320
C  -0.503050   4.856560  -2.306220
C   0.472300   4.693720   0.006130
C  -0.203390   0.089430   2.076090
C  -1.295970  -0.546610   2.604100
C  -1.457320  -0.489710   3.976860
C  -0.528480   0.183640   4.748840
C   0.759200   0.750630   2.799860
C   0.575920   0.793050   4.170200
O  -1.829530  -1.317310   0.477470
C  -2.224280  -1.327170   1.698610
O  -3.190530  -1.868830   2.161900
H  -1.241190   4.463050  -3.001730
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H  -0.722320   5.909460  -2.150310
H   0.475520   4.790940  -2.779730
H   0.449200   4.153410   0.947180
H   0.242610   5.737570   0.206680
H   1.486380   4.645660  -0.390140
H  -1.520480   4.175020  -0.553900
H   0.769670   2.508990  -1.602600
H  -0.949270   2.253400  -1.976970
H  -0.654970   0.224040   5.818870
H  -2.309510  -0.990650   4.406880
H   1.301330   1.298620   4.786510
H   1.617190   1.185410   2.314730
a5_ts
I   0.000000   0.000000   0.000000
O   1.812590   0.000000   0.000000
O  -0.424060   1.959500   0.000000
C  -0.311640   2.631860  -1.241180
C  -0.577160   4.114030  -1.005590
C  -0.203970   0.097760   2.075690
O  -1.832100  -1.310570   0.481150
C  -2.233420  -1.306750   1.700310
C  -1.302880  -0.526990   2.604160
O  -3.207050  -1.835780   2.162450
C  -1.470030  -0.457640   3.975650
C  -0.539750   0.215480   4.746190
C   0.571490   0.812210   4.167500
C   0.760190   0.757930   2.798230
C  -1.978400   4.302780  -0.440700
C  -0.461330   4.808770  -2.357170
C   0.459610   4.675260  -0.041950
H   0.692000   2.504080  -1.651630
H  -1.041040   2.238290  -1.953020
H   0.401740   4.179060   0.922190
H   1.297650   1.317760   4.782910
H  -0.670780   0.265760   5.815260
H  -2.327510  -0.948480   4.405970
H   0.292890   5.739250   0.111540
H   1.468450   4.547250  -0.430990
H   1.622380   1.184080   2.312870
H  -2.088030   3.787350   0.508780
H  -2.733300   3.918130  -1.124560
H  -2.181070   5.359650  -0.281540
H  -1.191200   4.423740  -3.067250
H  -0.640600   5.875510  -2.244690
H   0.530960   4.682870  -2.786860
a6_ts
I   0.000000   0.000000   0.000000
O   1.810830   0.000000   0.000000
O  -0.414830   1.946820   0.000000
H  -0.530290   1.901320  -2.071910
C  -0.716640   2.593300  -1.240790
C   0.265340   3.752310  -1.380160
C  -0.179060   0.075130   2.080770
O  -1.831420  -1.314940   0.495480
C  -2.196530  -1.351930   1.725410
C  -1.260640  -0.570530   2.620980
O  -3.142840  -1.917510   2.201390
C  -1.403650  -0.525510   3.996170
C  -0.469680   0.148760   4.761010
C   0.623350   0.767510   4.171500
C   0.790040   0.733720   2.798650
H   1.641950   1.174430   2.308770
H   1.354350   1.273090   4.781210
H  -0.582260   0.180940   5.832870
H  -2.245510  -1.036950   4.433340
H   0.198090   4.332930  -0.460010
C   1.686510   3.233300  -1.518620
C  -0.088120   4.651630  -2.555490
H  -2.390930   3.435610  -2.206460
C  -3.051530   1.685440  -1.208790
C  -2.573770   3.894100  -0.127070
H   1.961570   2.564010  -0.709400
H   1.808810   2.689870  -2.455840
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H   2.394250   4.058480  -1.526500
H  -0.136630   4.082920  -3.483850
H   0.676460   5.413870  -2.681600
H  -1.038840   5.159480  -2.421950
H  -2.958600   1.166210  -0.258320
H  -2.784630   0.987350  -2.001520
H  -4.102720   1.930320  -1.334900
H  -2.334010   3.453600   0.837310
H  -2.052350   4.845030  -0.202360
H  -3.640890   4.100910  -0.145940
a7_ts
C   0.000000   0.000000   0.000000
C   1.370550   0.000000   0.000000
I   2.301800   1.869300   0.000000
O   3.732240   1.359380  -0.996910
O   2.963770   1.380240   1.844570
C   4.147450   2.059330   2.222010
O   0.028510   2.317880  -0.154540
C  -0.756990   1.310030  -0.067790
O  -1.958380   1.300530  -0.044440
C  -0.632730  -1.230150   0.004090
C   0.120030  -2.389320  -0.002680
C   1.506800  -2.340440  -0.026830
C   2.161960  -1.123340  -0.027280
H  -1.710220  -1.242230   0.000430
H  -0.376260  -3.346320  -0.002700
H   2.081390  -3.251940  -0.048900
H   3.235280  -1.044580  -0.070240
H   4.990120   1.708760   1.628120
H   4.304030   1.751650   3.254240
C   4.009480   3.547140   2.105840
C   4.917240   4.287490   1.363620
C   4.768410   5.658270   1.241770
C   3.706050   6.295130   1.854590
C   2.792300   5.562010   2.594410
C   2.945000   4.196600   2.722880
H   2.232150   3.621870   3.294250
H   1.960820   6.056520   3.070200
H   3.584850   7.361600   1.753700
H   5.476690   6.225260   0.659630
H   5.735850   3.786820   0.869540
a8_ts
C   0.000000   0.000000   0.000000
C   1.370200   0.000000   0.000000
I   2.294370   1.873180   0.000000
O   3.676280   1.397510  -1.071480
O   2.972990   1.364130   1.815560
C   3.487750   2.381920   2.686210
O   0.027780   2.319550  -0.152830
C  -0.757350   1.309150  -0.062870
O  -1.958180   1.302520  -0.030640
C  -0.632030  -1.230950   0.004850
C   0.121980  -2.389690   0.000760
C   1.508480  -2.339460  -0.022340
C   2.163690  -1.121480  -0.027500
H  -1.709650  -1.244680   0.000180
H  -0.373410  -3.347400   0.001390
H   2.083990  -3.250560  -0.041970
H   3.236870  -1.042580  -0.071040
C   2.367980   3.317310   3.101590
C   4.630120   3.126560   2.020620
C   3.986980   1.573220   3.868280
H   1.548050   2.753230   3.536370
H   1.979160   3.882240   2.255160
H   2.722490   4.037380   3.834320
H   4.285450   3.743680   1.190650
H   5.367820   2.426760   1.639450
H   5.111350   3.793530   2.730700
H   3.172590   0.998150   4.297280
H   4.763840   0.885710   3.549110
H   4.391230   2.235110   4.630540
a9_ts
C   0.000000   0.000000   0.000000
C   1.370100   0.000000   0.000000
```

```
I   2.294900   1.872790   0.000000
O   3.678520   1.393880  -1.067890
O   2.952340   1.364930   1.821330
C   3.520070   2.363460   2.680470
O   0.028550   2.319160  -0.160360
C  -0.756840   1.309200  -0.069890
O  -1.957830   1.302520  -0.042810
C  -0.632080  -1.230890   0.007440
C   0.121910  -2.389720   0.006410
C   1.508380  -2.339670  -0.017220
C   2.163600  -1.121660  -0.025080
H  -1.709630  -1.244680   0.001880
H  -0.373450  -3.347430   0.009220
H   2.083830  -3.250890  -0.035270
H   3.236760  -1.042750  -0.069300
C   4.758790   2.959660   2.038890
C   2.490280   3.433330   2.994960
C   3.912510   1.559060   3.918420
C   2.767780   0.877120   4.640060
H   4.515270   3.537970   1.147710
H   5.450820   2.174630   1.749400
H   5.257570   3.633700   2.730140
H   1.560130   2.990640   3.336160
H   2.271740   4.044890   2.120470
H   2.861250   4.102380   3.767060
H   4.636370   0.813600   3.595350
H   4.435680   2.237030   4.593140
H   3.151280   0.261580   5.449400
H   2.075270   1.591740   5.077310
H   2.213220   0.235270   3.962590
a1_p
C   0.000000   0.000000   0.000000
C   1.370690   0.000000   0.000000
I   2.244000   1.896680   0.000000
O   3.931180   1.261910   0.282160
O   1.894040   2.426660   1.904660
C   2.860340   1.978030   2.821960
H   3.798380   1.711530   2.323120
H   2.484880   1.106260   3.352100
H   3.044350   2.798720   3.508660
O   0.069420   2.324970  -0.050900
C  -0.734700   1.317730  -0.024690
O  -1.932680   1.343090  -0.036920
C  -0.635650  -1.226720   0.030520
C   0.121160  -2.385110   0.061260
C   1.508200  -2.336440   0.065030
C   2.165960  -1.118320   0.032390
H  -1.713380  -1.242220   0.034030
H  -0.374010  -3.342660   0.085880
H   2.081180  -3.248950   0.093430
H   3.240520  -1.023510   0.043640
a2_p
I   0.000000   0.000000   0.000000
O   1.824010   0.000000   0.000000
O  -0.242650   1.974380   0.000000
C   0.907870   2.718820   0.364310
C   0.760380   4.070490  -0.283500
C  -0.149550  -0.389660   2.046920
C  -1.418460  -0.307600   2.559180
C  -1.571630  -0.530600   3.914320
C  -0.460620  -0.820540   4.687220
C   0.983380  -0.670270   2.769700
C   0.806770  -0.888800   4.125590
O  -2.182040   0.176480   0.415980
C  -2.566580   0.020420   1.634430
O  -3.684170   0.091300   2.062830
H   1.812830   2.207910   0.030750
H   0.946960   2.796260   1.450730
H   1.601330   4.700190  -0.002680
H  -0.156970   4.552700   0.038580
H   0.740210   3.975780  -1.364630
H  -2.563410  -0.467250   4.331720
H  -0.580040  -0.995370   5.744660
H   1.945940  -0.700310   2.282990
```

```
H   1.661030  -1.112520   4.743730
a3_p
I   0.000000   0.000000   0.000000
O   1.825990   0.000000   0.000000
O  -0.235510   1.977280   0.000000
C   0.946590   2.742530   0.224220
C   0.967320   3.197840   1.664800
C   0.902830   3.873470  -0.776480
C  -0.143220  -0.456410   2.033950
C  -1.408660  -0.377210   2.554020
C  -1.561370  -0.650960   3.900130
C  -0.452660  -0.988210   4.656530
C   0.987310  -0.785080   2.740340
C   0.811610  -1.054060   4.087090
O  -2.171580   0.200090   0.433840
C  -2.553710   0.003600   1.647820
O  -3.669010   0.075650   2.081550
H   1.818600   2.109330   0.032150
H   1.845620   3.810660   1.853280
H   0.999560   2.348820   2.342030
H   0.078850   3.782240   1.888830
H   1.776340   4.509370  -0.654990
H   0.010920   4.476020  -0.628310
H   0.893580   3.487380  -1.790990
H  -2.550730  -0.588960   4.323320
H  -0.570950  -1.201990   5.706800
H   1.947970  -0.809870   2.249790
H   1.664210  -1.316340   4.692200
a4_p
I   0.000000   0.000000   0.000000
O   1.826760   0.000000   0.000000
O  -0.233820   1.989100   0.000000
C   0.955380   2.735480  -0.154230
C   1.024280   3.377140  -1.525960
C  -0.108950   4.367820  -1.727160
C   1.052150   2.325540  -2.623200
C  -0.145540  -0.340120   2.052200
C  -1.412630  -0.229250   2.563200
C  -1.568540  -0.418380   3.923090
C  -0.461510  -0.706790   4.701910
C   0.983460  -0.620620   2.780730
C   0.804300  -0.804690   4.141330
O  -2.166420   0.230280   0.410790
C  -2.554200   0.099590   1.633210
O  -3.671990   0.194300   2.054930
H   1.826740   2.091780   0.011930
H   0.931290   3.481650   0.639090
H   1.972590   3.918510  -1.548730
H  -0.054580   4.831040  -2.709510
H  -0.077770   5.160280  -0.982190
H  -1.070240   3.866980  -1.639470
H   1.826550   1.582210  -2.443980
H   1.239970   2.780920  -3.591970
H   0.089670   1.819350  -2.695700
H  -2.558980  -0.330070   4.339320
H  -0.582350  -0.854800   5.763110
H   1.945680  -0.674550   2.296060
H   1.655940  -1.025390   4.764030
a5_p
I   0.000000   0.000000   0.000000
O   1.826760   0.000000   0.000000
O  -0.232890   1.990660   0.000000
C   0.955350   2.732270  -0.156980
C   1.036070   3.388760  -1.528060
C   2.355760   4.146620  -1.588480
C  -0.131870   4.348340  -1.706210
C   1.004410   2.319050  -2.612390
C  -0.144950  -0.339710   2.052410
C  -1.412690  -0.229410   2.563410
C  -1.567930  -0.419070   3.923250
C  -0.460600  -0.707430   4.701930
C   0.984190  -0.620380   2.780740
C   0.805200  -0.804860   4.141270
O  -2.166650   0.230120   0.411150
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C -2.554080  0.099110  1.633670
O -3.671780  0.193340  2.055770
H  1.827390  2.086110  0.001820
H  0.940460  3.477880  0.638280
H  3.204780  3.471660 -1.496310
H  2.423350  4.885260 -0.791210
H  2.448790  4.674860 -2.534830
H -0.109260  4.805020 -2.693760
H -0.095200  5.147730 -0.967910
H -1.079310  3.828570 -1.590180
H  1.779370  1.571060 -2.451720
H  1.164420  2.763610 -3.592010
H  0.034930  1.823790 -2.645040
H -2.558230 -0.331320  4.339550
H -0.581350 -0.855910  5.763070
H  1.946340 -0.674260  2.295980
H  1.656940 -1.025650  4.763800
a6_p
I  0.000000  0.000000  0.000000
O  1.826870  0.000000  0.000000
O -0.244020  1.981090  0.000000
C  0.923630  2.753940 -0.242250
C  0.878230  3.272870 -1.677240
C -0.289480  4.214150 -1.918970
C  0.852040  2.114790 -2.663670
C  0.984320  3.806130  0.864630
C  2.149870  4.758270  0.643400
C  1.086730  3.144760  2.228120
C -0.147770 -0.392400  2.042230
C -1.415450 -0.299250  2.556270
C -1.572000 -0.530710  3.909760
C -0.465160 -0.843030  4.679720
C  0.980430 -0.697260  2.762830
C  0.800800 -0.924490  4.116580
O -2.171430  0.224640  0.419720
C -2.558080  0.056550  1.636780
O -3.675490  0.137970  2.063680
H  1.802460  2.104460 -0.137180
H  1.811000  3.813620 -1.837600
H -0.324940  4.518660 -2.962480
H -0.220530  5.116430 -1.316660
H -1.228680  3.720980 -1.678910
H  1.635010  1.388830 -2.450530
H  0.997720  2.472300 -3.679680
H -0.115170  1.612100 -2.647260
H  0.055660  4.375200  0.830990
H  3.092630  4.214950  0.588430
H  2.221090  5.456820  1.473540
H  2.043970  5.342350 -0.266330
H  1.991370  2.541490  2.298510
H  0.232890  2.504520  2.424910
H  1.125640  3.895620  3.013590
H -2.562610 -0.456200  4.327900
H -0.586450 -1.023860  5.735800
H  1.942900 -0.735310  2.277120
H  1.652050 -1.165110  4.732420
a7_p
C  0.000000  0.000000  0.000000
C  1.370150  0.000000  0.000000
I  2.248160  1.893040  0.000000
O  3.936220  1.242450  0.262440
O  1.881500  2.370590  1.907700
C  3.064470  2.562210  2.662270
O  0.068500  2.324040 -0.020740
C -0.734940  1.317340 -0.010240
O -1.933490  1.342270 -0.023110
C -0.634920 -1.227230  0.021970
C  0.122390 -2.385430  0.044220
C  1.509350 -2.335870  0.049100
C  2.166340 -1.117290  0.024540
H -1.712600 -1.243040  0.026080
H -0.372210 -3.343410  0.061890
H  2.083120 -3.248030  0.072200
H  3.240590 -1.019550  0.038240
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H  3.789890  1.780680  2.439890
H  2.718460  2.438760  3.686720
C  3.658700  3.914370  2.429610
C  4.897780  4.042150  1.819180
C  5.437000  5.296660  1.589750
C  4.737780  6.428680  1.962740
C  3.495130  6.308140  2.564020
C  2.959260  5.057790  2.796690
H  1.988360  4.961100  3.257880
H  2.946750  7.190610  2.852580
H  5.156860  7.406100  1.783460
H  6.401170  5.387740  1.115510
H  5.424900  3.153520  1.507780
a8_p
I  0.000000  0.000000  0.000000
O  1.827000  0.000000  0.000000
O -0.415650  1.931760  0.000000
C  0.599140  2.961670 -0.020120
C  1.426120  2.883900 -1.289110
C  1.453000  2.900330  1.230760
C -0.279070  4.200760 -0.020870
C -0.141480 -0.403050  2.045750
C -1.412620 -0.368420  2.556870
C -1.557820 -0.600230  3.911700
C -0.438300 -0.855210  4.684300
C  0.999270 -0.653750  2.767170
C  0.830270 -0.883010  4.121930
O -2.201650  0.063430  0.413140
C -2.575240 -0.093300  1.632270
O -3.693090 -0.062670  2.067630
H  2.072050  3.755590 -1.357920
H  0.773750  2.878060 -2.159140
H  2.054110  1.998340 -1.295940
H  2.095200  3.776420  1.277530
H  2.084170  2.017590  1.226650
H  0.821540  2.893570  2.115610
H  0.352340  5.086390 -0.035810
H -0.902220  4.224430  0.867180
H -0.922390  4.209170 -0.894720
H -2.551730 -0.573580  4.327780
H -0.551950 -1.036320  5.741210
H  1.961640 -0.658220  2.279340
H  1.691270 -1.084430  4.738290
a9_p
I  0.000000  0.000000  0.000000
O  1.826200  0.000000  0.000000
O -0.418170  1.929390  0.000000
C  0.556900  2.953310 -0.289070
C  1.224270  2.712760 -1.630150
C  1.569430  3.047150  0.835640
C -0.333380  4.197760 -0.299490
C -1.420140  4.223360 -1.354610
C -0.143460 -0.347820  2.053550
C -1.415370 -0.304930  2.562260
C -1.560150 -0.497220  3.923210
C -0.439520 -0.721910  4.703700
C  0.998600 -0.567350  2.782590
C  0.829780 -0.756720  4.143630
O -2.202900  0.072520  0.407530
C -2.577920 -0.057880  1.629800
O -3.696740 -0.021050  2.061990
H  1.795090  3.592120 -1.917720
H  0.483400  2.525710 -2.402730
H  1.910650  1.872580 -1.575440
H  2.218110  3.905350  0.676230
H  2.185730  2.154900  0.874910
H  1.058540  3.176760  1.786390
H  0.333580  5.052910 -0.415170
H -0.782490  4.278180  0.688130
H -1.012690  4.245710 -2.362240
H -2.033660  5.112310 -1.234130
H -2.066180  3.355980 -1.261490
H -2.554290 -0.463670  4.338190
H -0.552940 -0.872320  5.765430
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H  1.961300 -0.578410  2.295500
H  1.691690 -0.932400  4.766540
```

b1-9(sm, ts, p)

```
b1_sm
C  0.000000  0.000000  0.000000
C  1.380980  0.000000  0.000000
I  2.084170  2.026270  0.000000
O  1.795930  2.709090 -1.663430
O  3.972970  1.502500 -0.413900
C  4.392110  1.437040 -1.757690
H  3.923190  0.609450 -2.290920
H  5.466950  1.282560 -1.731670
H  4.164720  2.352240 -2.295180
O  0.033520  2.290490  0.437510
C -0.756550  1.278650  0.215140
O -1.948680  1.309320  0.235780
C -0.681190 -1.194840 -0.097580
C  0.039070 -2.368380 -0.172840
C  1.417770 -2.339130 -0.113420
C  2.149010 -1.155590 -0.020490
H -1.758240 -1.167100 -0.093370
H -0.470850 -3.314990 -0.250620
H  1.968010 -3.267160 -0.129630
C  3.639100 -1.266320  0.082560
H  3.893510 -2.263560  0.426250
H  4.113320 -1.116850 -0.882890
H  4.068700 -0.539820  0.758910
b2_sm
C  0.000000  0.000000  0.000000
C  1.381470  0.000000  0.000000
I  2.087060  2.029290  0.000000
O  1.887300  2.646860 -1.702890
O  4.006590  1.534590 -0.264580
C  4.568170  1.482510 -1.564930
C  5.171680  2.805120 -1.960350
C  2.148330 -1.157130 -0.029820
C  3.639200 -1.269920  0.019560
C -0.763280  1.281400  0.166100
O  0.019810  2.306590  0.341530
O -1.955910  1.306230  0.182860
C -0.682230 -1.195860 -0.076990
C  0.035580 -2.371370 -0.139920
C  1.414670 -2.341280 -0.101480
H  3.818320  1.185270 -2.296860
H  5.334240  0.709760 -1.520070
H  5.691000  2.710920 -2.911900
H  5.886520  3.135330 -1.211290
H  4.394390  3.555030 -2.071370
H  3.907470 -2.274010  0.330650
H  4.070960 -1.101680 -0.963270
H  4.094190 -0.554450  0.691150
H  1.965440 -3.268840 -0.122480
H -0.475760 -3.318510 -0.200020
H -1.759180 -1.165220 -0.071940
b3_sm
C  0.000000  0.000000  0.000000
C  1.381110  0.000000  0.000000
I  2.095200  2.031960  0.000000
O  2.073570  2.559700 -1.744340
O  4.049590  1.573150  0.043600
C  4.912250  1.781190 -1.073470
C  6.214280  1.097320 -0.720780
C  5.119470  3.256950 -1.338380
C  2.145760 -1.158460 -0.030150
C  3.635380 -1.253460 -0.055050
C -0.773710  1.284150  0.061280
O -0.001740  2.326190  0.138030
O -1.967320  1.297290  0.070290
C -0.681040 -1.199800 -0.030140
C  0.034600 -2.376560 -0.057610
C  1.414600 -2.344440 -0.054220
H  4.470090  1.322900 -1.959190
```

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H   6.931990   1.225620  -1.527630
H   6.078610   0.035360  -0.547670
H   6.627730   1.539610   0.181980
H   5.846770   3.395230  -2.135040
H   5.499190   3.743880  -0.442210
H   4.193080   3.729030  -1.648740
H   3.931250  -2.289890   0.066210
H   4.026060  -0.901320  -1.005330
H   4.098920  -0.655200   0.718790
H   1.966630  -3.271040  -0.074350
H  -0.477480  -3.324920  -0.080130
H  -1.757960  -1.166860  -0.028200
b4_sm
C   0.000000   0.000000   0.000000
C   1.381620   0.000000   0.000000
I   2.091170   2.027810   0.000000
O   1.976000   2.605890  -1.723250
O   4.029230   1.526100  -0.119300
C   4.747830   1.650560  -1.332090
C   5.729120   2.806700  -1.264290
C   6.793780   2.566350  -0.208320
C   5.013870   4.128980  -1.045210
C   2.148430  -1.157900  -0.031040
C   3.639540  -1.268340  -0.016140
C  -0.768560   1.283250   0.118710
O   0.008670   2.317970   0.252940
O  -1.961630   1.303020   0.128900
C  -0.682060  -1.197420  -0.057540
C   0.034820  -2.373500  -0.105340
C   1.414260  -2.342410  -0.082150
H   4.059540   1.795330  -2.163450
H   5.288620   0.715220  -1.481080
H   6.211770   2.836830  -2.244020
H   7.352810   1.654100  -0.408420
H   6.336910   2.469790   0.773950
H   7.502560   3.390470  -0.171470
H   4.202220   4.266960  -1.755410
H   5.702820   4.964390  -1.142540
H   4.598010   4.175720  -0.038760
H   3.917200  -2.290600   0.217370
H   4.051840  -1.026250  -0.991750
H   4.102830  -0.598920   0.696250
H   1.965120  -3.269760  -0.103220
H  -0.476860  -3.321310  -0.149680
H  -1.758970  -1.165550  -0.054560
b5_sm
C   0.000000   0.000000   0.000000
C   1.381690   0.000000   0.000000
I   2.089150   2.028280   0.000000
O   1.936650   2.608130  -1.719870
O   4.026570   1.533030  -0.160350
C   4.709850   1.636810  -1.392180
C   5.704950   2.791840  -1.388690
C   6.353740   2.830740  -2.766500
C   6.762090   2.555640  -0.319350
C   4.978420   4.103430  -1.123440
C   2.148980  -1.156960  -0.035790
C   3.640040  -1.266820  -0.010280
C  -0.767540   1.281930   0.138360
O   0.011160   2.313580   0.289690
O  -1.960480   1.302820   0.150280
C  -0.681480  -1.196910  -0.069750
C   0.036120  -2.372350  -0.128100
C   1.415370  -2.341370  -0.099430
H   3.999660   1.770270  -2.207710
H   5.246920   0.698770  -1.542750
H   6.840670   1.885090  -3.001370
H   7.111000   3.610650  -2.810580
H   5.618880   3.034140  -3.543100
H   7.330130   1.649030  -0.523460
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H   7.463880   3.386540  -0.279080
H   4.149520   4.242900  -1.814070
H   5.659270   4.945670  -1.227460

H   4.587550   4.131590  -0.107260
H   3.916330  -2.283140   0.249530
H   4.057100  -1.049180  -0.989760
H   4.100400  -0.580430   0.687470
H   1.966580  -3.268440  -0.124650
H  -0.475280  -3.319780  -0.182530
H  -1.758410  -1.165820  -0.066500
b6_sm
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C   1.379680   0.000000   0.000000
I   2.122720   1.990060   0.000000
O   2.689780   2.259510  -1.704860
O   3.855600   1.345870   0.792520
C   4.434510   2.201420   1.762800
O   0.020040   2.318950  -0.275720
C  -0.760340   1.289030  -0.128520
O  -1.954310   1.315770  -0.102910
C  -0.670180  -1.205890   0.035430
C   0.060170  -2.375950   0.033270
C   1.438890  -2.336800  -0.049030
C   2.158720  -1.144610  -0.084350
H  -1.747310  -1.188760   0.039250
H  -0.443950  -3.328590   0.057820
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H   3.983060  -0.427590  -0.950880
H   4.162090  -1.042980   0.667990
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H   4.838750   4.389300   0.171660
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H   7.017420   1.071890   1.863780
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H   5.124690   1.738780   5.127690
H   4.676820   3.225900   4.310050
H   2.460570   1.909580   3.670660
H   3.126990   0.498030   4.468200
H   2.624050   0.382610   2.794330
b7_sm
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C   1.382080   0.000000   0.000000
I   2.089030   2.019640   0.000000
O   2.481130   2.459580  -1.722990
O   3.942840   1.377250   0.471720
C   4.999970   2.167540  -0.040540
C   4.963830   3.562860   0.511870
C   4.580590   4.630390  -0.287580
C   4.502670   5.909090   0.240290
C   5.264790   3.793450   1.849140
C   5.188390   5.067700   2.375550
C   4.806860   6.128400   1.569900
C   2.151310  -1.158540  -0.031290
C   3.636280  -1.266390  -0.166470
C  -0.775730   1.279830  -0.130850
O  -0.009860   2.321080  -0.251690
O  -1.970410   1.288350  -0.123110
C  -0.680040  -1.199700   0.051110
C   0.038400  -2.374520   0.080480
C   1.417420  -2.342340   0.022080
H   4.959290   2.194370  -1.127170
H   5.908670   1.652670   0.262500
H   4.323560   4.450920  -1.320470
H   4.201210   6.731020  -0.389260

H   5.558840   2.965240   2.475990
H   5.428970   5.236560   3.413120
H   4.747070   7.123530   1.981180
H   3.899220  -2.303220  -0.347310
H   4.000250  -0.666900  -0.992800
H   4.146260  -0.916130   0.723040
H  -1.756910  -1.169230   0.048970
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H   1.967250  -3.270090   0.000250
b8_sm
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C   1.380520   0.000000   0.000000
I   2.113750   1.995790   0.000000
O   2.714830   2.318520  -1.684790
O   3.823830   1.304400   0.800410
C   4.682230   2.213550   1.493520
O   0.004190   2.307850  -0.349260
C  -0.768260   1.282340  -0.166710
O  -1.963640   1.296740  -0.140390
C  -0.669560  -1.205290   0.058120
C   0.059770  -2.375610   0.076070
C   1.437710  -2.337320  -0.013130
C   2.158860  -1.146500  -0.070390
H  -1.746680  -1.186220   0.060690
H  -0.444480  -3.327600   0.118340
H   1.992500  -3.261280  -0.064440
C   3.638350  -1.213140  -0.266910
C   3.978240   2.772520   2.720300
C   5.144800   3.324700   0.566660
C   5.855010   1.347100   1.907950
H   3.595500   1.961060   3.333990
H   3.148990   3.424660   2.451940
H   4.665460   3.362910   3.320580
H   4.324700   3.977920   0.270430
H   5.574710   2.905290  -0.337450
H   5.889000   3.945710   1.059050
H   5.514480   0.533990   2.542720
H   6.331180   0.923250   1.029130
H   6.589120   1.932860   2.456510
H   3.896030  -2.180600  -0.685420
H   3.987570  -0.436710  -0.936420
H   4.165020  -1.079120   0.671330
b9_sm
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C   1.381280   0.000000   0.000000
I   2.099090   2.004780   0.000000
O   2.655030   2.387860  -1.689720
O   3.824470   1.330540   0.763500
C   4.983350   2.166020   0.844380
C   4.604290   3.614880   1.117020
C   5.757650   2.064760  -0.457930
C   5.798850   1.574170   1.989730
C   5.125780   1.601580   3.346840
C   2.154530  -1.152460  -0.049100
C   3.634860  -1.237730  -0.231340
C  -0.769350   1.279140  -0.177090
O   0.003140   2.305200  -0.361930
O  -1.964100   1.294480  -0.156070
C  -0.674250  -1.201890   0.067950
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H   5.494020   4.198290   1.337850
H   3.929200   3.703550   1.964560
H   4.142320   4.072730   0.242290
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O -1.990920  1.250120  0.031940
C -0.655580 -1.216030 -0.017160
C  0.081100 -2.381490 -0.023590
C  1.463290 -2.337350 -0.001950
C  2.170770 -1.140310  0.013570
H -1.732750 -1.203500 -0.020550
H -0.418940 -3.336810 -0.038670
H  2.027380 -3.256540  0.008480
C  3.663300 -1.165250  0.077020
H  4.713170  2.266010  1.991960
H  3.797070  2.104430  3.490930
C  3.316660  3.848190  2.331160
C  4.211460  4.810780  1.888190
C  3.819610  6.133020  1.780580
C  2.526880  6.499390  2.106400
C  1.625990  5.543200  2.544300
C  2.019610  4.225430  2.663180
```

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H   1.315900   3.479100   2.998080
H   0.614590   5.823200   2.789910
H   2.217790   7.528030   2.013050
H   4.520540   6.873760   1.430890
H   5.215800   4.522300   1.617070
H   4.009230  -2.192010   0.124630
H   4.105940  -0.666760  -0.777750
H   4.012660  -0.643570   0.964230
b8_ts
C   0.000000   0.000000   0.000000
C   1.376210   0.000000   0.000000
I   2.237510   1.936680   0.000000
O   3.714600   1.566650  -0.980590
O   2.800990   1.547570   1.878860
C   3.096180   2.646890   2.758660
O  -0.037220   2.325760   0.024800
C  -0.791280   1.292200   0.013420
O  -1.992140   1.249090   0.015120
C  -0.653230  -1.217600  -0.011060
C   0.085950  -2.381620  -0.010260
C   1.468080  -2.334850   0.009460
C   2.173990  -1.136810   0.017180
H  -1.730440  -1.207590  -0.016190
H  -0.412400  -3.337870  -0.019590
H   2.033680  -3.253390   0.023600
C   3.667320  -1.156750   0.068830
C   1.828650   3.429620   3.039020
C   4.188390   3.521650   2.172770
C   3.586010   1.932790   4.003580
H   1.060510   2.773100   3.436810
H   1.433040   3.895860   2.137960
H   2.020770   4.220590   3.759240
H   3.842230   4.075210   1.299920
H   5.043310   2.919380   1.879370
H   4.512570   4.257880   2.903120
H   2.821000   1.255960   4.370780
H   4.479450   1.357810   3.780740
H   3.817070   2.657630   4.780620
H   4.013860  -2.179280   0.171390
H   4.097750  -0.711210  -0.820910
H   4.031010  -0.582060   0.915880
b9_ts
C   0.000000   0.000000   0.000000
C   1.375860   0.000000   0.000000
I   2.236280   1.937240   0.000000
O   3.705250   1.565090  -0.992190
O   2.777690   1.541570   1.883120
C   3.175870   2.621600   2.744090
O  -0.036510   2.326550   0.025790
C  -0.790430   1.292650   0.016720
O  -1.991250   1.249960   0.023140
C  -0.653490  -1.217540  -0.013320
C   0.085840  -2.381480  -0.016420
C   1.468040  -2.334710   0.003020
C   2.173870  -1.136660   0.013830
H  -1.730670  -1.207680  -0.017750
H  -0.412350  -3.337790  -0.028550
H   2.033620  -3.253380   0.014410
C   3.667090  -1.156470   0.066720
C   4.432940   3.276800   2.205130
C   2.045960   3.623320   2.888590
C   3.483600   1.902700   4.056250
C   2.311980   1.184240   4.694480
H   4.251380   3.779980   1.255800
H   5.211790   2.536510   2.048790
H   4.796220   4.028430   2.901000
H   1.114600   3.128710   3.142640
H   1.886280   4.180290   1.966570
H   2.281400   4.348090   3.663670
H   4.281910   1.192210   3.850830
H   3.891200   2.645760   4.742100
H   2.644290   0.635640   5.571730
H   1.536710   1.873740   5.017860
H   1.869360   0.475300   4.001660
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H   4.014250  -2.179380   0.163410
H   4.098640  -0.704150  -0.818930
H   4.028510  -0.587810   0.918750
b1_p
C   0.000000   0.000000   0.000000
C   1.378310   0.000000   0.000000
I   2.159980   1.973930   0.000000
O   3.882310   1.553690   0.424250
O   1.657010   2.541940   1.864960
C   2.629150   2.283720   2.844200
H   3.612700   2.104470   2.396540
H   2.343540   1.407450   3.421590
H   2.681310   3.163700   3.478420
O   0.003150   2.324360  -0.137240
C  -0.768680   1.296480  -0.058350
O  -1.966540   1.292260  -0.059340
C  -0.669080  -1.205870   0.032680
C   0.061660  -2.375740   0.050160
C   1.443150  -2.337520   0.029840
C   2.165260  -1.146460   0.002670
H  -1.746230  -1.185480   0.037760
H  -0.442370  -3.328660   0.073760
H   1.999710  -3.261700   0.033370
C   3.660120  -1.217340  -0.018650
H   3.962730  -2.247610  -0.173530
H   4.092810  -0.603630  -0.800830
H   4.087380  -0.855510   0.909550
b2_p
C   0.000000   0.000000   0.000000
C   1.378040   0.000000   0.000000
I   2.159380   1.973130   0.000000
O   3.879260   1.548090   0.433880
O   1.631070   2.522310   1.861570
C   2.669830   2.516010   2.815390
C   3.035190   3.922900   3.209180
C   2.165230  -1.146020   0.004410
C   3.659990  -1.218360  -0.021950
C  -0.768500   1.295850  -0.065330
O   0.003380   2.323210  -0.148510
O  -1.966430   1.292050  -0.067670
C  -0.669030  -1.205550   0.039030
C   0.061760  -2.375260   0.061310
C   1.443130  -2.336960   0.037880
H   3.543360   1.988760   2.415880
H   2.288470   1.938590   3.656140
H   3.761670   3.906990   4.018600
H   2.158170   4.469470   3.542210
H   3.478240   4.457750   2.372590
H   3.960570  -2.246510  -0.194400
H   4.092520  -0.591970  -0.793780
H   4.089070  -0.873640   0.912020
H   1.999930  -3.261030   0.042960
H  -0.442120  -3.328150   0.089890
H  -1.746200  -1.185110   0.044590
b3_p
C   0.000000   0.000000   0.000000
C   1.378070   0.000000   0.000000
I   2.163910   1.974530   0.000000
O   3.889490   1.548500   0.406470
O   1.673120   2.583820   1.837700
C   2.623560   2.301600   2.857190
C   2.215510   1.038620   3.579470
C   2.656650   3.528020   3.739390
C   2.163950  -1.147720  -0.001890
C   3.658680  -1.220850  -0.023530
C  -0.769560   1.296480  -0.056700
O   0.000270   2.323540  -0.140750
O  -1.967730   1.289380  -0.050970
C  -0.669760  -1.205450   0.030060
C   0.059900  -2.375660   0.044780
C   1.441280  -2.338170   0.022990
H   3.602760   2.148090   2.393380
H   2.919280   0.815280   4.377740
H   2.198820   0.189830   2.900790
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H   1.223700   1.151710   4.009220
H   3.363050   3.379610   4.552520
H   1.673880   3.716860   4.162400
H   2.959930   4.400980   3.170140
H   3.959290  -2.251580  -0.179370
H   4.091770  -0.606750  -0.804980
H   4.087880  -0.859860   0.904290
H   1.997210  -3.262730   0.023140
H  -0.444600  -3.328360   0.066300
H  -1.746870  -1.184020   0.034970
b4_p
C   0.000000   0.000000   0.000000
C   1.378330   0.000000   0.000000
I   2.159590   1.971300   0.000000
O   3.883010   1.548110   0.422140
O   1.629000   2.501600   1.864010
C   2.675580   2.538640   2.806600
C   2.997190   3.965390   3.207750
C   1.810570   4.625860   3.887150
C   3.481030   4.772460   2.014230
C   2.165190  -1.146400   0.004440
C   3.659880  -1.219070  -0.018220
C  -0.769430   1.295870  -0.062220
O   0.001760   2.323650  -0.142820
O  -1.967380   1.291150  -0.063510
C  -0.668750  -1.205620   0.037490
C   0.061890  -2.375420   0.058460
C   1.443110  -2.337260   0.036370
H   3.565960   2.048140   2.396350
H   2.327820   1.950220   3.655450
H   3.816970   3.891210   3.925700
H   1.514760   4.081820   4.781920
H   0.955770   4.651020   3.215380
H   2.044790   5.646820   4.179470
H   4.294980   4.268900   1.496170
H   3.834440   5.751980   2.325540
H   2.667560   4.939540   1.308760
H   3.960690  -2.247410  -0.189050
H   4.094900  -0.592920  -0.788770
H   4.086160  -0.874120   0.917030
H   1.999900  -3.261280   0.041570
H  -0.442060  -3.328240   0.085650
H  -1.745870  -1.185150   0.043270
b5_p
C   0.000000   0.000000   0.000000
C   1.378310   0.000000   0.000000
I   2.159900   1.971020   0.000000
O   3.885320   1.544660   0.409850
O   1.645590   2.509100   1.867480
C   2.698770   2.539600   2.799190
C   3.056220   3.963820   3.202030
C   4.203150   3.877070   4.199990
C   1.848880   4.633530   3.842430
C   3.498130   4.747460   1.973160
C   2.164970  -1.146550  -0.000000
C   3.659540  -1.220350  -0.019710
C  -0.769740   1.295720  -0.052610
O   0.001020   2.324270  -0.126460
O  -1.967630   1.290830  -0.052350
C  -0.669010  -1.205640   0.029680
C   0.061420  -2.375490   0.044280
C   1.442560  -2.337300   0.024610
H   3.580970   2.035540   2.385350
H   2.352470   1.961260   3.656460
H   3.926980   3.279120   5.067250
H   4.473810   4.868450   4.556750
H   5.087450   3.429870   3.749300
H   1.549730   4.111700   4.750070
H   1.002200   4.633270   3.161010
H   2.075320   5.664060   4.109210
H   4.306400   4.238430   1.450520
H   3.851810   5.736270   2.257550
H   2.667690   4.893510   1.284130
H   3.959650  -2.248020  -0.195650
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H   4.097410  -0.589670  -0.784760
H   4.083370  -0.881850   0.919070
H   1.999170  -3.261360   0.025800
H  -0.442680  -3.328330   0.064800
H  -1.746100  -1.184960   0.034590
b6_p
C   0.000000   0.000000   0.000000
C   1.381500   0.000000   0.000000
I   2.201800   1.955030   0.000000
O   3.962210   1.536870   0.054820
O   2.018490   2.239560   1.939580
C   1.318470   3.369680   2.479250
O  -0.036110   2.326810   0.045350
C  -0.787840   1.288400   0.040330
O  -1.988450   1.256860   0.065100
C  -0.665920  -1.207940  -0.011720
C   0.062340  -2.379130  -0.025120
C   1.442870  -2.341300  -0.013540
C   2.165710  -1.150420   0.000860
H  -1.743010  -1.185640  -0.005040
H  -0.443170  -3.331510  -0.036460
H   2.000160  -3.264900  -0.010530
C   3.659190  -1.225590   0.043460
H   0.511290   3.637430   1.798470
C   2.273690   4.548510   2.636570
C   0.685810   2.850250   3.769430
C   2.830110   5.000210   1.293460
H   1.670060   5.369160   3.024100
C   3.407080   4.263360   3.607760
C  -0.288510   1.720280   3.481710
C  -0.014230   3.974500   4.520070
H   1.489300   2.457630   4.392220
H   3.959750  -2.267980   0.041780
H   4.119880  -0.721140  -0.798920
H   4.056420  -0.739320   0.927120
H   3.318870   5.966250   1.390620
H   2.046100   5.112810   0.544390
H   3.591580   4.312850   0.923990
H   4.093280   5.106030   3.649510
H   3.967810   3.388840   3.286730
H   3.047160   4.083620   4.617200
H   0.673820   4.739610   4.868470
H  -0.525300   3.572670   5.391330
H  -0.765070   4.452420   3.892100
H  -1.112900   2.059770   2.857470
H  -0.707480   1.341220   4.410970
H   0.202920   0.894830   2.977220
b7_p
C   0.000000   0.000000   0.000000
C   1.378200   0.000000   0.000000
I   2.171150   1.968250   0.000000
O   3.909840   1.562150   0.362190
O   1.698350   2.384190   1.911030
C   2.766250   2.990320   2.590980
C   3.000500   4.395230   2.125170
C   4.274020   4.944920   2.160090
C   4.486000   6.243240   1.739540
C   1.942610   5.157500   1.646230
C   2.158770   6.454560   1.215660
C   3.427930   7.000640   1.266110
C   2.166020  -1.145760  -0.006760
C   3.660810  -1.214710  -0.012150
C  -0.773220   1.294980  -0.024100
O  -0.005070   2.325250  -0.071130
O  -1.971920   1.285310  -0.021400
C  -0.667140  -1.207260   0.015380
C   0.063690  -2.376760   0.017530
C   1.444990  -2.337360   0.003720
H   3.677500   2.399550   2.486430
H   2.451750   2.954590   3.633790
H   5.103480   4.346090   2.503950
H   5.479700   6.661120   1.767390
H   0.953350   4.727430   1.611270
H   1.332040   7.038280   0.843450
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```
H   3.595290   8.011950   0.931200
H   3.966540  -2.246590  -0.149530
H   4.101680  -0.609570  -0.796350
H   4.075580  -0.839090   0.916350
H  -1.744280  -1.187010   0.022390
H  -0.439910  -3.330130   0.027360
H   2.002840  -3.260760   0.000790
b8_p
C   0.000000   0.000000   0.000000
C   1.379440   0.000000   0.000000
I   2.190050   1.961780   0.000000
O   3.962290   1.572130   0.026720
O   1.871270   2.154740   1.933820
C   2.073770   3.428090   2.582420
O  -0.045220   2.325660   0.004750
C  -0.793780   1.288260   0.021260
O  -1.994210   1.246540   0.043010
C  -0.660090  -1.211660  -0.006450
C   0.072510  -2.379960  -0.012360
C   1.453300  -2.338060  -0.001250
C   2.171040  -1.144580   0.007020
H  -1.737300  -1.192860  -0.001200
H  -0.429680  -3.334180  -0.018490
H   2.014030  -3.259590   0.006130
C   3.664960  -1.209170   0.051360
C   1.432430   4.548920   1.789210
C   3.557750   3.652270   2.790600
C   1.351630   3.213060   3.898280
H   0.419080   4.285320   1.502600
H   2.000720   4.776220   0.885590
H   1.416180   5.459260   2.381680
H   4.087650   3.715230   1.843180
H   3.986600   2.828990   3.353580
H   3.725920   4.577570   3.336480
H   0.294230   3.044140   3.722670
H   1.762260   2.349530   4.412030
H   1.474100   4.088430   4.531650
H   3.973110  -2.249360   0.051400
H   4.124700  -0.701790  -0.789590
H   4.056640  -0.721070   0.936720
b9_p
C   0.000000   0.000000   0.000000
C   1.379630   0.000000   0.000000
I   2.192290   1.959070   0.000000
O   3.963730   1.566320   0.006680
O   1.895910   2.152270   1.933840
C   2.127100   3.418500   2.588470
C   1.571970   4.563890   1.765100
C   3.614030   3.574290   2.834940
C   1.378810   3.235010   3.905480
C  -0.128100   3.135590   3.789120
C   2.170230  -1.145340   0.003750
C   3.664010  -1.211930   0.049410
C  -0.792970   1.288710   0.031510
O  -0.043800   2.325620   0.025080
O  -1.993460   1.246950   0.054890
C  -0.661140  -1.210780  -0.013170
C   0.070910  -2.379430  -0.025340
C   1.451610  -2.338240  -0.011820
H   1.542440   5.471070   2.362500
H   0.572620   4.340590   1.405550
H   2.213090   4.778230   0.908380
H   3.815050   4.509340   3.352460
H   4.171270   3.572830   1.901390
H   3.982420   2.751620   3.440460
H   1.659280   4.069490   4.549070
H   1.775470   2.334770   4.371050
H  -0.574520   4.067300   3.452300
H  -0.562180   2.897260   4.756550
H  -0.414570   2.357480   3.089240
H   3.970090  -2.252600   0.060220
H   4.123520  -0.714630  -0.797890
H   4.057330  -0.714170   0.928390
H  -1.738320  -1.191250  -0.008780
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H  -0.431690  -3.333370  -0.037660
H   2.011700  -3.260170  -0.007350
```

c1-7(sm, ts, p)

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c1_sm
O   0.000000   0.000000   0.000000
I   1.824600   0.000000   0.000000
O   2.037260   1.994560   0.000000
C   0.849460   2.708280  -0.242590
O   3.991670   0.217240  -0.415640
C   4.380360   0.065940  -1.635360
O   5.498110   0.152740  -2.058460
C   1.972020  -0.380050  -2.047830
C   3.239840  -0.278440  -2.560490
C   3.395300  -0.491650  -3.916920
C   2.287860  -0.792650  -4.690770
C   0.842740  -0.672240  -2.771480
C   1.021850  -0.880240  -4.128780
H  -0.037060   2.107230  -0.016610
H   0.871430   3.573280   0.413120
H   0.810120   3.015220  -1.284900
H   2.408690  -0.958560  -5.749360
H   4.385550  -0.411270  -4.334870
H   0.170220  -1.111110  -4.747850
H  -0.119640  -0.717220  -2.285980
c2_sm
O   0.000000   0.000000   0.000000
I   1.826000   0.000000   0.000000
O   2.050610   1.991520   0.000000
C   0.851110   2.736350   0.075670
C   0.745200   3.425420   1.409830
O   3.991330   0.230070  -0.409980
C   4.379440   0.103850  -1.632790
O   5.496980   0.202100  -2.054260
C   1.972940  -0.343010  -2.052370
C   3.238990  -0.225640  -2.563660
C   3.394790  -0.411070  -3.924080
C   2.288030  -0.701750  -4.702760
C   0.844350  -0.625890  -2.780320
C   1.023070  -0.806310  -4.141560
H   1.630260   4.023010   1.605210
H   0.631760   2.702330   2.213790
H  -0.123810   4.079490   1.422590
H  -0.010600   2.081250  -0.091050
H   0.897180   3.443560  -0.750620
H   4.384360  -0.318160  -4.341000
H   2.408650  -0.846580  -5.764450
H   0.171840  -1.028890  -4.764180
H  -0.117280  -0.684630  -2.294900
c3_sm
O   0.000000   0.000000   0.000000
I   1.825760   0.000000   0.000000
O   2.062710   1.976660   0.000000
C   0.885260   2.743260  -0.242530
C   0.939870   3.897660   0.730780
C   0.864370   3.166400  -1.692900
O   3.997460   0.200730  -0.436170
C   4.378650   0.003550  -1.650270
O   5.493110   0.078470  -2.085920
C   1.968660  -0.462570  -2.032770
C   3.233370  -0.382260  -2.554430
C   3.385090  -0.659350  -3.900030
C   2.276220  -1.001250  -4.654170
C   0.837910  -0.795320  -2.737030
C   1.012720  -1.068210  -4.083160
H   0.009640   2.120740  -0.033930
H   1.833080   4.492990   0.562640
H   0.954060   3.536160   1.754170
H   0.068010   4.533600   0.598400
H   1.756710   3.738760  -1.932280
H  -0.009670   3.781830  -1.892270
H   0.823140   2.303460  -2.351770
H   2.393710  -1.217810  -5.703960
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H   4.373780 -0.596320 -4.324600      C   0.848350  3.806630 -0.871940      C   0.830040 -0.450040 -2.813640
H   0.160010 -1.333890 -4.686580      C  -0.318220  4.759290 -0.658300      C   0.995030 -0.531240 -4.186280
H  -0.122240 -0.820180 -2.245430      C   0.754420  3.145360 -2.235990      H  -0.184800  1.543700 -0.010820
c4_sm                                 O   3.998180  0.224180 -0.419880      H   0.120190  3.098820  0.831870
O   0.000000  0.000000  0.000000      C   4.384860  0.055750 -1.636750      H   0.159510  2.992150 -1.001490
I   1.826540  0.000000  0.000000      O   5.502310  0.136310 -2.063670      H   2.357770 -0.426240 -5.826220
O   2.059880  1.988490  0.000000      C   1.974370 -0.391980 -2.042320      H   4.339100  0.045970 -4.389930
C   0.868760  2.736540  0.137090      C   3.242090 -0.299140 -2.556290      H   0.140270 -0.734040 -4.810920
C   0.796820  3.398620  1.498480      C   3.398490 -0.529740 -3.909880      H  -0.125000 -0.572890 -2.329040
C   1.929890  4.391830  1.687590      C   2.291480 -0.840550 -4.680110      c2_ts
C   0.765860  2.362550  2.610200      C   0.845990 -0.695580 -2.763170      O   0.000000  0.000000  0.000000
O   3.993910  0.230410 -0.408860      C   1.025490 -0.921610 -4.117100      I   1.852820  0.000000  0.000000
C   4.381620  0.104660 -1.631710      H   2.038600  5.117370  1.317650      O   1.743570  2.199890  0.000000
O   5.499080  0.202650 -2.053590      H   3.045010  3.722130  1.685420      C   0.453580  2.557500  0.058360
C   1.973500 -0.337920 -2.052460      H   2.133220  4.518960  2.963830      C   0.071680  3.271820  1.332650
C   3.240500 -0.222740 -2.562820      H   0.806550  2.472880  3.672580      O   3.995110  0.322630 -0.415050
C   3.397010 -0.407260 -3.923270      H   1.926390  1.613140  2.647460      C   4.364060  0.342160 -1.652470
C   2.290480 -0.695080 -4.703230      H   0.177810  1.388890  2.439280      O   5.469010  0.532740 -2.074240
C   0.845100 -0.617750 -2.782130      H   0.004620  3.813750  1.825700      C   1.965800 -0.142100 -2.081230
C   1.024770 -0.797220 -4.143270      H   0.023940  2.105050  0.125380      C   3.220010  0.065020 -2.593050
H   1.900250  5.173340  0.931080      H   1.776920  4.375390 -0.832660      C   3.364560  0.014970 -3.967070
H   2.891360  3.889770  1.609430      H  -0.217750  5.343600  0.251870      C   2.261240 -0.242870 -4.760530
H   1.873110  4.869230  2.662960      H  -1.261520  4.216390 -0.609100      C   0.841660 -0.402930 -2.823870
H   0.577150  2.831490  3.572260      H  -0.383940  5.457650 -1.489050      C   1.009990 -0.448880 -4.197720
H   1.727220  1.855520  2.690290      H   1.609020  2.504440 -2.427090      H   0.646620  4.187260  1.445560
H  -0.009370  1.617920  2.439980      H   0.721370  3.896280 -3.021660      H   0.267730  2.641280  2.196710
H  -0.151260  3.940790  1.510580      H  -0.150280  2.542940 -2.312460      H  -0.986090  3.521210  1.325400
H  -0.001160  2.088770 -0.019150      H   2.412640 -1.020440 -5.736360      H  -0.170110  1.562840  0.014660
H   0.893820  3.470150 -0.667680      H   4.389150 -0.455500 -4.327940      H   0.152410  3.054440 -0.868290
H   4.387180 -0.315900 -4.339040      H   0.174120 -1.161020 -4.733220      H   4.345440  0.183110 -4.380990
H   2.411850 -0.839500 -5.764860      H  -0.116520 -0.733560 -2.277550      H   2.373520 -0.283990 -5.832060
H   0.173610 -1.017270 -4.766840      c7_sm                                 H   0.159120 -0.648140 -4.828820
H  -0.117290 -0.674720 -2.298110      O   0.000000  0.000000  0.000000      H  -0.112750 -0.548090 -2.344170
c5_sm                                 I   1.824570  0.000000  0.000000      c3_ts
O   0.000000  0.000000  0.000000      O   2.039750  1.993560  0.000000      O   0.000000  0.000000  0.000000
I   1.826540  0.000000  0.000000      C   1.009660  2.624700  0.722480      I   1.852600  0.000000  0.000000
O   2.061040  1.989430  0.000000      C   1.144540  2.395560  2.196510      O   1.750310  2.197980  0.000000
C   0.870670  2.733720  0.131230      C   0.018600  2.247820  2.993110      C   0.458570  2.567760 -0.023330
C   0.780390  3.416090  1.488530      C   0.147790  2.046430  4.354050      C   0.061110  3.317070  1.234000
C   1.948890  4.376730  1.657850      C   2.404690  2.320350  2.777170      C   0.083030  3.225080 -1.340860
C   0.800690  2.366500  2.592550      C   2.532520  2.108530  4.137670      O   3.994800  0.321420 -0.429650
C  -0.538000  4.177720  1.523060      C   1.405080  1.976620  4.928360      C   4.357090  0.327920 -1.668610
O   3.994480  0.227990 -0.408990      O   4.005070  0.249890 -0.396900      O   5.457680  0.524360 -2.099650
C   4.381710  0.103010 -1.632010      C   4.398060  0.154030 -1.619370      C   1.961580 -0.185210 -2.079380
O   5.499220  0.199450 -2.054110      O   5.518590  0.252420 -2.034980      C   3.211590  0.024660 -2.599880
C   1.972770 -0.335250 -2.053050      C   1.986960 -0.249680 -2.064440      C   3.351670 -0.048940 -3.973570
C   3.239840 -0.221160 -2.563360      C   3.257230 -0.131890 -2.564870      C   2.248450 -0.332710 -4.758010
C   3.395770 -0.404060 -3.924070      C   3.415440 -0.269710 -3.930790      C   0.837780 -0.473130 -2.813220
C   2.288700 -0.688910 -4.704350      C   2.308140 -0.515580 -4.723900      C   1.001530 -0.542920 -4.186490
C   0.843770 -0.612230 -2.782900      C   0.857480 -0.489510 -2.805600      H  -0.154320  1.566940 -0.000990
C   1.022940 -0.789870 -4.144390      C   1.039200 -0.621410 -4.171910      H   0.602280  4.258720  1.295350
H   0.000510  2.083380 -0.019730      H   0.032250  2.292160  0.373020      H   0.299350  2.731120  2.117220
H   1.920680  5.161300  0.903450      H   1.132460  3.674800  0.458880      H  -1.005000  3.526490  1.235800
H   2.896260  3.852940  1.561020      H  -0.960630  2.274030  2.540560      H   0.599310  4.177440 -1.440490
H   1.917950  4.852990  2.635830      H  -0.732800  1.929640  4.965260      H  -0.987810  3.402110 -1.391140
H   0.634760  2.829370  3.562610      H   3.280610  2.422980  2.155120      H   0.371990  2.593540 -2.175060
H   1.768080  1.868690  2.640490      H   3.514150  2.049640  4.579970      H   2.357140 -0.391910 -5.829040
H   0.024580  1.618000  2.439680      H   1.505430  1.812390  5.989390      H   4.329320  0.121570 -4.394140
H  -0.596580  4.901720  0.711760      H   4.407920 -0.174740 -4.340230      H   0.150750 -0.763630 -4.810550
H  -0.637750  4.723470  2.458690      H   2.431350 -0.622790 -5.789750      H  -0.113790 -0.617400 -2.327410
H  -1.388030  3.503310  1.435880      H  -0.106420 -0.549860 -2.324460      c4_ts
H   0.891080  3.463620 -0.678170      H   0.187320 -0.806940 -4.805680      O   0.000000  0.000000  0.000000
H   2.409750 -0.832050 -5.766190      c1_ts                                 I   1.853210  0.000000  0.000000
H   4.386040 -0.313860 -4.339880      O   0.000000  0.000000  0.000000      O   1.746540  2.200370  0.000000
H   0.171330 -1.007700 -4.768140      I   1.853650  0.000000  0.000000      C   0.457630  2.560420  0.042220
H  -0.118610 -0.669000 -2.298830      O   1.732960  2.206350  0.000000      C   0.057700  3.308970  1.305910
c6_sm                                 C   0.441410  2.542660 -0.048950      C   0.733980  4.670070  1.349820
O   0.000000  0.000000  0.000000      O   3.996020  0.299060 -0.428410      C   0.367370  2.487740  2.545280
I   1.826670  0.000000  0.000000      C   4.365030  0.272210 -1.665870      O   3.998540  0.316170 -0.414120
O   2.071060  1.981180  0.000000      O   5.473440  0.426190 -2.092900      C   4.366160  0.342660 -1.651600
C   0.902250  2.754350  0.235500      C   1.958950 -0.186180 -2.079120      O   5.470820  0.534550 -2.073800
C   0.938480  3.273300  1.670920      C   3.214990 -0.009270 -2.597900      C   1.965840 -0.134500 -2.081520
C   2.104250  4.214890  1.920000      C   3.356460 -0.096210 -3.970520      C   3.220460  0.073050 -2.592710
C   0.958850  2.115340  2.657570      C   2.248050 -0.357020 -4.755860      C   3.364360  0.030620 -3.967090
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C   2.260450  -0.220480  -4.761950
C   0.841190  -0.389230  -2.825840
C   1.009080  -0.427590  -4.200030
H   0.481690   5.266280   0.475180
H   1.815110   4.553010   1.373690
H   0.430090   5.227780   2.233200
H   0.031550   3.001720   3.442180
H   1.439900   2.329970   2.640530
H  -0.126760   1.518650   2.510800
H  -1.022070   3.454570   1.245910
H  -0.170350   1.567900   0.017490
H   0.164320   3.047980  -0.893210
H   4.345490   0.199310  -4.380120
H   2.372440  -0.255610  -5.833770
H   0.157660  -0.621770  -4.832030
H  -0.113470  -0.535700  -2.347170
c5_ts
O   0.000000   0.000000   0.000000
I   1.852920   0.000000   0.000000
O   1.748760   2.200510   0.000000
C   0.461840   2.560570   0.043750
C   0.046780   3.310270   1.310340
C   0.794940   4.637290   1.359910
C   0.388830   2.470710   2.532690
C  -1.453410   3.553340   1.241170
O   3.999370   0.313420  -0.414540
C   4.367250   0.335340  -1.651950
O   5.472420   0.523490  -2.074640
C   1.965910  -0.138300  -2.081290
C   3.221140   0.065580  -2.592580
C   3.365420   0.019260  -3.966780
C   2.261260  -0.231520  -4.761370
C   0.840930  -0.392440  -2.825370
C   1.009210  -0.434480  -4.199380
H  -0.169350   1.570770   0.017670
H   0.553380   5.254770   0.496300
H   1.869160   4.471250   1.364620
H   0.527560   5.195970   2.255300
H   0.080650   2.980870   3.442530
H   1.461030   2.300180   2.598160
H  -0.119970   1.508410   2.500550
H  -1.721370   4.112130   0.345530
H  -1.786270   4.131500   2.100520
H  -2.005960   2.615580   1.232350
H   0.165990   3.054090  -0.889080
H   2.373590  -0.269660  -5.833020
H   4.347690   0.184690  -4.379880
H   0.157590  -0.628360  -4.831190
H  -0.114170  -0.536010  -2.346660
c6_ts
O   0.000000   0.000000   0.000000
I   1.855560   0.000000   0.000000
O   1.732940   2.216230   0.000000
C   0.450860   2.574640   0.137270
C   0.160010   3.122450   1.542070
C   0.845430   4.463560   1.757660
C   0.578040   2.124780   2.609230
C  -0.045480   3.402250  -1.064740
C  -1.531530   3.700080  -0.959260
C   0.276220   2.719510  -2.379050
O   4.001500   0.337330  -0.449070
C   4.369180   0.230480  -1.680150
O   5.466190   0.412250  -2.128340
C   1.985550  -0.377000  -2.049380
C   3.237150  -0.196800  -2.579890
C   3.396090  -0.424420  -3.934510
C   2.311900  -0.830320  -4.691070
C   0.881690  -0.786020  -2.756900
C   1.064920  -1.011960  -4.110140
H   0.484700   5.222830   1.068270
H   1.919540   4.363220   1.617430
H   0.667490   4.826090   2.767760
H   0.306180   2.488440   3.596900
H   1.657300   1.982100   2.603370

H   0.088600   1.163220   2.466230
H  -0.917450   3.258430   1.621050
H  -0.164850   1.572570   0.062700
H   0.501720   4.345430  -1.034480
H  -1.775960   4.298850  -0.086490
H  -2.111500   2.779280  -0.910820
H  -1.862920   4.253200  -1.835050
H   1.338370   2.519520  -2.474560
H  -0.023820   3.348480  -3.213620
H  -0.261230   1.777050  -2.464430
H   2.436320  -1.011120  -5.746670
H   4.374580  -0.277040  -4.361860
H   0.229530  -1.332180  -4.711400
H  -0.071560  -0.904760  -2.267620
c7_ts
O   0.000000   0.000000   0.000000
I   1.848460   0.000000   0.000000
O   1.759820   2.179010   0.000000
C   0.492110   2.555080   0.226500
C   0.232910   3.127640   1.580900
C  -1.057360   3.496080   1.939020
C  -1.312490   4.020590   3.190010
C   1.262290   3.285710   2.495780
C   1.004020   3.804430   3.751810
C  -0.281350   4.173390   4.101980
O   3.982740   0.380500  -0.391850
C   4.362600   0.417340  -1.626350
O   5.466840   0.636440  -2.035220
C   1.979860  -0.115250  -2.079930
C   3.233950   0.120960  -2.579270
C   3.390580   0.084580  -3.952330
C   2.298760  -0.189100  -4.756460
C   0.866530  -0.391050  -2.833150
C   1.046820  -0.422730  -4.205860
H  -0.166590   1.596210   0.132960
H   0.120320   3.159060  -0.605670
H  -1.866150   3.366690   1.234920
H  -2.317470   4.305320   3.457910
H   2.265240   3.016960   2.206600
H   1.812190   3.928560   4.455180
H  -0.480710   4.580570   5.080330
H   4.370950   0.275880  -4.357310
H   2.420610  -0.220370  -5.827290
H  -0.089170  -0.555750  -2.362150
H   0.205140  -0.632270  -4.845780
c1_p
O   0.000000   0.000000   0.000000
I   2.017110   0.000000   0.000000
O  -0.252530   2.890080   0.000000
C   0.318400   3.680470  -0.688230
O   4.144500   0.120630  -0.479850
C   4.465460   0.423310  -1.695780
O   5.576510   0.570160  -2.122380
C   2.008460   0.429740  -2.058500
C   3.265400   0.583530  -2.585720
C   3.370800   0.869310  -3.936440
C   2.228120   0.978220  -4.705230
C   0.846730   0.513840  -2.785940
C   0.976260   0.797560  -4.136000
H  -0.285010   0.908050   0.121410
H   0.092000   4.753310  -0.633450
H   1.091550   3.376460  -1.406710
H   2.308990   1.195590  -5.758070
H   4.358470   0.991850  -4.350710
H   0.090090   0.868420  -4.746310
H  -0.107180   0.350070  -2.314190
c2_p
O   0.000000   0.000000   0.000000
I   2.016210   0.000000   0.000000
O  -0.276320   2.823110   0.000000
C  -0.319970   3.487570  -0.997120
C  -0.270250   4.971840  -1.009220
O   4.145820   0.046210  -0.498430
C   4.462720   0.164520  -1.746120

O   5.572280   0.245220  -2.194680
C   2.004710   0.115570  -2.098640
C   3.259690   0.188540  -2.646410
C   3.361300   0.264730  -4.025170
C   2.217270   0.252210  -4.799260
C   0.841680   0.084270  -2.828110
C   0.967150   0.157430  -4.206100
H   0.585450   5.296980  -1.598850
H  -0.200230   5.360170  -0.000490
H  -1.159040   5.360280  -1.503800
H  -0.281780   0.917160   0.074290
H  -0.397510   3.001520  -1.982160
H   4.347990   0.324750  -4.455190
H   2.295730   0.305930  -5.873140
H   0.079840   0.129370  -4.818380
H  -0.109560  -0.011560  -2.332310
c3_p
O   0.000000   0.000000   0.000000
I   2.015520   0.000000   0.000000
O  -0.208970   2.814140   0.000000
C  -0.320490   4.010680   0.014880
C  -0.589140   4.773780   1.274570
C  -0.177150   4.815770  -1.238360
O   4.150350   0.073480  -0.469010
C   4.483400   0.345060  -1.689080
O   5.601270   0.442920  -2.113520
C   2.028360   0.427040  -2.058020
C   3.291000   0.535530  -2.582800
C   3.407190   0.813570  -3.934010
C   2.269610   0.964060  -4.702880
C   0.871040   0.560390  -2.783430
C   1.011830   0.835900  -4.133060
H  -0.273690   0.912790   0.116720
H   0.318260   5.300650   1.567930
H  -0.877710   4.094400   2.066940
H  -1.356710   5.527330   1.119720
H   0.470790   5.674390  -1.079780
H  -1.154430   5.203630  -1.521390
H   0.207640   4.194000  -2.037500
H   2.358020   1.177500  -5.755730
H   4.398890   0.899300  -4.347310
H   0.129210   0.945050  -4.742700
H  -0.087710   0.444880  -2.308220
c4_p
O   0.000000   0.000000   0.000000
I   2.018060   0.000000   0.000000
O  -0.030860   2.825050   0.000000
C  -0.462810   3.937520   0.105830
C   0.273240   5.178750  -0.289340
C  -0.607620   6.008370  -1.218930
C   1.638150   4.878990  -0.871200
O   4.151910   0.082580  -0.465310
C   4.484210   0.348790  -1.686420
O   5.601290   0.462200  -2.109630
C   2.030020   0.391350  -2.064170
C   3.292670   0.511230  -2.586230
C   3.411130   0.770610  -3.941160
C   2.275470   0.890900  -4.718060
C   0.874920   0.492660  -2.798340
C   1.017230   0.749430  -4.151970
H  -1.584600   6.205310  -0.782750
H  -0.755590   5.498430  -2.168390
H  -0.137030   6.965130  -1.424340
H   2.167480   5.801960  -1.090800
H   1.548460   4.310850  -1.793510
H   2.241460   4.293760  -0.184440
H   0.383490   5.741850   0.643520
H  -0.282920   0.909930   0.112450
H  -1.473170   4.100360   0.517690
H   4.403390   0.866800  -4.351280
H   2.366450   1.089410  -5.773840
H   0.135790   0.833060  -4.767530
H  -0.084550   0.364090  -2.327880
c5_p
```

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O   0.000000   0.000000   0.000000
I   2.017370   0.000000   0.000000
O  -0.381700   2.792870   0.000000
C  -1.240090   3.473310  -0.486040
C  -1.177780   4.965850  -0.640300
C  -1.328150   5.263800  -2.132810
C   0.132000   5.508380  -0.100910
C  -2.372770   5.542730   0.119720
O   4.150000   0.036630  -0.482350
C   4.476520   0.180670  -1.724980
O   5.590960   0.250380  -2.163910
C   2.020360   0.184700  -2.093580
C   3.280240   0.252650  -2.630930
C   3.391980   0.373560  -4.005680
C   2.252740   0.411780  -4.785720
C   0.861910   0.205970  -2.829290
C   0.997330   0.324460  -4.202710
H  -0.284090   0.915590   0.079790
H  -2.250070   4.846710  -2.534170
H  -0.493630   4.862320  -2.702980
H  -1.356160   6.339340  -2.289470
H   0.164710   6.589090  -0.216440
H   0.979870   5.081560  -0.629040
H   0.248930   5.272350   0.952920
H  -3.313560   5.126160  -0.235660
H  -2.412300   6.619630  -0.024680
H  -2.294400   5.348900   1.186910
H  -2.167230   3.008380  -0.865040
H   2.338770   0.502320  -5.856590
H   4.382310   0.429440  -4.427800
H   0.113290   0.340980  -4.820100
H  -0.094040   0.118050  -2.342230
c6_p
O   0.000000   0.000000   0.000000
I   2.016620   0.000000   0.000000
O  -0.047380   2.781070   0.000000
C  -0.484830   3.886450  -0.200590
C   0.415850   4.972850  -0.751640
C  -0.171030   5.590420  -2.018960
C   1.822530   4.456560  -0.982210
C  -1.935620   4.210030   0.094750
C  -2.052580   5.396580   1.048890
C  -2.677640   2.996420   0.619040
O   4.153830   0.116900  -0.459430
C   4.484610   0.468340  -1.658290
O   5.600460   0.619930  -2.073400
C   2.029970   0.514950  -2.035870
C   3.291850   0.680450  -2.547000
C   3.409660   1.029780  -3.881770
C   2.274180   1.188610  -4.651910
C   0.875220   0.649620  -2.765540
C   1.016510   0.995100  -4.099430
H  -1.130980   6.068840  -1.846070
H  -0.299050   4.835970  -2.792840
H   0.507520   6.345400  -2.406060
H   2.467220   5.264960  -1.316900
H   1.831830   3.677640  -1.740250
H   2.244640   4.035710  -0.075470
H   0.448860   5.752490   0.012560
H  -0.274550   0.908690   0.146580
H  -2.378560   4.506230  -0.858260
H  -1.628880   6.307020   0.634970
H  -1.551720   5.186360   1.991950
H  -3.098960   5.590360   1.267840
H  -2.618090   2.161070  -0.071720
H  -3.726620   3.236650   0.771300
H  -2.263940   2.667740   1.568960
H   2.364790   1.456710  -5.692290
H   4.401690   1.162580  -4.282220
H   0.135370   1.106410  -4.711250
H  -0.083060   0.480100  -2.305840
c7_p
O   0.000000   0.000000   0.000000
I   2.015690   0.000000   0.000000
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O  -0.285260   2.802110   0.000000
C  -1.152140   3.638170  -0.012870
C  -0.908590   5.079840  -0.064480
C  -1.986530   5.953300  -0.072100
C  -1.769910   7.315620  -0.124740
C   0.392430   5.571670  -0.109510
C   0.606120   6.931830  -0.162940
C  -0.475120   7.800870  -0.172370
O   4.149430   0.009620  -0.486140
C   4.473490   0.077270  -1.736420
O   5.587510   0.119000  -2.180000
C   2.017380   0.064230  -2.101500
C   3.276440   0.097660  -2.643590
C   3.385040   0.142690  -4.023240
C   2.243820   0.144450  -4.801490
C   0.857050   0.050960  -2.834040
C   0.989800   0.094200  -4.212060
H  -0.281390   0.920130   0.032780
H  -2.211620   3.342920   0.011490
H  -2.992360   5.562320  -0.035260
H  -2.604270   7.997440  -0.128990
H   1.213430   4.873330  -0.101740
H   1.610910   7.320600  -0.198570
H  -0.304420   8.864620  -0.217100
H   4.374380   0.173310  -4.449890
H   2.327090   0.177630  -5.875840
H  -0.098170   0.000640  -2.340550
H   0.104170   0.085110  -4.827200
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d1-7(sm, ts, p)

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d1_sm
O   0.000000   0.000000   0.000000
I   1.822720   0.000000   0.000000
O   1.995990   2.004750   0.000000
C   0.792700   2.701830  -0.193060
O   3.973730   0.325700  -0.248780
C   4.446300   0.262670  -1.445020
O   5.576510   0.465790  -1.785690
C   2.105080  -0.388770  -2.068070
C   3.406910  -0.154300  -2.455440
C   3.752200  -0.327640  -3.779580
C   2.787430  -0.744230  -4.673180
C   1.095970  -0.822280  -2.920820
C   1.496310  -0.988320  -4.244800
C  -0.327500  -1.115010  -2.563030
H  -0.076380   2.073220   0.026670
H   0.805820   3.544800   0.491390
H   0.725990   3.042780  -1.223710
H   3.037670  -0.887980  -5.712100
H   4.773030  -0.134390  -4.064620
H   0.756200  -1.323960  -4.954340
H  -0.865760  -0.209280  -2.307810
H  -0.413060  -1.761930  -1.697310
H  -0.812880  -1.592490  -3.407720
d2_sm
O   0.000000   0.000000   0.000000
I   1.823760   0.000000   0.000000
O   2.006230   2.003120   0.000000
C   0.797210   2.726370   0.057290
C   0.699190   3.475030   1.360510
O   3.973490   0.330000  -0.247830
C   4.441000   0.296030  -1.447260
O   5.569020   0.511650  -1.787730
C   2.100860  -0.354040  -2.073620
C   3.399070  -0.103060  -2.461980
C   3.738330  -0.243450  -3.791480
C   2.771490  -0.645760  -4.689380
C   1.090940  -0.777980  -2.929820
C   1.485010  -0.910460  -4.259480
C  -0.327560  -1.093100  -2.570980
H   1.573450   4.100990   1.511000
H   0.619320   2.787210   2.198480
H  -0.184530   4.109180   1.360030
```

```
H  -0.053330   2.045340  -0.062570
H   0.809300   3.395070  -0.802010
H   3.016830  -0.763370  -5.732720
H   4.756330  -0.036870  -4.077220
H   0.743780  -1.237030  -4.972090
H  -0.879190  -0.194980  -2.316800
H  -0.403760  -1.740480  -1.705010
H  -0.806010  -1.577600  -3.415700
d3_sm
O   0.000000   0.000000   0.000000
I   1.823430   0.000000   0.000000
O   2.020620   1.988030   0.000000
C   0.829520   2.726320  -0.239850
C   0.887280   3.912640   0.694860
C   0.762760   3.101940  -1.702010
O   3.984520   0.295920  -0.260800
C   4.454120   0.193660  -1.454030
O   5.585410   0.376890  -1.804360
C   2.104700  -0.449900  -2.058540
C   3.409500  -0.243610  -2.451230
C   3.754690  -0.463640  -3.768720
C   2.786860  -0.897740  -4.650280
C   1.092240  -0.900840  -2.899020
C   1.492480  -1.113930  -4.216190
C  -0.335680  -1.163460  -2.535710
H  -0.031070   2.097240   0.008420
H   1.765630   4.517030   0.485960
H   0.933650   3.583250   1.728000
H   0.001290   4.529400   0.565000
H   1.633980   3.688030  -1.982600
H  -0.131670   3.687250  -1.901690
H   0.730010   2.216370  -2.331390
H   3.036780  -1.077410  -5.683700
H   4.778210  -0.291090  -4.057470
H   0.749640  -1.464320  -4.915720
H  -0.862080  -0.245040  -2.302820
H  -0.430710  -1.787310  -1.653940
H  -0.827080  -1.655120  -3.369010
d4_sm
O   0.000000   0.000000   0.000000
I   1.824280   0.000000   0.000000
O   2.017360   1.999840   0.000000
C   0.817770   2.727120   0.136450
C   0.748290   3.413670   1.486600
C   1.864600   4.431090   1.643790
C   0.751370   2.397720   2.616990
O   3.978130   0.324540  -0.241340
C   4.448800   0.287250  -1.439160
O   5.579260   0.495300  -1.776810
C   2.104790  -0.344780  -2.074020
C   3.406710  -0.103450  -2.457170
C   3.749860  -0.244330  -3.785590
C   2.783560  -0.637660  -4.687980
C   1.094690  -0.757840  -2.935660
C   1.493030  -0.891470  -4.263810
C  -0.328680  -1.058510  -2.584020
H   1.813070   5.196180   0.871740
H   2.833980   3.944510   1.565690
H   1.809020   4.927500   2.609780
H   0.571060   2.881060   3.573620
H   1.721180   1.906280   2.688520
H  -0.015070   1.638640   2.472650
H  -0.209720   3.938140   1.500500
H  -0.041220   2.058700   0.004050
H   0.814450   3.446410  -0.682250
H   3.032240  -0.755950  -5.730470
H   4.770620  -0.045310  -4.066890
H   0.751570  -1.209420  -4.980060
H  -0.869010  -0.156390  -2.320020
H  -0.415310  -1.715400  -1.726130
H  -0.811360  -1.526340  -3.435670
d5_sm
O   0.000000   0.000000   0.000000
I   1.824300   0.000000   0.000000
```

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O   2.016740   2.001170   0.000000
C   0.816990   2.723810   0.130080
C   0.728630   3.429140   1.476400
C   1.880140   4.414980   1.614190
C   0.784120   2.399610   2.597720
C  -0.603900   4.165390   1.514570
O   3.978140   0.326170  -0.240790
C   4.449440   0.285940  -1.438230
O   5.580260   0.492380  -1.775660
C   2.105630  -0.345990  -2.073840
C   3.407700  -0.105800  -2.456300
C   3.751500  -0.247980  -3.784410
C   2.785470  -0.640930  -4.687210
C   1.095400  -0.758990  -2.935880
C   1.494510  -0.893520  -4.263780
C  -0.328680  -1.058070  -2.585750
H  -0.041210   2.052100   0.002800
H   1.827640   5.185020   0.846150
H   2.835800   3.907060   1.514810
H   1.851990   4.908350   2.583820
H   0.625190   2.876360   3.562300
H   1.759990   1.918410   2.636970
H   0.018440   1.635860   2.469510
H  -0.687110   4.873560   0.691460
H  -0.703060   4.725680   2.441690
H  -1.441350   3.472860   1.450100
H   0.809090   3.439540  -0.692770
H   3.034750  -0.759960  -5.729470
H   4.772580  -0.049890  -4.065180
H   0.753340  -1.211440  -4.980350
H  -0.869790  -0.154090  -2.329430
H  -0.417860  -1.709160  -1.723840
H  -0.809170  -1.531090  -3.435810
d6_sm
O   0.000000   0.000000   0.000000
I   1.823850   0.000000   0.000000
O   2.027940   1.992030   0.000000
C   0.851280   2.746370   0.236950
C   0.900750   3.293080   1.662110
C   2.054670   4.258180   1.874090
C   0.959450   2.152640   2.667220
C   0.756630   3.776500  -0.888820
C  -0.414220   4.721870  -0.667000
C   0.635690   3.086870  -2.236690
O   3.984790   0.315660  -0.240880
C   4.458000   0.255990  -1.435530
O   5.589930   0.454010  -1.775840
C   2.111710  -0.376140  -2.066630
C   3.416390  -0.147780  -2.449820
C   3.762910  -0.311820  -3.774860
C   2.797570  -0.714650  -4.673980
C   1.103110  -0.800100  -2.925270
C   1.504830  -0.956880  -4.249710
C  -0.322550  -1.088020  -2.573490
H   1.965570   5.146800   1.254240
H   2.999200   3.774900   1.635170
H   2.094560   4.584430   2.910890
H   0.821670   2.524560   3.679210
H   1.933880   1.665170   2.643400
H   0.185760   1.410690   2.476310
H  -0.039570   3.820420   1.823460
H  -0.296520   5.328110   0.226580
H  -1.350060   4.170690  -0.580220
H  -0.509540   5.400090  -1.511570
H   1.481110   2.433650  -2.427700
H   0.596400   3.820060  -3.038680
H  -0.276530   2.492850  -2.284880
H   1.679850   4.355350  -0.884320
H  -0.015760   2.077470   0.153670
H   3.048750  -0.849980  -5.713800
H   4.785570  -0.122370  -4.055840
H   0.764290  -1.282890  -4.963260
H  -0.414940  -1.729420  -1.704620
H  -0.805030  -1.567450  -3.418810
H  -0.858690  -0.178780  -2.325850
d7_sm
O   0.000000   0.000000   0.000000
I   1.822100   0.000000   0.000000
O   1.987700   2.004970   0.000000
C   0.952190   2.615550   0.726230
C   1.115080   2.421280   2.202730
C   0.003240   2.331920   3.027670
C   0.156190   2.165740   4.390540
C   2.384720   2.322920   2.757880
C   2.535860   2.146640   4.121550
C   1.423530   2.073330   4.939990
O   3.991040   0.340380  -0.203710
C   4.483460   0.313410  -1.391490
O   5.624250   0.504130  -1.706420
C   2.136370  -0.249320  -2.083740
C   3.450640  -0.030040  -2.435970
C   3.812630  -0.136710  -3.762800
C   2.852360  -0.471360  -4.694500
C   1.128980  -0.597420  -2.976720
C   1.546780  -0.697160  -4.301750
C  -0.310930  -0.854120  -2.660050
H  -0.020430   2.246070   0.399690
H   1.034320   3.664760   0.442260
H  -0.985030   2.377890   2.596390
H  -0.713820   2.094450   5.023620
H   3.249250   2.380060   2.114470
H   3.525040   2.069330   4.543870
H   1.542410   1.936860   6.003070
H   4.843000   0.044960  -4.019700
H   3.116310  -0.561490  -5.736030
H   0.807920  -0.962970  -5.041540
H  -0.809500   0.051110  -2.332560
H  -0.438190  -1.567190  -1.853340
H  -0.805580  -1.234240  -3.547670
d1_ts
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I   1.855400   0.000000   0.000000
O   1.707680   2.212210   0.000000
C   0.416250   2.535870  -0.034510
O   3.973550   0.450220  -0.282390
C   4.387640   0.587360  -1.496360
O   5.476190   0.939920  -1.849500
C   2.081010  -0.185810  -2.101370
C   3.338820   0.202020  -2.507670
C   3.635010   0.196680  -3.855270
C   2.672280  -0.218530  -4.751610
C   1.084360  -0.642580  -2.953090
C   1.434510  -0.636610  -4.301640
C  -0.274710  -1.136470  -2.568300
H  -0.191340   1.519370   0.011970
H   0.093370   3.090060   0.846940
H   0.111850   2.971670  -0.987150
H   2.886150  -0.233420  -5.808250
H   4.620680   0.510800  -4.156290
H   0.699930  -0.982590  -5.012100
H  -0.930460  -0.318310  -2.291790
H  -0.247630  -1.801240  -1.712240
H  -0.708820  -1.668470  -3.408460
d2_ts
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I   1.853550   0.000000   0.000000
O   1.718000   2.205580   0.000000
C   0.428870   2.551060   0.060140
C   0.039280   3.272500   1.327800
O   3.972870   0.458610  -0.269020
C   4.391990   0.607340  -1.479550
O   5.482550   0.962050  -1.824820
C   2.087380  -0.158220  -2.102290
C   3.346860   0.234010  -2.499190
C   3.647690   0.246090  -3.845740
C   2.687720  -0.156170  -4.750830
C   1.093200  -0.602040  -2.963590
C   1.447740  -0.578420  -4.310730
C  -0.268480  -1.096780  -2.589290
H   0.594890   4.201320   1.424960
H   0.256220   2.657680   2.197690
H  -1.023580   3.499060   1.325860
H  -0.177730   1.540130   0.030170
H   0.110730   3.029870  -0.870890
H   2.905220  -0.157030  -5.806840
H   4.634660   0.563360  -4.139110
H   0.714890  -0.913250  -5.028290
H  -0.920330  -0.280900  -2.297430
H  -0.245020  -1.777550  -1.745660
H  -0.704460  -1.611060  -3.439420
d3_ts
O   0.000000   0.000000   0.000000
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O   1.727410   2.201020   0.000000
C   0.436430   2.560520  -0.033080
C   0.027700   3.336400   1.204280
C   0.048830   3.172630  -1.368320
O   3.972600   0.456300  -0.282860
C   4.381860   0.607610  -1.496120
O   5.466390   0.972860  -1.849990
C   2.080390  -0.179140  -2.102350
C   3.333990   0.221560  -2.508640
C   3.626330   0.230280  -3.857220
C   2.664000  -0.183540  -4.754630
C   1.085070  -0.636620  -2.955580
C   1.430620  -0.615620  -4.305000
C  -0.270060  -1.140730  -2.570120
H  -0.162280   1.548250   0.013390
H   0.554720   4.287420   1.240660
H   0.276550   2.777200   2.101690
H  -1.041420   3.530280   1.202050
H   0.560120   4.123190  -1.504270
H  -1.023060   3.343380  -1.419080
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H   2.874620  -0.186640  -5.812010
H   4.608700   0.554510  -4.158290
H   0.696530  -0.960560  -5.016580
H  -0.928500  -0.328460  -2.282670
H  -0.235860  -1.813070  -1.720200
H  -0.704950  -1.667430  -3.413180
d4_ts
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C   0.022830   3.306430   1.303900
C   0.677250   4.678730   1.333050
C   0.351710   2.501800   2.549020
O   3.976570   0.457220  -0.268370
C   4.391060   0.619260  -1.478560
O   5.478130   0.984470  -1.824380
C   2.088040  -0.152610  -2.101980
C   3.345380   0.247380  -2.498510
C   3.643700   0.267510  -3.845460
C   2.684470  -0.135580  -4.751120
C   1.095290  -0.598300  -2.963830
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H   1.760110   4.578960   1.354740
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H   0.014550   3.019870   3.443040
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H   0.715800  -0.903410  -5.029310
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C  0.016480  3.299240  1.322760
C  0.743250  4.638550  1.363210
C  0.382970  2.468780  2.544070
C -1.487890  3.517740  1.265910
O  3.978060  0.453030 -0.266550
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O  5.485530  0.963820 -1.822340
C  2.090080 -0.157640 -2.101500
C  3.350450  0.233930 -2.496920
C  3.652310  0.246060 -3.843180
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C  1.096510 -0.600590 -2.964090
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d6_ts
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C  0.124980  3.150960  1.504850
C  0.801100  4.500820  1.693500
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C -0.068070  3.355940 -1.110820
C -1.563850  3.611000 -1.037180
C  0.298400  2.650750 -2.402040
O  3.976450  0.479450 -0.318630
C  4.380050  0.538120 -1.540260
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C  2.096800 -0.352130 -2.074050
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C  3.640480 -0.078350 -3.856850
C  2.694450 -0.606350 -4.710690
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C  1.472850 -1.030830 -4.222550
C -0.212470 -1.442000 -2.440590
H  0.442860  5.240910  0.982230
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H  0.611970  4.887280  2.692650
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H  1.621420  2.043810  2.599370
H  0.060090  1.212590  2.471430
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H -1.897090  4.137300 -1.928670
H  1.370230  2.506550 -2.486320
H -0.031240  3.234650 -3.258090
H -0.185210  1.677130 -2.459840
H  0.449040  4.316470 -1.096890
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C -1.083630  3.492380  1.942210
C -1.337930  4.016930  3.193530
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C -0.306300  4.169270  4.104930
O  3.960890  0.498950 -0.238470
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H -1.892650  3.364530  1.238010
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O  5.827210  0.378680 -1.649390
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C  3.004260  1.011440 -4.661600
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C  1.671220  0.925210 -4.310580
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H -0.299710  0.901160  0.107710
H  0.062280  4.684680  0.921680
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H  3.276580  1.227370 -5.682120
H  5.030160  0.861920 -3.920710
H  0.913910  1.073580 -5.064890
H -0.552870  1.431320 -2.153840
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d2_p
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O  4.174440  0.099700 -0.193000
C  4.654950  0.552060 -1.300140
O  5.814650  0.732640 -1.549860
C  2.252470  0.666920 -2.032850
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C  3.015410  0.682120 -4.717180
C  1.248770  0.439710 -3.052060
C  1.681560  0.626780 -4.363200
C -0.225410  0.412340 -2.796930
H -1.526450  4.683510  3.186590
H -0.831330  3.072640  3.352840
H -2.520650  3.348980  3.741550
H -3.386980  1.621200  2.166920
H -1.739580  1.145850  1.774250
H -2.851490  1.576360  0.491560
H -2.974420  3.904830  1.357850
H -2.464570  6.007620  1.044630
H -2.221680  5.721850 -0.677300
H -1.353740  7.012730  0.134980
H  1.383600  4.542130 -0.257960
H  0.916350  6.225710 -0.489360
```

```
H  0.195050  4.956210 -1.475100
H -0.161380  5.320260  1.527900
H -0.303170  0.912980  0.015700
H  3.290010  0.828890 -5.749330
H  5.039770  0.573920 -3.964670
H  0.925770  0.730050 -5.126500
H -0.523950 -0.430320 -2.187340
H -0.749260  0.375100 -3.746460
H -0.542660  1.309390 -2.271730
d7_p
O  0.000000  0.000000  0.000000
I  2.013710  0.000000  0.000000
O  0.068340  2.830100  0.000000
C -0.003440  4.003090  0.258510
C  0.830560  5.038160 -0.350120
C  0.645840  6.362810  0.022120
C  1.425870  7.353770 -0.540420
C  1.801850  4.702840 -1.287890
C  2.580840  5.692940 -1.845300
C  2.391170  7.015800 -1.472330
O  4.178790  0.102110 -0.193370
C  4.654520  0.650630 -1.256580
O  5.810590  0.877230 -1.486800
C  2.254570  0.754950 -1.997420
C  3.587590  0.992450 -2.260070
C  3.953220  1.520330 -3.484660
C  2.981230  1.786160 -4.422730
C  1.239250  0.972360 -2.920040
C  1.659260  1.503770 -4.138240
C -0.219300  0.689020 -2.744420
H -0.287590  0.899720  0.159220
H -0.733100  4.366120  0.999050
H -0.108700  6.612500  0.753250
H  1.285960  8.383250 -0.253920
H  1.932360  3.668740 -1.563870
H  3.338780  5.438520 -2.567920
H  3.003890  7.787480 -1.910740
H  5.002890  1.691470 -3.658640
H  3.246650  2.193720 -5.385010
H  0.904740  1.687330 -4.887580
H -0.686480  1.441320 -2.115900
H -0.401740 -0.266970 -2.271870
H -0.703590  0.708460 -3.715270
```

e4, 5(sm, ts, p)

```
e4_sm
I  0.000000  0.000000  0.000000
O  1.816860  0.000000  0.000000
O -0.432230  1.949320  0.000000
H -2.202870 -2.624580  3.654720
C  0.216220  3.126570  0.424780
H -0.415130  0.975890  5.119070
H -1.858480 -0.964370  5.494180
C -0.486570 -0.258410  2.039420
O -0.460650 -2.113860  0.121720
C -1.163120 -2.478800  1.153430
C -1.160910 -1.441660  2.242800
O -1.734080 -3.520340  1.284470
C -1.677480 -1.697130  3.496580
C -1.462590 -0.780080  4.508440
C -0.669300  0.331990  4.290650
C -0.127460  0.620920  3.041160
C  0.931350  1.676030  2.899920
H  1.633730  1.498740  3.712760
C  0.491540  3.130130  2.958890
H  1.507760  1.490580  1.996710
H  1.398440  3.731040  3.021240
H -0.060730  3.317060  3.879080
H -1.350510  3.237770  1.830200
H  1.300020  2.998600  0.440480
H -0.007150  3.860030 -0.347080
C -0.323900  3.593380  1.764030
H -0.373030  4.681130  1.775930
```

```
e5_sm
I  0.000000  0.000000  0.000000
O  1.818820  0.000000  0.000000
O -0.342730  1.973280  0.000000
C  0.597920  3.016760 -0.087370
C -0.579380 -0.125370  2.031740
O -0.392290 -2.111270  0.241070
C -1.129310 -2.430240  1.264140
C -1.221300 -1.321130  2.275750
O -1.666510 -3.482640  1.442110
C -1.810500 -1.515570  3.507580
C -1.701560 -0.523900  4.463980
C -0.942910  0.605060  4.218170
C -0.327080  0.838330  2.990330
C  0.695500  1.932940  2.871810
C  0.202840  3.368640  3.029070
C -0.011870  4.221790  0.604590
C -0.694110  3.910700  1.928900
H  1.552310  2.734780  0.354750
H  0.794610  3.245240 -1.134820
H -2.309720 -2.452140  3.693660
H -2.156020 -0.657360  5.432510
H -0.775280  1.315060  5.013770
H  1.408910  1.741340  3.673560
H  1.266380  1.800680  1.962910
H  1.081120  4.007580  3.128280
H -0.326540  3.446330  3.978750
H  0.767180  4.973340  0.741580
H -0.754000  4.658060 -0.061610
H -1.510690  3.215690  1.746330
H -1.147760  4.832580  2.290280
e4_ts
I -0.086840  0.115340  0.005900
O  1.708180  0.305660 -0.203440
O -0.678470  2.031910 -0.144770
H -2.183860 -1.240830  4.416360
C  0.294570  3.038830  0.077900
H  1.190270  1.347710  4.932540
H -0.633500  0.037630  5.915930
C -0.167070  0.142960  2.146890
O -1.836970 -1.274820  0.531740
C -2.132840 -1.402430  1.768760
C -1.204200 -0.606840  2.662660
O -3.014400 -2.052880  2.261190
C -1.373670 -0.643620  4.031960
C -0.512940  0.065290  4.844760
C  0.513220  0.804340  4.290900
C  0.726520  0.875140  2.916980
C  1.851850  1.730860  2.415310
H  2.687200  1.608320  3.101260
C  1.498430  3.216150  2.350030
H  2.195470  1.375550  1.451190
H  2.370210  3.741890  1.960620
H  1.335950  3.598060  3.357540
H -0.626270  3.182640  1.981070
H  1.285380  2.681220 -0.218650
H  0.014760  3.815230 -0.629730
C  0.279440  3.559300  1.508860
H  0.175250  4.642620  1.487380
e5_ts
I -0.099860  0.090680  0.028190
O  1.712650  0.206300 -0.047990
O -0.565390  2.051630  0.218880
C  0.513550  2.962760  0.126080
C -0.306170 -0.193870  2.133010
O -1.991940 -1.186070  0.238620
C -2.339100 -1.519670  1.423740
C -1.399060 -0.965150  2.473760
O -3.277150 -2.188440  1.762970
C -1.626160 -1.234550  3.807480
C -0.764340 -0.728050  4.759280
C  0.306590  0.054850  4.379440
C  0.576390  0.364320  3.048130
C  1.736740  1.276580  2.763460
```

```
C   1.484120   2.714080   3.226330
C   0.380660   3.976030   1.243500
C   0.259600   3.414890   2.651100
H   1.472410   2.439310   0.165650
H   0.459490   3.456240  -0.843370
H  -2.479900  -1.843450   4.054640
H  -0.925090  -0.941850   5.803890
H   0.972240   0.450280   5.131550
H   2.591890   0.889730   3.315900
H   2.025050   1.224070   1.723280
H   2.379380   3.298680   3.011560
H   1.387080   2.708430   4.311610
H   1.238830   4.647480   1.175510
H  -0.503120   4.578710   1.040730
H  -0.602590   2.751080   2.694430
H   0.021200   4.252360   3.304520
e4_p
I   0.000000   0.000000   0.000000
O   1.821450   0.000000   0.000000
O  -0.214170   1.987200   0.000000
H  -3.146000  -0.905090   3.823090
C   0.926740   2.653350   0.512630
H   0.848880  -0.134010   5.166910
H  -1.455020  -0.803520   5.671080
C  -0.389950  -0.186150   2.084740
O  -2.227150   0.000700   0.114860
C  -2.743020  -0.378570   1.228890
C  -1.718100  -0.456690   2.336730
O  -3.892530  -0.637220   1.452400
C  -2.105870  -0.690960   3.639820
C  -1.166160  -0.615320   4.649340
C   0.136740  -0.252530   4.364370
C   0.574250  -0.006950   3.065340
C   1.936580   0.569400   2.837760
H   2.593300   0.224900   3.632990
C   1.920750   2.107560   2.869980
H   2.347840   0.226590   1.895920
H   2.915960   2.446180   2.582990
H   1.775130   2.430100   3.900780
H  -0.128280   2.571290   2.358770
H   1.836810   2.131420   0.200600
H   0.902650   3.607230  -0.006940
C   0.875190   2.834110   2.028510
H   0.979230   3.896430   2.243460
e5_p
I   0.000000   0.000000   0.000000
O   1.822740   0.000000   0.000000
O  -0.213240   1.998150   0.000000
C   0.999670   2.704450   0.173280
C  -0.371930  -0.301150   2.066300
O  -2.222600   0.050080   0.135550
C  -2.726440  -0.442920   1.210780
C  -1.693080  -0.625090   2.298210
O  -3.873160  -0.727410   1.415900
C  -2.062810  -1.004740   3.571310
C  -1.111480  -1.020850   4.573600
C   0.177810  -0.592180   4.320700
C   0.595270  -0.191160   3.053790
C   1.921450   0.490130   2.898320
C   1.823240   1.959180   3.346490
C   0.958050   3.536930   1.436270
C   0.704590   2.819610   2.755460
H   1.847110   2.008900   0.170680
H   1.112660   3.344400  -0.700000
H  -3.096410  -1.257400   3.741550
H  -1.383950  -1.327460   5.570900
H   0.891650  -0.534750   5.128560
H   2.645460  -0.009100   3.538940
H   2.285250   0.406440   1.881980
H   2.788320   2.431400   3.161720
H   1.691130   1.959790   4.427840
H   1.902220   4.082510   1.486950
H   0.176950   4.284630   1.310940
H  -0.217260   2.245160   2.676890
```

```
H   0.488620   3.598430   3.484320
```

f2-5(sm, ts, p)

```
f2_p
I   0.000000   0.000000   0.000000
O   3.744400   0.000000   0.000000
C   3.793680   1.195850   0.000000
H   2.225050  -0.533540   1.033570
O   1.390780  -0.270770   1.434510
H   4.539070   1.712760  -0.623410
C   0.688960   1.941320  -0.628510
O  -1.456730   0.533020  -1.509610
C  -1.366990   1.698410  -2.051980
C  -0.173270   2.472380  -1.562760
O  -2.111400   2.166400  -2.866270
C   0.069300   3.732870  -2.078570
C   1.168640   4.442620  -1.653770
C   2.023560   3.882550  -0.724660
C   1.818050   2.617700  -0.180400
H  -0.629260   4.112310  -2.806250
H   1.367960   5.428520  -2.040900
H   2.886060   4.440020  -0.392680
C   2.857270   2.089910   0.772580
H   2.415390   1.538800   1.592200
H   3.428350   2.932260   1.152970
f3_p
O   0.000000   0.000000   0.000000
I   2.020720   0.000000   0.000000
O  -0.325330   2.779280   0.000000
C  -0.764690   3.337800  -0.963880
O   4.176190   0.082480  -0.161940
C   4.682190   0.756750  -1.136370
O   5.848730   0.940110  -1.344180
C   2.286880   1.128770  -1.823630
C   3.635180   1.321380  -2.055960
C   4.041830   2.030260  -3.169260
C   3.098720   2.523520  -4.043210
C   1.299570   1.600190  -2.677380
C   1.761970   2.298540  -3.793270
H  -0.282140   0.881370   0.254170
H  -1.111380   4.379690  -0.874880
C  -0.927230   2.734530  -2.320950
H   3.398490   3.067230  -4.924030
H   5.101950   2.159660  -3.313370
H   1.026160   2.659340  -4.497090
C  -0.193460   1.424130  -2.573990
H  -0.454980   0.689160  -1.825510
H  -0.536080   1.037020  -3.531570
H  -2.004510   2.593490  -2.448140
H  -0.656730   3.498050  -3.050950
f4_p
C   0.000000   0.000000   0.000000
H   2.671870   0.000000   0.000000
O   3.427450   0.595290   0.000000
I   4.130020   0.777050   1.881370
O   0.963380  -0.703240  -0.114940
H  -0.863900  -0.155260  -0.667210
C   2.998240   2.546320   2.414990
O   4.801910   1.140950   3.906630
C   4.332970   2.170450   4.522780
C   3.352170   2.948280   3.689870
O   4.608390   2.519070   5.636480
C   2.795820   4.094230   4.221930
C   1.905820   4.830250   3.471160
C   1.569990   4.399430   2.206490
C   2.089610   3.239940   1.627270
H   3.096660   4.372770   5.218560
H   1.476300   5.737720   3.863690
H   0.877460   4.981240   1.616210
C  -0.137730   1.123750   0.972280
H   0.549500   0.979930   1.802190
H  -1.153200   1.095980   1.363490
C   0.106390   2.474910   0.286550
```

```
H  -0.277590   2.445960  -0.733600
H  -0.477280   3.232030   0.804460
C   1.574590   2.901710   0.252360
H   2.193540   2.155230  -0.227470
H   1.645330   3.805810  -0.350000
f5_p
C   0.000000   0.000000   0.000000
H   2.702930   0.000000   0.000000
O   3.511350   0.525000   0.000000
I   3.802510   1.217180   1.874830
O   0.942380  -0.726340   0.157590
H  -1.009100  -0.371430   0.231810
O   3.884390   2.107460   3.851300
C   3.163480   3.157330   4.053770
C   2.597080   3.724850   2.781220
C   2.809280   3.108120   1.563040
O   2.957840   3.686020   5.110070
C   1.915290   4.924250   2.822940
C   1.486290   5.500180   1.646050
C   1.772330   4.888800   0.444260
C   2.451370   3.672010   0.347010
H   1.762640   5.376790   3.789000
H   0.960830   6.441490   1.658120
H   1.488950   5.375820  -0.476650
C   2.794350   3.196760  -1.042120
H   3.363840   4.007880  -1.494470
H   3.439110   2.328320  -1.010020
C   1.604280   2.897890  -1.958990
H   0.854960   3.686720  -1.882780
H   1.972590   2.933710  -2.982750
C   0.957320   1.537670  -1.752920
H   1.738420   0.783120  -1.751450
H   0.313020   1.317470  -2.602790
C   0.129200   1.414540  -0.473480
H   0.612830   1.952240   0.342750
H  -0.854890   1.859650  -0.596930
f2_sm
I   0.000000   0.000000   0.000000
O   1.998600   0.000000   0.000000
C   2.608080   1.268120   0.000000
H   2.093870   1.940770   0.689140
O  -0.204950   0.979110   1.515780
H   3.623960   1.133360   0.359930
C   0.079010   1.403960  -1.567320
O  -2.051280   0.119800  -0.563390
C  -2.368190   0.953920  -1.513380
C  -1.174590   1.674790  -2.070960
O  -3.467500   1.140630  -1.938430
C  -1.302530   2.597130  -3.087930
C  -0.170630   3.239340  -3.552260
C   1.066940   2.969760  -2.999640
C   1.238400   2.043240  -1.974790
H  -2.285830   2.792490  -3.482670
H  -0.250730   3.968180  -4.342720
H   1.937100   3.498730  -3.357670
C   2.609420   1.816930  -1.405510
H   3.151970   2.759580  -1.437520
H   3.145130   1.115610  -2.045450
f3_sm
O   0.000000   0.000000   0.000000
I   1.818890   0.000000   0.000000
O   2.151010   1.969090   0.000000
C   1.276800   2.940750  -0.514930
O   2.206760  -2.111260  -0.210750
C   2.857210  -2.467040  -1.278470
O   3.353540  -3.535660  -1.476480
C   2.327360  -0.158130  -2.041420
C   2.907340  -1.376060  -2.313230
C   3.413910  -1.608190  -3.577130
C   3.284010  -0.624520  -4.534600
C   2.059410   0.812040  -2.994730
C   2.588600   0.539160  -4.252470
H   0.238290   2.657480  -0.332870
H   1.479830   3.848400   0.049700
```

```
C  1.512550  3.164550 -1.985110
H  3.674800 -0.780660 -5.527140
H  3.870410 -2.563230 -3.777870
H  2.411250  1.252680 -5.042330
C  1.109030  1.970300 -2.843230
H  0.167010  1.571170 -2.464680
H  0.901710  2.321790 -3.849750
H  0.911180  4.017350 -2.298590
H  2.555140  3.427690 -2.152290
f4_sm
C  0.000000  0.000000  0.000000
H  1.094550  0.000000  0.000000
O  2.152590  1.858930  0.000000
I  0.639290  2.738240  0.505120
O -0.485190  1.102510  0.746460
H -0.327060 -0.852210  0.589340
C -0.194790  3.206540 -1.397780
O -1.247170  3.812310  1.014460
C -1.815450  4.455500  0.058150
C -1.243250  4.095540 -1.293080
O -2.713310  5.246240  0.140870
C -1.828660  4.560720 -2.452710
C -1.372450  4.100910 -3.672590
C -0.378810  3.141790 -3.730010
C  0.241240  2.642750 -2.587400
H -2.645210  5.257490 -2.358060
H -1.817180  4.461930 -4.586190
H -0.073220  2.741700 -4.684850
C -0.561080 -0.046830 -1.419840
H -1.365970  0.683520 -1.481320
H -1.040210 -1.014650 -1.558900
C  0.413830  0.134320 -2.580100
H  1.163870 -0.655590 -2.549650
H -0.155210 -0.021600 -3.496400
C  1.166220  1.471540 -2.695390
H  1.941680  1.521990 -1.940490
H  1.647380  1.501360 -3.670050
f5_sm
C  0.000000  0.000000  0.000000
H  1.090110  0.000000  0.000000
O  1.763760  2.197790  0.000000
I  0.386850  2.623650  1.115840
O -0.487520  0.828780  1.040330
H -0.336190 -0.981950  0.324650
O -1.406520  2.951450  2.347010
C -2.388190  3.582700  1.807230
C -2.125630  3.933140  0.363640
C -0.941050  3.581570 -0.253780
O -3.420540  3.897440  2.328280
C -3.096340  4.578590 -0.372050
C -2.861670  4.852120 -1.704510
C -1.677470  4.460280 -2.294000
C -0.666510  3.797290 -1.597590
H -4.013240  4.840800  0.129320
H -3.606950  5.363170 -2.292760
H -1.511060  4.661950 -3.341370
C  0.532520  3.354020 -2.388880
H  0.731500  4.146720 -3.107000
H  1.409020  3.243290 -1.762110
C  0.314250  2.050920 -3.176580
H -0.679140  2.055400 -3.628110
H  1.020610  2.068450 -4.005190
C  0.545320  0.755730 -2.408690
H  1.505560  0.836620 -1.906190
H  0.640610 -0.046900 -3.137940
C -0.532120  0.371230 -1.383240
H -1.256190  1.171700 -1.252420
H -1.114400 -0.463640 -1.766720
f2_ts
I  0.000000  0.000000  0.000000
O  2.261830  0.000000  0.000000
C  2.564360  1.296330  0.000000
H  1.730940  1.870940  0.600720
O  0.213600  1.684930  0.725440
```

```
H  3.449730  1.506300  0.603630
C  0.344280  0.649840 -1.965250
O -1.613390 -1.017190 -1.153120
C -1.714210 -0.701720 -2.402080
C -0.611110  0.219400 -2.859100
O -2.554500 -1.074350 -3.170300
C -0.515610  0.626260 -4.172940
C  0.534600  1.443260 -4.546730
C  1.485840  1.831240 -3.624510
C  1.435430  1.444810 -2.286330
H -1.265630  0.287930 -4.868410
H  0.624370  1.772340 -5.569470
H  2.312580  2.448720 -3.941920
C  2.555760  1.900240 -1.386770
H  2.531600  2.987290 -1.325460
H  3.485970  1.633380 -1.888590
f3_ts
O -0.004080  0.029060 -0.074420
I  1.835060  0.020100 -0.035260
O  1.727390  2.212600  0.129310
C  0.437940  2.564240 -0.058300
O  3.869570 -0.863360 -0.400540
C  4.303550 -0.852230 -1.608990
O  5.324010 -1.325330 -2.026180
C  2.172030  0.386440 -2.100030
C  3.366130 -0.128760 -2.547390
C  3.717110  0.058760 -3.871400
C  2.873390  0.768870 -4.695740
C  1.293740  1.133360 -2.876310
C  1.694110  1.294940 -4.198360
H -0.236200  1.660300  0.169450
H  0.156890  3.299710  0.699100
H  0.105520  2.949750 -1.487790
H  3.131220  0.927450 -5.730530
H  4.653930 -0.355110 -4.205520
H  1.048810  1.859890 -4.853100
C -0.005120  1.763850 -2.445990
H -0.651080  1.008930 -2.007850
H -0.490880  2.114230 -3.352300
H -0.858730  3.456440 -1.479530
H  0.845410  3.663020 -1.847670
f4_ts
C  0.000000  0.000000  0.000000
H  1.162260  0.000000  0.000000
O  2.344070  1.094760  0.000000
I  1.278470  2.551040  0.385040
O -0.402540  1.154650  0.563590
H -0.228770 -0.822760  0.680690
C  0.635700  2.992810 -1.608700
O -0.055430  4.281700  0.672930
C -0.506190  4.867740 -0.380700
C -0.126160  4.142050 -1.646560
O -1.164570  5.868120 -0.427130
C -0.604160  4.586110 -2.862490
C -0.324400  3.864130 -4.004360
C  0.395440  2.689440 -3.919620
C  0.897020  2.195810 -2.716250
H -1.197130  5.485770 -2.868020
H -0.684380  4.202640 -4.962660
H  0.581790  2.110760 -4.811630
C -0.478340 -0.180570 -1.440440
H -1.132660  0.660270 -1.662470
H -1.105520 -1.070830 -1.478810
C  0.574420 -0.314950 -2.534200
H  1.166620 -1.215230 -2.372390
H  0.036880 -0.469550 -3.469490
C  1.561330  0.851870 -2.724980
H  2.334500  0.801160 -1.971600
H  2.037890  0.724700 -3.694180
f5_ts
C  0.000000  0.000000  0.000000
H  1.159480  0.000000  0.000000
O  2.351230  1.071790  0.000000
I  1.321530  2.499060  0.559390
```

```
O -0.392940  1.137780  0.599240
H -0.240970 -0.850640  0.642200
O -0.118260  4.059680  1.080720
C -0.645430  4.732560  0.116970
C -0.171280  4.267810 -1.235490
C  0.721270  3.220630 -1.363810
O -1.423630  5.638230  0.213140
C -0.666630  4.871750 -2.371140
C -0.260160  4.416710 -3.608830
C  0.610290  3.351960 -3.697500
C  1.132670  2.695480 -2.580680
H -1.363520  5.683340 -2.242620
H -0.627410  4.884140 -4.508340
H  0.912100  2.992200 -4.669710
C  2.021280  1.510970 -2.858960
H  2.715140  1.833770 -3.632970
H  2.605230  1.230010 -1.992960
C  1.264720  0.285440 -3.399310
H  0.475680  0.617890 -4.075010
H  1.966960 -0.275980 -4.013950
C  0.678680 -0.689280 -2.384090
H  1.492550 -1.095810 -1.783410
H  0.284130 -1.531900 -2.948820
C -0.416970 -0.137660 -1.461720
H -0.750160  0.840540 -1.799730
H -1.295760 -0.778550 -1.506290
```

g1-13(sm, ts, p)

```
g01_sm
I  0.000000  0.000000  0.000000
O  1.818470  0.000000  0.000000
O -0.158420  2.007970  0.000000
H  1.875270  2.379790 -0.210270
C  0.983310  2.798820  0.247630
H  1.170570  2.906220  1.316480
H  0.778130  3.776430 -0.178850
C -0.685250  0.001190  1.986100
O -0.121120 -2.086070  0.432400
C -0.460740 -2.441230  1.641090
C -0.775180 -1.263260  2.514650
O -0.549200 -3.562800  2.038860
C -1.163590 -1.394260  3.834620
C -1.430620 -0.260420  4.579160
C -1.318380  1.001390  4.015500
C -0.935440  1.152080  2.693270
H -0.861950  2.116330  2.222100
H -1.530520  1.877660  4.606290
H -1.728880 -0.357030  5.610570
H -1.241070 -2.386350  4.248550
g02_sm
I  0.000000  0.000000  0.000000
O  1.817940  0.000000  0.000000
O -0.140800  2.012670  0.000000
H  1.890640  2.329560 -0.310810
C  1.017110  2.807690  0.124580
H  1.239580  3.024240  1.169690
H  0.813860  3.739220 -0.395640
C -0.648190  0.019380  1.996940
O -0.216190 -2.083630  0.415440
C -0.628050 -2.428320  1.604870
C -0.843310 -1.244330  2.500130
O -0.829560 -3.544620  1.975150
C -1.185520 -1.373040  3.833070
C -1.276510 -0.242060  4.622500
C -1.025010  1.014330  4.092150
C -0.695300  1.163260  2.756340
H -0.526290  2.127850  2.311920
H -1.085060  1.887740  4.721320
H -1.531990 -0.337790  5.665400
H -1.350150 -2.363470  4.224810
g03_sm
I  0.000000  0.000000  0.000000
O  1.816990  0.000000  0.000000
```

```
O  -0.136700   2.016860   0.000000
H   1.928610   2.237880  -0.088310
C   1.016680   2.826750  -0.002530
H   1.062880   3.404060   0.920930
H   0.952640   3.513710  -0.843220
C  -0.592350   0.041390   2.011710
O  -0.324660  -2.076720   0.409900
C  -0.803100  -2.392870   1.582190
C  -0.904750  -1.206930   2.495730
O  -1.124070  -3.488130   1.930780
C  -1.202550  -1.333530   3.839500
C  -1.110530  -0.226460   4.661820
C  -0.710230   1.000340   4.155070
C  -0.429220   1.148890   2.807890
H  -0.149200   2.097080   2.384950
H  -0.611010   1.849840   4.810920
H  -1.326690  -0.322520   5.713540
H  -1.463520  -2.309380   4.215130
g04_sm
I   0.000000   0.000000   0.000000
O   1.817760   0.000000   0.000000
O  -0.129890   2.021460   0.000000
H   1.931080   2.257390  -0.130570
C   1.005760   2.823970  -0.222800
H   1.007790   3.622990   0.516520
H   0.957240   3.266160  -1.216150
C  -0.546290   0.089920   2.020420
O  -0.452570  -2.058450   0.434660
C  -1.003000  -2.312430   1.590060
C  -0.987690  -1.120010   2.502700
O  -1.452980  -3.363820   1.932020
C  -1.255160  -1.228010   3.854600
C  -0.985220  -0.157730   4.686470
C  -0.428520   1.007480   4.181830
C  -0.182010   1.141090   2.826610
H   0.217960   2.047000   2.406590
H  -0.176940   1.818400   4.845660
H  -1.173490  -0.242420   5.744530
H  -1.621360  -2.169750   4.229450
g05_sm
I   0.000000   0.000000   0.000000
O   1.819340   0.000000   0.000000
O  -0.116820   2.022900   0.000000
H   1.758700   2.412760  -0.791830
C   0.720760   2.726550  -0.883100
H   0.642180   3.776480  -0.615710
H   0.400770   2.613550  -1.921180
C  -0.515670   0.192590   2.016300
O  -0.635220  -2.011340   0.500080
C  -1.250040  -2.153150   1.641400
C  -1.103300  -0.943650   2.522150
O  -1.838550  -3.127570   2.002090
C  -1.358480  -0.996130   3.879750
C  -0.922810   0.034520   4.691500
C  -0.205930   1.097010   4.162760
C   0.031470   1.178990   2.801980
H   0.562350   2.002650   2.358250
H   0.183000   1.864100   4.812230
H  -1.099760  -0.011270   5.753920
H  -1.839170  -1.875560   4.275870
g06_sm
I   0.000000   0.000000   0.000000
O   1.820070   0.000000   0.000000
O  -0.109480   2.023620   0.000000
H   1.712830   2.409680  -0.907760
C   0.667820   2.711520  -0.947220
H   0.594880   3.767000  -0.701670
H   0.289950   2.570600  -1.962390
C  -0.487340   0.208560   2.020050
O  -0.732630  -1.986730   0.505570
C  -1.366550  -2.086650   1.640030
C  -1.145020  -0.889600   2.523710
O  -2.020530  -3.020030   1.997390
C  -1.386320  -0.936680   3.884080

C  -0.863350   0.049700   4.699410
C  -0.071210   1.057700   4.171300
C   0.152730   1.135670   2.808160
H   0.743820   1.918640   2.366430
H   0.388040   1.782980   4.822830
H  -1.028640   0.005920   5.763800
H  -1.922590  -1.783820   4.279200
g07_sm
I   0.000000   0.000000   0.000000
O   1.819440   0.000000   0.000000
O  -0.387810   1.952670   0.000000
H   1.658960   2.343560   0.061700
C   0.702810   2.766490   0.378290
H   0.709470   2.915640   1.455230
H   0.545890   3.712930  -0.129890
C  -0.139180  -0.278800   2.070730
O  -2.209790  -0.305450   0.371290
C  -2.554300  -0.654700   1.558180
C  -1.400530  -0.562880   2.533220
O  -3.637950  -0.997490   1.942790
C  -1.583530  -0.615670   3.902440
C  -0.538260  -0.283270   4.745220
C   0.688550   0.115610   4.234910
C   0.901740   0.138970   2.867840
H   1.853670   0.396600   2.430190
H   1.482300   0.413310   4.900500
H  -0.688010  -0.300950   5.812910
H  -2.564150  -0.867440   4.272300
g08_sm
I   0.000000   0.000000   0.000000
O   1.820530   0.000000   0.000000
O  -0.357660   1.959860   0.000000
H   1.695110   2.311930   0.040930
C   0.751000   2.752420   0.367670
H   0.773520   2.898360   1.444940
H   0.605800   3.701910  -0.137040
C  -0.140210  -0.296850   2.066880
O  -2.211500  -0.195020   0.375490
C  -2.573500  -0.520720   1.564590
C  -1.412790  -0.511650   2.534490
O  -3.676460  -0.791320   1.951400
C  -1.586160  -0.584410   3.903880
C  -0.510730  -0.349890   4.742030
C   0.737590  -0.029320   4.228210
C   0.938950   0.016090   2.859680
H   1.899700   0.222640   2.413980
H   1.557480   0.190060   4.892550
H  -0.650560  -0.385560   5.810600
H  -2.577790  -0.778120   4.279260
g09_sm
I   0.000000   0.000000   0.000000
O   1.822120   0.000000   0.000000
O  -0.302340   1.971740   0.000000
H   1.761730   2.241510   0.017020
C   0.838030   2.732570   0.331110
H   0.874270   2.911850   1.402980
H   0.728810   3.669170  -0.205890
C  -0.144020  -0.329740   2.059670
O  -2.202520  -0.018550   0.385630
C  -2.587840  -0.283840   1.584650
C  -1.425700  -0.417060   2.540830
O  -3.711970  -0.415060   1.980780
C  -1.585380  -0.532610   3.908790
C  -0.473180  -0.493030   4.731270
C   0.800360  -0.327450   4.205470
C   0.984560  -0.231920   2.836750
H   1.953930  -0.121980   2.375490
H   1.653710  -0.268660   4.861270
H  -0.598700  -0.568610   5.799540
H  -2.587030  -0.616950   4.297800
g10_sm
I   0.000000   0.000000   0.000000
O   1.823510   0.000000   0.000000
O  -0.251230   1.984360   0.000000

H   1.820630   2.163630   0.020350
C   0.916560   2.718710   0.285170
H   0.950640   2.968790   1.342690
H   0.858850   3.618680  -0.318780
C  -0.146050  -0.358860   2.052920
O  -2.185150   0.119460   0.401000
C  -2.577110  -0.082320   1.611510
C  -1.423280  -0.337340   2.550970
O  -3.703250  -0.088670   2.022080
C  -1.576620  -0.506180   3.914010
C  -0.456160  -0.657970   4.712210
C   0.820490  -0.635460   4.168260
C   0.996940  -0.478280   2.803960
H   1.965280  -0.455490   2.328540
H   1.682640  -0.738580   4.806880
H  -0.574960  -0.783200   5.776580
H  -2.575480  -0.496020   4.318860
g11_sm
I   0.000000   0.000000   0.000000
O   1.825110   0.000000   0.000000
O  -0.204450   1.997190   0.000000
H   1.869840   2.095280   0.015300
C   0.987560   2.706560   0.231480
H   1.028570   3.027770   1.269510
H   0.973050   3.561950  -0.437000
C  -0.148490  -0.384180   2.046780
O  -2.163620   0.238400   0.418390
C  -2.550400   0.100820   1.640310
C  -1.412860  -0.262920   2.562530
O  -3.664830   0.209660   2.066850
C  -1.570940  -0.486550   3.917010
C  -0.469440  -0.822670   4.684680
C   0.792480  -0.937010   4.118400
C   0.973970  -0.717050   2.763340
H   1.934270  -0.778900   2.275670
H   1.638980  -1.198430   4.732260
H  -0.592200  -0.998820   5.741410
H  -2.558530  -0.389700   4.337720
g12_sm
I   0.000000   0.000000   0.000000
O   1.826270   0.000000   0.000000
O  -0.163320   2.007000   0.000000
H   1.910300   2.046340   0.008750
C   1.046120   2.694930   0.190880
H   1.097130   3.064720   1.212080
H   1.059450   3.515380  -0.520510
C  -0.150860  -0.415390   2.039430
O  -2.139900   0.342560   0.439860
C  -2.509470   0.266860   1.673040
C  -1.394480  -0.201190   2.575190
O  -3.599790   0.485480   2.118590
C  -1.567870  -0.483240   3.916730
C  -0.510500  -0.999750   4.645480
C   0.719940  -1.241870   4.051220
C   0.918120  -0.955640   2.710980
H   1.862860  -1.099830   2.210850
H   1.527960  -1.657720   4.630730
H  -0.647060  -1.228990   5.690200
H  -2.536750  -0.305700   4.354290
g13_sm
I   0.000000   0.000000   0.000000
O   1.827430   0.000000   0.000000
O  -0.123370   2.017680   0.000000
H   1.947590   2.002900   0.004490
C   1.100790   2.684730   0.149790
H   1.162500   3.103450   1.151420
H   1.139410   3.466190  -0.603830
C  -0.157290  -0.434860   2.035240
O  -2.114480   0.439270   0.458130
C  -2.456270   0.440720   1.702010
C  -1.371450  -0.118660   2.589450
O  -3.510260   0.772550   2.163950
C  -1.571070  -0.437070   3.919080
C  -0.584410  -1.118450   4.610560
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C  0.596290 -1.495280  3.987040
C  0.823420 -1.165510  2.661540
H  1.743210 -1.403440  2.151150
H  1.342030 -2.051740  4.530960
H -0.744620 -1.382250  5.643670
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g01_ts
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O  0.441200  2.311830  0.000000
H  2.205240  1.304080  0.043080
C  1.741500  2.467730  0.057840
H  2.128100  2.842680  1.008310
H  2.194770  2.895270 -0.837930
C -0.416980  0.130110  2.055460
O -0.837390 -2.119930  0.584870
C -0.869610 -2.339280  1.843580
C -0.725910 -1.066910  2.657920
O -1.046040 -3.383150  2.413450
C -1.045420 -1.033790  4.002560
C -1.121030  0.176470  4.667650
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H -1.005020  2.309770  4.509670
H -1.388140  0.195580  5.712070
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g02_ts
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H  2.224710  1.337010  0.015950
C  1.737590  2.468330  0.024640
H  2.133840  2.869900  0.960950
H  2.155240  2.910850 -0.881150
C -0.375820  0.131120  2.065400
O -1.103590 -1.958310  0.512570
C -1.184200 -2.225340  1.765550
C -0.848680 -1.029970  2.630220
O -1.527190 -3.255560  2.277640
C -1.131860 -1.010440  3.983010
C -0.998070  0.164560  4.699870
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H -0.013150  2.234250  2.197550
H -0.550930  2.257720  4.626030
H -1.233600  0.178030  5.751850
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g03_ts
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O  0.413480  2.283130  0.000000
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C  1.720880  2.475070 -0.016260
H  2.129240  2.905450  0.902350
H  2.096990  2.928500 -0.934760
C -0.354500  0.129530  2.069460
O -1.271360 -1.832880  0.468060
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H  0.313430  2.151250  2.273350
H -0.146910  2.147920  4.712690
H -1.110370  0.150180  5.779310
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O  0.376290  2.268790  0.000000
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C  1.683390  2.488940 -0.063430
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H  2.010160  2.950450 -0.996710
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O -1.420870 -1.709090  0.434650
C -1.655370 -1.960720  1.675240
C -1.070890 -0.912810  2.590190
O -2.279210 -2.879310  2.128090
C -1.305650 -0.914430  3.953040
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H  0.650620  2.006350  2.340630
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C  1.618510  2.512970 -0.093640
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O  0.064500  2.194990  0.000000
H  2.040480  1.648780 -0.025180
C  1.359540  2.580590  0.005140
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H  1.613270  3.141480 -0.894130
C -0.132020 -0.086380  2.088790
O -2.121730 -0.681240  0.399390
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H  1.779490  0.818740  2.413440
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g08_ts
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O  0.066550  2.197190  0.000000
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C  1.360340  2.567090  0.034270
H  1.621350  3.051610  0.974880
H  1.642120  3.134810 -0.852250
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C -1.378190 -0.343320  2.577440
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H  1.592940  0.535700  4.870300
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O  0.086180  2.202400  0.000000
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C  1.379220  2.555790  0.044030
H  1.648750  3.022170  0.991580
H  1.680660  3.120080 -0.838260
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H  1.991090  0.081350  2.385310
H  1.701450  0.130200  4.865120
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g10_ts
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O  0.104550  2.205150  0.000000
H  2.032810  1.559340  0.005350
C  1.396940  2.548120  0.045490
H  1.675230  3.003310  0.996230
H  1.709250  3.108590 -0.835510
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O -2.165350  0.160150  0.414380
C -2.542190  0.090790  1.647390
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H  2.006720 -0.246400  2.361150
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H -0.506180 -0.198140  5.839310
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g11_ts
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O  1.854190  0.000000  0.000000
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C   0.965950  -0.641730   2.796910
H   1.898110  -0.874170   2.308070
H   1.604520  -1.096760   4.779600
H  -0.541960  -0.495020   5.815640
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g13_ts
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O   0.151970   2.205410   0.000000
H   2.054050   1.525790  -0.005390
C   1.443620   2.535180   0.036210
H   1.741750   2.971910   0.990050
H   1.762540   3.094270  -0.843390
C  -0.114560  -0.196010   2.075890
O  -2.089520   0.539840   0.443270
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O  -3.430140   1.120750   2.127250
C  -1.481290   0.079450   3.973940
C  -0.492010  -0.524500   4.729250
C   0.667400  -1.001240   4.135330
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H   1.770150  -1.183540   2.282280
H   1.417360  -1.495500   4.731130
H  -0.632920  -0.648020   5.790990
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g01_p
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O   2.536170   2.839350   0.000000
H   2.350690   0.897880  -0.040560
C   3.558170   3.427670  -0.178700
H   3.626220   4.516820  -0.025660
H   4.472830   2.910220  -0.506140
C  -0.080710   0.745290   1.972350
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C  -1.705630  -1.161990   2.111660
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O  -2.209590  -2.038040   2.757820
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C  -0.912270   1.605690   4.438920
C  -0.456980   2.520040   3.506950
C  -0.102710   2.102490   2.233910

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H  -0.404520   3.568800   3.749870
H  -1.190790   1.936450   5.426680
H  -1.684540  -0.395450   4.679240
g02_p
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O   2.018280   0.000000   0.000000
O   2.529760   2.844570   0.000000
H   2.355810   0.898240   0.009910
C   3.419390   3.447540  -0.520530
H   3.502720   4.537160  -0.429440
H   4.192270   2.942490  -1.112150
C  -0.066680   0.566010   2.032360
O  -1.974700  -0.796380   0.733410
C  -1.876300  -1.164420   1.966390
C  -0.935480  -0.250530   2.732700
O  -2.516290  -2.010380   2.526780
C  -1.231770   0.065640   4.044760
C  -0.832020   1.284790   4.561500
C  -0.211710   2.207730   3.738580
C   0.120470   1.873390   2.435160
H   0.623100   2.587000   1.801490
H  -0.008800   3.205200   4.092960
H  -1.090640   1.553730   5.573050
H  -1.876470  -0.604180   4.590850
g03_p
I   0.000000   0.000000   0.000000
O   2.020850   0.000000   0.000000
O   2.602230   2.824990   0.000000
H   2.360790   0.897270   0.026390
C   3.437610   3.357020  -0.668100
H   4.089990   2.783240  -1.348880
H   3.587210   4.447370  -0.631540
C  -0.053790   0.458860   2.059010
O  -2.013830  -0.704460   0.651920
C  -2.016010  -1.079840   1.888540
C  -1.018710  -0.285670   2.706650
O  -2.769430  -1.856300   2.406970
C  -1.288150  -0.008770   4.034150
C  -0.730620   1.108980   4.626590
C   0.032580   1.981380   3.870210
C   0.334330   1.687760   2.549910
H   0.940940   2.360890   1.965050
H   0.376280   2.911210   4.293260
H  -0.961610   1.347880   5.652210
H  -2.015610  -0.623160   4.539380
g04_p
I   0.000000   0.000000   0.000000
O   2.018410   0.000000   0.000000
O   2.733340   2.790540   0.000000
H   2.362450   0.895340   0.013400
C   3.525960   3.281250  -0.745970
H   4.035410   2.691740  -1.519060
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C  -0.044930   0.424880   2.063770
O  -2.046600  -0.593360   0.602600
C  -2.144760  -0.907090   1.852490
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O  -3.000740  -1.576430   2.360130
C  -1.346310   0.083690   4.017970
C  -0.643920   1.098130   4.639980
C   0.257240   1.861130   3.916250
C   0.533110   1.558190   2.593200
H   1.243670   2.144060   2.032700
H   0.734450   2.714590   4.370010
H  -0.851450   1.345210   5.668630
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g05_p
I   0.000000   0.000000   0.000000
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O   2.824630   2.757550   0.000000
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C   3.612000   3.207540  -0.776580
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H   3.912500   4.262080  -0.738070
C  -0.034530   0.337830   2.078120
O  -2.071270  -0.501220   0.554600
C  -2.244850  -0.779920   1.805190
C  -1.158050  -0.191930   2.669350
O  -3.182780  -1.351010   2.287160
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C  -0.545890   0.934740   4.687390
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H   1.506690   1.830410   2.147580
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O   2.024240   0.000000   0.000000
O   3.707890   2.238060   0.000000
H   2.384590   0.874700   0.171160
C   4.510440   1.719400  -0.717690
H   5.432090   2.239280  -1.009210
H   4.356700   0.707050  -1.111310
C   0.000370  -0.546370   2.032660
O  -2.080870  -0.569870   0.345750
C  -2.307880  -1.250840   1.423790
C  -1.177540  -1.144130   2.411260
O  -3.311680  -1.850890   1.685680
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C  -0.416200  -1.041800   4.676090
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O   3.514270   2.385510   0.000000
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H   4.158030   1.068970  -1.401320
C   0.005820  -0.723910   1.974080
O  -2.095380  -0.491580   0.331050
C  -2.366950  -1.180920   1.392200
C  -1.208090  -1.240600   2.347310
O  -3.419930  -1.686420   1.656370
C  -1.362760  -1.661090   3.656390
C  -0.336570  -1.475460   4.560250
C   0.836680  -0.851040   4.169550
C   1.016260  -0.443130   2.859610
H   1.934430   0.007150   2.526520
H   1.618620  -0.670180   4.888420
H  -0.460360  -1.786340   5.584350
H  -2.310940  -2.085880   3.940680
g08_p
I   0.000000   0.000000   0.000000
O   2.025660   0.000000   0.000000
O   3.648670   2.279850   0.000000
H   2.369260   0.876940   0.194960
C   4.421750   1.811590  -0.781470
H   5.315690   2.364170  -1.098150
H   4.267930   0.813870  -1.211110
C   0.003760  -0.663590   1.996160
O  -2.107370  -0.374970   0.375160
C  -2.415180  -0.939650   1.500410
C  -1.239430  -1.051900   2.427600
O  -3.505670  -1.314570   1.826590
C  -1.374950  -1.440990   3.749310
C  -0.287430  -1.375120   4.597960
C   0.935470  -0.910510   4.138550
C   1.095910  -0.530560   2.816600
H   2.041770  -0.199270   2.424160
```

```
H  1.773730 -0.836770  4.812550
H -0.394010 -1.666240  5.630340
H -2.348890 -1.759430  4.083680
g09_p
I  0.000000  0.000000  0.000000
O  2.026690  0.000000  0.000000
O  3.588210  2.326690  0.000000
H  2.359020  0.879090  0.205480
C  4.370920  1.892940 -0.791930
H  5.234350  2.484450 -1.120440
H  4.256990  0.887210 -1.219130
C  0.001020 -0.649970  2.000000
O -2.114890 -0.266060  0.407000
C -2.443770 -0.733200  1.571060
C -1.257980 -0.925410  2.470560
O -3.555530 -0.981950  1.942200
C -1.382190 -1.325810  3.790060
C -0.258740 -1.410100  4.588660
C  0.992260 -1.092450  4.080400
C  1.140970 -0.696530  2.761310
H  2.099130 -0.468490  2.328510
H  1.863060 -1.151490  4.713160
H -0.354860 -1.716100  5.618030
H -2.370760 -1.547630  4.159320
g10_p
I  0.000000  0.000000  0.000000
O  2.026180  0.000000  0.000000
O  3.533270  2.361240  0.000000
H  2.352390  0.875840  0.227210
C  4.298150  1.964200 -0.827320
H  5.134820  2.584620 -1.173560
H  4.193600  0.966550 -1.271920
C  0.006060 -0.661980  1.995650
O -2.116600 -0.174690  0.442250
C -2.447700 -0.561650  1.634750
C -1.255600 -0.837770  2.503320
O -3.564960 -0.701090  2.044780
C -1.369580 -1.273870  3.812330
C -0.230510 -1.519320  4.554130
C  1.026280 -1.336560  3.997250
C  1.164830 -0.900970  2.689570
H  2.122940 -0.761500  2.219410
H  1.910110 -1.537190  4.581330
H -0.317730 -1.859180  5.573440
H -2.360270 -1.411130  4.214390
g11_p
I  0.000000  0.000000  0.000000
O  2.026370  0.000000  0.000000
O  3.504160  2.379040  0.000000
H  2.342480  0.880220  0.224330
C  4.284630  1.990630 -0.816690
H  5.115640  2.622360 -1.156590
H  4.201100  0.989610 -1.257700
C  0.011540 -0.587160  2.018470
O -2.115480 -0.055680  0.485290
C -2.436120 -0.305880  1.716600
C -1.244330 -0.636130  2.567190
O -3.545710 -0.307310  2.168820
C -1.358190 -1.052690  3.882630
C -0.228460 -1.434640  4.580040
C  1.016760 -1.415290  3.969910
C  1.155400 -0.994490  2.657380
H  2.104550 -0.965850  2.150020
H  1.890120 -1.737000  4.514400
H -0.316220 -1.766030  5.602140
H -2.343170 -1.082770  4.319610
g12_p
I  0.000000  0.000000  0.000000
O  2.025740  0.000000  0.000000
O  3.591620  2.293710  0.000000
H  2.330400  0.897490  0.168550
C  4.451170  1.776600 -0.640400
H  5.354590  2.319270 -0.914880
H  4.362410  0.732950 -0.976770
```

```
C  0.014710 -0.356390  2.065280
O -2.109230  0.110230  0.513570
C -2.411910  0.086170  1.771290
C -1.231560 -0.243820  2.637670
O -3.495290  0.264140  2.237210
C -1.364260 -0.555030  3.981950
C -0.269520 -1.023610  4.681030
C  0.956040 -1.198710  4.042370
C  1.111210 -0.882200  2.702480
H  2.049060 -0.997680  2.176700
H  1.797150 -1.599860  4.585020
H -0.374720 -1.281650  5.724470
H -2.342480 -0.454310  4.436590
g13_p
I  0.000000  0.000000  0.000000
O  2.019200  0.000000  0.000000
O  2.389870  2.835860  0.000000
H  2.287270  0.915410 -0.119510
C  2.358200  3.398950  1.052540
H  2.230130  2.856330  1.997720
H  2.453100  4.491130  1.118760
C  0.041910  0.463890  2.047410
O -2.105930  0.424870  0.454690
C -2.343000  0.994850  1.590340
C -1.159770  0.931180  2.519260
O -3.379970  1.484100  1.941920
C -1.277520  1.172770  3.877430
C -0.232840  0.850830  4.722410
C  0.919940  0.263360  4.222210
C  1.064070  0.037400  2.863290
H  1.954090 -0.399270  2.441050
H  1.707530 -0.040270  4.893170
H -0.330340  1.016400  5.783210
H -2.214120  1.562830  4.242000
```

h1, 2(sm, ts, p)

```
h1_sm
I  0.000000  0.000000  0.000000
O  2.004910  0.000000  0.000000
H  2.947790  2.322050  0.000000
O  2.169270  2.860440  0.117640
H  0.952010  2.198210 -0.481420
O  0.137770  1.701940 -0.820720
H  2.402150  3.766920 -0.062030
H  2.311480 -0.680850  0.599950
C -0.014650 -1.178470 -1.718190
C -1.275850 -1.247300 -2.258630
C -2.399370 -0.540290 -1.574410
O -1.993800  0.092400 -0.473190
O -3.517360 -0.555280 -1.954550
C -1.430150 -1.951680 -3.437020
C -0.323020 -2.544470 -4.019170
C  0.935240 -2.430280 -3.446960
C  1.116830 -1.727520 -2.265710
H -2.411880 -2.012630 -3.878060
H -0.437460 -3.093280 -4.939500
H  1.788870 -2.880440 -3.926470
H  2.087110 -1.589610 -1.821350
O  0.772570 -2.311260  1.155370
C  0.434440 -2.679150  2.493520
H  0.338370 -1.762850  3.063770
H -0.508240 -3.216940  2.521500
H  1.222650 -3.283170  2.931390
H  0.858030 -3.101860  0.628650
h1_ts
I  0.000000  0.000000  0.000000
O  2.139380  0.000000  0.000000
H  2.614850  1.195320  0.000000
O  2.606230  2.306740 -0.028660
H  1.624040  2.428560 -0.179020
O  0.157870  1.792420 -0.326030
H  3.114820  2.709110 -0.730990
H  2.475230 -0.744770  0.503560
```

```
C  0.075040 -0.907000 -1.887170
C -1.189010 -0.990500 -2.423660
C -2.350310 -0.516630 -1.620750
O -1.977860 -0.066700 -0.409970
O -3.473920 -0.550300 -1.974600
C -1.321980 -1.518150 -3.693630
C -0.190980 -1.934210 -4.373260
C  1.066440 -1.822180 -3.800540
C  1.224620 -1.293070 -2.528630
H -2.307870 -1.588830 -4.123930
H -0.287660 -2.346390 -5.364040
H  1.938010 -2.142880 -4.347280
H  2.192440 -1.176850 -2.074650
O  1.330070 -2.416330  0.996640
C  1.111190 -2.842470  2.338700
H  0.915040 -1.955330  2.929980
H  0.251850 -3.504720  2.403040
H  1.990990 -3.339150  2.736960
H  1.494310 -3.185640  0.458850
h1_p
I  0.000000  0.000000  0.000000
O  2.273550  0.000000  0.000000
H  2.602760  0.946380  0.000000
O  2.733910  2.474400  0.238720
H  1.821280  2.770590  0.260550
O  0.077810  1.796640  0.217060
H  3.265350  3.151240 -0.165680
H  2.629450 -0.442090  0.817290
C  0.150910 -0.396540 -2.061520
C -1.109060 -0.401810 -2.617290
C -2.293280 -0.240760 -1.736600
O -1.947610 -0.133700 -0.428040
O -3.416870 -0.237550 -2.082730
C -1.215300 -0.594270 -3.981020
C -0.064050 -0.768430 -4.729090
C  1.184420 -0.755510 -4.128760
C  1.318760 -0.560640 -2.761360
H -2.196250 -0.606070 -4.427840
H -0.139520 -0.919140 -5.793200
H  2.070830 -0.896910 -4.725260
H  2.279860 -0.546060 -2.280000
O  2.916730 -1.023880  2.255430
C  3.415500 -0.142640  3.260470
H  3.096020  0.856940  2.990790
H  3.001720 -0.399900  4.230040
H  4.500740 -0.169100  3.299780
H  3.248180 -1.903920  2.405820
h2_sm
I  0.000000  0.000000  0.000000
C  2.108800  0.000000  0.000000
O  0.272650  1.960040  0.000000
O -0.421130 -0.369660  1.706340
C  2.554740  1.301130  0.012880
C  1.570530  2.404000 -0.034600
O  1.797380  3.553610 -0.101180
C  3.917320  1.519660  0.081690
C  4.770660  0.431540  0.144370
C  4.276220 -0.862150  0.143860
C  2.910430 -1.106710  0.074770
H  4.282610  2.534070  0.093540
H  5.834250  0.593250  0.202800
H  4.953880 -1.697990  0.203370
H  2.510680 -2.105180  0.085140
O  0.647790  0.747930 -2.547870
C -0.049290  1.760360 -3.269420
H  0.642840  2.495910 -3.668320
H -0.709070  2.256250 -2.568000
H -0.636710  1.328360 -4.074580
H  1.296330  0.350030 -3.120170
O  0.120320 -2.553890  0.028710
H -0.175440 -2.818060  0.900900
H -0.103380 -3.250930 -0.584190
h2_ts
I  0.000000  0.000000  0.000000
```

```
C   2.109010   0.000000   0.000000
O   0.312510   1.970180   0.000000
O  -0.270430  -0.417640   1.725670
C   2.579970   1.287340   0.098390
C   1.611720   2.405630   0.091990
O   1.849920   3.552850   0.138600
C   3.944940   1.476150   0.217230
C   4.775010   0.370530   0.250940
C   4.256300  -0.912850   0.175100
C   2.890540  -1.125060   0.050550
H   4.327780   2.481500   0.290340
H   5.839170   0.507530   0.348640
H   4.916400  -1.763530   0.220050
H   2.479870  -2.119570   0.006900
O   0.621630  -1.624770  -2.020480
C  -0.299890  -2.373460  -2.805850
H  -0.189230  -2.132520  -3.858720
H  -1.295040  -2.089750  -2.487470
H  -0.163660  -3.439420  -2.649880
H   1.496750  -1.725640  -2.383990
O  -1.682930  -2.113130   0.205290
H  -1.768360  -2.148320   1.156550
H  -2.321990  -2.716650  -0.160490
h2_p
I   0.000000   0.000000   0.000000
C   2.103840   0.000000   0.000000
O   0.304580   1.962080   0.000000
O  -0.384240  -0.415380   1.708840
C   2.574940   1.294580   0.069310
C   1.600720   2.404480   0.075130
O   1.830610   3.555510   0.114730
C   3.939550   1.503130   0.126930
C   4.785780   0.408870   0.122190
C   4.279360  -0.879200   0.063700
C   2.912300  -1.108240   0.004970
H   4.312320   2.513390   0.177880
H   5.851560   0.559680   0.168820
H   4.951400  -1.721610   0.067360
H   2.510510  -2.104690  -0.032290
O   0.136050  -2.485650  -0.249460
C  -0.235710  -3.369410   0.821190
H  -1.238750  -3.748720   0.660210
H  -0.211040  -2.779180   1.727800
H   0.477060  -4.184630   0.882970
H   0.040590  -2.923840  -1.091780
O  -2.339390   1.071380   0.255770
H  -2.641590   0.969730   1.156630
H  -2.471430   1.988210   0.023960
```

i1-2

```
i1
C   0.000000   0.000000   0.000000
C   1.381800   0.000000   0.000000
C   2.030780   1.210430   0.000000
I   4.117040   1.003050  -0.042920
O   4.265610   3.003430  -0.086070
C   2.195870  -1.258150   0.021930
O   1.692240  -2.339010   0.041430
O   3.480670  -1.017650   0.050820
C  -0.677630   1.205430  -0.001810
C   0.011940   2.408300   0.000030
C   1.396960   2.428620   0.001510
H  -0.512250  -0.948300   0.001250
O   4.661090   0.867170  -1.775770
H   4.455920   3.262620  -0.988270
H   1.964080   3.343350   0.007770
H  -0.529060   3.340660   0.001040
H  -1.755680   1.211220  -0.003470
i2
O   0.000000   0.000000   0.000000
H   0.950340   0.000000   0.000000
H  -0.236700   0.920400   0.000000
```

j1-9

```
j1
C   0.000000   0.000000   0.000000
O   1.400400   0.000000   0.000000
H  -0.418020   1.008760   0.000000
H  -0.321000  -0.494380   0.910710
H  -0.418040  -0.549550  -0.845920
H   1.698230   0.429650  -0.792670
j2
C   0.000000   0.000000   0.000000
C   1.504810   0.000000   0.000000
O   1.938100   1.337600   0.000000
H  -0.376920   0.513880   0.880060
H  -0.386380  -1.016270  -0.000080
H  -0.376900   0.514010  -0.880000
H   2.887900   1.347270   0.000010
H   1.875090  -0.530010   0.881800
H   1.875080  -0.530010  -0.881800
j3
C   0.000000   0.000000   0.000000
C   1.514880   0.000000   0.000000
C   2.090240   1.394680   0.000000
O   2.020640  -0.640370  -1.151400
H  -0.394370   0.497970   0.883040
H  -0.373000   0.512020  -0.884260
H  -0.390790  -1.016760  -0.007350
H   3.175200   1.352520  -0.022240
H   1.753320   1.936160  -0.881100
H   1.780570   1.943150   0.885910
H   1.867780  -0.523660   0.894490
H   1.665470  -1.521700  -1.182900
j4
C   0.000000   0.000000   0.000000
C   1.520080   0.000000   0.000000
C   2.076870   1.414430   0.000000
C   2.065540  -0.801070   1.164980
O   1.654380  -0.195420   2.365960
H  -0.395240  -1.012870  -0.052960
H   1.865330  -0.506900  -0.903790
H   1.787170   1.935590   0.908370
H   1.703960   1.979300  -0.851450
H   3.164180   1.411180  -0.051370
H   1.994670  -0.701510   3.093470
H   1.695140  -1.828410   1.102080
H   3.157080  -0.834150   1.101380
H  -0.389100   0.555210  -0.850550
H  -0.378730   0.459040   0.909120
j5
C   0.000000   0.000000   0.000000
C   1.523820   0.000000   0.000000
C   2.043460   1.432470   0.000000
C   2.032760  -0.726030  -1.235590
O   1.571000  -0.068740  -2.388760
C   2.041430  -0.738440   1.227170
H  -0.384340   0.485100  -0.892200
H  -0.390040  -1.016710   0.025980
H   1.719120   1.958840  -0.892630
H   1.678240   1.972790   0.871490
H   3.132220   1.452450   0.026820
H   1.901000  -0.527960  -3.151410
H   3.126800  -0.745200  -1.211210
H   1.678710  -1.761400  -1.210680
H   3.130180  -0.756490   1.249620
H   1.686450  -1.767830   1.250020
H   1.699990  -0.250620   2.137810
H  -0.383310   0.526870   0.871970
j6
C   0.000000   0.000000   0.000000
C   1.523540   0.000000   0.000000
O   1.924690   1.354540   0.000000
C   2.179390  -0.762810   1.154360
C   1.751770  -0.237040   2.514650
C   3.694950  -0.728260   1.019690
```

```
C  -0.575260  -1.404090   0.089570
C  -0.525900   0.712060  -1.236390
H  -0.319340   0.568110   0.874670
H   2.848750   1.396530  -0.216400
H   1.849350  -0.475730  -0.934030
H   1.950280   0.829760   2.584410
H   2.299020  -0.737230   3.310740
H   0.691530  -0.391630   2.697730
H   1.871400  -1.804820   1.064080
H   4.018050  -1.067560   0.036170
H   4.165260  -1.370380   1.760310
H   4.084460   0.276470   1.181220
H  -0.200530  -2.031720  -0.719110
H  -0.338710  -1.894500   1.030080
H  -1.658700  -1.373340   0.001040
H  -0.112000   1.711370  -1.313580
H  -1.610740   0.787730  -1.205520
H  -0.259110   0.162430  -2.139430
j7
C   0.000000   0.000000   0.000000
C   1.382680   0.000000   0.000000
C   2.079220   1.195450   0.000000
C   1.384520   2.391570   0.004610
C  -0.704180   1.195490   0.003320
C   0.001550   2.389250   0.011240
C  -2.207280   1.193310  -0.024890
O  -2.779030   0.089240   0.621460
H   1.920090   3.327810   0.012310
H   3.157630   1.195040   0.000790
H   1.918250  -0.936380  -0.001710
H  -0.547680  -0.929060  -0.000430
H  -0.535810   3.326250   0.026510
H  -2.469460   0.084740   1.521490
H  -2.579230   2.134080   0.387540
H  -2.554560   1.139520  -1.054680
j8
C   0.000000   0.000000   0.000000
C   1.520320   0.000000   0.000000
C   2.058260   1.415710   0.000000
O   1.995300  -0.576340   1.204850
C   2.060010  -0.782810  -1.186320
H  -0.398010   0.476840  -0.893050
H  -0.372760   0.529470   0.872720
H  -0.384500  -1.019140   0.030980
H   3.144060   1.401570   0.039140
H   1.747540   1.949830  -0.894330
H   1.694480   1.952510   0.871900
H   1.676290  -1.471850   1.248280
H   1.696590  -1.809910  -1.166520
H   3.145950  -0.807060  -1.153960
H   1.749380  -0.339870  -2.130050
j9
C   0.000000   0.000000   0.000000
C   1.516520   0.000000   0.000000
C   2.158670   1.382180   0.000000
O   1.692220   2.017330  -1.178600
C   1.756210   2.201470   1.216170
C   3.671400   1.245640  -0.065970
H  -0.378300   0.603510  -0.819510
H  -0.380690  -1.011550  -0.118920
H  -0.408720   0.392950   0.927960
H   1.894730  -0.554270   0.858860
H   1.874420  -0.516780  -0.889740
H   2.052620   2.897520  -1.203200
H   2.252150   3.171700   1.199490
H   2.038690   1.702900   2.140960
H   0.684570   2.374490   1.226980
H   3.957700   0.690640  -0.955350
H   4.062540   0.729610   0.808260
H   4.143550   2.226550  -0.111450
```