Double-hybrid density functionals with long-range dispersion corrections: higher accuracy and extended applicability (Supplementary Material)

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Content

Table 1: Results for the S22 set of non-covalent bonding. Listed are the reference binding energies and for illustration the unscaled dispersion corrections (ΔE_{disp}, $s_6 = 1.0$). Further the deviations (dev) based on different methods with the aug-cc-pVTZ basis set are given. At the end statistical qualities are included: mean deviation (MD), mean absolute deviation (MAD), root mean square (RMS) and error spread ($\Delta_{min-max}$). All values in kcal mol^{-1}.

set entry	ΔE_{ref}[a]	ΔE_{disp}[b]	dev(mPW2PLYP)			dev(mPW2PLYP-D)			dev(B2PLYP)			dev(B2PLYP-D)		
			ΔE[c]	$\Delta E(CP)$[d]	$\Delta E(HCP)$[e]	ΔE[c]	$\Delta E(CP)$[d]	$\Delta E(HCP)$[e]	ΔE[c]	$\Delta E(CP)$[d]	$\Delta E(HCP)$[e]	ΔE[c]	$\Delta E(CP)$[d]	$\Delta E(HCP)$[e]
Hydrogen bonded complexes														
1 (NH$_3$)$_2$	-3.17	-1.39	-0.05	-0.16	-0.11	0.51	0.40	0.40	-0.47	-0.60	-0.54	0.29	0.16	0.23
2 (H$_2$O)$_2$	-5.02	-0.78	0.41	0.12	0.27	0.72	0.43	0.43	-0.05	-0.35	-0.20	0.38	0.08	0.23
3 Formic acid dimer (C$_{2h}$)	-18.61	-2.52	1.02	0.07	0.55	2.03	1.08	1.08	0.07	-0.92	-0.42	1.46	0.47	0.96
4 Formamide dimer (C$_{2h}$)	-15.96	-2.66	0.43	-0.45	-0.01	1.49	0.61	0.61	-0.41	-1.34	-0.87	1.05	0.12	0.59
5 Uracil dimer(C$_{2h}$)	-20.65	-3.33	0.61	-0.83	-0.11	1.94	0.50	0.50	-0.28	-1.81	-1.04	1.55	0.02	0.79
6 2-pyridoxine · 2-aminopyridine	-16.71	-3.97	0.50	-0.80	-0.15	2.09	0.79	0.79	-0.25	-1.63	-0.94	1.93	0.55	1.24
7 Adenine · thymine WC	-16.37	-4.24	0.42	-1.17	-0.38	2.12	0.53	0.53	-0.39	-2.08	-1.24	1.94	0.25	1.10
Complexes with predominant dispersion contribution														
8 (CH$_4$)$_2$ (D$_{3d}$)	-0.53	-0.83	-0.13	-0.25	-0.19	0.20	0.08	0.08	-0.44	-0.56	-0.50	0.02	-0.10	-0.04
9 (C$_2$H$_4$)$_2$ (D$_{2d}$)	-1.51	-2.14	-0.38	-0.68	-0.53	0.48	0.18	0.18	-0.88	-1.19	-1.04	0.30	-0.01	0.14
10 Benzene · CH$_4$ (C$_3$)	-1.50	-2.18	-0.35	-0.89	-0.62	0.52	-0.02	-0.02	-0.75	-1.32	-1.04	0.45	-0.12	0.16
11 Benzene dimer (C$_{2h}$)	-2.73	-5.71	-1.83	-2.79	-2.31	0.45	-0.51	-0.51	-2.39	-3.43	-2.91	0.75	-0.29	0.23
12 Pyrazine dimer (C$_s$)	-4.42	-6.21	-1.89	-2.91	-2.40	0.59	-0.43	-0.43	-2.51	-3.60	-3.06	0.91	-0.18	0.36
13 Uracil dimer (C$_s$)	-10.12	-9.01	-2.49	-4.16	-3.33	1.11	-0.56	-0.56	-3.48	-5.25	-4.37	1.48	-0.29	0.59
14 Indole · benzene	-5.22	-8.54	-3.24	-4.61	-3.93	0.18	-1.19	-1.19	-3.90	-5.37	-4.63	0.80	-0.67	0.06
15 Adenine · thymine stack	-12.23	-13.22	-3.82	-6.18	-5.00	1.47	-0.89	-0.89	-4.92	-7.42	-6.17	2.35	-0.15	1.10
Mixed complexes														
16 Ethene · ethine (C$_{2v}$)	-1.53	-0.99	0.22	-0.18	0.02	0.62	0.22	0.22	-0.08	-0.50	-0.29	0.46	0.04	0.25
17 Benzene · H$_2$O (C$_s$)	-3.28	-2.34	-0.19	-0.72	-0.45	0.75	0.22	0.22	-0.64	-1.21	-0.93	0.65	0.08	0.36
18 Benzene · NH$_3$(C$_s$)	-2.35	-2.28	-0.32	-0.85	-0.59	0.59	0.06	0.06	-0.74	-1.30	-1.02	0.51	-0.05	0.23
19 Benzene · HCN (C$_s$)	-4.46	-3.10	0.18	-0.76	-0.29	1.42	0.48	0.48	-0.31	-1.31	-0.81	1.40	0.40	0.90
20 Benzene dimer (C$_{2v}$)	-2.74	-3.64	-0.46	-1.52	-0.99	1.00	-0.06	-0.06	-0.94	-2.05	-1.49	1.06	-0.05	0.51
21 Indole · benzene T-shape	-5.73	-5.31	-0.85	-2.18	-1.52	1.27	-0.06	-0.06	-1.41	-2.85	-2.13	1.51	0.07	0.79
22 Phenol dimer	-7.05	-4.09	-0.51	-1.55	-1.03	1.13	0.09	0.09	-1.21	-2.30	-1.76	1.04	-0.05	0.49
MD			-0.6	-1.5	-1.1	1.0	0.1	0.6	-1.2	-2.2	-1.7	1.0	0.0	0.5
MAD			0.9	1.5	1.1	1.0	0.4	0.6	1.2	2.2	1.7	1.0	0.2	0.5
RMS			1.4	2.2	1.8	1.2	0.5	0.7	1.8	2.8	2.3	1.2	0.3	0.6
$\Delta_{min-max}$			4.8	6.3	5.6	1.9	2.3	2.1	5.0	7.8	6.4	2.4	1.2	1.3

[a] based on estimated CCSD(T) complete basis set limit. (P. Jurecka, J. Sponer, J. Cerny, and P. Hobza, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1985–1993.)

[b] unscaled dispersion correction based on the DFT-D model (S. Grimme, *J. Comput. Chem.*, 2004, **25**, 1463–1473; S. Grimme, *J. Comput. Chem.*, 2006, **27**, 1787–1799.)

[c] deviations based on binding energies

[d] deviations based on Counterpoise correceted binding energies

[e] deviations based on mean of binding energies with and without Counterpoise correction

Table 2: Results for the S22 set of non-covalent bonding. Listed are the reference binding energies and for illustration the unscaled dispersion corrections (ΔE_{disp}, $s_6 = 1.0$). Further the deviations (dev) based on different methods with the TZV(2df,2pd) basis set are given. At the end statistical qualities are included: mean deviation (MD), mean absolute deviation (MAD), root mean square (RMS) and error spread ($\Delta_{min-max}$). All values in kcal mol^{-1}.

	set entry	ΔE_{ref} [a]	ΔE_{disp} [b]	dev(mPW2PLYP)			dev(mPW2PLYP-D)			dev(B2PLYP)			dev(B2PLYP-D)		
				ΔE [c]	$\Delta E(CP)$ [d]	$\Delta E(HCP)$ [e]	ΔE [c]	$\Delta E(CP)$ [d]	$\Delta E(HCP)$ [e]	ΔE [c]	$\Delta E(CP)$ [d]	$\Delta E(HCP)$ [e]	ΔE [c]	$\Delta E(CP)$ [d]	$\Delta E(HCP)$ [e]
	Hydrogen bonded complexes														
1	$(NH_3)_2$	-3.17	-1.39	0.38	-0.09	0.14	0.94	0.47	0.47	-0.05	-0.51	-0.28	0.71	0.25	0.48
2	$(H_2O)_2$	-5.02	-0.78	0.85	0.13	0.49	1.16	0.44	0.44	0.38	-0.33	0.02	0.81	0.10	0.45
3	Formic acid dimer (C_{2h})	-18.61	-2.52	0.95	-0.08	0.44	1.96	0.93	0.93	-0.04	-1.09	-0.56	1.35	0.30	0.82
4	Formamide dimer (C_{2h})	-15.96	-2.66	0.29	-0.60	-0.16	1.35	0.46	0.46	-0.60	-1.50	-1.05	0.86	-0.04	0.41
5	Uracil dimer(C_{2h})	-20.65	-3.33	-0.24	-1.05	-0.64	1.09	0.28	0.28	-1.18	-2.03	-1.60	0.65	-0.20	0.23
6	2-pyridoxine · 2-aminopyridine	-16.71	-3.97	0.02	-0.96	-0.47	1.61	0.63	0.63	-0.79	-1.80	-1.30	1.39	0.38	0.89
7	Adenine · thymine WC	-16.37	-4.24	-0.46	-1.41	-0.93	1.24	0.29	0.29	-1.37	-2.33	-1.85	0.96	0.00	0.48
	Complexes with predominant dispersion contribution														
8	$(CH_4)_2$ (D_{3d})	-0.53	-0.83	-0.25	-0.28	-0.26	0.08	0.05	0.05	-0.56	-0.61	-0.59	-0.10	-0.15	-0.13
9	$(C_2H_4)_2$ (D_{2d})	-1.51	-2.14	-0.58	-0.76	-0.67	0.28	0.10	0.10	-1.10	-1.28	-1.19	0.08	-0.10	-0.01
10	Benzene · CH_4 (C_3)	-1.50	-2.18	-0.75	-0.93	-0.84	0.12	-0.06	-0.06	-1.18	-1.37	-1.27	0.02	-0.17	-0.08
11	Benzene dimer (C_{2h})	-2.73	-5.71	-2.42	-3.02	-2.72	-0.14	-0.74	-0.74	-3.03	-3.67	-3.35	0.11	-0.53	-0.21
12	Pyrazine dimer (C_s)	-4.42	-6.21	-2.56	-3.22	-2.89	-0.08	-0.74	-0.74	-3.23	-3.92	-3.58	0.19	-0.50	-0.16
13	Uracil dimer (C_s)	-10.12	-9.01	-3.15	-4.56	-3.86	0.45	-0.96	-0.96	-4.22	-5.66	-4.94	0.74	-0.70	0.02
14	Indole · benzene	-5.22	-8.54	-4.01	-4.94	-4.48	-0.59	-1.52	-1.52	-4.74	-5.72	-5.23	-0.04	-1.02	-0.53
15	Adenine · thymine stack	-12.23	-13.22	-4.78	-6.69	-5.73	0.51	-1.40	-1.40	-6.00	-7.97	-6.98	1.27	-0.70	0.29
	Mixed complexes														
16	Ethene · ethine (C_{2v})	-1.53	-0.99	-0.07	-0.24	-0.15	0.33	0.16	0.16	-0.40	-0.55	-0.48	0.14	-0.01	0.07
17	Benzene · H_2O (C_s)	-3.28	-2.34	-0.04	-0.80	-0.42	0.90	0.14	0.14	-0.52	-1.29	-0.90	0.77	0.00	0.38
18	Benzene · NH_3(C_s)	-2.35	-2.28	-0.45	-0.92	-0.68	0.46	-0.01	-0.01	-0.90	-1.37	-1.14	0.35	-0.12	0.12
19	Benzene · HCN (C_s)	-4.46	-3.10	-0.50	-0.78	-0.64	0.74	0.46	0.46	-1.06	-1.35	-1.21	0.65	0.36	0.50
20	Benzene dimer (C_{2v})	-2.74	-3.64	-1.17	-1.59	-1.38	0.29	-0.13	-0.13	-1.71	-2.13	-1.92	0.29	-0.13	0.08
21	Indole · benzene T-shape	-5.73	-5.31	-1.62	-2.27	-1.94	0.50	-0.15	-0.15	-2.28	-2.94	-2.61	0.64	-0.02	0.31
22	Phenol dimer	-7.05	-4.09	-0.84	-1.68	-1.26	0.80	-0.04	-0.04	-1.59	-2.44	-2.01	0.66	-0.19	0.23
	MD			-1.0	-1.7	-1.3	0.6	-0.1	0.3	-1.6	-2.4	-2.0	0.6	0.1	0.2
	MAD			1.2	1.7	1.4	0.7	0.5	0.5	1.7	2.4	2.0	0.6	0.3	0.3
	RMS			1.8	2.4	2.1	0.9	0.6	0.6	2.3	3.0	2.7	0.7	0.4	0.4
	$\Delta_{min-max}$			5.7	6.8	6.2	2.6	2.5	2.5	6.4	8.3	7.0	1.5	1.4	1.4

[a] based on estimated CCSD(T) complete basis set limit. (P. Jurecka, J. Sponer, J. Cerny, and P. Hobza, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1985–1993.)

[b] unscaled dispersion correction based on the DFT-D model (S. Grimme, *J. Comput. Chem.*, 2004, **25**, 1463–1473; S. Grimme, *J. Comput. Chem.*, 2006, **27**, 1787–1799.)

[c] deviations based on binding energies

[d] deviations based on Counterpoise correceted binding energies

[e] deviations based on mean of binding energies with and without Counterpoise correction

Table 3: Deviations from reference for relative energies of the phenylalanyl-glycyl-glycine conformers obtained with different methods and the TZVPP basis set. For illustration the unscaled dispersion corretions (E_{disp}, $s_6 = 1.0$) based on the DFT-D model are also given. All values in kcal mol^{-1}.

	label[a]	$E_{ref.}$[b]	B3LYP	B3LYP-D	B2PLYP	B2PLYP-D	mPW2PLYP	mPW2PLYP-D	E_{disp}
			deviation (reference - theory)							
1	FGG_099	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-36.66
2	FGG_444	0.14	4.37	0.75	2.05	0.16	1.74	0.36	-33.21
3	FGG_215	0.79	3.35	0.72	1.51	0.13	1.24	0.23	-34.15
4	FGG_357	0.90	2.02	0.98	0.91	0.36	0.68	0.28	-35.66
5	FGG_366	1.15	5.88	-0.35	2.86	-0.40	2.36	-0.01	-30.72
6	FGG_300	1.31	5.54	-0.19	2.62	-0.38	2.22	0.04	-31.20
7	FGG_114	1.87	1.91	1.17	0.98	0.60	0.75	0.47	-35.96
8	FGG_224	2.04	3.66	1.01	1.85	0.47	1.54	0.53	-34.14
9	FGG_691	2.07	5.45	-0.25	2.71	-0.27	2.18	0.01	-31.24
10	FGG_412	2.37	1.43	0.46	0.73	0.22	0.60	0.23	-35.73
11	FGG_470	2.51	4.31	0.74	2.17	0.30	1.87	0.51	-33.26

[a] labelling identical to D. Reha, H. Valdes, J. Vondrasek, P. Hobza, A. Abu-Riziq, B. Crews, and M. S. de Vries, *Chem. Eur. J.*, 2005, **11**, 6803–6817, see reference for geometries

[b] MP2 with extrapolated complete basis set limit and CCSD(T) correction, taken from D. Reha, H. Valdes, J. Vondrasek, P. Hobza, A. Abu-Riziq, B. Crews, and M. S. de Vries, *Chem. Eur. J.*, 2005, **11**, 6803–6817

Table 4: Experimental heats of formation for the G3/99, unscaled dispersion corrections to the total energies based on the DFT-D model ($E_{disp}, s_6 = 1.0$), and deviations from experiment (exp.- theo.) for various methods. Theoretical results are based on computations with CQZV3P basis set and B3LYP/TZV(2d,2p) frequencies. All values in kcal mol^{-1}.

	G3/99 entry	exp.[a]	E_{disp}	deviation					
				B3LYP	B3LYP-D	mPW2PLYP	mPW2PLYP-D	B2PLYP	B2PLYP-D
1	H_2	0.0	0.00	0.90	0.90	-1.00	-1.00	-0.80	-0.80
2	LiH	33.3	-0.50	-0.20	0.30	-1.20	-1.00	-1.00	-0.70
3	BeH	81.7	0.00	8.00	8.00	6.60	6.60	6.60	6.60
4	CH	142.5	0.00	1.50	1.50	-0.10	-0.10	-0.10	-0.10
5	$CH_2(^3B_1)$	93.7	-0.26	2.10	2.40	0.90	1.00	0.60	0.80
6	$CH_2(^1A_1)$	102.8	-0.08	-0.10	-0.10	-1.70	-1.70	-1.80	-1.80
7	CH_3	35.0	-0.49	2.60	3.10	1.20	1.40	0.70	1.00
8	CH_4	-17.9	-0.62	1.00	1.60	0.00	0.20	-0.60	-0.30
9	NH	85.2	0.00	4.10	4.10	1.30	1.30	1.40	1.40
10	NH_2	45.1	-0.04	5.70	5.80	2.30	2.30	2.40	2.40
11	NH_3	-11.0	-0.13	2.60	2.80	0.10	0.10	0.30	0.30
12	OH	9.4	0.00	1.80	1.80	0.20	0.20	0.60	0.60
13	H_2O	-57.8	-0.02	-1.80	-1.70	-2.40	-2.40	-1.70	-1.70
14	HF	-65.1	0.00	-1.40	-1.40	-1.50	-1.50	-0.80	-0.80
15	$SiH_2(^3B_1)$	65.2	-0.27	1.30	1.60	0.00	0.10	-0.30	-0.20
16	$SiH_2(^1A_1)$	86.2	-0.12	1.70	1.80	0.50	0.50	0.00	0.10
17	SiH_3	47.9	-0.47	2.40	2.90	1.30	1.50	0.50	0.80
18	SiH_4	8.2	-0.99	1.20	2.20	0.60	1.00	-0.50	0.10
19	PH_2	33.1	-0.28	5.50	5.80	2.60	2.70	2.20	2.30
20	PH_3	1.3	-0.85	2.70	3.60	0.00	0.30	-0.50	-0.10
21	H_2S	-4.9	-0.22	0.40	0.60	-0.20	-0.20	-0.30	-0.20
22	HCl	-22.1	0.00	-0.10	-0.10	0.20	0.20	0.30	0.30
23	Li_2	51.6	-0.97	-3.60	-2.60	-2.90	-2.50	-3.40	-2.80
24	LiF	-80.1	-0.10	-1.10	-1.00	-0.30	-0.30	0.20	0.30
25	C_2H_2	54.2	-0.33	-2.30	-1.90	-0.90	-0.70	-0.30	-0.10
26	$H_2C=CH_2$	12.5	-0.97	-0.20	0.80	-0.30	0.10	-0.80	-0.20
27	H_3C-CH_3	-20.1	-2.07	-0.50	1.60	-0.10	0.80	-1.40	-0.30
28	CN	104.9	0.00	-2.60	-2.60	-2.90	-2.90	-0.50	-0.50
29	HCN	31.5	-0.15	0.20	0.40	0.60	0.60	2.10	2.20
30	CO	-26.4	0.00	-4.10	-4.10	-2.10	-2.10	-0.40	-0.40
31	HCO	10.0	-0.07	1.60	1.70	0.80	0.90	2.30	2.30
32	$H_2C=O$	-26.0	-0.30	-0.20	0.10	-0.70	-0.60	0.30	0.50
33	CH_3OH	-48.0	-1.04	-1.00	0.10	-1.40	-0.90	-1.40	-0.80
34	N_2	0.0	0.00	-0.30	-0.30	-0.70	-0.70	1.60	1.60
35	H_2N-NH_2	22.8	-0.91	4.90	5.90	0.60	1.00	0.90	1.50
36	NO	24.6	0.00	4.70	4.80	2.70	2.70	5.00	5.00
37	O_2	0.0	0.00	3.30	3.30	0.60	0.60	3.20	3.20
38	HO-OH	-32.5	-0.24	-1.60	-1.40	-4.30	-4.20	-2.40	-2.20
39	F_2	0.0	0.00	-0.70	-0.70	-3.80	-3.80	-1.40	-1.40
40	CO_2	-94.0	-0.07	-1.60	-1.50	-0.10	-0.10	2.70	2.70

41	Na$_2$	34.0	-1.69	-0.10	1.60	0.70	1.40	0.00	0.90
42	Si$_2$	139.9	-0.01	-5.80	-5.80	-5.10	-5.10	-4.40	-4.40
43	P$_2$	34.3	-0.01	-2.30	-2.30	-2.00	-2.00	-0.70	-0.70
44	S$_2$	30.7	0.00	2.80	2.80	2.20	2.20	3.10	3.10
45	Cl$_2$	0.0	-0.01	-0.20	-0.20	-0.20	-0.20	0.30	0.40
46	NaCl	-43.6	-0.37	-4.40	-4.00	-2.40	-2.20	-2.20	-2.00
47	SiO	-24.6	0.00	-5.40	-5.40	-2.70	-2.60	-0.80	-0.80
48	CS	66.9	0.00	-4.90	-4.90	-2.50	-2.50	-0.90	-0.90
49	SO	1.2	0.00	2.20	2.20	1.40	1.40	3.20	3.20
50	ClO	24.2	0.00	2.60	2.60	-0.70	-0.70	0.70	0.70
51	ClF	-13.2	0.00	0.80	0.80	-0.40	-0.40	0.90	0.90
52	H$_3$Si-SiH$_3$	19.1	-2.62	-1.30	1.40	-0.40	0.70	-2.50	-1.00
53	CH$_3$Cl	-19.6	-0.73	-0.60	0.20	0.50	0.80	0.00	0.40
54	H$_3$CSH	-5.5	-1.15	-1.00	0.20	-0.40	0.00	-1.10	-0.50
55	HOCl	-17.8	-0.05	-0.40	-0.40	-1.30	-1.30	0.00	0.00
56	SO$_2$	-71.0	-0.14	-6.30	-6.20	-3.50	-3.50	0.20	0.30
57	BF$_3$	-271.4	-0.36	-4.60	-4.20	0.50	0.60	0.80	1.00
58	BCl$_3$	-96.3	-0.87	-6.00	-5.10	1.90	2.20	1.30	1.80
59	AlF$_3$	-289.0	-0.92	-10.60	-9.60	-4.00	-3.60	-2.70	-2.20
60	AlCl$_3$	-139.7	-1.48	-10.10	-8.50	-2.20	-1.60	-2.10	-1.30
61	CF$_4$	-223.0	-0.43	-6.40	-5.90	-2.20	-2.00	-1.20	-0.90
62	CCl$_4$	-22.9	-1.22	-12.20	-10.90	-2.70	-2.20	-2.30	-1.70
63	COS	-33.1	-0.14	0.00	0.10	2.00	2.10	4.40	4.50
64	CS$_2$	27.9	-0.28	-0.20	0.10	2.80	2.90	4.90	5.00
65	COF$_2$	-149.1	-0.19	-6.90	-6.70	-5.20	-5.10	-3.20	-3.00
66	SiF$_4$	-386.0	-1.86	-16.70	-14.70	-6.60	-5.90	-6.30	-5.30
67	SiCl$_4$	-158.4	-3.15	-16.60	-13.30	-3.40	-2.20	-4.60	-2.80
68	N$_2$O	19.6	-0.06	4.30	4.30	1.90	1.90	6.40	6.40
69	ClNO	12.4	-0.15	2.70	2.80	-0.90	-0.80	3.00	3.10
70	NF$_3$	-31.6	-0.20	3.70	3.90	-1.80	-1.70	1.70	1.80
71	PF$_3$	-229.1	-0.58	-4.70	-4.00	-2.30	-2.10	-1.30	-1.00
72	O$_3$	34.1	-0.04	-6.50	-6.50	-7.20	-7.20	-0.10	-0.10
73	F$_2$O	5.9	-0.09	1.30	1.40	-4.40	-4.40	-0.50	-0.50
74	ClF$_3$	-38.0	-0.43	5.10	5.60	0.30	0.50	4.30	4.50
75	C$_2$F$_4$	-157.4	-1.33	0.60	2.00	2.40	2.90	4.10	4.80
76	C$_2$Cl$_4$	-3.0	-2.18	-10.30	-8.00	0.40	1.30	0.90	2.10
77	CF$_3$CN	-118.4	-1.14	-5.50	-4.30	-0.70	-0.20	1.70	2.30
78	C$_3$H$_4$(propine)	44.2	-1.24	-2.40	-1.10	0.00	0.50	-0.20	0.50
79	C$_3$H$_4$(allene)	45.5	-1.13	1.10	2.20	0.90	1.30	0.70	1.30
80	C$_3$H$_4$(cyclopropene)	66.2	-1.81	-4.20	-2.30	-2.40	-1.70	-2.60	-1.60
81	C$_3$H$_6$(cyclopropylene)	4.8	-2.64	-1.90	0.80	-0.40	0.60	-1.70	-0.20
82	C$_3$H$_6$(cyclopropane)	12.7	-2.99	-3.70	-0.50	-1.00	0.20	-2.40	-0.80
83	C$_3$H$_8$(propane)	-25.0	-4.37	-3.10	1.50	-0.70	1.10	-2.80	-0.40
84	C$_4$H$_6$(buta-di-ene)	26.3	-3.32	-3.10	0.40	-0.70	0.60	-1.80	0.00
85	C$_4$H$_6$(but-2-ine)	34.8	-2.23	-3.70	-1.30	-0.10	0.80	-1.00	0.30
86	C$_4$H$_6$(methylencyclopropane)	47.9	-3.20	-1.60	1.70	1.20	2.50	0.10	1.90
87	C$_4$H$_6$(bicyclobutane)	51.9	-4.08	-8.90	-4.60	-3.80	-2.20	-5.00	-2.80
88	C$_4$H$_6$(cyclobutene)	37.4	-3.84	-7.60	-3.60	-3.30	-1.80	-4.60	-2.40
89	C$_4$H$_8$(cyclobutane)	6.8	-5.91	-7.10	-0.90	-2.10	0.30	-4.30	-1.00

90	C_4H_8(isobutene)	-4.0	-5.25	-5.00	0.60	-1.20	0.90	-3.30	-0.40
91	C_4H_{10}(butane)	-32.1	-6.82	-7.90	-0.70	-3.50	-0.80	-6.50	-2.70
92	C_4H_{10}(isobutane)	-32.1	-7.66	-7.10	1.00	-2.10	0.90	-5.10	-0.90
93	C_5H_8(spiropentane)	44.3	-6.11	-7.90	-1.50	-1.70	0.80	-3.80	-0.40
94	C_6H_6(benzene)	19.7	-4.41	-7.40	-2.70	0.90	2.70	-0.40	2.10
95	H_2CF_2	-107.7	-0.59	-0.90	-0.30	-0.10	0.10	0.30	0.60
96	CHF_3	-166.6	-0.50	-3.50	-3.00	-1.10	-0.90	-0.40	-0.10
97	H_2CCl_2	-22.8	-0.87	-3.50	-2.60	-0.10	0.20	-0.40	0.10
98	$CHCl_3$	-24.7	-1.03	-7.50	-6.40	-1.30	-0.90	-1.40	-0.80
99	CH_3NH_2	-5.5	-1.47	1.70	3.30	0.10	0.70	-0.50	0.30
100	CH_3CN	18.0	-1.00	-0.10	0.90	1.10	1.50	1.90	2.40
101	CH_3NO_2	-17.8	-1.70	0.80	2.60	-1.10	-0.50	1.90	2.90
102	CH_3-O-N=O	-15.9	-1.37	-0.40	1.00	-3.20	-2.70	-0.10	0.70
103	H_3C-SiH_3	-7.0	-2.35	-2.40	0.10	-1.10	-0.20	-2.90	-1.60
104	HCOOH	-90.5	-0.50	-2.40	-1.90	-1.80	-1.60	-0.20	0.00
105	$HCOOCH_3$	-85.0	-2.24	-2.60	-0.20	-0.80	0.10	0.00	1.20
106	CH_3CONH_2	-57.0	-2.90	-1.00	2.00	-0.40	0.80	-0.30	1.30
107	CH_2-NH-CH_2	30.2	-2.26	-0.90	1.50	-0.70	0.20	-1.10	0.10
108	NC-CN	73.3	-0.38	-0.20	0.20	1.50	1.60	4.90	5.10
109	$(CH_3)_2NH$	-4.4	-3.71	0.00	3.90	-0.20	1.30	-1.60	0.50
110	$C_2H_5NH_2$	-11.3	-3.58	0.20	4.00	0.50	1.90	-0.90	1.10
111	H_2C=C=O	-11.3	-0.56	1.30	1.90	1.40	1.60	2.70	3.00
112	H_2C-O-CH_2	-12.6	-1.56	-3.10	-1.40	-2.00	-1.30	-1.70	-0.90
113	CH_3CHO	-39.7	-1.52	-1.60	0.00	-0.80	-0.20	-0.60	0.30
114	O=CH-CH=O	-50.7	-1.12	-3.10	-1.90	-1.70	-1.20	0.30	0.90
115	C_2H_5OH	-56.2	-2.91	-3.50	-0.50	-2.10	-0.90	-2.90	-1.30
116	CH_3-O-CH_3	-44.0	-2.96	-1.80	1.30	-1.10	0.10	-2.00	-0.30
117	CH_2-S-CH_2(Thiiran)	19.6	-1.79	-3.60	-1.70	-0.40	0.40	-0.80	0.20
118	CH_3-SO-CH_3	-36.2	-3.88	-6.00	-1.90	-2.80	-1.20	-3.00	-0.90
119	C_2H_5SH	-11.1	-3.11	-3.40	-0.20	-0.80	0.40	-2.30	-0.60
120	CH_3-S-CH_3	-8.9	-2.67	-3.00	-0.20	-0.60	0.40	-2.00	-0.50
121	H_2C=CHF	-33.2	-1.04	0.40	1.50	0.70	1.10	0.80	1.40
122	C_2H_5Cl	-26.8	-2.53	-3.10	-0.50	-0.20	0.80	-1.50	-0.10
123	H_2C=CHCl	5.5	-1.22	-1.90	-0.60	0.20	0.70	0.00	0.60
124	H_2C=CHCN	43.2	-1.59	-3.00	-1.30	-1.00	-0.30	0.10	0.90
125	CH_3-CO-CH_3	-51.9	-3.57	-4.10	-0.40	-1.40	0.00	-2.00	-0.10
126	CH_3COOH	-103.4	-2.01	-4.90	-2.80	-2.60	-1.80	-1.90	-0.80
127	CH_3COF	-105.7	-1.67	-3.80	-2.00	-1.80	-1.10	-1.00	-0.10
128	CH_3COCl	-58.0	-1.91	-4.00	-2.00	-1.20	-0.40	-0.50	0.50
129	C_3H_7Cl	-31.5	-4.95	-5.60	-0.40	-0.70	1.30	-2.70	0.00
130	$(CH_3)_2CHOH$	-65.2	-5.58	-6.70	-0.80	-2.90	-0.60	-4.60	-1.50
131	$C_2H_5OCH_3$	-51.7	-4.85	-3.80	1.30	-1.20	0.70	-2.90	-0.20
132	$(CH_3)_3N$	-5.7	-7.01	-2.40	5.00	-0.20	2.60	-2.50	1.40
133	C_4H_4O(furane)	-8.3	-2.12	-6.70	-4.50	-1.40	-0.60	-1.20	-0.10
134	C_4H_4S(thiophene)	27.5	-2.28	-8.80	-6.40	-0.80	0.10	-1.00	0.20
135	C_4H_4NH(pyrrol)	25.9	-2.83	-3.60	-0.60	1.00	2.10	0.60	2.10
136	C_5H_5N(pryridine)	33.6	-3.62	-3.70	0.10	2.20	3.60	1.80	3.80
137	SH	34.2	0.00	2.10	2.10	1.10	1.10	1.00	1.00
138	CCH	135.1	-0.16	-3.50	-3.40	-2.90	-2.80	-2.10	-2.00

139	C$_2$H$_3$	71.6	-0.55	2.60	3.10	1.30	1.50	1.00	1.30
140	CH$_3$CO	-2.4	-1.04	0.80	1.90	1.00	1.40	1.60	2.20
141	H$_2$COH	-4.1	-0.70	1.60	2.30	0.20	0.50	0.30	0.70
142	CH$_3$O	4.1	-0.53	3.40	4.00	0.60	0.80	0.40	0.70
143	C$_2$H$_5$O	-3.7	-2.29	0.00	2.40	-1.10	-0.20	-2.10	-0.80
144	CH$_3$S	29.8	-0.68	2.10	2.80	1.90	2.20	1.30	1.70
145	C$_2$H$_5$	28.9	-1.48	2.00	3.50	1.40	2.00	0.10	1.00
146	(CH$_3$)$_2$CH	21.5	-3.20	0.70	4.00	1.40	2.70	-0.60	1.20
147	(CH$_3$)$_3$C	12.3	-5.81	-2.70	3.40	0.00	2.30	-2.80	0.40
148	NO$_2$	7.9	-0.04	4.50	4.50	0.90	0.90	5.50	5.50
149	CH$_3$-CH=C=CH$_2$	38.8	-2.68	-1.20	1.60	0.30	1.40	-0.60	0.90
150	C$_5$H$_8$(isoprene)	18.0	-6.39	-6.70	0.00	-1.80	0.80	-3.70	-0.20
151	C$_5$H$_1$0(cyclopentaane)	-18.3	-8.41	-11.30	-2.50	-3.20	0.10	-6.50	-1.90
152	C$_5$H$_1$2(n-pentane)	-35.1	-9.29	-8.70	1.10	-2.30	1.40	-6.00	-0.90
153	C$_5$H$_1$2(neopentane)n	-40.2	-11.99	-12.20	0.40	-4.10	0.70	-8.00	-1.40
154	C$_6$H$_8$(1.3-cyclohexadien)	25.4	-6.75	-11.70	-4.60	-3.20	-0.50	-5.40	-1.70
155	C$_6$H$_8$(1.4-cyclohexadien)	25.0	-6.34	-12.00	-5.30	-3.50	-1.00	-5.80	-2.30
156	C$_6$H$_{12}$(cyclohexane)	-29.5	-12.49	-15.80	-2.70	-4.90	0.10	-9.10	-2.30
157	C$_6$H$_{14}$(n-hexane)	-39.9	-11.78	-11.20	1.10	-2.80	1.90	-7.40	-0.90
158	C$_6$H$_{14}$(3-methyl-pentane)	-41.1	-13.94	-13.80	0.90	-4.40	1.20	-9.10	-1.40
159	C$_6$H$_5$CH$_3$(toluene)	12.0	-6.95	-10.40	-3.10	0.10	2.80	-2.00	1.80
160	C$_7$H$_{16}$(n-heptane)	-44.9	-14.27	-14.00	1.00	-3.60	2.10	-9.00	-1.10
161	C$_8$H$_8$(cyclooctatetraene)	70.7	-9.25	-15.00	-5.30	-3.90	-0.20	-5.80	-0.70
162	C$_8$H$_{18}$(n-octane)	-49.9	-16.79	-16.80	0.80	-4.40	2.30	-10.50	-1.30
163	C$_{10}$H$_8$(naphtalene)	35.9	-9.69	-16.10	-5.90	1.40	5.20	-0.70	4.60
164	C$_{10}$H$_8$(azulene)	69.1	-10.42	-15.90	-5.00	0.20	4.30	-1.20	4.50
165	CH$_3$COOCH$_3$	-98.4	-3.91	-6.20	-2.10	-2.60	-1.10	-2.70	-0.50
166	(CH$_3$)$_3$COH	-74.7	-9.30	-11.40	-1.60	-4.70	-1.00	-7.30	-2.20
167	C$_6$H$_5$NH$_2$	20.8	-6.20	-6.20	0.30	1.70	4.20	0.40	3.90
168	C$_6$H$_5$OH(phenol)	-23.0	-5.32	-10.40	-4.80	-1.30	0.80	-2.10	0.80
169	C$_4$H$_6$O	-3.3	-4.02	-4.60	-0.40	-1.90	-0.30	-2.40	-0.20
170	C$_4$H$_8$O(tetrahydrofuran)	-44.0	-6.12	-10.30	-3.90	-4.10	-1.70	-6.10	-2.70
171	C$_5$H$_8$O(cyclopentanone)	-45.9	-7.28	-11.40	-3.80	-3.20	-0.30	-4.90	-0.90
172	C$_6$H$_4$O$_2$(benzochinone)	-29.4	-5.11	-13.40	-8.00	-4.60	-2.50	-3.40	-0.60
173	C$_4$H$_4$N$_2$	46.8	-2.88	1.10	4.20	4.80	5.90	5.20	6.80
174	C$_2$H$_6$O$_2$S(dimethyl)	-89.2	-4.74	-14.20	-9.30	-7.80	-5.90	-7.40	-4.80
175	C$_6$H$_5$Cl	12.4	-5.09	-12.60	-7.30	-1.50	0.60	-2.50	0.20
176	NC-CH$_2$-CH$_2$-CN	50.1	-4.00	-5.30	-1.10	0.40	2.00	1.80	4.00
177	C$_4$H$_4$N$_2$	46.9	-2.88	-2.70	0.30	0.60	1.80	1.20	2.80
178	(acetyl	15.6	-2.66	-8.30	-5.60	-3.90	-2.80	-3.00	-1.50
179	CH$_3$-CH=CH-CHO	-24.0	-3.99	-3.40	0.80	-0.10	1.40	-0.50	1.70
180	(acetic	-136.8	-4.95	-8.70	-3.50	-2.70	-0.80	-1.90	0.80
181	C$_4$H$_6$S	20.8	-3.83	-9.60	-5.60	-2.20	-0.60	-3.60	-1.50
182	(CH$_3$)$_2$CH-CN	5.6	-5.88	-7.80	-1.60	-2.30	0.10	-3.10	0.20
183	CH$_3$-CO-CH$_2$-CH$_3$	-57.1	-5.88	-6.40	-0.20	-1.60	0.70	-3.00	0.20
184	(CH$_3$)$_2$-CH-CHO	-51.6	-6.76	-8.60	-1.50	-3.30	-0.60	-4.70	-1.00
185	C$_4$H$_8$O$_2$	-75.5	-7.47	-11.80	-4.00	-4.90	-1.90	-6.50	-2.40
186	C$_4$H$_8$S	-8.2	-6.53	-12.70	-5.80	-4.20	-1.50	-6.60	-3.00
187	(CH$_3$)$_3$C-Cl	-43.5	-8.94	-12.40	-3.00	-4.00	-0.40	-6.90	-2.00

188	(n-butyl	-37.0	-7.43	-8.90	-1.10	-2.00	1.00	-4.80	-0.70
189	C_4H_8NH	-0.8	-7.28	-8.00	-0.30	-2.40	0.50	-4.80	-0.80
190	CH_3-$CH(OCH_3)_2$-NO_2	-39.1	-10.03	-9.10	1.40	-4.10	-0.10	-3.50	2.00
191	(diethy	-60.3	-6.79	-6.80	0.30	-2.30	0.40	-4.80	-1.00
192	CH_3-$CH(OCH_3)_2$	-93.1	-8.52	-10.70	-1.80	-5.10	-1.70	-7.10	-2.50
193	$(CH_3)_3C$-SH	-26.2	-9.89	-12.50	-2.10	-4.10	-0.10	-7.20	-1.80
194	CH_3-CH_2-S-S-CH_2-CH_3	-17.9	-7.38	-12.10	-4.40	-4.30	-1.40	-7.10	-3.00
195	$(CH_3)_3C$-NH_2	-28.9	-10.74	-9.00	2.30	-3.10	1.20	-6.30	-0.30
196	$Si(CH_3)_4$	-55.7	-8.94	-17.50	-8.10	-9.60	-6.10	-13.60	-8.70
197	C_5H_6S	20.0	-4.33	-11.40	-6.90	-1.40	0.30	-2.40	0.00
198	C_5H_7N	24.6	-5.31	-6.10	-0.60	0.40	2.50	-0.80	2.20
199	$C_5H_{10}O$	-53.4	-9.93	-14.00	-3.60	-5.10	-1.10	-8.10	-2.60
200	CH_3-CH_3CO-C_2-CH_3	-61.6	-8.23	-8.60	0.00	-1.80	1.50	-4.00	0.50
201	CH_3-C(=O)-O-$CH(CH_3)_2$	-115.1	-9.04	-12.40	-2.90	-4.40	-0.80	-6.20	-1.20
202	C_5H_10S	-15.2	-10.35	-16.00	-5.20	-5.00	-0.80	-8.40	-2.70
203	cyc-$C_5H_{10}NH$	-11.3	-11.39	-12.40	-0.40	-4.20	0.40	-7.60	-1.40
204	$(CH_3)_3C$-O-CH_3	-67.8	-12.64	-13.40	-0.10	-5.10	0.00	-8.50	-1.50
205	$C_6H_4F_2$	-73.9	-4.98	-8.60	-3.40	0.40	2.40	0.10	2.80
206	$C_6H_4F_2$	-73.3	-4.98	-8.70	-3.50	0.30	2.30	0.00	2.80
207	C_6H_5F	-27.7	-4.69	-8.20	-3.30	0.40	2.30	-0.40	2.20
208	$(CH_3)_2CH$-O-$CH(CH_3)_2$	-76.3	-13.69	-14.90	-0.50	-5.10	0.40	-9.30	-1.80
209	PF_5	-381.1	-1.76	-17.00	-15.20	-8.10	-7.40	-7.50	-6.50
210	SF_6	-291.7	-1.78	-16.80	-14.90	-8.60	-7.80	-6.60	-5.60
211	P_4	14.1	-0.09	-14.80	-14.70	-9.10	-9.10	-7.60	-7.50
212	SO_3	-94.6	-0.42	-11.90	-11.50	-7.90	-7.70	-3.40	-3.20
213	SCl_2	-4.2	-0.49	-3.90	-3.40	-3.20	-3.00	-2.50	-2.20
214	$POCl_3$	-133.8	-2.28	-12.70	-10.30	-4.60	-3.70	-3.80	-2.50
215	PCl_5	-86.1	-3.27	-15.10	-11.70	-3.90	-2.60	-4.10	-2.30
216	Cl_2O_2S	-84.8	-1.64	-13.70	-11.90	-8.20	-7.50	-5.10	-4.20
217	PCl_3	-69.0	-1.38	-5.80	-4.30	-2.40	-1.90	-2.30	-1.50
218	Cl_2S_2	-4.0	-1.16	0.50	1.80	1.20	1.70	2.50	3.10
219	$SiCl_2$	-40.3	-0.51	-7.20	-6.60	-3.50	-3.30	-3.50	-3.20
220	CF_3Cl	-169.5	-0.60	-7.20	-6.60	-2.60	-2.40	-1.70	-1.40
221	C_2F_6	-321.3	-3.28	-12.10	-8.70	-4.10	-2.80	-3.00	-1.20
222	CF_3	-111.3	-0.23	0.50	0.70	1.50	1.60	2.60	2.70
223	C_6H_5	81.2	-3.71	-4.40	-0.50	2.40	3.90	1.40	3.40

[a]   Taken from L. A. Curtiss, K. Raghavachari, P. C. Redfern, and J. A. Pople, *J. Chem. Phys.*, 1997, **106**, 1063 for molecules 1 - 148, and from L. A. Curtiss, K. Raghavachari, P. C. Redfern, and J. A. Pople, *J. Chem. Phys.*, 2000, **112**, 7374 for molecules 149 - 223.

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------------------------ C14H30 folded
$coord
   -4.20336628844641     -0.47857244940978      0.31561295373445      c
   -3.09259323394575      0.85563850449661      2.64497009685014      c
   -2.90792708208878     -0.90401252255936      4.96308200629427      c
   -1.44396464940144      0.23225980454375      7.22983658041791      c
    1.44396464940144     -0.23225980454375      7.22983658041791      c
    2.90792708208878      0.90401252255936      4.96308200629427      c
    3.09259323394575     -0.85563850449661      2.64497009685014      c
    4.20336628844641      0.47857244940978      0.31561295373445      c
    4.38846028286657     -1.24609312858212     -2.01724428371430      c
    5.56551609578534      0.08214690404231     -4.32292858913966      c
    5.77521019800260     -1.66248272976288     -6.64449878127740      c
   -4.38846028286657      1.24609312858212     -2.01724428371430      c
   -5.56551609578534     -0.08214690404231     -4.32292858913966      c
   -5.77521019800260      1.66248272976288     -6.64449878127740      c
   -6.09607696815944     -1.22132840065008      0.77632977315704      h
   -3.01833270232908     -2.13073392453907     -0.14681751639287      h
   -1.22228545299416      1.61116250899120      2.15806725605052      h
   -4.27534782003023      2.49854654182249      3.13844748714238      h
   -2.01277421594515     -2.69874283259514      4.40105508625581      h
   -4.84429096271057     -1.38442387083902      5.55656381946714      h
   -1.79693343284761      2.28610268663703      7.30250810005767      h
   -2.20788140256853     -0.55781670076712      8.99683974826018      h
    1.79693343284761     -2.28610268663703      7.30250810005767      h
    2.20788140256853      0.55781670076712      8.99683974826018      h
    2.01277421594515      2.69874283259514      4.40105508625581      h
    4.84429096271057      1.38442387083902      5.55656381946714      h
    1.22228545299416     -1.61116250899120      2.15806725605052      h
    4.27534782003023     -2.49854654182249      3.13844748714238      h
    3.01833270232908      2.13073392453907     -0.14681751639287      h
    6.09607696815944      1.22132840065008      0.77632977315704      h
    2.48494269631577     -1.93813992170315     -2.51304714689889      h
    5.52577115170767     -2.92794463107058     -1.54258642262454      h
    4.42298539199471      1.75701060025708     -4.80060581580112      h
    7.45593350301369      0.78497618346235     -3.80077559721321      h
    3.89745979210746     -2.34063465043966     -7.22989821600000      h
    6.63906957942461     -0.68219181739803     -8.26135482617856      h
    6.94215623888575     -3.32728274254683     -6.20355571244688      h
   -2.48494269631577      1.93813992170315     -2.51304714689889      h
   -5.52577115170767      2.92794463107058     -1.54258642262454      h
   -4.42298539199471     -1.75701060025708     -4.80060581580112      h
   -7.45593350301369     -0.78497618346235     -3.80077559721321      h
   -3.89745979210746      2.34063465043966     -7.22989821600000      h
   -6.63906957942461      0.68219181739803     -8.26135482617856      h
   -6.94215623888575      3.32728274254683     -6.20355571244688      h


------------------------ C14H30 linear
$coord
  -15.78861044310000     -0.35170123370000      0.00000000000000      c
  -13.32756923630000      1.20474635170000      0.00000000000000      c
  -10.94620879730000     -0.46784100960000      0.00000000000000      c
   -8.47063183560000      1.05858877460000      0.00000000000000      c
   -6.09211029520000     -0.61590201660000      0.00000000000000      c
   -3.61637934540000      0.91073432410000      0.00000000000000      c
   -1.23779951780000     -0.76343009550000      0.00000000000000      c
    1.23779951780000      0.76343009550000      0.00000000000000      c
    3.61637934540000     -0.91073432410000      0.00000000000000      c
    6.09211029520000      0.61590201660000      0.00000000000000      c
    8.47063183560000     -1.05858877460000      0.00000000000000      c
   10.94620879730000      0.46784100960000      0.00000000000000      c
   13.32756923630000     -1.20474635170000      0.00000000000000      c
   15.78861044310000      0.35170123370000      0.00000000000000      c
  -17.46808428500000      0.87330902150000      0.00000000000000      h
  -15.88267589000000     -1.57516910390000     -1.68025715870000      h
  -15.88267589000000     -1.57516910390000      1.68025715870000      h
  -13.28345174300000      2.44975184090000      1.66957093730000      h
  -13.28345174300000      2.44975184090000     -1.66957093730000      h
  -10.98516045090000     -1.71549747340000      1.66995808840000      h
  -10.98516045090000     -1.71549747340000     -1.66995808840000      h
   -8.43220583780000      2.30579825340000      1.66993212280000      h
   -8.43220583780000      2.30579825340000     -1.66993212280000      h
   -6.12997243260000     -1.86315898950000      1.66984844730000      h
   -6.12997243260000     -1.86315898950000     -1.66984844730000      h
   -3.57834095090000      2.15800281910000      1.66985837620000      h
   -3.57834095090000      2.15800281910000     -1.66985837620000      h
   -1.27559238840000     -2.01070833090000      1.66986085730000      h
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   -1.27559238840000       -2.01070833090000       -1.66986085730000           h
    1.27559238840000        2.01070833090000        1.66986085730000           h
    1.27559238840000        2.01070833090000       -1.66986085730000           h
    3.57834095090000       -2.15800281910000        1.66985837620000           h
    3.57834095090000       -2.15800281910000       -1.66985837620000           h
    6.12997243260000        1.86315898950000        1.66984844730000           h
    6.12997243260000        1.86315898950000       -1.66984844730000           h
    8.43220583780000       -2.30579825340000        1.66993212280000           h
    8.43220583780000       -2.30579825340000       -1.66993212280000           h
   10.98516045090000        1.71549747340000        1.66995808840000           h
   10.98516045090000        1.71549747340000       -1.66995808840000           h
   13.28345174300000       -2.44975184090000        1.66957093730000           h
   13.28345174300000       -2.44975184090000       -1.66957093730000           h
   15.88267589000000        1.57516910390000        1.68025715870000           h
   17.46808428500000       -0.87330902150000        0.00000000000000           h
   15.88267589000000        1.57516910390000       -1.68025715870000           h


----------------------- C22H46 folded
$coord
    3.54786454630000        0.79403301320000        5.21024670874118           c
    3.02109448510000       -0.69480021010000        7.65242229304118           c
    2.90715145960000        0.99365311360000       10.03623778524118           c
    1.45188746270000       -0.19920914480000       12.28123641704117           c
   -1.45188746270000        0.19920914480000       12.28123641704117           c
   -2.90715145960000       -0.99365311360000       10.03623778524118           c
   -3.02109448510000        0.69480021010000        7.65242229304118           c
   -3.54786454630000       -0.79403301320000        5.21024670874118           c
   -3.28066119510000        0.82866323320000        2.81300825714118           c
   -3.57137827870000       -0.70238273710000        0.35998432514118           c
   -3.22859869610000        0.90447352420000       -2.03755909935882           c
   -3.51758555220000       -0.63183914120000       -4.48766132455882           c
   -3.19776189860000        0.97165697940000       -6.89051656355882           c
   -3.51097472150000       -0.56622680460000       -9.33875196505882           c
   -3.22034004960000        1.06167313140000      -11.73345472565882           c
    3.28066119510000       -0.82866323320000        2.81300825714118           c
    3.57137827870000        0.70238273710000        0.35998432514118           c
    3.22859869610000       -0.90447352420000       -2.03755909935882           c
    3.51758555220000        0.63183914120000       -4.48766132455882           c
    3.19776189860000       -0.97165697940000       -6.89051656355882           c
    3.51097472150000        0.56622680460000       -9.33875196505882           c
    3.22034004960000       -1.06167313140000      -11.73345472565882           c
    5.44763020500000        1.64737070510000        5.28169045594118           h
    2.19566291550000        2.37598944370000        5.09480203874118           h
    1.22758812110000       -1.70432760410000        7.41741863484118           h
    4.47723395710000       -2.16007552790000        7.91603469914118           h
    2.01899659670000        2.81419958140000        9.55145069574118           h
    4.85177797920000        1.44015154820000       10.62736483294118           h
    1.85002739890000       -2.24515306210000       12.33830220724118           h
    2.18724484080000        0.59371618460000       14.05913722184118           h
   -1.85002739890000        2.24515306210000       12.33830220724118           h
   -2.18724484080000       -0.59371618460000       14.05913722184118           h
   -2.01899659670000       -2.81419958140000        9.55145069574118           h
   -4.85177797920000       -1.44015154820000       10.62736483294118           h
   -1.22758812110000        1.70432760410000        7.41741863484118           h
   -4.47723395710000        2.16007552790000        7.91603469914118           h
   -2.19566291550000       -2.37598944370000        5.09480203874118           h
   -5.44763020500000       -1.64737070510000        5.28169045594118           h
   -1.40592037060000        1.73218617040000        2.82459644374118           h
   -4.68541506500000        2.36749593240000        2.84419192654118           h
   -2.16688676910000       -2.24193663460000        0.35431471944118           h
   -5.44676838700000       -1.61099358780000        0.32241470914118           h
   -1.34539934230000        1.78719104350000       -2.00201666515882           h
   -4.61735785660000        2.45841169580000       -2.03091719115882           h
   -2.11251494830000       -2.16968009900000       -4.49745892895882           h
   -5.39220599960000       -1.54283932350000       -4.51227086475882           h
   -1.31622155280000        1.85780558760000       -6.87696340925882           h
   -4.58887061860000        2.52388730040000       -6.87103924925882           h
   -2.10112117390000       -2.09747595260000       -9.35775528605882           h
   -5.38174322520000       -1.48178298510000       -9.33152834735882           h
   -1.34047988800000        1.94328906500000      -11.79395169615882           h
   -3.45001028270000       -0.07293169100000      -13.45971444615882           h
   -4.64278706870000        2.57931463440000      -11.76329460915882           h
    1.40592037060000       -1.73218617040000        2.82459644374118           h
    4.68541506500000       -2.36749593240000        2.84419192654118           h
    2.16688676910000        2.24193663460000        0.35431471944118           h
    5.44676838700000        1.61099358780000        0.32241470914118           h
    1.34539934230000       -1.78719104350000       -2.00201666515882           h
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     4.61735785660000        -2.45841169580000        -2.03091719115882       h
     2.11251494830000         2.16968009900000        -4.49745892895882       h
     5.39220599960000         1.54283932350000        -4.51227086475882       h
     1.31622155280000        -1.85780658760000        -6.87696340925882       h
     4.58887061860000        -2.52388730040000        -6.87103924925882       h
     2.10112117390000         2.09747595260000        -9.35775528605882       h
     5.38174322520000         1.48178298510000        -9.33152834735882       h
     1.34047988800000        -1.94328906500000       -11.79395169615882       h
     3.45001028270000         0.07293169100000       -13.45971444615882       h
     4.64278706870000        -2.57931463440000       -11.76329460915882       h


------------------------ C22H46 linear
$coord
   -11.55170306087300        -6.74765542705506         0.00000000000000       c
   -10.10690673337319        -4.22386585951680         0.00000000000000       c
    -7.21762398036493        -4.55828507276439         0.00000000000000       c
    -5.77449813132640        -2.03340374368110         0.00000000000000       c
    -2.88476697767487        -2.36252046905555         0.00000000000000       c
    -1.44488772695360         0.16431936024356         0.00000000000000       c
     1.44488772695360        -0.16431936024356         0.00000000000000       c
     2.88476697767487         2.36252046905555         0.00000000000000       c
     5.77449813132640         2.03340374368110         0.00000000000000       c
     7.21762398036493         4.55828507276439         0.00000000000000       c
    10.10690673337319         4.22386585951680         0.00000000000000       c
    11.55170306087300         6.74765542705506         0.00000000000000       c
    14.44124459076912         6.41576952651132         0.00000000000000       c
    15.88261315112483         8.94176233411131         0.00000000000000       c
    18.77222975484635         8.61310931282639         0.00000000000000       c
    20.21202971775118        11.14149975981365         0.00000000000000       c
    23.10196585138743        10.78768548681581         0.00000000000000       c
   -14.44124459076912        -6.41576952651132         0.00000000000000       c
   -15.88261315112483        -8.94176233411131         0.00000000000000       c
   -18.77222975484635        -8.61310931282639         0.00000000000000       c
   -20.21202971775118       -11.14149975981365         0.00000000000000       c
   -23.10196585138743       -10.78768548681581         0.00000000000000       c
   -10.98848363567879        -7.86131242048638         1.66973978330924       h
   -10.98848363567879        -7.86131242048638        -1.66973978330924       h
   -10.66944266326372        -3.10984460200088        -1.66977744111016       h
   -10.66944266326372        -3.10984460200088         1.66977744111016       h
    -6.65486233949992        -5.67212536435000        -1.66978822939742       h
    -6.65486233949992        -5.67212536435000         1.66978822939742       h
    -6.33902026022685        -0.92035843059257        -1.66968678001954       h
    -6.33902026022685        -0.92035843059257         1.66968678001954       h
    -2.31957911870797        -3.47512039179578        -1.66977758553821       h
    -2.31957911870797        -3.47512039179578         1.66977758553821       h
    -2.00979414111968         1.27712731710287        -1.66974516457237       h
    -2.00979414111968         1.27712731710287         1.66974516457237       h
     2.00979414111968        -1.27712731710287        -1.66974516457237       h
     2.00979414111968        -1.27712731710287         1.66974516457237       h
     2.31957911870797         3.47512039179578        -1.66977758553821       h
     2.31957911870797         3.47512039179578         1.66977758553821       h
     6.33902026022685         0.92035843059257        -1.66968678001954       h
     6.33902026022685         0.92035843059257         1.66968678001954       h
     6.65486233949992         5.67212536435000        -1.66978822939742       h
     6.65486233949992         5.67212536435000         1.66978822939742       h
    10.66944266326372         3.10984460200088        -1.66977744111016       h
    10.66944266326372         3.10984460200088         1.66977744111016       h
    10.98848363567879         7.86131242048638        -1.66973978330924       h
    10.98848363567879         7.86131242048638         1.66973978330924       h
    15.00530510853647         5.30282856667778        -1.66983957108604       h
    15.00530510853647         5.30282856667778         1.66983957108604       h
    15.31818284503017        10.05455933229918        -1.66992590078608       h
    15.31818284503017        10.05455933229918         1.66992590078608       h
    19.33846414404447         7.50074304075667        -1.67003061349925       h
    19.33846414404447         7.50074304075667         1.67003061349925       h
    19.63984968900944        12.24798438533498        -1.66952387867955       h
    19.63984968900944        12.24798438533498         1.66952387867955       h
    23.71049817950964         9.72222842941824        -1.68034360259377       h
    24.09484323074180        12.61405003041146         0.00000000000000       h
    23.71049817950964         9.72222842941824         1.68034360259377       h
   -15.00530510853647        -5.30282856667778        -1.66983957108604       h
   -15.00530510853647        -5.30282856667778         1.66983957108604       h
   -15.31818284503017       -10.05455933229918        -1.66992590078608       h
   -15.31818284503017       -10.05455933229918         1.66992590078608       h
   -19.33846414404447        -7.50074304075667        -1.67003061349925       h
   -19.33846414404447        -7.50074304075667         1.67003061349925       h
   -19.63984968900944       -12.24798438533498        -1.66952387867955       h
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  -19.63984968900944    -12.24798438533498     1.66952387867955      h
  -23.71049817950964     -9.72222842941824    -1.68034360259377      h
  -24.09484323074180    -12.61405003041146     0.00000000000000      h
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------------------------ C30H62 folded
$coord
    2.54378414010000    -2.59440078520000   -10.06852531030217      c
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    1.89277141670000    -2.41967063170000   -14.89552339000217      c
    1.32442254740000    -0.62719149730000   -17.14176686010217      c
   -1.32442254740000     0.62719149730000   -17.14176686010217      c
   -1.89277141670000     2.41967063170000   -14.89552339000217      c
   -2.91306085040000     1.06501666000000   -12.51430582830217      c
   -2.54378414010000     2.59440078520000   -10.06852531030217      c
   -3.20432991820000     1.08192928190000    -7.67432283760217      c
   -2.62892165400000     2.52537917570000    -5.21837031730217      c
   -3.20225909780000     0.98392563180000    -2.82128640700217      c
   -2.63170049260000     2.44113223240000    -0.37202640120217      c
   -3.20160826180000     0.91356973920000     2.03427269109783      c
   -2.65763866450000     2.39376670030000     4.47610197939783      c
   -3.21470429690000     0.86939119040000     6.88738335189783      c
    3.20432991820000    -1.08192928190000    -7.67432283760217      c
    2.62892165400000    -2.52537917570000    -5.21837031730217      c
    3.20225909780000    -0.98392563180000    -2.82128640700217      c
    2.63170049260000    -2.44113223240000    -0.37202640120217      c
    3.20160826180000    -0.91356973920000     2.03427269109783      c
    2.65763866450000    -2.39376670030000     4.47610197939783      c
    3.21470429690000    -0.86939119040000     6.88738335189783      c
    2.68012045170000    -2.35614178530000     9.32745480739783      c
    3.24022349420000    -0.83170274270000    11.73819280569783      c
   -2.68012045170000     2.35614178530000     9.32745480739783      c
   -3.24022349420000     0.83170274270000    11.73819280569783      c
   -2.70228265920000     2.31302921530000    14.18251062689783      c
    2.70228265920000    -2.31302921530000    14.18251062689783      c
    3.30755399490000    -0.77778364890000    16.58013946429782      c
   -3.30755399490000     0.77778364890000    16.58013946429782      c
    3.67259740770000    -4.34472486030000   -10.13542536320217      h
    0.54839463920000    -3.18430342290000    -9.95153430020217      h
    1.96404785410000     0.76170064070000   -12.28201536930217      h
    4.93317766870000    -0.63510412090000   -12.78082343430217      h
    0.15473649470000    -3.45918510660000   -14.40905374920217      h
    3.27721905050000    -3.85620494300000   -15.48715039720217      h
    2.77667975520000     0.86775444400000   -17.20112297610217      h
    1.50549643150000    -1.69498395410000   -18.91869631140218      h
   -2.77667975520000    -0.86775444400000   -17.20112297610217      h
   -1.50549643150000     1.69498395410000   -18.91869631140218      h
   -0.15473649470000     3.45918510660000   -14.40905374920217      h
   -3.27721905050000     3.85620494300000   -15.48715039720217      h
   -1.96404785410000    -0.76170064070000   -12.28201536930217      h
   -4.93317766870000     0.63510412090000   -12.78082343430217      h
   -0.54839463920000     3.18430342290000    -9.95153430020217      h
   -3.67259740770000     4.34472486030000   -10.13542536320217      h
   -2.11626307360000    -0.69192764300000    -7.68445393060217      h
   -5.21794361300000     0.54745751620000    -7.71265649980217      h
   -0.61771749900000     3.07061062300000    -5.21083891350217      h
   -3.72352454180000     4.29847829600000    -5.17919249550217      h
   -2.08008122310000    -0.76742624690000    -2.85238667000217      h
   -5.20575061530000     0.41040156000000    -2.83142471760217      h
   -0.62583178970000     3.00333027580000    -0.36519619580217      h
   -3.74065818370000     4.20576150930000    -0.34658368920217      h
   -2.06547258860000    -0.82822127170000     2.02397894639783      h
   -5.20016137480000     0.32310024800000     2.01809671749783      h
   -0.65973612470000     2.98281374340000     4.48607397399783      h
   -3.79038514560000     4.14335327950000     4.48834903179783      h
   -2.06594899660000    -0.86407330960000     6.87956996819783      h
   -5.20877613720000     0.26399013220000     6.87356448969783      h
    5.21794361300000    -0.54745751620000    -7.71265649980217      h
    2.11626307360000     0.69192764300000    -7.68445393060217      h
    3.72352454180000    -4.29847829600000    -5.17919249550217      h
    0.61771749900000    -3.07061062300000    -5.21083891350217      h
    5.20575061530000    -0.41040156000000    -2.83142471760217      h
    2.08008122310000     0.76742624690000    -2.85238667000217      h
    3.74065818370000    -4.20576150930000    -0.34658368920217      h
    0.62583178970000    -3.00333027580000    -0.36519619580217      h
    5.20016137480000    -0.32310024800000     2.01809671749783      h
    2.06547258860000     0.82822127170000     2.02397894639783      h
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     3.79038514560000       -4.14335327950000        4.48834903179783        h
     0.65973612470000       -2.98281374340000        4.48607397399783        h
     5.20877613720000       -0.26399013220000        6.87356448969783        h
     2.06594899660000        0.86407330960000        6.87956996819783        h
     3.81808496840000       -4.10238819210000        9.33490259019783        h
     0.68396633670000       -2.95057134460000        9.34086337669783        h
     5.23629457160000       -0.23171235880000       11.72339950229783        h
     2.09632056260000        0.90556497040000       11.72890930279783        h
    -3.81808496840000        4.10238819210000        9.33490259019783        h
    -0.68396633670000        2.95057134460000        9.34086337669783        h
    -5.23629457160000        0.23171235880000       11.72339950229783        h
    -2.09632056260000       -0.90556497040000       11.72890930279783        h
    -3.81664261790000        4.07261449760000       14.17219633929783        h
    -0.69937463340000        2.87880164970000       14.20088507959783        h
     0.69937463340000       -2.87880164970000       14.20088507959783        h
     3.81664261790000       -4.07261449760000       14.17219633929783        h
     2.17340383480000        0.96166618940000       16.63897211559782        h
     2.90187008320000       -1.86445105310000       18.30480704989782        h
     5.31586528170000       -0.23650740050000       16.61405815409783        h
    -5.31586528170000        0.23650740050000       16.61405815409783        h
    -2.17340383480000       -0.96166618940000       16.63897211559782        h
    -2.90187008320000        1.86445105310000       18.30480704989782        h

------------------------ C30H62 linear
$coord
    35.19926364893623       -0.73544620799695        0.00000000000000        c
    32.78063284088273        0.88618765191658        0.00000000000000        c
    30.35436077419187       -0.72036270144675        0.00000000000000        c
    27.92219950137341        0.87443874111054        0.00000000000000        c
    25.49799614162571       -0.73290220381679        0.00000000000000        c
    23.06581214203849        0.86216632244530        0.00000000000000        c
    20.64170974180661       -0.74511413741156        0.00000000000000        c
    18.20941548351852        0.84972535658132        0.00000000000000        c
    15.78539323517770       -0.75766890631386        0.00000000000000        c
    13.35298031889182        0.83698149746443        0.00000000000000        c
    10.92905321182937       -0.77056782963899        0.00000000000000        c
     8.49653150433373        0.82391460050978        0.00000000000000        c
     6.07269435220320       -0.78376777109877        0.00000000000000        c
     3.64010142033653        0.81059691711033        0.00000000000000        c
     1.21631001732626       -0.79716252416452        0.00000000000000        c
    -1.21631001732626        0.79716252416452        0.00000000000000        c
    -3.64010142033653       -0.81059691711033        0.00000000000000        c
    -6.07269435220320        0.78376777109877        0.00000000000000        c
    -8.49653150433373       -0.82391460050978        0.00000000000000        c
   -10.92905321182937        0.77056782963899        0.00000000000000        c
   -13.35298031889182       -0.83698149746443        0.00000000000000        c
   -15.78539323517770        0.75766890631386        0.00000000000000        c
   -18.20941548351852       -0.84972535658132        0.00000000000000        c
   -20.64170974180661        0.74511413741156        0.00000000000000        c
   -23.06581214203849       -0.86216632244530        0.00000000000000        c
   -25.49799614162571        0.73290220381679        0.00000000000000        c
   -27.92219950137341       -0.87443874111054        0.00000000000000        c
   -30.35436077419187        0.72036270144675        0.00000000000000        c
   -32.78063284088273       -0.88618765191658        0.00000000000000        c
   -35.19926364893623        0.73544620799695        0.00000000000000        c
    36.91029248208727        0.44507183683268        0.00000000000000        h
    35.26112120421837       -1.96093118376189        1.68025406128442        h
    35.26112120421837       -1.96093118376189       -1.68025406128442        h
    32.77030380954928        2.13193129204813       -1.66955666773415        h
    32.77030380954928        2.13193129204813        1.66955666773415        h
    30.35860206508062       -1.96857624057291       -1.66997355431251        h
    30.35860206508062       -1.96857624057291        1.66997355431251        h
    27.91883013550126        2.12222071615847       -1.66991909869615        h
    27.91883013550126        2.12222071615847        1.66991909869615        h
    25.50109743167375       -1.98070308650213       -1.66983896755940        h
    25.50109743167375       -1.98070308650213        1.66983896755940        h
    23.06266335029123        2.11000028505253       -1.66984452339031        h
    23.06266335029123        2.11000028505253        1.66984452339031        h
    20.64488894675895       -1.99295410203508       -1.66984146031557        h
    20.64488894675895       -1.99295410203508        1.66984146031557        h
    18.20618225186930        2.09756664087096       -1.66984522544412        h
    18.20618225186930        2.09756664087096        1.66984522544412        h
    15.78866662270358       -2.00552336673496       -1.66983506526917        h
    15.78866662270358       -2.00552336673496        1.66983506526917        h
    13.34966180890807        2.08482780211082       -1.66984407255083        h
    13.34966180890807        2.08482780211082        1.66984407255083        h
    10.93241351819821       -2.01842359499278       -1.66983543956048        h
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   10.93241351819821      -2.01842359499278       1.66983543956048        h
    8.49311613908074       2.07177082406079      -1.66983799501153        h
    8.49311613908074       2.07177082406079       1.66983799501153        h
    6.07611845400582      -2.03162282063192      -1.66983728060346        h
    6.07611845400582      -2.03162282063192       1.66983728060346        h
    3.63663028495393       2.05845781913482      -1.66983508365967        h
    3.63663028495393       2.05845781913482       1.66983508365967        h
    1.21976954816661      -2.04501607686152      -1.66983933137965        h
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   -1.21976954816661       2.04501607686152       1.66983933137965        h
   -3.63663028495393      -2.05845781913482      -1.66983508365967        h
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   -6.07611845400582       2.03162282063192      -1.66983728060346        h
   -6.07611845400582       2.03162282063192       1.66983728060346        h
   -8.49311613908074      -2.07177082406079      -1.66983799501153        h
   -8.49311613908074      -2.07177082406079       1.66983799501153        h
  -10.93241351819821       2.01842359499278      -1.66983543956048        h
  -10.93241351819821       2.01842359499278       1.66983543956048        h
  -13.34966180890807      -2.08482780211082      -1.66984407255083        h
  -13.34966180890807      -2.08482780211082       1.66984407255083        h
  -15.78866662270358       2.00552336673496      -1.66983506526917        h
  -15.78866662270358       2.00552336673496       1.66983506526917        h
  -18.20618225186930      -2.09756664087096      -1.66984522544412        h
  -18.20618225186930      -2.09756664087096       1.66984522544412        h
  -20.64488894675895       1.99295410203508      -1.66984146031557        h
  -20.64488894675895       1.99295410203508       1.66984146031557        h
  -23.06266335029123      -2.11000028505253      -1.66984452339031        h
  -23.06266335029123      -2.11000028505253       1.66984452339031        h
  -25.50109743167375       1.98070308650213      -1.66983896755940        h
  -25.50109743167375       1.98070308650213       1.66983896755940        h
  -27.91883013550126      -2.12222071615847      -1.66991909869615        h
  -27.91883013550126      -2.12222071615847       1.66991909869615        h
  -30.35860206508062       1.96857624057291      -1.66997355431251        h
  -30.35860206508062       1.96857624057291       1.66997355431251        h
  -32.77030380954928      -2.13193129204813      -1.66955666773415        h
  -32.77030380954928      -2.13193129204813       1.66955666773415        h
  -35.26112120421837       1.96093118376189      -1.68025406128442        h
  -36.91029248208727      -0.44507183683268       0.00000000000000        h
  -35.26112120421837       1.96093118376189       1.68025406128442        h

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$coord
   -2.65430198986241       0.00000000000000       0.00000000000000        c
    2.65430198986241       0.00000000000000       0.00000000000000        c
   -1.36159508253642      -2.30597037599152       0.00000000000000        c
    1.36159508253642       2.30597037599152       0.00000000000000        c
   -1.36159508253642       2.30597037599152       0.00000000000000        c
    1.36159508253642      -2.30597037599152       0.00000000000000        c
   -4.70310708254382       0.00000000000000       0.00000000000000        h
    4.70310708254382       0.00000000000000       0.00000000000000        h
   -2.65577378894885      -4.66229575041726       0.00000000000000        c
    2.65577378894885       4.66229575041726       0.00000000000000        c
   -2.65577378894885       4.66229575041726       0.00000000000000        c
    2.65577378894885      -4.66229575041726       0.00000000000000        c
   -1.34107377427652      -6.89853099781233       0.00000000000000        c
    1.34107377427652       6.89853099781233       0.00000000000000        c
   -1.34107377427652       6.89853099781233       0.00000000000000        c
    1.34107377427652      -6.89853099781233       0.00000000000000        c
   -4.70153615782784      -4.66052617732141       0.00000000000000        h
    4.70153615782784       4.66052617732141       0.00000000000000        h
   -4.70153615782784       4.66052617732141       0.00000000000000        h
    4.70153615782784      -4.66052617732141       0.00000000000000        h
   -2.35177317390589      -8.67378650579427       0.00000000000000        h
    2.35177317390589       8.67378650579427       0.00000000000000        h
   -2.35177317390589       8.67378650579427       0.00000000000000        h
    2.35177317390589      -8.67378650579427       0.00000000000000        h

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$coord
   -2.63372797028676      -4.41766633177002       3.43123719140841        c
   -1.31812349118051      -6.53091038128144       4.30064764006822        c
    1.31812349118051      -6.53091038128144       4.30064764006822        c
    2.63372797028676      -4.41766633177002       3.43123719140841        c
    1.32513012917128      -2.30929267572259       2.54944660299566        c
   -1.32513012917128      -2.30929267572259       2.54944660299566        c
    2.62402884094061       0.00000000000000       1.52072438198238        c
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15

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   -2.62402884094061        0.00000000000000        1.52072438198238        c
   -1.32513012917128        2.30929267572259        2.54944660299566        c
    1.32513012917128        2.30929267572259        2.54944660299566        c
   -2.63372797028676        4.41766633177002        3.43123719140841        c
    2.63372797028676        4.41766633177002        3.43123719140841        c
   -1.31812349118051        6.53091038128144        4.30064764006822        c
    1.31812349118051        6.53091038128144        4.30064764006822        c
   -2.63372797028676        4.41766633177002       -3.43123719140841        c
   -1.31812349118051        6.53091038128144       -4.30064764006822        c
    1.31812349118051        6.53091038128144       -4.30064764006822        c
    2.63372797028676        4.41766633177002       -3.43123719140841        c
    1.32513012917128        2.30929267572259       -2.54944660299566        c
   -1.32513012917128        2.30929267572259       -2.54944660299566        c
    2.62402884094061        0.00000000000000       -1.52072438198238        c
   -2.62402884094061        0.00000000000000       -1.52072438198238        c
   -1.32513012917128       -2.30929267572259       -2.54944660299566        c
    1.32513012917128       -2.30929267572259       -2.54944660299566        c
   -2.63372797028676       -4.41766633177002       -3.43123719140841        c
    2.63372797028676       -4.41766633177002       -3.43123719140841        c
   -1.31812349118051       -6.53091038128144       -4.30064764006822        c
    1.31812349118051       -6.53091038128144       -4.30064764006822        c
   -4.68032751110567       -4.40681060589470        3.43377363512053        h
   -2.34237424688077       -8.16125997781747        4.98293654157568        h
    2.34237424688077       -8.16125997781747        4.98293654157568        h
    4.68032751110567       -4.40681060589470        3.43377363512053        h
    4.59809699520696        0.00000000000000        2.11365497665152        h
   -4.59809699520696        0.00000000000000        2.11365497665152        h
   -4.68032751110567        4.40681060589470        3.43377363512053        h
    4.68032751110567        4.40681060589470        3.43377363512053        h
   -2.34237424688077        8.16125997781747        4.98293654157568        h
    2.34237424688077        8.16125997781747        4.98293654157568        h
   -4.68032751110567        4.40681060589470       -3.43377363512053        h
   -2.34237424688077        8.16125997781747       -4.98293654157568        h
    2.34237424688077        8.16125997781747       -4.98293654157568        h
    4.68032751110567        4.40681060589470       -3.43377363512053        h
    4.59809699520696        0.00000000000000       -2.11365497665152        h
   -4.59809699520696        0.00000000000000       -2.11365497665152        h
   -4.68032751110567       -4.40681060589470       -3.43377363512053        h
    4.68032751110567       -4.40681060589470       -3.43377363512053        h
   -2.34237424688077       -8.16125997781747       -4.98293654157568        h
    2.34237424688077       -8.16125997781747       -4.98293654157568        h


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$coord
   -1.22579692459838        2.30753138104892        2.91510953619209        c
   -2.66756550451085        0.10072220898200        2.63538591502519        c
   -1.40787342478674       -2.21178553238024        2.92390209010301        c
    1.22579692459838       -2.30753138104892        2.91510953619209        c
    2.66756550451085       -0.10072220898200        2.63538591502519        c
    5.27776327059377       -0.22611292170812        1.49973372106320        c
   -5.27776327059377        0.22611292170812        1.49973372106320        c
    5.27776327059377        0.22611292170812       -1.49973372106320        c
   -5.27776327059377       -0.22611292170812       -1.49973372106320        c
    2.66756550451085        0.10072220898200       -2.63538591502519        c
    1.40787342478674       -2.21178553238024       -2.92390209010301        c
   -1.22579692459838       -2.30753138104892       -2.91510953619209        c
   -2.66756550451085       -0.10072220898200       -2.63538591502519        c
   -1.40787342478674        2.21178553238024       -2.92390209010301        c
    1.22579692459838        2.30753138104892       -2.91510953619209        c
    1.40787342478674        2.21178553238024        2.92390209010301        c
   -2.17205873995502        4.14031983098413        2.84354201109636        h
   -2.48540517203529       -3.97104796873235        2.86132995753878        h
    2.17205873995502       -4.14031983098413        2.84354201109636        h
    6.53839082018647        1.19038237122145        2.35033396980888        h
    6.09965180150989       -2.09648551042666        1.87520622029760        h
   -6.09965180150989        2.09648551042666        1.87520622029760        h
   -6.53839082018647       -1.19038237122145        2.35033396980888        h
    6.09965180150989        2.09648551042666       -1.87520622029760        h
    6.53839082018647       -1.19038237122145       -2.35033396980888        h
   -6.53839082018647        1.19038237122145       -2.35033396980888        h
   -6.09965180150989       -2.09648551042666       -1.87520622029760        h
    2.48540517203529       -3.97104796873235       -2.86132995753878        h
   -2.17205873995502       -4.14031983098413       -2.84354201109636        h
   -2.48540517203529        3.97104796873235       -2.86132995753878        h
    2.17205873995502        4.14031983098413       -2.84354201109636        h
    2.48540517203529        3.97104796873235        2.86132995753878        h
```

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----------------------- p-xylene
$coord
    0.00000000000000      2.68673819497727      0.01299104725543      c
    0.00000000000000      1.31646208389457     -2.25907726110522      c
    0.00000000000000     -1.31646208389457     -2.25907726110522      c
    0.00000000000000     -2.68673819497727      0.01299104725543      c
    0.00000000000000     -1.32131621310295      2.27629754894597      c
    0.00000000000000      1.32131621310295      2.27629754894597      c
    0.00000000000000      5.53386506184282     -0.00165486485627      c
    0.00000000000000     -5.53386506184282     -0.00165486485627      c
    0.00000000000000      2.33599210624993     -4.05420419327648      h
    0.00000000000000     -2.33599210624993     -4.05420419327648      h
    0.00000000000000     -2.34367121952440      4.06923527613470      h
    0.00000000000000      2.34367121952440      4.06923527613470      h
    0.00000000000000      6.29223524533602      1.93072941624223      h
   -1.67352314164156      6.27997657379230     -0.98715848467016      h
    1.67352314164156      6.27997657379230     -0.98715848467016      h
    0.00000000000000     -6.29223524533602      1.93072941624223      h
   -1.67352314164156     -6.27997657379230     -0.98715848467016      h
    1.67352314164156     -6.27997657379230     -0.98715848467016      h

----------------------- h2
$coord
    0.00000000000000      0.00000000000000      0.70940103395743      h
    0.00000000000000      0.00000000000000     -0.70940103395743      h


----------------------- branched oktane
$coord
    1.47807934191286      0.00000000000000      0.00000000000000      c
   -1.47807934191286      0.00000000000000      0.00000000000000      c
    2.52617919842986     -1.63599355693769      2.14835190336600      c
    2.52617919842986      2.67852410305245      0.34263602905270      c
    2.52617919842986     -1.04253054611476     -2.49098793241870      c
   -2.52617919842986      1.63599355693769      2.14835190336600      c
   -2.52617919842986     -2.67852410305245      0.34263602905270      c
   -2.52617919842986      1.04253054611476     -2.49098793241870      c
    1.69324181759085     -1.14578623404091      3.97102774120850      h
    2.20273286072211     -3.64363307102095      1.80733987079338      h
    4.56629756232587     -1.35126588264652      2.29870905388167      h
    2.20273286072211      3.38701877689003      2.25180886617656      h
    4.56629756232587      2.66637337789408      0.02087605469825      h
    1.69324181759085      4.01190402003975     -0.99323388461832      h
    1.69324181759085     -2.86611778599884     -2.97779385659018      h
    2.20273286072211      0.25661429413092     -4.05914873696994      h
    4.56629756232587     -1.31510749524756     -2.31958510857992      h
   -1.69324181759085      1.14578623404091      3.97102774120850      h
   -2.20273286072211      3.64363307102095      1.80733987079338      h
   -4.56629756232587      1.35126588264652      2.29870905388167      h
   -2.20273286072211     -3.38701877689003      2.25180886617656      h
   -4.56629756232587     -2.66637337789408      0.02087605469825      h
   -1.69324181759085     -4.01190402003975     -0.99323388461832      h
   -1.69324181759085      2.86611778599884     -2.97779385659018      h
   -2.20273286072211     -0.25661429413092     -4.05914873696994      h
   -4.56629756232587      1.31510749524756     -2.31958510857992      h

----------------------- n oktane
$coord
   -8.42906726792371     -0.50685360354785      0.00000000000000      c
   -5.98272469198327      1.01405603367231      0.00000000000000      c
   -3.63574237133041     -0.65521350484313      0.00000000000000      c
   -1.17249224414226      0.83573198687852      0.00000000000000      c
    1.17249224414226     -0.83573198687852      0.00000000000000      c
    3.63574237133041      0.65521350484313      0.00000000000000      c
    5.98272469198327     -1.01405603367231      0.00000000000000      c
    8.42906726792371      0.50685360354785      0.00000000000000      c
  -10.08545056110654      0.71990189016964      0.00000000000000      h
   -8.53638759674950     -1.71748743405413     -1.66657845920882      h
   -8.53638759674950     -1.71748743405413      1.66657845920882      h
   -5.92982746947456      2.24653286192231      1.65854269640428      h
   -5.92982746947456      2.24653286192231     -1.65854269640428      h
   -3.68035469173524     -1.89028402392402      1.66006925656190      h
   -3.68035469173524     -1.89028402392402     -1.66006925656190      h
   -1.12521678629703      2.07015416073293      1.66023924286326      h
   -1.12521678629703      2.07015416073293     -1.66023924286326      h
    1.12521678629703     -2.07015416073293      1.66023924286326      h
    1.12521678629703     -2.07015416073293     -1.66023924286326      h
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    3.68035469173524        1.89028402392402         1.66006925656190       h
    3.68035469173524        1.89028402392402        -1.66006925656190       h
    5.92982746947456       -2.24653286192231         1.65854269640428       h
    5.92982746947456       -2.24653286192231        -1.65854269640428       h
    8.53638759674950        1.71748743405413         1.66657845920882       h
   10.08545056110654       -0.71990189016964         0.00000000000000       h
    8.53638759674950        1.71748743405413        -1.66657845920882       h


------------------------ branched undecane
$coord
   -4.78241723399452       -0.74980806803302        -1.25915936597097       c
   -2.55133179387184        0.00165815633773         0.45442160851874       c
    0.00000000000000        0.00000000000000        -1.11100932617491       c
    2.55133179387184       -0.00165815633773         0.45442160851874       c
    4.78241723399452        0.74980806803302        -1.25915936597097       c
   -2.60656957737364       -1.89415940777408         2.64206224055004       c
   -3.24906044565675        2.61304691836495         1.51740561709597       c
    0.01121397158445       -2.32630617764317        -2.85192286506392       c
   -0.01121397158445        2.32630617764317        -2.85192286506392       c
    3.24906044565675       -2.61304691836495         1.51740561709597       c
    2.60656957737364        1.89415940777408         2.64206224055004       c
   -4.72432546173171       -2.74045058593334        -1.78161958812072       h
   -6.54164401860800       -0.43556096429068        -0.22701935600371       h
   -4.87599029315811        0.37265856570727        -2.98381301694102       h
    4.87599029315811       -0.37265856570727        -2.98381301694102       h
    4.72432546173171        2.74045058593334        -1.78161958812072       h
    6.54164401860800        0.43556096429068        -0.22701935600371       h
   -2.14859109872724       -3.80323053697783         2.01594834187628       h
   -1.33991727322146       -1.38210368447951         4.17864393142505       h
   -4.51890928460903       -1.95074337335186         3.42005143908457       h
   -3.62839025558735        3.96707341749478         0.01186983843478       h
   -4.98508466861374        2.43139870196252         2.62099324750301       h
   -1.81856890042780        3.40802168568809         2.75365619322623       h
   -0.44183673690581       -4.06623663752089        -1.84490165154458       h
   -1.35327428895573       -2.10030621696241        -4.37717224178524       h
    1.85474974507291       -2.57635256624139        -3.73393970919699       h
    0.44183673690581        4.06623663752089        -1.84490165154458       h
    1.35327428895573        2.10030621696241        -4.37717224178524       h
   -1.85474974507291        2.57635256624139        -3.73393970919699       h
    3.62839025558735       -3.96707341749478         0.01186983843478       h
    4.98508466861374       -2.43139870196252         2.62099324750301       h
    1.81856890042780       -3.40802168568809         2.75365619322623       h
    2.14859109872724        3.80323053697783         2.01594834187628       h
    1.33991727322146        1.38210368447951         4.17864393142505       h
    4.51890928460903        1.95074337335186         3.42005143908457       h


------------------------ n undecane
$coord
    0.00000000000000      -11.99493525602856        -0.69507912857104       c
    0.00000000000000       -9.61157066554375         0.91822657189101       c
    0.00000000000000       -7.20874099444937        -0.66388714109116       c
    0.00000000000000       -4.80282401952191         0.91169959183365       c
    0.00000000000000       -2.40418943496772        -0.67715780078414       c
    0.00000000000000        0.00000000000000         0.90227384366287       c
    0.00000000000000        2.40418943496772        -0.67715780078414       c
    0.00000000000000        4.80282401952191         0.91169959183365       c
    0.00000000000000        7.20874099444937        -0.66388714109116       c
    0.00000000000000        9.61157066554375         0.91822657189101       c
    0.00000000000000       11.99493525602856        -0.69507912857104       c
    0.00000000000000      -13.69681448759782         0.46423117743508       h
   -1.66656648360998      -12.04900059358410        -1.90685843312713       h
    1.66656648360998      -12.04900059358410        -1.90685843312713       h
    1.65840609849402       -9.60416319312329         2.15002758418078       h
   -1.65840609849402       -9.60416319312329         2.15002758418078       h
    1.65797871679860       -7.20826161049998        -1.90048876449906       h
   -1.65797871679860       -7.20826161049998        -1.90048876449906       h
    1.65923301011441       -4.79772622131999         2.14641260421142       h
   -1.65923301011441       -4.79772622131999         2.14641260421142       h
    1.65911944309760       -2.40716107708723        -1.91233133231710       h
   -1.65911944309760       -2.40716107708723        -1.91233133231710       h
    1.65907370468613        0.00000000000000         2.13730649055737       h
   -1.65907370468613        0.00000000000000         2.13730649055737       h
    1.65911944309760        2.40716107708723        -1.91233133231710       h
   -1.65911944309760        2.40716107708723        -1.91233133231710       h
    1.65923301011441        4.79772622131999         2.14641260421142       h
   -1.65923301011441        4.79772622131999         2.14641260421142       h
    1.65797871679860        7.20826161049998        -1.90048876449906       h
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18

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    -1.65797871679860      7.20826161049998     -1.90048876449906      h
     1.65840609849402      9.60416319312329      2.15002758418078      h
    -1.65840609849402      9.60416319312329      2.15002758418078      h
     1.66656648360998     12.04900059358410     -1.90685843312713      h
     0.00000000000000     13.69681448759782      0.46423117743508      h
    -1.66656648360998     12.04900059358410     -1.90685843312713      h


---------------------- peptid conformer 114
$coord
     7.83000362538377      2.45470317428441     -0.83336922505927      o
     7.05332618434213      0.35332771336398     -0.39117330972170      c
     7.68827416533967     -1.64789226245863     -1.79523982722519      o
     6.90970699816412     -3.17101152639916     -1.05257745659414      h
     5.30721923659890     -0.23059766201769      1.82925489763577      c
     4.88581030873446      1.52495791639515      2.79679467820345      h
     6.29743573077363     -1.50427307628062      3.11615839483615      h
     2.94695129533125     -1.42112512638808      1.09793088380825      n
     1.39170668711406     -0.34020177778512      0.85037676026456      h
     2.86947252384048     -3.87398964821786      0.45353427214110      c
     4.78376509750271     -5.21191575103411      0.34770960864151      o
     0.31078333851111     -4.99459724563317     -0.15873699524938      c
     0.24086347155602     -6.83141104780462      0.77100826263987      h
     0.22007648408289     -5.32151986680154     -2.19019258921473      h
    -1.80570993148070     -3.42612455447853      0.49699797322129      n
    -2.13074282651515     -2.84219917909686      2.28656862204472      h
    -3.56882441442922     -2.73448478946335     -1.23210143931665      c
    -3.49701482134022     -3.29951290350580     -3.47520636028118      o
    -5.65886151854613     -1.05640798254128     -0.18141370885644      c
    -5.61728754359986     -1.00160592465756      2.58514535120427      n
    -6.53191499241775     -2.53417381926770      3.28056456848729      h
    -6.58860677643538      0.52151333928297      3.21820360606789      h
    -7.42575545376250     -1.79718062703841     -0.95431169763023      h
    -5.27902656562796      1.60432641401984     -1.28312404493253      c
    -5.66642042308181      1.48338394144888     -3.30135155596043      h
    -6.69821089220282      2.85532511467571     -0.45353427214110      h
    -2.67498395308447      2.67013195355143     -0.89384046134475      c
    -0.85895713838615      2.45092372201656     -2.80624330887306      c
    -1.35217565933960      1.48338394144888     -4.54101189981277      h
     1.55233340849737      3.46948610820012     -2.50199740131174      c
     2.93750266466165      3.29374157774544     -3.99488104710952      h
     2.18728138949491      4.72615398725775     -0.27401028941858      c
     4.05999998821087      5.51039033283507     -0.05291233174979      h
     0.40149019293933      4.92835468358733      1.65540009331502      c
     0.87392172641964      5.90345336869069      3.39016868425473      h
    -2.00602090167635      3.90412311900201      1.34737473348585      c
    -3.38741070557278      4.10254436306374      2.84403783155148      h


---------------------- peptid conformer 215
$coord
     6.41199399343269     -4.04186883206108      0.65486671592265      o
     6.20979329710312     -1.84033788604282      0.07472079280883      c
     6.52915701373581     -1.02964537459060     -2.29121632686058      o
     6.43467070703975      0.83551431958967     -2.30255468366410      h
     5.66177271826596      0.21568414766350      2.02680788914948      c
     7.37764404786645      1.34385064961449      2.24790584681827      h
     5.24603296880328     -0.71406111022575      3.80692990730330      h
     3.57173561414905      1.88809177618381      1.41075716949116      n
     1.97869648325343      1.88809177618381      2.48034216129058      h
     3.78149521501431      3.69089050794468     -0.35802649185914      c
     5.64287545692674      3.89687065654210     -1.76209300936263      o
     1.55917728152292      5.50502759650909     -0.53566074844773      c
     1.96168894804814      6.81271808118259     -2.06255946465611      h
     1.39666083400569      6.54248724403185      1.23879209130432      h
    -0.81431874268218      4.24269053904969     -1.03076899553510      n
    -1.60989344506302      4.22568300384440     -2.76742731260873      h
    -2.19570854657861      3.18255417791987      0.81927288957380      c
    -1.48139206795638      3.06728088375067      3.03970109693127      o
    -4.74872855350622      2.15076670879886     -0.03299359682468      c
    -4.85266349087189      2.04871849756712     -2.79199375234971      n
    -6.67058003170413      2.00714452262085     -3.38158830613314      h
    -4.04008125328575      0.41599511785915     -3.39103693680275      h
    -6.13956698807226      3.54538159563275      0.59250575350325      h
    -5.30808748914691     -0.36446177545032      1.32571949346470      c
    -5.30808748914691     -0.01675216680881      3.35528536129612      h
    -7.20159307533601     -0.96728441217120      0.77580918849361      h
    -3.39757436775253     -2.35623312060332      0.67376397726187      c
    -3.61300314701955     -3.79242498238347     -1.53910532555992      c
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19

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    -5.28730050167378      -3.60345236899135      -2.70506635018933        h
    -1.73272564376790      -5.50640658585005      -2.22885536444118        c
    -1.92736743556179      -6.58732993445300      -3.95228559857736        h
     0.37998817395606      -5.83332920701843      -0.69439774369712        c
     1.86531291521816      -7.12968133488840      -1.22919023959683        h
     0.57085051348210      -4.48406474739865       1.56004553407093        c
     2.18845608411869      -4.78264147655821       2.76947025978053        h
    -1.29241945456425      -2.75496533486071       2.22900858547906        c
    -1.14691054225232      -1.70049815213265       3.97511553322229        h


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$coord
     6.85112548801256      -2.29683443158305       3.01171272067752        o
     6.57522547246005      -0.83985558232976       1.27127495133605        c
     6.71317548023631      -1.57873850069297      -1.13812586941355        o
     6.28042819556834      -0.12742882984145      -2.23416702708787        h
     6.06688914243524       1.96827745267722       1.66433798719167        c
     7.55599333596518       3.05109052741410       0.73270300316849        h
     6.11413229578327       2.33677404879186       3.67878604595172        h
     3.63103215581074       2.77708023799551       0.69301875435615        n
     2.21751700763765       3.32510081683268       1.88354621872654        h
     3.20395404954454       3.03030353994096      -1.78819165948246        c
     4.75352947935997       2.42181172481832      -3.43603284826179        o
     0.68494911302751       4.23594881338272      -2.48361087676548        c
     0.59802171086713       4.30208922806997      -4.53018427980219        h
     0.66605185168830       6.15969001771456      -1.74094850613443        h
    -1.52414073752643       2.92069942417353      -1.54819644047446        n
    -2.63529970427213       1.89457813345429      -2.71604719123779        h
    -2.30648735696983       3.07187751488723       0.86309410640906        c
    -1.09139345285846       4.13012414988313       2.55628872240250        o
    -4.81793338895117       1.79820210062431       1.41300441138014        c
    -6.28058141660622       1.49773564533083      -0.90946900720907        n
    -7.00623625203198       3.18904053519035      -1.44615122924271        h
    -7.77913424080577       0.35067188204063      -0.58065665990678        h
    -5.73445056390298       2.99061929112862       2.83029901182108        h
    -4.31337651119420      -0.78883297671389       2.64321612456288        c
    -3.44221276345650      -0.43923364193846       4.47814020060041        h
    -6.14452113496389      -1.67889398579080       2.99470518547223        h
    -2.65041751334350      -2.50092485404654       1.10686877768490        c
    -0.11251531548726      -2.83540637975060       1.77394210295910        c
     0.62447787674203      -1.89621249119174       3.43690110080980        h
     1.46729573247091      -4.39820989250348       0.35853722865209        c
     3.40804447200804      -4.66655100352030       0.92923452109630        h
     0.52810184391205      -5.62275242728445      -1.77496357654501        c
     1.75453410482694      -6.82650797459229      -2.88045336488894        h
    -1.99657227100674      -5.31472706745528      -2.45715471089058        c
    -2.74490382003956      -6.28604630029081      -4.09365754286638        h
    -3.57449359283099      -3.77648999444339      -1.01718339684259        c
    -5.53980877210909      -3.57806875038165      -1.54441698820662        h


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$coord
    -2.99874000613655      -2.88367100668454       0.53254525401073        o
    -4.84311271284369      -3.87577722699320      -0.39153082547677        c
    -5.28341890204734      -6.37966435443885      -0.30460342331639        o
    -3.88124211067777      -7.11287809440030       0.61758293003718        h
    -6.92559091242491      -2.52651276737342      -1.82394323498907        c
    -8.72461019191795      -3.11988677342470      -1.02836853260823        h
    -6.86134022387158      -3.14634293929959      -3.78358923586541        h
    -6.68559569341691       0.16823669959828      -1.67276514427537        n
    -5.32499287699361       1.02239291213069      -2.72156314860167        h
    -7.18070394050428       1.27750594021006       0.60813429936758        c
    -8.34288551286585       0.22870793588376       2.30699809376278        o
    -5.99773538066957       3.88154855275354       0.89159321945576        c
    -6.86700940227335       4.83586025038377       2.48274262421746        h
    -6.22639224287404       5.00026642403492      -0.82049865787689        h
    -3.31810372276924       3.55462593158517       1.36591447907000        n
    -2.69260437244130       3.07085604130133       3.10824197454539        h
    -1.70049815213265       3.01605398341761      -0.52948083325302        c
    -2.28064407524647       3.12943755145288      -2.78392411102107        o
     0.94133898308926       2.26583270825087       0.34924181902037        c
     0.79205061850949       1.20758607325497       2.89470292141229        n
     2.55705482759193       1.00727510305932       3.60901940003452        h
     0.03804989107491      -0.55552840969356       2.78131935337702        h
     2.04493904529927       4.01004992986019       0.47207401772525        h
     2.16966097013808       0.54429220024861      -1.63686034773087        c
     1.01125885004435      -1.15079214187875      -1.82394323498907        h
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20

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     2.14887398266494      1.51750115921806      -3.44910771016135      h
     4.81149810535999     -0.13978866023088      -0.87530071576061      c
     5.31983443538480     -2.40746002093638       0.38136716329703      c
     3.79104599304251     -3.73026831468126       0.70262060606364      h
     7.75947087427714     -2.98949567018413       1.19016994861532      c
     8.11851883972218     -4.75827933153442       2.15015082464732      h
     9.72856550582308     -1.29819078032461       0.75742266394736      c
    11.62396081814609     -1.74794560019787       1.37914256200745      h
     9.24857506780709      0.96759085424697      -0.49546576284243      c
    10.77358405788154      2.28284024345616      -0.85262400215355      h
     6.80893862891475      1.53828814669119      -1.30048909589289      c
     6.44800093733579      3.29573345123795      -2.28692613779978      h

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$coord
    -7.37922733192460      3.06048808440441       0.87535178943990      o
    -6.89167798937292      0.87974412585929       0.40480998209351      c
    -7.78551845071767     -1.03832790007078       1.78242033372211      o
    -7.19214444466640     -2.64270538776992       1.03975796309105      h
    -5.23249844379006      0.10117695868373      -1.82317712979964      c
    -4.58810183212291      1.80004075307894      -2.76804019676027      h
    -6.37200330254458     -1.02321009099941      -3.12330870993746      h
    -3.04041612844141     -1.38414778257837      -1.09941202050780      n
    -1.35667014311757     -0.51865321324244      -0.87264488443725      h
    -3.25017572930667     -3.82945339987247      -0.45312568270674      c
    -5.30619776301299     -4.93494318821640      -0.33218321013578      o
    -0.81809819495002     -5.21651238217067       0.15725585854983      c
    -0.92959203685137     -7.05710563660997      -0.75926131640198      h
    -0.76140641093238     -5.52642746813375       2.19249090478302      h
     1.43634508281804     -3.86913764868482      -0.52871472806359      n
     2.02782936273539     -3.72173901023896      -2.33907236436014      h
     3.11442188974011     -3.04143760202731       1.22684085034926      c
     2.86875749233034     -3.33812460505294       3.50774029399221      o
     5.33673982323150     -1.56556149143481       0.11946133587140      c
     5.17044392344643     -1.41816285298895      -2.63575936738578      n
     4.21613222581620      0.16542764723706      -3.14220597127668      h
     6.91844059732359     -1.27454366681094      -3.39731899935605      h
     7.02993443922494     -2.63136703096640       0.61079013069093      h
     5.44445421286501      1.01958385976946       1.46683606935726      c
     5.71090559774791      0.68132288179756       3.47939440198339      h
     7.08095704484082      2.05137432889046       0.75440931686894      h
     3.06339928412423      2.50679832716549       1.03408878468929      c
     1.01682588108752      2.27436201269317       2.70082723480783      c
     1.20768822061356      1.07816536992102       4.34866842358717      h
    -1.23950712281446      3.55559633149178       2.25107241493458      c
    -2.80231063556733      3.37229289650142       3.55687317347416      h
    -1.50028932929559      5.08249504770015       0.11757160973748      c
    -3.26718326451196      6.05192455440175      -0.21879964210050      h
     0.52738681240191      5.34894643258305      -1.54160793584538      c
     0.36298063875076      6.56404033669441      -3.17811076782118      h
     2.79316844697349      4.07716074445405      -1.07862503303467      c
     4.38620757786911      4.36061966454223      -2.33529291209230      h

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$coord
    -4.32716640460389      3.06748517846785       0.70410174276320      o
    -6.46255693593491      3.55881397328738       0.05025650042644      c
    -7.55859809360923      5.82648533399288       0.42442227494285      o
    -6.31326857135513      6.85827580311388       1.28235793974310      h
    -8.24645840635657      1.77680222899964      -1.30845658986294      c
    -8.64897007288180      2.55536939617519      -3.16794710564145      h
   -10.00768316317117      1.71633099271416      -0.25020995486704      h
    -7.21277821110165     -0.71952599391034      -1.52388536912996      n
    -5.78225552772326     -0.99353628332892      -2.77488406978583      h
    -7.05404121585227     -2.12737196368167       0.63796132807595      c
    -8.26913511996363     -1.66816851313880       2.55036417560426      o
    -5.09061576270808     -4.22118852006642       0.49245241576402      c
    -5.15675617739532     -5.18872830063410      -1.32168467280038      h
    -5.41564865774253     -5.54966599221305       2.01935113197239      h
    -2.61507452727124     -3.07790420904406       0.77780106198613      n
    -1.98390599854154     -2.55822952221571       2.50879020065799      h
    -1.49446692985593     -1.85714112653093      -1.15916822528316      c
    -2.25413683569228     -1.94028907642346      -3.36258889743534      o
     0.87713936821524     -0.41339036021509      -0.43918256825916      c
     0.77887360925133      0.32171310588027       2.21588264990020      n
     2.49852439111967      0.96988916981526       2.75823405033560      h
    -0.46834563913669      1.76546387219611       2.41997307236369      h
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21

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     0.97540512717914        1.18153849681444       -1.74876277906659        h
     3.17126689479564       -2.12548223754775       -0.90972437560555        c
     3.01819907794801       -3.76954397405924        0.32426678984503        h
     3.08811894490310       -2.77365830148274       -2.86559092421405        h
     5.59956497688444       -0.74598215978523       -0.41650585465211        c
     6.89024792635266       -1.03699998440911        1.86817304125869        c
     6.17026226932866       -2.35413909975222        3.26090120195865        h
     9.08799942010308        0.32927201041596        2.36139156221213        c
    10.06876728360821        0.07415898233659        4.13773412809811        h
    10.02530358252802        2.00923854347195        0.56615173498695        c
    11.73361600759283        3.06559545233393        0.94031750950335        h
     8.75540762053293        2.31348445103327       -1.72419633932561        c
     9.48106245595869        3.60416740050149       -3.13204230909694        h
     6.55954585291644        0.94721245620821       -2.20607650347553        c
     5.58255744167915        1.17964877068052       -3.98997797389719        h

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$coord
     6.88309761125133        0.01460707227842        0.98076786350513        o
     4.89699544450010       -1.04552928885140        0.60471236285481        c
     2.79939943584751       -0.64301762232617        1.99933024968869        o
     3.27183096932782        0.68923930208831        3.17096045271987        h
     4.51716049158193       -2.95415268411186       -1.50044255033347        c
     5.84185851146072       -4.48672057872200       -1.13950485875451        h
     5.07840915335654       -2.03574578302614       -3.25221867647847        h
     2.01327336413627       -3.96515616575973       -1.73476859093970        n
     0.66400890451649       -2.97682939771892       -2.66829330109680        h
     1.20825003108581       -5.72260147030650       -0.03401507041058        c
     2.61420627472322       -6.82431180638259        1.43052268337839        o
    -1.63956725273351       -6.12889258909957       -0.07180959308900        c
    -2.07609398966932       -7.71059336319166        1.15651239395981        h
    -2.28774331666850       -6.52573507722303       -1.98610216675124        h
    -2.93969883287133       -3.89145684653681        0.82014114212183        n
    -3.18347350414718       -3.56264449923451        2.68719056243601        h
    -3.44803516289615       -1.92992111952655       -0.71242675248831        c
    -2.98505226008544       -1.92614166725870       -2.99899537453302        o
    -4.74249756463221        0.29428654009877        0.59715345831912        c
    -4.13589547564349        0.26405092195603        3.29001319915689        n
    -2.37467071882888        0.98025712671218        3.54323650110235        h
    -5.33965102295132        1.39788660230878        4.25188380132281        h
    -6.77017370632971       -0.07421005601588        0.42707810626621        h
    -4.18313862899152        2.77549695393737       -0.80691305918437        c
    -4.73493866009652        2.53361200879545       -2.77600769073031        h
    -5.38500445016543        4.24003470772634        0.01322808293745        h
    -1.46571244841276        3.58052028698782       -0.65384524233675        c
    -0.57754116546977        4.94868200794681        1.43052268337839        c
    -1.88712137627720        5.50237176518574        2.90261934170304        h
     1.95091240171687        5.68567520017610        1.59492885702954        c
     2.59341928725009        6.76092937037729        3.21253442766612        h
     3.62898920863894        5.08096283732130       -0.34015070410582        c
     5.58863520951527        5.64032177296199       -0.21920823153486        h
     2.75782546090124        3.75059563904074       -2.44152616502625        c
     4.04283923196769        3.31028944983708       -3.97031460736854        h
     0.24071025051813        2.99281545933831       -2.58892480347211        c
    -0.43581170542568        1.96102499021731       -4.21786873091224        h

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$coord
     4.89500357100758       -5.15205739890017        2.15357276116009        o
     5.48081867252317       -3.39650182048733        0.81186720607600        c
     5.34097893861300       -3.52311347146005       -1.70713773044103        o
     5.86821252997702       -1.88094146108248       -2.42334393519718        h
     6.42757146561772       -0.88505578850598        1.85877548426838        c
     8.33808458701210       -0.54868453646680        1.15579736244967        h
     6.46914544056398       -1.02867497468400        3.90345916117117        h
     4.84209123925779        1.24088611215543        1.15957681471751        n
     3.57408500339663        1.99677656572393        2.39734743243593        h
     4.86854740513268        2.20842589272311       -1.18368359134484        c
     6.13466391485992        1.30891625297659       -2.93356999135592        o
     3.21314731181767        4.53089931131232       -1.54462128292380        c
     3.59487199086976        5.26789250354161       -3.41922960777368        h
     3.70258638050327        5.94630418561934       -0.12732668248286        h
     0.54296428458694        3.95831229273419       -1.34620003886207        n
    -0.63055564457816        4.05468832556417       -2.85042204146338        h
    -0.61543783550679        3.65973556357463        0.89123570370069        c
     0.51083894031028        3.61060268409267        2.93780910673741        o
    -3.48782155906709        3.44052733203976        0.74950624365660        c
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    -4.34386749773342         3.41029171389702        -1.87721308249394       n
    -6.05406964893215         4.24744039122414        -2.03028089934156       h
    -4.56307572926829         1.59048544693086        -2.45357955333992       h
    -4.17757159794835         5.17151647071163         1.63578780046567       h
    -4.38355174654577         1.18041487586995         2.35388373135574       c
    -3.44624758412083         1.28812926550346         4.18313862899152       h
    -6.41500734051111         1.37505666766383         2.65623991278314       h
    -3.84120034611037        -1.28945718116513         1.06509050802145       c
    -5.68557305281751        -2.42518258765180        -0.45424930365124       c
    -7.54506356859602        -1.57669555352116        -0.57141232395435       h
    -5.17723672279269        -4.65316969954496        -1.76382951445866       c
    -6.63043611977813        -5.50921563821129        -2.91845218228455       h
    -2.80752015085544        -5.77755674922810        -1.56540827039693       c
    -2.40689821046414        -7.51232534016781        -2.56885284750912       h
    -0.95558853961262        -4.68340531768770        -0.04228900645640       c
     0.87366635802316        -5.57157660063069         0.15613223760533       h
    -1.47148377417312        -2.44974902739278         1.25217339527965       c
    -0.03907136466081        -1.62393870686919         2.45970839485533       h


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$coord
    -5.25696273617244         1.54651100905772         3.46621739272523       o
    -6.18481826792778         1.75438088378905         1.38940837154578       c
    -7.74195260227889         3.66489400518344         0.73178367694118       o
    -7.91958685886749         4.70046392657228         2.23222622727465       h
    -5.76718879233118        -0.00684387302555        -0.79511503926719       c
    -4.98484217288778         1.07785892784525        -2.37114663495751       h
    -7.58888478543127        -0.72493980391563        -1.43762192480042       h
    -4.12312705581969        -2.02696111018737        -0.04300403796653       n
    -3.20660988086789        -1.94192343416092         1.63885222122338       h
    -3.53542222817018        -3.86188518622491        -1.72297057102253       c
    -4.45571885538983        -3.98660711106371        -3.84702274555001       o
    -1.60034266703482        -5.75917022468184        -0.75543079045484       c
    -1.50585636033876        -7.29551757155982        -2.11036442847638       h
    -2.18048859014865        -6.48104560783976         1.08516246398445       h
     0.88086774680378        -4.63289344886478        -0.49653831010763       n
     2.23580138482532        -4.83698387132827        -1.82501578225427       h
     1.54416161981014        -3.31386460738774         1.56893235426830       c
     0.10419030576215        -2.90379403632683         3.35661327695780       o
     4.27670560946027        -2.38033989723065         1.57649125880398       c
     5.41810019434871        -2.69025498319373        -0.91983696410599       n
     5.00802962328780        -1.15768708858360        -1.99887058657503       h
     7.32105441120741        -2.76395430241666        -0.77054859952621       h
     5.27070155590285        -3.63511805015436         2.88040229120964       h
     4.38630972522771         0.31818902200890         2.66308378580870       c
     3.45656446733845         0.30496093907145         4.49989758798016       h
     6.37052216584502         0.81518699523019         2.94276325362905       h
     3.15042883364321         2.20413570366231         0.94154327780644       c
     0.57851156537638         2.77672272224045         1.17964877068052       c
    -0.50430150936049         1.92256650970804         2.68953995168360       h
    -0.57044192404774         4.46991733823389        -0.47575132263450       c
    -2.54709546012937         4.94423859784813        -0.24520473429611       h
     0.81661705825046         5.59619411405096        -2.41461033603770       c
    -0.08478230762998         6.90766405099231        -3.69584465483631       h
     3.37908569584768         5.05384271361556        -2.66027473344747       c
     4.48268575805769         5.94579344882639        -4.13237139177212       h
     4.53370836367356         3.37954535896133        -0.98408765265932       c
     6.54437697016577         3.01671794124845        -1.14093492177478       h
---------------------- peptid conformer 691
$coord
     5.98935929726517        -2.66303271212940         0.46568980781335       o
     7.93766694133798        -1.85234020067719        -0.40736366605827       c
    10.13163998282055        -3.15436150694893        -0.41492257059396       o
     9.76881156510767        -4.74929036397847         0.40710829766179       h
     8.27214846704204         0.70067980625042        -1.66025209284806       c
     8.82772795041489         0.39643389868910        -3.61800836759048       h
     9.80471636165218         1.68333739588947        -0.70783012135175       h
     6.01203601087222         2.19167372591429        -1.52608153733965       n
     4.49836537760130         1.62664561187184        -2.56543091099634       h
     5.42055173095487         3.26881762224940         0.74347954949977       c
     6.93422236422580         3.55227654233759         2.46690978363595       o
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     1.96424263201290         4.85429784860933        -0.77208080990507       h
     2.42722553482361         5.29649376394691         2.53493992445712       h
     1.16677820349814         1.73624972763927         1.44834739745240       n
     0.97780559010601         1.02571270128488         3.21335160653485       h
     0.59041173265215         0.10919552633307        -0.41303284446003       c
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    -1.18593083323382        -2.26996967627378         3.16610845318682        n
    -1.14813631055540        -4.02741498082055         3.91444000221963        h
    -2.96605285138764        -1.59722717259782         3.40610367219482        h
     0.92300353222229        -3.75151496526805         0.21246650586790        h
    -2.81298503454002        -3.06932383092247        -1.26340960472460        c
    -2.15536033993543        -2.96727861969073        -3.21171724879741        h
    -3.36289533951111        -5.01574174886136        -0.86278766433329        h
    -5.02396461122789        -1.34022441838453        -0.85522875979761        c
    -6.98550033823815        -2.02052582659618         0.78127407217820        c
    -6.95904417236325        -3.87245743783901         1.65621727218374        h
    -8.98483058792683        -0.37457436395077         1.26504396246204        c
   -10.48905259052815        -0.94149220412714         2.52927074605535        h
    -9.04719155034623         1.98947302958472         0.11231102077007        c
   -10.59676698016166         3.27070734838333         0.47702816461688        h
    -7.11022226307695         2.68678197300166        -1.53364044187534        c
    -7.15746541642498         4.51225741836959        -2.45015761682714        h
    -5.11467146565611         1.04083051035625        -2.01174115375741        c
    -3.61233918918871         1.58129218465773        -3.29108574642210        h


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     2.21429936584205         0.37799630046354        -2.20004980931870        o
     4.12670221337036         0.46114425035608        -0.95094083479675        c
     6.24508520949608        -0.82386952071037        -1.53297648404449        o
     5.83690436456909        -1.80274765808158        -3.02586012984228        h
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     6.16382698573747         3.16723207413131         1.18822914880211        h
     4.84479814426043         0.69924974323016         2.99480733283083        h
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     1.85147194812917         5.50104384952406         0.34919074534107        c
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    -1.53491728385771         6.68779186162660         2.32584428142270        h
    -2.46088308947913         4.47492255880482        -0.75629904300286        n
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    -4.59249416854230        -0.60844074144335        -4.72661365037141        h
    -6.56347852622216         1.03751072120206        -1.13991344818887        h
    -4.55092019359603        -2.12211137471427         0.35863937601068        c
    -5.33704626530727        -1.85377026369746         2.24269633153017        h
    -5.80569834651974        -3.39011761057543        -0.67693054537817        h
    -1.97333374692744        -3.29941075614721         0.53816335873320        c
    -1.04169876290427        -4.79985330648069        -1.42715182054490        c
    -2.21710841820329        -5.14945264125612        -3.06554437865463        h
     1.34880479650612        -5.89778419028893        -1.28542236050081        c
     2.02343702631600        -7.06941439332011        -2.81987998124487        h
     2.84735762070567        -5.51983896350468         0.84618871856236        c
     4.69550977968065        -6.38155408057278         0.97469009566901        h
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     3.06089667383877        -3.79073955096674         4.51603687063743        h
    -0.45588366138868        -2.94414224297002         2.67544361619813        c
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24