

Supporting Information

For

Coupling Constants, High Spin, and Broken Symmetry States of Organic Radicals: An Assessment of the Molecules-in-Molecules Fragmentation-Based Method

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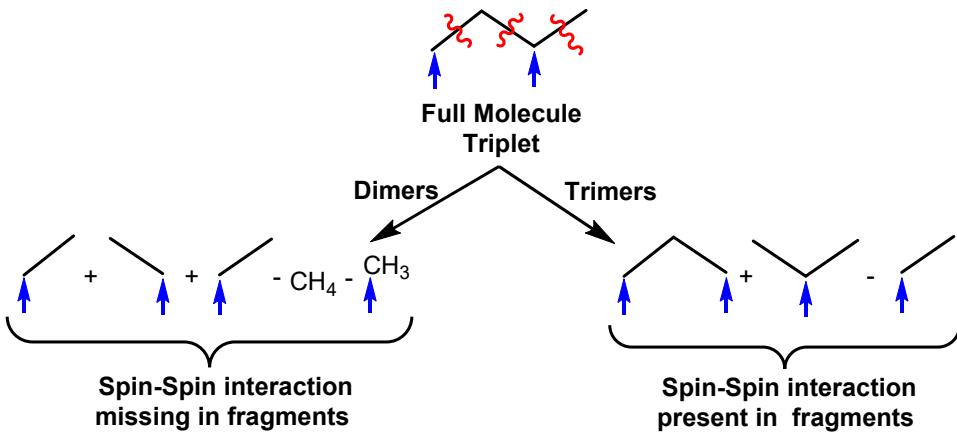
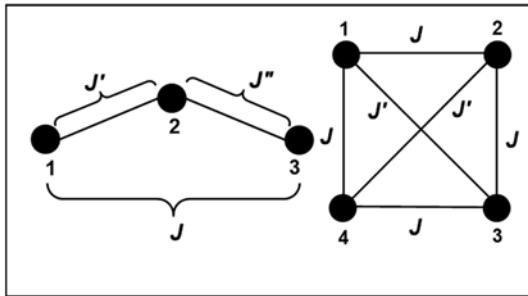


Figure S1. An example of the MIM method applied to a small diradical molecule, illustrating the composition of individual subsystems and their spins.

Section 1. Calculation of Inter-Site Coupling Constants.



To determine the inter-site coupling constants in a polyyradical, the Heisenberg-Dirac-van Vleck (HDvV) Hamiltonian can be used. Determination of the inter-site coupling constant is particularly important when the unpaired electrons are localized on specific atoms. The HDvV Hamiltonian is written as:

$$H_{HDVV} = -2 \sum_{(i < j)}^{atom} J_{ij} S(i) \cdot S(j) \quad (S1)$$

where i and j are the radical sites with local spin $S(i)$ and $S(j)$ respectively. Generally, the HDvV Hamiltonian has been used for transition metal complexes. However, this technique can also be applied to polyyradical systems, due to the unique exchange interactions if sites are close enough to couple, allowing us to easily compute their coupling constants.^{1,2}

The following expressions can be used to determine the energy expression for different spin states of a molecule:

$$\begin{aligned}
S_1 \cdot S_2 &= S_{1z}S_{2z} + \frac{1}{2}(S_{1+}S_{2-} + S_{1-}S_{2+}) \\
S_1 \cdot S_2 |\alpha\alpha\rangle &= \frac{1}{4}|\alpha\alpha\rangle ; S_1 \cdot S_2 |\beta\beta\rangle = \frac{1}{4}|\beta\beta\rangle ; \\
S_1 \cdot S_2 |\alpha\beta\rangle &= -\frac{1}{4}|\alpha\beta\rangle + \frac{1}{2}|\beta\alpha\rangle ; S_1 \cdot S_2 |\beta\alpha\rangle = -\frac{1}{4}|\beta\alpha\rangle + \frac{1}{2}|\alpha\beta\rangle
\end{aligned} \tag{S2}$$

Since the total spin operator commutes with the Hamiltonian, the above expressions can be used to determine the energy of a particular spin state.

For a linear triradical, as modelled in Figure 9(a), the energy expressions can be written as,

$$\begin{aligned}
E_{HS} &= E_0 - J'/2 - J''/2 - J/2 \\
E_{BS1} &= E_0 + J'/2 - J''/2 + J/2 \\
E_{BS2} &= E_0 + J'/2 + J''/2 - J/2 \\
E_{BS3} &= E_0 - J'/2 + J''/2 + J/2
\end{aligned} \tag{S3}$$

For the tetra- and octa-radical, due to symmetry, J and J' can be calculated from the approximate model represented in Figure 9(b) and the HS and distinct BS states shown in **Table S1**.

Table S1. Different high spin (HS) and broken symmetry states (BS) computed for tetraradicals and octaradicals.

Tetraradical	Octaradical
HS $ \uparrow\uparrow\uparrow\uparrow\rangle$	$ \uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle$
BS1 $ \downarrow\uparrow\uparrow\uparrow\rangle = \uparrow\downarrow\uparrow\uparrow\rangle = \uparrow\uparrow\downarrow\uparrow\rangle = \uparrow\uparrow\uparrow\downarrow\rangle$	$ \downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle = \uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle = \uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle = \uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\rangle$
BS2 $ \uparrow\uparrow\downarrow\downarrow\rangle = \uparrow\downarrow\downarrow\uparrow\rangle$	$ \uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle = \uparrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle$
BS3 $ \uparrow\downarrow\uparrow\downarrow\rangle$	$ \uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\rangle$

The energy expressions can be written as,

$$\begin{aligned}
E_{HS} &= E_0 - 2J - J' \\
E_{BS1} &= E_0 \\
E_{BS2} &= E_0 + J' \\
E_{BS3} &= E_0 + 2J - J'
\end{aligned} \tag{S4}$$

Following the procedure of Pantazis *et al.*³, we have determined the J values. Since there are more equations than J values, the system as defined by the HDvV Hamiltonian is over-determined and the solutions are not unique in principle. Hence, the linear equations are solved by singular value decomposition (SVD). This method guarantees that the J values are unique and represents the best possible solution in the least squares sense. For each system, the total energies of each states obtained from full (or MIM2) calculation was used in the equations to obtain the set of J values for full (or MIM2) set.

References

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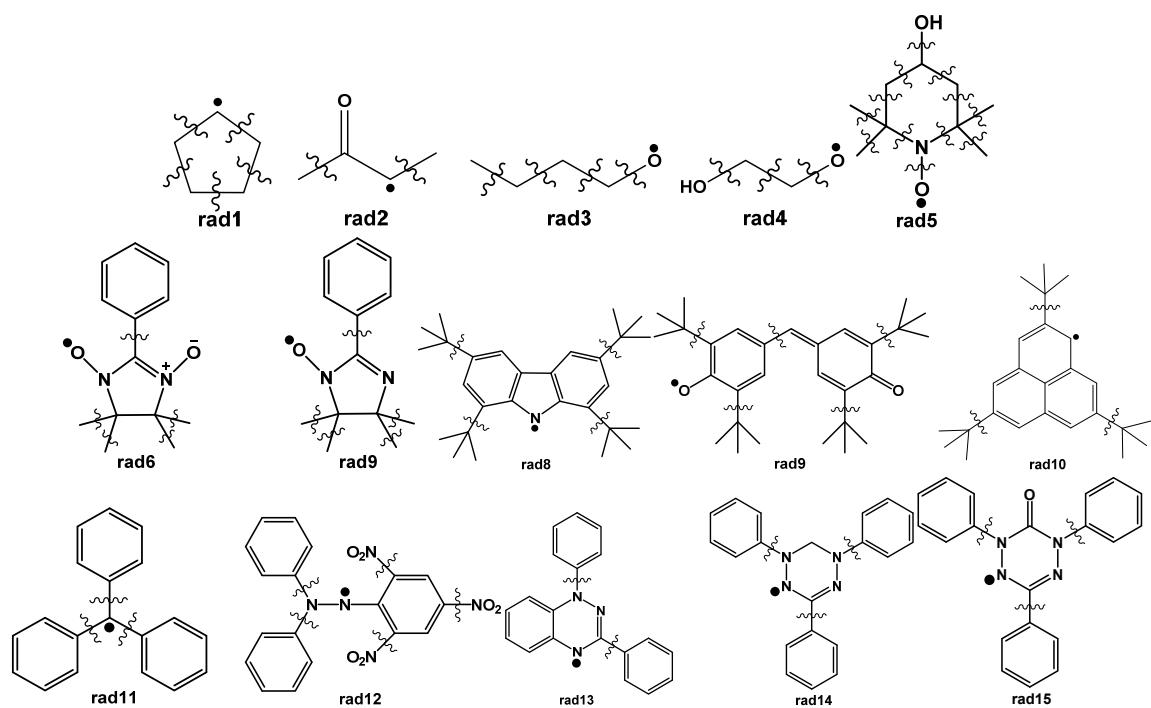
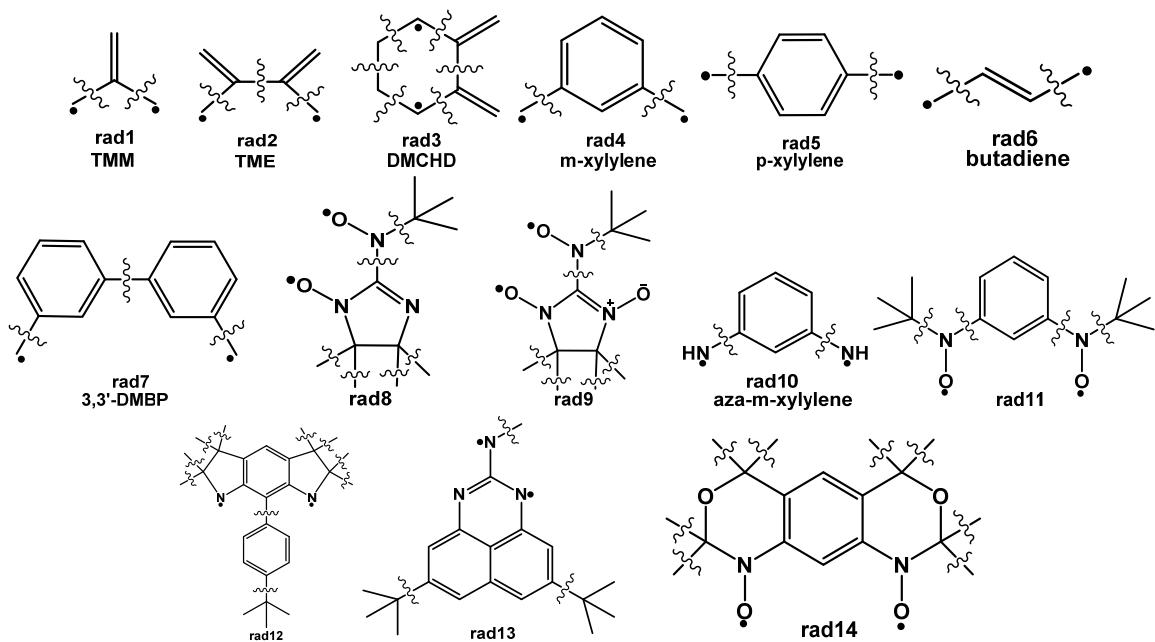


Figure S2. Fragmentation scheme of 15 monoradicals included in the Mono15 test set.



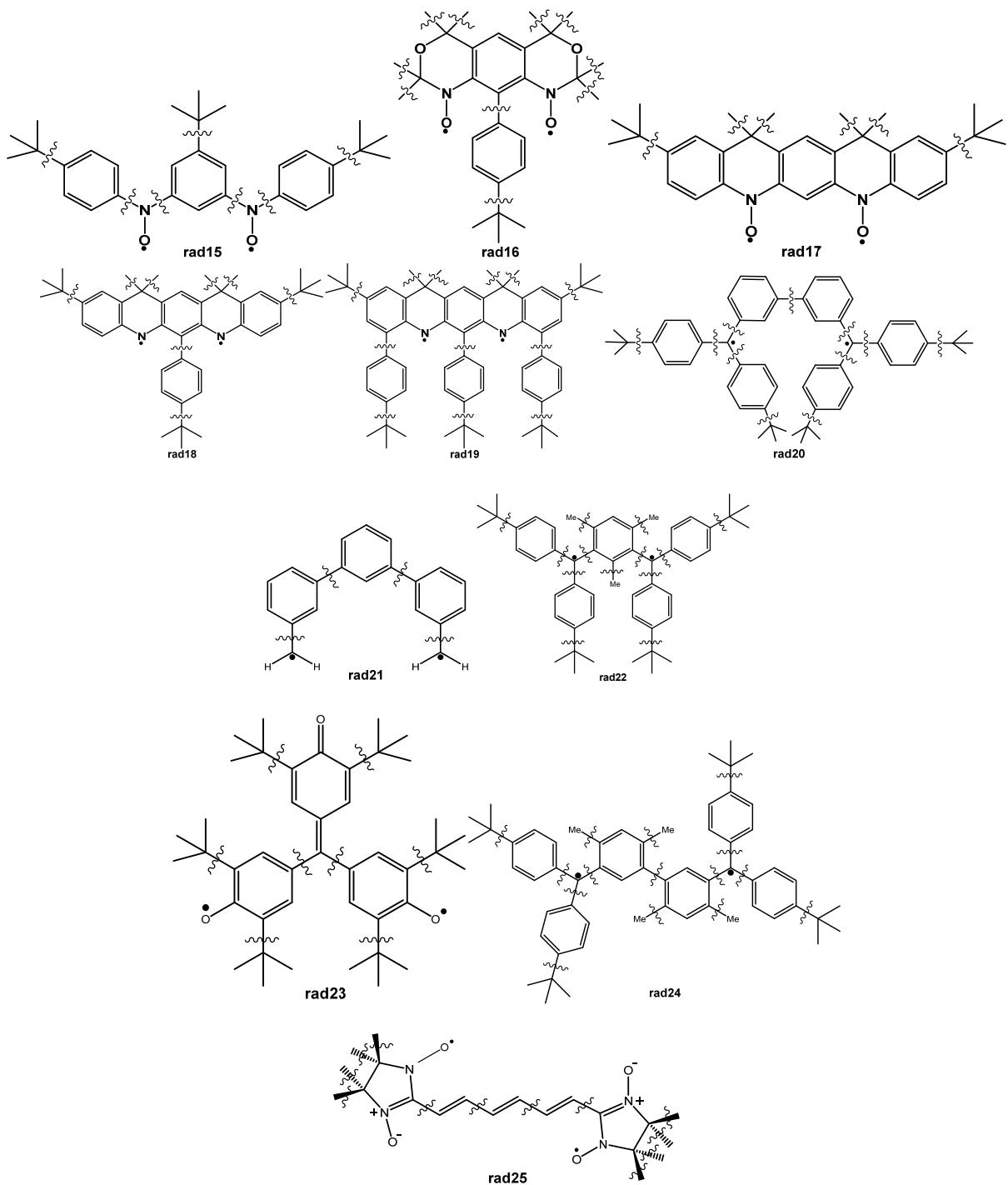


Figure S3. Fragmentation scheme of 25 diradicals included in the Di25 test set.

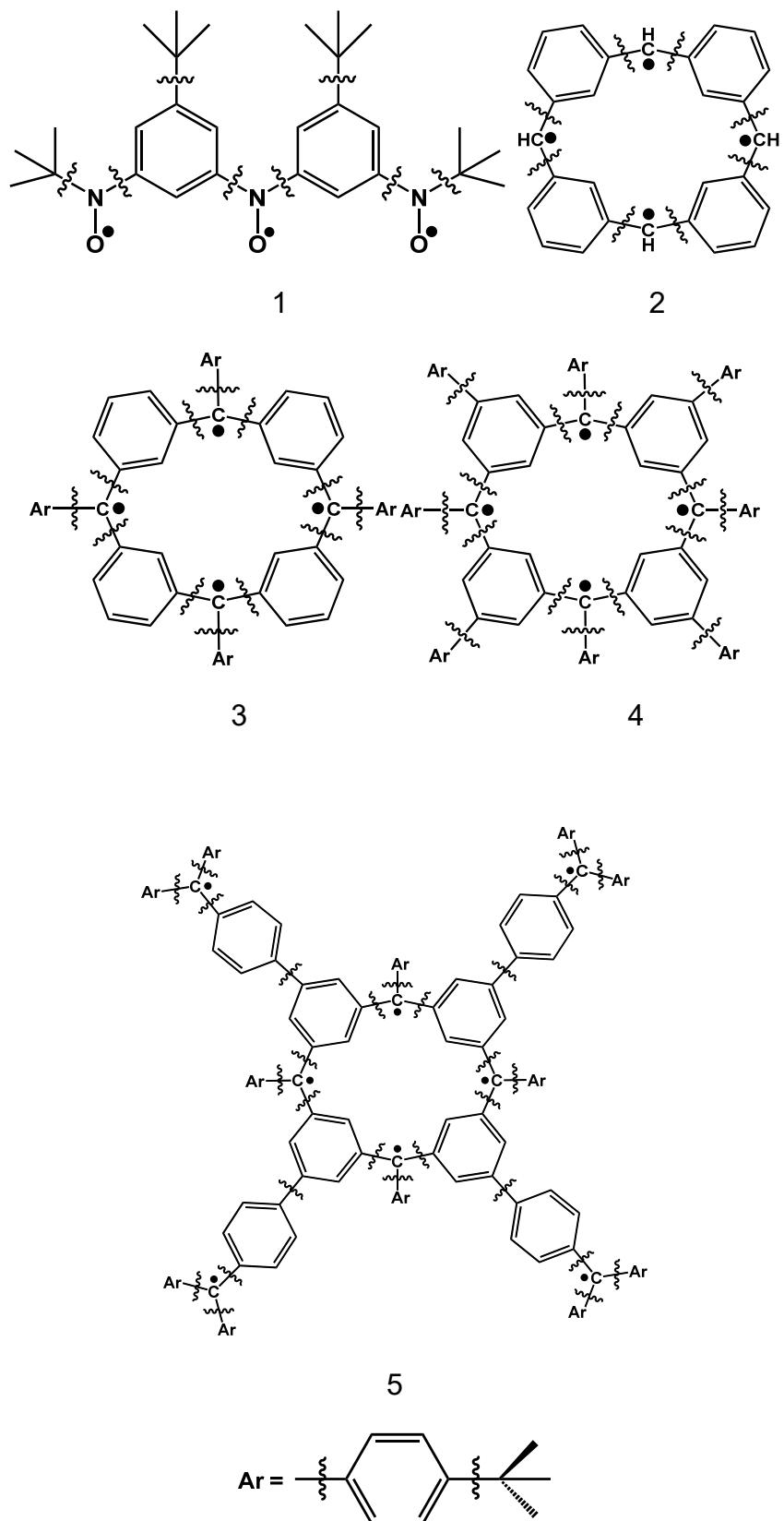


Figure S4. Fragmentation scheme of examined polyradicals.

Table S2. Energies of the full high level calculation (E_{high}), MIM2 with dimer subsystem ($E_{\text{MIM2-dimers}}$), MIM2 with trimer subsystem ($E_{\text{MIM2-trimers}}$), full low level calculation (E_{low}) in a.u. and $\langle S^2 \rangle$ of the full high level calculation ($\langle S^2 \rangle_{\text{high}}$) and full low level calculation ($\langle S^2 \rangle_{\text{low}}$) for the doublet state of the Mono15 test set. E_{high} and $\langle S^2 \rangle_{\text{high}}$ correspond to the high level quantities. All high-level calculations are carried out at the B3LYP-D3BJ/6-311++G(d,p) level of theory while all MIM2 calculations are carried out at the B3LYP-D3BJ/6-311++G(d,p):B3LYP-D3BJ/6-31G(d) level of theory.

	E_{high}	$\langle S^2 \rangle_{\text{high}}$	$E_{\text{MIM2-dimers}}$	$E_{\text{MIM2-trimers}}$	E_{low}	$\langle S^2 \rangle_{\text{low}}$
rad1	-195.967696	0.754	-195.967577	-195.969063	-195.912954	0.754
rad2	-231.904891	0.763	-231.904934	NA	-231.833250	0.763
rad3	-233.086763	0.754	-233.087112	-233.087049	-233.013404	0.753
rad4	-229.667406	0.754	-229.668422	-229.668064	-229.580642	0.753
rad5	-559.153969	0.754	-559.155416	-559.156584	-558.983414	0.754
rad6	-765.741802	0.808	-765.741799	-765.741836	-765.532428	0.812
rad7	-690.541466	0.768	-690.5417037	-690.541258	-690.357698	0.768
rad8	-1146.285461	0.775	-1146.285459	-1146.285570	-1145.998002	0.775
rad9	-1280.706049	0.818	-1280.706474	-1280.706612	-1280.371515	0.824
rad10	-972.944301	0.797	-972.9443668	-972.944332	-972.701813	0.800
rad11	-733.295288	0.776	-733.297563	-733.295260	-733.114323	0.778
rad12	-1418.367287	0.762	-1418.367865	-1418.367704	-1417.978692	0.762
rad13	-896.981194	0.766	-896.981181	NA	-896.761152	0.766
rad14	-991.639442	0.774	-991.639107	-991.639499	-991.391080	0.775
rad15	-1065.703313	0.773	-1065.703236	-1065.703299	-1065.433720	0.773

Table S3. Energies of the full high level calculation (E_{high}), MIM2 with dimer subsystem ($E_{\text{MIM2-dimers}}$), MIM2 with trimer subsystem ($E_{\text{MIM2-trimmers}}$) in a.u. and $\langle S^2 \rangle$ of full high level calculation ($\langle S^2 \rangle_{\text{high}}$) and error in energies with respect to full calculation (ΔE) for the doublet state of Mono15 test set. All high-level calculations are carried out at the CAM-B3LYP/6-311++G(d,p) level of theory while all MIM2 calculations are carried out at the CAM-B3LYP/6-311++G(d,p):CAM-B3LYP/6-31G(d) level of theory.

	E_{high}	$\langle S^2 \rangle_{\text{high}}$	$E_{\text{MIM2-dimers}}$	ΔE_{dimers} (kcal/mol)	$E_{\text{MIM2-trimmers}}$	$\Delta E_{\text{trimers}}$ (kcal/mol)
rad1	-195.8244059	0.7547	-195.8239368	-0.29	-195.8255766	0.73
rad2	-231.7668996	0.7675	-231.7669156	0.01	NA	-
rad3	-232.9432373	0.7541	-232.9432841	0.03	-232.9435001	0.16
rad4	-229.5623936	0.7541	-229.5632783	0.56	-229.5630806	0.43
rad5	-558.8161019	0.7547	-558.8155525	-0.34	-558.8187323	1.65
rad6	-765.2765629	0.8648	-765.2763634	-0.13	-765.2766427	0.05
rad7	-690.1030349	0.7774	-690.1030722	0.02	-690.1028586	-0.11
rad8	-1145.443973	0.8057	-1145.443905	-0.04	-1145.444059	0.05
rad9	-1279.811436	0.9406	-	-	-	-
rad10	-972.2245851	0.8628	-972.224646	0.04	-972.2246044	0.01
rad11	-732.7768222	0.8056	-732.778681	1.17	-732.7768300	0.005
rad12	-1417.614105	0.7738	-1417.614457	0.22	-1417.614497	0.25
rad13	-896.400218	0.7804	-896.4002166	-0.0009	NA	-
rad14	-991.0022245	0.8001	-991.0019509	-0.17	-991.0022729	0.03
rad15	-1065.05176	0.7904	-1065.051674	-0.05	-1065.051746	-0.01

Table S4. Energies of full high level calculation (E_{high}), MIM2 with dimer subsystem ($E_{\text{MIM2-dimers}}$), MIM2 with trimer subsystem ($E_{\text{MIM2-trimmers}}$), full-low level calculation (E_{low}) in a.u. and $\langle \mathbf{S}^2 \rangle$ of full-high level calculation ($\langle \mathbf{S}^2 \rangle_{\text{high}}$) and full-low level calculation ($\langle \mathbf{S}^2 \rangle_{\text{low}}$) for the triplet state of Di25 test set. E_{high} and $\langle \mathbf{S}^2 \rangle_{\text{high}}$ correspond to the optimized results. All high-level calculations are carried out at the B3LYP-D3BJ/6-311++G(d,p) level of theory while all MIM2 calculations are carried out at the B3LYP-D3BJ/6-311++G(d,p):B3LYP-D3BJ/6-31G(d) level of theory.

	E_{high}	$\langle \mathbf{S}^2 \rangle_{\text{high}}$	$E_{\text{MIM2-dimers}}$	$E_{\text{MIM2-trimmers}}$	E_{low}	$\langle \mathbf{S}^2 \rangle_{\text{low}}$
rad1	-155.985820	2.033	-155.986161	NA	-155.938574	2.036
rad2	-233.413071	2.050	-233.413586	-233.413153	-233.345129	2.056
rad3	-310.873714	2.045	-310.874181	-310.872997	-310.790031	2.049
rad4	-309.694442	2.064	-309.694619	NA	-309.612857	2.070
rad5	-309.676657	2.008	-309.676661	NA	-309.594927	2.008
rad6	-155.957934	2.007	-155.957420	NA	-155.909614	2.006
rad7	-540.828318	2.055	-540.828287	-540.828284	-540.692252	2.060
rad8	-746.665384	2.021	-746.666156	-746.665720	-746.454771	2.020
rad9	-821.861964	2.052	-821.863527	-821.862333	-821.625190	2.053
rad10	-341.783377	2.071	-341.783593	NA	-341.686194	2.076
rad11	-806.857994	2.028	-806.858001	-806.857857	-806.634914	2.027
rad12	-1199.798816	2.065	-1199.799608	-1199.797502	-1199.498255	2.067
rad13	-941.756392	2.078	-941.756548	-941.756390	-941.521566	2.082
rad14	-1112.267149	2.033	-1112.266382	-1112.266802	-1111.964682	2.033
rad15	-1426.454922	2.029	-1426.454721	-1426.455315	-1426.082006	2.028
rad16	-1500.708825	2.026	-1500.708183	-1500.709766	-1500.310827	2.025
rad17	-1502.727401	2.037	-1502.727230	-1502.727229	-1502.346667	2.036
rad18	-1740.755319	2.072	-1740.755483	-1740.754999	-1740.328525	2.075
rad19	-2517.677262	2.071	-2517.679466	-2517.678708	-2517.062066	2.074
rad20	-2094.692223	2.050	-2094.699045	-2094.694087	-2094.177061	2.053
rad21	-771.969940	2.070	-771.969887	-771.969870	-771.780020	2.076
rad22	-1981.546957	2.054	-1981.552110	-1981.547046	-1981.055402	2.056
rad23	-1901.103180	2.121	-1901.104995	-1901.104246	-1900.611835	2.128
rad24	-2252.019791	2.051	-2252.027713	-2252.022061	-2251.466415	2.053
rad25	-1300.326908	2.132	-1300.327229	-1300.326962	-1299.961679	2.144

Table S5. Energies of full high level calculation (E_{high}) in a.u. and $\langle \mathbf{S}^2 \rangle_{\text{high}}$ of triplet and broken symmetry, J in kcal mol⁻¹ obtained from Eq. (3) and error in MIM2 energy with trimer model of triplet state ($\Delta E_{\text{MIM2-trimers-triplet}}$) of Di25 test set. All high-level calculations are carried out at the CAM-B3LYP/6-311++G(d,p) level of theory while all MIM2 calculations are carried out at the CAM-B3LYP/6-311++G(d,p):CAM-B3LYP/6-31G(d) level of theory

	$E_{\text{high-triplet}}$	$\langle \mathbf{S}^2 \rangle_{\text{high-triplet}}$	$E_{\text{high-BS}}$	$\langle \mathbf{S}^2 \rangle_{\text{high-BS}}$	J from Eq. (3) (kcal/mol)	$\Delta E_{\text{MIM2-trimers-triplet}}$ (kcal/mol)
rad1	-155.8725915	2.048	-	-	-	NA
rad2	-233.242197	2.079	-233.243655	1.072	-0.91	0.03
rad3	-310.6497149	2.072	-	-	-	-0.41
rad4	-309.4761604	2.113	-309.4625729	1.018	7.78	NA
rad5	-309.4561774	2.010	-	-	-	NA
rad6	-155.8425888	2.008	-	-	-	NA
rad7	-540.4473386	2.106	-540.4481253	1.135	-0.51	-0.03
rad8	-746.2185997	2.032	-746.2162564	1.012	1.44	0.20
rad9	-821.3883457	2.098	-821.3855175	1.097	1.77	0.25
rad10	-341.5729732	2.121	-341.5560015	0.993	9.44	NA
rad11	-806.3557307	2.048	-806.3539992	1.011	1.05	-0.09
rad12	-1198.943315	2.122	-1198.928765	0.990	8.07	-0.87
rad13	-941.1175709	2.161	-941.1060094	1.053	6.55	-0.002
rad14	-1111.613837	2.060	-1111.610923	1.010	1.74	-0.23
rad15	-1425.50359	2.052	-1425.502153	1.027	0.88	0.22
rad16	-1499.765067	2.045	-	-	-	0.63
rad17	-1501.724246	2.072	-1501.722127	1.032	1.28	-0.13
rad18	-1739.508627	2.161	-1739.500107	1.086	4.97	-0.24
rad19	-2515.839395	2.164	-2515.834286	1.090	2.99	0.65
rad20	-2093.150715	2.110	-2093.150762	1.122	-0.03	1.05
rad21	-771.4268551	2.143	-771.4263554	1.123	0.31	-0.04
rad22	-1980.072203	2.118	-1980.072352	1.107	-0.09	-0.14
rad23	-1899.767404	2.297	-1899.757917	1.179	5.33	0.55
rad24	-2250.345698	2.112	-2250.346151	1.114	-0.28	1.12
rad25	-1299.551609	2.262	-1299.555656	1.564	-3.64	-0.05

Table S6. Energies of full high level calculation (E_{high}), MIM2 with dimer subsystem ($E_{\text{MIM2-dimers}}$), MIM2 with trimer subsystem ($E_{\text{MIM2-trimmers}}$), full-low level calculation (E_{low}) in a.u. and $\langle \mathbf{S}^2 \rangle$ of full-high level calculation ($\langle \mathbf{S}^2 \rangle_{\text{high}}$) and full-low level calculation ($\langle \mathbf{S}^2 \rangle_{\text{low}}$) for the broken symmetry state of Di25 test set. E_{high} and $\langle \mathbf{S}^2 \rangle_{\text{high}}$ correspond to the optimized results. All high-level calculations are carried out at the B3LYP-D3BJ/6-311++G(d,p) level of theory while all MIM2 calculations are carried out at the B3LYP-D3BJ/6-311++G(d,p):B3LYP-D3BJ/6-31G(d) level of theory.

	E_{high}	$\langle \mathbf{S}^2 \rangle_{\text{high}}$	$E_{\text{MIM2-dimers}}$	$E_{\text{MIM2-trimmers}}$	E_{low}	$\langle \mathbf{S}^2 \rangle_{\text{low}}$
rad1	—	—	—	—	—	—
rad2	-233.414453	1.021	-233.414922	-233.414470	-233.346479	1.072
rad3	-310.876872	1.038	-310.877356	-310.876222	-310.793256	1.056
rad4	-309.684233	1.012	-309.683912	NA	-309.602144	1.012
rad5	—	—	—	—	—	—
rad6	—	—	—	—	—	—
rad7	-540.828757	1.069	-540.828769	-540.828752	-540.692783	1.075
rad8	-746.663243	1.004	-746.663455	-746.662986	-746.452068	0.994
rad9	-821.859462	1.051	-821.858738	-821.857570	-821.620239	1.039
rad10	-341.771359	0.973	-341.771030	NA	-341.673777	0.979
rad11	-806.856437	1.009	-806.856923	-806.856524	-806.633005	1.008
rad12	-1199.789317	0.968	-1199.789101	-1199.786935	-1199.487327	0.979
rad13	-941.748197	1.016	-941.747641	-941.747470	-941.512300	1.018
rad14	-1112.265012	1.004	-1112.264217	-1112.264621	-1111.962309	1.005
rad15	-1426.453838	1.015	-1426.453475	-1426.454151	-1426.080760	1.013
rad16	-1500.707295	1.009	-1500.706561	-1500.708158	-1500.309185	1.008
rad17	-1502.726115	1.008	-1502.725877	-1502.725883	-1502.345119	1.011
rad18	-1740.749579	1.037	-1740.749260	-1740.748772	-1740.322115	1.036
rad19	-2517.671789	1.037	-2517.673512	-2517.672735	-2517.055934	1.036
rad20	-2094.692350	1.055	-2094.699181	-2094.694223	-2094.177198	1.058
rad21	-771.969568	1.061	-771.969475	-771.969459	-771.779609	1.067
rad22	-1981.547006	1.039	-1981.552084	-1981.547066	-1981.055376	1.043
rad23	-1901.096157	1.054	-1901.095199	-1901.095045	-1900.602039	1.054
rad24	-2252.019834	1.051	-2252.027757	-2252.022105	-2251.466459	1.053
rad25	-1300.328927	1.275	-1300.329391	-1300.329125	-1299.963841	1.276

Table S7. Energies of the full high level calculations (E_{high}), MIM2 with dimer subsystems ($E_{\text{MIM2-dimers}}$), MIM2 with trimer subsystems ($E_{\text{MIM2-trimmers}}$), MIM2 with tetramer subsystems ($E_{\text{MIM2-tetramers}}$), full low level calculation (E_{low}), all in a.u., and $\langle \mathbf{S}^2 \rangle$ of the full high level calculation ($\langle \mathbf{S}^2 \rangle_{\text{high}}$) and full-low level calculation ($\langle \mathbf{S}^2 \rangle_{\text{low}}$) for the high spin and broken symmetry (BS) states of polyradicals. All high-level calculations are carried out at the B3LYP-D3BJ/6-311++G(d,p) level of theory while all MIM2 calculations are carried out at the B3LYP-D3BJ/6-311++G(d,p):B3LYP-D3BJ/6-31G(d) level of theory.

	Multiplicity	E_{high}	$\langle \mathbf{S}^2 \rangle_{\text{high}}$	$E_{\text{MIM2-dimers}}$	$E_{\text{MIM2-trimmers}}$	$E_{\text{MIM2-tetramers}}$	E_{low}	$\langle \mathbf{S}^2 \rangle_{\text{low}}$	
1	HS	4	-1482.581632	3.780	-1482.583376	-1482.582148	-	-1482.182707	3.778
	BS1	2	-1482.580947	1.773	-1482.582685	-1482.583177	-	-1482.182017	1.770
	BS2	2	-1482.580182	1.763	-1482.581891	-1482.580692	-	-1482.181223	1.761
	BS3	2	-1482.580881	1.771	-1482.582594	-1482.581392	-	-1482.181925	1.769
2	HS	5	-1079.297196	6.161	-1079.301152	-1079.296730	-	-1079.041577	6.173
	BS1	3	-1079.287257	3.074	-1079.290524	-1079.287022	-	-1079.030949	3.085
	BS2	1	-1079.287504	2.075	-1079.290805	-1079.288221	-	-1079.031229	2.085
	BS3	1	-1079.276792	1.983	-1079.279296	-1079.275793	-	-1079.019721	1.994
3	HS	5	-2633.144877	6.127	-2633.15358	-2633.145017	-	-2632.507097	6.135
	BS1	3	-2633.140579	3.086	-2633.149014	-2633.140833	-	-2632.502531	3.092
	BS2	1	-2633.140685	2.085	-2633.149110	-2633.140929	-	-2632.502627	2.091
	BS3	1	-2633.136044	2.049	-2633.144212	-2633.136413	-	-2632.497729	2.052
4	HS	5	-4186.988749	6.132	-4186.997614	-4186.988457	-	-4185.970677	6.139
	BS1	3	-4186.984272	3.088	-4186.992891	-4186.984134	-	-4185.965954	3.093
	BS2	1	-4186.984373	2.086	-4186.992984	-4186.984231	-	-4185.966047	2.092
	BS3	1	-4186.979524	2.048	-4186.987907	-4186.979560	-	-4185.960970	2.051
5	HS	9	-6820.146574	20.258	-6820.165795	-6820.147346	-6820.147288	-6818.493011	20.271
	BS1	7	-6820.145576	13.244	-6820.164783	-6820.146718	-6820.146512	-6818.491999	13.256
	BS2	5	-6820.144839	8.232	-6820.164018	-6820.145899	-6820.145767	-6818.491234	8.244
	BS3	5	-6820.145091	8.235	-6820.164274	-6820.146592	-6820.146240	-6818.491490	8.246

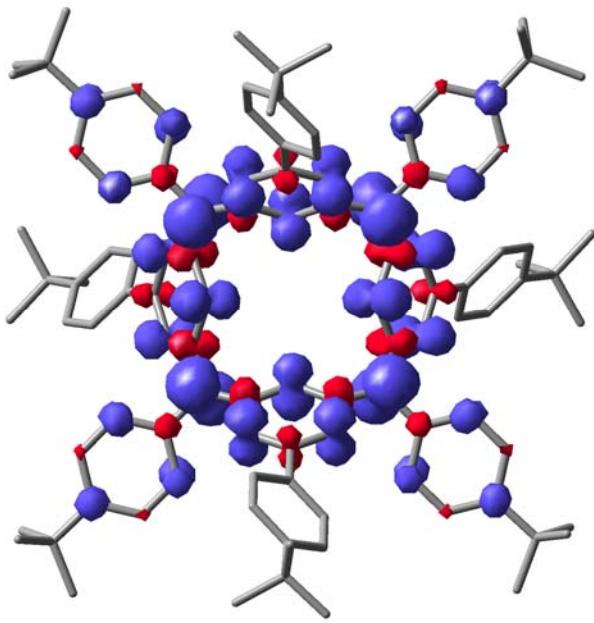


Figure S5: Spin Density plot of high spin state of polyyradical **3**.

Table S8. Lowest energy levels of the different S states, relative to the ground state of polyyradicals in kcal mol⁻¹.

		GS	ES1	ES2	ES3	ES4
1	Full	0.0 ($S = 3/2$)	0.45 ($S = 1/2$)	1.37 ($S = 1/2$)	-	-
	MIM2	0.0 ($S = 1/2$)	1.02 ($S = 3/2$)	2.79 ($S = 1/2$)	-	-
2	Full	0.0 ($S = 2$)	5.76 ($S = 0$)	6.08 ($S = 1$)	12.80 ($S = 1$)	19.21 ($S = 0$)
	MIM2	0.0 ($S = 2$)	4.16 ($S = 0$)	5.36 ($S = 1$)	13.14 ($S = 1$)	19.70 ($S = 0$)
3	Full	0.0 ($S = 2$)	2.49 ($S = 0$)	2.63 ($S = 1$)	5.54 ($S = 1$)	8.32 ($S = 0$)
	MIM2	0.0 ($S = 2$)	2.43 ($S = 0$)	2.56 ($S = 1$)	5.40 ($S = 1$)	8.10 ($S = 0$)
4	Full	0.0 ($S = 2$)	2.59 ($S = 0$)	2.74 ($S = 1$)	5.79 ($S = 1$)	8.68 ($S = 0$)
	MIM2	0.0 ($S = 2$)	2.51 ($S = 0$)	2.65 ($S = 1$)	5.58 ($S = 1$)	8.38 ($S = 0$)
5	Full	0.0 ($S = 4$)	0.93 ($S = 3$)	1.06 ($S = 3$)	1.40 ($S = 2$)	1.66 ($S = 2$)
	MIM2	0.0 ($S = 4$)	0.66 ($S = 3$)	0.93 ($S = 3$)	0.98 ($S = 2$)	1.52 ($S = 2$)

XYZ Coordinates of the geometries optimized at the B3LYP-D3BJ/6-311++G(d,p) level of theory for Mono15 and Di25. All the polyyradicals were optimized at the B3LYP-D3BJ/6-311G(d) level of theory.

Mono15 test set

rad1

C	-0.73623900	-0.98796200	0.22463200
C	0.73624400	-0.98794300	-0.22469400
C	1.23228200	0.43421400	0.12138700
C	0.00000600	1.27630500	0.00000300
C	-1.23228900	0.43422700	-0.12130300
H	-1.32739100	-1.77506900	-0.24837300
H	-0.79028700	-1.13945000	1.30783300
H	0.79029900	-1.13932000	-1.30790900
H	1.32739100	-1.77509600	0.24824100
H	1.63085300	0.45919600	1.14933400
H	2.05174900	0.76930200	-0.52508100
H	0.00003500	2.35881500	-0.00031800
H	-2.05167400	0.76925900	0.52530500
H	-1.63099900	0.45932100	-1.14919000

rad2

C	-0.50335500	0.13216900	-0.00880700
O	-0.43523400	1.36736200	-0.00173600
C	-1.85452500	-0.55981200	0.00256900
H	-2.52886600	-0.04639700	-0.68458800
H	-1.79085700	-1.61592400	-0.26525400
H	-2.28601600	-0.48243600	1.00525500
C	0.68804400	-0.67737100	-0.00920100
H	0.58056800	-1.75796900	-0.01680000
C	2.04860500	-0.09154000	0.00588000
H	1.99997400	0.99705700	0.00138900
H	2.60504400	-0.42271300	0.89221400
H	2.62941300	-0.43119200	-0.86097900

rad3

C	2.46156300	-0.25857600	-0.00074700
H	3.32440400	0.41218200	0.01017000
H	2.53537200	-0.91293500	0.87287900
H	2.53828600	-0.88763400	-0.89255300
C	1.14637700	0.52272400	0.00805400
H	1.11135200	1.16920400	0.89354200
H	1.11431600	1.19289800	-0.85956400
C	-0.08518700	-0.38608600	-0.00575300
H	-0.07796000	-1.04684300	0.86751700
H	-0.06280700	-1.03251800	-0.88993100
C	-1.39600000	0.39904700	-0.01272700
H	-1.44383900	1.11469000	-0.85704900
H	-1.46070800	1.06346500	0.87640300
O	-2.54236700	-0.34189600	0.00570300

rad4

C	-0.53011500	0.52343200	-0.00000100
H	-0.48329900	1.16291300	0.88986100
H	-0.48315800	1.16291400	-0.88985700
C	0.66153100	-0.42952700	0.00008800
H	0.61049700	-1.11862700	-0.86629700
H	0.61054100	-1.11853600	0.86653300
O	-1.70139000	-0.28912100	-0.00009700
H	-2.47949100	0.27515400	0.00069400
O	1.88094200	0.17321600	-0.00008500

rad5

C	1.80415800	-0.11631000	0.19968800
C	1.04671900	-1.30585500	-0.35980700
C	1.19716200	1.16191200	-0.36386300
H	1.48830600	-2.23517800	0.00801400
H	1.32138000	1.13497400	-1.45102600
C	-0.44947100	-1.29947100	-0.01432000
C	-0.28936400	1.34391700	-0.01826700
H	1.17374700	-1.29642400	-1.44693600
H	1.73937800	2.04079600	0.00196700
N	-1.03117900	0.06253900	-0.25869900
O	-2.30752700	0.14179100	-0.22585300
C	-1.18454000	-2.27978100	-0.93562800
H	-0.75169500	-3.27660400	-0.82167300
H	-2.24436100	-2.32041800	-0.68891000
H	-1.08393600	-1.97342200	-1.97900300
C	-0.69599400	-1.69717100	1.45312400
H	-0.41842600	-2.74367800	1.60122100
H	-0.11468000	-1.09342200	2.15093700
H	-1.75415000	-1.57919500	1.69077600
C	-0.89881200	2.40440800	-0.94243000
H	-1.94616700	2.57322200	-0.69681600
H	-0.34940800	3.34244200	-0.83004500
H	-0.83569700	2.08574300	-1.98505000
C	-0.48339800	1.77335300	1.44817600
H	-0.07868300	2.77809900	1.59445700
H	-1.54802500	1.78870100	1.68553100
H	0.01669600	1.10248400	2.14747800
H	1.74878900	-0.11436100	1.29523300
O	3.17012600	-0.27164800	-0.19894100
H	3.67564200	0.47730300	0.13305800

rad6

C	-2.01680400	0.76840200	-0.11189200
C	0.22506800	-0.00000300	0.00001300
C	-2.01680900	-0.76839900	0.11188600
N	-0.57186900	1.08909600	0.17062200
N	-0.57186800	-1.08909900	-0.17060300
O	-0.21105500	2.28854400	0.39461400
O	-0.21105900	-2.28854900	-0.39459000

C	1.68341800	-0.00000200	0.00000800
C	2.39950900	1.20686800	-0.11916900
C	2.39951300	-1.20686900	0.11917700
C	3.78895600	1.19718400	-0.12482800
H	1.86035100	2.13835800	-0.19101200
C	3.78896100	-1.19718300	0.12481900
H	1.86035700	-2.13836000	0.19102900
C	4.49048400	0.00000100	-0.00000900
H	4.32507900	2.13412900	-0.22088300
H	4.32508600	-2.13412700	0.22086800
H	5.57446700	0.00000300	-0.00001600
C	-2.91700900	-1.56332900	-0.82393800
H	-2.80369200	-2.62722800	-0.61933800
H	-3.95898900	-1.28261500	-0.65375400
H	-2.67302200	-1.39447600	-1.87146800
C	-2.26537200	-1.18218400	1.56903400
H	-3.30891700	-1.01992100	1.84357900
H	-2.03878400	-2.24414100	1.67285800
H	-1.63043100	-0.62402300	2.25929800
C	-2.26534000	1.18218300	-1.56904600
H	-3.30888100	1.01992200	-1.84360800
H	-2.03874900	2.24413900	-1.67286900
H	-1.63038800	0.62401800	-2.25929600
C	-2.91702000	1.56333700	0.82391300
H	-2.80369600	2.62723500	0.61931100
H	-3.95899800	1.28262600	0.65370800
H	-2.67305500	1.39448700	1.87144800

rad7

C	2.05501000	-0.59793900	0.10388300
C	-0.18392300	0.15209100	-0.00313400
C	1.93167500	0.95965900	-0.00939400
N	0.63999500	-0.96749100	-0.22757500
N	0.49039700	1.23226900	0.20260100
O	0.28769500	-2.15182800	-0.50230300
C	-1.65555600	0.09292400	-0.00241600
C	-2.35258900	1.31028700	-0.05291800
C	-2.37583900	-1.10640500	0.07613100
C	-3.73998800	1.32749200	-0.02470700
H	-1.78543600	2.23005500	-0.10969200
C	-3.76827200	-1.07965000	0.10839900
H	-1.84824100	-2.04752000	0.10358900
C	-4.45352800	0.13074700	0.05669800
H	-4.26740600	2.27336400	-0.06665600
H	-4.31713800	-2.01199400	0.17138400
H	-5.53724600	0.14412800	0.07744800
C	2.30498500	-1.09389800	1.53609300
H	2.15971800	-2.17545400	1.56631500
H	3.32694500	-0.87183300	1.84799900
H	1.61567400	-0.63245600	2.24522000
C	3.01538000	-1.28089300	-0.86073000
H	4.03940900	-0.96783900	-0.64427400

H	2.95097200	-2.36281000	-0.73749200
H	2.79012800	-1.04600100	-1.90004300
C	2.75674000	1.73450400	1.01663500
H	3.82298600	1.52156100	0.89909400
H	2.60175900	2.80437100	0.86581800
H	2.46257800	1.49555100	2.03807900
C	2.25991300	1.47719200	-1.42101300
H	1.99595400	2.53437200	-1.47839400
H	3.32421900	1.37158000	-1.64326800
H	1.68677900	0.94544200	-2.18304800

rad8

C	-3.04154100	-1.34702700	-0.00000100
C	-3.39029500	0.01567700	0.00000900
C	-2.46607900	1.06387300	0.00004100
C	-1.10359200	0.68270900	0.00003100
C	-0.73123700	-0.69503300	0.00001800
C	-1.67853900	-1.69798600	0.00001300
H	-4.44119400	0.26286200	0.00000400
H	-1.37256500	-2.73540600	0.00001000
C	1.10359200	0.68271000	-0.00000300
C	2.46608100	1.06387300	-0.00001900
C	3.39029600	0.01567700	-0.00001000
C	3.04154100	-1.34702700	0.00000700
C	1.67853900	-1.69798600	0.00001700
C	0.73123700	-0.69503300	0.00001500
H	4.44119400	0.26286100	-0.00001800
H	1.37256500	-2.73540600	0.00002500
N	0.00000100	1.50474100	0.00000300
C	-2.89209100	2.53334500	0.00003100
C	2.89209000	2.53334600	-0.00003400
C	-4.42056600	2.69705100	-0.00036600
H	-4.87924300	2.25208500	0.88680700
H	-4.66685000	3.76167300	-0.00029400
H	-4.87876000	2.25232200	-0.88790800
C	-2.33242600	3.22714100	-1.26205000
H	-1.24445000	3.18611100	-1.27720900
H	-2.71155800	2.74520300	-2.16763600
H	-2.64439000	4.27576400	-1.27838100
C	-2.33311000	3.22699000	1.26249900
H	-2.71269200	2.74490700	2.16782000
H	-1.24514300	3.18601100	1.27821700
H	-2.64513600	4.27559600	1.27881600
C	2.33282700	3.22703800	-1.26235100
H	1.244485600	3.18603700	-1.27783700
H	2.64482700	4.27565100	-1.27868600
H	2.71222300	2.74500400	-2.16777500
C	4.42056400	2.69705700	0.00003600
H	4.66684500	3.76167900	-0.00000500
H	4.87895700	2.25225600	0.88744000
H	4.87904700	2.25216500	-0.88727500
C	2.33270200	3.22709100	1.26219800

H	1.24472900	3.18607200	1.27758900
H	2.71202400	2.74510800	2.16768000
H	2.64468100	4.27571000	1.27850900
C	4.15653100	-2.39931700	0.00001900
C	-4.15653000	-2.39931800	-0.00002600
C	-5.03018000	-2.21873400	-1.26073100
H	-5.82838000	-2.96674600	-1.27692100
H	-5.49444300	-1.23126400	-1.29289600
H	-4.43062600	-2.33745200	-2.16689600
C	-5.03036100	-2.21861400	1.26053200
H	-5.49461300	-1.23113300	1.29255000
H	-5.82857900	-2.96660900	1.27666400
H	-4.43094600	-2.33727100	2.16679700
C	-3.60689700	-3.83461600	0.00008300
H	-3.00021800	-4.03627800	-0.88650900
H	-3.00037900	-4.03620300	0.88680200
H	-4.43853200	-4.54356800	0.00003700
C	3.60690200	-3.83461700	0.00002100
H	3.00030100	-4.03624100	0.88667500
H	3.00030700	-4.03624400	-0.88663600
H	4.43853800	-4.54356600	0.00002600
C	5.03028500	-2.21867900	-1.26060300
H	5.49454200	-1.23120300	-1.29269600
H	5.82849600	-2.96668100	-1.27675100
H	4.43081200	-2.33737300	-2.16682500
C	5.03025900	-2.21866300	1.26065900
H	5.82847100	-2.96666200	1.27683200
H	5.49451100	-1.23118400	1.29274800
H	4.43076600	-2.33734700	2.16686900

rad9

C	2.78214000	1.03019200	0.43043500
C	1.52996300	0.49706100	0.40754800
C	1.27815900	-0.86950800	0.05871100
C	2.40520600	-1.72137300	-0.18595800
C	3.68812300	-1.26953200	-0.21884500
C	3.93352200	0.17094700	0.04551100
H	2.19012000	-2.76282300	-0.38617700
C	3.04152400	2.47880700	0.84940700
C	1.74537500	3.18924800	1.27367600
H	1.98221400	4.21131500	1.57738400
H	1.02654900	3.25110200	0.45295200
H	1.26363600	2.69582200	2.12229500
C	3.64294100	3.26539200	-0.33886700
H	2.95994700	3.25152100	-1.19321500
H	3.79477800	4.30834600	-0.04586500
H	4.59816100	2.84596500	-0.64676400
C	4.01268200	2.51268900	2.05210400
H	3.59633100	1.95893400	2.89865700
H	4.97893200	2.08465400	1.79414400
H	4.16347400	3.54845300	2.36935900
C	4.87290500	-2.18741900	-0.52633300

C	4.42452200	-3.64383500	-0.73473600
H	3.93377200	-4.05224400	0.15316300
H	3.74623000	-3.74669500	-1.58621000
H	5.30250900	-4.26082800	-0.93870300
C	5.57615100	-1.71856200	-1.82124700
H	5.97271500	-0.71143400	-1.71251400
H	6.40167700	-2.39737800	-2.05445900
H	4.87902700	-1.73361400	-2.66403300
C	5.87161300	-2.16603400	0.65412600
H	6.69739000	-2.85237400	0.44579500
H	6.27901000	-1.16938500	0.80976900
H	5.38455100	-2.49546800	1.57654300
O	5.07321300	0.64260900	-0.03245600
H	0.69084500	1.09684100	0.71952100
C	-0.00000600	-1.45059200	0.00009900
H	-0.00001100	-2.53836600	0.00012600
C	-1.27815500	-0.86949700	-0.05855800
C	-1.52993500	0.49707400	-0.40741800
C	-2.40522500	-1.72135100	0.18606300
C	-2.78210900	1.03020300	-0.43040200
H	-0.69079600	1.09684800	-0.71934300
C	-3.68813800	-1.26950400	0.21887600
H	-2.19015400	-2.76279900	0.38631300
C	-3.93351300	0.17097600	-0.04551000
C	-3.04148000	2.47881900	-0.84939300
C	-4.01215900	2.51267000	-2.05247800
H	-4.97846400	2.08451100	-1.79493200
H	-4.16293700	3.54843600	-2.36973000
H	-3.59540500	1.95901200	-2.89889600
C	-3.64348000	3.26524200	0.33869000
H	-4.59874800	2.84563900	0.64620100
H	-2.96081200	3.25143900	1.19330000
H	-3.79537900	4.30818600	0.04568600
C	-1.74524900	3.18945600	-1.27308800
H	-1.02677600	3.25137600	-0.45206000
H	-1.26308500	2.69613400	-2.12152700
H	-1.98210100	4.21150300	-1.57685200
C	-4.87293900	-2.18739000	0.52630300
C	-4.42458900	-3.64384700	0.73448400
H	-3.93393000	-4.05216300	-0.15351000
H	-3.74622400	-3.74683200	1.58588500
H	-5.30257800	-4.26083600	0.93844900
C	-5.87170300	-2.16580900	-0.65410600
H	-6.69749600	-2.85214500	-0.44582600
H	-6.27906900	-1.16912200	-0.80959300
H	-5.38469800	-2.49513700	-1.57659000
C	-5.57610700	-1.71870500	1.82132200
H	-5.97268300	-0.71156600	1.71275000
H	-6.40161600	-2.39755600	2.05449400
H	-4.87893200	-1.73386800	2.66406400
O	-5.07324000	0.64260100	0.03213700

rad10

C	0	2.33692100	-0.65706300	-0.00002400	H
C	0	1.35542300	0.35962200	-0.00001700	H
C	0	1.68099600	1.73564400	-0.00001000	H
C	0	-0.01653100	-0.01693400	-0.00001200	H
C	0	0.69922100	2.73424100	0.00001400	H
C	0	-0.63940000	2.34763900	0.00003800	H
C	0	-1.02656800	0.98199200	0.00001600	H
C	0	2.00189900	-2.01621300	-0.00002900	H
C	0	0.65241400	-2.36570000	-0.00003300	H
C	0	-0.37529700	-1.38912800	-0.00002600	H
H	0	0.35490700	-3.40570300	-0.00004800	H
C	0	-1.74882000	-1.73705100	-0.00002800	H
C	0	-2.75368900	-0.77140000	-0.00000800	H
C	0	-2.37880900	0.57788500	0.00002000	H
H	0	-1.99903400	-2.78948000	-0.00004900	H
H	0	2.73036200	2.00660600	-0.00002400	H
H	0	-1.42563200	3.09050500	0.00007700	H
H	0	-3.13806500	1.35137300	0.00005000	H
H	0	3.37777100	-0.35495600	-0.00002200	H
C	0	3.12327000	-3.06568600	0.00000800	H
C	0	-4.24560100	-1.13583800	0.00000200	H
C	0	2.58008700	-4.50309300	0.00004400	H
H	0	1.97398000	-4.70666900	0.88651000	H
H	0	1.97391800	-4.70668600	-0.88637700	H
H	0	3.41490200	-5.20853000	0.00002400	H
C	0	3.99470900	-2.88072200	1.26029800	H
H	0	4.79835800	-3.62298200	1.27791500	H
H	0	4.45231000	-1.88992700	1.29331500	H
H	0	3.39495500	-3.00307700	2.16591000	H
C	0	3.99475800	-2.88081200	-1.26026000	H
H	0	4.79838500	-3.62309600	-1.27780400	H
H	0	3.39503500	-3.00320500	-2.16588800	H
H	0	4.45239400	-1.89003600	-1.29332200	H
C	0	-4.47741700	-2.65484900	0.00004100	H
H	0	-4.04906600	-3.12961000	-0.88638500	H
H	0	-4.04911800	-3.12955800	0.88651900	H
H	0	-5.55094400	-2.86009500	0.00001700	H
C	0	-4.91422100	-0.54714100	-1.26028000	H
H	0	-5.97877000	-0.79918900	-1.27758100	H
H	0	-4.82637800	0.54065800	-1.29355200	H
H	0	-4.45197600	-0.94845400	-2.16586900	H
C	0	-4.91421100	-0.54707400	1.26025800	H
H	0	-4.82634500	0.54072500	1.29348000	H
H	0	-5.97876400	-0.79910000	1.27757000	H
H	0	-4.45197300	-0.94835500	2.16586400	H
C	0	1.12924600	4.20871000	0.00000200	H
C	0	-0.07053400	5.16882900	0.00045100	H
H	0	0.28847000	6.20115600	0.00036000	H
H	0	-0.69609700	5.03534600	-0.88583300	H
H	0	-0.69547700	5.03527900	0.88716300	H
C	0	1.97283700	4.49368300	-1.26055700	H

H	0	2.28588700	5.54190700	-1.27822900 H
H	0	2.87150100	3.87450500	-1.29377500 H
H	0	1.39414700	4.29322400	-2.16595100 H
C	0	1.97362500	4.49352100	1.26006300 H
H	0	1.39548500	4.29301000	2.16579900 H
H	0	2.87228800	3.87430800	1.29268200 H
H	0	2.28673500	5.54172700	1.27763300 H

rad11

C		-0.00019800	0.00009700	-0.00064100
C		-1.36092700	0.52331100	-0.00057700
C		-1.68552700	1.71964000	0.67526800
C		-2.40374400	-0.14729400	-0.67599200
C		-2.98296100	2.21345000	0.67842300
H		-0.90940700	2.24496600	1.21726400
C		-3.69798200	0.35484000	-0.67760300
H		-2.17975200	-1.05696000	-1.21859400
C		-3.99827100	1.53688800	0.00086100
H		-3.20682300	3.12643100	1.21857900
H		-4.47618200	-0.17305500	-1.21718800
H		-5.00979400	1.92558700	0.00147600
C		1.13334700	0.91693100	-0.00023000
C		2.33069600	0.60078200	0.67771200
C		1.07502500	2.15414300	-0.67781100
C		3.40737500	1.47712700	0.68041400
H		2.39664000	-0.33310600	1.22141800
C		2.15727800	3.02359200	-0.67981600
H		0.17585200	2.41418400	-1.22186300
C		3.33026500	2.69344100	0.00046500
H		4.30930000	1.21519300	1.22202100
H		2.09010700	3.96052600	-1.22116600
H		4.17287500	3.37481800	0.00073600
C		0.22732700	-1.43998300	-0.00031900
C		1.32918500	-2.00747400	-0.67640700
C		-0.64584100	-2.31938600	0.67603700
C		1.54148100	-3.37938800	-0.67859200
H		2.00463600	-1.35836700	-1.21912000
C		-0.42487400	-3.68993600	0.67845300
H		-1.48848800	-1.91001200	1.21867300
C		0.66826100	-4.23069000	-0.00002800
H		2.38746000	-3.78919800	-1.21876900
H		-1.10328200	-4.34049800	1.21877400
H		0.83736700	-5.30105000	0.00005200

rad12

N		-0.60052200	-1.09828500	-0.02231800
N		-1.57031000	-0.20574600	0.12696500
C		0.67978200	-0.67773400	-0.17714600
C		1.69361200	-1.47993100	0.41549800
C		1.17509000	0.42356200	-0.93930700
C		3.04165400	-1.24676200	0.28651100
C		2.52605200	0.71070200	-1.04118400

C	3.44872200	-0.12378200	-0.43126000
H	3.76821600	-1.89599800	0.75433100
H	2.85499100	1.56021400	-1.62201000
C	-2.87435300	-0.61146500	-0.23599200
C	-3.99010100	-0.10033000	0.43769600
C	-3.03090400	-1.54432500	-1.26673100
C	-5.26060100	-0.52482300	0.06975200
H	-3.86139700	0.60494300	1.24717400
C	-4.30692100	-1.96190400	-1.61858400
H	-2.15459400	-1.91320100	-1.77996900
C	-5.42552900	-1.45445600	-0.95663300
H	-6.12425000	-0.13571400	0.59528200
H	-4.42977800	-2.67882100	-2.42133800
H	-6.41900000	-1.78105200	-1.23894400
C	-1.34161500	1.04025400	0.80160400
C	-1.84024900	2.22627100	0.26407000
C	-0.60599400	1.03687300	1.98866300
C	-1.59064100	3.42498300	0.92255000
H	-2.38668200	2.20519000	-0.66958900
C	-0.36189800	2.24349500	2.63466100
H	-0.24767800	0.09862500	2.39392900
C	-0.85081300	3.43713800	2.10419500
H	-1.95974400	4.35164600	0.50081400
H	0.20324800	2.24924800	3.55878900
H	-0.65395600	4.37486400	2.60957200
N	4.87855600	0.17066400	-0.55539200
N	0.29204800	1.24035600	-1.78343300
N	1.29371500	-2.58483600	1.31088400
O	-0.70363200	0.70070300	-2.25345300
O	0.62675100	2.39790800	-1.99846200
O	5.19896100	1.16969200	-1.18794700
O	5.66122400	-0.60198400	-0.01427900
O	1.81964200	-3.66990800	1.12201700
O	0.50261100	-2.32161200	2.20522900

rad13

C	1.55624200	4.05364500	-0.14663300
C	0.28400800	3.53439200	0.01854800
C	0.07142800	2.14370100	0.04158000
C	1.19865400	1.28488900	-0.07308900
C	2.47790500	1.81627700	-0.27734100
C	2.65030900	3.19361500	-0.30889900
H	1.70518300	5.12653600	-0.16583000
H	-0.58436900	4.17330400	0.11901200
H	3.32431100	1.15918300	-0.41618600
H	3.64196100	3.60049300	-0.46561400
C	-1.32766400	0.32358500	0.05640300
N	-1.19875100	1.64922200	0.14059700
N	-0.33874700	-0.57037900	-0.01745100
N	0.92906400	-0.08040200	-0.00148100
C	1.94623800	-1.07969100	0.01629000
C	2.98988000	-1.00454700	0.93939800

C	1.85871100	-2.15516700	-0.86748300
C	3.96220100	-1.99977000	0.95768400
H	3.02749700	-0.18458000	1.64485400
C	2.83342500	-3.14682200	-0.83839600
H	1.02649200	-2.20398100	-1.55676800
C	3.88982500	-3.07064500	0.06837700
H	4.76890200	-1.94448400	1.67895000
H	2.76828200	-3.98003900	-1.52805300
H	4.64742300	-3.84485400	0.08739500
C	-2.70075700	-0.24396600	0.05653100
C	-2.91085500	-1.62888000	0.04531100
C	-3.80610500	0.61453200	0.06704300
C	-4.20321700	-2.14219100	0.04210700
H	-2.05528700	-2.29061800	0.04385100
C	-5.09742300	0.09686500	0.06376800
H	-3.63325800	1.68213100	0.07800100
C	-5.30095700	-1.28202400	0.05100800
H	-4.35504800	-3.21549000	0.03529900
H	-5.94648200	0.77071600	0.07126400
H	-6.30764400	-1.68419200	0.04893200

rad14

C	-1.33621800	0.00001500	-0.21689700
N	-0.72440200	1.19005000	-0.20030500
C	1.14949000	-0.00001100	-1.08304200
N	-0.72442900	-1.19003500	-0.20030900
H	2.22910500	-0.00002400	-1.00179700
N	0.60573000	-1.16211400	-0.40466600
N	0.60575800	1.16209700	-0.40465400
C	-2.81565500	0.00003000	-0.12429200
C	-3.52495400	-1.20663500	-0.08144400
C	-3.52492600	1.20670900	-0.08136200
C	-4.91287700	-1.20421400	0.01206400
H	-2.97821400	-2.13922600	-0.12304000
C	-4.91284800	1.20431300	0.01214500
H	-2.97816400	2.13928900	-0.12289500
C	-5.61343000	0.00005600	0.06021100
H	-5.44925000	-2.14572600	0.04497000
H	-5.44919900	2.14583600	0.04511700
H	-6.69503000	0.00006700	0.13074800
C	1.36229400	2.29948400	-0.09194400
C	2.63412600	2.50547500	-0.64706000
C	0.83385900	3.25554000	0.78969500
C	3.36767900	3.63726200	-0.30412400
H	3.05078700	1.80915400	-1.36257500
C	1.57426000	4.38440500	1.11081000
H	-0.14794000	3.09054800	1.20921500
C	2.84720700	4.58357300	0.57425400
H	4.34858900	3.78221000	-0.74153700
H	1.15559900	5.11250000	1.79598400
H	3.42149500	5.46409600	0.83458300
C	1.36224300	-2.29951300	-0.09194200

C	0.83377800	-3.25556000	0.78968900
C	2.63408000	-2.50552700	-0.64704000
C	1.57415400	-4.38443900	1.11081400
H	-0.14802400	-3.09055000	1.20919600
C	3.36760700	-3.63732700	-0.30409400
H	3.05076500	-1.80921400	-1.36254800
C	2.84710500	-4.58362900	0.57427700
H	1.15547000	-5.11252600	1.79598200
H	4.34852000	-3.78229200	-0.74149300
H	3.42137300	-5.46416400	0.83461300
H	0.84367400	-0.00000300	-2.13930600

rad15

C	0.00002700	1.29805100	0.00000400
N	1.18464300	0.69609800	0.02845900
C	-0.00003800	-1.43906100	0.00001500
N	-1.18461900	0.69615600	-0.02845300
N	-1.16551800	-0.66615100	-0.05922600
N	1.16548100	-0.66620900	0.05923900
C	0.00006300	2.78178100	0.00000100
C	1.19157100	3.48869700	0.20032500
C	-1.19141200	3.48875300	-0.20032600
C	1.18866500	4.87963900	0.20010400
H	2.11019000	2.93990100	0.35897100
C	-1.18843900	4.87969400	-0.20011000
H	-2.11005600	2.93999900	-0.35896900
C	0.00013000	5.58000000	-0.00000500
H	2.11594000	5.41782100	0.35883100
H	-2.11568800	5.41792000	-0.35883900
H	0.00015500	6.66385200	-0.00000700
C	2.45908200	-1.28494600	0.04567500
C	2.72196500	-2.43233900	0.79491400
C	3.46820600	-0.68311900	-0.70763800
C	4.00191900	-2.97801600	0.77516300
H	1.93866200	-2.89525300	1.37503100
C	4.74275200	-1.23843000	-0.71697900
H	3.24627900	0.21415200	-1.26843600
C	5.01459000	-2.38840600	0.02174900
H	4.20558400	-3.86877700	1.35740200
H	5.52289700	-0.77177700	-1.30666300
H	6.00801600	-2.82075700	0.01140500
C	-2.45914400	-1.28483600	-0.04567100
C	-2.72206700	-2.43220100	-0.79493600
C	-3.46824200	-0.68299100	0.70766100
C	-4.00203900	-2.97783400	-0.77519600
H	-1.93877800	-2.89512800	-1.37506300
C	-4.74280900	-1.23825700	0.71699100
H	-3.24628100	0.21425900	1.26848000
C	-5.01468700	-2.38820600	-0.02176500
H	-4.20573800	-3.86857500	-1.35745500
H	-5.52293600	-0.77159200	1.30668800
H	-6.00812900	-2.82052100	-0.01143000

O -0.00007300 -2.65032900 0.00000700

Di25 test set

Triplet

rad1

C	0.00000000	0.00003200	0.00000000
C	0.00761100	-1.41286800	0.00000000
H	-0.91700300	-1.97579700	0.00000000
H	0.93824000	-1.96579700	0.00000000
C	-1.22736300	0.69982300	0.00000000
C	1.21975200	0.71300500	0.00000000
H	2.16959800	0.19378800	0.00000000
H	1.23329000	1.79542500	0.00000000
H	-2.17155800	0.17040100	0.00000000
H	-1.25256400	1.78203300	0.00000000

rad2

C	0.00000000	0.00000000	-0.75236500
C	-0.49889400	1.10575100	-1.42692200
H	-0.50213100	1.13646800	-2.50989200
H	-0.91372600	1.95161000	-0.89518000
C	0.49889400	-1.10575100	-1.42692200
H	0.50213100	-1.13646800	-2.50989200
H	0.91372600	-1.95161000	-0.89518000
C	0.00000000	0.00000000	0.75236500
C	-0.49889400	-1.10575100	1.42692200
H	-0.50213100	-1.13646800	2.50989200
H	-0.91372600	-1.95161000	0.89518000
C	0.49889400	1.10575100	1.42692200
H	0.50213100	1.13646800	2.50989200
H	0.91372600	1.95161000	0.89518000

rad3

C	-0.08114900	1.41403500	-0.55222000
C	-0.35323100	0.68253100	-1.82830500
C	0.35323100	-0.68253100	-1.82830500
H	-0.01586000	2.49688400	-0.56595600
H	-1.43707600	0.52157900	-1.94412800
H	1.43707600	-0.52157900	-1.94412800
C	0.08114900	-1.41403500	-0.55222000
H	-0.03790500	1.28018000	-2.68792200
H	0.03790500	-1.28018000	-2.68792200
H	0.01586000	-2.49688400	-0.56595600
C	0.08114900	0.74782000	0.66273300
C	-0.08114900	-0.74782000	0.66273300
C	0.40318900	1.43362000	1.82292400
H	0.59642300	0.92664300	2.75770900
H	0.50136300	2.51227800	1.80951200
C	-0.40318900	-1.43362000	1.82292400
H	-0.59642300	-0.92664300	2.75770900

H	-0.50136300	-2.51227800	1.80951200
rad4			
C	1.24090200	-0.33714600	-0.00002300
C	1.20929300	1.09394300	-0.00002600
C	0.00000000	1.77705200	-0.00000400
C	-1.20929300	1.09394300	0.00002100
C	-1.24090200	-0.33714600	0.00002500
C	0.00000000	-1.02137100	0.00000200
H	2.14607500	1.63894700	-0.00004500
H	0.00000000	2.86139000	-0.00000700
H	-2.14607500	1.63894800	0.00003700
H	0.00000000	-2.10623400	0.00000400
C	-2.45497500	-1.03358500	0.00005000
C	2.45497500	-1.03358500	-0.00004400
H	-3.40079900	-0.50688100	0.00006500
H	-2.47833400	-2.11596200	0.00005100
H	2.47833400	-2.11596200	-0.00004300
H	3.40079900	-0.50688100	-0.00006400
rad5			
C	-1.42626700	0.00000000	0.00001300
C	-0.69372600	1.20624500	0.00000300
C	0.69372600	1.20624500	-0.00001000
C	1.42626700	0.00000000	-0.00001300
C	0.69372600	-1.20624500	-0.00000300
C	-0.69372600	-1.20624500	0.00001000
H	-1.23002800	2.14884900	0.00000500
H	1.23002800	2.14884900	-0.00001700
H	-1.23002800	-2.14884900	0.00001700
C	-2.86229600	0.00000000	0.00002600
H	-3.41706300	-0.92894800	0.00004500
H	-3.41706300	0.92894800	0.00001700
H	1.23002800	-2.14884900	-0.00000500
C	2.86229600	0.00000000	-0.00002600
H	3.41706300	0.92894800	-0.00003700
H	3.41706300	-0.92894800	-0.00002500
rad6			
C	-0.32499700	0.59476200	0.00000000
H	-1.41283200	0.58892300	0.00000000
C	0.32499700	-0.59476200	0.00000000
H	1.41283200	-0.58892300	0.00000000
C	0.32499700	1.89305100	0.00000000
C	-0.32499700	-1.89305100	0.00000000
H	1.40519500	1.96955600	0.00000000
H	-0.25422100	2.80563800	0.00000000
H	0.25422100	-2.80563800	0.00000000
H	-1.40519500	-1.96955600	0.00000000
rad7			
C	2.89741000	0.79064800	-0.23483200

C	1.47869000	0.75985700	-0.33014800
C	0.74057800	-0.35322700	0.05235600
C	1.42023900	-1.48360400	0.54213700
C	2.81415000	-1.48086000	0.64565000
C	3.54748000	-0.37122100	0.26836300
H	0.96723800	1.62589500	-0.73494700
H	0.85500700	-2.34957500	0.86423100
H	3.32252900	-2.35632600	1.03359900
H	4.62846200	-0.37438800	0.35155300
C	-0.74057700	-0.35322700	-0.05235200
C	-1.42023700	-1.48360400	-0.54213500
C	-1.47869200	0.75985500	0.33015200
C	-2.81414700	-1.48086100	-0.64565300
H	-0.85500400	-2.34957600	-0.86422400
C	-2.89741100	0.79064700	0.23483100
H	-0.96724200	1.62589300	0.73495700
C	-3.54747900	-0.37122200	-0.26836800
H	-3.32252500	-2.35632700	-1.03360400
H	-4.62846000	-0.37438800	-0.35156500
C	3.62798200	1.92320800	-0.63065600
C	-3.62798500	1.92320600	0.63065400
H	3.12858500	2.80266200	-1.01677900
H	4.70797400	1.94295200	-0.55969000
H	-4.70797700	1.94294900	0.55968200
H	-3.12859100	2.80265900	1.01678400

rad8

C	-2.12415500	-0.45896300	-0.05500700
C	-1.67145600	1.04502100	-0.03547900
C	0.20147000	-0.19223600	-0.11229400
N	-0.80292400	-1.09984000	0.25817500
N	-0.21830600	0.99984500	-0.35572900
N	1.52656100	-0.61688200	-0.20794400
O	1.74150200	-1.78741700	-0.67280500
C	2.69017400	0.31307000	0.05746100
C	3.91927400	-0.56706500	0.29374600
H	4.15057600	-1.17225300	-0.58102100
H	4.77031000	0.08198400	0.51085800
H	3.76518400	-1.23777700	1.14117200
C	2.39700900	1.14840800	1.30954000
H	1.56475000	1.83201500	1.15203100
H	2.17196400	0.50171300	2.16146800
H	3.28401000	1.73626200	1.55553600
C	2.88994400	1.20368300	-1.17759100
H	3.76053700	1.84725200	-1.02650600
H	3.06756700	0.58747800	-2.06184400
H	2.01374300	1.82815500	-1.34971400
C	-2.53502500	-0.95886600	-1.44716500
H	-2.62048000	-2.04686400	-1.42186700
H	-3.50059100	-0.54138900	-1.73841300
H	-1.79555800	-0.69097700	-2.20363100
C	-2.38474900	1.92838800	-1.05579300

H	-3.46144900	1.94639800	-0.86612000
H	-2.00555300	2.94892500	-0.97606200
H	-2.21514600	1.58677700	-2.07625900
C	-3.16161200	-0.86787300	0.98029900
H	-4.10217900	-0.34837000	0.78298700
H	-3.33979200	-1.94200600	0.91684200
H	-2.84120700	-0.64087500	1.99605300
C	-1.78606300	1.67644400	1.36179100
H	-1.30525900	2.65608100	1.34791700
H	-2.83096600	1.80809300	1.65081900
H	-1.28829000	1.06553600	2.11756600
O	-0.66504500	-2.26359300	0.72150800

rad9

C	2.10773200	-0.62522900	-0.00449900
C	1.81337000	0.90601100	0.10274300
C	-0.20695300	-0.25342500	-0.19330900
N	0.71661500	-1.18608500	0.16464600
N	0.38125400	0.94771700	-0.37272200
N	-1.53522700	-0.54687200	-0.44242300
O	-1.77145600	-1.53666500	-1.21887600
C	-2.69904200	0.16429900	0.21082300
C	-3.65304200	-0.92937500	0.70648000
H	-3.16124400	-1.56925800	1.44248300
H	-4.51924900	-0.45684100	1.17495000
H	-3.99249900	-1.55245700	-0.11942200
C	-3.36745200	1.04104200	-0.85372800
H	-2.67538800	1.80744500	-1.20326900
H	-3.67913200	0.42696400	-1.70075400
H	-4.25253900	1.52279300	-0.43074700
C	-2.19627100	0.99710200	1.39212400
H	-3.06068300	1.42908600	1.90033300
H	-1.66437200	0.37343600	2.11538800
H	-1.55663500	1.81671300	1.06663700
C	3.02406200	-1.18485400	1.07311300
H	3.12020100	-2.26233400	0.94320900
H	4.01419200	-0.73242300	0.98239700
H	2.64203300	-1.00056600	2.07592200
C	1.80688000	1.43404700	1.54261600
H	2.82184600	1.47858400	1.94054500
H	1.38939000	2.44202300	1.54480900
H	1.20149100	0.80730800	2.19951000
C	2.57807200	-1.06626800	-1.39638900
H	3.59843900	-0.72775500	-1.58385200
H	2.55779300	-2.15593100	-1.44294200
H	1.92818100	-0.67844600	-2.18261900
C	2.67125300	1.79315900	-0.78743600
H	2.35444400	2.83009500	-0.68030300
H	3.71711900	1.71331400	-0.48243100
H	2.58825200	1.52310900	-1.83870900
O	0.49683500	-2.38379100	0.50058200
O	-0.17310300	2.02080200	-0.77206300

rad10

C	1.24724300	-0.34806800	-0.00004400
C	-0.00000100	-1.03991900	-0.00004400
C	-1.24724100	-0.34806600	0.00001600
C	-1.20988100	1.08907100	0.00006000
C	0.00000100	1.77059600	0.00005700
C	1.20988200	1.08907000	0.00000900
H	-0.00000100	-2.12623000	-0.00008900
H	-2.15778800	1.61164500	0.00010200
H	0.00000100	2.85446900	0.00009200
H	2.15779000	1.61164400	0.00001000
N	-2.43683900	-0.94975900	0.00002900
N	2.43683700	-0.94976100	-0.00007600
H	-2.30999300	-1.96549200	-0.00001300
H	2.30999200	-1.96549400	-0.00010400

rad11

C	-1.20942300	0.18687100	-0.11675700
C	0.00001200	-0.50470400	0.00004800
C	1.20943500	0.18688700	0.11685600
C	1.20697000	1.59190300	0.12603600
C	-0.00000400	2.26878800	0.00006100
C	-1.20697000	1.59188800	-0.12592200
H	0.00002000	-1.58249100	0.00004700
H	2.11491200	2.15756500	0.25041600
H	-0.00001400	3.35249800	0.00007100
H	-2.11491400	2.15754900	-0.25028400
N	2.38592300	-0.58951800	0.26632300
N	-2.38589500	-0.58955500	-0.26622400
O	2.25178400	-1.79299900	0.67451300
O	-2.25171500	-1.79307900	-0.67427200
C	3.78318400	-0.12118800	-0.08238700
C	-3.78319500	-0.12118500	0.08229500
C	4.66139300	-1.37067400	-0.22025200
H	4.27503500	-2.03974900	-0.98994700
H	5.66700300	-1.05147100	-0.50342500
H	4.71507400	-1.92700300	0.71343300
C	4.33211000	0.74585400	1.06354900
H	5.37699100	0.99477500	0.86186100
H	3.78543100	1.67934900	1.19264500
H	4.28722800	0.19175500	2.00329200
C	3.77648500	0.61815000	-1.42909900
H	3.34013500	-0.01459000	-2.20502900
H	3.22578500	1.55594700	-1.40892600
H	4.80751800	0.84149300	-1.71235700
C	-3.77665100	0.61816800	1.42900100
H	-3.22593100	1.55595400	1.40889200
H	-4.80771600	0.84153300	1.71213000
H	-3.34041000	-0.01457600	2.20498900
C	-4.66146500	-1.37063800	0.22006800
H	-5.66710200	-1.05139200	0.50309900

H	-4.71504100	-1.92698300	-0.71361300
H	-4.27523600	-2.03971200	0.98982800
C	-4.33195600	0.74585000	-1.06372500
H	-3.78522400	1.67931600	-1.19279500
H	-4.28699700	0.19172100	-2.00344600
H	-5.37684800	0.99482100	-0.86215500

rad12

C	-0.18571300	-0.01455700	0.02369600
C	-0.98375600	-1.21182100	0.02151400
C	-2.42247900	-1.15805600	0.06044600
C	-3.11570700	0.04207400	0.07642500
C	-2.37922900	1.21413500	0.04211400
C	-0.93939500	1.21226800	-0.00243600
H	-4.19946400	0.06228700	0.13522400
C	1.27666800	-0.03529100	0.01961100
C	2.00114100	-1.05505200	-0.61941100
C	2.01736200	0.97371100	0.66702900
C	3.39159500	-1.06057400	-0.61657800
H	1.46664800	-1.84788900	-1.12007400
C	3.40139500	0.94689600	0.67797900
H	1.49449400	1.77894500	1.16086200
C	4.12793600	-0.06609900	0.03348900
H	3.89887700	-1.86302800	-1.13481600
H	3.92659800	1.73760600	1.20065300
C	5.65933200	-0.04590800	0.06464500
C	6.16501900	1.26110900	-0.58296900
H	7.25866900	1.29235800	-0.56823300
H	5.83362700	1.33080700	-1.62223000
H	5.79613900	2.14225800	-0.05424200
C	6.27529000	-1.23022500	-0.69619500
H	7.36550800	-1.17069300	-0.64460700
H	5.97405900	-2.18830500	-0.26501900
H	5.99197700	-1.22379200	-1.75182300
C	6.13920900	-0.11098500	1.53072100
H	5.77003800	0.73516500	2.11371700
H	5.78910500	-1.02803800	2.01153300
H	7.23253300	-0.09716800	1.57198400
C	-2.83229600	2.64861500	0.16036300
C	-1.52239400	3.38518300	-0.34613000
N	-0.41787600	2.43289400	-0.12101400
C	-2.93107900	-2.56661200	0.24745100
C	-1.64227700	-3.37940000	-0.19134200
N	-0.50794900	-2.45787500	0.01038300
C	-4.20255900	-2.88144600	-0.54766400
H	-4.47015600	-3.93721300	-0.44678900
H	-5.04280600	-2.29558300	-0.16437800
H	-4.09374300	-2.65347100	-1.60812700
C	-3.23229600	-2.75519400	1.75348700
H	-4.02184900	-2.06380700	2.05821400
H	-3.57247800	-3.77230000	1.96250400
H	-2.35199600	-2.55052100	2.36550500

C	-1.65652300	-3.69577800	-1.70182200
H	-0.68195500	-4.09068500	-1.99434500
H	-2.41759800	-4.44272100	-1.93888400
H	-1.84943900	-2.79666300	-2.29100100
C	-1.39807300	-4.67432100	0.58367100
H	-2.24569100	-5.35752900	0.47698600
H	-0.50774800	-5.16993300	0.19162300
H	-1.23352300	-4.48520100	1.64424400
C	-4.10620900	2.96877600	-0.62830000
H	-4.96070900	2.43850500	-0.19834700
H	-4.33111000	4.03816700	-0.58195100
H	-4.02680000	2.67887000	-1.67613600
C	-3.09742400	2.92913000	1.65885300
H	-3.39592000	3.96812100	1.81829700
H	-3.90565000	2.28516700	2.01438700
H	-2.21399500	2.72439600	2.26647600
C	-1.21238000	4.70915500	0.35269900
H	-1.03887300	4.57266800	1.42015500
H	-0.30971300	5.14502600	-0.07992800
H	-2.03324900	5.42002500	0.22094500
C	-1.55471400	3.62032300	-1.87082500
H	-2.28978100	4.38452200	-2.13402200
H	-0.57005700	3.95482600	-2.20120800
H	-1.79585500	2.69934900	-2.40585100

rad13

C	-2.42502300	0.26452000	-0.00003700
C	-1.29079300	1.12215800	-0.00003200
C	-2.28386800	-1.12027700	-0.00002200
C	0.00274800	0.54358400	-0.00000800
C	0.17162200	-0.85952300	0.00000700
C	-0.98905600	-1.66805600	0.00000100
C	1.49060500	-1.37110400	0.00002700
H	1.61930400	-2.44687800	0.00003600
C	2.61723300	-0.53110300	0.00003100
C	2.42556300	0.84813200	0.00001100
C	1.12105800	1.41456400	-0.00000600
C	-0.31649900	3.22193800	-0.00003500
H	-0.85949700	-2.74375300	0.00001600
H	3.25349300	1.54195700	0.00001000
C	-3.49252000	-2.06697100	-0.00001600
C	4.01679000	-1.16235200	0.00004800
C	5.13146700	-0.10520000	-0.00007100
H	6.10421500	-0.60288200	-0.00002600
H	5.08514200	0.53260900	-0.88611800
H	5.08515500	0.53279400	0.88584400
C	4.17883300	-2.03743500	-1.26102800
H	5.17397400	-2.49069700	-1.27888600
H	3.44373700	-2.84445100	-1.29367200
H	4.06012600	-1.43729300	-2.16670900
C	4.17889900	-2.03722200	1.26126400
H	4.06021300	-1.43693100	2.16684900

H	3.44382300	-2.84424900	1.29407000
H	5.17405100	-2.49045800	1.27916100
C	-4.82712100	-1.30612700	0.00001700
H	-5.65324300	-2.02122500	0.00000000
H	-4.93427500	-0.67586100	0.88630200
H	-4.93428400	-0.67580300	-0.88622500
C	-3.44133400	-2.95531300	-1.26120000
H	-2.53452900	-3.56288400	-1.29430700
H	-4.29905200	-3.63358200	-1.27849200
H	-3.47010600	-2.34426900	-2.16692700
C	-3.44128300	-2.95534100	1.26114700
H	-3.47003800	-2.34431800	2.16688900
H	-4.29898800	-3.63362600	1.27844900
H	-2.53446300	-3.56289400	1.29421100
N	-1.44631800	2.45818300	-0.00005400
N	0.96313600	2.75026200	-0.00001500
N	-0.41589800	4.56967300	-0.00002400
C	-1.74605900	5.12611700	-0.00004900
H	-1.67325500	6.21387900	-0.00034700
H	-2.32054700	4.79639500	-0.87505100
H	-2.32026800	4.79691500	0.87533900
H	-3.39468300	0.74074700	-0.00005600

rad14

C	-2.52537000	1.46510400	-0.10726300
C	-1.22331900	0.68599200	-0.09810400
C	-1.20469300	-0.71343500	-0.27127500
C	-3.64169300	-0.73759900	0.20450700
C	0.00000000	1.34472200	-0.00564000
C	0.00000000	-1.41044000	-0.36275400
C	1.20469300	-0.71343500	-0.27127500
C	1.22331900	0.68599200	-0.09810400
C	2.52537000	1.46510400	-0.10726400
C	3.64169300	-0.73759900	0.20450800
H	0.00000000	2.42166900	0.10834400
H	0.00000000	-2.48371200	-0.47335800
N	2.41029900	-1.42194100	-0.30324500
N	-2.41029900	-1.42194100	-0.30324500
O	2.43098900	-2.68306400	-0.47782600
O	-2.43098900	-2.68306400	-0.47782600
O	-3.65430600	0.58401700	-0.29711300
O	3.65430700	0.58401700	-0.29711200
C	4.87035900	-1.40689500	-0.38863500
H	5.75570400	-0.88201300	-0.02737800
H	4.91671300	-2.45355800	-0.09573700
H	4.83722200	-1.34148700	-1.47614300
C	3.62736500	-0.82693900	1.73495500
H	3.71563400	-1.87345100	2.03131800
H	4.46987400	-0.26628700	2.14305800
H	2.70019800	-0.43413800	2.15223000
C	2.57999100	2.37546400	-1.34239000
H	1.80113900	3.13887700	-1.29874700

H	3.55376800	2.86758100	-1.38698100
H	2.44353100	1.78343000	-2.24809400
C	2.71895800	2.30367900	1.16597300
H	3.70134800	2.77910500	1.13431300
H	1.95937800	3.08610800	1.22757000
H	2.65149000	1.69775800	2.06788300
C	-2.57999100	2.37546600	-1.34238800
H	-3.55376800	2.86758300	-1.38697700
H	-1.80113900	3.13888000	-1.29874300
H	-2.44353000	1.78343400	-2.24809300
C	-2.71895900	2.30367500	1.16597600
H	-1.95937800	3.08610500	1.22757500
H	-3.70134800	2.77910200	1.13431600
H	-2.65149200	1.69775300	2.06788400
C	-4.87035800	-1.40689500	-0.38863600
H	-4.91671200	-2.45355800	-0.09573900
H	-5.75570400	-0.88201300	-0.02738000
H	-4.83722100	-1.34148700	-1.47614500
C	-3.62736600	-0.82693800	1.73495400
H	-4.46987600	-0.26628700	2.14305600
H	-3.71563400	-1.87345000	2.03131800
H	-2.70020000	-0.43413500	2.15222900

rad15

C	0.01076900	-1.76702200	-0.58589200
C	1.20376100	-1.06215500	-0.70675700
C	1.20805900	0.31396500	-0.98290300
C	0.00953200	1.00931800	-1.12802100
C	-1.19099200	0.30579300	-0.98763900
C	-1.18701800	-1.06424200	-0.71018600
H	0.01161100	-2.83084500	-0.40507600
H	2.15292200	0.81738700	-1.10939700
H	-2.13539600	0.81243900	-1.12003800
N	2.42204100	-1.78367100	-0.59389400
N	-2.40358300	-1.78909700	-0.59424500
C	3.63842400	-1.18074800	-0.16095600
C	4.84418100	-1.66672900	-0.67322500
C	3.65642600	-0.17083300	0.80040200
C	6.04260600	-1.12066600	-0.24244800
H	4.81888100	-2.46991600	-1.39709000
C	4.87127300	0.36336300	1.22166900
H	2.73125700	0.18514100	1.23367300
C	6.09048200	-0.09046800	0.71007300
H	6.96277200	-1.50872000	-0.66207200
H	4.85107700	1.13911500	1.97456500
C	-3.61975700	-1.18798700	-0.15899100
C	-3.63689200	-0.17143800	0.79575800
C	-4.82635500	-1.68136200	-0.66232500
C	-4.85164000	0.36128800	1.21908900
H	-2.71130300	0.19140500	1.22232100
C	-6.02462300	-1.13648900	-0.22951800
H	-4.80167400	-2.48914400	-1.38105600

C	-6.07173800	-0.10016700	0.71633300
H	-4.83040400	1.14219800	1.96661700
H	-6.94535800	-1.53043600	-0.64235200
C	7.44317900	0.47812900	1.15192400
C	8.17831500	1.05645700	-0.07620500
H	9.14822000	1.46513400	0.22180500
H	8.35586100	0.29392000	-0.83727100
H	7.59468300	1.85905900	-0.53458200
C	7.29283400	1.59724600	2.19398000
H	6.80651400	1.23993900	3.10533700
H	8.28092200	1.97203900	2.47206800
H	6.71704900	2.44019000	1.80288600
C	8.29153100	-0.65192800	1.77368200
H	8.47378400	-1.45893200	1.06118400
H	9.26181800	-0.26281100	2.09578500
H	7.78771700	-1.08036600	2.64382500
C	-7.42430000	0.46690300	1.16050700
C	-8.16599000	1.03629500	-0.06787700
H	-8.34392700	0.26911900	-0.82418700
H	-9.13606500	1.44347200	0.23162800
H	-7.58672400	1.83833100	-0.53275900
C	-7.27298000	1.59213200	2.19580400
H	-8.26101200	1.96544700	2.47606300
H	-6.78166000	1.24124700	3.10697100
H	-6.70144000	2.43471000	1.79775800
C	-8.26696500	-0.66208800	1.79185100
H	-7.75837800	-1.08446200	2.66217800
H	-9.23694400	-0.27383800	2.11591000
H	-8.45006500	-1.47341200	1.08449600
C	-0.03534500	2.50770300	-1.45503300
C	-0.75332600	2.71323000	-2.80546400
H	-1.77833400	2.33770600	-2.77964700
H	-0.79184500	3.77754600	-3.05471300
H	-0.22513400	2.19200200	-3.60775200
C	-0.81079000	3.24387400	-0.34178900
H	-0.85384300	4.31546700	-0.55635300
H	-1.83643400	2.87910600	-0.25372600
H	-0.32068900	3.10875000	0.62614900
C	1.36899800	3.12299300	-1.55363000
H	1.92372100	3.02008400	-0.61725900
H	1.95681300	2.66603300	-2.35364400
H	1.28495800	4.18993200	-1.77387300
O	2.43445400	-3.02833900	-0.89536800
O	-2.41359200	-3.03302000	-0.89896600

rad16

C	-0.94770900	3.65939200	-0.33846800
C	-1.02148200	1.19264800	0.12805800
C	-2.42679100	1.21144200	0.09530600
C	-3.09704000	2.56452300	0.23988900
C	-0.28374300	-0.00147800	0.00656500
C	-3.11646700	0.01010400	-0.00311700

C	-2.43603700	-1.19677600	-0.09786100
C	-1.03056600	-1.18910800	-0.12178600
C	-0.97803900	-3.65685900	0.34073100
C	-3.11593400	-2.54448400	-0.24772000
H	-4.19707500	0.01455700	-0.00640200
C	1.20416600	-0.00894200	0.01410300
C	1.92475300	0.52102600	-1.05641000
C	1.90775700	-0.54456400	1.08747100
C	3.31147200	0.51077800	-1.04630400
H	1.39445900	0.93420200	-1.90656900
C	3.29991000	-0.55027400	1.09404900
H	1.36604800	-0.95239100	1.93304600
C	4.03436600	-0.02416100	0.02884800
H	3.83843300	0.92555000	-1.89761400
H	3.80740400	-0.97124300	1.95137500
C	5.56734400	-0.01317700	-0.00250000
C	6.05863700	-0.81641000	-1.22557600
H	5.69068500	-0.39033700	-2.16122200
H	7.15231400	-0.81950600	-1.26396800
H	5.71300000	-1.85189500	-1.17137400
C	6.06541500	1.44373200	-0.11074500
H	5.72289300	2.03310100	0.74362100
H	7.15920300	1.47101500	-0.13234500
H	5.69932900	1.92761100	-1.01860800
C	6.18109500	-0.63777800	1.26012100
H	5.89020300	-0.09369500	2.16241600
H	5.88541200	-1.68347700	1.37801300
H	7.27159500	-0.60684800	1.19067100
N	-0.40104500	2.44130400	0.34239700
N	-0.41888100	-2.44219100	-0.33561300
O	0.70069900	-2.55634300	-0.93319900
O	0.71816200	2.54809100	0.94204100
O	-2.34527600	3.51087200	-0.55726400
O	-2.37580100	-3.49789900	0.55190600
C	-3.15945000	2.97907100	1.71966300
H	-3.54599000	3.99719300	1.80464900
H	-3.82814100	2.30339300	2.25811800
H	-2.18095200	2.92850700	2.19708600
C	-4.49131700	2.61280800	-0.37862700
H	-5.19118800	1.98428300	0.17458100
H	-4.85596800	3.64061000	-0.34597500
H	-4.46080900	2.28748600	-1.41938100
C	-4.51371800	-2.58260400	0.36356500
H	-5.20571300	-1.94771300	-0.19228200
H	-4.88636900	-3.60742000	0.32753200
H	-4.48594700	-2.25901100	1.40493400
C	-3.17386900	-2.95659100	-1.72835300
H	-3.56776000	-3.97161100	-1.81663700
H	-3.83455200	-2.27513000	-2.26940300
H	-2.19253500	-2.91294900	-2.20061300
C	-0.69174600	-4.88959300	-0.51126400
H	0.38020900	-5.06092800	-0.59256300

H	-1.16371400	-5.74668000	-0.02870100
H	-1.10227700	-4.77941900	-1.51379800
C	-0.33781300	-3.76203100	1.72431100
H	-0.73601300	-4.63489300	2.24454300
H	0.74456500	-3.85971800	1.62741500
H	-0.57245900	-2.87063700	2.30813300
C	-0.29883300	3.75792700	-1.71853300
H	-0.68775200	4.63288400	-2.24224700
H	0.78363300	3.84801600	-1.61550300
H	-0.53664600	2.86740300	-2.30243400
C	-0.65662700	4.89098500	0.51361200
H	0.41615300	5.05407700	0.60068300
H	-1.11921400	5.75108600	0.02734100
H	-1.07366200	4.78534400	1.51394500

rad17

C	3.65539400	1.19713400	-0.00003800
C	1.20447300	1.10404100	-0.00001200
C	1.23046500	-0.30130800	-0.00000800
C	2.52441200	-1.10758600	0.00002600
C	3.74943400	-0.19775600	-0.00000700
C	0.00000100	1.80351200	0.00000100
C	0.00000000	-0.95556400	-0.00000900
C	-1.23046500	-0.30130600	-0.00000500
C	-1.20447200	1.10404200	0.00000900
C	-3.65539300	1.19713600	0.00002300
C	-3.74943400	-0.19775500	-0.00000800
C	-2.52441100	-1.10758700	-0.00002000
H	0.00000300	2.88149600	0.00000300
H	-0.00000200	-2.03736300	-0.00001100
C	5.03088100	-0.76100700	-0.00000100
C	6.19853000	-0.00136400	-0.00004400
C	6.05628900	1.39631000	-0.00006800
H	6.93309600	2.03203400	-0.00007500
C	4.81066800	1.99126200	-0.00006600
C	-5.03088000	-0.76100600	-0.00002600
C	-6.19853100	-0.00136300	-0.00002100
C	-6.05628800	1.39630900	0.00002500
H	-6.93309300	2.03203700	0.00005500
C	-4.81066700	1.99126200	0.00004600
N	2.40096600	1.84828500	-0.00003600
N	-2.40096500	1.84828700	0.00003500
O	2.35358400	3.12417400	-0.00006000
O	-2.35358300	3.12417500	0.00006700
C	-7.59686400	-0.62786200	-0.00001200
C	7.59686300	-0.62786100	0.00000700
H	5.10741600	-1.83836000	0.00002500
H	-5.10741300	-1.83835800	-0.00005400
H	4.69409900	3.06530600	-0.00008300
H	-4.69410100	3.06530600	0.00008000
C	7.55036500	-2.16369000	0.00046000
H	7.04445000	-2.55351200	0.88770300

H	7.04390900	-2.55401200	-0.88625700
H	8.56874600	-2.55990100	0.00026800
C	8.36015300	-0.16750100	-1.26045300
H	8.46615700	0.91861800	-1.29406400
H	9.36340400	-0.60334000	-1.27565900
H	7.83603700	-0.48154700	-2.16678400
C	8.36035500	-0.16675200	1.26007000
H	9.36366800	-0.60244900	1.27529600
H	8.46621300	0.91940200	1.29308800
H	7.83646700	-0.48039200	2.16667300
C	-7.55036700	-2.16369100	0.00021800
H	-7.04400000	-2.55388500	-0.88660500
H	-7.04436300	-2.55363800	0.88735500
H	-8.56874800	-2.55990100	0.00007000
C	-8.36031800	-0.16693500	1.26014100
H	-8.46619900	0.91921100	1.29330600
H	-9.36362100	-0.60265600	1.27534900
H	-7.83638800	-0.48068400	2.16668300
C	-8.36019300	-0.16731900	-1.26038200
H	-9.36345300	-0.60313800	-1.27560900
H	-8.46617800	0.91880600	-1.29384100
H	-7.83611700	-0.48125300	-2.16677500
C	2.56058100	-1.99948800	-1.26644600
H	2.53562400	-1.38355200	-2.16745700
H	3.46839500	-2.60499400	-1.28989800
H	1.70437300	-2.67648400	-1.29015000
C	2.56056500	-1.99936600	1.26658900
H	3.46837900	-2.60486900	1.29011000
H	2.53559800	-1.38334200	2.16753900
H	1.70435100	-2.67635300	1.29034500
C	-2.56056700	-1.99940600	-1.26655100
H	-2.53560000	-1.38341100	-2.16752100
H	-1.70435700	-2.67639800	-1.29028800
H	-3.46838100	-2.60491000	-1.29005300
C	-2.56057800	-1.99944400	1.26648500
H	-1.70436700	-2.67643600	1.29021200
H	-2.53562200	-1.38347600	2.16747400
H	-3.46839200	-2.60495000	1.28995800

rad18

C	-3.57219200	-0.12167400	-0.06835400
C	-1.23077200	-0.19806800	-0.01746300
C	-1.21374200	-1.62610700	0.00358900
C	-2.50630800	-2.43435300	0.01125700
C	-3.72683100	-1.52593000	-0.01161100
C	0.00354600	0.52137400	-0.00660200
C	0.01101600	-2.28233800	0.00364100
C	1.23219900	-1.61948700	-0.00108300
C	1.24187100	-0.19112900	0.00991300
C	3.58290700	-0.10266800	0.05972800
C	3.74476200	-1.50642500	0.01212000
C	2.52890200	-2.42117800	-0.00361500

H	0.01397500	-3.36531400	0.00746500
C	-5.01395800	-2.06169900	0.00578900
C	-6.16494400	-1.27032400	-0.03242600
C	-5.99244400	0.12672600	-0.09514800
H	-6.85781900	0.77743300	-0.12968900
C	-4.73444600	0.68646400	-0.11440800
C	5.03460700	-2.03572200	-0.00256400
C	6.18155400	-1.23824800	0.02958900
C	6.00190700	0.15826700	0.08335700
H	6.86394800	0.81362800	0.11302400
C	4.74106600	0.71164600	0.09990600
N	-2.37291900	0.52457000	-0.08192700
N	2.38038900	0.53760800	0.06974100
C	7.59716000	-1.82248800	0.01160700
C	-7.57754000	-1.86171800	-0.01165900
H	-5.12105600	-3.13651300	0.04817900
H	5.14716600	-3.11023600	-0.03788000
H	-4.59158800	1.75917600	-0.16315400
H	4.59274600	1.78390700	0.14169900
C	-7.57157900	-3.39672800	0.05795700
H	-7.07261000	-3.83969800	-0.80793100
H	-7.07859900	-3.75924400	0.96378200
H	-8.60020100	-3.76556000	0.07114000
C	-8.33482500	-1.32545900	1.22266400
H	-8.41338900	-0.23665800	1.20669800
H	-9.34876400	-1.73532400	1.25167400
H	-7.82275200	-1.61149100	2.14502400
C	-8.32472800	-1.43931000	-1.29531400
H	-9.33864000	-1.85026800	-1.29520300
H	-8.40277600	-0.35355100	-1.37851300
H	-7.80555400	-1.80736800	-2.18398200
C	7.59905700	-3.35792600	-0.04798600
H	7.10325100	-3.79781500	0.82128400
H	7.10704200	-3.72886000	-0.95092200
H	8.62955800	-3.72151600	-0.05982800
C	8.35077700	-1.29044100	-1.22678000
H	8.42377600	-0.20117200	-1.21799900
H	9.36678200	-1.69529100	-1.25389200
H	7.83949800	-1.58511600	-2.14685600
C	8.34312200	-1.38785200	1.29188900
H	9.35912600	-1.79361100	1.29369900
H	8.41566600	-0.30118000	1.36790100
H	7.82648900	-1.75271800	2.18335100
C	-2.54477100	-3.30752000	1.29224000
H	-2.52538000	-2.67745500	2.18361300
H	-3.45231800	-3.91378400	1.32006800
H	-1.68653300	-3.98149100	1.32987200
C	-2.54055800	-3.35007500	-1.24016200
H	-3.45200300	-3.95098100	-1.25299700
H	-2.51250900	-2.74993000	-2.15170600
H	-1.68649700	-4.03028100	-1.25020800
C	2.56846300	-3.32773700	1.25429900

H	2.53775300	-2.72125000	2.16155200
H	1.71793700	-4.01226300	1.26964700
H	3.48302800	-3.92378900	1.27094500
C	2.57126600	-3.30325400	-1.27836000
H	1.71640900	-3.98176300	-1.31093300
H	2.54847000	-2.67963700	-2.17417300
H	3.48181500	-3.90516900	-1.30220900
C	-0.00133200	1.99885700	-0.01270200
C	0.71430800	2.72015700	-0.97080500
C	-0.72449700	2.72375200	0.94324900
C	0.69918500	4.11222000	-0.98267300
H	1.28480900	2.18714300	-1.71979100
C	-0.71674600	4.11055900	0.94129000
H	-1.29069700	2.19168400	1.69609300
C	-0.01057300	4.84122600	-0.02492600
H	1.25864700	4.62388800	-1.75415300
H	-1.27885800	4.63125400	1.70782300
C	-0.04115300	6.37371500	0.00370800
C	0.78657200	6.99606000	-1.13148500
H	0.41027900	6.70095800	-2.11434700
H	0.73307800	8.08614500	-1.06855900
H	1.83968000	6.71062800	-1.06683700
C	0.53313300	6.87066200	1.34761900
H	0.51878700	7.96428100	1.38612100
H	-0.04476500	6.49647800	2.19509800
H	1.56609700	6.53586100	1.47301700
C	-1.49948800	6.85866000	-0.14112200
H	-1.92807100	6.51494300	-1.08611800
H	-2.13028200	6.48458100	0.66782700
H	-1.54017200	7.95213600	-0.12238200

rad19

C	-3.52194100	-1.72067700	0.02529100
C	-1.16927600	-1.76511400	0.09924200
C	-1.13383400	-3.19066700	0.04651600
C	-2.41399600	-4.01558300	0.11237000
C	-3.65173600	-3.12856900	0.13041300
C	0.06540200	-1.03594700	0.19991200
C	0.09582700	-3.82632300	-0.02890300
C	1.30793600	-3.15423500	-0.04045600
C	1.31120700	-1.73051400	0.06323700
C	3.65415100	-1.61431000	-0.13183800
C	3.82201800	-3.02246300	-0.16993900
C	2.60920000	-3.94474800	-0.12763500
H	0.11024900	-4.90784200	-0.09064800
C	-4.91737800	-3.69730300	0.23697900
C	-6.08801500	-2.93819400	0.20937100
C	-5.95070700	-1.55342000	0.02618300
H	-6.83463600	-0.93003200	-0.05163100
C	-4.71407700	-0.93607500	-0.07845100
C	5.10138100	-3.56159200	-0.25092200
C	6.25179400	-2.76922400	-0.30141800

C	6.07559400	-1.37874100	-0.27874800
H	6.93796100	-0.72537600	-0.34666300
C	4.82276500	-0.78763600	-0.20314400
N	-2.33004500	-1.05639200	0.06516200
N	2.44768900	-0.98902600	-0.00751100
C	7.66784900	-3.35368600	-0.39347500
C	-7.48847900	-3.55120400	0.34011100
H	-4.98865100	-4.77149100	0.33884700
H	5.20186600	-4.63753200	-0.27540800
C	-7.44908300	-5.07227100	0.55702700
H	-6.99035200	-5.59320700	-0.28760300
H	-6.90238000	-5.33803200	1.46570000
H	-8.46914000	-5.45347500	0.66086600
C	-8.21741100	-2.91804400	1.54441100
H	-8.32570700	-1.83761900	1.43011400
H	-9.21992200	-3.34597300	1.64553300
H	-7.67191200	-3.10485600	2.47335700
C	-8.29568900	-3.26998600	-0.94575700
H	-9.29885800	-3.70083700	-0.86434700
H	-8.40439800	-2.19853400	-1.12682700
H	-7.80532900	-3.71008900	-1.81824600
C	7.67531600	-4.89048100	-0.37726100
H	7.23545600	-5.28863600	0.54105400
H	7.13473700	-5.30937900	-1.23009800
H	8.70628200	-5.25186400	-0.43298200
C	8.33330600	-2.88585900	-1.70553700
H	8.40626600	-1.79748900	-1.75567300
H	9.34617600	-3.29436400	-1.78172100
H	7.76289400	-3.22447100	-2.57464400
C	8.50757200	-2.86080200	0.80408200
H	9.52090600	-3.27149800	0.74882400
H	8.58862200	-1.77198000	0.81994600
H	8.06221000	-3.17900200	1.75060100
C	-2.37280300	-4.88104100	1.39833100
H	-2.32205000	-4.24904100	2.28742300
H	-3.26519300	-5.50729000	1.47208400
H	-1.49914500	-5.53718200	1.39339200
C	-2.49770600	-4.94782400	-1.12298800
H	-3.39934100	-5.56266600	-1.08202000
H	-2.52316300	-4.36551800	-2.04650100
H	-1.63740900	-5.62012400	-1.16559000
C	2.71704500	-4.86439800	1.11906800
H	2.73238100	-4.27102400	2.03578200
H	1.86956000	-5.55205100	1.16997100
H	3.63214000	-5.45949800	1.08135900
C	2.59469400	-4.82420100	-1.40347700
H	1.74632700	-5.51218600	-1.39330000
H	2.52119500	-4.20378200	-2.29925500
H	3.50720900	-5.42036800	-1.47402900
C	0.05072800	0.41508200	0.51967900
C	-0.79674600	1.33931400	-0.10459900
C	0.83402900	0.87498000	1.58721900

C	-0.88655500	2.65113200	0.35940300
H	-1.42183900	1.02977800	-0.92929300
C	0.74339200	2.18067300	2.04107800
H	1.50850000	0.19199000	2.08667100
C	-0.14199900	3.09228400	1.46084600
H	-1.56374400	3.32306300	-0.14835100
H	1.37204800	2.48316100	2.87160800
C	-0.29410500	4.48693100	2.07441000
C	-1.23354700	5.38711500	1.26318700
H	-2.23497000	4.95657600	1.22325000
H	-1.31229500	6.36803300	1.74040300
H	-0.89642600	5.53660700	0.23482200
C	1.09408700	5.15389300	2.20295500
H	1.00989800	6.14604700	2.65684600
H	1.74726000	4.55893100	2.84979400
H	1.59533200	5.25231400	1.23775600
C	-0.91089200	4.33901900	3.48661200
H	-1.89257400	3.86193200	3.43015200
H	-0.27382100	3.72610100	4.12724400
H	-1.03270800	5.31891200	3.96270300
C	-4.67253100	0.52276300	-0.36073000
C	-4.05237800	0.98452400	-1.52526800
C	-5.30866800	1.45909100	0.45048700
C	-4.08837600	2.33053800	-1.87111200
H	-3.54404700	0.28101900	-2.17664900
C	-5.34150000	2.80974700	0.09953500
H	-5.79482200	1.13647100	1.36475200
C	-4.73981400	3.28070000	-1.07132600
H	-3.61426000	2.63262900	-2.79747500
H	-5.85706100	3.49209700	0.76262800
C	4.73243100	0.69248100	-0.21532700
C	5.55298100	1.47158400	0.60746600
C	3.86680100	1.35665500	-1.08564300
C	5.51904000	2.86191000	0.54305900
H	6.22193400	0.98786000	1.31126100
C	3.84311100	2.74574700	-1.15320500
H	3.20219800	0.78012400	-1.72002000
C	4.67698000	3.53160500	-0.35182900
H	6.15966400	3.42436200	1.21299800
H	3.16184900	3.21168200	-1.85601200
C	-4.84313900	4.74379000	-1.53241500
C	-3.47849000	5.27216800	-2.01500800
H	-3.10876500	4.70741100	-2.87339700
H	-3.58168800	6.31626700	-2.32982800
H	-2.71399300	5.23429700	-1.23730000
C	-5.83529100	4.82064400	-2.71529800
H	-6.82540800	4.46209300	-2.41995000
H	-5.93613400	5.85411300	-3.06211400
H	-5.49739000	4.21454900	-3.55921800
C	-5.36287400	5.67294700	-0.42341100
H	-4.73338000	5.63843700	0.46744900
H	-5.37054200	6.70598200	-0.78323800

H	-6.38503400	5.42039500	-0.13058600
C	5.97478400	5.56140800	-1.04125100
H	6.12017800	5.14522500	-2.04123200
H	5.97100300	6.65326300	-1.12488000
H	6.83181100	5.27191500	-0.42972500
C	3.48709600	5.54000500	-1.29887600
H	2.52884200	5.22922500	-0.88267300
H	3.49584800	6.63438200	-1.34793500
H	3.54963900	5.15774400	-2.31989200
C	4.64995600	5.06098900	-0.42441700
C	4.48205300	5.67700200	0.97756400
H	4.47276400	6.76898900	0.90732700
H	3.54336300	5.36713700	1.43929200
H	5.30148900	5.38757800	1.64330200

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C	0.36455800	-3.13213700	-1.51008100
C	1.17058100	-2.03249400	-1.20896900
C	2.57184900	-2.11723700	-1.13285900
C	3.15573400	-3.38628700	-1.33441700
C	2.36334900	-4.48978000	-1.62580200
C	0.97646500	-4.37340600	-1.72356100
C	-1.09717400	-2.91641300	-1.63267000
C	-1.72992700	-2.03752200	-0.75437700
C	-3.07439400	-1.64201400	-0.90925500
C	-3.80197200	-2.23809800	-1.96547000
C	-3.19718000	-3.15835800	-2.80926400
C	-1.85044700	-3.49507800	-2.66218100
H	0.70253500	-1.07148900	-1.05053600
H	4.23266200	-3.49122200	-1.29243300
H	2.83208900	-5.45351200	-1.79186700
H	0.37223100	-5.24500000	-1.94849900
H	-1.16610600	-1.64553200	0.07964600
H	-4.83039600	-1.94752700	-2.13763800
H	-3.77049100	-3.59340300	-3.62064100
H	-1.37977800	-4.17102400	-3.36700500
C	3.37308700	-0.91910100	-0.88461200
C	-3.64407300	-0.63196900	-0.03211200
C	4.60443900	-1.01882000	-0.11379700
C	5.72353400	-0.20193800	-0.38780800
C	4.74125800	-1.94197900	0.94203600
C	6.89046100	-0.30672900	0.34961900
H	5.67450200	0.50363700	-1.20776100
C	5.91419200	-2.03305200	1.68154800
H	3.90354100	-2.57885400	1.19810600
C	7.02078200	-1.22081500	1.40775900
H	7.72448000	0.33374400	0.08623200
H	5.95142900	-2.74978900	2.49110500
C	-5.07274900	-0.59301900	0.25524400
C	-5.85687300	-1.76004400	0.33756700
C	-5.73865500	0.63259300	0.47740500
C	-7.21589300	-1.70474900	0.62417400

H	-5.38544300	-2.72548200	0.20433000
C	-7.09415300	0.67735500	0.75534100
H	-5.17744400	1.55655500	0.40980700
C	-7.87331600	-0.48830700	0.83900000
H	-7.76056500	-2.63722800	0.69077500
H	-7.55792500	1.64605900	0.90146900
C	-2.74805400	0.33580800	0.60157700
C	-1.61680100	0.86026500	-0.05991500
C	-2.93372200	0.72844300	1.93862700
C	-0.69526400	1.65822700	0.59817100
H	-1.45980200	0.62462800	-1.10586900
C	-2.01212000	1.53847100	2.59148600
H	-3.79438200	0.35976000	2.48355700
C	-0.85563100	1.99992600	1.95348100
H	0.16680500	2.00933300	0.04324300
H	-2.19548900	1.78144600	3.62990500
C	2.93137800	0.36700900	-1.41256600
C	2.20465100	0.46515500	-2.61757400
C	3.20006100	1.58417600	-0.74725300
C	1.76138600	1.68556000	-3.10838400
H	1.99587600	-0.43347700	-3.18342100
C	2.75179400	2.79825600	-1.24425500
H	3.74818700	1.56470100	0.18584500
C	2.01387700	2.88741800	-2.43581500
H	1.20920100	1.68712400	-4.03835500
H	2.97351100	3.69672400	-0.68020400
C	0.22946300	2.79227700	2.68992300
C	0.54949200	4.09595500	1.93149300
H	1.31940900	4.66361400	2.46290600
H	0.92010000	3.88805600	0.92792200
H	-0.33971600	4.72588900	1.84093600
C	1.49982200	1.91885400	2.76415700
H	1.84957800	1.64809100	1.76715200
H	2.30469600	2.45566700	3.27734400
H	1.30036100	0.99397700	3.31195000
C	-0.19179000	3.15987700	4.12068800
H	0.61098700	3.72335700	4.60353700
H	-1.09006500	3.78322100	4.12687800
H	-0.38304500	2.27292600	4.72990800
C	1.54065900	4.24834200	-2.95734500
C	2.77558800	5.13311900	-3.23539000
H	3.41849200	4.67563900	-3.99219100
H	2.46452600	6.11782300	-3.59869200
H	3.37134600	5.27892600	-2.33142000
C	0.72935000	4.12088300	-4.25706100
H	-0.15726300	3.49626600	-4.11782500
H	0.39358600	5.11125000	-4.57473800
H	1.32435300	3.69852800	-5.07062900
C	0.64849300	4.93285400	-1.89920100
H	1.19258700	5.12749600	-0.97206400
H	0.28830900	5.89381100	-2.27792400
H	-0.21840800	4.31300500	-1.65733200

C	8.33217800	-1.29465800	2.19666500
C	9.48513500	-1.65983100	1.23670700
H	9.59795300	-0.91931100	0.44185600
H	10.43147700	-1.71228400	1.78386000
H	9.30482800	-2.63104700	0.76844800
C	8.28365000	-2.34877700	3.31375600
H	9.23895100	-2.36327100	3.84511200
H	7.50098200	-2.12769600	4.04422300
H	8.11000100	-3.35187700	2.91524200
C	8.61740700	0.07957000	2.84000400
H	7.81256500	0.35971400	3.52478900
H	9.55396200	0.04632300	3.40521600
H	8.70747600	0.86573100	2.08714700
C	-9.37116500	-0.38848700	1.14781600
C	-10.05926800	0.45936400	0.05625400
H	-11.13079300	0.54546200	0.26197100
H	-9.64378800	1.46851500	0.00945000
H	-9.93416200	-0.00189400	-0.92695900
C	-9.56871800	0.28759600	2.52181100
H	-10.63509800	0.36764000	2.75458700
H	-9.08754900	-0.29536900	3.31159200
H	-9.14514900	1.29389000	2.54133900
C	-10.05109200	-1.76594000	1.18842800
H	-9.97001100	-2.28536300	0.22986300
H	-9.62152100	-2.40533300	1.96423900
H	-11.11462800	-1.64341900	1.41006300

rad21

C	0.54496100	1.14321700	-0.25366900
C	-0.55523800	0.29294300	-0.08488500
C	-1.87400300	0.75434700	-0.18413300
C	-2.08234300	2.11472000	-0.46197000
C	-1.00167000	2.97192900	-0.63315100
C	0.30087300	2.49784000	-0.53056400
H	-0.38123300	-0.74055400	0.19049800
H	-3.09216300	2.49187900	-0.57673100
H	-1.17642100	4.01694900	-0.86738500
H	1.13368600	3.17122200	-0.69834900
C	-3.01027000	-0.16427100	0.00823600
C	-4.20389700	0.26826700	0.62214800
C	-2.94322800	-1.50778800	-0.41534300
C	-5.26823700	-0.58617400	0.80735400
H	-4.27255400	1.28765300	0.98604800
C	-4.00211200	-2.37106000	-0.24105000
H	-2.04916400	-1.85973600	-0.91845800
C	-5.21267300	-1.94570500	0.38099100
H	-6.16867200	-0.22826400	1.29669100
H	-3.92610400	-3.39595200	-0.59055600
C	1.92057500	0.62850700	-0.13319700
C	2.95089200	1.41850800	0.41733500
C	2.25424400	-0.67211600	-0.56446800
C	4.23781000	0.94199800	0.53556000

H	2.71696300	2.41129100	0.78605600
C	3.53814900	-1.15881500	-0.45693700
H	1.48892300	-1.29081100	-1.02036500
C	4.58718800	-0.37030000	0.10080600
H	5.00659000	1.56817700	0.97738300
H	3.76765600	-2.15900900	-0.81087200
C	5.89135300	-0.85888000	0.21553200
H	6.68259400	-0.25385100	0.64146700
C	-6.28981200	-2.81700000	0.56346100
H	-6.23990100	-3.84837900	0.23589900
H	-7.20576300	-2.48629700	1.03801100
H	6.14881900	-1.85698400	-0.11770300

rad22

C	1.55895000	-1.41458100	2.35147500
C	1.69413900	-0.84065100	1.06956900
C	0.58726000	-0.20957300	0.46351200
C	-0.64141100	-0.12370200	1.14996300
C	-0.77636300	-0.70225600	2.42807900
C	0.32689800	-1.33503100	2.99529200
H	0.23142200	-1.75572100	3.99270700
C	-1.77716800	0.61474500	0.54636600
C	3.00550600	-0.87119200	0.37981800
C	0.69770500	0.32938700	-0.94352000
H	1.43784500	-0.22626300	-1.51898700
H	-0.25988400	0.26547300	-1.46070500
H	1.00138700	1.37963900	-0.95491800
C	-2.06646300	-0.61252000	3.20320000
H	-2.49283500	0.39234900	3.15864200
H	-2.82559900	-1.29009100	2.80231200
H	-1.90739800	-0.87070600	4.25196200
C	2.72176400	-2.06989200	3.05327600
H	2.93652000	-3.05998500	2.64153000
H	3.63746500	-1.48402000	2.94694800
H	2.51308400	-2.18850300	4.11832000
C	3.63628400	0.38822500	0.05298900
C	4.54440200	0.53784700	-1.01653900
C	3.30590000	1.56448500	0.76635300
C	5.09009200	1.77269300	-1.33911500
H	4.78666500	-0.32019500	-1.63136800
C	3.85775500	2.78813300	0.43731200
H	2.60733000	1.49758400	1.59187300
C	4.76853600	2.93146200	-0.62289800
H	5.76794300	1.82551800	-2.18178700
H	3.57085000	3.65592300	1.02150100
C	3.59049700	-2.15430300	0.05546900
C	4.98582000	-2.36452200	-0.03161500
C	2.77067100	-3.28462800	-0.13892300
C	5.50852000	-3.61491900	-0.30757000
H	5.65973000	-1.53945100	0.16438300
C	3.30619000	-4.53320200	-0.42376800
H	1.69494500	-3.16736600	-0.07310700

C	4.68775300	-4.73552900	-0.51936400
H	6.58715300	-3.72430300	-0.34496400
H	2.62341800	-5.35967100	-0.57551600
C	-1.60322800	2.02963400	0.29761800
C	-2.29022800	2.72395200	-0.71974000
C	-0.66142600	2.77598300	1.04357700
C	-2.05983200	4.07141800	-0.96239300
H	-2.97899200	2.18487200	-1.35863000
C	-0.44636100	4.11914400	0.79806300
H	-0.10643300	2.28052700	1.83137200
C	-1.13852900	4.80977100	-0.21059000
H	-2.60490800	4.54391500	-1.76983200
H	0.27900400	4.64454700	1.41002900
C	-2.99070700	-0.10330000	0.23298700
C	-4.26377200	0.51233800	0.19557300
C	-2.95779400	-1.49389800	-0.00204400
C	-5.40722800	-0.21720900	-0.07347800
H	-4.34995700	1.56735300	0.42494300
C	-4.11152500	-2.21406800	-0.27829500
H	-2.00247800	-2.00563100	0.02473800
C	-5.36806500	-1.59918000	-0.32546700
H	-6.35992300	0.30168300	-0.07285700
H	-4.01882900	-3.27702500	-0.46213200
C	5.34725600	4.30931300	-0.95560700
C	6.32211000	4.26298000	-2.14112500
C	4.19611800	5.27124100	-1.31351900
C	6.10632300	4.85555200	0.27146000
H	7.17622000	3.61090400	-1.94098400
H	5.83474100	3.91570700	-3.05571400
H	6.71262500	5.26461300	-2.33794500
H	3.49180500	5.38534400	-0.48834500
H	4.58609800	6.26398200	-1.55782100
H	3.63514400	4.90396200	-2.17654500
H	6.52584400	5.84238900	0.05387200
H	5.45337400	4.95685300	1.14077600
H	6.92805600	4.19050500	0.54909700
C	5.31616500	-6.09796500	-0.82541700
C	6.21922900	-6.52052800	0.35209600
C	4.26062300	-7.19301200	-1.03746200
C	6.16559400	-5.99282100	-2.10905000
H	7.02323000	-5.80231900	0.52547800
H	5.64114200	-6.60149200	1.27615400
H	6.67917000	-7.49300200	0.15225400
H	3.59940500	-6.96376300	-1.87705100
H	4.75305900	-8.14361500	-1.25724200
H	3.64330600	-7.34168500	-0.14783900
H	6.62400100	-6.95789800	-2.34495800
H	5.54917800	-5.69229500	-2.96012500
H	6.96881100	-5.26034100	-2.00593500
C	-0.86914000	6.29899800	-0.44322600
C	0.63025400	6.51167700	-0.73353900
C	-1.67096200	6.85976500	-1.62666400

C	-1.26001500	7.08783400	0.82399500
H	1.25422400	6.19075300	0.10245100
H	0.94307500	5.94669700	-1.61471800
H	0.83996600	7.57005100	-0.91469700
H	-2.74870000	6.77520900	-1.46591700
H	-1.44213000	7.92022900	-1.75897400
H	-1.42447500	6.35067000	-2.56199800
H	-1.07078300	8.15654100	0.68446200
H	-2.32088200	6.95726100	1.05226600
H	-0.69028600	6.75941600	1.69592400
C	-6.66317300	-2.36043300	-0.62161700
C	-6.41685900	-3.85499800	-0.87425700
C	-7.62160800	-2.22665700	0.58015300
C	-7.33132800	-1.76308300	-1.87742800
H	-5.76121100	-4.02000500	-1.73305900
H	-5.97171500	-4.34699700	-0.00568200
H	-7.36534100	-4.35568300	-1.08431600
H	-7.87597000	-1.18437800	0.78321800
H	-8.55443000	-2.76516000	0.38771500
H	-7.17056800	-2.64096100	1.48543900
H	-8.26101000	-2.29304100	-2.10550100
H	-7.57518100	-0.70709600	-1.74420200
H	-6.67188100	-1.84476100	-2.74522500

rad23

C	-1.19541800	-1.84319400	-0.44095200
C	-1.04176400	-0.54594400	0.12869900
C	-2.14898000	0.02452000	0.82130800
C	-3.34549300	-0.61694300	0.96432300
C	-3.50340400	-1.96422200	0.36794500
C	-2.35469500	-2.55904200	-0.35506500
H	-0.35979100	-2.23806700	-0.99900100
H	-1.99747100	0.98848000	1.28328800
C	0.20140400	0.17108000	0.00745500
C	1.44546200	-0.55063500	-0.06575300
C	1.60041100	-1.80710400	0.58869300
C	2.55242600	-0.02569400	-0.79385700
C	2.76025500	-2.52599400	0.55013500
H	0.76519200	-2.16485600	1.17181400
C	3.74943600	-0.67425300	-0.89452800
H	2.40011600	0.90603800	-1.31757100
C	3.90789000	-1.97993800	-0.21186900
C	0.20008100	1.61071600	-0.03998900
C	1.29673000	2.35929900	0.47736200
C	-0.89856200	2.32152200	-0.60429400
C	1.33825500	3.72377100	0.45946800
H	2.09829200	1.80295500	0.93945100
C	-0.94512100	3.68425300	-0.67139900
H	-1.69808400	1.73448100	-1.03061600
C	0.19482800	4.46010600	-0.12888800
O	0.19189500	5.69904500	-0.16629900
C	2.52179600	4.50339700	1.03345200

C	2.04375600	5.42696500	2.17544800
C	3.60029000	3.56668900	1.60244100
C	3.17292100	5.34592400	-0.08724800
H	1.32630100	6.16095300	1.81657000
H	1.57759600	4.84437900	2.97533400
H	2.89886400	5.95759700	2.60378700
H	4.01044700	2.89620100	0.84220100
H	4.42861500	4.16469300	1.98834900
H	3.22575000	2.95821900	2.43003700
H	4.04415400	5.87555300	0.30849700
H	3.51514400	4.70542500	-0.90552400
H	2.47549900	6.07789300	-0.48751100
C	-2.13191500	4.42228100	-1.29187200
C	-2.78813800	5.32664500	-0.22359400
C	-1.65799200	5.27857500	-2.48680500
C	-3.20513600	3.44791600	-1.80476600
H	-3.12855100	4.73399200	0.63069800
H	-2.09438900	6.08403700	0.13341300
H	-3.66119200	5.82813300	-0.65076800
H	-1.18945400	4.65162700	-3.25096000
H	-2.51557100	5.77899100	-2.94550000
H	-0.94382100	6.03588200	-2.17266300
H	-4.03554800	4.01764900	-2.22723100
H	-2.82622800	2.79244600	-2.59358500
H	-3.61367200	2.82249800	-1.00622100
C	4.91737700	-0.09479600	-1.69343400
C	5.31501900	-1.06407300	-2.82848200
C	4.55792100	1.25760400	-2.33066700
C	6.12092400	0.13369000	-0.75064800
H	5.64674200	-2.02127800	-2.43350200
H	4.47153400	-1.23758800	-3.50297800
H	6.12881600	-0.63017900	-3.41648000
H	4.29042300	2.01012100	-1.58372800
H	5.42264100	1.63780300	-2.87873100
H	3.73296800	1.17358700	-3.04328500
H	6.94644600	0.58405000	-1.30911700
H	5.85431800	0.81785700	0.06037900
H	6.46635600	-0.80157700	-0.31673800
C	2.90414000	-3.86607500	1.27227200
C	4.04407800	-3.78862600	2.31162900
C	1.61451800	-4.25635000	2.01308900
C	3.20835700	-4.97502100	0.23909800
H	4.99991300	-3.58226400	1.83622200
H	3.84382100	-3.00552400	3.04862800
H	4.12063100	-4.73922000	2.84711800
H	0.76227400	-4.36066700	1.33594400
H	1.75942900	-5.22163400	2.50287400
H	1.34860800	-3.53441000	2.78997200
H	3.27495800	-5.94234500	0.74511400
H	2.40926100	-5.04211900	-0.50510700
H	4.14777600	-4.78857900	-0.27581400
O	4.97772100	-2.60238600	-0.27709100

O	-4.57385100	-2.58045000	0.47125600
C	-4.51394700	0.01301900	1.72327900
C	-4.91376500	-0.88116900	2.91758600
C	-4.15432100	1.40326400	2.27299300
C	-5.71601100	0.18125300	0.76600400
H	-5.24529300	-1.86164900	2.58440600
H	-4.07142000	-1.01110800	3.60322100
H	-5.72831100	-0.41007800	3.47510500
H	-3.88622800	2.10651100	1.47970400
H	-5.01908000	1.81800700	2.79533200
H	-3.32966900	1.36444200	2.98984000
H	-6.54208300	0.66696700	1.29314400
H	-5.44766000	0.81181300	-0.08682000
H	-6.06144500	-0.77972600	0.39242000
C	-2.49771400	-3.94378800	-0.98760900
C	-3.63389700	-3.93309600	-2.03397900
C	-1.20602900	-4.38344200	-1.69646900
C	-2.80729600	-4.98231500	0.11479500
H	-4.59107500	-3.69482800	-1.57646200
H	-3.42986100	-3.20009000	-2.81984800
H	-3.71007600	-4.91656000	-2.50647600
H	-0.35613600	-4.44260600	-1.01096000
H	-1.35002800	-5.37922000	-2.12115300
H	-0.93704200	-3.71529000	-2.51904800
H	-2.87316900	-5.98055600	-0.32719300
H	-2.01110700	-5.00143500	0.86487900
H	-3.74841000	-4.76165600	0.61273900

rad24

C	-3.22051400	-1.27340300	0.45734700
C	-3.07367400	-1.59398700	-0.94779400
C	-2.57141100	-2.85085300	-1.36335300
C	-3.35088200	-0.66505600	-1.97438400
C	-2.34386800	-3.13518100	-2.69676800
H	-2.36206900	-3.60591100	-0.61548000
C	-3.11520600	-0.96102600	-3.31002000
H	-3.71675200	0.31965000	-1.71680800
C	-2.59684500	-2.19693500	-3.71186000
H	-1.95643300	-4.11504900	-2.95434300
H	-3.32739500	-0.19498200	-4.04509900
C	-4.07598500	-0.18687700	0.90314100
C	-3.69374800	0.62658200	1.99114300
C	-5.29539100	0.12849500	0.27558900
C	-4.46401600	1.70380700	2.38946300
H	-2.75772500	0.41993900	2.49714800
C	-6.06570200	1.20843500	0.68781900
H	-5.64981200	-0.49655100	-0.53574300
C	-5.66706300	2.03396000	1.74485200
H	-4.10982400	2.31343400	3.21368300
H	-6.99696500	1.39925200	0.16959500
C	-2.34063000	-1.93670300	1.43379000
C	-2.78955200	-2.45350200	2.67240000

C	-0.97547800	-2.03313000	1.13979400
C	-1.84482300	-2.99884200	3.54010700
C	-0.03592800	-2.58488300	2.01210900
H	-0.62632100	-1.63722400	0.19461800
C	-0.47637900	-3.06783000	3.25482800
H	-2.18952400	-3.38769500	4.49541600
C	-2.29061800	-2.54204800	-5.17109400
C	-0.78482000	-2.84892600	-5.31202300
C	-3.10788100	-3.78151100	-5.58993900
C	-2.63746300	-1.39159600	-6.12737600
H	-0.18264400	-1.98557600	-5.01761000
H	-0.48258600	-3.69231900	-4.68781500
H	-0.53982400	-3.09702800	-6.34909700
H	-4.18008600	-3.59053000	-5.49744300
H	-2.89776900	-4.04402500	-6.63105800
H	-2.87124600	-4.65187400	-4.97454300
H	-2.40412300	-1.68208500	-7.15474900
H	-3.70014600	-1.13820300	-6.09124300
H	-2.06341400	-0.48874600	-5.90394300
C	-6.46873400	3.25581500	2.20179400
C	-5.59991200	4.52008100	2.03333200
C	-7.75684700	3.44675200	1.38813500
C	-6.85538200	3.09397000	3.68625600
H	-4.68604100	4.46662100	2.62844100
H	-5.30679900	4.65441900	0.98896000
H	-6.15234700	5.40999400	2.34954100
H	-8.42949200	2.59049200	1.48351800
H	-8.29422600	4.32790900	1.74753200
H	-7.54863400	3.60029800	0.32618700
H	-7.42767700	3.96096200	4.02954700
H	-7.46935000	2.20174500	3.83344600
H	-5.97671000	3.00184600	4.32783000
C	0.47279600	-3.62086500	4.28608600
H	0.18834100	-3.29705100	5.29024500
H	0.47025400	-4.71567300	4.28932600
H	1.49763600	-3.29580500	4.10300200
C	-4.24577700	-2.45207900	3.06199300
H	-4.44419000	-3.21540300	3.81723200
H	-4.55576000	-1.48699400	3.47306700
H	-4.89021500	-2.64458800	2.20214400
C	1.37916700	-2.54908200	1.54686300
C	2.16112300	-3.68946300	1.29129400
C	1.88148400	-1.30400700	1.17839600
C	3.40030400	-3.50797700	0.66803200
C	3.10068200	-1.12057000	0.50789600
H	1.27530500	-0.43131700	1.38474800
C	3.88889000	-2.26977600	0.25129500
H	3.98847600	-4.39248500	0.43590900
C	1.68047400	-5.08389800	1.59837800
H	2.01828600	-5.41829700	2.58461400
H	0.59097000	-5.14413900	1.59264100
H	2.06535300	-5.79908200	0.86793700

C	5.17612000	-2.21679700	-0.53185600
H	6.02593600	-1.92563500	0.09147500
H	5.40085400	-3.19331700	-0.96579200
H	5.12342300	-1.48597500	-1.34075600
C	3.42395300	0.23164100	0.03464000
C	4.74902900	0.78805700	0.21669300
C	5.28990600	1.74900400	-0.66017500
C	5.56829500	0.37933900	1.29159900
C	6.56789200	2.26065600	-0.47712200
H	4.70531800	2.07255300	-1.51359600
C	6.83679500	0.90115000	1.46940600
H	5.18036400	-0.34464400	1.99961100
C	7.37699400	1.85446200	0.59031500
H	6.93544800	2.98471400	-1.19333800
H	7.41934700	0.56223400	2.31946200
C	2.33074400	1.02744500	-0.50623200
C	1.23631700	0.41598100	-1.16176100
C	2.24815700	2.42125600	-0.31991300
C	0.11770200	1.13673300	-1.53773500
H	1.26944700	-0.64862900	-1.35975500
C	1.12388300	3.13951500	-0.70898100
H	3.05323300	2.93622900	0.19069200
C	0.01973000	2.51914100	-1.30487200
H	-0.70221600	0.60310000	-2.00456100
H	1.10587700	4.20351500	-0.50846700
C	8.78957400	2.39771500	0.82473300
C	8.84993100	3.08701000	2.20376800
C	9.79842300	1.23090600	0.79192500
C	9.20581500	3.42150700	-0.24148300
H	8.14212600	3.91829800	2.25447800
H	8.60872800	2.39609400	3.01417200
H	9.85292900	3.48223600	2.39097600
H	9.77364500	0.72235500	-0.17524700
H	10.81556200	1.59887700	0.95703000
H	9.58504500	0.48789300	1.56309600
H	10.21709400	3.78063600	-0.03450400
H	9.21091000	2.98613300	-1.24402400
H	8.54416900	4.29142400	-0.25086700
C	-1.28069700	3.26477800	-1.61859200
C	-2.33133900	2.85253100	-0.56520800
C	-1.10709200	4.79025800	-1.56475000
C	-1.79078700	2.89372500	-3.02544700
H	-2.48422800	1.77396300	-0.54993900
H	-2.01413800	3.14643400	0.43804200
H	-3.29696400	3.32705300	-0.76584200
H	-0.33490500	5.13470500	-2.25809000
H	-2.04513000	5.27891500	-1.84067200
H	-0.84562700	5.13886400	-0.56292300
H	-2.71493700	3.43591200	-3.24612200
H	-1.05451300	3.15432400	-3.79047000
H	-2.00622700	1.82889800	-3.11847400

rad25

C	2.42637500	-0.74955900	-0.01868000
H	2.31888900	-1.82963000	-0.02897100
C	1.33792600	0.06035700	-0.00409800
H	1.48491300	1.13425500	0.00974900
C	-0.00343900	-0.44394600	-0.00200900
H	-0.13597000	-1.52471900	-0.01492100
C	-1.10408400	0.34906800	0.01437200
H	-0.97166800	1.42983900	0.02813100
C	-2.44533700	-0.15555800	0.01387900
H	-2.59188900	-1.22953800	0.00125200
C	-3.53415300	0.65374100	0.03234300
H	-3.42727100	1.73380300	0.04900100
C	3.78346000	-0.31323600	-0.01973800
C	5.74714900	0.98575800	-0.21989500
C	6.13765600	-0.47121100	0.17560600
C	-4.89093700	0.21637300	0.03451200
C	-6.85552700	-1.07904200	-0.17896900
C	-7.24306500	0.36684600	0.25784400
N	4.25639300	0.95539900	0.00161500
N	4.83204500	-1.18327900	-0.04509600
N	-5.36266500	-1.05286300	0.02816300
N	-5.94034100	1.08570800	0.04211900
C	7.22077800	-1.11406000	-0.67989100
H	8.16845500	-0.58784100	-0.54496100
H	7.35275700	-2.15069200	-0.37244000
H	6.96622800	-1.11105100	-1.73851100
C	6.46725500	-0.64475400	1.66392000
H	6.51846200	-1.71104400	1.88633200
H	7.42900400	-0.19096200	1.90872600
H	5.70029700	-0.20163000	2.30131200
C	5.94425200	1.30016400	-1.70806100
H	5.45515900	2.24898500	-1.93052600
H	7.00385000	1.38785000	-1.95389800
H	5.50111800	0.53247600	-2.34463700
C	6.36461800	2.08353800	0.63514300
H	7.44837600	2.10063700	0.49939400
H	5.96118300	3.04742300	0.32777500
H	6.14630000	1.95401400	1.69395700
C	-7.46351000	-2.19913900	0.65360900
H	-8.54858000	-2.21369000	0.52843400
H	-7.06260900	-3.15437500	0.31729200
H	-7.23453800	-2.09689700	1.71315700
C	-7.06721700	-1.35540000	-1.67272900
H	-6.57922800	-2.29749600	-1.92430500
H	-8.12908300	-1.43838300	-1.91025800
H	-6.63133100	-0.57104600	-2.29379900
C	-7.55744200	0.50173200	1.75345500
H	-7.60727500	1.56190100	2.00367400
H	-8.51620000	0.04068800	1.99645300
H	-6.78353400	0.04327900	2.37129100
C	-8.33543300	1.03028600	-0.56967000

H	-9.28114800	0.49952300	-0.43883300
H	-8.46538200	2.05842200	-0.23410900
H	-8.09166400	1.05507800	-1.63054300
O	4.75134700	-2.44886800	-0.05703500
O	3.56965800	2.02574800	0.01200200
O	-4.67505200	-2.12242900	0.00407100
O	-5.86065400	2.35124900	0.06257800

Polyradicals

High-Spin State

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C	-1.29801000	-0.70577500	0.47863700
C	-2.39561100	-1.45925800	0.06596200
C	-3.66940400	-0.93367300	0.24641800
C	-3.85020700	0.30574800	0.87089100
C	-2.75534100	1.05187100	1.30736600
C	-1.47504400	0.53073500	1.10253200
H	-2.25641500	-2.43660000	-0.37123300
H	-4.85474500	0.65607500	1.04520200
H	-0.60707500	1.06788700	1.45779300
N	0.00223600	-1.25022500	0.28444600
C	1.15773900	-0.43471800	0.11527800
C	1.07485100	0.80476100	-0.53311800
C	2.37960100	-0.93058900	0.55379500
C	2.21195200	1.58815100	-0.71355000
H	0.11585300	1.13562800	-0.90125100
C	3.52260300	-0.15883000	0.35612800
H	2.43910500	-1.89170700	1.04212600
C	3.43654500	1.09475000	-0.24622200
H	4.33106500	1.69462700	-0.33030300
N	4.77231700	-0.65926000	0.84936000
N	-4.79189300	-1.72273300	-0.16672500
C	-5.70392300	-1.31118100	-1.30366800
C	-5.94055100	0.19833200	-1.35045100
C	-5.01971800	-1.77469900	-2.59872200
C	-7.03298500	-2.04030200	-1.09493100
H	-6.45119600	0.55972800	-0.45587100
H	-5.01619200	0.76216300	-1.47881400
H	-6.58419800	0.41832400	-2.20508100
H	-4.82997300	-2.84759300	-2.55814000
H	-5.65426900	-1.56304900	-3.46275100
H	-4.06665400	-1.25873100	-2.74136100
H	-7.70874700	-1.82263700	-1.92521900
H	-6.87698300	-3.11547700	-1.03837400
H	-7.50994200	-1.71395000	-0.16748900
C	5.88386900	-1.10088900	-0.07883300
C	5.54249300	-2.53181000	-0.52126700
C	6.01275400	-0.19057900	-1.30022900
C	7.18060900	-1.07245700	0.73259000
H	5.42925800	-3.17639500	0.35098600

H	4.61009600	-2.55305000	-1.09097600
H	6.33709600	-2.93524100	-1.15362700
H	6.27239000	0.83218600	-1.01938400
H	6.81947100	-0.57136200	-1.93039000
H	5.10459900	-0.16927500	-1.90310700
H	8.00781600	-1.43682300	0.11918500
H	7.41225700	-0.05410000	1.05437000
H	7.09473600	-1.69864400	1.61804300
C	-2.90865100	2.39808400	2.02667800
C	-2.35481600	2.27350800	3.46057600
C	-2.11482200	3.47727300	1.26226300
C	-4.37406600	2.84900400	2.10988400
H	-2.89640800	1.50864800	4.02234100
H	-1.29730400	2.00144900	3.46530800
H	-2.45682800	3.22340000	3.99325200
H	-2.47650300	3.57577600	0.23523900
H	-2.22107800	4.44853500	1.75334400
H	-1.04853700	3.24533300	1.22055700
H	-4.43361300	3.81915400	2.60873100
H	-4.82287200	2.96057200	1.11919900
H	-4.98462200	2.14938900	2.68605900
C	2.15999700	2.96456500	-1.38838700
C	0.75415100	3.30799000	-1.90254600
C	2.57862000	4.04091600	-0.36604900
C	3.13002900	2.98661500	-2.58668900
H	0.40364700	2.58456000	-2.64323400
H	0.02064100	3.35186700	-1.09409900
H	0.76777700	4.28905900	-2.38319600
H	3.59092000	3.87447700	0.00818400
H	2.55151900	5.03390800	-0.82385100
H	1.90374900	4.04558600	0.49379900
H	3.10053700	3.96063500	-3.08300400
H	4.16224500	2.80349800	-2.28139900
H	2.85993600	2.22365600	-3.32125200
O	-4.68827300	-2.98565300	0.01804500
O	0.14210000	-2.52065800	0.26313300
O	4.72574000	-1.26142500	1.97932700

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C	1.21513500	1.77167500	-0.10925300
H	0.63853600	1.08545700	0.49690900
C	2.53554500	1.42500300	-0.47273600
C	3.31918200	2.39426700	-1.15787300
H	4.33460000	2.13820400	-1.44109100
C	2.81113300	3.64863900	-1.45358900
C	1.53082700	3.99159900	-1.05078000
H	1.14606300	4.98610600	-1.25020700
C	0.70150800	3.06297000	-0.36317500
C	-0.54701800	3.55597500	0.12180100
C	-2.09779600	1.57547000	0.24401100
H	-1.44925400	0.99364400	-0.39759400
C	-1.73127100	2.89955000	0.57303500

C	-2.65781400	3.68900900	1.30873000
H	-2.38621000	4.70727500	1.56606700
C	-3.89106600	3.18291900	1.68551100
C	-4.25634600	1.89856400	1.31663200
H	-5.23628800	1.51500500	1.58017500
C	-3.37044700	1.06337500	0.58138800
C	-3.89061700	-0.19008400	0.13939700
C	-1.91941000	-1.74075900	-0.08891800
H	-1.30005100	-1.08570400	0.50949300
C	-3.26158300	-1.37822700	-0.33978500
C	-4.09347900	-2.31231900	-1.01683400
H	-5.12590300	-2.04381500	-1.21396700
C	-3.60996600	-3.54890100	-1.41193400
C	-2.30502700	-3.90983000	-1.11883900
H	-1.93715600	-4.89206300	-1.39587800
C	-1.42743500	-3.01632500	-0.44474300
C	-0.14861200	-3.53144800	-0.07546000
C	1.41053200	-1.55702500	0.03883800
H	0.71912700	-0.94390800	-0.52405700
C	1.06586200	-2.89706800	0.32399300
C	2.04078900	-3.72182500	0.95029400
H	1.78630000	-4.75257300	1.17311300
C	3.29852500	-3.23358000	1.26448300
C	3.63904000	-1.93114800	0.93770100
H	4.63586500	-1.55989900	1.15071200
C	2.70481300	-1.06068800	0.31123400
C	3.19469200	0.21487300	-0.10114300
H	-4.58137000	3.80170300	2.24951400
H	3.42543100	4.37172200	-1.98018600
H	4.02594300	-3.87943100	1.74537100
H	-4.26131100	-4.24500600	-1.93029500
H	4.27929800	0.27677600	-0.13908100
H	-4.97530000	-0.25194100	0.17513100
H	-0.60787200	4.64085100	0.15308100
H	-0.08774900	-4.61638500	-0.10453400

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C	2.01108300	1.31413700	-0.07512200
H	1.55596200	1.05183500	0.87252900
C	2.97701000	0.45557800	-0.62829300
C	3.57887700	0.82829600	-1.85136500
H	4.30213600	0.16338600	-2.30755900
C	3.24373500	2.02626900	-2.46825600
C	2.34877200	2.90193100	-1.86793100
H	2.11492400	3.84975000	-2.33732500
C	1.72468600	2.56695800	-0.64510100
C	0.88326000	3.53090500	0.04997300
C	-1.16853200	2.13022200	0.22292300
H	-0.90151200	1.65902300	-0.71551000
C	-0.31275700	3.10551200	0.76380400
C	-0.69156600	3.72817400	1.97452400
H	-0.02901300	4.45929500	2.42153000

C	-1.89255800	3.40345900	2.59111600
C	-2.76520200	2.49828200	2.00181600
H	-3.71532500	2.27237800	2.47044100
C	-2.42419400	1.85350500	0.79145500
C	-3.38464300	1.00022500	0.10607400
C	-1.98297300	-1.05395400	-0.02431200
H	-1.51636400	-0.77041600	0.91156500
C	-2.95559200	-0.20783400	-0.58492100
C	-3.57224300	-0.60781100	-1.79184200
H	-4.30116100	0.04674100	-2.25397600
C	-3.24465500	-1.81954500	-2.38554800
C	-2.34272100	-2.68179000	-1.77639600
H	-2.11503800	-3.64029500	-2.22668000
C	-1.70373700	-2.31945700	-0.56918800
C	-0.85372800	-3.26753800	0.13734200
C	1.19981500	-1.86343600	0.25346300
H	0.92105900	-1.41310700	-0.69178200
C	0.35084100	-2.82630500	0.82648700
C	0.74475700	-3.42209300	2.04590200
H	0.08766200	-4.14263200	2.51751600
C	1.95349800	-3.08429900	2.64000300
C	2.81863900	-2.19262600	2.01992500
H	3.77457100	-1.95665700	2.47145900
C	2.46242300	-1.57455400	0.79999800
C	3.41437600	-0.73699700	0.08398400
H	-2.15602700	3.86859900	3.53568200
H	3.69267700	2.28498500	-3.42193000
H	2.22879400	-3.52854500	3.59122900
H	-3.70520500	-2.09961100	-3.32758500
C	-4.79562300	1.35884100	0.11324300
C	-5.21837900	2.70609100	0.15310800
C	-5.80952200	0.38146700	0.07987900
C	-6.56092800	3.04011900	0.15454600
H	-4.47369400	3.49299500	0.15790200
C	-7.15447200	0.72764500	0.08938900
H	-5.53252300	-0.66592900	0.07047600
C	-7.56952200	2.06325100	0.12504300
H	-6.82959000	4.09096600	0.16958500
H	-7.88663100	-0.06982700	0.07775000
C	1.24197800	4.94173400	0.02991400
C	2.58845800	5.36389700	-0.03473300
C	0.26553300	5.95607100	0.07507700
C	2.92270800	6.70631800	-0.04790800
H	3.37499700	4.61895400	-0.04942600
C	0.61180000	7.30086600	0.05359500
H	-0.78161200	5.67941700	0.10344700
C	1.94671200	7.71533400	-0.00643100
H	3.97319800	6.97462400	-0.08195400
H	-0.18518600	8.03333300	0.07530400
C	4.82514200	-1.09656800	0.08117900
C	5.24738900	-2.44305400	0.14513300
C	5.83925100	-0.12116300	0.01378400

C	6.58958700	-2.77829800	0.13707400
H	4.50223300	-3.22890200	0.17644700
C	7.18398800	-0.46839000	0.01403300
H	5.56289800	0.92605200	-0.01497700
C	7.59843900	-1.80332700	0.07364700
H	6.85775400	-3.82879700	0.17170300
H	7.91657200	0.32788600	-0.02405500
C	-1.21394700	-4.67803000	0.15604200
C	-0.23316600	-5.69305900	0.21227200
C	-2.55696200	-5.10141200	0.11886400
C	-0.58181000	-7.03179600	0.22587700
H	0.81396300	-5.41510200	0.22037500
C	-2.89615300	-6.44802600	0.14084600
H	-3.34433000	-4.35748500	0.09677000
C	-1.92188100	-7.45073400	0.19322300
H	0.21242000	-7.77011100	0.25338000
H	-3.94656500	-6.70993300	0.12571600
C	-9.04244800	2.48259100	0.13214800
C	-9.33711300	3.29273400	1.41158100
C	-9.33051700	3.35795600	-1.10528500
C	-9.99286300	1.27679900	0.09815800
H	-9.13863400	2.69520900	2.30499300
H	-8.72350500	4.19390200	1.47190500
H	-10.38624700	3.60233100	1.43556400
H	-9.12754800	2.80737900	-2.02738500
H	-10.37955500	3.66851300	-1.11844800
H	-8.71689400	4.26102900	-1.11609500
H	-11.02947600	1.62297000	0.10351800
H	-9.85318700	0.67331700	-0.80237200
H	-9.85922500	0.62815200	0.96766400
C	2.36627300	9.18806400	-0.02737100
C	1.16154300	10.13903800	0.02363700
C	3.26339000	9.48129700	1.19316600
C	3.15388700	9.47675500	-1.32214800
H	0.49786500	10.00202100	-0.83391400
H	0.57377100	10.00326900	0.93509000
H	1.50785400	11.17549600	0.00796400
H	4.16632600	8.86737600	1.19085600
H	3.57448100	10.53025600	1.19615100
H	2.72907700	9.28270600	2.12572900
H	3.46323800	10.52568100	-1.35627400
H	4.05372800	8.86260600	-1.39553200
H	2.54073400	9.27444300	-2.20403600
C	9.07096600	-2.22409500	0.07187700
C	9.34272800	-3.12810700	-1.14855700
C	10.02192400	-1.02056000	-0.00171500
C	9.38087500	-3.00500500	1.36582700
H	8.72811800	-4.03041900	-1.13099100
H	9.12891300	-2.59866300	-2.08053200
H	10.39120500	-3.44026200	-1.16756300
H	9.89993100	-0.35216500	0.85443700
H	11.05820500	-1.36773900	-0.00168700

H	9.87123900	-0.43758300	-0.91390100
H	10.42995300	-3.31520400	1.38383800
H	9.19412300	-2.38689300	2.24768800
H	8.76725700	-3.90384500	1.45453900
C	-2.25780000	-8.94476900	0.21441200
C	-1.62328300	-9.62841200	-1.01462300
C	-1.69046300	-9.57826000	1.50166600
C	-3.77110300	-9.20346300	0.17917100
H	-2.00748600	-9.19621400	-1.94208100
H	-0.53671800	-9.52095600	-1.02362400
H	-1.85173500	-10.69841800	-1.01776900
H	-2.12307800	-9.10986400	2.38940200
H	-1.91984700	-10.64753600	1.53531600
H	-0.60580200	-9.46933300	1.56414300
H	-3.96265300	-10.27930500	0.19577100
H	-4.27915400	-8.76638500	1.04258300
H	-4.23196600	-8.80217400	-0.72703300

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C	0.05064500	2.38268000	0.06912200
H	0.20690600	1.65119900	0.85258700
C	1.11947500	2.72244100	-0.77720500
C	0.90245300	3.69863100	-1.77212100
H	1.70286000	3.92031700	-2.46632800
C	-0.32204600	4.35558700	-1.89912000
C	-1.33979400	4.05460700	-0.99175800
H	-2.27622300	4.59582200	-1.04021400
C	-1.16988900	3.07797200	0.01174400
C	-2.19484100	2.87555200	1.02534400
C	-2.50123300	0.42094000	0.71709500
H	-2.25365800	0.53355100	-0.33142600
C	-2.48099900	1.54973500	1.55345900
C	-2.83577800	1.38628800	2.90888400
H	-2.76382100	2.23919800	3.57155000
C	-3.24382300	0.15185600	3.41560600
C	-3.33118900	-0.93378000	2.54187400
H	-3.70071900	-1.88415900	2.90571500
C	-2.97662700	-0.81781200	1.18163200
C	-3.20163000	-1.92562800	0.26427800
C	-0.88494000	-2.09413200	-0.63949400
H	-0.50110800	-1.74691300	0.31201800
C	-2.27371500	-2.20644100	-0.82088900
C	-2.75115900	-2.68944200	-2.05734600
H	-3.81999400	-2.72100400	-2.22562400
C	-1.88157800	-3.09470900	-3.07059200
C	-0.50683800	-3.04721400	-2.83113400
H	0.17976800	-3.41176200	-3.58465700
C	0.01452100	-2.56158400	-1.61364100
C	1.44075100	-2.64506900	-1.33575600
C	1.82482600	-0.24603200	-0.77626900
H	1.03697200	0.02952400	-1.46672000
C	2.12411700	-1.60477700	-0.58119000

C	3.17299900	-1.94027900	0.30025400
H	3.36783900	-2.98575200	0.50217300
C	3.93759200	-0.96121600	0.93584400
C	3.66910200	0.38079800	0.65917200
H	4.28930500	1.15162300	1.09888000
C	2.62256600	0.76158300	-0.20648200
C	2.44615300	2.15722000	-0.58125700
C	-4.37574000	-2.77178000	0.43284200
C	-5.59094400	-2.26216600	0.93994000
C	-4.35808700	-4.13915000	0.09479400
C	-6.70487200	-3.06965300	1.08761900
H	-5.65686400	-1.21164500	1.19657600
C	-5.47984400	-4.94267000	0.25372700
H	-3.43979400	-4.57940700	-0.27518400
C	-6.68415000	-4.43269000	0.75114400
H	-7.61716900	-2.62270100	1.46760700
H	-5.39878300	-5.99003300	-0.00838900
C	-2.95012200	4.01723000	1.52400600
C	-2.37662900	5.30431600	1.61482000
C	-4.28884500	3.89291700	1.94456200
C	-3.09749200	6.38163800	2.09893200
H	-1.34347200	5.44407000	1.32019800
C	-5.00576200	4.98232500	2.42249700
H	-4.77795300	2.92896200	1.87034900
C	-4.43235100	6.25523500	2.51581100
H	-2.60293900	7.34496700	2.16108400
H	-6.03647200	4.82650400	2.71502100
C	3.615558100	3.00642300	-0.76495500
C	4.84010900	2.48984100	-1.24187100
C	3.58200200	4.38559400	-0.47993000
C	5.94379100	3.30443000	-1.42327800
H	4.90785700	1.43785700	-1.49189700
C	4.69781900	5.19316200	-0.65885000
H	2.67057300	4.82155300	-0.08856900
C	5.90798400	4.67856900	-1.13688700
H	6.85492700	2.85789100	-1.80652500
H	4.61413300	6.24264600	-0.40621100
C	2.20302500	-3.79139000	-1.81298900
C	3.56330800	-3.67577500	-2.17590200
C	1.62639600	-5.07055500	-1.93042600
C	4.28555700	-4.76826300	-2.62204900
H	4.04225100	-2.70523700	-2.12560700
C	2.36248200	-6.16252700	-2.37259000
H	0.59025200	-5.21078200	-1.64653000
C	3.70964200	-6.04467800	-2.73032300
H	5.32252700	-4.61963800	-2.90358900
H	1.86664700	-7.12337400	-2.42689800
C	-7.94211300	-5.28624000	0.93604600
C	-8.35894800	-5.26693500	2.42132900
C	-9.08410300	-4.70538400	0.07643000
C	-7.72269600	-6.74747200	0.51785500
H	-7.56491500	-5.67196300	3.05381100

H	-8.57612500	-4.25505500	2.76930700
H	-9.25779700	-5.87172400	2.57442300
H	-8.81304100	-4.70516800	-0.98244200
H	-9.99352800	-5.30211000	0.19461500
H	-9.32246900	-3.67774200	0.35806600
H	-8.64400300	-7.31651100	0.66541200
H	-7.44996000	-6.83265200	-0.53719000
H	-6.94149200	-7.22839000	1.11205800
C	-5.18988000	7.47845300	3.04029200
C	-6.63267900	7.14232900	3.44472600
C	-4.46041600	8.03854600	4.27910300
C	-5.23639200	8.56023500	1.94130100
H	-7.21541700	6.76601100	2.60008400
H	-6.66862700	6.39677700	4.24324200
H	-7.13237200	8.04179400	3.81304600
H	-3.43797500	8.34246700	4.04583300
H	-4.98694300	8.91460000	4.66945700
H	-4.41116200	7.28965100	5.07371900
H	-5.77393500	9.44436100	2.29699700
H	-4.23574900	8.87803900	1.64148100
H	-5.74718400	8.18768100	1.04975000
C	7.15726100	5.53804900	-1.35086700
C	7.57198800	5.47512100	-2.83561200
C	6.92373800	7.00988100	-0.98014500
C	8.30622500	4.99651300	-0.47517500
H	7.79919400	4.45484000	-3.15117100
H	6.77296900	5.85167900	-3.47939500
H	8.46444000	6.08366000	-3.00971700
H	6.65357100	7.12698900	0.07243900
H	7.83849500	7.58334800	-1.14966100
H	6.13550500	7.46272500	-1.58709400
H	9.20967300	5.59779500	-0.61439600
H	8.03679300	5.02801500	0.58359000
H	8.55378200	3.96250000	-0.72353200
C	4.55161900	-7.22469100	-3.22403500
C	5.06070900	-6.92725200	-4.64982500
C	5.75680400	-7.42258400	-2.28133300
C	3.75278900	-8.53556200	-3.26327800
H	4.22493100	-6.77979400	-5.33847700
H	5.67925700	-6.02792700	-4.68112000
H	5.66523700	-7.75989800	-5.02180700
H	5.42321300	-7.63104300	-1.26155600
H	6.37109000	-8.26350600	-2.61683900
H	6.39581700	-6.53776200	-2.24745900
H	4.39203200	-9.34747500	-3.61906400
H	3.38431800	-8.81746800	-2.27362800
H	2.89719200	-8.47091700	-3.94023200
C	-0.52701500	5.37119900	-2.95720000
C	0.49790200	6.24573000	-3.32861100
C	-1.75602800	5.49669100	-3.61808000
C	0.30406900	7.20614200	-4.31790900
H	1.45657000	6.19226800	-2.82320000

C	-1.94319000	6.45482700	-4.60378700
H	-2.56592400	4.81769700	-3.37358200
C	-0.91939200	7.33549200	-4.97996600
H	1.12878200	7.86357300	-4.56194000
H	-2.90877800	6.50869500	-5.09478200
C	-2.40829100	-3.59380400	-4.36153000
C	-3.56324800	-4.37881000	-4.41579000
C	-1.76443500	-3.30506500	-5.57189900
C	-4.05430100	-4.85736400	-5.62759800
H	-4.07606000	-4.64062000	-3.49608800
C	-2.25910300	-3.78334200	-6.77663400
H	-0.87989600	-2.67707300	-5.56993600
C	-3.41590100	-4.57290700	-6.83733700
H	-4.94806400	-5.46797700	-5.61260400
H	-1.73271100	-3.52627500	-7.68944400
C	-1.17115200	8.37810900	-6.07509600
C	-1.54756200	7.65966800	-7.38720100
C	-2.32997100	9.30118500	-5.64582800
C	0.06302100	9.25147500	-6.34407100
H	-0.74275600	6.99530800	-7.71194700
H	-2.45067500	7.05625700	-7.27528100
H	-1.73032400	8.38747800	-8.18347200
H	-2.08951300	9.82046400	-4.71458600
H	-2.52464100	10.05453100	-6.41505100
H	-3.25522800	8.74403100	-5.48533000
H	-0.16215200	9.97747500	-7.12936200
H	0.36667700	9.81216700	-5.45627600
H	0.91649600	8.65776200	-6.68131000
C	-3.92632600	-5.07964300	-8.19105300
C	-4.25302400	-3.87460700	-9.09696300
C	-2.83578400	-5.94189600	-8.85909500
C	-5.19513400	-5.93379800	-8.05351200
H	-5.02242700	-3.24428400	-8.64391000
H	-3.37506400	-3.25014400	-9.27441000
H	-4.62116500	-4.21523600	-10.06939300
H	-2.58329100	-6.80273200	-8.23467400
H	-3.18199500	-6.31420300	-9.82793200
H	-1.91797600	-5.37564800	-9.03004600
H	-5.52074500	-6.27334000	-9.03999300
H	-5.02337600	-6.82254900	-7.44082000
H	-6.02046900	-5.36926700	-7.61220400
C	5.02925300	-1.34028600	1.86189100
C	5.83330200	-2.45613000	1.61362500
C	5.29949100	-0.59154800	3.01487100
C	6.86458400	-2.80970000	2.47968100
H	5.66738000	-3.04715200	0.71893600
C	6.32775500	-0.94910900	3.87482500
H	4.67914900	0.26597200	3.25274400
C	7.13812000	-2.06671100	3.63082500
H	7.46198600	-3.67905300	2.23630600
H	6.49384900	-0.34516800	4.76026400
C	-3.60462400	0.00424500	4.84425500

C	-4.27836900	1.01941800	5.52884900
C	-3.29153900	-1.16014900	5.55780900
C	-4.62653100	0.87777000	6.86954000
H	-4.55641900	1.92662300	5.00253300
C	-3.63997700	-1.29538300	6.89380400
H	-2.74606000	-1.95809900	5.06540500
C	-4.31718400	-0.28138100	7.58549200
H	-5.15470900	1.69135500	7.35020000
H	-3.36887700	-2.21103100	7.40800200
C	-4.68286800	-0.47503900	9.06148300
C	-5.59880700	-1.70797100	9.20348500
C	-3.39552000	-0.69618000	9.88206100
C	-5.41981300	0.73963100	9.64432700
H	-6.51890900	-1.57778900	8.62803600
H	-5.11194800	-2.61864800	8.84862200
H	-5.87206000	-1.86363100	10.25146200
H	-2.72593800	0.16325800	9.79506200
H	-3.63534600	-0.83509100	10.94051700
H	-2.84689400	-1.57898200	9.54748600
H	-5.65931100	0.55736300	10.69498200
H	-4.81043500	1.64587500	9.59925100
H	-6.36035100	0.93442400	9.12259800
C	8.26227300	-2.42497100	4.60946800
C	9.25393200	-1.24721500	4.70280800
C	7.65871300	-2.69793600	6.00255500
C	9.04100600	-3.67396800	4.17158000
H	9.69454300	-1.03086300	3.72621500
H	8.76931200	-0.33519200	5.05728700
H	10.06552300	-1.48401600	5.39734500
H	6.94815800	-3.52745900	5.96320600
H	8.44591100	-2.95763400	6.71673200
H	7.12969400	-1.82660300	6.39390900
H	9.82985900	-3.89058700	4.89632700
H	8.39763200	-4.55565600	4.11384300
H	9.51871800	-3.53575700	3.19821200

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C	0.39454000	-1.37923700	-1.85158700
H	-0.52142600	-1.05505500	-1.37345700
C	0.90036600	-0.64254400	-2.93547200
C	2.07219800	-1.10267500	-3.57112000
H	2.49922000	-0.50424800	-4.36559300
C	2.70801900	-2.28215200	-3.17348800
C	2.13821900	-3.03232300	-2.14030300
H	2.58470000	-3.97630300	-1.85553500
C	0.96821500	-2.60813300	-1.47592700
C	0.30517300	-3.46798400	-0.51256000
C	0.12374400	-1.85286700	1.38008700
H	1.08211300	-1.43346800	1.09841900
C	-0.41739300	-2.90244900	0.62127600
C	-1.65224400	-3.45133300	1.01769000
H	-2.10106100	-4.21997600	0.40093800

C	-2.33033800	-2.98674300	2.14720600
C	-1.72524700	-2.00116100	2.93182800
H	-2.20721900	-1.67273200	3.84453400
C	-0.48702300	-1.43238700	2.57442200
C	0.18731600	-0.50121800	3.46984000
C	0.38791100	1.38891700	1.86653400
H	-0.52699100	1.06051500	1.38926900
C	0.89851400	0.65415900	2.94950600
C	2.06923500	1.11931300	3.58338700
H	2.50050100	0.52236500	4.37668200
C	2.69923900	2.30166000	3.18500300
C	2.12420200	3.05010900	2.15346900
H	2.56566300	3.99645800	1.86869000
C	0.95522700	2.62064700	1.49064000
C	0.28655700	3.47665400	0.52755100
C	0.11352000	1.86032300	-1.36533900
H	1.07425300	1.44600500	-1.08421300
C	-0.43311400	2.90663200	-0.60582100
C	-1.67149000	3.44835500	-1.00139600
H	-2.12517300	4.21316000	-0.38349800
C	-2.34674300	2.98174600	-2.13175700
C	-1.73633500	2.00008300	-2.91710000
H	-2.21634400	1.66991300	-3.83020100
C	-0.49531800	1.43718300	-2.55976700
C	0.18308700	0.50929700	-3.45542700
C	0.14387200	-0.72651500	4.90677300
C	0.07895000	-2.02777500	5.45152300
C	0.17176000	0.34167200	5.82454400
C	0.05298300	-2.23466400	6.81920200
H	0.07264300	-2.88057800	4.78320500
C	0.13828700	0.12312900	7.19547700
H	0.19531800	1.35856200	5.45069200
C	0.08103000	-1.16789500	7.73183900
H	0.01894200	-3.25541600	7.18472900
H	0.14610400	0.98539300	7.85034800
C	0.32125600	-4.91337400	-0.68298700
C	0.36186600	-5.51552600	-1.95949100
C	0.28286200	-5.78290300	0.42456500
C	0.36390200	-6.89122600	-2.10605600
H	0.36660900	-4.88627100	-2.84147300
C	0.29211900	-7.16256500	0.26651800
H	0.26875900	-5.36367800	1.42382400
C	0.33262600	-7.75566600	-1.00007500
H	0.38053500	-7.30138600	-3.11012600
H	0.27748600	-7.77903600	1.15666200
C	0.13694300	0.73359100	-4.89249100
C	0.06634600	2.03422500	-5.43800100
C	0.16772200	-0.33506600	-5.80960200
C	0.03783200	2.24012400	-6.80578600
H	0.05768500	2.88742700	-4.77022100
C	0.13162800	-0.11756200	-7.18064000
H	0.19568800	-1.35160700	-5.43510300

C	0.06872200	1.17287800	-7.71776400
H	-0.00047600	3.26050100	-7.17193900
H	0.14187700	-0.98021800	-7.83496300
C	0.28985300	4.92213100	0.69940300
C	0.24480800	5.79252800	-0.41231700
C	0.32197800	5.52458600	1.97166000
C	0.23642300	7.16643400	-0.25151800
H	0.23912400	5.37227000	-1.41115400
C	0.30639500	6.90524800	2.12214800
H	0.33320100	4.89648000	2.85441300
C	0.26418600	7.76424400	1.01906000
H	0.21728200	7.78912000	-1.13961500
H	0.31760400	7.30882500	3.12678900
C	0.05294200	-1.44702300	9.23624000
C	-1.23093700	-2.22642600	9.58825500
C	1.28603500	-2.29144000	9.61918500
C	0.07608700	-0.15633200	10.06826400
H	-2.12120200	-1.65015900	9.32393000
H	-1.28511900	-3.18096800	9.06075300
H	-1.26802000	-2.43691700	10.66123300
H	2.21103800	-1.75980400	9.38162600
H	1.28350300	-2.50720000	10.69177100
H	1.30563400	-3.24547000	9.08813600
H	0.05215800	-0.40276000	11.13265500
H	0.98127500	0.42916000	9.88761900
H	-0.78842400	0.47896400	9.85892200
C	0.34060200	-9.27096100	-1.21374000
C	0.30757500	-10.04583700	0.11175400
C	-0.89700100	-9.67516700	-2.04134200
C	1.62013100	-9.67206200	-1.97668500
H	1.17460600	-9.81947400	0.73776100
H	-0.59531500	-9.82888500	0.68839900
H	0.31847900	-11.12014800	-0.08818300
H	-0.90999500	-9.18671900	-3.01794700
H	-0.90791900	-10.75615000	-2.20965700
H	-1.81905300	-9.40280900	-1.52146500
H	1.64382200	-10.75340600	-2.14142600
H	1.68087100	-9.18613000	-2.95268500
H	2.51345200	-9.39456200	-1.41130300
C	0.03781900	1.45090200	-9.22231900
C	1.26764200	2.29915700	-9.60728600
C	0.06424000	0.15972200	-10.05349100
C	-1.24906100	2.22577700	-9.57337400
H	1.28474600	3.25351000	-9.07672600
H	2.19469000	1.77069800	-9.37061200
H	1.26304800	2.51434900	-10.67997900
H	-0.79764900	-0.47851500	-9.84227800
H	0.03770400	0.40532000	-11.11801100
H	0.97181200	-0.42240400	-9.87393900
H	-1.28813000	2.43529600	-10.64647100
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C	0.24848500	9.28919100	1.14707400
C	1.48564100	9.87317100	0.43390000
C	-1.03147700	9.84361300	0.48807600
C	0.27475800	9.75056900	2.61159800
H	2.40788200	9.49539800	0.88268500
H	1.50285000	9.61521300	-0.62710900
H	1.49168700	10.96451500	0.51119100
H	-1.92463000	9.44311600	0.97438600
H	-1.06091600	10.93435200	0.56788900
H	-1.08704500	9.58685300	-0.57192000
H	0.26282700	10.84245000	2.65493400
H	-0.59450300	9.39041900	3.16783600
H	1.17547600	9.41130100	3.12961700
C	3.93346700	-2.74359000	-3.85306900
C	4.13535300	-2.50853800	-5.22396300
C	4.93394600	-3.44748100	-3.16223100
C	5.27276900	-2.95453100	-5.87115400
H	3.36709600	-2.00087500	-5.79737000
C	6.07029500	-3.90158000	-3.80572300
H	4.83212600	-3.60722700	-2.09428300
C	6.27995700	-3.67236200	-5.18531900
H	5.38005400	-2.78482300	-6.93581400
H	6.83525900	-4.41510700	-3.23577300
C	3.92526700	2.76609000	3.86151700
C	4.13093200	2.53178300	5.23197900
C	4.92349500	3.47016200	3.16765100
C	5.27042300	2.97750800	5.87561300
H	3.36422200	2.02443200	5.80773300
C	6.06214200	3.92374400	3.80754300
H	4.81831300	3.62979500	2.09999800
C	6.27631200	3.69400100	5.18639500
H	5.38078500	2.80810400	6.93999800
H	6.82565000	4.43661600	3.23505800
C	7.46712800	-4.15160800	-5.86415000
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H	-3.24480200	5.54484400	-1.91280000
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H	-5.48171900	6.39991000	-2.42508600
H	-6.69912700	2.46802600	-3.65532400
C	-3.66208600	-3.52094500	2.49284500
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C	-5.23510500	-5.36876500	2.60973900
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C	-6.26112300	-4.52320000	3.08803400
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C	-7.59742000	-5.02412800	3.36242100
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C	-8.94484400	7.11863500	-3.52178400
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H	-9.68630200	6.69847200	-2.85244800
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H	-5.99048800	6.39547000	-5.01313400
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H	-9.99575400	8.95711300	-3.70082700
H	-6.29499400	8.65370700	-5.85794000
C	-8.77556800	4.14471700	-3.10867200
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H	-9.94106400	4.88112200	-4.76404300
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H	-7.94843000	3.16574900	-1.37192700
C	-11.04542300	2.47581000	-2.61936600
H	-11.87153000	3.46241700	-4.35006800
H	-9.87895200	1.74814000	-0.95446000
C	-8.75532500	-4.17434200	3.11427800
C	-9.90610900	-4.23239700	3.92241500
C	-8.78156600	-3.25895800	2.03940800
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H	-9.92254400	-4.90831100	4.76954500
C	-9.88720400	-2.46327400	1.79813700
H	-7.92710900	-3.19927200	1.37584300
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H	-11.85742600	-3.49903500	4.34414000
H	-9.86203600	-1.79116600	0.94694800
C	-7.78123800	-6.37369300	3.87551400
C	-8.91368800	-7.14712900	3.54029600
C	-6.83786800	-6.97286000	4.73179200
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H	-9.65547900	-6.73280400	2.86770000
C	-7.01538300	-8.26028800	5.22157400
H	-5.96501500	-6.40593800	5.03408600
C	-8.13590200	-9.02621800	4.88318900
H	-9.95778200	-8.98888400	3.72538800
H	-6.26229400	-8.66169500	5.88807300
C	8.00569600	3.43892700	7.00147200
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C	7.94039800	2.03127100	7.07668400
C	9.12992800	3.40387600	9.16685100
H	8.67744300	5.18450700	8.06943600
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H	9.57796300	3.97035700	9.97359000
H	8.39527700	0.26103600	8.16145700
C	8.13017800	5.38715400	5.40910200
C	7.40732800	6.47394500	4.88297200
C	9.53170500	5.53444100	5.48392400
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C	9.43431000	7.77372400	4.52798400
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H	6.32204600	-6.39066100	-4.83064800
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C	9.42565400	-7.76285600	-4.53924600
H	7.42391000	-8.42309700	-4.08122000
H	11.23258400	-6.74081300	-5.13207800
C	8.00416100	-3.42123900	-7.00587400
C	8.61462400	-4.08552600	-8.08567900
C	7.94149000	-2.01342200	-7.08064000
C	9.12194900	-3.38802900	-9.17462900
H	8.66893100	-5.16797400	-8.07636400
C	8.45735200	-1.32702500	-8.16584900
H	7.50174300	-1.46014400	-6.25902200
C	9.05928200	-1.99248000	-9.24575600
H	9.56637000	-3.95526000	-9.98284000
H	8.39676300	-0.24389800	-8.16639700
C	-12.24452900	1.57419200	-2.31643900
C	-13.37705400	1.75094600	-3.33820600
C	-11.79889500	0.09714800	-2.34066700
C	-12.79624000	1.92067000	-0.91820100
H	-13.76805000	2.77166600	-3.34108400
H	-13.05122200	1.50781000	-4.35288000
H	-14.20588200	1.08326300	-3.09007800
H	-11.02074400	-0.10589900	-1.60211700
H	-12.64398700	-0.56143300	-2.12026900
H	-11.40313300	-0.17422400	-3.32261900
H	-13.65880400	1.29129600	-0.68084300
H	-12.04884000	1.76787200	-0.13727500
H	-13.11479200	2.96528800	-0.87390000
C	-8.40225900	10.43143000	-5.36418600
C	-8.48706700	11.39446000	-4.16183800
C	-7.27060200	10.91034700	-6.28534200
C	-9.72494800	10.48388700	-6.15634400
H	-9.30395800	11.13072600	-3.48683800
H	-7.55977100	11.37743300	-3.58348400

H	-8.65592000	12.41985800	-4.50405700
H	-7.17443000	10.28084100	-7.17375400
H	-7.47691300	11.92833200	-6.62510500
H	-6.30575700	10.92503600	-5.77187000
H	-9.90886400	11.49670500	-6.52701700
H	-9.69137500	9.80854500	-7.01509400
H	-10.57931700	10.19555200	-5.54043200
C	-12.23203600	-1.62086300	2.30134600
C	-13.36675300	-1.79739500	3.32072500
C	-11.79184000	-0.14210500	2.32032000
C	-12.77863600	-1.97546700	0.90313900
H	-13.75372400	-2.81963600	3.32717300
H	-13.04479900	-1.54832700	4.33519300
H	-14.19747700	-1.13411200	3.06720400
H	-11.01219600	0.06039400	1.58316400
H	-12.63864000	0.51243200	2.09449900
H	-11.39994800	0.13507800	3.30220200
H	-13.64287400	-1.35034500	0.66072500
H	-12.02975000	-1.82326800	0.12352500
H	-13.09318400	-3.02144400	0.86251800
C	-8.36192000	-10.44957700	5.39846100
C	-8.44181200	-11.41827000	4.20033800
C	-7.22976200	-10.92033500	6.32319700
C	-9.68544300	-10.50317000	6.18916000
H	-9.25880300	-11.16049400	3.52315900
H	-7.51386400	-11.40053100	3.62304600
H	-8.60741700	-12.44271900	4.54694800
H	-7.13711100	-10.28663500	7.20899600
H	-7.43278000	-11.93759200	6.66710300
H	-6.26416500	-10.93367900	5.81110500
H	-9.86631000	-11.51498300	6.56405500
H	-9.65531900	-9.82394400	7.04496800
H	-10.54001100	-10.22051700	5.57089800
C	10.15868500	-9.02539500	-4.07934900
C	11.14817700	-8.65919600	-2.95376800
C	9.19531900	-10.09469100	-3.54351600
C	10.93580800	-9.62700600	-5.26845600
H	11.89035000	-7.93036200	-3.28609700
H	10.62194500	-8.23037700	-2.09716100
H	11.68532700	-9.54913100	-2.61243600
H	8.48014500	-10.41709900	-4.30470600
H	9.75979200	-10.97611800	-3.22924800
H	8.63296800	-9.73877200	-2.67643200
H	11.46999400	-10.53017900	-4.95865700
H	10.25647600	-9.89596500	-6.08139900
H	11.67190900	-8.92676800	-5.66882400
C	9.60972100	-1.19018900	-10.42736400
C	10.22081100	-2.09236100	-11.50956000
C	8.46682400	-0.37455200	-11.06646400
C	10.70610900	-0.22808600	-9.92512300
H	11.05814500	-2.68030700	-11.12481300
H	9.48401600	-2.78232000	-11.92894400

H	10.60040100	-1.47896200	-12.33051200
H	8.01786800	0.32202500	-10.35529500
H	8.84048200	0.20890500	-11.91324100
H	7.67488900	-1.03385500	-11.43096500
H	11.10986500	0.35838300	-10.75581800
H	10.32272600	0.47202400	-9.18000000
H	11.53016400	-0.78171200	-9.46785800
C	9.61674900	1.20529400	10.41866700
C	10.23297700	2.10640600	11.49883000
C	8.47393800	0.39232200	11.06130700
C	10.70956000	0.24066800	9.91348300
H	11.07039600	2.69249600	11.11144400
H	9.49890200	2.79801000	11.92026600
H	10.61371900	1.49238100	12.31878000
H	8.02138700	-0.30343400	10.35161400
H	8.84878500	-0.19174900	11.90713500
H	7.68451600	1.05344600	11.42795400
H	11.11444200	-0.34646900	10.74315600
H	10.32249100	-0.45880000	9.16966700
H	11.53349300	0.79237100	9.45368200
C	10.17059800	9.03325200	4.06505000
C	11.15529900	8.66265200	2.93671000
C	9.20960300	10.10579000	3.53145100
C	10.95356200	9.63272800	5.25140200
H	11.89575700	7.93127100	3.26726700
H	10.62488600	8.23525300	2.08197700
H	11.69472300	9.55036000	2.59317600
H	8.49797800	10.43136100	4.29462600
H	9.77639400	10.98490600	3.21489900
H	8.64332400	9.75143000	2.66628500
H	11.49011900	10.53373200	4.93940000
H	10.27772200	9.90469000	6.06625400
H	11.68830400	8.93003400	5.64995600