Supporting Information

Electrochemical control of the regioselectivity in the exohedral functionalization of C_{60}. The role of aromaticity

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Computational details

All Density Functional Theory (DFT) calculations were performed with the Amsterdam Density Functional (ADF) program.[1] The molecular orbitals (MOs) were expanded in an uncontracted set of Slater type orbitals (STOs) of double-ζ (DZP) and triple-ζ (TZP) quality containing diffuse functions and one set of polarization functions. In order to reduce the computational time needed to carry out the calculations, the frozen core approximation has been used.[2] In this approximation, the core density is obtained and included explicitly, albeit with core orbitals (*1s* for C) frozen during the SCF procedure. It was shown that the frozen core approximation has a negligible effect on the optimized equilibrium geometries.[3] Scalar relativistic corrections have been included self-consistently using the Zeroth Order Regular Approximation (ZORA).[4] An auxiliary set of *s*, *p*,

d, *f*, and *g* STOs was used to fit the molecular density and to represent the Coulomb and exchange potentials accurately for each SCF cycle.[5] Energies and gradients were calculated using the local density approximation (Slater exchange) with non-local corrections for exchange (Becke88)[6] and correlation (Perdew86)[7] included self-consistently (i.e. the BP86 functional). Open-shell systems were treated with the unrestricted formalism (UBP86). Moreover, energy dispersion corrections were introduced using Grimme's methodology[8,9] (D_2) implemented in ADF 2010.01 version.[1] All the structures were fully optimized using these corrections in each optimization step. It was shown that dispersion corrections are essential for a correct description of the thermodynamics and kinetics of fullerene and nanotube reactions.[10,11] All energies reported here were obtained with the TZP basis in single-point energy calculations at geometries that were optimized with the DZP basis (i.e., BP86-D_2/TZP//BP86-D_2/DZP). The actual geometry optimizations and transition state (TS) searches were performed with the QUILD[12] (QUantum-regions Interconnected by Local Descriptions) program, which functions as a wrapper around the ADF program. The QUILD program constructs all input files for ADF, runs ADF, and collects all data; ADF is used only for the generation of the energy and gradients. Furthermore, the QUILD program uses improved geometry optimization techniques, such as adapted delocalized coordinates[13] and specially constructed model Hessians with the appropriate number of eigenvalues.[13] The latter is particularly useful for TS searches. All TSs were characterized by computing the analytical[14] vibrational frequencies, to have one and only one imaginary frequency corresponding to the approach of the reacting carbons.

As a structure-based measure of aromaticity, we have employed the harmonic oscillator model of aromaticity (HOMA) index, defined by Kruszewski and Krygowski as:[15,16]

$$HOMA = 1 - \frac{\alpha}{n}\sum_{i=1}^{n}\left(R_{opt} - R_i\right)^2 \quad , \qquad (1)$$

where n is the number of bonds considered, and α is an empirical constant (for C–C bonds α = 257.7) fixed to give HOMA = 0 for a model nonaromatic system, and HOMA = 1 for a system with all bonds equal to an optimal value R_{opt} (1.388Å for C–C bonds), assumed to be achieved for fully aromatic systems. R_i stands for a running bond length.

As magnetic indices of aromaticity, we have used the nucleus-independent chemical shift (NICS) index, proposed by Schleyer and co-workers.[17,18] NICS is defined as the negative value of the absolute shielding computed at a ring center or at some other interesting point of the system. Rings with large negative NICS values are considered aromatic. NICS values have been obtained at the BP86/cc-pVDZ[19]//BP86-D_2/DZP level of theory using the Gaussian09 package.[20]

For the aromaticity analysis we have also applied the multicenter index (MCI).[21,22] MCI is a particular extension of the I_{ring} index.[23]

$$I_{ring}(\mathcal{A}) = \sum_{i_1,i_2,\ldots,i_N} n_{i_1} n_{i_N} S_{i_1 i_2}(A_1) S_{i_2 i_3}(A_2) \ldots S_{i_N i_1}(A_N) \qquad (2)$$

n_i being the occupancy of MO i and $\mathcal{A}$ = { A_1, A_2, ..., A_N } a string containing the set of N atoms forming the ring structure. The MCI index[22] is defined as the sum of all I_{ring} values resulting from the permutations of indices A_1, A_2, ..., A_N:

$$MCI(\mathcal{A}) = \frac{1}{2N} \sum_{P(\mathcal{A})} I_{ring}(\mathcal{A}) \qquad (3)$$

where $P(\mathcal{A})$ stands for a permutation operator which interchanges the atomic labels A_1, A_2, ..., A_N to generate the N! permutations of the elements in the string $\mathcal{A}$.[22] MCI and I_{ring} give a measure of the electron sharing between all atoms in the ring. MCI values were computed at the BP86/cc-pVDZ//BP86-D_2/DZP level of theory with the help of the ESI-3D program.[24] The more positive the HOMA and MCI values and the more negative the NICS values, the more aromatic the rings.

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Table S1. Reaction energies (ΔE_R, kcal·mol^{-1}) and reaction barriers ($\Delta E^{\ddagger}$, kcal·mol^{-1}) for the Diels-Alder cycloaddition of cyclopentadiene on C_{60} at BP86-D_2/TZP//BP86-D_2/DZP level.

n	ΔE_R [6,6]	ΔE_R [5,6]	$\Delta E^{\ddagger}$ [6,6]	$\Delta E^{\ddagger}$ [5,6]	$\Delta\Delta E_R$ ([6,6]-[5,6])	$\Delta\Delta E^{\ddagger}$ ([6,6]-[5,6])
0	-24.69	-7.94	-3.02	9.33	-16.75	-12.35
1	-22.77	-12.33	0.34	8.53	-10.44	-8.19
2	-20.44	-16.76	2.26	5.86	-3.68	-3.60
3	-18.08	-15.34	2.90	4.37	-2.74	-1.47
4	-20.20	-18.53	-1.62[a]	-1.47[a]	-1.67	-0.15
5	-17.98	-21.33	-7.04[a]	-11.62[a]	3.35	4.58
6	-20.75	-27.41	-15.95[a]	-23.79[a]	6.66	7.84

[a]In the present model used here, we have not considered the formation of the initial intermediate because the charge transfer from C_{60}^{n-} to the Cp molecule does not allow to correctly optimization of the intermediate.. This fact implies having negative barriers for the charged studied systems.

Table S2. Reaction energies (ΔE_R, kcal·mol^{-1}) for the 1,3-dipolar cycloaddition of N-methyl azomethine on C_{60} at BP86-D_2/TZP//BP86-D_2/DZP level.

n	ΔE_R [6,6]	ΔE_R [5,6]	$\Delta\Delta E_R$ ([6,6]-[5,6])
0	-54.87	-40.39	-14.48
1	-53.07	-45.59	-7.48
2	-50.94	-50.33	-0.61
3	-49.23	-49.26	0.03
4	-51.57	-53.01	1.44
5	-48.80	-55.70	6.90
6	-47.10	-64.20	17.10

Table S3. Reaction energies (ΔE_R, kcal·mol^{-1}) for the carbene addition of dichlorocarbene on C_{60} at BP86-D_2/TZP//BP86-D_2/DZP level.

n	ΔE_R [6,6]	ΔE_R [5,6]	$\Delta\Delta E_R$ ([6,6]-[5,6])
0	-74.70	-71.81	-2.89
1	-77.67	-76.75	-0.92
2	-80.24	-83.30	3.06
3	-82.79	-91.06	8.27

Table S4. Bond distances (Å) and pyramidalization angles (deg.) of C_{60}^{n-} (n = 0 – 6) optimized at BP86-D_2/DZP level.

n	[6,6]	[5,6]	Pyr. Angle
0	1.394	1.447	11.64
1	1.400	1.447	11.64
2	1.405	1.446	11.64
3	1.411	1.446	11.64
4	1.418	1.447	11.64
5	1.425	1.448	11.64
6	1.432	1.449	11.64

Table S5. HOMA and MCI (electrons) values for the 5-MRs and 6-MRs of the C_{60} molecule when it is reduced by n electrons (n = 0 – 6). NICS(1) values (ppm) for the neutral and hexaanionic cases are also included.

n =	0	1	2	3	4	5	6
HOMA 5-MR	0.0950	0.1163	0.1250	0.1219	0.1070	0.0808	0.0430
HOMA 6-MR	0.5426	0.5410	0.5241	0.4907	0.4388	0.3664	0.2709
MCI 5-MR	0.0094	0.0103	0.0103	0.0112	0.0115	0.0121	0.0130
MCI 6-MR	0.0130	0.0119	0.0116	0.0105	0.0091	0.0090	0.0080
NICS(1) 5-MR[a]	7.3837						-8.1921
NICS(1) 6-MR[a]	0.4417						-6.3419

[a] Only calculated for closed shell species.

Table S6. MCI index average (ΣMCI 6-MR / nº 6-MR) for the 6-MR (the most aromatic ring in the neutral C_{60} species) and 5-MR (the most aromatic ring in the C_{60}^{6-} species) for the [6,6] and [5,6] products, and the % of the average MCI reduction with respect the reactant MCI ($\frac{\sum MCI\ 6-MR_{prod.} - \sum MCI\ 6-MR_{react.}}{\sum MCI\ 6-MR_{react.}} \times 100\ (\%)$). Units are electrons.

n = 0	**[6,6]**	**[5,6]**
ΣMCI 6-MR$_{prod.}$ / nº 6-MR	0.0120	0.0110
$\frac{\sum MCI\ 6-MR_{prod.} - \sum MCI\ 6-MR_{react.}}{\sum MCI\ 6-MR_{react.}} \times 100\ (\%)$	-7.5	-15.3
n = 6	**[6,6]**	**[5,6]**
ΣMCI 5-MR$_{prod.}$ / nº 5-MR	0.0099	0.0121
$\frac{\sum MCI\ 5-MR_{prod.} - \sum MCI\ 5-MR_{react.}}{\sum MCI - 5MR_{react.}} \times 100\ (\%)$	-31.9	-9.3

Results presented in the table above show equivalent but opposite tendencies for the [5,6] and [6,6] products of C_{60} and C_{60}^{6-}. Average MCI values show that the most 6-MR aromatic product is the C_{60} – [6,6] that is in agreement with the energetically most stable, and the 5-MR most aromatic product is the C_{60}^{6-} – [5,6], that coincides with the major C_{60}^{6-} product. Moreover, the percentages of aromaticity average reduction with respect to the reactant for 6-MR or 5-MR depending on the case, indicate that the most stable product of each case is the one that loses less aromaticity due to the addition reaction.

Table S7. Xyz Cartesian coordinates of all optimized species and BP86-D/TZP//BP86-D/DZP energies.

c60	-12055.9512		
C	3.022400	-0.249100	-1.824100
C	2.591600	-1.575000	-1.824100
C	1.420700	-1.955500	-2.585000
C	3.022400	1.742900	-0.593000
C	3.469600	0.366500	-0.593000
C	3.469600	-0.366500	0.593000
C	0.697100	-2.951400	-1.824100
C	-0.697100	-2.951400	-1.824100
C	2.591600	2.335900	0.593000
C	1.420700	-3.186600	-0.593000
C	-2.298800	-1.978000	1.824100
C	-1.170900	-2.797500	1.824100
C	0.000000	-2.417100	2.585000
C	0.000000	-1.231100	3.317900
C	-1.170900	-0.380400	3.317900
C	-3.022400	-1.742900	0.593000
C	-2.591600	-2.335900	-0.593000
C	-1.420700	-3.186600	-0.593000
C	-0.723600	-3.413100	0.593000
C	1.170900	-2.797500	1.824100
C	2.298800	-1.978000	1.824100
C	2.298800	-0.746900	2.585000
C	1.170900	-0.380400	3.317900
C	0.723600	0.996000	3.317900
C	-0.723600	0.996000	3.317900
C	1.420700	1.955500	2.585000
C	2.591600	1.575000	1.824100
C	3.022400	0.249100	1.824100
C	0.723600	-3.413100	0.593000
C	3.022400	-1.742900	0.593000
C	-2.298800	-0.746900	2.585000
C	2.591600	-2.335900	-0.593000
C	2.298800	0.746900	-2.585000
C	1.170900	0.380400	-3.317900
C	0.723600	-0.996000	-3.317900
C	2.298800	1.978000	-1.824100
C	1.170900	2.797500	-1.824100
C	-0.723600	-0.996000	-3.317900
C	-1.420700	-1.955500	-2.585000
C	-1.170900	0.380400	-3.317900
C	-3.469600	-0.366500	0.593000
C	-3.469600	0.366500	-0.593000
C	-3.022400	1.742900	-0.593000
C	-2.591600	2.335900	0.593000
C	-2.591600	1.575000	1.824100
C	-2.591600	-1.575000	-1.824100
C	-3.022400	-0.249100	-1.824100
C	-2.298800	1.978000	-1.824100
C	-1.170900	2.797500	-1.824100
C	-0.723600	3.413100	-0.593000
C	-1.420700	3.186600	0.593000
C	-0.697100	2.951400	1.824100
C	-1.420700	1.955500	2.585000
C	0.697100	2.951400	1.824100
C	1.420700	3.186600	0.593000
C	0.723600	3.413100	-0.593000
C	-2.298800	0.746900	-2.585000
C	0.000000	2.417100	-2.585000
C	-3.022400	0.249100	1.824100
C	0.000000	1.231100	-3.317900

c60_1	-12122.1913		
C	3.025800	0.247400	1.825800
C	2.593300	1.578400	1.825800
C	1.423100	1.958700	2.586300
C	3.025800	-1.743700	0.595300
C	3.472800	-0.367900	0.595300
C	3.472800	0.367900	-0.595300
C	0.699800	2.954200	1.825800
C	-0.699800	2.954200	1.825800
C	2.593300	-2.338900	-0.595300
C	1.423100	3.189200	0.595300
C	-2.302500	1.978700	-1.825800
C	-1.170300	2.801300	-1.825800
C	0.000000	2.421000	-2.586300
C	0.000000	1.230500	-3.322100
C	-1.170300	0.380300	-3.322100
C	-3.025800	1.743700	-0.595300
C	-2.593300	2.338900	0.595300
C	-1.423100	3.189200	0.595300
C	-0.723300	3.416600	-0.595300
C	1.170300	2.801300	-1.825800
C	2.302500	1.978700	-1.825800
C	2.302500	0.748100	-2.586300
C	1.170300	0.380300	-3.322100
C	0.723300	-0.995500	-3.322100
C	-0.723300	-0.995500	-3.322100
C	1.423100	-1.958700	-2.586300
C	2.593300	-1.578400	-1.825800
C	3.025800	-0.247400	-1.825800
C	0.723300	3.416600	-0.595300
C	3.025800	1.743700	-0.595300
C	-2.302500	0.748100	-2.586300
C	2.593300	2.338900	0.595300
C	2.302500	-0.748100	2.586300
C	1.170300	-0.380300	3.322100
C	0.723300	0.995500	3.322100
C	2.302500	-1.978700	1.825800
C	1.170300	-2.801300	1.825800
C	-0.723300	0.995500	3.322100
C	-1.423100	1.958700	2.586300
C	-1.170300	-0.380300	3.322100
C	-3.472800	0.367900	-0.595300
C	-3.472800	-0.367900	0.595300
C	-3.025800	-1.743700	0.595300
C	-2.593300	-2.338900	-0.595300
C	-2.593300	-1.578400	-1.825800
C	-2.593300	1.578400	1.825800
C	-3.025800	0.247400	1.825800
C	-2.302500	-1.978700	1.825800
C	-1.170300	-2.801300	1.825800
C	-0.723300	-3.416600	0.595300
C	-1.423100	-3.189200	-0.595300
C	-0.699800	-2.954200	-1.825800
C	-1.423100	-1.958700	-2.586300
C	0.699800	-2.954200	-1.825800
C	1.423100	-3.189200	-0.595300
C	0.723300	-3.416600	0.595300
C	-2.302500	-0.748100	2.586300
C	0.000000	-2.421000	2.586300
C	-3.025800	-0.247400	-1.825800
C	0.000000	-1.230500	3.322100

c60_2_t	-12119.9386		
C	3.030100	0.245700	1.828000
C	2.595800	1.582200	1.828000
C	1.425800	1.962400	2.588300
C	3.030100	-1.744900	0.597700
C	3.477000	-0.369400	0.597700
C	3.477000	0.369400	-0.597700
C	0.702600	2.957700	1.828000
C	-0.702600	2.957700	1.828000
C	2.595800	-2.342600	-0.597700
C	1.425800	3.192700	0.597700
C	-2.306900	1.979800	-1.828000
C	-1.170100	2.805800	-1.828000
C	0.000000	2.425700	-2.588300
C	0.000000	1.230300	-3.327100
C	-1.170100	0.380200	-3.327100
C	-3.030100	1.744900	-0.597700
C	-2.595800	2.342600	0.597700
C	-1.425800	3.192700	0.597700
C	-0.723100	3.421000	-0.597700
C	1.170100	2.805800	-1.828000
C	2.306900	1.979800	-1.828000
C	2.306900	0.749600	-2.588300
C	1.170100	0.380200	-3.327100
C	0.723100	-0.995300	-3.327100
C	-0.723100	-0.995300	-3.327100
C	1.425800	-1.962400	-2.588300
C	2.595800	-1.582200	-1.828000
C	3.030100	-0.245700	-1.828000
C	0.723100	3.421000	-0.597700
C	3.030100	1.744900	-0.597700
C	-2.306900	0.749600	-2.588300
C	2.595800	2.342600	0.597700
C	2.306900	-0.749600	2.588300
C	1.170100	-0.380200	3.327100
C	0.723100	0.995300	3.327100

C	2.306900	-1.979800	1.828000
C	1.170100	-2.805800	1.828000
C	-0.723100	0.995300	3.327100
C	-1.425800	1.962400	2.588300
C	-1.170100	-0.380200	3.327100
C	-3.477000	0.369400	-0.597700
C	-3.477000	-0.369400	0.597700
C	-3.030100	-1.744900	0.597700
C	-2.595800	-2.342600	-0.597700
C	-2.595800	-1.582200	-1.828000
C	-2.595800	1.582200	1.828000
C	-3.030100	0.245700	1.828000
C	-2.306900	-1.979800	1.828000
C	-1.170100	-2.805800	1.828000
C	-0.723100	-3.421000	0.597700
C	-1.425800	-3.192700	-0.597700
C	-0.702600	-2.957700	-1.828000
C	-1.425800	-1.962400	-2.588300
C	0.702600	-2.957700	-1.828000
C	1.425800	-3.192700	-0.597700
C	0.723100	-3.421000	0.597700
C	-2.306900	-0.749600	2.588300
C	0.000000	-2.425700	2.588300
C	-3.030100	-0.245700	-1.828000
C	0.000000	-1.230300	3.327100

c60_3_q -12049.9855

C	-2.311900	0.751200	-2.591000
C	-1.170100	0.380200	-3.333000
C	-0.723200	-0.995400	-3.333000
C	-3.035100	1.746600	-0.600300
C	-2.311900	1.981600	-1.830600
C	-1.170100	2.811100	-1.830600
C	0.723200	-0.995400	-3.333000
C	1.428900	-1.966700	-2.591000
C	-2.599000	2.346900	0.600300
C	1.170100	0.380200	-3.333000
C	3.482100	-0.371000	0.600300
C	3.482100	0.371000	-0.600300
C	3.035100	1.746600	-0.600300
C	2.599000	2.346900	0.600300
C	2.599000	1.586500	1.830600
C	3.035100	-1.746600	0.600300
C	2.599000	-2.346900	-0.600300
C	2.599000	-1.586500	-1.830600
C	3.035100	-0.244200	-1.830600
C	2.311900	1.981600	-1.830600
C	1.170100	2.811100	-1.830600
C	0.723200	3.426300	-0.600300
C	1.428900	3.197000	0.600300
C	0.705700	2.962000	1.830600
C	1.428900	1.966700	2.591000
C	-0.705700	2.962000	1.830600
C	-1.428900	3.197000	0.600300
C	-0.723200	3.426300	-0.600300
C	2.311900	0.751200	-2.591000
C	0.000000	2.430900	-2.591000
C	3.035100	0.244200	1.830600
C	0.000000	1.230400	-3.333000
C	-3.035100	-0.244200	-1.830600
C	-2.599000	-1.586500	-1.830600
C	-1.428900	-1.966700	-2.591000
C	-3.482100	0.371000	-0.600300
C	-3.482100	-0.371000	0.600300
C	-0.705700	-2.962000	-1.830600
C	0.705700	-2.962000	-1.830600
C	-1.428900	-3.197000	-0.600300
C	2.311900	-1.981600	1.830600
C	1.170100	-2.811100	1.830600
C	0.000000	-2.430900	2.591000
C	0.000000	-1.230400	3.333000
C	1.170100	-0.380200	3.333000
C	1.428900	-3.197000	-0.600300
C	0.723200	-3.426300	0.600300
C	-1.170100	-2.811100	1.830600
C	-2.311900	-1.981600	1.830600
C	-2.311900	-0.751200	2.591000
C	-1.170100	-0.380200	3.333000
C	-0.723200	0.995400	3.333000
C	0.723200	0.995400	3.333000
C	-1.428900	1.966700	2.591000
C	-2.599000	1.586500	1.830600
C	-3.035100	0.244200	1.830600
C	-0.723200	-3.426300	0.600300
C	-3.035100	-1.746600	0.600300
C	2.311900	-0.751200	2.591000
C	-2.599000	-2.346900	-0.600300

c60_4_t -11909.1623

C	-2.317600	1.983800	-1.833800
C	-1.170500	2.817200	-1.833800
C	0.000000	2.436900	-2.594500
C	-3.488100	0.372700	-0.603000
C	-3.041000	1.748800	-0.603000
C	-2.602900	2.351800	0.603000
C	1.170500	2.817200	-1.833800
C	2.317600	1.983800	-1.833800
C	-3.488100	-0.372700	0.603000
C	0.723400	3.432600	-0.603000
C	3.041000	0.242700	1.833800
C	2.602900	1.591100	1.833800
C	1.432400	1.971500	2.594500
C	0.723400	0.995700	3.339900
C	1.170500	-0.380300	3.339900
C	3.488100	-0.372700	0.603000
C	3.488100	0.372700	-0.603000
C	3.041000	1.748800	-0.603000
C	2.602900	2.351800	0.603000
C	0.708900	2.967200	1.833800
C	-0.708900	2.967200	1.833800
C	-1.432400	1.971500	2.594500
C	-0.723400	0.995700	3.339900
C	-1.170500	-0.380300	3.339900
C	0.000000	-1.230800	3.339900
C	-2.317600	-0.753000	2.594500
C	-3.041000	0.242700	1.833800
C	-2.602900	1.591100	1.833800
C	1.432400	3.202200	0.603000
C	-1.432400	3.202200	0.603000
C	2.317600	-0.753000	2.594500
C	-0.723400	3.432600	-0.603000
C	-2.317600	0.753000	-2.594500
C	-1.170500	0.380300	-3.339900
C	0.000000	1.230800	-3.339900
C	-3.041000	-0.242700	-1.833800
C	-2.602900	-1.591100	-1.833800
C	1.170500	0.380300	-3.339900
C	2.317600	0.753000	-2.594500
C	0.723400	-0.995700	-3.339900
C	3.041000	-1.748800	0.603000
C	2.602900	-2.351800	-0.603000
C	1.432400	-3.202200	-0.603000
C	0.723400	-3.432600	0.603000
C	1.170500	-2.817200	1.833800
C	3.041000	-0.242700	-1.833800
C	2.602900	-1.591100	-1.833800
C	0.708900	-2.967200	-1.833800
C	-0.708900	-2.967200	-1.833800
C	-1.432400	-3.202200	-0.603000
C	-0.723400	-3.432600	0.603000
C	-1.170500	-2.817200	1.833800
C	0.000000	-2.436900	2.594500
C	-2.317600	-1.983800	1.833800
C	-3.041000	-1.748800	0.603000
C	-2.602900	-2.351800	-0.603000
C	1.432400	-1.971500	-2.594500
C	-1.432400	-1.971500	-2.594500
C	2.317600	-1.983800	1.833800
C	-0.723400	-0.995700	-3.339900

c60_5 -11702.4703

C	3.047700	0.241200	1.837500
C	2.607500	1.596300	1.837500
C	1.436200	1.976800	2.598600
C	3.047700	-1.751400	0.606000
C	3.495100	-0.374500	0.606000
C	3.495100	0.374500	-0.606000
C	0.712400	2.973100	1.837500
C	-0.712400	2.973100	1.837500
C	2.607500	-2.357400	-0.606000
C	1.436200	3.208300	0.606000
C	-2.323900	1.986600	-1.837500
C	-1.171200	2.824000	-1.837500
C	0.000000	2.443500	-2.598600
C	0.000000	1.231500	-3.347600
C	-1.171200	0.380600	-3.347600
C	-3.047700	1.751400	-0.606000
C	-2.607500	2.357400	0.606000
C	-1.436200	3.208300	0.606000
C	-0.723900	3.439800	-0.606000
C	1.171200	2.824000	-1.837500
C	2.323900	1.986600	-1.837500
C	2.323900	0.755100	-2.598600
C	1.171200	0.380600	-3.347600
C	0.723900	-0.996300	-3.347600
C	-0.723900	-0.996300	-3.347600

C	1.436200	-1.976800	-2.598600
C	2.607500	-1.596300	-1.837500
C	3.047700	-0.241200	-1.837500
C	0.723900	3.439800	-0.606000
C	3.047700	1.751400	-0.606000
C	-2.323900	0.755100	-2.598600
C	2.607500	2.357400	0.606000
C	2.323900	-0.755100	2.598600
C	1.171200	-0.380600	3.347600
C	0.723900	0.996300	3.347600
C	2.323900	-1.986600	1.837500
C	1.171200	-2.824000	1.837500
C	-0.723900	0.996300	3.347600
C	-1.436200	1.976800	2.598600
C	-1.171200	-0.380600	3.347600
C	-3.495100	0.374500	-0.606000
C	-3.495100	-0.374500	0.606000
C	-3.047700	-1.751400	0.606000
C	-2.607500	-2.357400	-0.606000
C	-2.607500	-1.596300	-1.837500
C	-2.607500	1.596300	1.837500
C	-3.047700	0.241200	1.837500
C	-2.323900	-1.986600	1.837500
C	-1.171200	-2.824000	1.837500
C	-0.723900	-3.439800	0.606000
C	-1.436200	-3.208300	-0.606000
C	-0.712400	-2.973100	-1.837500
C	-1.436200	-1.976800	-2.598600
C	0.712400	-2.973100	-1.837500
C	1.436200	-3.208300	-0.606000
C	0.723900	-3.439800	0.606000
C	-2.323900	-0.755100	2.598600
C	0.000000	-2.443500	2.598600
C	-3.047700	-0.241200	-1.837500
C	0.000000	-1.231500	3.347600

c60_6 -11430.8042

C	2.330800	1.989900	-1.841700
C	1.172200	2.831600	-1.841700
C	0.724500	3.447900	-0.609100
C	3.055300	-0.239800	-1.841700
C	2.330800	0.757300	-2.603400
C	1.172200	0.380900	-3.356300
C	-0.724500	3.447900	-0.609100
C	-1.440500	3.215200	0.609100
C	2.612700	-1.601800	-1.841700
C	-1.172200	2.831600	-1.841700
C	-3.503000	-0.376500	0.609100
C	-3.503000	0.376500	-0.609100
C	-3.055300	-0.239800	-1.841700
C	-2.612700	-1.601800	-1.841700
C	-2.612700	-2.363600	-0.609100
C	-3.055300	0.239800	1.841700
C	-2.612700	1.601800	1.841700
C	-2.612700	2.363600	0.609100
C	-3.055300	1.754500	-0.609100
C	-2.330800	0.757300	-2.603400
C	-1.172200	0.380900	-3.356300
C	-0.724500	-0.997100	-3.356300
C	-1.440500	-1.982700	-2.603400
C	-0.716100	-2.979900	-1.841700
C	-1.440500	-3.215200	-0.609100
C	0.716100	-2.979900	-1.841700
C	1.440500	-1.982700	-2.603400
C	0.724500	-0.997100	-3.356300
C	-2.330800	1.989900	-1.841700
C	0.000000	1.232500	-3.356300
C	-3.055300	-1.754500	0.609100
C	0.000000	2.450800	-2.603400
C	3.055300	1.754500	-0.609100
C	2.612700	2.363600	0.609100
C	1.440500	3.215200	0.609100
C	3.503000	0.376500	-0.609100
C	3.503000	-0.376500	0.609100
C	0.716100	2.979900	1.841700
C	-0.716100	2.979900	1.841700
C	1.440500	1.982700	2.603400
C	-2.330800	-0.757300	2.603400
C	-1.172200	-0.380900	3.356300
C	0.000000	-1.232500	3.356300
C	0.000000	-2.450800	2.603400
C	-1.172200	-2.831600	1.841700
C	-1.440500	1.982700	2.603400
C	-0.724500	0.997100	3.356300
C	1.172200	-0.380900	3.356300
C	2.330800	-0.757300	2.603400
C	2.330800	-1.989900	1.841700
C	1.172200	-2.831600	1.841700
C	0.724500	-3.447900	0.609100
C	-0.724500	-3.447900	0.609100
C	1.440500	-3.215200	-0.609100
C	2.612700	-2.363600	-0.609100
C	3.055300	-1.754500	0.609100
C	0.724500	0.997100	3.356300
C	3.055300	0.239800	1.841700
C	-2.330800	-1.989900	1.841700
C	2.612700	1.601800	1.841700

c60_int -13562.4359

C	1.307400	3.325500	-1.171100
C	1.585700	2.555600	-2.300300
C	0.506700	1.919000	-3.023900
C	1.307400	3.325500	1.171100
C	2.152000	3.224100	0.000000
C	3.243100	2.356000	0.000000
C	0.971000	0.623400	-3.471100
C	0.100700	-0.466700	-3.470200
C	1.585700	2.555600	2.300300
C	2.337400	0.458500	-3.023000
C	1.129700	-3.335900	-0.724100
C	2.170000	-2.721800	-1.420900
C	3.249900	-2.085400	-0.697400
C	3.249900	-2.085400	0.697400
C	2.170000	-2.721800	1.420900
C	-0.236300	-3.172600	-1.171500
C	-0.513500	-2.399300	-2.298400
C	0.565400	-1.762600	-3.022200
C	1.882600	-1.920900	-2.591700
C	3.629600	-0.891300	-1.420900
C	3.995100	0.259500	-0.723500
C	3.995100	0.259500	0.723500
C	3.629600	-0.891300	1.420900
C	2.785200	-0.789700	2.592600
C	1.882600	-1.920900	2.591700
C	2.337400	0.458500	3.023000
C	2.717400	1.653200	2.299100
C	3.530700	1.555400	1.171000
C	2.785200	-0.789700	-2.592600
C	3.530700	1.555400	-1.171000
C	1.129700	-3.335900	0.724100
C	2.717400	1.653200	-2.299100
C	-0.059000	3.489500	-0.724200
C	-1.098900	2.876000	-1.420800
C	-0.810200	2.076600	-2.592300
C	-0.059000	3.489500	0.724200
C	-1.098900	2.876000	1.420800
C	-1.711600	0.944800	-2.590100
C	-1.266300	-0.302500	-3.025200
C	-2.557200	1.047900	-1.419700
C	-1.080800	-3.070500	0.000000
C	-2.168800	-2.198500	0.000000
C	-2.457100	-1.397100	1.170900
C	-1.646300	-1.497500	2.299500
C	-0.513500	-2.399300	2.298400
C	-1.646300	-1.497500	-2.299500
C	-2.457100	-1.397100	-1.170900
C	-2.933200	-0.103600	0.724200
C	-2.557200	1.047900	1.419700
C	-1.711600	0.944800	2.590100
C	-1.266300	-0.302500	3.025200
C	0.100700	-0.466700	3.470200
C	0.565400	-1.762600	3.022200
C	0.971000	0.623400	3.471100
C	0.506700	1.919000	3.023900
C	-0.810200	2.076600	2.592300
C	-2.933200	-0.103600	-0.724200
C	-2.182200	2.239600	0.699200
C	-0.236300	-3.172600	1.171500
C	-2.182200	2.239600	-0.699200
C	-5.767500	-0.721700	1.176800
C	-5.945000	0.546200	0.727800
C	-5.945000	0.546200	-0.727800
C	-5.767500	-0.721700	-1.176800
H	-5.714400	-1.047600	2.214100
H	-6.047500	1.437100	1.346700
H	-6.047500	1.437100	-1.346700
H	-5.714400	-1.047600	-2.214100
C	-5.680700	-1.643000	0.000000
H	-6.535800	-2.348600	0.000000
H	-4.774700	-2.273800	0.000000

c60_DA_prod56 -13564.75

C	1.68690710	-1.57883209	2.27992529
C	2.50588238	-1.48611678	1.16965530
C	3.28816242	-0.22826891	0.81697321

C	2.62279055	0.95811283	1.43387964
C	1.76176465	0.85536290	2.59582562
C	1.31388525	-0.38004805	3.03330078
C	2.25691763	2.08869289	0.71823030
C	2.25680594	2.08868541	-0.71847614
C	2.62255745	0.95803582	-1.43409233
C	3.28803228	-0.22832133	-0.81728464
C	1.16533921	2.76493314	-1.43118586
C	0.86767571	1.99128327	-2.60806877
C	1.76143596	0.85526739	-2.59593043
C	1.31351939	-0.38016700	-3.03333700
C	-0.05414853	-0.53968028	-3.47571586
C	-0.92334155	0.55455245	-3.48604095
C	-0.45114945	1.84612779	-3.04077902
C	-0.52423659	-1.82803031	-3.01737368
C	-1.84246657	-1.98469100	-2.59282137
C	-2.74120773	-0.84944565	-2.59789254
C	-2.28893111	0.39419855	-3.03079319
C	-2.13619919	-2.78592108	-1.42185955
C	-3.20908266	-2.14112486	-0.70033917
C	-3.58260128	-0.94765705	-1.42099343
C	-3.93833324	0.20627262	-0.72175566
C	-3.93832025	0.20621759	0.72201512
C	-3.58254598	-0.94771908	1.42112829
C	-3.20899551	-2.14107324	0.70033928
C	-2.13608243	-2.78580808	1.42196692
C	-1.84210965	-1.98452658	2.59289999
C	-2.74106428	-0.84949141	2.59802362
C	-2.28866820	0.39407118	3.03116028
C	-0.92292538	0.55458288	3.48625743
C	-0.05373871	-0.53957678	3.47581104
C	-0.52391759	-1.82792541	3.01746171
C	0.54935772	-2.46180199	2.28141228
C	0.86800295	1.99140360	2.60807759
C	-0.45082656	1.84619550	3.04093129
C	0.26445602	-3.24949257	1.16482241
C	-1.10244083	-3.41124081	0.72526651
C	-3.46473443	1.49925718	1.17198181
C	-2.65861424	1.59286959	2.30435270
C	-1.51982174	2.48541988	2.31076132
C	-1.10250987	-3.41122457	-0.72501251
C	-2.65862157	1.59292462	-2.30364936
C	-3.46468779	1.49939707	-1.17127970
C	-3.16860376	2.29653388	0.00040544
C	-1.52003175	2.48529752	-2.31033556
C	-1.22576447	3.24404904	-1.17344498
C	-2.06774346	3.15149666	0.00037144
C	1.68666833	-1.57904995	-2.27999229
C	0.54909530	-2.46201460	-2.28133141
C	0.26439622	-3.24972673	-1.16462989
C	0.14059392	3.37896629	-0.73161796
C	2.50572445	-1.48622879	-1.16975891
C	-1.22542233	3.24432734	1.17389750
C	0.14078688	3.37906263	0.73169190
C	1.16556036	2.76496546	1.43108342
C	2.18842725	-2.24461270	0.00000317
C	1.10062459	-3.14094068	0.00008217
C	4.83960012	-0.33239619	-1.12787049
C	4.83982289	-0.33227299	1.12724724
C	5.43937895	0.98242079	0.67032504
C	5.43922838	0.98235277	-0.67125054
C	5.29912861	-1.27083565	-0.00030743
H	5.02418183	-0.63798599	-2.16572218
H	5.69592031	1.81068872	-1.33105426
H	5.69622186	1.81085384	1.32993227
H	5.02457893	-0.63777509	2.16509292
H	4.79755397	-2.24976927	-0.00018054
H	6.39153849	-1.39647924	-0.00041462

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C	1.68550129	1.57341927	-2.28485433
C	2.50020947	1.47864343	-1.16871987
C	3.28918545	0.22127120	-0.81655070
C	2.62877953	-0.97086449	-1.44459672
C	1.77181948	-0.86074129	-2.58708435
C	1.32311351	0.38386209	-3.05086679
C	2.24522487	-2.10662001	-0.71206496
C	2.24514067	-2.10651729	0.71208773
C	2.62865138	-0.97077965	1.44472438
C	3.28915069	0.22138072	0.81680223
C	1.15981552	-2.77689977	1.42050345
C	0.86432595	-1.99086867	2.59278123
C	1.77159947	-0.86058992	2.58714465
C	1.32288472	0.38395988	3.05104423
C	-0.04153883	0.53975219	3.47668107
C	-0.92373128	-0.55355737	3.48570925
C	-0.45176760	-1.84644818	3.03094824
C	-0.51958183	1.83149318	3.01487566
C	-1.84072019	1.98833607	2.59264531
C	-2.74557028	0.85946812	2.60227983
C	-2.28232961	-0.39080590	3.03377039
C	-2.13222852	2.79262479	1.42086913
C	-3.20618598	2.15044711	0.70017515
C	-3.58193241	0.95684388	1.42786060
C	-3.93649899	-0.19828294	0.72082906
C	-3.93641944	-0.19828065	-0.72100682
C	-3.58175219	0.95679864	-1.42814048
C	-3.20605067	2.15041446	-0.70050117
C	-2.13196268	2.79260908	-1.42109548
C	-1.84037090	1.98829167	-2.59282069
C	-2.74525450	0.85943214	-2.60247365
C	-2.28208868	-0.39086915	-3.03406026
C	-0.92347032	-0.55365854	-3.48580061
C	-0.04122147	0.53966629	-3.47670636
C	-0.51920332	1.83144175	-3.01487088
C	0.55028720	2.46840065	-2.28503360
C	0.86453234	-1.99100628	-2.59292477
C	-0.45154212	-1.84658830	-3.03116203
C	0.26941800	3.25731455	-1.16565435
C	-1.09695161	3.42138297	-0.72508385
C	-3.46360867	-1.49290853	-1.17065054
C	-2.65412955	-1.58814481	-2.30157596
C	-1.52391740	-2.49275188	-2.31076826
C	-1.09704778	3.42132215	0.72503814
C	-2.65421641	-1.58809324	2.30128711
C	-3.46373069	-1.49292625	1.17042390
C	-3.17381432	-2.29599172	-0.00011927
C	-1.52402810	-2.49271743	2.31052493
C	-1.23449880	-3.25793201	1.17312229
C	-2.07778734	-3.15977698	-0.00013394
C	1.68533278	1.57352696	2.28512369
C	0.55005624	2.46832885	2.28523907
C	0.26925472	3.25706750	1.16584702
C	0.12821379	-3.40577024	0.72735840
C	2.50010113	1.47866885	1.16904408
C	-1.23447821	-3.25799516	-1.17333243
C	0.12827826	-3.40578503	-0.72754652
C	1.15995458	-2.77698839	-1.42056594
C	2.17941733	2.23537621	0.00016685
C	1.10457923	3.15110871	0.00016966
C	4.83248281	0.34125929	1.12677062
C	4.83249945	0.34111805	-1.12649739
C	5.43817213	-0.97379413	-0.67053492
C	5.43816569	-0.97369939	0.67097545
C	5.29535452	1.28085091	0.00007890
H	5.01768563	0.64705697	2.16486262
H	5.67185396	-1.81006656	1.32922723
H	5.67188367	-1.81026132	-1.32864743
H	5.01766361	0.64678777	-2.16463657
H	4.78448863	2.25515812	0.00002551
H	6.38778948	1.41344912	0.00006485

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C	1.68038049	1.56970097	-2.29152647
C	2.49005928	1.47398257	-1.16866919
C	3.28663595	0.21841518	-0.81608844
C	2.63603245	-0.98023401	-1.45516569
C	1.78374629	-0.86500065	-2.58232608
C	1.33099784	0.39000415	-3.06945363
C	2.24152603	-2.12278667	-0.70755443
C	2.24152603	-2.12278667	0.70755443
C	2.63603245	-0.98023401	1.45516569
C	3.28663595	0.21841518	0.81608844
C	1.16144147	-2.78897349	1.41327793
C	0.86683575	-1.99039911	2.58207040
C	1.78374629	-0.86500065	2.58232608
C	1.33099784	0.39000415	3.06945363
C	-0.02972964	0.54109144	3.48048926
C	-0.92356856	-0.55299787	3.48627657
C	-0.44853392	-1.84737030	3.02218236
C	-0.51866853	1.83659110	3.01422537
C	-1.84370999	1.98986780	2.59366034
C	-2.75321421	0.86626263	2.60880409
C	-2.27656075	-0.39138081	3.04025156
C	-2.13386573	2.79639488	1.42031583
C	-3.20851522	2.15526304	0.70054277
C	-3.58421032	0.96089954	1.43628155
C	-3.93458029	-0.19642019	0.71977274
C	-3.93458029	-0.19642019	-0.71977274
C	-3.58421032	0.96089954	-1.43628155
C	-3.20851522	2.15526304	-0.70054277
C	-2.13386573	2.79639488	-1.42031583
C	-1.84370999	1.98986780	-2.59366034
C	-2.75321421	0.86626263	-2.60880409
C	-2.27656075	-0.39138081	-3.04025156
C	-0.92356856	-0.55299787	-3.48627657

C	-0.02972964	0.54109144	-3.48048926
C	-0.51866853	1.83659110	-3.01422537
C	0.54554304	2.47672353	-2.29021218
C	0.86683575	-1.99039911	-2.58207040
C	-0.44853392	-1.84737030	-3.02218236
C	0.26791065	3.26480195	-1.16714351
C	-1.09820250	3.43006506	-0.72527066
C	-3.45734900	-1.49174176	-1.16924880
C	-2.64562969	-1.58679756	-2.29947496
C	-1.52208086	-2.50207662	-2.31185569
C	-1.09820250	3.43006506	0.72527066
C	-2.64562969	-1.58679756	2.29947496
C	-3.45734900	-1.49174176	1.16924880
C	-3.17271740	-2.30030059	0.00000000
C	-1.52208086	-2.50207662	2.31185569
C	-1.23580069	-3.27250294	1.17291574
C	-2.07919403	-3.17141107	0.00000000
C	1.68038049	1.56970097	2.29152647
C	0.54554304	2.47672353	2.29021218
C	0.26791065	3.26480195	1.16714351
C	0.12423105	-3.42920404	0.72499314
C	2.49005928	1.47398257	1.16866919
C	-1.23580069	-3.27250294	-1.17291574
C	0.12423105	-3.42920404	-0.72499314
C	1.16144147	-2.78897349	-1.41327793
C	2.16464437	2.22818408	0.00000000
C	1.10298234	3.16330565	0.00000000
C	4.82673001	0.35568274	1.12617630
C	4.82673001	0.35568274	-1.12617630
C	5.44031339	-0.95688093	-0.67110401
C	5.44031339	-0.95688093	0.67110401
C	5.28752685	1.29851542	0.00000000
H	5.00956253	0.66163399	2.16523880
H	5.65335980	-1.80077420	1.32714632
H	5.65335980	-1.80077420	-1.32714632
H	5.00956253	0.66163399	-2.16523880
H	4.76146242	2.26500948	0.00000000
H	6.37974138	1.44410835	0.00000000

c60_DA_prod56_3e_d -13566.19

C	1.68772766	1.57025112	-2.29166598
C	2.50551681	1.48285095	-1.16764657
C	3.29480524	0.22095155	-0.81613092
C	2.64675593	-0.97991019	-1.45634256
C	1.78543186	-0.86579568	-2.58011138
C	1.33414406	0.39237338	-3.06510215
C	2.24701587	-2.12158616	-0.70725547
C	2.24712402	-2.12154427	0.70692060
C	2.64696617	-0.97991405	1.45606063
C	3.29486487	0.22099785	0.81589095
C	1.16793923	-2.79024345	1.42159532
C	0.87771925	-1.99889440	2.58680324
C	1.78576237	-0.86580013	2.57992671
C	1.33443464	0.39230933	3.06511785
C	-0.03209456	0.54733037	3.47964160
C	-0.92318389	-0.55855001	3.48753578
C	-0.45040915	-1.84796743	3.03152077
C	-0.51781382	1.83951410	3.02576648
C	-1.85514873	1.99860371	2.59789803
C	-2.75639109	0.86727965	2.60594992
C	-2.28158846	-0.39307125	3.03656798
C	-2.14251684	2.79812525	1.42916024
C	-3.21476193	2.15285763	0.70082156
C	-3.59585712	0.95872958	1.43578699
C	-3.95010417	-0.20101341	0.72082251
C	-3.95024753	-0.20090126	-0.72022058
C	-3.59595011	0.95880832	-1.43524896
C	-3.21475540	2.15287103	-0.70030512
C	-2.14247802	2.79806964	-1.42869441
C	-1.85517852	1.99862574	-2.59747212
C	-2.75652215	0.86741139	-2.60548013
C	-2.28185414	-0.39290313	-3.03628964
C	-0.92351933	-0.55838162	-3.48741836
C	-0.03236357	0.54744506	-3.47952768
C	-0.51791342	1.83961929	-3.02551392
C	0.54424770	2.47221087	-2.28823839
C	0.87739841	-1.99889250	-2.58705071
C	-0.45078060	-1.84787528	-3.03162400
C	0.26857931	3.25824866	-1.16210728
C	-1.10394460	3.43463385	-0.72052037
C	-3.47359480	-1.49668069	-1.16808360
C	-2.65614346	-1.58717553	-2.30167273
C	-1.52198815	-2.49592349	-2.31039724
C	-1.10404754	3.43468105	0.72077140
C	-2.65584728	-1.58733759	2.30186702
C	-3.47340263	-1.49683101	1.16836319
C	-3.19116588	-2.30387967	0.00001497
C	-1.52167771	-2.49597731	2.31028231
C	-1.23691830	-3.26503582	1.16879825
C	-2.08689097	-3.17510748	-0.00014739
C	1.68784725	1.57026658	2.29173971
C	0.54425742	2.47215933	2.28842548
C	0.26845307	3.25825280	1.16240058
C	0.12714950	-3.43221438	0.72134728
C	2.50558963	1.48283847	1.16770883
C	-1.23703731	-3.26513829	-1.16902922
C	0.12707686	-3.43230632	-0.72162426
C	1.16775400	-2.79033368	-1.42190154
C	2.18685352	2.23605575	0.00007930
C	1.10952164	3.16975055	0.00017700
C	4.83857381	0.35393045	1.12555120
C	4.83848420	0.35379977	-1.12605819
C	5.44778335	-0.96096228	-0.67195167
C	5.44784687	-0.96087127	0.67149856
C	5.30503517	1.29525993	-0.00032364
H	5.01935763	0.66000872	2.16557044
H	5.62948160	-1.81555912	1.32376524
H	5.62936978	-1.81573492	-1.32413318
H	5.01915514	0.65975127	-2.16614050
H	4.77369035	2.25873937	-0.00030544
H	6.39964814	1.43921750	-0.00041263

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C	-1.69596210	1.56946974	2.29301527
C	-2.52158364	1.48990638	1.16737705
C	-3.30248143	0.22152309	0.81623168
C	-2.65816693	-0.98182214	1.45789288
C	-1.78750515	-0.86846822	2.57865296
C	-1.33837168	0.39368049	3.06189510
C	-2.25241239	-2.12267477	0.70677723
C	-2.25238355	-2.12275570	-0.70667750
C	-2.65812698	-0.98186309	-1.45757499
C	-3.30242606	0.22137321	-0.81571944
C	-1.17367388	-2.79334920	-1.43049612
C	-0.88822005	-2.00838240	-2.59271584
C	-1.78767491	-0.86854720	-2.57841754
C	-1.33858775	0.39356116	-3.06148431
C	0.03403773	0.55350848	-3.48041878
C	0.92324616	-0.56401559	-3.49005595
C	0.45356523	-1.84969464	-3.04240831
C	0.51596209	1.84313920	-3.03861289
C	1.86611173	2.00751414	-2.60320812
C	2.75955721	0.86983761	-2.60450837
C	2.28751473	-0.39414510	-3.03428640
C	2.15048016	2.80054310	-1.43744515
C	3.22065170	2.15170073	-0.70098505
C	3.60758266	0.95825481	-1.43591501
C	3.96525728	-0.20357817	-0.72165561
C	3.96527172	-0.20358917	0.72132904
C	3.60769808	0.95827977	1.43568823
C	3.22070834	2.15178099	0.70088583
C	2.15067891	2.80070634	1.43751629
C	1.86633357	2.00765504	2.60327250
C	2.75977268	0.86993262	2.60431565
C	2.28771578	-0.39408253	3.03388726
C	0.92353923	-0.56396254	3.48984986
C	0.03433750	0.55359078	3.48058300
C	0.51623874	1.84330671	3.03887931
C	-0.54390094	2.46747827	2.28787122
C	-0.88794472	-2.00822365	2.59252275
C	0.45387980	-1.84962217	3.04204432
C	-0.27060731	3.25144653	1.15809612
C	1.10856479	3.43966360	0.71674233
C	3.49095815	-1.50068096	1.16735118
C	2.66809160	-1.58711601	2.30496612
C	1.52353516	-2.48985232	2.30964682
C	1.10851511	3.43952872	-0.71648284
C	2.66799836	-1.58724924	-2.30563613
C	3.49097384	-1.50064779	-1.16799296
C	3.21198581	-2.30667799	-0.00042550
C	1.52332023	-2.49000942	-2.31034561
C	1.24057596	-3.25717552	-1.16537798
C	2.09677177	-3.17825001	-0.00050379
C	-1.69601817	1.56920322	-2.29230029
C	-0.54398869	2.46719986	-2.28729571
C	-0.27066438	3.25120648	-1.15756986
C	-0.12801658	-3.43601196	-0.71829233
C	-2.52153148	1.48979715	-1.16657420
C	1.24094524	-3.25703490	1.16464984
C	-0.12784364	-3.43577344	0.71806879
C	-1.17359222	-2.79310780	1.43029940
C	-2.20987569	2.24246080	0.00042393
C	-1.11718362	3.17519679	0.00033027
C	-4.85121700	0.35258546	-1.12569528
C	-4.85135940	0.35307399	1.12573532
C	-5.45850623	-0.96282544	0.67293190

C	-5.45837736	-0.96315465	-0.67242873
C	-5.32056528	1.29373666	-0.00022586
H	-5.02830286	0.65977296	-2.16683157
H	-5.60548479	-1.82910085	-1.31959969
H	-5.60579085	-1.82838555	1.32057087
H	-5.02866007	0.66070361	2.16669612
H	-4.78151689	2.25313879	-0.00040944
H	-6.41807169	1.43924571	-0.00042328

c60_DA_prod56_5e -13224.66

C	1.70031208	1.57284067	-2.30378857
C	2.53616440	1.49381098	-1.17406905
C	3.30356175	0.21956955	-0.81836645
C	2.66150287	-0.98451903	-1.46186985
C	1.79033110	-0.86780149	-2.58182959
C	1.34550003	0.39786747	-3.07324667
C	2.25001355	-2.12990789	-0.70892719
C	2.25001355	-2.12990789	0.70892719
C	2.66150287	-0.98451903	1.46186985
C	3.30356175	0.21956955	0.81836645
C	1.17312220	-2.79703814	1.43217064
C	0.88751671	-2.00823251	2.59499167
C	1.79033110	-0.86780149	2.58182959
C	1.34550003	0.39786747	3.07324667
C	-0.03040601	0.55512542	3.49274960
C	-0.92004105	-0.56257401	3.50522986
C	-0.45502887	-1.84755427	3.04858353
C	-0.50983484	1.84802066	3.05171983
C	-1.86539436	2.00946742	2.61577029
C	-2.75523266	0.87201371	2.61271375
C	-2.28974363	-0.39614097	3.04406469
C	-2.15313877	2.79750837	1.43923716
C	-3.23412362	2.16372692	0.71112910
C	-3.60559005	0.96599667	1.43595944
C	-3.96831019	-0.20437827	0.72872932
C	-3.96831019	-0.20437827	-0.72872932
C	-3.60559005	0.96599667	-1.43595944
C	-3.23412362	2.16372692	-0.71112910
C	-2.15313877	2.79750837	-1.43923716
C	-1.86539436	2.00946742	-2.61577029
C	-2.75523266	0.87201371	-2.61271375
C	-2.28974363	-0.39614097	-3.04406469
C	-0.92004105	-0.56257401	-3.50522986
C	-0.03040601	0.55512542	-3.49274960
C	-0.50983484	1.84802066	-3.05171983
C	0.55282649	2.47191093	-2.30516568
C	0.88751671	-2.00823251	-2.59499167
C	-0.45502887	-1.84755427	-3.04858353
C	0.27129378	3.25262646	-1.16267512
C	-1.10405203	3.43617135	-0.72073605
C	-3.50849048	-1.49614597	-1.17590757
C	-2.67763801	-1.59282428	-2.32893941
C	-1.53430448	-2.48655036	-2.32059300
C	-1.10405203	3.43617135	0.72073605
C	-2.67763801	-1.59282428	2.32893941
C	-3.50849048	-1.49614597	1.17590757
C	-3.21436507	-2.29173353	0.00000000
C	-1.53430448	-2.48655036	2.32059300
C	-1.25087853	-3.26382150	1.17108092
C	-2.10352559	-3.16943760	0.00000000
C	1.70031208	1.57284067	2.30378857
C	0.55282649	2.47191093	2.30516568
C	0.27129378	3.25262646	1.16267512
C	0.11539912	-3.43513200	0.71969658
C	2.53616440	1.49381098	1.17406905
C	-1.25087853	-3.26382150	-1.17108092
C	0.11539912	-3.43513200	-0.71969658
C	1.17312220	-2.79703814	-1.43217064
C	2.20891024	2.23308283	0.00000000
C	1.11484348	3.16677440	0.00000000
C	4.86652067	0.34464480	1.12633024
C	4.86652067	0.34464480	-1.12633024
C	5.47266680	-0.97000908	-0.67640568
C	5.47266680	-0.97000908	0.67640568
C	5.33177346	1.28624195	0.00000000
H	5.03770711	0.65716014	2.16780472
H	5.55909335	-1.85227593	1.31439947
H	5.55909335	-1.85227593	-1.31439947
H	5.03770711	0.65716014	-2.16780472
H	4.77983759	2.23931224	0.00000000
H	6.43186321	1.44062226	0.00000000

c60_DA_prod56_6e -12959.07

C	-1.70673591	1.57154051	2.31618388
C	-2.54833910	1.48419663	1.17906804
C	-3.30315873	0.20921896	0.82022155
C	-2.65754363	-0.99111831	1.46360822
C	-1.78843675	-0.87178483	2.58545947
C	-1.34944342	0.39770651	3.08463538
C	-2.24501744	-2.14246717	0.71219097
C	-2.24505975	-2.14252501	-0.71217964
C	-2.65766335	-0.99120826	-1.46356871
C	-3.30327031	0.20912743	-0.82018796
C	-1.16636115	-2.80434679	-1.43443057
C	-0.88109075	-2.01124206	-2.59817036
C	-1.78862618	-0.87192123	-2.58545585
C	-1.34974254	0.39763367	-3.08456362
C	0.02837067	0.55553060	-3.50505312
C	0.92123896	-0.56094878	-3.51952345
C	0.46237778	-1.84725744	-3.05476201
C	0.50222528	1.85207998	-3.06261926
C	1.86158306	2.01443598	-2.62613784
C	2.75229055	0.87892179	-2.62059977
C	2.29462654	-0.39469107	-3.05373152
C	2.15102997	2.80017517	-1.44036660
C	3.24170051	2.18062072	-0.71999285
C	3.60480207	0.97968972	-1.43799763
C	3.97362586	-0.19741242	-0.73486255
C	3.97373834	-0.19739073	0.73460484
C	3.60506455	0.97972840	1.43782766
C	3.24181966	2.18066831	0.72000754
C	2.15127488	2.80020849	1.44061082
C	1.86196455	2.01447907	2.62632129
C	2.75269209	0.87897601	2.62055804
C	2.29497323	-0.39464567	3.05361239
C	0.92158226	-0.56087871	3.51943701
C	0.02871276	0.55561716	3.50509638
C	0.50266492	1.85216899	3.06288435
C	-0.56585054	2.47426359	2.32124427
C	-0.88095112	-2.01111271	2.59808839
C	0.46257108	-1.84714226	3.05462292
C	-0.27851703	3.25401063	1.16763431
C	1.09323628	3.43683816	0.72472542
C	3.52766872	-1.48704499	1.18224003
C	2.69101544	-1.59353491	2.34861322
C	1.55049854	-2.48377920	2.33120203
C	1.09309208	3.43674869	-0.72421421
C	2.69081043	-1.59356363	-2.34880514
C	3.52759529	-1.48706079	-1.18253128
C	3.22370165	-2.27617879	-0.00013544
C	1.55036020	-2.48384609	-2.33138042
C	1.26714522	-3.27000553	-1.17667866
C	2.11654607	-3.16096705	-0.00010185
C	-1.70702359	1.57143036	-2.31602459
C	-0.56619633	2.47424389	-2.32083467
C	-0.27868973	3.25393951	-1.16711538
C	-0.09663918	-3.43623355	-0.72198162
C	-2.54850621	1.48414388	-1.17891263
C	1.26720263	-3.26996581	1.17652701
C	-0.09662947	-3.43619692	0.72191278
C	-1.16629697	-2.80426680	1.43437697
C	-2.21125579	2.21569393	0.00007593
C	-1.11828635	3.15412918	0.00029003
C	-4.89384528	0.33467743	-1.12871327
C	-4.89374082	0.33486827	1.12853472
C	-5.52625149	-0.96589725	0.68839154
C	-5.52627299	-0.96606414	-0.68848132
C	-5.33966962	1.28197594	-0.00015212
H	-5.04959514	0.66403090	-2.16896176
H	-5.48772113	-1.87448517	-1.29923269
H	-5.48764487	-1.87419267	1.29930335
H	-5.04946193	0.66439478	2.16872468
H	-4.76952145	2.22535798	-0.00018179
H	-6.44155130	1.45498345	-0.00019326

c60_DA_prod66 -13581.5

C	-1.98165534	2.42006260	-0.73581803
C	-2.47013563	1.33616595	-1.43066263
C	-3.26666806	0.20802927	-0.80045515
C	-0.02643356	3.47431429	0.00000000
C	-0.77247336	3.07399929	-1.17254521
C	-0.09277529	2.62309759	-2.30911297
C	-2.60425448	-0.99773183	-1.43598446
C	-2.24282971	-2.12784524	-0.73618014
C	1.36618549	3.41164185	0.00000000
C	-1.83917414	-0.59380331	-2.57591780
C	1.72278354	-3.09616355	-1.17244257
C	1.05415096	-2.63038900	-2.30550752
C	1.57310069	-1.48835148	-3.03072974
C	2.73752800	-0.85619174	-2.59515481
C	3.42907374	-1.34276120	-1.42209423
C	0.97127584	-3.49361323	0.00000000
C	-0.41906189	-3.39621878	0.00000000
C	-1.11481284	-2.91365429	-1.17255353
C	-0.38808638	-2.54441914	-2.30982892
C	0.44813076	-0.69831301	-3.48059305

C	0.52696290	0.69331431	-3.47994642
C	1.73467266	1.35014886	-3.03031406
C	2.81988528	0.58971250	-2.59511519
C	3.56240158	0.99448451	-1.42202901
C	3.94000860	-0.19951513	-0.69733206
C	3.19246377	2.14510326	-0.72508264
C	2.06736772	2.93086534	-1.17239521
C	1.34982364	2.54410529	-2.30529118
C	-0.76027670	-1.35747942	-3.03093301
C	-0.59870066	1.48551837	-3.02868981
C	2.93000878	-2.44363921	-0.72507772
C	-4.81671709	0.32594949	-1.12411321
C	-5.43792319	-0.97671421	-0.67072462
C	-5.24837272	1.28117328	0.00000000
H	-4.70006435	2.23628711	0.00000000
H	-6.33443253	1.45441369	0.00000000
H	-5.70289932	-1.80102338	-1.33262984
H	-4.99113847	0.63228631	-2.16330781
C	-1.75764733	0.84960165	-2.57404379
C	-1.98165534	2.42006260	0.73581803
C	-2.47013563	1.33616595	1.43066263
C	-3.26666806	0.20802927	0.80045515
C	-0.77247336	3.07399929	1.17254521
C	-0.09277529	2.62309759	2.30911297
C	-2.60425448	-0.99773183	1.43598446
C	-2.24282971	-2.12784524	0.73618014
C	-1.83917414	-0.59380331	2.57591780
C	1.72278354	-3.09616355	1.17244257
C	1.05415096	-2.63038900	2.30550752
C	1.57310069	-1.48835148	3.03072974
C	2.73752800	-0.85619174	2.59515481
C	3.42907374	-1.34276120	1.42209423
C	-1.11481284	-2.91365429	1.17255353
C	-0.38808638	-2.54441914	2.30982892
C	0.44813076	-0.69831301	3.48059305
C	0.52696290	0.69331431	3.47994642
C	1.73467266	1.35014886	3.03031406
C	2.81988528	0.58971250	2.59511519
C	3.56240158	0.99448451	1.42202901
C	3.94000860	-0.19951513	0.69733206
C	3.19246377	2.14510326	0.72508264
C	2.06736772	2.93086534	1.17239521
C	1.34982364	2.54410529	2.30529118
C	-0.76027670	-1.35747942	3.03093301
C	-0.59870066	1.48551837	3.02868981
C	2.93000878	-2.44363921	0.72507772
C	-4.81671709	0.32594949	1.12411321
C	-5.43792319	-0.97671421	0.67072462
H	-5.70289932	-1.80102338	1.33262984
H	-4.99113847	0.63228631	2.16330781
C	-1.75764733	0.84960165	2.57404379

c60_DA_prod66_1e -13645.82

C	1.99217034	-2.41705092	-0.73363530
C	2.47861142	-1.33368634	-1.43404143
C	3.27263655	-0.20427796	-0.80045186
C	0.03736106	-3.48631424	0.00000000
C	0.77615881	-3.07411175	-1.16625939
C	0.09950778	-2.61619361	-2.30600810
C	2.61151697	1.00182303	-1.43979650
C	2.24792499	2.12972211	-0.73379765
C	-1.37174268	-3.42402072	0.00000000
C	1.85246611	0.59331395	-2.58087796
C	-1.72761711	3.09631942	-1.16643014
C	-1.06086144	2.62300162	-2.30279793
C	-1.57867546	1.48951979	-3.03064401
C	-2.75303179	0.85077040	-2.60001728
C	-3.43941550	1.33879144	-1.42458924
C	-0.98365925	3.50472532	0.00000000
C	0.42328744	3.40938209	0.00000000
C	1.11165656	2.91704962	-1.16624711
C	0.38802531	2.53843580	-2.30658301
C	-0.44858995	0.69781754	-3.47003440
C	-0.52629251	-0.69391599	-3.46961786
C	-1.73763417	-1.35448953	-3.03047433
C	-2.83364850	-0.58860714	-2.59999843
C	-3.57003758	-0.99675459	-1.42458258
C	-3.95085556	0.19602708	-0.69767350
C	-3.19802342	-2.14633091	-0.72335574
C	-2.06518872	-2.93445040	-1.16624505
C	-1.34981937	-2.53851367	-2.30245687
C	0.76494664	1.36211680	-3.03352976
C	0.60581254	-1.48878967	-3.03101926
C	-2.94107501	2.43945244	-0.72345913
C	4.81944942	-0.32358877	-1.12322620
C	5.44371780	0.97841482	-0.67087932
C	5.25394544	-1.27935406	0.00000000
H	4.69705996	-2.22965750	0.00000000
H	6.34030104	-1.45598584	0.00000000
H	5.68561501	1.81156732	-1.33069144
H	4.99098302	-0.62957457	-2.16317294
C	1.77223421	-0.84548261	-2.57848685
C	1.99217034	-2.41705092	0.73363530
C	2.47861142	-1.33368634	1.43404143
C	3.27263655	-0.20427796	0.80045186
C	0.77615881	-3.07411175	1.16625939
C	0.09950778	-2.61619361	2.30600810
C	2.61151697	1.00182303	1.43979650
C	2.24792499	2.12972211	0.73379765
C	1.85246611	0.59331395	2.58087796
C	-1.72761711	3.09631942	1.16643014
C	-1.06086144	2.62300162	2.30279793
C	-1.57867546	1.48951979	3.03064401
C	-2.75303179	0.85077040	2.60001728
C	-3.43941550	1.33879144	1.42458924
C	1.11165656	2.91704962	1.16624711
C	0.38802531	2.53843580	2.30658301
C	-0.44858995	0.69781754	3.47003440
C	-0.52629251	-0.69391599	3.46961786
C	-1.73763417	-1.35448953	3.03047433
C	-2.83364850	-0.58860714	2.59999843
C	-3.57003758	-0.99675459	1.42458258
C	-3.95085556	0.19602708	0.69767350
C	-3.19802342	-2.14633091	0.72335574
C	-2.06518872	-2.93445040	1.16624505
C	-1.34981937	-2.53851367	2.30245687
C	0.76494664	1.36211680	3.03352976
C	0.60581254	-1.48878967	3.03101926
C	-2.94107501	2.43945244	0.72345913
C	4.81944942	-0.32358877	1.12322620
C	5.44371780	0.97841482	0.67087932
H	5.68561501	1.81156732	1.33069144
H	4.99098302	-0.62957457	2.16317294
C	1.77223421	-0.84548261	2.57848685

c60_DA_prod66_2e_s -13641.24

C	2.00306121	-2.41437783	-0.73134382
C	2.48800808	-1.33115043	-1.43787356
C	3.27915280	-0.20038364	-0.80063774
C	0.04837552	-3.49936715	0.00000000
C	0.77987685	-3.07508776	-1.16036633
C	0.10612492	-2.60968421	-2.30365215
C	2.61991906	1.00636572	-1.44388008
C	2.25345481	2.13200975	-0.73153649
C	-1.37752812	-3.43741568	0.00000000
C	1.86533545	0.59374507	-2.58548332
C	-1.73316879	3.09700307	-1.16065315
C	-1.06816987	2.61572773	-2.30025977
C	-1.58508740	1.49097291	-3.03153511
C	-2.76960952	0.84546617	-2.60561904
C	-3.45047744	1.33429131	-1.42743334
C	-0.99651530	3.51604321	0.00000000
C	0.42724336	3.42252917	0.00000000
C	1.10823912	2.92057315	-1.16017601
C	0.38772401	2.53270786	-2.30380220
C	-0.44989919	0.69755932	-3.45978650
C	-0.52582613	-0.69461218	-3.45955979
C	-1.74122146	-1.35960196	-3.03152661
C	-2.84805506	-0.58839237	-2.60557996
C	-3.57809982	-0.99988198	-1.42736757
C	-3.96207652	0.19175735	-0.69817393
C	-3.20375066	-2.14857863	-0.72183752
C	-2.06362848	-2.93969033	-1.16063248
C	-1.35047838	-2.53406930	-2.30065487
C	0.76943759	1.36739184	-3.03661395
C	0.61308691	-1.49237862	-3.03461287
C	-2.95295925	2.43517847	-0.72182713
C	4.82502486	-0.32114324	-1.12261413
C	5.45190605	0.98014262	-0.67128440
C	5.26145991	-1.27765608	0.00000000
H	4.69602070	-2.22316342	0.00000000
H	6.34870085	-1.45768092	0.00000000
H	5.67070937	1.82198931	-1.32858815
H	4.99277470	-0.62683718	-2.16361084
C	1.78711408	-0.84154814	-2.58324829
C	2.00306121	-2.41437783	0.73134382
C	2.48800808	-1.33115043	1.43787356
C	3.27915280	-0.20038364	0.80063774
C	0.77987685	-3.07508776	1.16036633
C	0.10612492	-2.60968421	2.30365215
C	2.61991906	1.00636572	1.44388008
C	2.25345481	2.13200975	0.73153649
C	1.86533545	0.59374507	2.58548332
C	-1.73316879	3.09700307	1.16065315
C	-1.06816987	2.61572773	2.30025977
C	-1.58508740	1.49097291	3.03153511

C	-2.76960952	0.84546617	2.60561904
C	-3.45047744	1.33429131	1.42743334
C	1.10823912	2.92057315	1.16017601
C	0.38772401	2.53270786	2.30380220
C	-0.44989919	0.69755932	3.45978650
C	-0.52582613	-0.69461218	3.45955979
C	-1.74122146	-1.35960196	3.03152661
C	-2.84805506	-0.58839237	2.60557996
C	-3.57809982	-0.99988198	1.42736757
C	-3.96207652	0.19175735	0.69817393
C	-3.20375066	-2.14857863	0.72183752
C	-2.06362848	-2.93969033	1.16063248
C	-1.35047838	-2.53406930	2.30065487
C	0.76943759	1.36739184	3.03661395
C	0.61308691	-1.49237862	3.03461287
C	-2.95295925	2.43517847	0.72182713
C	4.82502486	-0.32114324	1.12261413
C	5.45190605	0.98014262	0.67128440
H	5.67070937	1.82198931	1.32858815
H	4.99277470	-0.62683718	2.16361084
C	1.78711408	-0.84154814	2.58324829

c60_DA_prod66_3e_d -13568.93

C	2.00987628	2.43276475	0.72855835
C	2.48961073	1.33906288	1.44270157
C	3.26960104	0.20041525	0.79954957
C	0.04970921	3.51274382	0.00000000
C	0.78419245	3.08681895	1.16028062
C	0.10522798	2.61770526	2.30223550
C	2.62284373	-1.01355180	1.44915429
C	2.26192193	-2.14820346	0.72885151
C	-1.37727755	3.44894634	0.00000000
C	1.86450998	-0.59795628	2.57894306
C	-1.73373552	-3.10669117	1.15989671
C	-1.06500645	-2.62497092	2.29932641
C	-1.57902037	-1.49342935	3.03457241
C	-2.76765770	-0.85027846	2.59955965
C	-3.45250119	-1.34136453	1.43195305
C	-0.99390470	-3.52834233	0.00000000
C	0.43113346	-3.43622011	0.00000000
C	1.11450599	-2.93184310	1.16022775
C	0.38829249	-2.54145917	2.30256417
C	-0.44959848	-0.70648740	3.47203636
C	-0.52655389	0.70239611	3.47138587
C	-1.73565153	1.36125955	3.03467074
C	-2.84688583	0.59165662	2.59966661
C	-3.58123293	1.00471691	1.43216963
C	-3.95135640	-0.19225024	0.69843523
C	-3.21106395	2.16417672	0.71864891
C	-2.06593724	2.94755301	1.15974670
C	-1.34869745	2.54192359	2.29941541
C	0.76467490	-1.36937393	3.03806686
C	0.60793280	1.49313294	3.03571669
C	-2.95780547	-2.45340127	0.71860593
C	4.81805545	0.32390101	1.12204618
C	5.44828892	-0.97574690	0.67195446
C	5.25400680	1.28196589	0.00000000
H	4.67918537	2.22223856	0.00000000
H	6.34243354	1.46776859	0.00000000
H	5.63932114	-1.82748888	1.32598244
H	4.97999384	0.62993778	2.16434777
C	1.78530884	0.84526082	2.57607318
C	2.00987628	2.43276475	-0.72855835
C	2.48961073	1.33906288	-1.44270157
C	3.26960104	0.20041525	-0.79954957
C	0.78419245	3.08681895	-1.16028062
C	0.10522798	2.61770526	-2.30223550
C	2.62284373	-1.01355180	-1.44915429
C	2.26192193	-2.14820346	-0.72885151
C	1.86450998	-0.59795628	-2.57894306
C	-1.73373552	-3.10669117	-1.15989671
C	-1.06500645	-2.62497092	-2.29932641
C	-1.57902037	-1.49342935	-3.03457241
C	-2.76765770	-0.85027846	-2.59955965
C	-3.45250119	-1.34136453	-1.43195305
C	1.11450599	-2.93184310	-1.16022775
C	0.38829249	-2.54145917	-2.30256417
C	-0.44959848	-0.70648740	-3.47203636
C	-0.52655389	0.70239611	-3.47138587
C	-1.73565153	1.36125955	-3.03467074
C	-2.84688583	0.59165662	-2.59966661
C	-3.58123293	1.00471691	-1.43216963
C	-3.95135640	-0.19225024	-0.69843523
C	-3.21106395	2.16417672	-0.71864891
C	-2.06593724	2.94755301	-1.15974670
C	-1.34869745	2.54192359	-2.29941541
C	0.76467490	-1.36937393	-3.03806686
C	0.60793280	1.49313294	-3.03571669
C	-2.95780547	-2.45340127	-0.71860593
C	4.81805545	0.32390101	-1.12204618
C	5.44828892	-0.97574690	-0.67195446
H	5.63932114	-1.82748888	-1.32598244
H	4.97999384	0.62993778	-2.16434777
C	1.78530884	0.84526082	-2.57607318

c60_DA_prod66_4e_s -13430.22

C	-2.01878148	-2.45055709	0.72566106
C	-2.49406986	-1.34576111	1.44812565
C	-3.26117565	-0.19841262	0.79845284
C	-0.05286713	-3.52592134	0.00000000
C	-0.79019294	-3.09762405	1.16026739
C	-0.10611650	-2.62601053	2.30163383
C	-2.62749617	1.02292135	1.45512965
C	-2.27016643	2.16702158	0.72612645
C	1.37539835	-3.46140566	0.00000000
C	-1.86454179	0.60379760	2.57259860
C	1.73699968	3.11567436	1.15967858
C	1.06404804	2.63423568	2.29983764
C	1.57429251	1.49545180	3.03943353
C	2.76662264	0.85347690	2.59500488
C	3.45575624	1.34604740	1.43692478
C	0.99449117	3.53982581	0.00000000
C	-0.43208294	3.45003876	0.00000000
C	-1.11854406	2.94378580	1.16030884
C	-0.38715341	2.55106669	2.30199970
C	0.44857329	0.71567909	3.48501489
C	0.52569348	-0.71051893	3.48401011
C	1.72927362	-1.36427495	3.03922350
C	2.84550024	-0.59693100	2.59500841
C	3.58364305	-1.01195747	1.43714504
C	3.94143095	0.19004683	0.69882346
C	3.21665238	-2.18191280	0.71633490
C	2.06685862	-2.95747985	1.15952138
C	1.34551474	-2.55133014	2.29967328
C	-0.75993737	1.37269874	3.04101652
C	-0.60444096	-1.49387093	3.03827927
C	2.96433128	2.46934920	0.71623001
C	-4.81357455	-0.32488835	1.12172438
C	-5.44780736	0.97289400	0.67296435
C	-5.24832847	-1.28448977	0.00000000
H	-4.66545629	-2.22032193	0.00000000
H	-6.33901560	-1.47481024	0.00000000
H	-5.60839885	1.83496266	1.32281570
H	-4.96820771	-0.63267550	2.16528061
C	-1.78479669	-0.84777256	2.56875159
C	-2.01878148	-2.45055709	-0.72566106
C	-2.49406986	-1.34576111	-1.44812565
C	-3.26117565	-0.19841262	-0.79845284
C	-0.79019294	-3.09762405	-1.16026739
C	-0.10611650	-2.62601053	-2.30163383
C	-2.62749617	1.02292135	-1.45512965
C	-2.27016643	2.16702158	-0.72612645
C	-1.86454179	0.60379760	-2.57259860
C	1.73699968	3.11567436	-1.15967858
C	1.06404804	2.63423568	-2.29983764
C	1.57429251	1.49545180	-3.03943353
C	2.76662264	0.85347690	-2.59500488
C	3.45575624	1.34604740	-1.43692478
C	-1.11854406	2.94378580	-1.16030884
C	-0.38715341	2.55106669	-2.30199970
C	0.44857329	0.71567909	-3.48501489
C	0.52569348	-0.71051893	-3.48401011
C	1.72927362	-1.36427495	-3.03922350
C	2.84550024	-0.59693100	-2.59500841
C	3.58364305	-1.01195747	-1.43714504
C	3.94143095	0.19004683	-0.69882346
C	3.21665238	-2.18191280	-0.71633490
C	2.06685862	-2.95747985	-1.15952138
C	1.34551474	-2.55133014	-2.29967328
C	-0.75993737	1.37269874	-3.04101652
C	-0.60444096	-1.49387093	-3.03827927
C	2.96433128	2.46934920	-0.71623001
C	-4.81357455	-0.32488835	-1.12172438
C	-5.44780736	0.97289400	-0.67296435
H	-5.60839885	1.83496266	-1.32281570
H	-4.96820771	-0.63267550	-2.16528061
C	-1.78479669	-0.84777256	-2.56875159

c60_DA_prod66_5e -13221.31

C	2.02240465	-2.43914632	-0.72591443
C	2.50629343	-1.33364094	-1.45255843
C	3.26517129	-0.18283216	-0.80230435
C	0.05929876	-3.51747270	0.00000000
C	0.79974201	-3.09660779	-1.16437210
C	0.11007249	-2.62637156	-2.31109070
C	2.63270741	1.03564935	-1.46126577

C	2.25874518	2.17730822	-0.72647601
C	-1.36996442	-3.45575173	0.00000000
C	1.86465920	0.61393755	-2.57732193
C	-1.76109883	3.11574655	-1.16570417
C	-1.07733081	2.63890564	-2.31743754
C	-1.57991192	1.49676477	-3.05066652
C	-2.77411123	0.84190328	-2.61040255
C	-3.46623437	1.32625426	-1.43822129
C	-1.01738370	3.53086243	0.00000000
C	0.41171110	3.45033570	0.00000000
C	1.10506080	2.95410098	-1.16345197
C	0.37213222	2.55718630	-2.30877945
C	-0.44889580	0.71762671	-3.49533670
C	-0.52056551	-0.71061596	-3.49447982
C	-1.72378213	-1.37250834	-3.04960097
C	-2.84679932	-0.60229776	-2.61084150
C	-3.58509931	-1.01569633	-1.43868759
C	-3.96709926	0.17677141	-0.71083973
C	-3.20675593	-2.18878968	-0.72155714
C	-2.06832091	-2.96869678	-1.16668074
C	-1.33809257	-2.56128894	-2.31844305
C	0.75711484	1.37940520	-3.04903178
C	0.61248965	-1.49029365	-3.04716298
C	-2.97484011	2.45614997	-0.72123419
C	4.83508804	-0.32157370	-1.12341239
C	5.49948865	0.95751868	-0.68050455
C	5.24745104	-1.28946172	0.00000000
H	4.64303571	-2.21210177	0.00000000
H	6.33755172	-1.50172687	0.00000000
H	5.59557142	1.84146101	-1.31600434
H	4.97534381	-0.64154306	-2.16629812
C	1.79029858	-0.83917540	-2.57475843
C	2.02240465	-2.43914632	0.72591443
C	2.50629343	-1.33364094	1.45255843
C	3.26517129	-0.18283216	0.80230435
C	0.79974201	-3.09660779	1.16437210
C	0.11007249	-2.62637156	2.31109070
C	2.63270741	1.03564935	1.46126577
C	2.25874518	2.17730822	0.72647601
C	1.86465920	0.61393755	2.57732193
C	-1.76109883	3.11574655	1.16570417
C	-1.07733081	2.63890564	2.31743754
C	-1.57991192	1.49676477	3.05066652
C	-2.77411123	0.84190328	2.61040255
C	-3.46623437	1.32625426	1.43822129
C	1.10506080	2.95410098	1.16345197
C	0.37213222	2.55718630	2.30877945
C	-0.44889580	0.71762671	3.49533670
C	-0.52056551	-0.71061596	3.49447982
C	-1.72378213	-1.37250834	3.04960097
C	-2.84679932	-0.60229776	2.61084150
C	-3.58509931	-1.01569633	1.43868759
C	-3.96709926	0.17677141	0.71083973
C	-3.20675593	-2.18878968	0.72155714
C	-2.06832091	-2.96869678	1.16668074
C	-1.33809257	-2.56128894	2.31844305
C	0.75711484	1.37940520	3.04903178
C	0.61248965	-1.49029365	3.04716298
C	-2.97484011	2.45614997	0.72123419
C	4.83508804	-0.32157370	1.12341239
C	5.49948865	0.95751868	0.68050455
H	5.59557142	1.84146101	1.31600434
H	4.97534381	-0.64154306	2.16629812
C	1.79029858	-0.83917540	2.57475843

c60_DA_prod66_6e -12952.41

C	2.03287619	-2.41785413	-0.72712142
C	2.51831085	-1.30705889	-1.45227171
C	3.27203459	-0.15423111	-0.80527554
C	0.07805568	-3.50727371	0.00000000
C	0.81987305	-3.09054027	-1.16839536
C	0.12245228	-2.62586428	-2.32140982
C	2.63199182	1.05601813	-1.46382547
C	2.23968621	2.19522677	-0.72765867
C	-1.35272734	-3.45599059	0.00000000
C	1.86171714	0.63166682	-2.58174177
C	-1.79518310	3.11087729	-1.17056779
C	-1.10079200	2.64026877	-2.33175759
C	-1.59334664	1.49330292	-3.06075677
C	-2.78706737	0.82356995	-2.62311361
C	-3.48496111	1.29889115	-1.44067091
C	-1.05123255	3.52215285	0.00000000
C	0.38090841	3.45330581	0.00000000
C	1.08195034	2.96824247	-1.16629413
C	0.34831441	2.56587593	-2.31551037
C	-0.45467253	0.71955280	-3.50454742
C	-0.51607899	-0.71095925	-3.50387198
C	-1.71664156	-1.38423317	-3.05917359
C	-2.84906094	-0.61721370	-2.62409664
C	-3.58807116	-1.03323767	-1.44134417
C	-3.99046883	0.15075911	-0.72083147
C	-3.19321039	-2.20781756	-0.72570839
C	-2.05974279	-2.98632844	-1.17294367
C	-1.32329852	-2.57344751	-2.33421211
C	0.74772879	1.39012205	-3.05548729
C	0.62348976	-1.48315202	-3.05463350
C	-2.99686249	2.43664855	-0.72499668
C	4.87181666	-0.31112423	-1.12685148
C	5.59826656	0.93320490	-0.69862464
C	5.24631017	-1.29230409	0.00000000
H	4.61475058	-2.19697397	0.00000000
H	6.33345344	-1.53602667	0.00000000
H	5.55898549	1.85361054	-1.29403243
H	4.98646390	-0.65372508	-2.16764619
C	1.79710426	-0.82233622	-2.58056662
C	2.03287619	-2.41785413	0.72712142
C	2.51831085	-1.30705889	1.45227171
C	3.27203459	-0.15423111	0.80527554
C	0.81987305	-3.09054027	1.16839536
C	0.12245228	-2.62586428	2.32140982
C	2.63199182	1.05601813	1.46382547
C	2.23968621	2.19522677	0.72765867
C	1.86171714	0.63166682	2.58174177
C	-1.79518310	3.11087729	1.17056779
C	-1.10079200	2.64026877	2.33175759
C	-1.59334664	1.49330292	3.06075677
C	-2.78706737	0.82356995	2.62311361
C	-3.48496111	1.29889115	1.44067091
C	1.08195034	2.96824247	1.16629413
C	0.34831441	2.56587593	2.31551037
C	-0.45467253	0.71955280	3.50454742
C	-0.51607899	-0.71095925	3.50387198
C	-1.71664156	-1.38423317	3.05917359
C	-2.84906094	-0.61721370	2.62409664
C	-3.58807116	-1.03323767	1.44134417
C	-3.99046883	0.15075911	0.72083147
C	-3.19321039	-2.20781756	0.72570839
C	-2.05974279	-2.98632844	1.17294367
C	-1.32329852	-2.57344751	2.33421211
C	0.74772879	1.39012205	3.05548729
C	0.62348976	-1.48315202	3.05463350
C	-2.99686249	2.43664855	0.72499668
C	4.87181666	-0.31112423	1.12685148
C	5.59826656	0.93320490	0.69862464
H	5.55898549	1.85361054	1.29403243
H	4.98646390	-0.65372508	2.16764619
C	1.79710426	-0.82233622	2.58056662

c60_DA_ts56 -13547.48

C	1.68654551	-1.55442020	2.28612110
C	2.50007914	-1.45149225	1.16725298
C	3.12180049	-0.17258819	0.75544103
C	2.59038474	0.98644204	1.41675010
C	1.73957614	0.87869851	2.58166978
C	1.30314635	-0.36210764	3.02609353
C	2.22833037	2.15375234	0.70934426
C	2.22835342	2.15380703	-0.70905506
C	2.59026807	0.98642797	-1.41640929
C	3.12162503	-0.17259550	-0.75508360
C	1.13354803	2.80180423	-1.42535757
C	0.84105036	2.01092964	-2.59696592
C	1.73963421	0.87870730	-2.58138602
C	1.30333877	-0.36217229	-3.02577826
C	-0.06141187	-0.53198988	-3.47245419
C	-0.93671698	0.55604843	-3.47842355
C	-0.47513241	1.85232688	-3.03155507
C	-0.52143196	-1.82705266	-3.01935296
C	-1.83872956	-1.99116729	-2.59183976
C	-2.74541714	-0.86293375	-2.59559598
C	-2.30135063	0.38550935	-3.02628356
C	-2.12506478	-2.79371907	-1.42089848
C	-3.20590769	-2.15918443	-0.69877104
C	-3.58805548	-0.96753845	-1.42089971
C	-3.95382620	0.18319121	-0.72255848
C	-3.95393393	0.18319127	0.72267435
C	-3.58820379	-0.96753876	1.42099290
C	-3.20597521	-2.15917063	0.69888185
C	-2.12515280	-2.79358513	1.42110411
C	-1.83896438	-1.99101142	2.59206225
C	-2.74574017	-0.86285457	2.59583538
C	-2.30169600	0.38560488	3.02664563
C	-0.93694246	0.55610648	3.47869975
C	-0.06165574	-0.53184111	3.47267307
C	-0.52170932	-1.82686617	3.01960279

C	0.55735924	-2.45578391	2.28878587
C	0.84094907	2.01087330	2.59721518
C	-0.47525501	1.85228811	3.03181469
C	0.28122449	-3.23924202	1.16852559
C	-1.08480716	-3.40846632	0.72472423
C	-3.49187493	1.48060069	1.17136605
C	-2.68277372	1.58071107	2.30136173
C	-1.55263553	2.48489832	2.30602571
C	-1.08473800	-3.40850484	-0.72435622
C	-2.68256144	1.58063669	-2.30104591
C	-3.49171598	1.48058702	-1.17111700
C	-3.20361369	2.28066647	0.00018114
C	-1.55251620	2.48488004	-2.30568722
C	-1.26870966	3.24939403	-1.17193658
C	-2.11148007	3.14746588	0.00020557
C	1.68659716	-1.55448736	-2.28559985
C	0.55752770	-2.45594208	-2.28832274
C	0.28135941	-3.23932292	-1.16793708
C	0.09736720	3.41002203	-0.72798232
C	2.49997210	-1.45155653	-1.16663197
C	-1.26875929	3.24942284	1.17233763
C	0.09733107	3.41005051	0.72831615
C	1.13347800	2.80171284	1.42561468
C	2.20629070	-2.24087324	0.00037350
C	1.12222873	-3.12908639	0.00036457
C	5.19646113	-0.35341016	-1.15519205
C	5.19747671	-0.35356909	1.15367770
C	5.61909331	0.91230782	0.69632007
C	5.61849488	0.91239476	-0.69805384
C	5.37139366	-1.30186374	-0.00091938
H	5.20387885	-0.66911750	-2.19945225
H	5.76026647	1.79114783	-1.32656680
H	5.76137038	1.79102128	1.32475631
H	5.20590066	-0.66945006	2.19786139
H	4.73785125	-2.19687376	-0.00074200
H	6.43132950	-1.62837630	-0.00146089

c60_DA_ts56_1e -13614.52

C	1.68776204	2.28618583	1.54353343
C	2.49587491	1.16218928	1.43296546
C	3.10231385	0.74791353	0.14843967
C	2.58151619	1.42727910	-1.01064265
C	1.73901717	2.58223228	-0.89428026
C	1.30410667	3.03785239	0.35984084
C	2.19620239	0.70810875	-2.17783982
C	2.19638515	-0.70377450	-2.17910798
C	2.58188580	-1.42494308	-1.01317938
C	3.10253444	-0.74751550	0.14710355
C	1.10462189	-1.41836511	-2.82110765
C	0.82117377	-2.58720892	-2.01880250
C	1.73972527	-2.58036941	-0.89894488
C	1.30488961	-3.03833447	0.35440361
C	-0.05355314	-3.47396416	0.53078807
C	-0.94879338	-3.47845428	-0.55113559
C	-0.49380332	-3.02241227	-1.85144359
C	-0.51118143	-3.01673775	1.83178809
C	-1.82937360	-2.59178737	2.00486767
C	-2.75079678	-2.59950225	0.88841449
C	-2.30556061	-3.03208237	-0.37086671
C	-2.10845265	-1.42284307	2.81542673
C	-3.19248829	-0.70123976	2.18730006
C	-3.58706076	-1.42964350	0.99862490
C	-3.96197835	-0.72045108	-0.15147523
C	-3.96216181	0.71966208	-0.15019789
C	-3.58740397	1.42693886	1.00118549
C	-3.19266593	0.69653380	2.18860204
C	-2.10875747	1.41724781	2.81801891
C	-1.82995742	2.58771778	2.00961403
C	-2.75140843	2.59718874	0.89312589
C	-2.30634690	3.03212775	-0.36545411
C	-0.94966642	3.47910511	-0.54488247
C	-0.05439960	3.47286509	0.53703523
C	-0.51181320	3.01323640	1.83727186
C	0.56879682	2.28830643	2.46316898
C	0.82043045	2.59089237	-2.01412404
C	-0.49459893	3.02555943	-1.84606278
C	0.30122885	1.16493764	3.25182843
C	-1.06322977	0.72106508	3.42941743
C	-3.50392833	1.16958821	-1.45131183
C	-2.69413495	2.29969620	-1.55633836
C	-1.57700882	2.30762893	-2.47856389
C	-1.06310264	-0.72752213	3.42811392
C	-2.69346135	-2.29763020	-1.56040469
C	-3.50365729	-1.16800646	-1.45336268
C	-3.22762094	0.00153883	-2.26111171
C	-1.57636445	-2.30366097	-2.48264649
C	-1.30232262	-1.16875403	-3.25608580
C	-2.14407741	0.00248878	-3.14438142
C	1.68833396	-2.28863230	1.53939912
C	0.56927713	-2.29265878	2.45897500
C	0.30142360	-1.17084416	3.24966235
C	0.05998869	-0.72301782	-3.43077156
C	2.49615259	-1.16424367	1.43087416
C	-1.30265896	1.17412926	-3.25404777
C	0.05980682	0.72904296	-3.42948053
C	1.10423749	1.42356425	-2.81853575
C	2.21164732	-0.00181193	2.22888876
C	1.14046849	-0.00275909	3.13957954
C	5.21940787	-1.15460531	0.33371717
C	5.21931288	1.15515827	0.33580469
C	5.63264509	0.70070007	-0.93008302
C	5.63272132	-0.69780268	-0.93135211
C	5.38483748	-0.00057246	1.28407220
H	5.21261885	-2.19821420	0.65038508
H	5.74649489	-1.32305994	-1.81640459
H	5.74628129	1.32755651	-1.81402398
H	5.21241934	2.19819524	0.65435022
H	4.72598704	-0.00141165	2.16239999
H	6.43616032	-0.00081758	1.64072449

c60_DA_ts56_2e_s -13614.94

C	1.68392689	2.28816334	1.53382108
C	2.48632100	1.15843342	1.42074614
C	3.09050389	0.74252700	0.13557805
C	2.58381285	1.43712653	-1.02718734
C	1.74756608	2.58414975	-0.90857307
C	1.30720129	3.05103367	0.35685958
C	2.18254669	0.70560130	-2.19473102
C	2.18265129	-0.70114641	-2.19592152
C	2.58418189	-1.43480307	-1.02974008
C	3.09079762	-0.74221798	0.13426380
C	1.09538400	-1.41441012	-2.83720390
C	0.81661922	-2.58058515	-2.02469274
C	1.74830271	-2.58240401	-0.91325129
C	1.30809593	-3.05168314	0.35141601
C	-0.04549467	-3.47668429	0.52797814
C	-0.95484030	-3.47946688	-0.55243683
C	-0.49896529	-3.01486981	-1.85538312
C	-0.50719556	-3.01334120	1.83314053
C	-1.82786550	-2.59058796	2.00718398
C	-2.75808314	-2.60373659	0.89811235
C	-2.30598124	-3.04019707	-0.37069790
C	-2.10368176	-1.42213731	2.82361465
C	-3.18756454	-0.70148291	2.19515341
C	-3.58835984	-1.43752101	1.00808355
C	-3.96557374	-0.71759883	-0.14405751
C	-3.96563236	0.71735290	-0.14290136
C	-3.58870202	1.43496842	1.01057352
C	-3.18780857	0.69675739	2.19633225
C	-2.10412688	1.41644664	2.82608365
C	-1.82860858	2.58640104	2.01172511
C	-2.75870007	2.60140518	0.90263548
C	-2.30671792	3.04027876	-0.36540046
C	-0.95576169	3.48002667	-0.54627208
C	-0.04645531	3.47543104	0.53413077
C	-0.50807305	3.00970435	1.83846548
C	0.57083419	2.29102096	2.46703292
C	0.81585025	2.58398002	-2.01989455
C	-0.49977189	3.01783352	-1.85003772
C	0.30791322	1.16470350	3.26048151
C	-1.05644561	0.72099582	3.44021813
C	-3.50264341	1.16701792	-1.44599964
C	-2.69272410	2.29753256	-1.55255184
C	-1.58351935	2.30778953	-2.48709812
C	-1.05622189	-0.72762008	3.43895391
C	-2.69223035	-2.29525311	-1.55649904
C	-3.50246965	-1.16489098	-1.44799192
C	-3.23479162	0.00181734	-2.26281050
C	-1.58294956	-2.30385733	-2.49108318
C	-1.31414188	-1.16792467	-3.27232793
C	-2.15493163	0.00248516	-3.15794615
C	1.68466889	-2.29083529	1.52974069
C	0.57156056	-2.29553819	2.46291371
C	0.30824344	-1.17074134	3.25833134
C	0.04628931	-0.72178899	-3.45297246
C	2.48675004	-1.16070168	1.41869273
C	-1.31443749	1.17327464	-3.27030343
C	0.04615791	0.72784124	-3.45173810
C	1.09512808	1.41966813	-2.83480798
C	2.20719387	-0.00193682	2.22162681
C	1.14558443	-0.00286994	3.15150421
C	5.24309183	-1.15474407	0.34653335
C	5.24297899	1.15542107	0.34861395
C	5.66605848	0.70258084	-0.91289900
C	5.66613126	-0.69952399	-0.91418449
C	5.39083678	-0.00051551	1.30032689

H	5.21716697	-2.19778796	0.66399419
H	5.75929282	-1.32266585	-1.80351254
H	5.75911954	1.32739008	-1.80107180
H	5.21685290	2.19790916	0.66792313
H	4.70022927	-0.00144543	2.15612515
H	6.43052389	-0.00077503	1.69652839

c60_DA_ts56_3e_d -13546.48

C	1.69204388	2.29064764	1.53322352
C	2.50058660	1.15780239	1.42446883
C	3.10621747	0.74599806	0.13751201
C	2.59406325	1.43809302	-1.02598898
C	1.74875949	2.58111946	-0.90905427
C	1.31062883	3.04846598	0.35905154
C	2.18445588	0.70507987	-2.19233685
C	2.18472440	-0.69999514	-2.19346223
C	2.59477832	-1.43501275	-1.02870433
C	3.10718659	-0.74485583	0.13622997
C	1.10012717	-1.42194553	-2.83804250
C	0.82593088	-2.58376398	-2.03270011
C	1.74998919	-2.57850481	-0.91370866
C	1.31215426	-3.04829502	0.35357844
C	-0.04721832	-3.47667853	0.53391156
C	-0.95380507	-3.48048183	-0.55810585
C	-0.50131267	-3.02507922	-1.85618619
C	-0.50614081	-3.02503787	1.83513218
C	-1.83889451	-2.59574050	2.01565018
C	-2.76063455	-2.60162776	0.89905475
C	-2.31044773	-3.03606038	-0.37205437
C	-2.11189552	-1.43080312	2.82395732
C	-3.19406694	-0.70178558	2.19293744
C	-3.59967767	-1.43715562	1.00612427
C	-3.98003558	-0.71955065	-0.14768187
C	-3.98045193	0.71812916	-0.14636643
C	-3.60042937	1.43397116	1.00874947
C	-3.19441484	0.69664310	2.19416032
C	-2.11251904	1.42500534	2.82652787
C	-1.84014886	2.59154527	2.02031482
C	-2.76187887	2.59899565	0.90370585
C	-2.31193189	3.03582444	-0.36662771
C	-0.95551890	3.48117716	-0.55186534
C	-0.04894915	3.47593796	0.54012109
C	-0.50760969	3.02180989	1.84053216
C	0.56954436	2.29004178	2.46087013
C	0.82471505	2.58788345	-2.02798978
C	-0.50275531	3.02823840	-1.85071281
C	0.30859963	1.16044506	3.25101661
C	-1.06172614	0.71670297	3.44221616
C	-3.52058669	1.16599279	-1.45017333
C	-2.70436655	2.29975488	-1.55266131
C	-1.58495367	2.30642072	-2.48046251
C	-1.06136519	-0.72310762	3.44097368
C	-2.70326117	-2.29811809	-1.55678616
C	-3.52000031	-1.16492659	-1.45230518
C	-3.25559726	0.00134396	-2.26537922
C	-1.58382953	-2.30258951	-2.48463162
C	-1.31750551	-1.16401547	-3.26392319
C	-2.16526663	0.00240918	-3.16028869
C	1.69304523	-2.29220581	1.52915140
C	0.57064158	-2.29386296	2.45679376
C	0.30919721	-1.16570719	3.24890211
C	0.04670509	-0.71749776	-3.45598360
C	2.50105636	-1.15883435	1.42252675
C	-1.31801235	1.16937706	-3.26186405
C	0.04637059	0.72388337	-3.45473647
C	1.09960306	1.42769567	-2.83555194
C	2.22521894	-0.00122474	2.22158056
C	1.15208002	-0.00231226	3.15463883
C	5.24260785	-1.15352907	0.34650865
C	5.24592333	1.15362406	0.34903371
C	5.68856955	0.70175979	-0.91135311
C	5.68708594	-0.70006695	-0.91293014
C	5.40582665	-0.00118706	1.30360675
H	5.21066599	-2.19663639	0.66547174
H	5.75409765	-1.31961503	-1.80790832
H	5.75725055	1.32311582	-1.80496356
H	5.21538037	2.19610751	0.67002819
H	4.70834470	-0.00105239	2.15456569
H	6.44793015	-0.00339441	1.70192027

c60_DA_ts56_4e_s -13411.49

C	-1.68726032	1.55246937	2.31479661
C	-2.50224496	1.43508789	1.17223899
C	-3.11558299	0.15766282	0.75867016
C	-2.59008528	-1.01680700	1.44168298
C	-1.75474683	-0.89518084	2.59116495
C	-1.31910548	0.37349832	3.07484555
C	-2.19254459	-2.18981762	0.71233166
C	-2.59008528	-1.01680700	-1.44168298
C	-3.11558299	0.15766282	-0.75867016
C	-1.10979462	-2.82525511	-1.41938819
C	-0.82344431	-2.00943965	-2.59049571
C	-1.75474683	-0.89518084	-2.59116495
C	-1.31910548	0.37349832	-3.07484555
C	0.03997082	0.53897159	-3.50073399
C	0.94508198	-0.54588108	-3.50733703
C	0.49291004	-1.84700144	-3.03214854
C	0.50279772	1.84616223	-3.03480511
C	1.83084791	2.00724959	-2.61012699
C	2.75048608	0.89630210	-2.61794409
C	2.30277661	-0.37592799	-3.05703671
C	2.12129978	2.81515759	-1.42267574
C	3.21668914	2.20806615	-0.71781359
C	3.58414357	1.01194197	-1.43662383
C	3.95886978	-0.15832073	-0.73026643
C	3.95886978	-0.15832073	0.73026643
C	3.58414357	1.01194197	1.43662383
C	3.21668914	2.20806615	0.71781359
C	2.12129978	2.81515759	1.42267574
C	1.83084791	2.00724959	2.61012699
C	2.75048608	0.89630210	2.61794409
C	2.30277661	-0.37592799	3.05703671
C	0.94508198	-0.54588108	3.50733703
C	0.03997082	0.53897159	3.50073399
C	0.50279772	1.84616223	3.03480511
C	-0.57994812	2.47962346	2.32828930
C	-0.82344431	-2.00943965	2.59049571
C	0.49291004	-1.84700144	3.03214854
C	-0.29593480	3.26671954	1.17753111
C	1.06062463	3.43015373	0.73228578
C	3.51981403	-1.44899725	1.18164336
C	2.69475956	-1.57030807	2.33436359
C	1.59005220	-2.48904601	2.33461030
C	1.06062463	3.43015373	-0.73228578
C	2.69475956	-1.57030807	-2.33436359
C	3.51981403	-1.44899725	-1.18164336
C	3.22254587	-2.24623212	0.00000000
C	1.59005220	-2.48904601	-2.33461030
C	1.30988628	-3.27899623	-1.18284265
C	2.14283301	-3.13793434	0.00000000
C	-1.68726032	1.55246937	-2.31479661
C	-0.57994812	2.47962346	-2.32828930
C	-0.29593480	3.26671954	-1.17753111
C	-0.04146197	-3.43859688	-0.72991616
C	-2.50224496	1.43508789	-1.17223899
C	1.30988628	-3.27899623	1.18284265
C	-0.04146197	-3.43859688	0.72991616
C	-1.10979462	-2.82525511	1.41938819
C	-2.18687031	2.20705005	0.00000000
C	-1.12364665	3.13875380	0.00000000
C	-5.19536857	0.32463413	-1.15025082
C	-5.19536857	0.32463413	1.15025082
C	-5.67171320	-0.93602762	0.70151979
C	-5.67171320	-0.93602762	-0.70151979
C	-5.39256355	1.28358425	0.00000000
H	-5.17927477	0.65039521	-2.19324915
H	-5.70090335	-1.83758437	-1.31684191
H	-5.70090335	-1.83758437	1.31684191
H	-5.17927477	0.65039521	2.19324915
H	-4.70154050	2.14206561	0.00000000
H	-6.44471509	1.66589327	0.00000000

c60_DA_ts56_5e -13214.95

C	-1.70874068	-1.53366687	-2.30802715
C	-2.52796913	-1.42279465	-1.16373849
C	-3.14647190	-0.13666772	-0.76042756
C	-2.60692913	1.03264793	-1.44099596
C	-1.75192866	0.91220550	-2.58154866
C	-1.32430990	-0.36164679	-3.05976152
C	-2.18585253	2.19836253	-0.70664276
C	-2.18585253	2.19836253	0.70664276
C	-2.60692913	1.03264793	1.44099596
C	-3.14647190	-0.13666772	0.76042756
C	-1.10167144	2.83700881	1.43345902
C	-0.83171457	2.03646303	2.59515907
C	-1.75192866	0.91220550	2.58154866
C	-1.32430990	-0.36164679	3.05976152
C	0.04508635	-0.54649068	3.49065619
C	0.95138233	0.55531364	3.49674478
C	0.50890216	1.85112026	3.04611228
C	0.49657801	-1.84855511	3.04990176
C	1.84722291	-2.03344706	2.61269196
C	2.75852413	-0.91296941	2.60962803
C	2.31816016	0.36526344	3.04177436
C	2.11972320	-2.82887234	1.43817961

C	3.21154312	-2.21306609	0.70995811
C	3.60719182	-1.02284333	1.43517207
C	3.99228518	0.14061448	0.72721987
C	3.99228518	0.14061448	-0.72721987
C	3.60719182	-1.02284333	-1.43517207
C	3.21154312	-2.21306609	-0.70995811
C	2.11972320	-2.82887234	-1.43817961
C	1.84722291	-2.03344706	-2.61269196
C	2.75852413	-0.91296941	-2.60962803
C	2.31816016	0.36526344	-3.04177436
C	0.95138233	0.55531364	-3.49674478
C	0.04508635	-0.54649068	-3.49065619
C	0.49657801	-1.84855511	-3.04990176
C	-0.58119124	-2.45673758	-2.30818443
C	-0.83171457	2.03646303	-2.59515907
C	0.50890216	1.85112026	-3.04611228
C	-0.31460689	-3.24415526	-1.16420694
C	1.05775145	-3.44518631	-0.72050973
C	3.55479029	1.44265169	-1.17378111
C	2.72500448	1.55360535	-2.32419585
C	1.59981604	2.47045104	-2.31844451
C	1.05775145	-3.44518631	0.72050973
C	2.72500448	1.55360535	2.32419585
C	3.55479029	1.44265169	1.17378111
C	3.27903921	2.24527202	0.00000000
C	1.59981604	2.47045104	2.31844451
C	1.33258786	3.25448406	1.16963864
C	2.18320287	3.14576018	0.00000000
C	-1.70874068	-1.53366687	2.30802715
C	-0.58119124	-2.45673758	2.30818443
C	-0.31460689	-3.24415526	1.16420694
C	-0.03117839	3.45370345	0.71953363
C	-2.52796913	-1.42279465	1.16373849
C	1.33258786	3.25448406	-1.16963864
C	-0.03117839	3.45370345	-0.71953363
C	-1.10167144	2.83700881	-1.43345902
C	-2.23790077	-2.20232174	0.00000000
C	-1.15810426	-3.14742878	0.00000000
C	-5.21080682	-0.32928763	1.14803741
C	-5.21080682	-0.32928763	-1.14803741
C	-5.71999055	0.92904449	-0.70070060
C	-5.71999055	0.92904449	0.70070060
C	-5.42193828	-1.29070616	0.00000000
H	-5.19947612	-0.65778406	2.19173405
H	-5.72893571	1.83635963	1.31023694
H	-5.72893571	1.83635963	-1.31023694
H	-5.19947612	-0.65778406	-2.19173405
H	-4.72562296	-2.14537061	0.00000000
H	-6.48040629	-1.67648818	0.00000000

c60_DA_ts56_6e -12955.45

C	-1.71392465	-1.54211497	-2.32182573
C	-2.53863739	-1.42668284	-1.17013646
C	-3.17461813	-0.14584266	-0.77318926
C	-2.61604937	1.03078666	-1.44577531
C	-1.75891576	0.90711353	-2.58653161
C	-1.33320518	-0.36793482	-3.07257301
C	-2.19694931	2.19856691	-0.71200760
C	-2.19694931	2.19856691	0.71200760
C	-2.61604937	1.03078666	1.44577531
C	-3.17461813	-0.14584266	0.77318926
C	-1.11222933	2.83388224	1.43470552
C	-0.83886536	2.03348478	2.60073060
C	-1.75891576	0.90711353	2.58653161
C	-1.33320518	-0.36793482	3.07257301
C	0.03962353	-0.54850769	3.50354104
C	0.94479087	0.55507345	3.51063392
C	0.50353624	1.85092077	3.05450229
C	0.49126947	-1.85290534	3.06223246
C	1.84749359	-2.03262783	2.62445305
C	2.75446068	-0.91164808	2.62009454
C	2.31614816	0.36981218	3.05184016
C	2.12570392	-2.82388621	1.43955112
C	3.22593418	-2.22070933	0.72025584
C	3.60627114	-1.02572491	1.43695043
C	3.98886992	0.14690180	0.73376570
C	3.98886992	0.14690180	-0.73376570
C	3.60627114	-1.02572491	-1.43695043
C	3.22593418	-2.22070933	-0.72025584
C	2.12570392	-2.82388621	-1.43955112
C	1.84749359	-2.03262783	-2.62445305
C	2.75446068	-0.91164808	-2.62009454
C	2.31614816	0.36981218	-3.05184016
C	0.94479087	0.55507345	-3.51063392
C	0.03962353	-0.54850769	-3.50354104
C	0.49126947	-1.85290534	-3.06223246
C	-0.58803622	-2.46223782	-2.32451199
C	-0.83886536	2.03348478	-2.60073060
C	0.50353624	1.85092077	-3.05450229
C	-0.31146487	-3.24880189	-1.16948449
C	1.05717602	-3.44340741	-0.72493986
C	3.56336168	1.44505073	-1.18159864
C	2.72613795	1.56305954	-2.34513543
C	1.60131961	2.47178859	-2.33216064
C	1.05717602	-3.44340741	0.72493986
C	2.72613795	1.56305954	2.34513543
C	3.56336168	1.44505073	1.18159864
C	3.27116700	2.23805538	0.00000000
C	1.60131961	2.47178859	2.33216064
C	1.32857154	3.26093217	1.17574612
C	2.17627391	3.13979093	0.00000000
C	-1.71392465	-1.54211497	2.32182573
C	-0.58803622	-2.46223782	2.32451199
C	-0.31146487	-3.24880189	1.16948449
C	-0.03186538	3.45073089	0.72238912
C	-2.53863739	-1.42668284	1.17013646
C	1.32857154	3.26093217	-1.17574612
C	-0.03186538	3.45073089	-0.72238912
C	-1.11222933	2.83388224	-1.43470552
C	-2.22920999	-2.19122730	0.00000000
C	-1.15042396	-3.14028247	0.00000000
C	-5.16833881	-0.32373953	1.14395699
C	-5.16833881	-0.32373953	-1.14395699
C	-5.72733747	0.93181822	-0.70348881
C	-5.72733747	0.93181822	0.70348881
C	-5.41588364	-1.28757686	0.00000000
H	-5.17703679	-0.66044480	2.18791748
H	-5.67717936	1.84988185	1.29906056
H	-5.67717936	1.84988185	-1.29906056
H	-5.17703679	-0.66044480	-2.18791748
H	-4.72870835	-2.15094950	0.00000000
H	-6.48742402	-1.65401301	0.00000000

c60_DA_ts66 -13559.83

C	-2.00229651	-2.39899583	0.72843023
C	-2.46844998	-1.28563400	1.41608290
C	-3.06018170	-0.14307947	0.71988285
C	-0.06144403	-3.48318214	0.00000000
C	-0.80306097	-3.07016747	1.17265325
C	-0.11943770	-2.61615573	2.30452954
C	-2.56477132	1.04624806	1.41877780
C	-2.19388295	2.19204054	0.73061986
C	1.33236927	-3.42925544	0.00000000
C	-1.82002034	0.63236945	2.57947287
C	1.78810507	3.08184211	1.17173098
C	1.11027067	2.62442608	2.30211112
C	1.60913164	1.47300396	3.02630055
C	2.76408591	0.82292607	2.59281099
C	3.46635855	1.29941328	1.42108073
C	1.04433325	3.49422570	0.00000000
C	-0.34874313	3.43048396	0.00000000
C	-1.05364701	2.95818121	1.17305773
C	-0.33403154	2.56514724	2.30651540
C	0.47071220	0.70117614	3.47508660
C	0.52807758	-0.69165033	3.47441847
C	1.72617356	-1.36694422	3.02555614
C	2.82387436	-0.62377875	2.59266447
C	3.56315879	-1.04043460	1.42101674
C	3.96093207	0.14826197	0.69731580
C	3.17762151	-2.18551291	0.72440113
C	2.03891425	-2.95578178	1.17145828
C	1.32491362	-2.55562802	2.30141921
C	-0.72797405	1.37967424	3.02617498
C	-0.61074459	-1.46602893	3.02407975
C	2.98654050	2.40870120	0.72435181
C	-5.27476368	-0.33040356	1.15901341
C	-5.62711044	0.93904022	0.70404077
C	-5.38034210	-1.27753648	0.00000000
H	-4.68366319	-2.12669327	0.00000000
H	-6.41225487	-1.68810060	0.00000000
H	-5.75525602	1.81970660	1.33254265
H	-5.25269721	-0.64582454	2.20199549
C	-1.76038535	-0.81148717	2.57921969
C	-2.00229651	-2.39899583	-0.72843023
C	-2.46844998	-1.28563400	-1.41608290
C	-3.06018170	-0.14307947	-0.71988285
C	-0.80306097	-3.07016747	-1.17265325
C	-0.11943770	-2.61615573	-2.30452954
C	-2.56477132	1.04624806	-1.41877780
C	-2.19388295	2.19204054	-0.73061986
C	-1.82002034	0.63236945	-2.57947287
C	1.78810507	3.08184211	-1.17173098
C	1.11027067	2.62442608	-2.30211112
C	1.60913164	1.47300396	-3.02630055
C	2.76408591	0.82292607	-2.59281099
C	3.46635855	1.29941328	-1.42108073

C	-1.05364701	2.95818121	-1.17305773
C	-0.33403154	2.56514724	-2.30651540
C	0.47071220	0.70117614	-3.47508660
C	0.52807758	-0.69165033	-3.47441847
C	1.72617356	-1.36694422	-3.02555614
C	2.82387436	-0.62377875	-2.59266447
C	3.56315879	-1.04043460	-1.42101674
C	3.96093207	0.14826197	-0.69731580
C	3.17762151	-2.18551291	-0.72440113
C	2.03891425	-2.95578178	-1.17145828
C	1.32491362	-2.55562802	-2.30141921
C	-0.72797405	1.37967424	-3.02617498
C	-0.61074459	-1.46602893	-3.02407975
C	2.98654050	2.40870120	-0.72435181
C	-5.27476368	-0.33040356	-1.15901341
C	-5.62711044	0.93904022	-0.70404077
H	-5.75525602	1.81970660	-1.33254265
H	-5.25269721	-0.64582454	-2.20199549
C	-1.76038535	-0.81148717	-2.57921969

c60_DA_ts66_1e -13622.71

C	-2.01144696	2.38891697	-0.72646586
C	-2.47523471	1.27713814	-1.42058451
C	-3.06600206	0.13285649	-0.72040077
C	-0.07447170	3.49310781	0.00000000
C	-0.80787756	3.06700541	-1.16695214
C	-0.12716125	2.60888269	-2.30285356
C	-2.56581008	-1.05470285	-1.42210986
C	-2.18985001	-2.19621206	-0.72965158
C	1.33504934	3.44500313	0.00000000
C	-1.82837685	-0.63406967	-2.58498379
C	1.80066629	-3.07354670	-1.16582521
C	1.12512396	-2.61195165	-2.30018517
C	1.62152574	-1.46984466	-3.02853912
C	2.78597679	-0.81028671	-2.59865210
C	3.48239820	-1.28537267	-1.42482264
C	1.06506330	-3.49963759	0.00000000
C	-0.34372774	-3.44141068	0.00000000
C	-1.04240181	-2.96312618	-1.16784537
C	-0.32677800	-2.55925396	-2.30496307
C	0.47713525	-0.69870137	-3.46465386
C	0.52836766	0.69474924	-3.46446754
C	1.73057416	1.37671581	-3.02567364
C	2.83914888	0.63006849	-2.59749106
C	3.57207239	1.05226099	-1.42326935
C	3.97529996	-0.13410269	-0.69751971
C	3.18137642	2.19504295	-0.72335781
C	2.03503801	2.96489732	-1.16616355
C	1.32496129	2.55486844	-2.30052880
C	-0.72600005	-1.38450321	-3.02731775
C	-0.61695706	1.46893206	-3.02846221
C	3.00418129	-2.39486758	-0.72239888
C	-5.25330252	0.31490204	-1.15769380
C	-5.63088650	-0.94952152	-0.70362006
C	-5.36917080	1.26578297	0.00000000
H	-4.66907584	2.11229774	0.00000000
H	-6.40357720	1.67070553	0.00000000
H	-5.74357810	-1.83346174	-1.33053493
H	-5.21909714	0.63013915	-2.20040716
C	-1.77543297	0.80444548	-2.58607081
C	-2.01144696	2.38891697	0.72646586
C	-2.47523471	1.27713814	1.42058451
C	-3.06600206	0.13285649	0.72040077
C	-0.80787756	3.06700541	1.16695214
C	-0.12716125	2.60888269	2.30285356
C	-2.56581008	-1.05470285	1.42210986
C	-2.18985001	-2.19621206	0.72965158
C	-1.82837685	-0.63406967	2.58498379
C	1.80066629	-3.07354670	1.16582521
C	1.12512396	-2.61195165	2.30018517
C	1.62152574	-1.46984466	3.02853912
C	2.78597679	-0.81028671	2.59865210
C	3.48239820	-1.28537267	1.42482264
C	-1.04240181	-2.96312618	1.16784537
C	-0.32677800	-2.55925396	2.30496307
C	0.47713525	-0.69870137	3.46465386
C	0.52836766	0.69474924	3.46446754
C	1.73057416	1.37671581	3.02567364
C	2.83914888	0.63006849	2.59749106
C	3.57207239	1.05226099	1.42326935
C	3.97529996	-0.13410269	0.69751971
C	3.18137642	2.19504295	0.72335781
C	2.03503801	2.96489732	1.16616355
C	1.32496129	2.55486844	2.30052880
C	-0.72600005	-1.38450321	3.02731775
C	-0.61695706	1.46893206	3.02846221
C	3.00418129	-2.39486758	0.72239888
C	-5.25330252	0.31490204	1.15769380
C	-5.63088650	-0.94952152	0.70362006
H	-5.74357810	-1.83346174	1.33053493
H	-5.21909714	0.63013915	2.20040716
C	-1.77543297	0.80444548	2.58607081

c60_DA_ts66_2e_s -13618.54

C	-2.01923652	2.38202038	-0.72397707
C	-2.48490089	1.27275797	-1.42668725
C	-3.07580398	0.12799162	-0.72142986
C	-0.08204594	3.50244002	0.00000000
C	-0.80870040	3.06381811	-1.16123668
C	-0.13221403	2.60001812	-2.30120783
C	-2.57566604	-1.05968383	-1.42536255
C	-2.19658489	-2.19815626	-0.72909592
C	1.34318596	3.45842372	0.00000000
C	-1.84210599	-0.63390712	-2.58984916
C	1.79993198	-3.07174280	-1.16007971
C	1.12814176	-2.60465488	-2.29871397
C	1.62563088	-1.47298623	-3.03293520
C	2.80239745	-0.80711728	-2.60553482
C	3.49087869	-1.28132078	-1.42952004
C	1.07103209	-3.51041323	0.00000000
C	-0.35333059	-3.45500342	0.00000000
C	-1.04502972	-2.96958911	-1.16324937
C	-0.33161291	-2.55645259	-2.30424669
C	0.47856399	-0.69969306	-3.45519909
C	0.52521010	0.69477966	-3.45497324
C	1.73422067	1.38074968	-3.02452888
C	2.85087293	0.62818213	-2.60206949
C	3.57922333	1.05473225	-1.42487539
C	3.98440833	-0.13077166	-0.69793284
C	3.18650820	2.19695220	-0.72274668
C	2.03589921	2.97069223	-1.16146832
C	1.32787243	2.55108752	-2.30009246
C	-0.73237306	-1.38992057	-3.02758967
C	-0.62383534	1.47147965	-3.03447697
C	3.01125713	-2.39055690	-0.72007580
C	-5.24248996	0.31534069	-1.15648039
C	-5.64949243	-0.94270298	-0.70356677
C	-5.36227167	1.27047639	0.00000000
H	-4.65022110	2.10758233	0.00000000
H	-6.39468518	1.68318932	0.00000000
H	-5.74805208	-1.83021886	-1.32827273
H	-5.19657117	0.63092528	-2.19886395
C	-1.79448207	0.80082075	-2.59408506
C	-2.01923652	2.38202038	0.72397707
C	-2.48490089	1.27275797	1.42668725
C	-3.07580398	0.12799162	0.72142986
C	-0.80870040	3.06381811	1.16123668
C	-0.13221403	2.60001812	2.30120783
C	-2.57566604	-1.05968383	1.42536255
C	-2.19658489	-2.19815626	0.72909592
C	-1.84210599	-0.63390712	2.58984916
C	1.79993198	-3.07174280	1.16007971
C	1.12814176	-2.60465488	2.29871397
C	1.62563088	-1.47298623	3.03293520
C	2.80239745	-0.80711728	2.60553482
C	3.49087869	-1.28132078	1.42952004
C	-1.04502972	-2.96958911	1.16324937
C	-0.33161291	-2.55645259	2.30424669
C	0.47856399	-0.69969306	3.45519909
C	0.52521010	0.69477966	3.45497324
C	1.73422067	1.38074968	3.02452888
C	2.85087293	0.62818213	2.60206949
C	3.57922333	1.05473225	1.42487539
C	3.98440833	-0.13077166	0.69793284
C	3.18650820	2.19695220	0.72274668
C	2.03589921	2.97069223	1.16146832
C	1.32787243	2.55108752	2.30009246
C	-0.73237306	-1.38992057	3.02758967
C	-0.62383534	1.47147965	3.03447697
C	3.01125713	-2.39055690	0.72007580
C	-5.24248996	0.31534069	1.15648039
C	-5.64949243	-0.94270298	0.70356677
H	-5.74805208	-1.83021886	1.32827273
H	-5.19657117	0.63092528	2.19886395
C	-1.79448207	0.80082075	2.59408506

c60_DA_ts66_3e_d -13547.95

C	-2.02997127	2.39517650	-0.72194419
C	-2.49096241	1.27722201	-1.43221550
C	-3.07193484	0.12456815	-0.72321682
C	-0.08995662	3.51455524	0.00000000
C	-0.81788804	3.07312191	-1.16095787
C	-0.13638507	2.60736563	-2.30004146
C	-2.58079957	-1.06868935	-1.43169731
C	-2.20380942	-2.21492960	-0.72556073
C	1.33687324	3.46958332	0.00000000

C	-1.84382849	-0.64089902	-2.58414893
C	1.80339985	-3.08183285	-1.15972078
C	1.12633451	-2.61398370	-2.29800370
C	1.61876777	-1.47440671	-3.03450257
C	2.79806390	-0.80973014	-2.59957980
C	3.49231726	-1.28656498	-1.43355049
C	1.07248031	-3.52279479	0.00000000
C	-0.35285366	-3.46771558	0.00000000
C	-1.04717562	-2.97850735	-1.16232917
C	-0.33046974	-2.56471772	-2.30267979
C	0.47508038	-0.70863646	-3.46742019
C	0.52321432	0.70233866	-3.46713900
C	1.72475170	1.38277361	-3.02887864
C	2.84739348	0.63307368	-2.59707209
C	3.57864520	1.06091598	-1.43023792
C	3.97214973	-0.12931415	-0.69828974
C	3.18891565	2.21300070	-0.71924520
C	2.03190484	2.97789283	-1.16031183
C	1.32097002	2.55831982	-2.29896069
C	-0.72884407	-1.39312156	-3.03168530
C	-0.62284194	1.47126504	-3.03586376
C	3.01662484	-2.40648769	-0.71773317
C	-5.21947702	0.31746434	-1.15483230
C	-5.65591143	-0.93511889	-0.70342231
C	-5.34753815	1.27687191	0.00000000
H	-4.63007329	2.10994397	0.00000000
H	-6.38223439	1.69008598	0.00000000
H	-5.73809710	-1.82662582	-1.32563930
H	-5.16046615	0.63320971	-2.19691748
C	-1.79532259	0.80181333	-2.58781251
C	-2.02997127	2.39517650	0.72194419
C	-2.49096241	1.27722201	1.43221550
C	-3.07193484	0.12456815	0.72321682
C	-0.81788804	3.07312191	1.16095787
C	-0.13638507	2.60736563	2.30004146
C	-2.58079957	-1.06868935	1.43169731
C	-2.20380942	-2.21492960	0.72556073
C	-1.84382849	-0.64089902	2.58414893
C	1.80339985	-3.08183285	1.15972078
C	1.12633451	-2.61398370	2.29800370
C	1.61876777	-1.47440671	3.03450257
C	2.79806390	-0.80973014	2.59957980
C	3.49231726	-1.28656498	1.43355049
C	-1.04717562	-2.97850735	1.16232917
C	-0.33046974	-2.56471772	2.30267979
C	0.47508038	-0.70863646	3.46742019
C	0.52321432	0.70233866	3.46713900
C	1.72475170	1.38277361	3.02887864
C	2.84739348	0.63307368	2.59707209
C	3.57864520	1.06091598	1.43023792
C	3.97214973	-0.12931415	0.69828974
C	3.18891565	2.21300070	0.71924520
C	2.03190484	2.97789283	1.16031183
C	1.32097002	2.55831982	2.29896069
C	-0.72884407	-1.39312156	3.03168530
C	-0.62284194	1.47126504	3.03586376
C	3.01662484	-2.40648769	0.71773317
C	-5.21947702	0.31746434	1.15483230
C	-5.65591143	-0.93511889	0.70342231
H	-5.73809710	-1.82662582	1.32563930
H	-5.16046615	0.63320971	2.19691748
C	-1.79532259	0.80181333	2.58781251

c60_DA_ts66_4e_s -13411.64

C	-2.04260325	2.40461116	-0.72037806
C	-2.49871940	1.27792340	-1.43729201
C	-3.07075455	0.11647787	-0.72608331
C	-0.10188339	3.52522906	0.00000000
C	-0.83037003	3.08058889	-1.16087118
C	-0.14320375	2.61347140	-2.29969640
C	-2.58737736	-1.08187347	-1.43951332
C	-2.20863967	-2.23612210	-0.72167320
C	1.32722287	3.48003627	0.00000000
C	-1.84547077	-0.65155904	-2.57864913
C	1.81275218	-3.09393279	-1.15985315
C	1.12962362	-2.62502908	-2.29867554
C	1.61512052	-1.47602294	-3.03629505
C	2.79529724	-0.81110982	-2.59438111
C	3.49645042	-1.29061454	-1.43705291
C	1.08058120	-3.53688232	0.00000000
C	-0.34643595	-3.48291397	0.00000000
C	-1.04394625	-2.98903077	-1.16102838
C	-0.32461868	-2.57432327	-2.30108646
C	0.47217048	-0.71858457	-3.48060047
C	0.52204099	0.70894785	-3.48112297
C	1.71540583	1.38535729	-3.03637151
C	2.84634143	0.63934269	-2.59450866
C	3.57832595	1.06822176	-1.43659580
C	3.96164376	-0.12606908	-0.69878290
C	3.19007775	2.22995677	-0.71609120
C	2.02512586	2.98487009	-1.15933951
C	1.31198463	2.56478127	-2.29890138
C	-0.72358813	-1.39922957	-3.03816322
C	-0.62331698	1.46928183	-3.03754010
C	3.02592194	-2.42129321	-0.71639058
C	-5.20028419	0.32593259	-1.15285201
C	-5.67167711	-0.92009894	-0.70339043
C	-5.33420500	1.28988726	0.00000000
H	-4.60797500	2.11615374	0.00000000
H	-6.36990686	1.71100157	0.00000000
H	-5.73505136	-1.81663806	-1.32191738
H	-5.12937456	0.64219553	-2.19471243
C	-1.79528813	0.79953596	-2.58068831
C	-2.04260325	2.40461116	0.72037806
C	-2.49871940	1.27792340	1.43729201
C	-3.07075455	0.11647787	0.72608331
C	-0.83037003	3.08058889	1.16087118
C	-0.14320375	2.61347140	2.29969640
C	-2.58737736	-1.08187347	1.43951332
C	-2.20863967	-2.23612210	0.72167320
C	-1.84547077	-0.65155904	2.57864913
C	1.81275218	-3.09393279	1.15985315
C	1.12962362	-2.62502908	2.29867554
C	1.61512052	-1.47602294	3.03629505
C	2.79529724	-0.81110982	2.59438111
C	3.49645042	-1.29061454	1.43705291
C	-1.04394625	-2.98903077	1.16102838
C	-0.32461868	-2.57432327	2.30108646
C	0.47217048	-0.71858457	3.48060047
C	0.52204099	0.70894785	3.48112297
C	1.71540583	1.38535729	3.03637151
C	2.84634143	0.63934269	2.59450866
C	3.57832595	1.06822176	1.43659580
C	3.96164376	-0.12606908	0.69878290
C	3.19007775	2.22995677	0.71609120
C	2.02512586	2.98487009	1.15933951
C	1.31198463	2.56478127	2.29890138
C	-0.72358813	-1.39922957	3.03816322
C	-0.62331698	1.46928183	3.03754010
C	3.02592194	-2.42129321	0.71639058
C	-5.20028419	0.32593259	1.15285201
C	-5.67167711	-0.92009894	0.70339043
H	-5.73505136	-1.81663806	1.32191738
H	-5.12937456	0.64219553	2.19471243
C	-1.79528813	0.79953596	2.58068831

c60_DA_ts66_5e -13210.37

C	-2.03845981	2.40087244	-0.72347388
C	-2.50264583	1.27203616	-1.43980339
C	-3.10170795	0.11550414	-0.74288338
C	-0.10154852	3.51648039	0.00000000
C	-0.83435607	3.08304967	-1.16575962
C	-0.13922768	2.61878942	-2.31303746
C	-2.59072914	-1.07954101	-1.44373214
C	-2.20281199	-2.23367334	-0.72444482
C	1.32853007	3.47329599	0.00000000
C	-1.84417915	-0.65297174	-2.58517089
C	1.82323785	-3.09859335	-1.16502489
C	1.13164466	-2.63121918	-2.31325589
C	1.61718582	-1.47940969	-3.04602901
C	2.79901975	-0.80882034	-2.60468343
C	3.50196452	-1.28379467	-1.43840489
C	1.08724660	-3.53023462	0.00000000
C	-0.34199172	-3.47667363	0.00000000
C	-1.04406796	-2.99242187	-1.16518035
C	-0.31829209	-2.57899313	-2.31174492
C	0.47352598	-0.71999723	-3.49254475
C	0.52270007	0.70918998	-3.49276474
C	1.71570214	1.38907028	-3.04568052
C	2.84885406	0.63950198	-2.60485160
C	3.58294791	1.06549657	-1.43835313
C	3.97828203	-0.12367425	-0.70793446
C	3.18729479	2.23256465	-0.72018467
C	2.03246815	2.99192572	-1.16538177
C	1.30993185	2.57220081	-2.31428075
C	-0.72229916	-1.40258445	-3.04725642
C	-0.62333119	1.47092729	-3.04686888
C	3.02802138	-2.42074862	-0.72016547
C	-5.17154582	0.31553475	-1.14978291
C	-5.72918758	-0.90880311	-0.70703596
C	-5.32228283	1.28894424	0.00000000
H	-4.59330382	2.11346145	0.00000000
H	-6.36399525	1.70568242	0.00000000
H	-5.78279268	-1.81264669	-1.31882109
H	-5.11179098	0.63886783	-2.19217307
C	-1.79398578	0.79810380	-2.58680193

C	-2.03845981	2.40087244	0.72347388
C	-2.50264583	1.27203616	1.43980339
C	-3.10170795	0.11550414	0.74288338
C	-0.83435607	3.08304967	1.16575962
C	-0.13922768	2.61878942	2.31303746
C	-2.59072914	-1.07954101	1.44373214
C	-2.20281199	-2.23367334	0.72444482
C	-1.84417915	-0.65297174	2.58517089
C	1.82323785	-3.09859335	1.16502489
C	1.13164466	-2.63121918	2.31325589
C	1.61718582	-1.47940969	3.04602901
C	2.79901975	-0.80882034	2.60468343
C	3.50196452	-1.28379467	1.43840489
C	-1.04406796	-2.99242187	1.16518035
C	-0.31829209	-2.57899313	2.31174492
C	0.47352598	-0.71999723	3.49254475
C	0.52270007	0.70918998	3.49276474
C	1.71570214	1.38907028	3.04568052
C	2.84885406	0.63950198	2.60485160
C	3.58294791	1.06549657	1.43835313
C	3.97828203	-0.12367425	0.70793446
C	3.18729479	2.23256465	0.72018467
C	2.03246815	2.99192572	1.16538177
C	1.30993185	2.57220081	2.31428075
C	-0.72229916	-1.40258445	3.04725642
C	-0.62333119	1.47092729	3.04686888
C	3.02802138	-2.42074862	0.72016547
C	-5.17154582	0.31553475	1.14978291
C	-5.72918758	-0.90880311	0.70703596
H	-5.78279268	-1.81264669	1.31882109
H	-5.11179098	0.63886783	2.19217307
C	-1.79398578	0.79810380	2.58680193

c60_DA_ts66_6e -12947.61

C	-2.03738690	2.39460382	-0.72675206
C	-2.50948901	1.26453263	-1.44220600
C	-3.14240104	0.11238690	-0.76144107
C	-0.10345055	3.50658075	0.00000000
C	-0.84042080	3.08317735	-1.17034683
C	-0.13788076	2.62234823	-2.32611529
C	-2.59622975	-1.07942842	-1.44805457
C	-2.19858651	-2.23249044	-0.72743129
C	1.32786277	3.46699274	0.00000000
C	-1.84474917	-0.65596200	-2.59126621
C	1.83399284	-3.10343068	-1.17012257
C	1.13460250	-2.63785314	-2.32806246
C	1.61963409	-1.48339079	-3.05658132
C	2.80343640	-0.80640547	-2.61560078
C	3.50884418	-1.27684474	-1.44053988
C	1.09431028	-3.52475417	0.00000000
C	-0.33734363	-3.47139910	0.00000000
C	-1.04410341	-2.99673229	-1.16909524
C	-0.31260972	-2.58412413	-2.32188410
C	0.47443996	-0.72266659	-3.50483377
C	0.52210435	0.70843995	-3.50454123
C	1.71505895	1.39237850	-3.05618483
C	2.85151668	0.64001719	-2.61597917
C	3.58812783	1.06405445	-1.44095479
C	3.99473537	-0.12022876	-0.71708281
C	3.18410654	2.23607049	-0.72425958
C	2.03806702	2.99927306	-1.17154376
C	1.30701451	2.57882179	-2.32994879
C	-0.72169820	-1.40681556	-3.05585693
C	-0.62526540	1.47084228	-3.05562083
C	3.03107718	-2.41985157	-0.72384061
C	-5.13745036	0.30761313	-1.14648723
C	-5.79311805	-0.88860835	-0.71556996
C	-5.30947696	1.29178964	0.00000000
H	-4.58124805	2.11775857	0.00000000
H	-6.35884364	1.69812737	0.00000000
H	-5.79544131	-1.81001388	-1.30904448
H	-5.09309298	0.64373969	-2.18885966
C	-1.79504276	0.79522037	-2.59210557
C	-2.03738690	2.39460382	0.72675206
C	-2.50948901	1.26453263	1.44220600
C	-3.14240104	0.11238690	0.76144107
C	-0.84042080	3.08317735	1.17034683
C	-0.13788076	2.62234823	2.32611529
C	-2.59622975	-1.07942842	1.44805457
C	-2.19858651	-2.23249044	0.72743129
C	-1.84474917	-0.65596200	2.59126621
C	1.83399284	-3.10343068	1.17012257
C	1.13460250	-2.63785314	2.32806246
C	1.61963409	-1.48339079	3.05658132
C	2.80343640	-0.80640547	2.61560078
C	3.50884418	-1.27684474	1.44053988
C	-1.04410341	-2.99673229	1.16909524
C	-0.31260972	-2.58412413	2.32188410
C	0.47443996	-0.72266659	3.50483377
C	0.52210435	0.70843995	3.50454123
C	1.71505895	1.39237850	3.05618483
C	2.85151668	0.64001719	2.61597917
C	3.58812783	1.06405445	1.44095479
C	3.99473537	-0.12022876	0.71708281
C	3.18410654	2.23607049	0.72425958
C	2.03806702	2.99927306	1.17154376
C	1.30701451	2.57882179	2.32994879
C	-0.72169820	-1.40681556	3.05585693
C	-0.62526540	1.47084228	3.05562083
C	3.03107718	-2.41985157	0.72384061
C	-5.13745036	0.30761313	1.14648723
C	-5.79311805	-0.88860835	0.71556996
H	-5.79544131	-1.81001388	1.30904448
H	-5.09309298	0.64373969	2.18885966
C	-1.79504276	0.79522037	2.59210557

c60_prato_56_1 13512.88

C	1.986700	-2.280100	-1.166800
C	2.769900	-1.161000	-0.928800
C	3.319900	-0.801300	0.450700
C	2.452100	-1.430500	1.499300
C	1.635900	-2.577400	1.241700
C	1.419400	-3.046300	-0.061700
C	1.873300	-0.703300	2.555200
C	1.868000	0.718900	2.553800
C	2.441400	1.448200	1.496400
C	3.313900	0.823400	0.449100
C	0.678800	1.424600	3.019100
C	0.523700	2.593000	2.188500
C	1.616600	2.588400	1.236500
C	1.396500	3.053200	-0.067800
C	0.080600	3.474700	-0.464500
C	-0.982400	3.479700	0.454300
C	-0.746900	3.026900	1.811200
C	-0.157700	3.010600	-1.820200
C	-1.428400	2.583000	-2.209400
C	-2.520200	2.589200	-1.259700
C	-2.288600	3.023200	0.052800
C	-1.567900	1.410300	-3.051800
C	-2.736500	0.685400	-2.610100
C	-3.321800	1.412300	-1.503300
C	-3.874500	0.704000	-0.429200
C	-3.869000	-0.737600	-0.427700
C	-3.311000	-1.443900	-1.500400
C	-2.731200	-0.714800	-2.608700
C	-1.557200	-1.431900	-3.048900
C	-1.408900	-2.601700	-2.204200
C	-2.500500	-2.614200	-1.254300
C	-2.265700	-3.043800	0.059000
C	-0.956200	-3.489500	0.461400
C	0.106700	-3.478600	-0.457500
C	-0.135100	-3.019000	-1.814000
C	1.028300	-2.285500	-2.250600
C	0.543200	-2.588300	2.193900
C	-0.724200	-3.032500	1.817400
C	0.887100	-1.168200	-3.077300
C	-0.429200	-0.732100	-3.483500
C	-3.631800	-1.184900	0.930900
C	-2.848100	-2.312500	1.170000
C	-1.897400	-2.316800	2.262100
C	-0.434700	0.718100	-3.485100
C	-2.865400	2.289600	1.165300
C	-3.640700	1.155800	0.928500
C	-3.494500	-0.013200	1.771800
C	-1.914700	2.303100	2.257100
C	-1.762900	1.167900	3.063900
C	-2.570600	-0.008700	2.817700
C	1.969500	2.288900	-1.171400
C	1.011100	2.284900	-2.255200
C	0.878300	1.164800	-3.079800
C	-0.446600	0.727100	3.454000
C	2.761100	1.176200	-0.931100
C	-1.754000	-1.178600	3.066300
C	-0.441200	-0.727200	3.455400
C	0.689500	-1.417100	3.022100
C	2.574000	0.006000	-1.729000
C	1.684500	0.001500	-2.822100
C	4.838000	1.162300	0.643900
C	4.846400	-1.128300	0.646300
N	5.617500	0.019300	0.191600
C	5.920500	0.019500	-1.241700
H	6.523000	0.912400	-1.470500
H	6.522100	-0.874000	-1.470600
H	5.031400	0.020000	-1.896300

H	5.133300	-2.049900	0.119000
H	5.007700	-1.260300	1.730700
H	5.118100	2.084700	0.114200
H	4.998400	1.298200	1.727900

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C	1.983800	-2.286300	-1.158800
C	2.760800	-1.160100	-0.918900
C	3.322400	-0.802300	0.460000
C	2.457200	-1.442300	1.515800
C	1.645500	-2.573400	1.252600
C	1.428900	-3.065200	-0.061600
C	1.863400	-0.699600	2.572600
C	1.858200	0.714700	2.571200
C	2.446100	1.459700	1.512800
C	3.316400	0.824200	0.458500
C	0.673500	1.417500	3.032700
C	0.522700	2.582600	2.191100
C	1.626200	2.584300	1.247500
C	1.406000	3.071900	-0.067700
C	0.093400	3.478600	-0.461300
C	-0.983100	3.480800	0.454300
C	-0.747000	3.018000	1.813000
C	-0.152200	3.009700	-1.822500
C	-1.426200	2.583800	-2.211600
C	-2.524100	2.595500	-1.269900
C	-2.283100	3.029700	0.052400
C	-1.562500	1.409800	-3.056700
C	-2.732000	0.685800	-2.617600
C	-3.320300	1.420700	-1.511500
C	-3.871800	0.702800	-0.435600
C	-3.865900	-0.736200	-0.434100
C	-3.309500	-1.452300	-1.508700
C	-2.726600	-0.715100	-2.616200
C	-1.551900	-1.431200	-3.053800
C	-1.406900	-2.602300	-2.206400
C	-2.504500	-2.620500	-1.264800
C	-2.260400	-3.050500	0.058400
C	-0.957100	-3.491000	0.461200
C	0.119400	-3.482600	-0.454400
C	-0.129700	-3.018100	-1.816500
C	1.030200	-2.289800	-2.255100
C	0.542000	-2.578100	2.196100
C	-0.724500	-3.023800	1.819000
C	0.893600	-1.169200	-3.082100
C	-0.421600	-0.732200	-3.491700
C	-3.626800	-1.183400	0.926200
C	-2.841600	-2.310600	1.167000
C	-1.900800	-2.317600	2.269400
C	-0.427000	0.718300	-3.493100
C	-2.858700	2.287700	1.162500
C	-3.635600	1.154300	0.923900
C	-3.496800	-0.013200	1.772000
C	-1.918000	2.303800	2.264800
C	-1.771400	1.167200	3.076500
C	-2.578300	-0.008700	2.826100
C	1.966600	2.294800	-1.163200
C	1.013100	2.289100	-2.259600
C	0.884900	1.166000	-3.084500
C	-0.459800	0.724600	3.475500
C	2.752400	1.175300	-0.921200
C	-1.762700	-1.178300	3.078800
C	-0.454400	-0.725100	3.476900
C	0.684000	-1.410200	3.035400
C	2.561500	0.006000	-1.717200
C	1.690600	0.001600	-2.829300
C	4.831300	1.163900	0.633200
C	4.840200	-1.130500	0.634100
N	5.631300	0.019600	0.188200
C	5.911900	0.020500	-1.250800
H	6.509000	0.916800	-1.488700
H	6.515300	-0.871600	-1.488400
H	5.016400	0.017400	-1.896600
H	5.121300	-2.047400	0.093500
H	5.014400	-1.278500	1.715700
H	5.105900	2.082900	0.092700
H	5.003700	1.313500	1.714900

c60_prato_56_3_d -13444.35

C	-1.987300	2.323100	-1.093200
C	-2.773800	1.189100	-0.895300
C	-3.332200	0.791800	0.475900
C	-2.468600	1.398300	1.554400
C	-1.647000	2.533000	1.326800
C	-1.430300	3.062900	0.025500
C	-1.873300	0.621700	2.587600
C	-1.869500	-0.791300	2.542800
C	-2.460700	-1.504200	1.462400
C	-3.327900	-0.835300	0.424400
C	-0.687000	-1.518300	2.987000
C	-0.539200	-2.654200	2.118000
C	-1.633300	-2.618000	1.163900
C	-1.413900	-3.063500	-0.168300
C	-0.095600	-3.462100	-0.576700
C	0.978400	-3.496000	0.352100
C	0.742000	-3.084100	1.719200
C	0.150400	-2.964600	-1.919300
C	1.436800	-2.520700	-2.300300
C	2.525800	-2.555900	-1.348500
C	2.284400	-3.029200	-0.038000
C	1.574300	-1.326100	-3.101200
C	2.742200	-0.608900	-2.634100
C	3.332500	-1.377100	-1.550900
C	3.886300	-0.694700	-0.450900
C	3.882700	0.745400	-0.405400
C	3.324800	1.492900	-1.460300
C	2.738500	0.791300	-2.589800
C	1.566600	1.530200	-3.011000
C	1.422900	2.671200	-2.136200
C	2.511800	2.652100	-1.183900
C	2.268000	3.040300	0.153900
C	0.959700	3.474500	0.572500
C	-0.114300	3.493600	-0.356800
C	0.134200	3.083200	-1.728100
C	-1.022200	2.356900	-2.184200
C	-0.552900	2.514600	2.281400
C	0.725800	2.975700	1.910700
C	-0.886700	1.258400	-3.042100
C	0.433000	0.833400	-3.474600
C	3.642800	1.149300	0.968200
C	2.851500	2.272800	1.238500
C	1.897200	2.243600	2.334400
C	0.436900	-0.607500	-3.520200
C	2.863800	-2.328500	1.093100
C	3.648900	-1.185700	0.894400
C	3.512400	-0.045200	1.775500
C	1.909600	-2.373900	2.188400
C	1.764100	-1.259300	3.032200
C	2.581000	-0.081200	2.829100
C	-1.975200	-2.257500	-1.238000
C	-1.010000	-2.217100	-2.328700
C	-0.880500	-1.065900	-3.115600
C	0.450100	-0.828400	3.453600
C	-2.767900	-1.142500	-0.969100
C	1.757800	1.077200	3.106100
C	0.446200	0.613500	3.499200
C	-0.694600	1.325500	3.076900
C	-2.581000	0.048900	-1.726100
C	-1.693600	0.086400	-2.838600
C	-4.840800	-1.178200	0.590700
C	-4.846900	1.116100	0.662600
N	-5.653900	-0.019400	0.187900
C	-5.923100	0.025200	-1.253200
H	-6.519400	-0.864500	-1.523500
H	-6.525200	0.926400	-1.467100
H	-5.021500	0.048200	-1.890200
H	-5.126600	2.049700	0.148300
H	-5.020100	1.232200	1.749100
H	-5.116000	-2.079300	0.019200
H	-5.013000	-1.362600	1.667800

c60_prato_56_4_s -13307.27

C	1.996300	-2.288400	-1.158300
C	2.789900	-1.158200	-0.931000
C	3.340100	-0.804100	0.456700
C	2.478100	-1.445500	1.519000
C	1.648300	-2.570300	1.254900
C	1.435600	-3.057800	-0.066100
C	1.875000	-0.699100	2.572800
C	1.869600	0.713900	2.571400
C	2.466200	1.462200	1.515500
C	3.334000	0.825500	0.455500
C	0.686100	1.434900	3.038400
C	0.541300	2.593900	2.211700
C	1.629000	2.580800	1.249700
C	1.413100	3.064400	-0.072200
C	0.089500	3.478300	-0.475400
C	-0.985400	3.483600	0.464800
C	-0.752100	3.038500	1.814600
C	-0.151800	3.034100	-1.829900
C	-1.449100	2.593500	-2.233100
C	-2.532200	2.591500	-1.273800
C	-2.295600	3.023100	0.054000
C	-1.582900	1.426700	-3.063500
C	-2.749100	0.686200	-2.615500
C	-3.346400	1.420000	-1.511300

C	-3.904700	0.704800	-0.431900
C	-3.899400	-0.738000	-0.430500
C	-3.335900	-1.451400	-1.508500
C	-2.743900	-0.715400	-2.614100
C	-1.572300	-1.448300	-3.060600
C	-1.430000	-2.612500	-2.228000
C	-2.513100	-2.616400	-1.268700
C	-2.273300	-3.043700	0.059900
C	-0.959700	-3.493700	0.471600
C	0.115200	-3.482400	-0.468500
C	-0.129500	-3.042700	-1.823900
C	1.023000	-2.288200	-2.248600
C	0.560500	-2.589400	2.216700
C	-0.729700	-3.044100	1.820500
C	0.889000	-1.160200	-3.070100
C	-0.435300	-0.723900	-3.503200
C	-3.662900	-1.181800	0.931200
C	-2.864100	-2.316000	1.164700
C	-1.899300	-2.315200	2.257600
C	-0.440500	0.709800	-3.504600
C	-2.881100	2.293400	1.160300
C	-3.671500	1.152900	0.929000
C	-3.537700	-0.013100	1.773500
C	-1.916300	2.302000	2.253300
C	-1.772300	1.159400	3.061300
C	-2.596400	-0.008500	2.831500
C	1.979500	2.296800	-1.162700
C	1.006200	2.287200	-2.253100
C	0.880500	1.156700	-3.072400
C	-0.455600	0.717900	3.482700
C	2.782500	1.173500	-0.933700
C	-1.763800	-1.170100	3.063400
C	-0.450300	-0.718200	3.484100
C	0.696700	-1.427700	3.041200
C	2.603200	0.006000	-1.724600
C	1.701900	0.001500	-2.840800
C	4.845200	1.165100	0.637800
C	4.854500	-1.133000	0.635700
N	5.675000	0.019800	0.207600
C	5.936400	0.022000	-1.237200
H	6.524600	0.926400	-1.483900
H	6.545000	-0.869300	-1.483000
H	5.028200	0.011800	-1.866400
H	5.133900	-2.046400	0.083700
H	5.027000	-1.291600	1.717900
H	5.119200	2.082800	0.090300
H	5.014200	1.320200	1.721000

c60_prato_56_5 -13103.27

C	2.000300	-2.298100	-1.164700
C	2.806100	-1.165900	-0.940000
C	3.346400	-0.807800	0.454200
C	2.486300	-1.451100	1.520300
C	1.654300	-2.573600	1.251800
C	1.444900	-3.068600	-0.071700
C	1.874300	-0.701500	2.576100
C	1.869000	0.715700	2.574900
C	2.474400	1.467600	1.517200
C	3.340300	0.829200	0.453100
C	0.689000	1.435600	3.039800
C	0.544100	2.595500	2.209700
C	1.635000	2.583800	1.247100
C	1.422200	3.075100	-0.077300
C	0.094100	3.489900	-0.476800
C	-0.979500	3.498600	0.465300
C	-0.749700	3.045200	1.812800
C	-0.146500	3.047800	-1.833900
C	-1.451600	2.607100	-2.233100
C	-2.528200	2.600100	-1.271000
C	-2.297000	3.032600	0.059200
C	-1.591900	1.428900	-3.058100
C	-2.766500	0.697200	-2.626300
C	-3.345300	1.420000	-1.513800
C	-3.907800	0.712500	-0.425200
C	-3.902400	-0.745900	-0.423900
C	-3.334700	-1.451300	-1.511300
C	-2.761200	-0.726300	-2.625000
C	-1.581100	-1.450100	-3.055400
C	-1.432400	-2.625900	-2.228400
C	-2.508900	-2.625000	-1.266400
C	-2.274600	-3.053400	0.064600
C	-0.953600	-3.508900	0.471600
C	0.119900	-3.494200	-0.470500
C	-0.123900	-3.056200	-1.828500
C	1.028700	-2.305500	-2.254000
C	0.563400	-2.591500	2.214200
C	-0.727100	-3.051400	1.818200
C	0.884100	-1.164500	-3.072300
C	-0.438200	-0.727700	-3.497800
C	-3.679800	-1.191300	0.928700
C	-2.873200	-2.341800	1.172900
C	-1.906800	-2.327600	2.254100
C	-0.443500	0.714200	-3.499200
C	-2.890300	2.318600	1.168800
C	-3.688600	1.161900	0.926700
C	-3.534300	-0.013500	1.761900
C	-1.923900	2.313500	2.250100
C	-1.779200	1.165400	3.067200
C	-2.596500	-0.009100	2.822100
C	1.983400	2.306700	-1.168800
C	1.011800	2.304800	-2.258100
C	0.875500	1.161400	-3.074400
C	-0.463600	0.718900	3.479800
C	2.798700	1.181400	-0.942500
C	-1.770500	-1.177100	3.069100
C	-0.458300	-0.720200	3.481000
C	0.699700	-1.429200	3.042400
C	2.598600	0.006100	-1.721300
C	1.693800	0.001700	-2.836700
C	4.852200	1.165000	0.643700
C	4.861600	-1.132400	0.641300
N	5.694500	0.020300	0.214800
C	5.931500	0.022800	-1.235300
H	6.522300	0.926400	-1.491700
H	6.531000	-0.874400	-1.493900
H	5.009700	0.019200	-1.845900
H	5.142700	-2.047900	0.090800
H	5.031300	-1.286800	1.726200
H	5.127500	2.085100	0.097800
H	5.018300	1.316200	1.729600

c60_prato_56_6 -12840.1

C	-1.995000	2.322900	-1.159000
C	-2.821800	1.190000	-0.956000
C	-3.356700	0.813200	0.439100
C	-2.503700	1.444200	1.522100
C	-1.665000	2.566700	1.266500
C	-1.448600	3.080100	-0.053000
C	-1.892700	0.679300	2.576300
C	-1.890400	-0.743500	2.559800
C	-2.498700	-1.485600	1.487900
C	-3.354000	-0.832300	0.420100
C	-0.717300	-1.469300	3.020800
C	-0.569300	-2.622500	2.176400
C	-1.656600	-2.599200	1.206500
C	-1.438700	-3.081100	-0.124500
C	-0.104800	-3.497400	-0.516500
C	0.961800	-3.522900	0.434100
C	0.727300	-3.074700	1.783300
C	0.143700	-3.042500	-1.869700
C	1.459400	-2.601100	-2.252500
C	2.524100	-2.601800	-1.280800
C	2.290000	-3.050000	0.045900
C	1.612800	-1.402500	-3.058600
C	2.793600	-0.686900	-2.626600
C	3.349000	-1.413300	-1.511400
C	3.908900	-0.725200	-0.402000
C	3.906700	0.748500	-0.384900
C	3.344500	1.460600	-1.478100
C	2.791300	0.758400	-2.609800
C	1.608200	1.480100	-3.025100
C	1.451000	2.659000	-2.191400
C	2.515800	2.640700	-1.220000
C	2.280300	3.057200	0.116800
C	0.950600	3.516600	0.515800
C	-0.116000	3.509700	-0.435100
C	0.133900	3.087200	-1.798500
C	-1.019500	2.348400	-2.241300
C	-0.577600	2.570800	2.236600
C	0.717500	3.036400	1.854200
C	-0.862300	1.203000	-3.068800
C	0.459700	0.767200	-3.483400
C	3.690200	1.181100	0.963700
C	2.876100	2.346300	1.224500
C	1.901800	2.310700	2.289500
C	0.462000	-0.682900	-3.500300
C	2.883500	-2.363100	1.169900
C	3.693900	-1.189500	0.936300
C	3.517300	-0.014000	1.775000
C	1.909200	-2.355500	2.235400
C	1.760900	-1.210200	3.073800
C	2.576200	-0.028000	2.832900
C	-1.987700	-2.300300	-1.212700
C	-1.012000	-2.297400	-2.295200
C	-0.858500	-1.132600	-3.096000
C	0.444900	-0.760700	3.472900

C	-2.818500	-1.175200	-0.983500
C	1.757100	1.145700	3.101100
C	0.442600	0.682800	3.489600
C	-0.721900	1.397900	3.053900
C	-2.589000	0.016700	-1.735300
C	-1.672400	0.031000	-2.842300
C	-4.870700	-1.162700	0.605900
C	-4.874800	1.134700	0.631100
N	-5.718900	-0.010700	0.187600
C	-5.930800	0.004900	-1.266700
H	-6.522200	-0.896700	-1.545400
H	-6.526000	0.909900	-1.525600
H	-4.994800	0.013200	-1.858100
H	-5.152100	2.059300	0.090900
H	-5.046900	1.273300	1.719900
H	-5.145500	-2.076400	0.046300
H	-5.041700	-1.325000	1.691600

c60_prato_56 -13441.44

C	2.046000	-2.352500	-0.929500
C	2.821600	-1.218600	-0.760400
C	3.317900	-0.747800	0.600300
C	2.433100	-1.287300	1.666700
C	1.620500	-2.471700	1.484200
C	1.439900	-3.017900	0.222900
C	1.839100	-0.496300	2.647200
C	1.829900	0.930600	2.532400
C	2.414500	1.562100	1.437400
C	3.307300	0.870600	0.470300
C	0.620700	1.668900	2.909200
C	0.480600	2.772700	1.994900
C	1.587500	2.692000	1.069000
C	1.401500	3.027800	-0.263000
C	0.093100	3.425100	-0.732100
C	-0.982200	3.498900	0.157700
C	-0.782600	3.165000	1.549900
C	-0.100300	2.859400	-2.049300
C	-1.356200	2.394100	-2.436400
C	-2.468400	2.466300	-1.512500
C	-2.283100	3.003300	-0.241000
C	-1.472400	1.158600	-3.184600
C	-2.650500	0.464600	-2.716800
C	-3.264900	1.267100	-1.685700
C	-3.845500	0.651200	-0.576600
C	-3.836400	-0.788300	-0.460900
C	-3.247000	-1.566100	-1.457900
C	-2.641600	-0.930900	-2.604500
C	-1.454400	-1.675800	-2.956500
C	-1.323500	-2.774400	-2.020800
C	-2.435700	-2.712100	-1.096300
C	-2.244800	-3.036700	0.244500
C	-0.938100	-3.446000	0.715900
C	0.137000	-3.501500	-0.175400
C	-0.062300	-3.156000	-1.565800
C	1.113400	-2.448100	-2.025100
C	0.513600	-2.417200	2.412100
C	-0.744200	-2.891500	2.036600
C	0.988600	-1.401900	-2.939400
C	-0.318600	-1.006100	-3.411500
C	-3.635900	-1.125900	0.933700
C	-2.858000	-2.228500	1.280300
C	-1.927000	-2.140000	2.384800
C	-0.327800	0.439300	-3.528000
C	-2.887000	2.363100	0.911300
C	-3.650500	1.209600	0.746000
C	-3.517500	0.110000	1.678500
C	-1.956300	2.463900	2.014800
C	-1.817800	1.396700	2.906900
C	-2.615900	0.200800	2.738000
C	2.017300	2.194300	-1.295100
C	1.084700	2.102100	-2.390800
C	0.973900	0.921800	-3.126300
C	-0.506100	0.996800	3.356400
C	2.807300	1.112000	-0.948000
C	-1.802800	-0.942400	3.095000
C	-0.496800	-0.459300	3.473500
C	0.638900	-1.180000	3.138200
C	2.656200	-0.118900	-1.659100
C	1.777300	-0.212600	-2.754500
C	4.847000	1.223700	0.665200
C	4.862700	-1.045900	0.847500
N	5.579100	0.053200	0.248200
C	5.846500	-0.064700	-1.196000
H	5.455000	0.809700	-1.738200
H	6.933600	-0.130700	-1.369200
H	5.367900	-0.963400	-1.616300
H	5.157400	-2.018600	0.430700
H	5.021300	-1.041800	1.938600
H	5.130000	2.121700	0.099400
H	5.004700	1.394600	1.743000

c60_prato_66_1 -13520.36

C	2.439000	-1.937700	-0.732500
C	2.730700	-0.785300	-1.431200
C	3.309000	0.471800	-0.795900
C	0.710600	-3.343000	0.000000
C	1.362600	-2.803000	-1.166000
C	0.615700	-2.475600	-2.306200
C	2.433000	1.531600	-1.434300
C	1.874400	2.581000	-0.732600
C	-0.686500	-3.534700	0.000000
C	1.763400	0.996400	-2.577900
C	-2.210200	2.817000	-1.166400
C	-1.468800	2.471000	-2.302500
C	-1.773500	1.262400	-3.029500
C	-2.813300	0.422800	-2.599400
C	-3.577000	0.779800	-1.424100
C	-1.552000	3.352500	0.000000
C	-0.150700	3.512300	0.000000
C	0.615200	3.151300	-1.166100
C	-0.028100	2.647600	-2.305700
C	-0.518800	0.686800	-3.468800
C	-0.345300	-0.696200	-3.467600
C	-1.418200	-1.564000	-3.030500
C	-2.634600	-1.007700	-2.600000
C	-3.285500	-1.541300	-1.424900
C	-3.874600	-0.436600	-0.697600
C	-2.712800	-2.605300	-0.723100
C	-1.456700	-3.177200	-1.166400
C	-0.824200	-2.659000	-2.302400
C	0.555000	1.557800	-3.031600
C	0.911900	-1.274500	-3.028500
C	-3.285300	1.952200	-0.723600
C	4.840900	0.679400	-1.130600
C	1.944300	-0.432600	-2.576100
C	2.439000	-1.937700	0.732500
C	2.730700	-0.785300	1.431200
C	3.309000	0.471800	0.795900
C	1.362600	-2.803000	1.166000
C	0.615700	-2.475600	2.306200
C	2.433000	1.531600	1.434300
C	1.874400	2.581000	0.732600
C	1.763400	0.996400	2.577900
C	-2.210200	2.817000	1.166400
C	-1.468800	2.471000	2.302500
C	-1.773500	1.262400	3.029500
C	-2.813300	0.422800	2.599400
C	-3.577000	0.779800	1.424100
C	0.615200	3.151300	1.166100
C	-0.028100	2.647600	2.305700
C	-0.518800	0.686800	3.468800
C	-0.345300	-0.696200	3.467600
C	-1.418200	-1.564000	3.030500
C	-2.634600	-1.007700	2.600000
C	-3.285500	-1.541300	1.424900
C	-3.874600	-0.436600	0.697600
C	-2.712800	-2.605300	0.723100
C	-1.456700	-3.177200	1.166400
C	-0.824200	-2.659000	2.302400
C	0.555000	1.557800	3.031600
C	0.911900	-1.274500	3.028500
C	-3.285300	1.952200	0.723600
C	4.840900	0.679400	1.130600
C	1.944300	-0.432600	2.576100
N	5.592000	0.163200	0.000000
C	5.733000	-1.310300	0.000000
H	5.252000	-1.755900	-0.884800
H	6.801100	-1.586400	0.000000
H	5.252000	-1.755900	0.884800
H	5.019100	1.765000	-1.215000
H	5.118200	0.191100	-2.075200
H	5.019100	1.765000	1.215000
H	5.118200	0.191100	2.075200

c60_prato_66_2_s -13515.98

C	2.447300	-1.937200	-0.730800
C	2.739200	-0.786400	-1.435100
C	3.318300	0.471800	-0.797100
C	0.720400	-3.355500	0.000000
C	1.363900	-2.806300	-1.160100
C	0.619000	-2.470000	-2.303900
C	2.442000	1.532400	-1.438700
C	1.883600	2.580300	-0.730400
C	-0.693300	-3.548100	0.000000
C	1.778000	0.995300	-2.582700
C	-2.211500	2.819500	-1.160800

C	-1.471000	2.464400	-2.300600
C	-1.777800	1.264700	-3.030100
C	-2.827000	0.418000	-2.604800
C	-3.585300	0.778100	-1.426800
C	-1.561700	3.363000	0.000000
C	-0.143900	3.525100	0.000000
C	0.616000	3.152300	-1.160100
C	-0.023200	2.641000	-2.303200
C	-0.517800	0.686400	-3.458400
C	-0.345000	-0.697000	-3.457800
C	-1.421800	-1.568000	-3.031900
C	-2.649600	-1.007000	-2.605800
C	-3.294200	-1.541500	-1.428000
C	-3.884700	-0.437700	-0.698100
C	-2.720900	-2.604900	-0.721500
C	-1.457300	-3.179600	-1.160500
C	-0.828000	-2.653800	-2.300300
C	0.561100	1.562200	-3.035300
C	0.919100	-1.279200	-3.031900
C	-3.292600	1.950100	-0.722200
C	4.842000	0.682500	-1.130100
C	1.958200	-0.430200	-2.581000
C	2.447300	-1.937200	0.730800
C	2.739200	-0.786400	1.435100
C	3.318300	0.471800	0.797100
C	1.363900	-2.806300	1.160100
C	0.619000	-2.470000	2.303900
C	2.442000	1.532400	1.438700
C	1.883600	2.580300	0.730400
C	1.778000	0.995300	2.582700
C	-2.211500	2.819500	1.160800
C	-1.471000	2.464400	2.300600
C	-1.777800	1.264700	3.030100
C	-2.827000	0.418000	2.604800
C	-3.585300	0.778100	1.426800
C	0.616000	3.152300	1.160100
C	-0.023200	2.641000	2.303200
C	-0.517800	0.686400	3.458400
C	-0.345000	-0.697000	3.457800
C	-1.421800	-1.568000	3.031900
C	-2.649600	-1.007000	2.605800
C	-3.294200	-1.541500	1.428000
C	-3.884700	-0.437700	0.698100
C	-2.720900	-2.604900	0.721500
C	-1.457300	-3.179600	1.160500
C	-0.828000	-2.653800	2.300300
C	0.561100	1.562200	3.035300
C	0.919100	-1.279200	3.031900
C	-3.292600	1.950100	0.722200
C	4.842000	0.682500	1.130100
C	1.958200	-0.430200	2.581000
N	5.610900	0.170000	0.000000
C	5.727400	-1.306700	0.000000
H	5.235000	-1.746700	-0.881700
H	6.792300	-1.601900	0.000000
H	5.235000	-1.746700	0.881700
H	5.020800	1.768800	-1.214000
H	5.119000	0.194600	-2.075800
H	5.020800	1.768800	1.214000
H	5.119000	0.194600	2.075800

c60_prato_66_3_d -13444.32

C	2.457800	-1.954900	-0.727700
C	2.745700	-0.795800	-1.441300
C	3.313600	0.470000	-0.797100
C	0.724700	-3.369700	0.000000
C	1.370700	-2.817900	-1.159900
C	0.620600	-2.479700	-2.302800
C	2.444700	1.538200	-1.443400
C	1.892300	2.597000	-0.728200
C	-0.690400	-3.560700	0.000000
C	1.778000	0.997200	-2.575600
C	-2.210800	2.827000	-1.159900
C	-1.466900	2.472100	-2.299500
C	-1.770300	1.266800	-3.034000
C	-2.824500	0.421900	-2.599200
C	-3.586600	0.783200	-1.431500
C	-1.558300	3.373500	0.000000
C	-0.139300	3.537700	0.000000
C	0.623200	3.163700	-1.160400
C	-0.021500	2.648300	-2.302100
C	-0.517700	0.693700	-3.470900
C	-0.342300	-0.706200	-3.469700
C	-1.414700	-1.570000	-3.034900
C	-2.646100	-1.011000	-2.599800
C	-3.295100	-1.548100	-1.432500
C	-3.873000	-0.436500	-0.698400
C	-2.723800	-2.622700	-0.718600
C	-1.457400	-3.189700	-1.160000
C	-0.824000	-2.663100	-2.299700
C	0.558200	1.561700	-3.036400
C	0.915800	-1.282500	-3.033500
C	-3.298500	1.965600	-0.718800
C	4.833000	0.688100	-1.128400
C	1.959900	-0.436100	-2.574000
C	2.457800	-1.954900	0.727700
C	2.745700	-0.795800	1.441300
C	3.313600	0.470000	0.797100
C	1.370700	-2.817900	1.159900
C	0.620600	-2.479700	2.302800
C	2.444700	1.538200	1.443400
C	1.892300	2.597000	0.728200
C	1.778000	0.997200	2.575600
C	-2.210800	2.827000	1.159900
C	-1.466900	2.472100	2.299500
C	-1.770300	1.266800	3.034000
C	-2.824500	0.421900	2.599200
C	-3.586600	0.783200	1.431500
C	0.623200	3.163700	1.160400
C	-0.021500	2.648300	2.302100
C	-0.517700	0.693700	3.470900
C	-0.342300	-0.706200	3.469700
C	-1.414700	-1.570000	3.034900
C	-2.646100	-1.011000	2.599800
C	-3.295100	-1.548100	1.432500
C	-3.873000	-0.436500	0.698400
C	-2.723800	-2.622700	0.718600
C	-1.457400	-3.189700	1.160000
C	-0.824000	-2.663100	2.299700
C	0.558200	1.561700	3.036400
C	0.915800	-1.282500	3.033500
C	-3.298500	1.965600	0.718800
C	4.833000	0.688100	1.128400
C	1.959900	-0.436100	2.574000
N	5.617100	0.175600	0.000000
C	5.708400	-1.303900	0.000000
H	5.203900	-1.737100	-0.878900
H	6.770100	-1.619000	0.000000
H	5.203900	-1.737100	0.878900
H	5.010800	1.775800	-1.204900
H	5.109400	0.204200	-2.077400
H	5.010800	1.775800	1.204900
H	5.109400	0.204200	2.077400

c60_prato_66_4_s -13305.83

C	2.468800	-1.974100	-0.724500
C	2.754600	-0.806200	-1.448500
C	3.309300	0.467600	-0.797200
C	0.727300	-3.384100	0.000000
C	1.376300	-2.829300	-1.159700
C	0.621400	-2.490000	-2.302100
C	2.448000	1.543400	-1.448700
C	1.901300	2.613700	-0.726200
C	-0.689100	-3.573900	0.000000
C	1.778000	0.998300	-2.569100
C	-2.210800	2.835000	-1.159600
C	-1.463300	2.480300	-2.299500
C	-1.763400	1.269400	-3.039200
C	-2.822800	0.426100	-2.594900
C	-3.588200	0.788500	-1.436600
C	-1.555700	3.384300	0.000000
C	-0.135100	3.550300	0.000000
C	0.630000	3.174700	-1.160800
C	-0.020100	2.655700	-2.301500
C	-0.516800	0.701500	-3.484300
C	-0.338700	-0.715400	-3.482000
C	-1.408100	-1.572100	-3.038300
C	-2.643000	-1.015100	-2.594900
C	-3.296500	-1.554700	-1.437300
C	-3.862000	-0.435300	-0.698800
C	-2.727300	-2.640100	-0.716600
C	-1.458900	-3.200700	-1.159800
C	-0.820700	-2.673100	-2.299600
C	0.555500	1.561500	-3.039200
C	0.912800	-1.286900	-3.037100
C	-3.304600	1.981300	-0.716200
C	4.826000	0.695000	-1.126500
C	1.961600	-0.443200	-2.567200
C	2.468800	-1.974100	0.724500
C	2.754600	-0.806200	1.448500
C	3.309300	0.467600	0.797200
C	1.376300	-2.829300	1.159700
C	0.621400	-2.490000	2.302100
C	2.448000	1.543400	1.448700
C	1.901300	2.613700	0.726200
C	1.778000	0.998300	2.569100

C	-2.210800	2.835000	1.159600
C	-1.463300	2.480300	2.299500
C	-1.763400	1.269400	3.039200
C	-2.822800	0.426100	2.594900
C	-3.588200	0.788500	1.436600
C	0.630000	3.174700	1.160800
C	-0.020100	2.655700	2.301500
C	-0.516800	0.701500	3.484300
C	-0.338700	-0.715400	3.482000
C	-1.408100	-1.572100	3.038300
C	-2.643000	-1.015100	2.594900
C	-3.296500	-1.554700	1.437300
C	-3.862000	-0.435300	0.698800
C	-2.727300	-2.640100	0.716600
C	-1.458900	-3.200700	1.159800
C	-0.820700	-2.673100	2.299600
C	0.555500	1.561500	3.039200
C	0.912800	-1.286900	3.037100
C	-3.304600	1.981300	0.716200
C	4.826000	0.695000	1.126500
C	1.961600	-0.443200	2.567200
N	5.624400	0.181400	0.000000
C	5.690600	-1.301000	0.000000
H	5.173800	-1.726600	-0.876500
H	6.749400	-1.636100	0.000000
H	5.173800	-1.726600	0.876500
H	5.001800	1.784800	-1.193700
H	5.101300	0.215600	-2.079600
H	5.001800	1.784800	1.193700
H	5.101300	0.215600	2.079600

c60_prato_66_5 -13096.37

C	2.464800	-1.976900	-0.723900
C	2.772100	-0.812200	-1.458900
C	3.318200	0.466100	-0.802900
C	0.718100	-3.382000	0.000000
C	1.374100	-2.836200	-1.163200
C	0.616200	-2.494900	-2.310100
C	2.460600	1.545300	-1.457300
C	1.899100	2.609800	-0.726400
C	-0.700400	-3.566000	0.000000
C	1.783500	0.996800	-2.574900
C	-2.221700	2.838500	-1.167000
C	-1.464300	2.487500	-2.320900
C	-1.760800	1.274300	-3.051400
C	-2.823100	0.422200	-2.612400
C	-3.589400	0.779300	-1.437600
C	-1.560500	3.372700	0.000000
C	-0.138900	3.543700	0.000000
C	0.630000	3.178300	-1.165000
C	-0.023600	2.655700	-2.309700
C	-0.511200	0.701600	-3.495600
C	-0.333400	-0.716500	-3.492300
C	-1.405500	-1.577500	-3.050500
C	-2.645100	-1.011100	-2.612500
C	-3.301300	-1.544800	-1.438600
C	-3.888000	-0.437400	-0.712300
C	-2.726400	-2.634100	-0.722700
C	-1.472000	-3.207500	-1.167300
C	-0.822200	-2.681600	-2.320600
C	0.560700	1.561100	-3.047900
C	0.917400	-1.289400	-3.045500
C	-3.300100	1.977400	-0.722200
C	4.834100	0.702300	-1.125200
C	1.967400	-0.446500	-2.572600
C	2.464800	-1.976900	0.723900
C	2.772100	-0.812200	1.458900
C	3.318200	0.466100	0.802900
C	1.374100	-2.836200	1.163200
C	0.616200	-2.494900	2.310100
C	2.460600	1.545300	1.457300
C	1.899100	2.609800	0.726400
C	1.783500	0.996800	2.574900
C	-2.221700	2.838500	1.167000
C	-1.464300	2.487500	2.320900
C	-1.760800	1.274300	3.051400
C	-2.823100	0.422200	2.612400
C	-3.589400	0.779300	1.437600
C	0.630000	3.178300	1.165000
C	-0.023600	2.655700	2.309700
C	-0.511200	0.701600	3.495600
C	-0.333400	-0.716500	3.492300
C	-1.405500	-1.577500	3.050500
C	-2.645100	-1.011100	2.612500
C	-3.301300	-1.544800	1.438600
C	-3.888000	-0.437400	0.712300
C	-2.726400	-2.634100	0.722700
C	-1.472000	-3.207500	1.167300
C	-0.822200	-2.681600	2.320600
C	0.560700	1.561100	3.047900
C	0.917400	-1.289400	3.045500
C	-3.300100	1.977400	0.722200
C	4.834100	0.702300	1.125200
C	1.967400	-0.446500	2.572600
N	5.645800	0.188300	0.000000
C	5.686600	-1.297100	0.000000
H	5.158300	-1.714400	-0.874900
H	6.743000	-1.652300	0.000000
H	5.158300	-1.714400	0.874900
H	5.006200	1.794700	-1.185100
H	5.109600	0.226400	-2.081600
H	5.006200	1.794700	1.185100
H	5.109600	0.226400	2.081600

c60_prato_66_6 -12823.00

C	2.459300	-1.980100	-0.723200
C	2.794000	-0.820300	-1.471600
C	3.327800	0.463400	-0.809700
C	0.708300	-3.380800	0.000000
C	1.371600	-2.844400	-1.166700
C	0.610200	-2.500800	-2.318500
C	2.473100	1.545000	-1.465600
C	1.896700	2.603700	-0.727300
C	-0.712500	-3.560000	0.000000
C	1.788300	0.993400	-2.581500
C	-2.232400	2.843700	-1.174600
C	-1.465200	2.494800	-2.342400
C	-1.759400	1.279200	-3.064500
C	-2.824400	0.418900	-2.630600
C	-3.592500	0.771600	-1.439400
C	-1.564900	3.362800	0.000000
C	-0.141500	3.536600	0.000000
C	0.631000	3.182400	-1.169700
C	-0.026800	2.655400	-2.318800
C	-0.506600	0.701100	-3.507300
C	-0.329400	-0.717500	-3.501900
C	-1.404500	-1.582900	-3.063100
C	-2.648700	-1.007300	-2.630600
C	-3.308800	-1.535600	-1.440600
C	-3.912400	-0.438100	-0.725800
C	-2.727000	-2.628200	-0.728800
C	-1.486200	-3.216000	-1.174600
C	-0.824800	-2.690500	-2.340900
C	0.565300	1.560100	-3.056900
C	0.921300	-1.292700	-3.053700
C	-3.296000	1.974600	-0.728200
C	4.844700	0.711700	-1.124100
C	1.972700	-0.450600	-2.578700
C	2.459300	-1.980100	0.723200
C	2.794000	-0.820300	1.471600
C	3.327800	0.463400	0.809700
C	1.371600	-2.844400	1.166700
C	0.610200	-2.500800	2.318500
C	2.473100	1.545000	1.465600
C	1.896700	2.603700	0.727300
C	1.788300	0.993400	2.581500
C	-2.232400	2.843700	1.174600
C	-1.465200	2.494800	2.342400
C	-1.759400	1.279200	3.064500
C	-2.824400	0.418900	2.630600
C	-3.592500	0.771600	1.439400
C	0.631000	3.182400	1.169700
C	-0.026800	2.655400	2.318800
C	-0.506600	0.701100	3.507300
C	-0.329400	-0.717500	3.501900
C	-1.404500	-1.582900	3.063100
C	-2.648700	-1.007300	2.630600
C	-3.308800	-1.535600	1.440600
C	-3.912400	-0.438100	0.725800
C	-2.727000	-2.628200	0.728800
C	-1.486200	-3.216000	1.174600
C	-0.824800	-2.690500	2.340900
C	0.565300	1.560100	3.056900
C	0.921300	-1.292700	3.053700
C	-3.296000	1.974600	0.728200
C	4.844700	0.711700	1.124100
C	1.972700	-0.450600	2.578700
N	5.669400	0.197100	0.000000
C	5.685500	-1.291400	0.000000
H	5.145800	-1.699000	-0.874500
H	6.739800	-1.666900	0.000000
H	5.145800	-1.699000	0.874500
H	5.011300	1.807400	-1.175600
H	5.120900	0.238600	-2.083800
H	5.011300	1.807400	1.175600
H	5.120900	0.238600	2.083800

c60_prato_66 -13455.92

C	-2.517800	-1.869000	0.733900
C	-2.777300	-0.706900	1.427800
C	-3.318200	0.565000	0.795000
C	-0.827000	-3.310100	0.000000
C	-1.472700	-2.760700	1.172000
C	-0.715100	-2.462900	2.308900
C	-2.414000	1.599100	1.430100
C	-1.825700	2.634100	0.734900
C	0.548000	-3.539100	0.000000
C	-1.753100	1.046900	2.573400
C	2.254300	2.752500	1.172300
C	1.502700	2.436000	2.304800
C	1.771200	1.210700	3.029800
C	2.778500	0.349700	2.594700
C	3.556900	0.681400	1.422000
C	1.602500	3.298300	0.000000
C	0.222400	3.495100	0.000000
C	-0.558800	3.167700	1.172300
C	0.074100	2.653200	2.308600
C	0.505800	0.672800	3.479100
C	0.292400	-0.704400	3.478300
C	1.337300	-1.598800	3.029600
C	2.557500	-1.081600	2.594800
C	3.200000	-1.632500	1.422000
C	3.818500	-0.543400	0.697300
C	2.598200	-2.680700	0.725100
C	1.333900	-3.215000	1.172600
C	0.712500	-2.686500	2.305100
C	-0.538500	1.569200	3.028300
C	-0.974000	-1.244100	3.026800
C	3.299200	1.862200	0.725000
C	-4.855200	0.814000	1.131500
C	-1.975900	-0.380900	2.572200
C	-2.517800	-1.869000	-0.733900
C	-2.777300	-0.706900	-1.427800
C	-3.318200	0.565000	-0.795000
C	-1.472700	-2.760700	-1.172000
C	-0.715100	-2.462900	-2.308900
C	-2.414000	1.599100	-1.430100
C	-1.825700	2.634100	-0.734900
C	-1.753100	1.046900	-2.573400
C	2.254300	2.752500	-1.172300
C	1.502700	2.436000	-2.304800
C	1.771200	1.210700	-3.029800
C	2.778500	0.349700	-2.594700
C	3.556900	0.681400	-1.422000
C	-0.558800	3.167700	-1.172300
C	0.074100	2.653200	-2.308600
C	0.505800	0.672800	-3.479100
C	0.292400	-0.704400	-3.478300
C	1.337300	-1.598800	-3.029600
C	2.557500	-1.081600	-2.594800
C	3.200000	-1.632500	-1.422000
C	3.818500	-0.543400	-0.697300
C	2.598200	-2.680700	-0.725100
C	1.333900	-3.215000	-1.172600
C	0.712500	-2.686500	-2.305100
C	-0.538500	1.569200	-3.028300
C	-0.974000	-1.244100	-3.026800
C	3.299200	1.862200	-0.725000
C	-4.855200	0.814000	-1.131500
C	-1.975900	-0.380900	-2.572200
N	-5.600300	0.314400	0.000000
C	-5.815200	-1.148800	0.000000
H	-5.360900	-1.614500	0.888200
H	-6.894800	-1.369100	0.000000
H	-5.360900	-1.614500	-0.888200
H	-5.000300	1.904000	1.215000
H	-5.146700	0.333400	2.075100
H	-5.000300	1.904000	-1.215000
H	-5.146700	0.333400	-2.075100

c60_Car_56_1e -12409.69

C	-1.611400	-1.490900	-2.314600
C	-2.488100	-1.361900	-1.232200
C	-3.209800	-0.098500	-1.095900
C	-2.537800	1.055900	-1.550000
C	-1.611100	0.930100	-2.628100
C	-1.204600	-0.333600	-3.081400
C	-2.092200	2.171400	-0.705800
C	-2.092200	2.171400	0.705800
C	-2.537800	1.055900	1.550000
C	-3.209800	-0.098500	1.095900
C	-0.963800	2.791400	1.401000
C	-0.672600	2.014600	2.581200
C	-1.611100	0.930100	2.628100
C	-1.204600	-0.333600	3.081400
C	0.156300	-0.534200	3.501900
C	1.068500	0.530800	3.488900
C	0.635700	1.838700	3.026000
C	0.582900	-1.838400	3.029600
C	1.891600	-2.039300	2.596100
C	2.837000	-0.943600	2.601000
C	2.420300	0.327200	3.038600
C	2.138400	-2.849100	1.419600
C	3.237500	-2.247600	0.697500
C	3.663800	-1.068300	1.428900
C	4.063300	0.073900	0.720000
C	4.063300	0.073900	-0.720000
C	3.663800	-1.068300	-1.428900
C	3.237500	-2.247600	-0.697500
C	2.138400	-2.849100	-1.419600
C	1.891600	-2.039300	-2.596100
C	2.837000	-0.943600	-2.601000
C	2.420300	0.327200	-3.038600
C	1.068500	0.530800	-3.488900
C	0.156300	-0.534200	-3.501900
C	0.582900	-1.838400	-3.029600
C	-0.516800	-2.421000	-2.297300
C	-0.672600	2.014600	-2.581200
C	0.635700	1.838700	-3.026000
C	-0.290300	-3.189000	-1.159700
C	1.070300	-3.417600	-0.721000
C	3.630400	1.384700	-1.167200
C	2.826400	1.506400	-2.299900
C	1.724400	2.447100	-2.303300
C	1.070300	-3.417600	0.721000
C	2.826400	1.506400	2.299900
C	3.630400	1.384700	1.167200
C	3.368800	2.198900	0.000000
C	1.724400	2.447100	2.303300
C	1.455700	3.218800	1.169000
C	2.295900	3.100500	0.000000
C	-1.611400	-1.490900	2.314600
C	-0.516800	-2.421000	2.297300
C	-0.290300	-3.189000	1.159700
C	0.090500	3.395400	0.719500
C	-2.488100	-1.361900	1.232200
C	1.455700	3.218800	-1.169000
C	0.090500	3.395400	-0.719500
C	-0.963800	2.791400	-1.401000
C	-2.210700	-2.098000	0.000000
C	-1.135600	-3.024200	0.000000
C	-4.198200	-0.023900	0.000000
Cl	-5.191200	1.487900	0.000000
Cl	-5.368300	-1.455400	0.000000

c60_Car_56 -12338.51

C	-1.649300	-1.447600	-2.317300
C	-2.529400	-1.299200	-1.241600
C	-3.201700	-0.013400	-1.097900
C	-2.504500	1.115900	-1.539500
C	-1.572600	0.967600	-2.622700
C	-1.204400	-0.294700	-3.067700
C	-2.045500	2.227700	-0.706800
C	-2.045500	2.227700	0.706800
C	-2.504500	1.115900	1.539500
C	-3.201700	-0.013400	1.097900
C	-0.898200	2.815900	1.404300
C	-0.621900	2.039900	2.587300
C	-1.572600	0.967600	2.622700
C	-1.204400	-0.294700	3.067700
C	0.155200	-0.529000	3.500600
C	1.080000	0.515800	3.488000
C	0.681300	1.831100	3.031900
C	0.545200	-1.840000	3.034900
C	1.846000	-2.071600	2.598000
C	2.809800	-0.991700	2.597000
C	2.432300	0.279800	3.031000
C	2.075700	-2.881200	1.420400
C	3.190500	-2.308500	0.697300
C	3.640500	-1.138100	1.421300
C	4.066000	-0.008100	0.723200
C	4.066000	-0.008100	-0.723200
C	3.640500	-1.138100	-1.421300
C	3.190500	-2.308500	-0.697300
C	2.075700	-2.881200	-1.420400
C	1.846000	-2.071600	-2.598000
C	2.809800	-0.991700	-2.597000
C	2.432300	0.279800	-3.031000
C	1.080000	0.515800	-3.488000
C	0.155200	-0.529000	-3.500600

C	0.545200	-1.840000	-3.034900
C	-0.571400	-2.393300	-2.298400
C	-0.621900	2.039900	-2.587300
C	0.681300	1.831100	-3.031900
C	-0.359300	-3.155900	-1.160300
C	0.994900	-3.419100	-0.720700
C	3.671900	1.310900	-1.170700
C	2.870900	1.452300	-2.302600
C	1.785200	2.409100	-2.303100
C	0.994900	-3.419100	0.720700
C	2.870900	1.452300	2.302600
C	3.671900	1.310900	1.170700
C	3.421600	2.124600	0.000000
C	1.785200	2.409100	2.303100
C	1.530600	3.179400	1.170200
C	2.369400	3.041800	0.000000
C	-1.649300	-1.447600	2.317300
C	-0.571400	-2.393300	2.298400
C	-0.359300	-3.155900	1.160300
C	0.168700	3.386900	0.719800
C	-2.529400	-1.299200	1.241600
C	1.530600	3.179400	-1.170200
C	0.168700	3.386900	-0.719800
C	-0.898200	2.815900	-1.404300
C	-2.267500	-2.036100	0.000000
C	-1.203200	-2.965600	0.000000
C	-4.200600	0.088100	0.000000
Cl	-5.138200	1.619900	0.000000
Cl	-5.377500	-1.298200	0.000000

c60_Car_56_2_s -12413.99

C	-1.604700	-1.485500	-2.313300
C	-2.475100	-1.354600	-1.224100
C	-3.216300	-0.098100	-1.094700
C	-2.545700	1.066200	-1.564700
C	-1.624100	0.939700	-2.635600
C	-1.208400	-0.334700	-3.096500
C	-2.084500	2.172500	-0.705000
C	-2.084500	2.172500	0.705000
C	-2.545700	1.066200	1.564700
C	-3.216300	-0.098100	1.094700
C	-0.959700	2.796200	1.397300
C	-0.671900	2.013700	2.576000
C	-1.624100	0.939700	2.635600
C	-1.208400	-0.334700	3.096500
C	0.148300	-0.533300	3.505900
C	1.073500	0.531100	3.492000
C	0.637200	1.840700	3.021600
C	0.581400	-1.840600	3.026400
C	1.893100	-2.040800	2.595300
C	2.845800	-0.951000	2.605700
C	2.420000	0.328400	3.047400
C	2.138200	-2.855500	1.419300
C	3.236000	-2.251500	0.697900
C	3.666400	-1.073700	1.436800
C	4.066200	0.071400	0.717100
C	4.066200	0.071400	-0.717100
C	3.666400	-1.073700	-1.436800
C	3.236000	-2.251500	-0.697900
C	2.138200	-2.855500	-1.419300
C	1.893100	-2.040800	-2.595300
C	2.845800	-0.951000	-2.605700
C	2.420000	0.328400	-3.047400
C	1.073500	0.531100	-3.492000
C	0.148300	-0.533300	-3.505900
C	0.581400	-1.840600	-3.026400
C	-0.515100	-2.425700	-2.297700
C	-0.671900	2.013700	-2.576000
C	0.637200	1.840700	-3.021600
C	-0.291300	-3.201600	-1.159300
C	1.069600	-3.429000	-0.721300
C	3.625700	1.383800	-1.164300
C	2.821600	1.504700	-2.298200
C	1.725000	2.454400	-2.304300
C	1.069600	-3.429000	0.721300
C	2.821600	1.504700	2.298200
C	3.625700	1.383800	1.164300
C	3.370700	2.204100	0.000000
C	1.725000	2.454400	2.304300
C	1.459200	3.232800	1.168300
C	2.298100	3.114400	0.000000
C	-1.604700	-1.485500	2.313300
C	-0.515100	-2.425700	2.297700
C	-0.291300	-3.201600	1.159300
C	0.095000	3.410300	0.719200
C	-2.475100	-1.354600	1.224100
C	1.459200	3.232800	-1.168300
C	0.095000	3.410300	-0.719200
C	-0.959700	2.796200	-1.397300
C	-2.198300	-2.094500	0.000000
C	-1.134100	-3.041200	0.000000
C	-4.185000	-0.022400	0.000000
Cl	-5.205200	1.491100	0.000000
Cl	-5.407000	-1.500500	0.000000

c60_Car_56_3_d -12351.8

C	-1.604400	-1.485700	-2.326200
C	-2.479300	-1.349200	-1.230100
C	-3.219400	-0.099100	-1.112000
C	-2.549700	1.073300	-1.586000
C	-1.628200	0.944900	-2.659300
C	-1.209400	-0.333700	-3.111000
C	-2.085400	2.167900	-0.714600
C	-2.085400	2.167900	0.714600
C	-2.549700	1.073300	1.586000
C	-3.219400	-0.099100	1.112000
C	-0.961700	2.787300	1.398500
C	-0.669500	2.014700	2.589100
C	-1.628200	0.944900	2.659300
C	-1.209400	-0.333700	3.111000
C	0.148100	-0.532000	3.522200
C	1.074500	0.533200	3.508300
C	0.641300	1.841300	3.032700
C	0.578400	-1.839400	3.037300
C	1.891800	-2.036400	2.603600
C	2.843400	-0.948900	2.614400
C	2.421800	0.331500	3.056600
C	2.141800	-2.848300	1.420200
C	3.246100	-2.257900	0.706800
C	3.664300	-1.077200	1.436600
C	4.063300	0.075200	0.722400
C	4.063300	0.075200	-0.722400
C	3.664300	-1.077200	-1.436600
C	3.246100	-2.257900	-0.706800
C	2.141800	-2.848300	-1.420200
C	1.891800	-2.036400	-2.603600
C	2.843400	-0.948900	-2.614400
C	2.421800	0.331500	-3.056600
C	1.074500	0.533200	-3.508300
C	0.148100	-0.532000	-3.522200
C	0.578400	-1.839400	-3.037300
C	-0.521000	-2.423700	-2.313200
C	-0.669500	2.014700	-2.589100
C	0.641300	1.841300	-3.032700
C	-0.290000	-3.198900	-1.164500
C	1.065000	-3.421100	-0.725300
C	3.637500	1.382500	-1.172100
C	2.827700	1.512300	-2.315400
C	1.735500	2.454600	-2.319400
C	1.065000	-3.421100	0.725300
C	2.827700	1.512300	2.315400
C	3.637500	1.382500	1.172100
C	3.368700	2.194100	0.000000
C	1.735500	2.454600	2.319400
C	1.461100	3.232700	1.174200
C	2.297100	3.101800	0.000000
C	-1.604400	-1.485700	2.326200
C	-0.521000	-2.423700	2.313200
C	-0.290000	-3.198900	1.164500
C	0.103000	3.399300	0.721400
C	-2.479300	-1.349200	1.230100
C	1.461100	3.232700	-1.174200
C	0.103000	3.399300	-0.721400
C	-0.961700	2.787300	-1.398500
C	-2.197100	-2.082300	0.000000
C	-1.127900	-3.024800	0.000000
C	-4.137000	0.008300	0.000000
Cl	-5.196100	1.498900	0.000000
Cl	-5.511000	-1.602300	0.000000

c60_Car_66_1 -12410.61

C	0.731600	-2.278400	2.016900
C	1.458600	-1.183100	2.456100
C	0.818400	0.000000	3.086000
C	0.000000	-3.452800	0.117600
C	1.164400	-2.997800	0.832800
C	2.300800	-2.577100	0.130200
C	1.458600	1.183100	2.456100
C	0.731600	2.278400	2.016900
C	0.000000	-3.468200	-1.292500
C	2.590300	0.720400	1.702800
C	1.165400	3.019200	-2.013800
C	2.300100	2.583600	-1.322500
C	3.029100	1.424700	-1.777100
C	2.599600	0.720800	-2.914200
C	1.424200	1.169700	-3.627000

C	0.000000	3.468200	-1.292500
C	0.000000	3.452800	0.117600
C	1.164400	2.997800	0.832800
C	2.300800	2.577100	0.130200
C	3.467900	0.696700	-0.605500
C	3.467900	-0.696700	-0.605500
C	3.029100	-1.424700	-1.777100
C	2.599600	-0.720800	-2.914200
C	1.424200	-1.169700	-3.627000
C	0.697500	0.000000	-4.074700
C	0.722900	-2.296200	-3.190900
C	1.165400	-3.019200	-2.013800
C	2.300100	-2.583600	-1.322500
C	3.029200	1.423500	0.569900
C	3.029200	-1.423500	0.569900
C	0.722900	2.296200	-3.190900
C	0.000000	0.000000	4.333400
C	2.590300	-0.720400	1.702800
C	-0.731600	-2.278400	2.016900
C	-1.458600	-1.183100	2.456100
C	-0.818400	0.000000	3.086000
C	-1.164400	-2.997800	0.832800
C	-2.300800	-2.577100	0.130200
C	-1.458600	1.183100	2.456100
C	-0.731600	2.278400	2.016900
C	-2.590300	0.720400	1.702800
C	-1.165400	3.019200	-2.013800
C	-2.300100	2.583600	-1.322500
C	-3.029100	1.424700	-1.777100
C	-2.599600	0.720800	-2.914200
C	-1.424200	1.169700	-3.627000
C	-1.164400	2.997800	0.832800
C	-2.300800	2.577100	0.130200
C	-3.467900	0.696700	-0.605500
C	-3.467900	-0.696700	-0.605500
C	-3.029100	-1.424700	-1.777100
C	-2.599600	-0.720800	-2.914200
C	-1.424200	-1.169700	-3.627000
C	-0.697500	0.000000	-4.074700
C	-0.722900	-2.296200	-3.190900
C	-1.165400	-3.019200	-2.013800
C	-2.300100	-2.583600	-1.322500
C	-3.029200	1.423500	0.569900
C	-3.029200	-1.423500	0.569900
C	-0.722900	2.296200	-3.190900
C	-2.590300	-0.720400	1.702800
Cl	0.000000	1.487100	5.324100
Cl	0.000000	-1.487100	5.324100

c60_Car_66 -12341.4

C	0.734100	2.280200	-2.006200
C	1.454300	1.182800	-2.444100
C	0.818800	0.000000	-3.078000
C	0.000000	3.441500	-0.107000
C	1.170800	2.997400	-0.829700
C	2.303900	2.584300	-0.123600
C	1.454300	-1.182800	-2.444100
C	0.734100	-2.280200	-2.006200
C	0.000000	3.457200	1.286800
C	2.584200	-0.722400	-1.684500
C	1.171500	-3.017800	2.015800
C	2.302900	-2.590300	1.322500
C	3.029100	-1.421900	1.776000
C	2.594800	-0.724100	2.902900
C	1.421600	-1.170800	3.621300
C	0.000000	-3.457200	1.286800
C	0.000000	-3.441500	-0.107000
C	1.170800	-2.997400	-0.829700
C	2.303900	-2.584300	-0.123600
C	3.478500	-0.696700	0.608600
C	3.478500	0.696700	0.608600
C	3.029100	1.421900	1.776000
C	2.594800	0.724100	2.902900
C	1.421600	1.170800	3.621300
C	0.697000	0.000000	4.067100
C	0.724500	2.298100	3.186100
C	1.171500	3.017800	2.015800
C	2.302900	2.590300	1.322500
C	3.027000	-1.420100	-0.560800
C	3.027000	1.420100	-0.560800
C	0.724500	-2.298100	3.186100
C	0.000000	0.000000	-4.329400
C	2.584200	0.722400	-1.684500
C	-0.734100	2.280200	-2.006200
C	-1.454300	1.182800	-2.444100
C	-0.818800	0.000000	-3.078000
C	-1.170800	2.997400	-0.829700
C	-2.303900	2.584300	-0.123600
C	-1.454300	-1.182800	-2.444100
C	-0.734100	-2.280200	-2.006200
C	-2.584200	-0.722400	-1.684500
C	-1.171500	-3.017800	2.015800
C	-2.302900	-2.590300	1.322500
C	-3.029100	-1.421900	1.776000
C	-2.594800	-0.724100	2.902900
C	-1.421600	-1.170800	3.621300
C	-1.170800	-2.997400	-0.829700
C	-2.303900	-2.584300	-0.123600
C	-3.478500	-0.696700	0.608600
C	-3.478500	0.696700	0.608600
C	-3.029100	1.421900	1.776000
C	-2.594800	0.724100	2.902900
C	-1.421600	1.170800	3.621300
C	-0.697000	0.000000	4.067100
C	-0.724500	2.298100	3.186100
C	-1.171500	3.017800	2.015800
C	-2.302900	2.590300	1.322500
C	-3.027000	-1.420100	-0.560800
C	-3.027000	1.420100	-0.560800
C	-0.724500	-2.298100	3.186100
C	-2.584200	0.722400	-1.684500
Cl	0.000000	-1.486200	-5.302800
Cl	0.000000	1.486200	-5.302800

c60_Car_66_2_s -12410.93

C	0.729100	-2.277400	2.024800
C	1.463300	-1.183900	2.465500
C	0.818800	0.000000	3.091200
C	0.000000	-3.465500	0.124600
C	1.158100	-2.999500	0.832700
C	2.297400	-2.570000	0.133100
C	1.463300	1.183900	2.465500
C	0.729100	2.277400	2.024800
C	0.000000	-3.479900	-1.302200
C	2.596100	0.718900	1.717300
C	1.159600	3.021800	-2.016200
C	2.297400	2.577000	-1.326400
C	3.029800	1.427500	-1.782200
C	2.605200	0.718000	-2.929900
C	1.426900	1.168800	-3.637000
C	0.000000	3.479900	-1.302200
C	0.000000	3.465500	0.124600
C	1.158100	2.999500	0.832700
C	2.297400	2.570000	0.133100
C	3.457500	0.696800	-0.606200
C	3.457500	-0.696800	-0.606200
C	3.029800	-1.427500	-1.782200
C	2.605200	-0.718000	-2.929900
C	1.426900	-1.168800	-3.637000
C	0.698000	0.000000	-4.086300
C	0.721300	-2.295000	-3.200200
C	1.159600	-3.021800	-2.016200
C	2.297400	-2.577000	-1.326400
C	3.032100	1.427200	0.575700
C	3.032100	-1.427200	0.575700
C	0.721300	2.295000	-3.200200
C	0.000000	0.000000	4.334700
C	2.596100	-0.718900	1.717300
C	-0.729100	-2.277400	2.024800
C	-1.463300	-1.183900	2.465500
C	-0.818800	0.000000	3.091200
C	-1.158100	-2.999500	0.832700
C	-2.297400	-2.570000	0.133100
C	-1.463300	1.183900	2.465500
C	-0.729100	2.277400	2.024800
C	-2.596100	0.718900	1.717300
C	-1.159600	3.021800	-2.016200
C	-2.297400	2.577000	-1.326400
C	-3.029800	1.427500	-1.782200
C	-2.605200	0.718000	-2.929900
C	-1.426900	1.168800	-3.637000
C	-1.158100	2.999500	0.832700
C	-2.297400	2.570000	0.133100
C	-3.457500	0.696800	-0.606200
C	-3.457500	-0.696800	-0.606200
C	-3.029800	-1.427500	-1.782200
C	-2.605200	-0.718000	-2.929900
C	-1.426900	-1.168800	-3.637000
C	-0.698000	0.000000	-4.086300
C	-0.721300	-2.295000	-3.200200
C	-1.159600	-3.021800	-2.016200
C	-2.297400	-2.577000	-1.326400
C	-3.032100	1.427200	0.575700
C	-3.032100	-1.427200	0.575700
C	-0.721300	2.295000	-3.200200
C	-2.596100	-0.718900	1.717300

Cl	0.000000	1.490100	5.346200
Cl	0.000000	-1.490100	5.346200
c60_Car_66_3_d	-12343.53		
C	0.725600	-2.292500	2.030600
C	1.470500	-1.191000	2.469500
C	0.821400	0.000000	3.083400
C	0.000000	-3.477800	0.125100
C	1.157500	-3.008500	0.835700
C	2.296100	-2.578300	0.131300
C	1.470500	1.191000	2.469500
C	0.725600	2.292500	2.030600
C	0.000000	-3.491100	-1.302600
C	2.589400	0.722800	1.714200
C	1.159000	3.030700	-2.019400
C	2.296400	2.585400	-1.325200
C	3.032500	1.428800	-1.777200
C	2.599600	0.721800	-2.929100
C	1.431400	1.174600	-3.640200
C	0.000000	3.491100	-1.302600
C	0.000000	3.477800	0.125100
C	1.157500	3.008500	0.835700
C	2.296100	2.578300	0.131300
C	3.469700	0.704900	-0.606700
C	3.469700	-0.704900	-0.606700
C	3.032500	-1.428800	-1.777200
C	2.599600	-0.721800	-2.929100
C	1.431400	-1.174600	-3.640200
C	0.698400	0.000000	-4.076600
C	0.718300	-2.311000	-3.206900
C	1.159000	-3.030700	-2.019400
C	2.296400	-2.585400	-1.325200
C	3.034300	1.428600	0.569900
C	3.034300	-1.428600	0.569900
C	0.718300	2.311000	-3.206900
C	0.000000	0.000000	4.320700
C	2.589400	-0.722800	1.714200
C	-0.725600	-2.292500	2.030600
C	-1.470500	-1.191000	2.469500
C	-0.821400	0.000000	3.083400
C	-1.157500	-3.008500	0.835700
C	-2.296100	-2.578300	0.131300
C	-1.470500	1.191000	2.469500
C	-0.725600	2.292500	2.030600
C	-2.589400	0.722800	1.714200
C	-1.159000	3.030700	-2.019400
C	-2.296400	2.585400	-1.325200
C	-3.032500	1.428800	-1.777200
C	-2.599600	0.721800	-2.929100
C	-1.431400	1.174600	-3.640200
C	-1.157500	3.008500	0.835700
C	-2.296100	2.578300	0.131300
C	-3.469700	0.704900	-0.606700
C	-3.469700	-0.704900	-0.606700
C	-3.032500	-1.428800	-1.777200
C	-2.599600	-0.721800	-2.929100
C	-1.431400	-1.174600	-3.640200
C	-0.698400	0.000000	-4.076600
C	-0.718300	-2.311000	-3.206900
C	-1.159000	-3.030700	-2.019400
C	-2.296400	-2.585400	-1.325200
C	-3.034300	1.428600	0.569900
C	-3.034300	-1.428600	0.569900
C	-0.718300	2.311000	-3.206900
C	-2.589400	-0.722800	1.714200
Cl	0.000000	1.497000	5.360400
Cl	0.000000	-1.497000	5.360400

Figure S1. Schematic representation of the reaction energies and reaction barrier differences between the Diels-Alder cycloaddition of cyclopentadiene on C_{60}^{n-} (n = 0 – 6) for the [6,6] and [5,6] positions, obtained at BP86-D_2/TZP//BP86-D_2/DZP level.

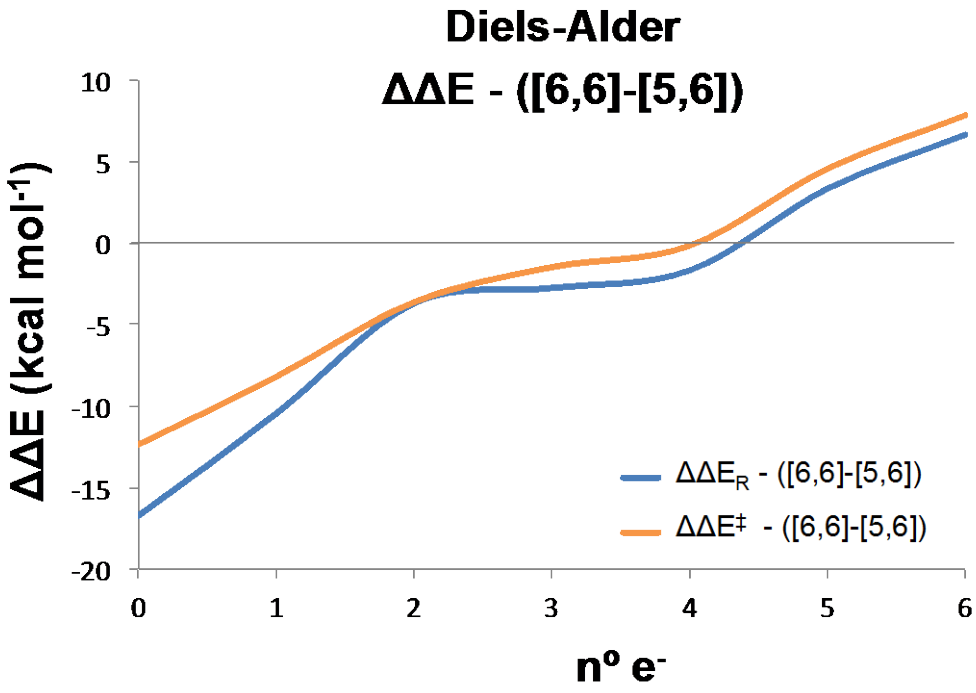


Figure S2. Schematic representation of the reaction energies found for the 1,3-dipolar cycloaddition of N-methyl azomethine ylide on [6,6] and [5,6] positions of C_{60}^{n-} (n = 0 – 6) fullerene, obtained at BP86-D_2/TZP//BP86-D_2/DZP level.

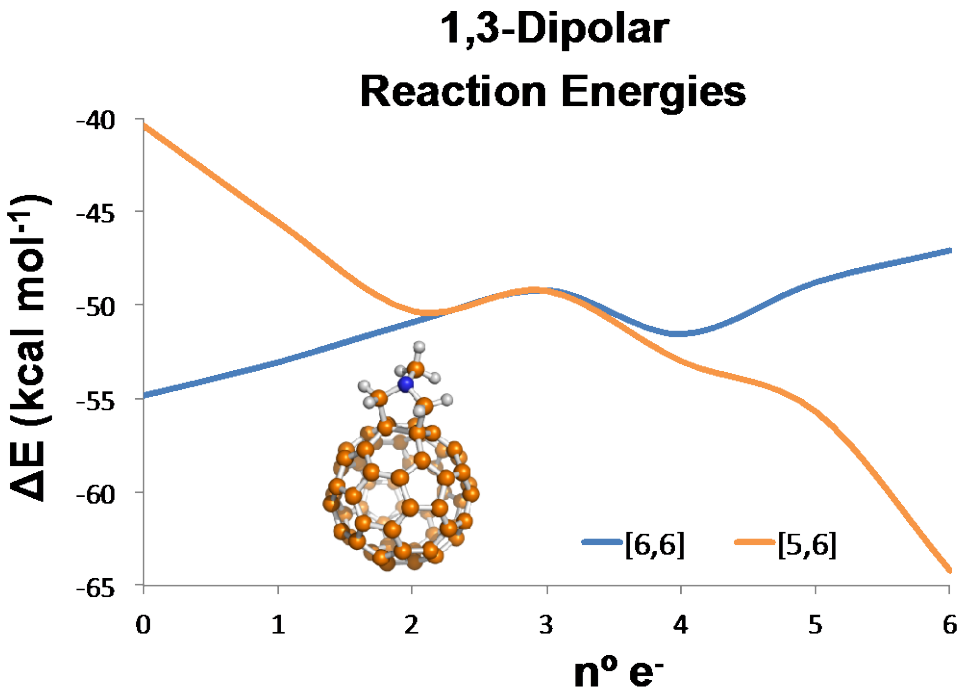


Figure S3. Schematic representation of the reaction energies found for the carbene addition of dichlorocarbene on [6,6] and [5,6] positions of C_{60}^{n-} (n = 0 – 6) fullerene, obtained at BP86-D_2/TZP//BP86-D_2/DZP level.

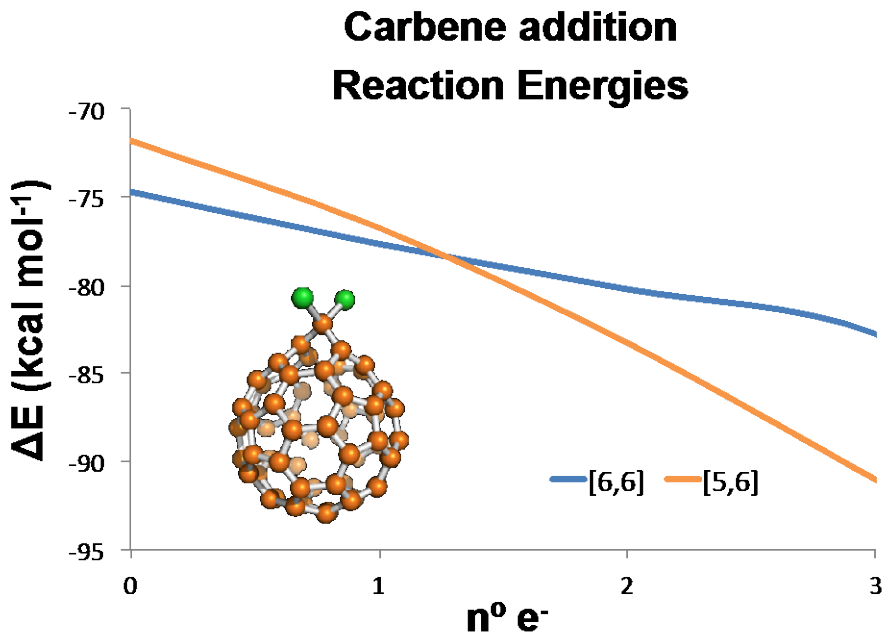


Figure S4. Schematic representation of [5,6] and [6,6] bond distances (Å) evolution when C_{60} fullerene is reduced with n electrons (n = 0 – 6) calculated at the BP86-D_2/DZP level.

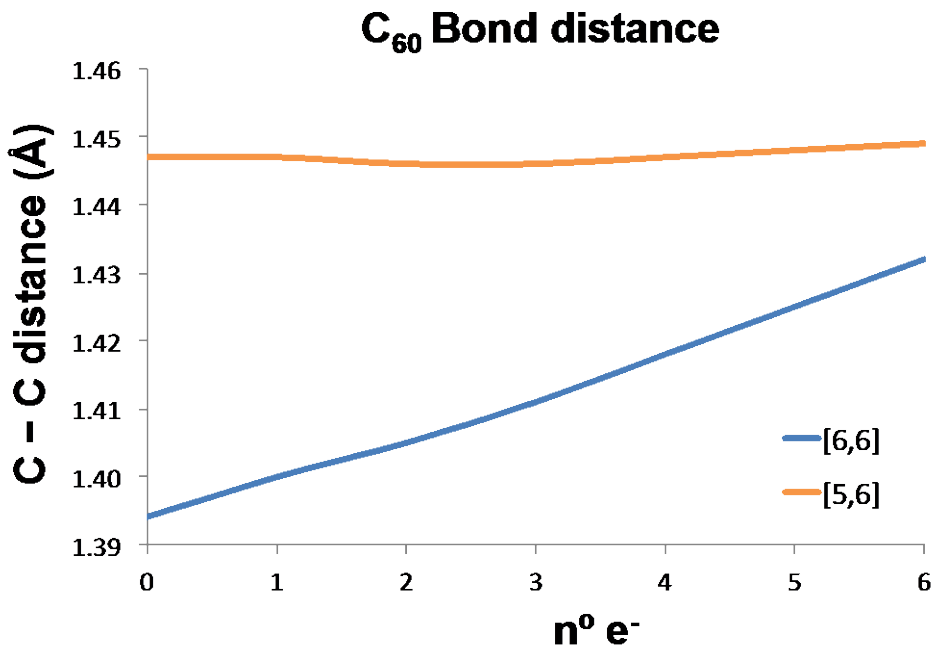


Figure S5. Schematic representation of 5-MRs and 6-MRs BP86-D_2/DZP HOMA indexes evolution when C_{60} fullerene is reduced with n electrons (n = 0 – 6).

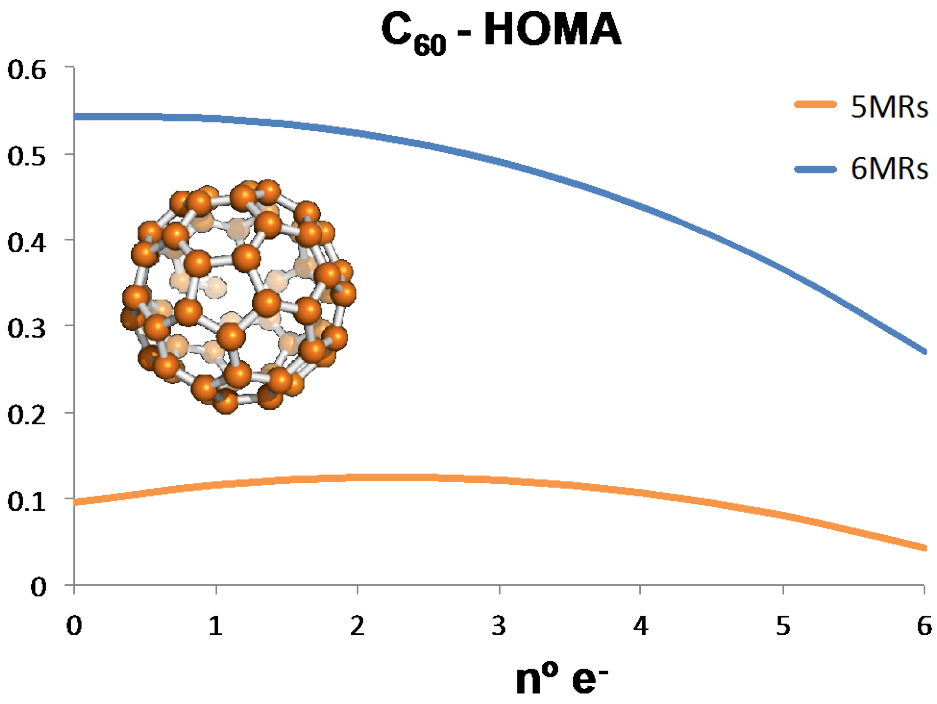
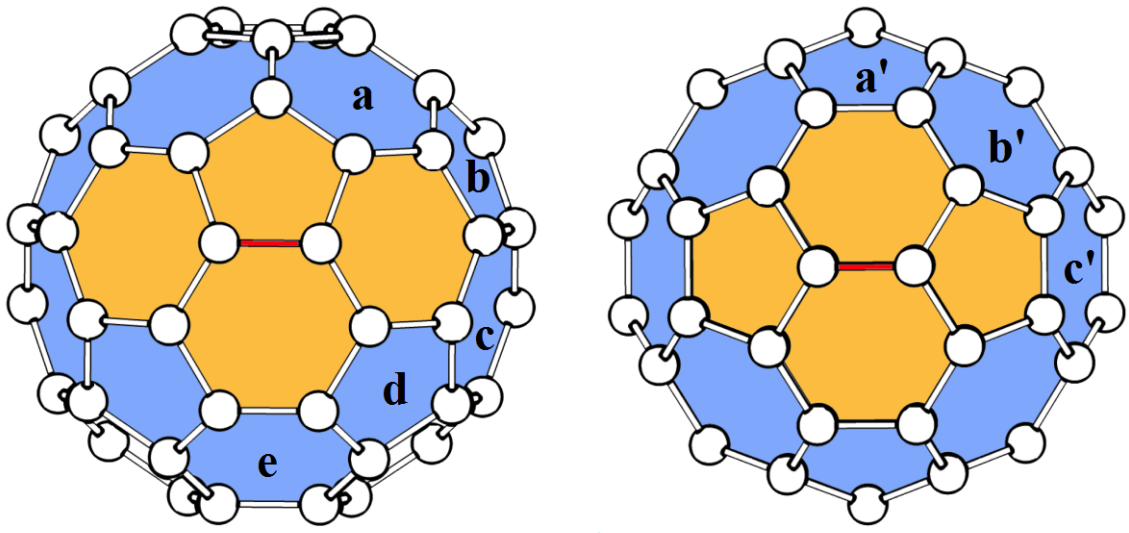


Figure S6. MCI indexes for the second ring crown (represented in blue) and pyracylenic or corannulenic units (orange) for the neutral [5,6] and [6,6] C_{60}-Cp products. There are also presented the MCI increments from reactants to products (ΔMCI) and the relative variation of the MCIs in % calculated as: $\%\Delta MCI = \Delta MCI/MCI_{reactant} \cdot 100$.



[5,6] **[6,6]**

MCI	[5,6]	[6,6]
a	0.0149	0.0079
b	0.0085	0.0165
c	0.0131	0.0110
d	0.0107	
e	0.0057	
C_{60}-Cp Σ[blue crown]	0.1002	0.1037
C_{60}-Cp Σ[4 rings orange unit]	0.0096	0.0091
$\Delta MCI_{blue\ crown}$	0.0036	0.0012
$\Delta MCI_{4\ rings\ orange\ unit}$	-0.0387	-0.0357
$\%\Delta MCI_{blue\ crown}$	3.7	1.1
$\%\Delta MCI_{4\ rings\ orange\ unit}$	*-80.1*	*-79.7*