Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information

Aromaticity as a Driving Force for the Stability of non-IPR Endohedral Metallofullerene Bingel-Hirsch Adducts

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(26) Baerends, E. J.; Ziegler, T.; Autschbach, J.; Bashford, D.; Bérces, A.; Bickelhaupt, F. M.; Bo, C.; Boerrigter, P. M.; Cavallo, L.; Chong, D. P.; Deng, L.; Dickson, R. M.; Ellis, D. E.; Faassen, M. v.; Fan, L.; Fischer, T. H.; Fonseca Guerra, C.; Ghysels, A.; Giammona, A.; van Gisbergen, S. J. A.; Götz, A. W.; Groeneveld, J. A.; Gritsenko, O. V.; Grüning, M.; Gusarov, S.; Harris, F. E.; van den Hoek, P.; Jacob, C. R.; Jacobsen, H.; Jensen, L.; Kaminski, J. W.; van Kessel, G.; Kootstra, F.; Kovalenko, A.; Krykunov, M. V.; van Lenthe, E.; McCormack, D. A.; Michalak, A.; Mitoraj, M.; Neugebauer, J.; Nicu, V. P.; Noodleman, L.; Osinga, V. P.; Patchkovskii, S.; Philipsen, P. H. T.; Post, D.; Pye, C. C.; Ravenek, W.; Rodríguez, J. I.; Ros, P.; Schipper, P. R. T.; Schreckenbach, G.; Seldenthuis, J. S.; Seth, M.; Snijders, J. G.; Solà, M.; Swart, M.; Swerhone, D.; te Velde, G.; Vernooijs, P.; Versluis, L.; Visscher, L.; Visser, O.; Wang, F.; Wesolowski, T. A.; van Wezenbeek, E. M.; Wiesenekker, G.; Wolff, S. K.; Woo, T. K.; Yakovlev, A. L. ADF2010.01; SCM: Amsterdam, 2010.

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 second period, 1s2s2p for third to fourth period, 1s2s2p3s3p4s3d for fifth period, 1s2s2p3s3p4s3d4p5s4d for sixth period) 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). We should mention here that the optimization of the gadolinium-based compounds has been a difficult task. Gadolinium atoms have

an incomplete f Shell ([Xe]$4f^7 5d^1 6s^2$), and therefore different spin configurations for $Gd_3N@C_{80}$ are possible. The seven unpaired electrons of the gadolinium atoms can be coupled either ferromagnetically (S=21/2) or antiferromagnetically (S=7/2). The difference in energy between the latter two configurations was found to be extremely low (0.1 kcal·mol^{-1}).[8] It was also recently published that the low-spin state in the case of the related compound Gd3N@C78 is 4.5 meV (0.1 kcal·mol^{-1}) lower in energy than the high-spin state.[9] All calculations reported here have been performed considering the ferromagnetic coupling (i.e., S=21/2).

Moreover, energy dispersion corrections were introduced using Grimme's methodology[10,11] (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.[12,13] 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 were performed with the QUILD[14] (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[15] and specially constructed model Hessians with the appropriate number of eigenvalues.[15] In all cases, we have started the geometry optimization of adducts from close- and open-cage structures, and for a given bond the optimizations have yielded always a single close- or open-cage adduct.

We define the Additive Local Aromaticity (ALA) index[16] as the sum of the local aromaticities of all rings in the fullerene cage:

$$ALA = \sum_{i=1}^{n} A_i \qquad (1)$$

where A_i is the local aromaticity of ring *i* and *n* is the total number of rings in the fullerene including both 5- and 6-MRs.

Local aromaticity of each ring (A_i) can be computed using different aromaticity indices.[17] We have chosen the low-computational cost option of calculating the harmonic oscillator model of aromaticity (HOMA) index[18] from the optimized geometries obtained with the BP86-D/DZP method. The HOMA index was defined by Kruszewski and Krygowski as:[18,19]

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

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.

In a previous work,[16] we have checked that aromaticity trends given by the HOMA index are equal to those delivered by the electronic multicenter index (MCI).[20,21] MCI is a particular extension of the I_{ring} index.[22] Our results confirm that HOMA indices give the same trends as those provided by the MCI index.

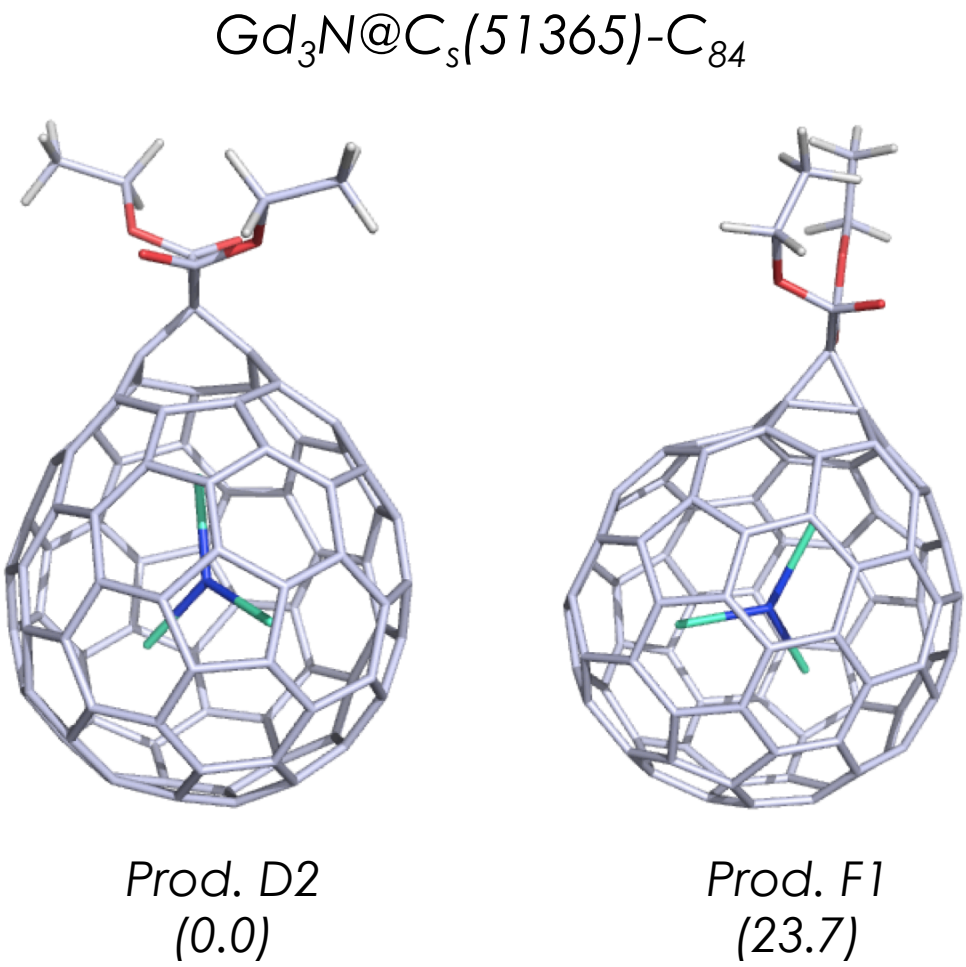
References

(1) Baerends, E. J.; Ziegler, T.; Autschbach, J.; Bashford, D.; Bérces, A.; Bickelhaupt, F. M.; Bo, C.; Boerrigter, P. M.; Cavallo, L.; Chong, D. P.; Deng, L.; Dickson, R. M.; Ellis, D. E.; Faassen, M. v.; Fan, L.; Fischer, T. H.; Fonseca Guerra, C.; Ghysels, A.; Giammona, A.; van Gisbergen, S. J. A.; Götz, A. W.; Groeneveld, J. A.; Gritsenko, O. V.; Grüning, M.; Gusarov, S.; Harris, F. E.; van den Hoek, P.; Jacob, C. R.; Jacobsen, H.; Jensen, L.; Kaminski, J. W.; van Kessel, G.; Kootstra, F.; Kovalenko, A.; Krykunov, M. V.; van Lenthe, E.; McCormack,

D. A.; Michalak, A.; Mitoraj, M.; Neugebauer, J.; Nicu, V. P.; Noodleman, L.; Osinga, V. P.; Patchkovskii, S.; Philipsen, P. H. T.; Post, D.; Pye, C. C.; Ravenek, W.; Rodríguez, J. I.; Ros, P.; Schipper, P. R. T.; Schreckenbach, G.; Seldenthuis, J. S.; Seth, M.; Snijders, J. G.; Solà, M.; Swart, M.; Swerhone, D.; te Velde, G.; Vernooijs, P.; Versluis, L.; Visscher, L.; Visser, O.; Wang, F.; Wesolowski, T. A.; van Wezenbeek, E. M.; Wiesenekker, G.; Wolff, S. K.; Woo, T. K.; Yakovlev, A. L. In *ADF2010.01*; ADF2010.01 ed.; SCM: Amsterdam, 2010.
(2) te Velde, G.; Bickelhaupt, F. M.; Baerends, E. J.; Fonseca Guerra, C.; van Gisbergen, S. J. A.; Snijders, J. G.; Ziegler, T. *J. Comput. Chem.* **2001**, *22*, 931.
(3) Swart, M.; Snijders, J. G. *Theor. Chem. Acc.* **2003**, *110*, 34.
(4) van Lenthe, E.; Baerends, E. J.; Snijders, J. G. *J. Chem. Phys.* **1993**, *99*, 4597.
(5) Baerends, E. J.; Ellis, D. E.; Ros, P. *Chem. Phys.* **1973**, *2*, 41.
(6) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098.
(7) Perdew, J. P. *Phys. Rev. B* **1986**, *33*, 8822.
(8) Osuna, S.; Valencia, R.; Rodríguez-Fortea, A.; Swart, M.; Solà, M.; Poblet, J. M. *Chem. Eur. J.* **2012**, *18*, 8944.
(9) Yang, T.; Zhao, X.; Li, L.-S.; Zheng, J.-J.; Gao, W.-Y. *ChemPhysChem* **2012**, *13*, 449.
(10) Grimme, S. *J. Comput. Chem.* **2006**, *27*, 1787.
(11) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.
(12) Osuna, S.; Swart, M.; Solà, M. *J. Phys. Chem. A* **2010**, *115*, 3491.
(13) Garcia-Borràs, M.; Osuna, S.; Luis, J. M.; Swart, M.; Solà, M. *Chem. Eur. J.* **2012**, *18*, 7141.
(14) Swart, M.; Bickelhaupt, F. M. *J. Comput. Chem.* **2008**, *29*, 724.
(15) Swart, M.; Bickelhaupt, F. M. *Int. J. Quant. Chem.* **2006**, *106*, 2536.
(16) Garcia-Borràs, M.; Osuna, S.; Swart, M.; Luis, J. M.; Solà, M. **2013**, submitted for publication.
(17) Feixas, F.; Matito, E.; Poater, J.; Solà, M. *J. Comput. Chem.* **2008**, *29*, 1543.
(18) Kruszewski, J.; Krygowski, T. M. *Tetrahedron Lett.* **1972**, *13*, 3839.
(19) Krygowski, T. M. *J. Chem. Inf. Comp. Sci.* **1993**, *33*, 70.
(20) Bultinck, P.; Ponec, R.; Van Damme, S. *J. Phys. Org. Chem.* **2005**, *18*, 706.
(21) Poater, J.; Duran, M.; Solà, M.; Silvi, B. *Chem. Rev.* **2005**, *105*, 3911.
(22) Giambiagi, M.; de Giambiagi, M. S.; dos Santos, C. D.; de Figueiredo, A. P. *Phys. Chem. Chem. Phys.* **2000**, *2*, 3381.

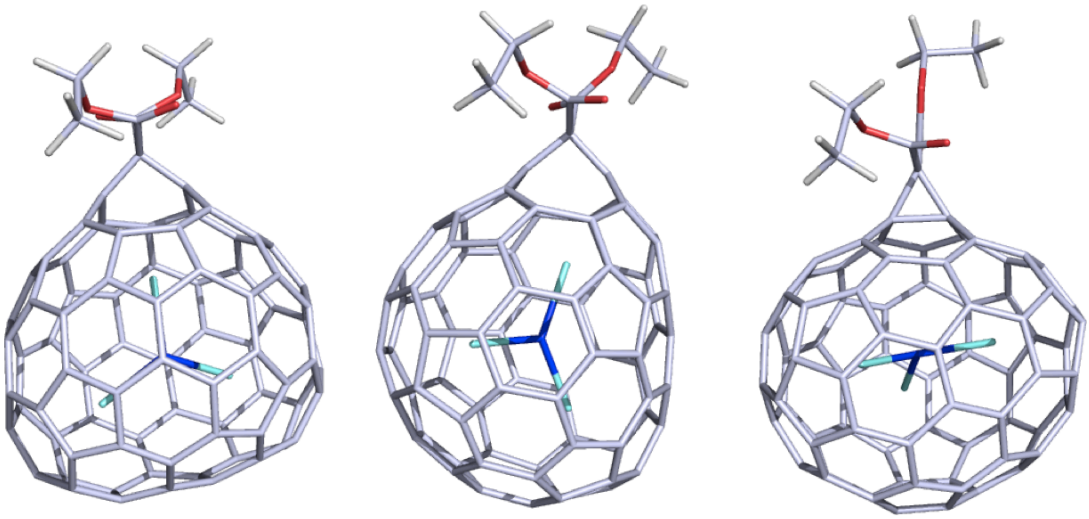
Figure S1. Representation of the most stable and less stable optimized Bingel-Hirsch monoadducts of: **a)** $Gd_3N@C_s(51365)$-C_{84} with 1 APP; **b)** $Y_3N@C_2(22010)$-C_{78} with 2 APPs; and **c)** $Sc_3N@D_3(6140)$-C_{68} with 3 APPs. Geometries are optimized at BP86-D_2/DZP level. It should be emphasized here that for the three explored systems, always for the most stable adducts an open-cage structure is obtained, while a closed-cage structure is found for the less stable ones.

a)



b)

$Y_3N@C_2(22010)\text{-}C_{78}$



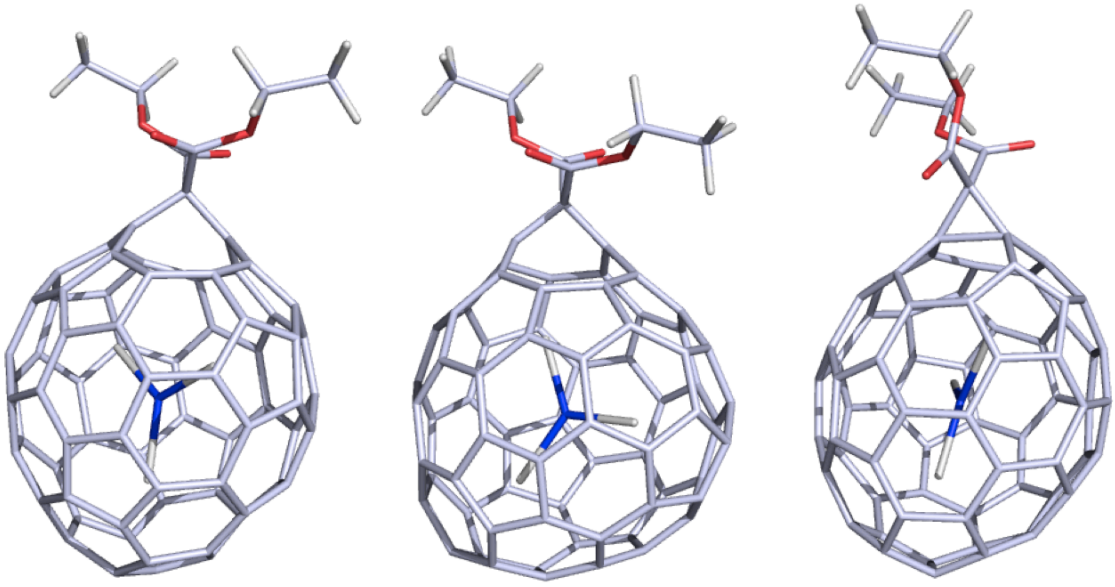
Prod. DI
(0.0)

Prod. B3
(3.9)

Prod. Ds
(29.1)

c)

$Sc_3N@D_3(6140)\text{-}C_{68}$



Prod. C
(0.0)

Prod. D
(0.2)

Prod. A
(19.4)

Figure S2. Representation of superimposed structures of: **a)** $C_s(51365)$-C_{84} (lila) and $Gd_3N@C_s(51365)$-C_{84} (gray); **b)** $C_2(22010)$-C_{78} (lila); $Y_3N@C_2(22010)$-C_{78} (gray); and **c)** $D_3(6140)$-C_{68} (lila) and $Sc_3N@D_3(6140)$-C_{68} (gray). Geometries are optimized at BP86-D_2/DZP level.

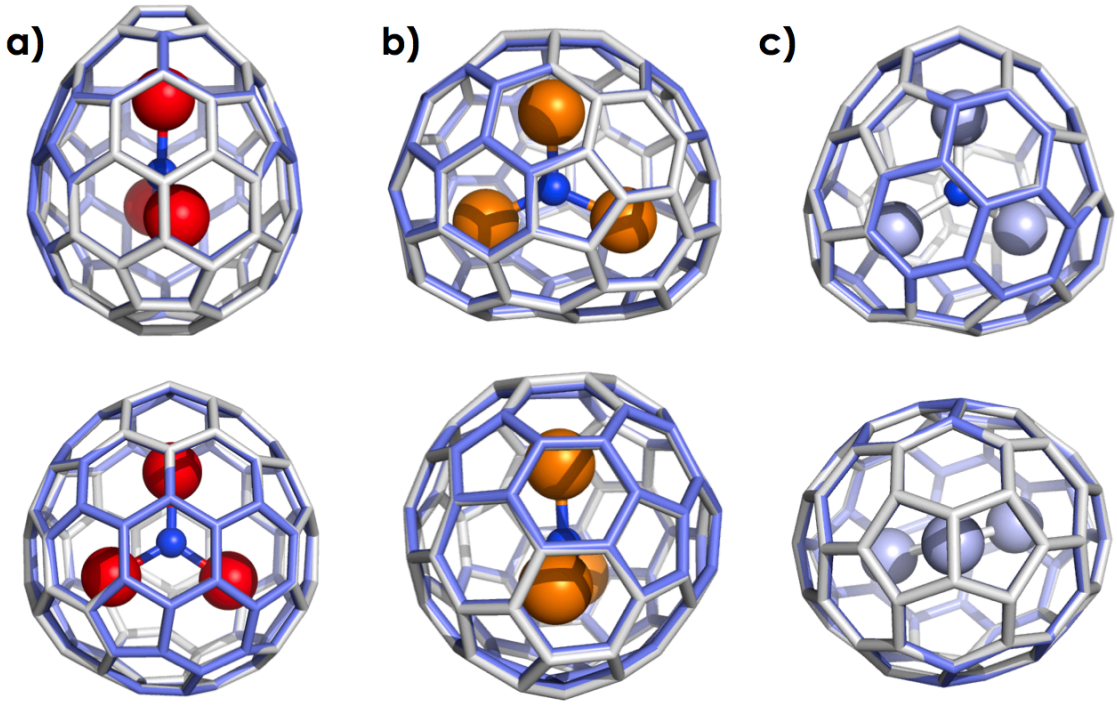


Figure S3. Representation of the endohedral metal orientations and Metal–C_{cage} distances (in Å) of: **a)** $Gd_3N@C_s(51365)$-C_{84} with 1 APP; **b)** $Y_3N@C_2(22010)$-C_{78} with 2 APPs; and **c)** $Sc_3N@D_3(6140)$-C_{68} with 3 APPs. Geometries are optimized at BP86-D_2/DZP level.

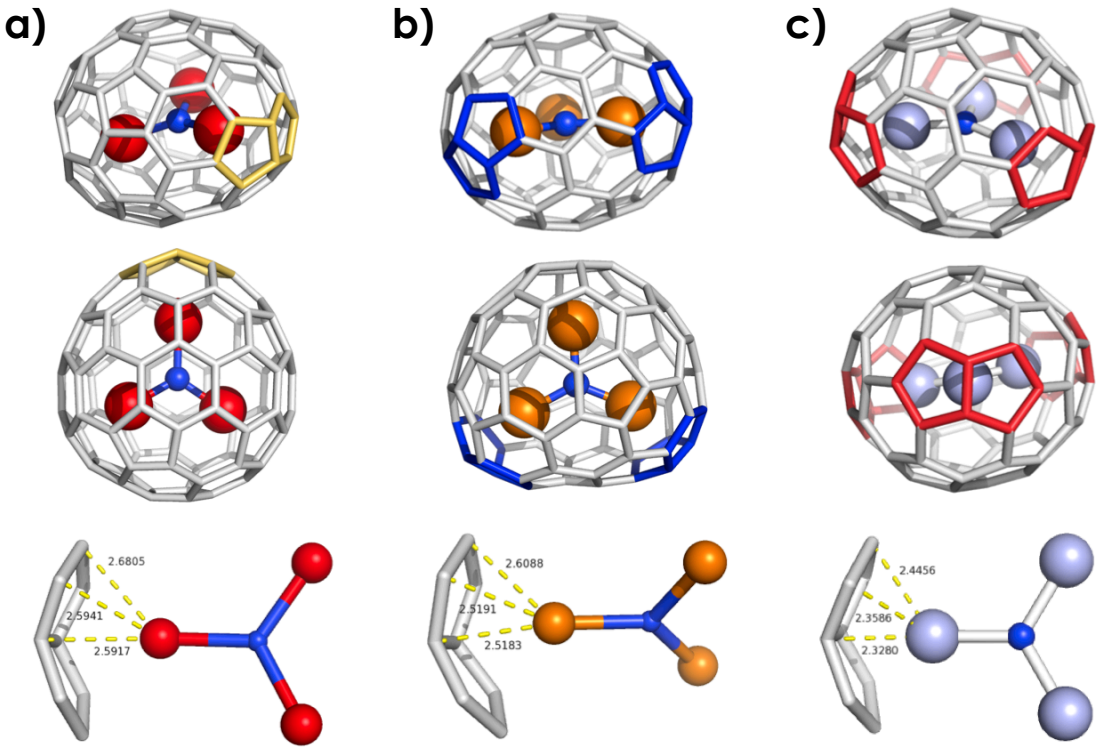


Table S1. C–C bond distances (d_{C-C}, in Å) and pyramidalization angles (θ_{Pyr}, in deg.) of the $C_s(51365)$-C_{84}, $C_2(22010)$-C_{78}, and $D_3(6140)$-C_{68} empty cages and $Gd_3N@C_s(51365)$-C_{84}, $Y_3N@C_2(22010)$-C_{78}, and $Sc_3N@D_3(6140)$-C_{68} obtained at BP86-D_2/DZP level. Bond pyramidalization angles are calculated as the average over the two atoms that constitute the bond under consideration. For the EMF systems, shortest C– C bonds and largest pyramidalization angles are highlighted in bold.

	d_{C-C}			θ_{Pyr}		
	C_{84}	$Gd_3N@C_{84}$	$\Delta(Gd_3N@C_{84} - C_{84})$	C_{84}	$Gd_3N@C_{84}$	$\Delta(Gd_3N@C_{84} - C_{84})$
E	1.445	**1.443**	-0.002	16.08	**15.63**	-0.45
D_1	1.455	1.458	0.003	11.39	11.30	-0.09
D_2	1.447	1.456	0.009	11.53	11.47	-0.05
F_1	1.399	**1.423**	0.024	13.72	**14.08**	0.37
F_2	1.400	**1.424**	0.024	13.96	**14.18**	0.22
B_1	1.417	1.462	0.046	9.77	11.53	1.77
B_2	1.427	1.463	0.036	9.73	11.81	2.08
	d_{C-C}			θ_{Pyr}		
	C_{78}	$Y_3N@C_{78}$	$\Delta(Y_3N@C_{78} - C_{78})$	C_{78}	$Y_3N@C_{78}$	$\Delta(Y_3N@C_{78} - C_{78})$
E	1.440	1.434	-0.007	15.75	**16.03**	0.28
F	1.395	1.429	0.034	13.68	**13.48**	-0.20
A	1.387	1.418	0.032	11.88	**12.07**	0.19
B_1	1.422	**1.412**	-0.010	9.62	9.38	-0.24
B_2	1.408	**1.413**	0.005	8.96	8.84	-0.13
B_3	1.433	1.455	0.022	11.04	11.43	0.39
D_s	1.433	**1.416**	-0.016	9.81	9.62	-0.19
D_l	1.443	1.476	0.033	10.63	**12.15**	1.52
	d_{C-C}			θ_{Pyr}		
	C_{68}	$Sc_3N@C_{68}$	$\Delta(Sc_3N@C_{68} - C_{68})$	C_{68}	$Sc_3N@C_{68}$	$\Delta(Sc_3N@C_{68} - C_{68})$
E	1.426	**1.438**	0.012	16.17	**16.55**	0.38
D	1.442	1.463	0.021	11.31	11.41	0.09
F_1	1.421	1.452	0.031	13.79	**14.65**	0.86
F_2	1.418	1.443	0.025	14.26	**14.69**	0.44
B	1.438	**1.441**	0.003	10.27	10.71	0.44
C	1.481	1.457	-0.024	8.55	9.12	0.57
A	1.390	**1.413**	0.023	11.47	11.66	0.19

Table S2. Relative energies (ΔE, in kcal·mol^{-1}) with respect the most stable EMF Bingel-Hirsch monoadduct of the $Gd_3N@C_s(51365)$-C_{84}, $Y_3N@C_2(22010)$-C_{78}, and $Sc_3N@D_3(6140)$-C_{68} systems computed at BP86-D_2/TZP//BP86-D_2/DZP level.

$Gd_3N@C_s(51365)$-C_{84}				
Bond Type		**ΔE**	**ALA**	**Final Bond**
E	[5,5]	11.5 (10.0)[a]	12.83	Open
D_1	[5,6]	**1.9** (0.0)[a]	**13.16**	Open
D_2	[5,6]	**0.0** (4.4)[a,b]	**13.37**	Open
F_1	[5,6]	23.7	5.81	Closed
F_2	[5,6]	23.7	5.47	Closed
B_1	[6,6]	**2.8** (3.2)[a]	**14.37**	Open
B_2	[6,6]	**4.3** (3.7)[a]	**13.82**	Open
$Y_3N@C_2(22010)$-C_{78}				
Bond Type		**ΔE**	**ALA**	**Final Bond**
E	[5,5]	14.1	6.96	Open
F	[5,6]	16.8	6.61	Open
D_s	[5,6]	29.1	3.61	Closed
D_l	[5,6]	**0.0**	**8.13**	Open
A	[6,6]	17.8	7.42	Open
B_1	[6,6]	25.1	5.00	Closed
B_2	[6,6]	26.7	4.17	Closed
B_3	[6,6]	**3.9**	**8.40**	Open
$Sc_3N@D_3(6140)$-C_{68}				
Bond Type		**ΔE**	**ALA**	**Final Bond**
E	[5,5]	16.6 [13.5][d]	8.02	Open
D	[5,6]	**0.2** (2.7)[c]	**9.57**	Open
F_1	[5,6]	**2.4** (5.4)[c]	**9.70**	Open
F_2	[5,6]	11.1 (14.0)[c]	9.16	Open
B	[6,6]	11.0 (13.6)[c] [11.3][d]	9.25	Open
C	[6,6]	**0.0** (0.0)[c] [0.0][d]	**9.56**	Open
A	[6,6]	19.4 (18.8)[c] [23.3][d]	7.90	Closed

[a] In parenthesis relative energies obtained by M. Alegret et al. *J. Org. Chem.* **2010**, *75*, 8299.
[b] $Y_3N@C_s(51365)$-C_{84} has been considered instead of $Gd_3N@C_s(51365)$-C_{84}.
[c] In parenthesis relative energies obtained by M. Alegret et al. *Chem. Eur. J.* **2013**, *19,* 5061. Solvent effects (*ortho*-dichloroebenzene) included by means of single point energy calculations.
[d] In brackets relative energies obtained by T. Cai et al. *J. Phys. Chem. C* **2008**, *112*, 19203.

Table S3. Xyz coordinates of all presented structures (in Å).

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109
gd3n_c84_prode_opt
C      -4.216105   -0.235212    1.042645
C      -3.467390    0.919223    1.448495
C      -3.271991    1.939378    0.395429
C      -4.217392    0.189904   -1.043476
C      -3.466962    1.408468   -0.971652
C      -3.478058   -0.968370   -1.451947
C      -3.474400   -1.459495    0.969069
C      -3.282401   -1.988065   -0.399912
C      -2.432643   -1.687427    1.950197
C      -2.431933    0.750868    2.439907
C      -1.901621   -0.580613    2.737869
C      -1.632539    1.886433    2.702219
C      -2.290819    2.978290    0.601759
C      -1.598557    3.026320    1.833131
C      -1.599382    3.504435   -0.522178
C      -2.432664    1.637924   -1.952724
C      -1.632261    2.789460   -1.760635
C      -2.441967   -0.796713   -2.447894
C      -1.908527    0.530931   -2.745396
C      -1.637452   -1.923097   -2.712256
C      -2.286532   -3.019655   -0.608273
C      -1.595610   -3.060423   -1.838346
C      -1.627016   -2.831006    1.755707
C      -1.594802   -3.545253    0.513016
C      -0.370352   -2.978373    2.397166
C      -0.558782   -0.697107    3.316796
C       0.204815   -1.918868    3.147229
C      -0.385680    1.778353    3.347684
C       0.163857    0.509439    3.659070
C      -0.302047    3.636462    1.960176
C       0.425672    2.891966    2.946533
C      -0.308878    4.127168   -0.410184
C       0.376102    4.227267    0.844578
C      -0.389960    2.947471   -2.407623
C       0.429572    3.835425   -1.614780
C      -0.569261    0.651357   -3.328960
C       0.153117    1.900005   -3.189451
C      -0.385173   -1.807213   -3.364617
C       0.193772   -0.541514   -3.637983
C      -0.285256   -3.655533   -1.964837
C       0.398292   -2.938420   -2.982123
C      -0.290827   -4.150142    0.396244
C       0.407077   -3.889483    1.612725
C       0.431493   -4.192086   -0.846233
C       1.813302   -3.839003    1.635853
C       1.654561   -1.912682    3.246202
C       2.427046   -2.863120    2.476343
C       1.570009    0.480432    3.793087
C       2.306200   -0.709255    3.571951
C       1.838465    2.800024    2.914951
C       2.395528    1.595153    3.405693
C       1.832146    4.236292    0.830311
C       2.542158    3.512737    1.868616
C       1.859202    3.793999   -1.653574
C       2.587837    4.073612   -0.417812
C       1.561794    1.930715   -3.327925
C       2.398698    2.828097   -2.557231
C       1.642472   -0.495448   -3.726977
C       2.294651    0.746986   -3.577322
C       1.787410   -2.864728   -2.982103
C       2.409237   -1.659769   -3.399466
C       1.920986   -4.150036   -0.835488
C       2.613641   -4.052740    0.447588
C       2.562404   -3.484913   -1.940810
C       3.682346   -2.500990    1.871684
C       3.807461   -3.202825    0.609642
C       3.587693   -0.354698    3.029649
C       3.623849    1.071610    2.896507
C       4.242647   -1.200861    2.107607
C       3.729524    2.933045    1.296237
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C	3.759394	3.262408	-0.112820
C	4.277689	1.696734	1.800878
C	3.636689	2.135792	-2.300124
C	3.580201	0.866089	-2.957201
C	4.295329	2.289277	-1.042771
C	3.656665	-1.553347	-2.701142
C	3.757202	-2.657002	-1.779653
C	4.376213	-2.476816	-0.504202
C	4.223105	-0.280095	-2.425906
C	4.951023	-0.581066	1.046467
C	4.948889	0.843036	0.884960
C	4.941679	1.129129	-0.518138
C	4.967837	-1.190554	-0.251132
C	4.931693	-0.125835	-1.211522
Gd	-1.532319	-0.062477	0.000167
Gd	1.801545	-1.728212	-0.001176
Gd	1.558176	1.858615	0.052527
N	0.589058	-0.010319	0.072481
C	-5.251782	-0.018615	0.000707
C	-6.158127	1.192584	0.304558
O	-6.494722	1.504617	1.425418
O	-6.526651	1.776349	-0.841961
C	-6.168525	-1.221597	-0.304135
O	-6.505137	-1.530505	-1.425872
O	-6.545754	-1.802270	0.840813
C	-7.453950	-2.945390	0.667318
C	-7.752287	-3.473215	2.047726
H	-6.944213	-3.681278	0.028425
H	-8.350259	-2.582660	0.142949
H	-8.436699	-4.331260	1.969022
H	-6.826797	-3.803822	2.541740
H	-8.227044	-2.695322	2.663607
C	-7.421595	2.930369	-0.674318
C	-7.698102	3.465752	-2.056509
H	-6.909313	3.657994	-0.028023
H	-8.328060	2.577719	-0.160631
H	-8.371930	4.332585	-1.983291
H	-6.762866	3.785232	-2.539459
H	-8.176041	2.695785	-2.679859

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C	-4.102765	-1.007440	-0.559958
C	-3.912589	0.382172	0.323097
C	-3.445540	1.361510	-0.721999
C	-3.625676	-0.644567	-1.920212
C	-3.228187	0.713213	-1.997679
C	-2.748916	-1.660908	-2.370346
C	-3.298714	-2.150695	-0.116466
C	-2.641000	-2.653112	-1.311756
C	-2.570488	-2.174248	1.129438
C	-3.040180	0.287190	1.523387
C	-2.396341	-0.949961	1.947901
C	-2.475365	1.537058	1.890566
C	-2.725156	2.515169	-0.341145
C	-2.403610	2.689583	1.027809
C	-1.868845	3.110378	-1.299595
C	-2.067648	1.094665	-2.789768
C	-1.506732	2.360638	-2.468891
C	-1.575886	-1.339815	-3.151731
C	-1.195587	0.061559	-3.353980
C	-0.566704	-2.333894	-3.176756
C	-1.505392	-3.509966	-1.235098
C	-0.554016	-3.450977	-2.272075
C	-1.541642	-3.162938	1.199126
C	-1.066801	-3.891580	0.048789
C	-0.471665	-3.096106	2.127455
C	-1.214333	-0.854158	2.829696
C	-0.261815	-1.943554	2.927660
C	-1.405321	1.616934	2.803867
C	-0.777882	0.449336	3.288903
C	-1.266372	3.468045	1.419371
C	-0.694377	2.843607	2.577194
C	-0.752590	3.915962	-0.912676
C	-0.421092	4.137399	0.468929
C	-0.173011	2.693010	-2.800101
C	0.292378	3.710048	-1.884103
C	0.214635	0.381563	-3.606603
C	0.690839	1.729246	-3.365875

C	0.778356	-2.020896	-3.502704
C	1.203617	-0.679651	-3.673114
C	0.817818	-3.821330	-2.038450
C	1.611668	-3.009521	-2.891156
C	0.293349	-4.286460	0.284544
C	0.609676	-3.886041	1.613731
C	1.299902	-4.221342	-0.747322
C	1.940204	-3.608946	1.970172
C	1.099192	-1.712264	3.380371
C	2.173180	-2.539970	2.881109
C	0.536687	0.640254	3.776207
C	1.469102	-0.421657	3.799959
C	0.679095	2.970334	2.894272
C	1.262998	1.865651	3.558931
C	0.975533	4.365776	0.807720
C	1.509484	3.779138	2.025071
C	1.675067	3.884665	-1.570130
C	2.029072	4.295201	-0.212834
C	2.071695	1.978530	-3.166945
C	2.555200	3.004759	-2.267995
C	2.607581	-0.407697	-3.415636
C	3.010710	0.922374	-3.173907
C	2.928843	-2.716425	-2.552615
C	3.443145	-1.432053	-2.863366
C	2.713608	-3.942599	-0.377193
C	3.036979	-3.715024	1.028568
C	3.507320	-3.199294	-1.326772
C	3.474505	-1.998978	2.588710
C	4.015888	-2.691564	1.435731
C	2.781141	0.118344	3.580281
C	2.642646	1.532055	3.394384
C	3.762575	-0.627033	2.890055
C	2.872400	3.375714	1.783728
C	3.196639	3.681074	0.406119
C	3.451352	2.240759	2.463659
C	3.780537	2.519496	-1.687072
C	4.075653	1.248951	-2.274107
C	4.080670	2.790423	-0.318041
C	4.451283	-1.124338	-1.890106
C	4.486191	-2.190884	-0.919050
C	4.735417	-1.900965	0.459527
C	4.733850	0.224866	-1.547940
C	4.615217	0.082208	2.006525
C	4.443673	1.487318	1.779027
C	4.743643	1.751898	0.404100
C	5.044720	-0.533575	0.784407
C	5.090431	0.502603	-0.207692
Gd	-1.398799	-0.431538	-0.535262
Gd	2.067241	-1.541651	0.235677
Gd	1.248216	1.960707	0.145092
N	0.638987	-0.039410	-0.110694
C	-5.240664	-0.310675	0.107943
C	-5.859840	-1.005542	1.297926
O	-5.221919	-1.621199	2.126029
O	-7.192884	-0.841174	1.286456
C	-6.219438	0.394962	-0.824226
O	-6.596550	-0.070968	-1.877830
O	-6.574816	1.567258	-0.277006
C	-7.895179	-1.481470	2.406596
H	-7.471151	-1.083318	3.339539
H	-7.690664	-2.560631	2.356390
C	-9.357819	-1.152794	2.239004
H	-9.931381	-1.614124	3.057202
H	-9.514288	-0.064566	2.270399
H	-9.734225	-1.540705	1.280996
C	-7.638210	2.281880	-0.995501
H	-7.544004	3.313541	-0.635133
H	-7.424401	2.230699	-2.072255
C	-8.978563	1.667291	-0.654304
H	-9.784894	2.251177	-1.125756
H	-9.024482	0.633670	-1.026568
H	-9.127480	1.667860	0.435530

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C	3.674316	-1.992135	-0.102115
C	4.028632	-0.895976	-0.940703
C	4.083206	0.532506	0.798904
C	3.516822	-1.759657	1.337935

C	3.525199	-0.378690	1.773792	C	-2.169711	-4.069029	0.250195
C	2.450556	-2.620475	1.776168	C	-2.831733	-2.994434	-2.353876
C	2.684834	-2.911041	-0.522721	C	-1.628490	-1.128687	-3.570592
C	2.030067	-3.422163	0.650835	C	-2.842798	-1.767013	-3.090305
C	1.923496	-2.684484	-1.725578	C	-0.534760	1.074060	-3.672723
C	3.046405	-0.434867	-1.882866	C	-1.695182	0.262588	-3.763366
C	2.014895	-1.379893	-2.372376	C	-0.092971	3.188796	-2.460727
C	2.740265	0.979698	-1.931000	C	-0.946190	2.378636	-3.234146
C	3.356365	1.707549	0.464353	C	0.019521	4.291241	-0.214814
C	2.938897	1.986256	-0.878069	C	-0.680866	4.018847	-1.440971
C	2.622465	2.303180	1.512812	C	-0.644898	3.760550	2.137088
C	2.445339	0.086261	2.646680	C	-0.965092	4.394928	0.859977
C	2.172770	1.483559	2.598768	C	-1.379798	1.778295	3.506180
C	1.433816	-2.195763	2.710980	C	-1.669380	3.009087	2.791473
C	1.382952	-0.799100	3.125585	C	-2.417261	-0.454230	3.472562
C	0.232801	-2.948978	2.701116	C	-2.525133	0.953514	3.435911
C	0.749987	-4.025483	0.567453	C	-3.287424	-2.488938	2.352600
C	-0.093701	-3.907080	1.679180	C	-3.486040	-1.183759	2.867881
C	0.715596	-3.424528	-1.820269	C	-3.500375	-3.436646	0.034561
C	0.163452	-4.155259	-0.713696	C	-3.848050	-2.960768	-1.310328
C	-0.359354	-2.996265	-2.643431	C	-4.020228	-2.654432	1.126348
C	0.852256	-0.889642	-3.113869	C	-3.937634	-0.976993	-2.590471
C	-0.333704	-1.720271	-3.271406	C	-4.535890	-1.675460	-1.477548
C	1.646255	1.425667	-2.720061	C	-2.829812	1.048803	-3.360858
C	0.725804	0.529955	-3.333224	C	-2.356839	2.352928	-3.007976
C	1.967703	3.029751	-1.088793	C	-3.916779	0.452261	-2.688459
C	1.225294	2.714716	-2.260386	C	-2.091039	3.965564	-1.165894
C	1.686080	3.344162	1.301750	C	-2.285178	4.192703	0.258921
C	1.347994	3.752036	-0.017754	C	-2.940643	3.092094	-1.939906
C	0.953868	2.036682	3.063418	C	-2.996038	2.882746	2.234356
C	0.673965	3.245269	2.317691	C	-3.530311	1.623124	2.667418
C	0.099866	-0.228335	3.553695	C	-3.308496	3.416892	0.936353
C	-0.077106	1.208726	3.553319	C	-4.451164	-0.533601	2.030575
C	-0.986625	-2.410730	3.188542	C	-4.765680	-1.413120	0.941173
C	-1.095016	-1.051983	3.568560	C	-4.996253	-0.886335	-0.358782
C	-1.525920	-3.951943	1.531201	C	-4.442311	0.876466	1.879934
C	-2.057796	-3.104069	2.538712	C	-4.542288	1.204106	-1.660632
C	-1.266014	-4.203091	-0.871158	C	-4.046904	2.493436	-1.279561
C	-1.569852	-3.583313	-2.125245	C	-4.210743	2.634001	0.141999

C	-5.029348	0.540433	-0.492082
C	-4.795679	1.411432	0.619016
Gd	1.450872	-0.709119	0.209803
Gd	-2.106639	-1.378808	-0.503121
Gd	-1.084549	1.962205	0.331572
N	-0.572342	-0.065771	0.089055
C	5.012997	-0.000852	-0.258424
C	5.658646	1.044575	-1.193972
O	5.783495	0.874608	-2.386113
O	6.086168	2.093526	-0.479577
C	6.187146	-0.792887	0.378743
O	6.549865	-0.636129	1.523242
O	6.706422	-1.623209	-0.534771
C	6.674767	3.171063	-1.286790
H	7.565102	2.765634	-1.789498
H	5.934326	3.453898	-2.049948
C	6.992882	4.297438	-0.336308
H	7.707805	3.966596	0.431348
H	7.435919	5.133638	-0.897855
H	6.076209	4.650833	0.158669
C	7.760189	-2.515502	-0.027089
H	8.276729	-2.843100	-0.937501
H	8.435567	-1.925951	0.608691
C	7.125890	-3.663404	0.726719
H	6.611525	-3.288826	1.624003
H	6.404315	-4.187766	0.081795
H	7.905696	-4.376010	1.039632

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C	3.735987	-0.324352	1.691389
C	2.933877	-1.389706	2.170267
C	2.836048	-2.381677	1.111416
C	4.168966	-0.653927	0.310043
C	3.405019	-1.831558	-0.105956
C	3.866914	0.736405	-0.557913
C	3.277920	1.014525	1.802191
C	3.393020	1.678159	0.519488
C	2.124492	1.312923	2.649253
C	1.789584	-1.151789	3.010182
C	1.340385	0.225723	3.243071
C	0.851530	-2.217736	3.076453
C	1.770142	-3.317542	1.085054
C	0.868944	-3.331686	2.169290
C	1.296203	-3.720724	-0.181828
C	2.627954	-1.896425	-1.314960
C	1.665625	-2.955989	-1.341341
C	2.945386	0.586488	-1.721518
C	2.351352	-0.684092	-2.120514
C	2.276709	1.790306	-2.048976
C	2.568006	2.778175	0.179278
C	2.166745	2.928815	-1.169445
C	1.465723	2.535764	2.364042
C	1.723620	3.312032	1.179494
C	0.118854	2.775360	2.756170
C	-0.075120	0.453128	3.560886
C	-0.680683	1.748579	3.315970
C	-0.485039	-1.998229	3.464013
C	-0.961436	-0.686108	3.707870
C	-0.475169	-3.805891	2.004973
C	-1.308404	-3.014046	2.863326
C	-0.037620	-4.213934	-0.355697
C	-0.964823	-4.286804	0.742304
C	0.561808	-2.960498	-2.218639
C	-0.482034	-3.792043	-1.658410
C	1.125182	-0.660389	-2.944410
C	0.280822	-1.834497	-3.026559
C	1.153547	1.801594	-2.917363
C	0.540496	0.604611	-3.347875
C	0.949567	3.618232	-1.500059
C	0.414675	2.994107	-2.658558
C	0.529315	4.032407	0.848527
C	-0.410953	3.785660	1.890525
C	0.071560	4.179447	-0.511399
C	-1.789556	3.859405	1.631727
C	-2.118509	1.880195	3.137115
C	-2.640491	2.923683	2.286419
C	-2.358338	-0.522672	3.572178
C	-2.926772	0.739292	3.272085

C	-2.671551	-2.779564	2.557545
C	-3.196551	-1.537492	2.985888
C	-2.382699	-4.149415	0.444905
C	-3.218559	-3.391141	1.361962
C	-1.863315	-3.602349	-1.968669
C	-2.846490	-3.854767	-0.917269
C	-1.068384	-1.725536	-3.443615
C	-2.121038	-2.562184	-2.908342
C	-0.859486	0.701854	-3.733897
C	-1.633302	-0.473113	-3.778905
C	-0.948189	3.053490	-2.930654
C	-1.574432	1.923912	-3.516135
C	-1.384342	4.272634	-0.791575
C	-2.320124	4.191913	0.326215
C	-1.857591	3.717206	-2.037148
C	-3.782117	2.710282	1.436421
C	-3.596869	3.465702	0.212037
C	-4.107373	0.531647	2.482144
C	-4.247437	-0.878435	2.275375
C	-4.492139	1.466363	1.494740
C	-4.202772	-2.669980	0.596123
C	-3.973438	-2.941834	-0.806446
C	-4.726037	-1.401526	1.044044
C	-3.320965	-1.765485	-2.868379
C	-3.025485	-0.488775	-3.439209
C	-4.227180	-1.894761	-1.774806
C	-2.942857	1.917786	-3.085238
C	-3.129464	3.001293	-2.150169
C	-4.003080	2.840093	-1.028456
C	-3.660801	0.695699	-2.988654
C	-5.032386	0.954298	0.287183
C	-5.122815	-0.457743	0.057957
C	-4.863625	-0.697249	-1.329326
C	-4.740398	1.605587	-0.957531
C	-4.607907	0.572137	-1.944690
Gd	1.457958	-0.123338	0.406577
Gd	-1.683953	1.806597	-0.131787
Gd	-1.719468	-1.792490	-0.076685
N	-0.650997	0.000381	0.209136
C	5.232568	0.115100	-0.409937
C	6.214118	0.925880	0.431077
O	6.456219	2.093924	0.221697
O	6.746327	0.150388	1.387268
C	5.829253	-0.552639	-1.628207
O	5.181465	-1.193645	-2.428949
O	7.153099	-0.335625	-1.673397
C	7.823239	-0.942957	-2.833059
C	9.289213	-0.613013	-2.707472
H	7.366269	-0.519876	-3.739088
H	7.623406	-2.023771	-2.806465
H	9.832188	-1.042245	-3.562814
H	9.440148	0.476499	-2.703528
H	9.702477	-1.036344	-1.780038
C	7.726946	0.836133	2.239099
C	8.176806	-0.162910	3.275392
H	7.232275	1.714052	2.679692
H	8.546127	1.181485	1.591159
H	8.916628	0.308798	3.939529
H	7.322781	-0.499180	3.881746
H	8.639958	-1.037644	2.795267

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C	3.406442	-1.805662	1.412113
C	2.337776	-2.687490	1.788387
C	1.970112	-3.467209	0.627057
C	3.613488	-1.985135	-0.023245
C	2.646984	-2.894693	-0.502734
C	4.046824	-0.893149	-0.818502
C	3.445601	-0.452966	1.909133
C	4.064973	0.483933	0.993310
C	2.326429	-0.011613	2.752200
C	1.295433	-2.286252	2.685276
C	1.239115	-0.903706	3.147441
C	0.091018	-3.041869	2.613365
C	0.702817	-4.064880	0.476529
C	-0.194612	-3.975524	1.561662
C	0.158376	-4.145350	-0.830676
C	1.952248	-2.635198	-1.723168

C	0.750470	-3.373133	-1.887528	C	-1.434732	-1.059544	-3.697602
C	3.129231	-0.402440	-1.813751	C	-2.695978	-1.613890	-3.268911
C	2.090441	-1.311451	-2.340002	C	-0.497906	1.208074	-3.594812
C	2.814073	1.014031	-1.811250	C	-1.585596	0.341984	-3.817818
C	3.348475	1.669730	0.656508	C	0.074420	3.295743	-2.399065
C	2.965074	1.977941	-0.699903	C	-0.836014	2.531646	-3.161721
C	2.060085	1.384078	2.737056	C	-0.079957	4.234696	-0.109307
C	2.557724	2.233355	1.683017	C	-1.035207	4.292245	0.984200
C	0.817105	1.931698	3.166881	C	-0.638142	4.059175	-1.416155
C	-0.054918	-0.336231	3.545649	C	-2.915587	3.210353	1.891763
C	-0.263172	1.098171	3.540755	C	-2.476886	4.056906	0.785860
C	-1.136655	-2.516930	3.069608	C	-3.868961	1.068066	2.585153
C	-1.230604	-1.180740	3.532047	C	-4.395440	-0.192715	2.161958
C	-1.618385	-4.030460	1.360390	C	-3.948743	2.221784	1.765008
C	-2.205649	-3.157375	2.348060	C	-4.781866	-1.631388	0.229817
C	-1.264898	-4.199414	-1.045513	C	-4.573561	-1.723242	-1.188517
C	-2.209723	-4.194847	0.050911	C	-4.948725	-0.356431	0.868793
C	-0.281473	-2.916091	-2.731592	C	-3.596360	-0.516710	-3.070480
C	-1.530150	-3.471709	-2.267920	C	-2.929550	0.688304	-3.452341
C	0.958009	-0.788052	-3.102752	C	-4.511786	-0.531285	-1.989013
C	-0.196944	-1.635696	-3.338106	C	-2.162678	2.877033	-2.728159
C	1.742822	1.501260	-2.631038	C	-2.064758	3.820648	-1.634990
C	0.801168	0.641008	-3.266515	C	-3.005653	3.790402	-0.541461
C	1.990530	3.032408	-0.915851	C	-3.210877	1.920997	-2.814965
C	1.349875	2.783638	-2.149039	C	-4.567137	2.077383	0.491147
C	1.609285	3.270920	1.457868	C	-5.037393	0.801241	0.045085
C	0.613739	3.159231	2.463058	C	-4.811077	0.714179	-1.364810
C	1.276485	3.696141	0.140436	C	-4.053559	2.805031	-0.647785
C	-0.673506	3.649337	2.221489	C	-4.189875	1.930538	-1.786459
C	-1.598956	1.664955	3.406563	Gd	1.532127	-0.301001	0.178236
C	-1.782937	2.932916	2.742058	Gd	-1.383753	1.913549	0.094748
C	-2.520639	-0.604713	3.459127	Gd	-1.886232	-1.664542	-0.140809
C	-2.701061	0.797784	3.377405	N	-0.574608	-0.035315	0.116801
C	-3.440123	-2.495346	2.117170	C	5.012118	-0.033819	-0.060745
C	-3.597749	-1.231583	2.739908	C	6.161756	-0.853791	0.585769
C	-3.503557	-3.568309	-0.184016	O	6.510631	-0.714298	1.736545
C	-4.102979	-2.735707	0.854888	O	6.698375	-1.669133	-0.328718
C	-2.765541	-2.800180	-2.489457	C	5.704830	1.035738	-0.934213
C	-3.776706	-2.894418	-1.456118	O	5.874971	0.903058	-2.125784

O	6.118934	2.054048	-0.169744
C	6.769146	3.140459	-0.915877
C	7.092589	4.219457	0.086262
H	6.065073	3.476021	-1.691878
H	7.662223	2.723846	-1.404541
H	7.584901	5.058306	-0.428381
H	6.172483	4.588872	0.562734
H	7.767653	3.834852	0.864885
C	7.826915	-2.473051	0.162468
C	8.300133	-3.307802	-1.000581
H	7.461570	-3.079104	1.004331
H	8.595113	-1.778534	0.533154
H	9.152797	-3.926014	-0.681926
H	7.495050	-3.969707	-1.352084
H	8.619802	-2.663099	-1.832497

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C	2.680116	-4.255579	-0.346429
C	1.589922	-4.333616	0.565055
C	0.372322	-4.372374	-0.235467
C	2.159459	-4.130461	-1.682825
C	0.739571	-4.128425	-1.623014
C	2.868393	-3.099356	-2.358585
C	3.724181	-3.305866	-0.170720
C	3.925821	-2.662429	-1.461757
C	3.781104	-2.504294	1.034071
C	1.610672	-3.559297	1.783266
C	2.700173	-2.592610	2.024432
C	0.331084	-3.308407	2.346303
C	-0.875508	-3.932206	0.290626
C	-0.906005	-3.536367	1.637794
C	-1.796551	-3.321325	-0.595142
C	-0.016114	-3.169924	-2.386950
C	-1.325359	-2.913889	-1.889575
C	2.147840	-2.116421	-3.139532
C	0.676929	-2.116002	-3.143217
C	2.827866	-0.887375	-3.333187
C	4.476085	-1.352244	-1.555267
C	4.014414	-0.524229	-2.599158
C	4.495926	-1.282752	0.911879
C	4.904034	-0.735004	-0.356988
C	4.279365	-0.196716	1.802598
C	2.434021	-1.429418	2.884013
C	3.244943	-0.226944	2.770344
C	0.116927	-2.244687	3.242422
C	1.145324	-1.308748	3.532168
C	-1.889860	-2.609990	2.108958
C	-1.261751	-1.862972	3.162299
C	-2.835853	-2.416383	-0.152077
C	-2.919549	-2.044335	1.262520
C	-2.026739	-1.755645	-2.251204
C	-3.060966	-1.509001	-1.280091
C	-0.028044	-0.852805	-3.399206
C	-1.411022	-0.720775	-2.993386
C	2.132782	0.310357	-3.651340
C	0.717657	0.369699	-3.639004
C	4.038235	0.908677	-2.472540
C	2.939263	1.407954	-3.218315
C	4.937164	0.695654	-0.232324
C	4.673828	1.006003	1.131794
C	4.466162	1.565833	-1.273112
C	4.108809	2.243128	1.481338
C	2.743709	1.065265	3.217844
C	3.172943	2.276144	2.552237
C	0.709492	-0.049276	4.009309
C	1.484812	1.124627	3.832890
C	-1.655274	-0.550390	3.470266
C	-0.672487	0.331122	3.962240
C	-3.465175	-0.752998	1.706842
C	-2.748443	-0.015608	2.727971
C	-3.743675	-0.264404	-1.272603
C	-4.079799	0.256186	0.871099
C	-1.973213	0.565965	-2.788295
C	-3.029567	0.821505	-1.839820
C	0.127239	1.672358	-3.372567
C	-1.208453	1.734176	-2.928432
C	2.357886	2.624509	-2.879024
C	0.955266	2.773990	-3.006384

C	3.864161	2.871792	-0.906675
C	3.774455	3.244666	0.496362
C	2.825977	3.383700	-1.756455
C	2.273394	3.377606	2.305943
C	2.615942	3.979023	1.029367
C	0.594211	2.241568	3.655357
C	-0.739118	1.732523	3.701640
C	0.932547	3.326555	2.814226
C	-2.771218	1.373799	2.399521
C	-3.482421	1.538685	1.148363
C	-1.749448	2.253815	2.855860
C	-2.793804	2.144375	-1.247593
C	-1.692852	2.709096	-2.001130
C	-2.933034	2.479441	0.167864
C	0.524314	3.726083	-2.024903
C	1.668244	4.103864	-1.232334
C	1.529790	4.387323	0.162116
C	-0.784600	3.659204	-1.475420
C	-0.102762	3.889632	2.012683
C	-1.422882	3.340644	2.013956
C	-1.961811	3.416760	0.682008
C	0.190766	4.352139	0.687858
C	-0.948734	4.026552	-0.125049
Gd	1.519666	-1.905292	-0.426743
Gd	1.752253	1.724421	0.213748
Gd	-1.505105	0.083325	0.278617
N	0.613761	-0.050732	0.124260
C	-4.884123	-0.032469	-0.340573
C	-5.784703	1.164161	-0.742601
O	-6.169109	2.007677	0.035471
O	-6.069613	1.076855	-2.046081
C	-5.804894	-1.273192	-0.237771
O	-5.977382	-2.050488	-1.149860
O	-6.383976	-1.301602	0.967711
C	-7.308230	-2.428324	1.169362
C	-7.823910	-2.315196	2.581401
H	-6.744163	-3.355688	0.992747
H	-8.102204	-2.346842	0.412432
H	-8.525232	-3.139677	2.779560
H	-6.993284	-2.377949	3.299747
H	-8.349313	-1.359699	2.725637
C	-6.916177	2.165304	-2.557259
C	-7.085791	1.919877	-4.034970
H	-6.404569	3.113628	-2.337041
H	-7.866030	2.137027	-2.003438
H	-7.716710	2.712103	-4.465150
H	-6.108849	1.932462	-4.540277
H	-7.566846	0.946746	-4.212192

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C	-2.258295	4.363208	-0.949125
C	-3.169752	3.439439	-1.525309
C	-4.027816	2.968214	-0.444578
C	-2.458641	4.387411	0.477566
C	-3.494051	3.472170	0.814996
C	-1.190779	4.333593	1.116592
C	-0.861841	4.284040	-1.214853
C	-0.185490	4.392802	0.064441
C	-0.354829	3.353634	-2.196628
C	-2.710768	2.509573	-2.530990
C	-1.273628	2.430143	-2.863650
C	-3.512147	1.345965	-2.668265
C	-4.677420	1.705900	-0.517786
C	-4.525511	0.969060	-1.713028
C	-4.858457	0.989069	0.693261
C	-3.326680	2.561062	1.928735
C	-4.127548	1.385954	1.869312
C	-0.987434	3.452253	2.245250
C	-2.040417	2.506602	2.642895
C	0.363069	3.109147	2.488250
C	1.118936	3.860081	0.258758
C	1.416373	3.377870	1.542719
C	1.010399	2.973974	-2.029665
C	1.775469	3.269459	-0.853598
C	1.546278	1.802652	-2.619903
C	-0.735305	1.170367	-3.388149
C	0.684339	0.877430	-3.285813
C	-3.001652	0.162953	-3.242339

C	-1.640831	0.059232	-3.620078	C	-0.934126	-3.336605	-2.674752
C	-4.625645	-0.457941	-1.714134	C	1.439406	-3.063565	-2.043599
C	-3.732762	-0.953761	-2.712016	C	-2.527803	-3.967354	-0.907811
C	-4.960876	-0.436087	0.693499	C	-2.744674	-4.008692	0.531439
C	-4.854063	-1.192268	-0.512347	C	-1.211456	-4.084131	-1.491495
C	-3.776568	0.211205	2.573578	C	-1.597553	-3.283476	2.596612
C	-4.353335	-0.925563	1.898606	C	-0.390945	-2.726717	3.133853
C	-1.646961	1.249200	3.297753	C	-1.588055	-4.079989	1.403766
C	-2.563459	0.126520	3.292802	C	1.876855	-1.967699	2.670690
C	0.721341	1.940957	3.210433	C	2.924694	-1.735374	1.688465
C	-0.246802	0.971836	3.570638	C	2.890984	-2.492276	0.445705
C	2.433219	2.392198	1.711444	C	0.874186	-2.957264	2.534194
C	2.042648	1.571050	2.803589	C	1.202712	-3.843632	-0.889650
C	2.826938	2.280256	-0.711384	C	-0.114411	-4.329672	-0.611554
C	2.748560	1.430444	-1.896708	C	-0.300080	-4.299090	0.812655
C	3.208881	1.852240	0.637162	C	1.855594	-3.503141	0.343459
C	3.227299	0.087477	-2.018265	C	0.907404	-3.766587	1.380783
C	1.149554	-0.490847	-3.349856	Gd	-1.497921	2.009421	-0.079410
C	2.358254	-0.846727	-2.666910	Gd	1.477824	-0.185166	-0.141661
C	-1.146065	-1.263809	-3.707327	Gd	-1.856025	-1.644557	0.216990
C	0.230555	-1.534337	-3.550970	N	-0.632668	0.059205	0.023224
C	-3.152886	-2.238875	-2.618943	C	4.890440	0.036253	-0.071773
C	-1.876675	-2.394656	-3.196261	C	5.745211	1.120020	-0.779302
C	-4.308285	-2.529146	-0.418790	O	5.984468	1.120659	-1.965464
C	-3.487020	-3.055201	-1.478007	O	6.181397	1.995908	0.133421
C	-3.789756	-2.232220	1.994287	C	5.888786	-0.921266	0.629946
C	-3.850026	-3.103685	0.833331	O	6.175725	-0.849382	1.803748
C	-2.086394	-1.193561	3.510001	O	6.389619	-1.772775	-0.271880
C	-2.664013	-2.345873	2.857519	C	7.385736	-2.710023	0.269686
C	0.223834	-0.396933	3.719900	C	7.818415	-3.588791	-0.876205
C	-0.708716	-1.447838	3.691182	H	6.904247	-3.272601	1.082687
C	2.436503	0.238835	2.842290	H	8.209122	-2.114286	0.690579
C	1.553734	-0.738083	3.329728	H	8.570307	-4.308169	-0.518386
C	3.884624	0.579404	0.892476	H	6.959843	-4.146131	-1.278768
C	3.956606	-0.629808	-1.012894	H	8.260515	-2.983838	-1.681461
C	3.304589	-0.308394	1.849428	C	7.002669	3.085591	-0.414453
C	2.470044	-2.096926	-1.973941	C	7.352503	3.984958	0.743821
C	3.335071	-1.918374	-0.826064	H	6.406357	3.593998	-1.186249
C	0.372920	-2.820274	-2.927274	H	7.884818	2.631677	-0.889549

H	7.972550	4.819040	0.382296
H	6.439818	4.395277	1.200593
H	7.915101	3.429315	1.508409

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C	2.794425	-2.531513	-0.332057
C	2.978054	-1.937635	-1.660029
C	3.148313	-1.770621	0.857560
C	1.672956	-3.446801	-0.166264
C	3.489135	-0.576976	-1.890228
C	1.879585	-2.111748	-2.624517
C	3.672622	-0.403559	0.871423
C	3.835073	0.462827	-0.923937
C	0.730058	-3.735616	-1.210434
C	2.286122	-1.838457	2.023630
C	0.961118	-3.615046	1.076144
C	0.775109	-2.998465	-2.426550
C	2.611234	0.055596	-2.814328
C	1.231452	-2.780187	2.181217
C	1.641945	-0.853529	-3.289618
C	2.819164	0.408374	1.709979
C	-0.525768	-4.101184	-0.620596
C	-0.393533	-4.050336	0.815773
C	2.135831	-0.526510	2.562602
C	2.889956	1.572268	-1.062525
C	2.206269	1.337441	-2.335305
C	-0.452659	-2.668169	-3.048196
C	0.146332	-2.476762	3.064275
C	0.347082	-0.391035	-3.654757
C	-1.762201	-3.771165	-1.238296
C	2.213565	1.693291	1.391063
C	-1.506387	-3.796308	1.710625
C	1.021241	-0.170636	3.344045
C	-0.658661	-1.382690	-3.670196
C	2.155572	2.231294	0.008912
C	-1.708463	-3.080128	-2.483809
C	-1.196864	-2.991852	2.880536
C	0.059195	-1.177166	3.654109
C	0.919793	1.834040	-2.634709
C	-0.013727	1.005245	-3.415182
C	-2.888125	-3.530617	-0.363062
C	-2.818419	-3.597931	1.095620
C	1.172824	2.068962	2.291864
C	0.617054	1.175374	3.277504
C	-2.683843	-2.091051	-2.820556
C	-2.024141	-1.035457	-3.541779
C	-2.118894	-1.961558	3.374028
C	-1.313872	-0.844443	3.836632
C	0.993896	3.036348	-0.396919
C	0.449061	2.902100	-1.770978
C	-3.857833	-2.541954	-0.733953
C	-3.751928	-2.570688	1.609883
C	-0.741554	1.533219	3.512447
C	-1.413597	1.362825	-3.432511
C	0.160937	2.999168	1.945181
C	-3.761809	-1.800605	-1.959159
C	-3.391378	-1.712862	2.733005
C	-2.434184	0.315989	-3.459370
C	-1.730549	0.525000	3.734874
C	0.070474	3.535857	0.635706
C	-4.376691	-1.939381	0.458115
C	-1.022596	2.697362	2.727223
C	-0.834870	3.428629	-2.091833
C	-1.782976	2.652578	-2.898609
C	-4.294868	-0.487362	-2.000706
C	-3.808481	-0.331162	2.672312
C	-3.025840	0.756282	3.212660
C	-3.688960	0.543695	-2.800220
C	-1.221298	4.061675	0.270013
C	-4.815999	-0.564696	0.421134
C	-1.596915	4.149456	-1.106586
C	-2.322556	2.938654	2.225204
C	-4.566497	0.218142	1.576354
C	-4.854794	0.119447	-0.830436
C	-3.329537	1.954809	2.486482
C	-3.108814	2.902027	-2.349343

C	-3.991788	1.803092	-2.193035
C	-2.425562	3.716417	1.020580
C	-2.986064	3.828404	-1.244995
C	-4.304928	1.631172	1.483548
C	-4.664506	1.548686	-0.928921
C	-3.511337	3.506364	0.068236
C	-4.364568	2.341903	0.237496
Y	1.350325	-0.362823	-0.545361
Y	-1.832433	1.680138	-0.525452
Y	-1.659913	-1.459264	0.892657
N	-0.690877	-0.033441	-0.234848
C	4.816081	0.226268	0.163836
C	5.380797	1.417982	0.952021
O	5.865297	1.269952	2.053615
O	5.237484	2.563917	0.273264
C	5.924711	-0.737452	-0.281847
O	5.781216	-1.937178	-0.352746
O	7.007655	-0.027012	-0.626586
C	8.151323	-0.827244	-1.097301
H	7.767801	-1.605325	-1.772002
H	8.754338	-0.099920	-1.654725
C	5.582191	3.780547	1.025681
H	6.477915	3.575233	1.627871
H	5.805216	4.514261	0.241243
C	4.402255	4.188505	1.881190
H	3.512485	4.355902	1.254840
H	4.181594	3.407069	2.624355
H	4.639601	5.122994	2.414873
C	8.893460	-1.413294	0.081871
H	9.193729	-0.616069	0.778469
H	9.796641	-1.931881	-0.276587
H	8.256532	-2.138164	0.608949

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C	0.554304	4.051448	-0.926406
C	-0.413014	4.545665	0.038707
C	1.755250	3.435684	-0.416024
C	0.072569	3.537446	-2.181010
C	-0.148394	4.384760	1.462696
C	-1.820516	4.217364	-0.169585
C	1.914638	3.148264	0.996657
C	0.946267	3.565714	1.942290
C	-1.329827	3.368834	-2.433775
C	2.397891	2.352339	-1.129765
C	0.768607	2.507483	-2.915082
C	-2.285506	3.624165	-1.398615
C	-1.343107	3.900738	2.088005
C	1.927855	1.887213	-2.397913
C	-2.373365	3.768948	1.106358
C	2.557900	1.866751	1.126400
C	-1.492528	2.269752	-3.344043
C	-0.191292	1.737074	-3.673910
C	2.932256	1.449291	-0.177973
C	0.419339	2.573175	2.872911
C	-1.025915	2.781248	2.939794
C	-3.404228	2.761803	-1.321199
C	2.136496	0.500045	-2.750038
C	-3.295419	2.668010	1.179273
C	-2.624235	1.420112	-3.276585
C	2.146126	0.924287	2.151113
C	0.025691	0.365622	-4.076820
C	3.297140	0.079882	-0.538969
C	-3.910903	2.302885	-0.046221
C	0.975803	1.241633	2.972084
C	-3.600514	1.704894	-2.274019
C	1.279067	-0.256927	-3.654376
C	2.734976	-0.397608	-1.816281
C	-1.918654	1.678810	3.056974
C	-3.143939	1.645247	2.228482
C	-2.437147	0.057680	-3.686279
C	-1.154015	-0.476925	-4.111801
C	2.460364	-0.423057	1.921283
C	3.125112	-0.943079	0.698180
C	-4.292260	0.646722	-1.615984
C	-4.470323	1.014494	-0.236144
C	1.327451	-1.661756	-3.203464
C	2.211199	-1.696740	-2.030739
C	0.111469	0.188799	3.462565

C	-1.344293	0.441489	3.573313
C	-3.171702	-0.984349	-3.041271
C	-1.106841	-1.881901	-3.685133
C	2.462201	-2.228721	0.388960
C	-3.851530	0.388065	2.073212
C	1.666296	-1.453008	2.446286
C	-4.092801	-0.702869	-1.983574
C	0.118791	-2.482681	-3.187375
C	-4.495036	0.058473	0.803936
C	2.035185	-2.608435	-0.906486
C	0.547582	-1.195133	3.282378
C	-2.370786	-2.169382	-3.026790
C	1.695384	-2.580888	1.536410
C	-2.235366	-0.661392	3.692884
C	-3.486539	-0.713096	2.935678
C	-4.288591	-1.682930	-0.977733
C	-0.040338	-3.382591	-2.067545
C	0.916765	-3.484270	-0.990046
C	-4.569192	-1.317229	0.386493
C	-0.383209	-2.276636	3.419550
C	-2.508814	-3.104429	-1.948815
C	-1.736103	-2.007898	3.785196
C	0.610474	-3.486724	1.469876
C	-1.324702	-3.750367	-1.512750
C	-3.537006	-2.899321	-0.976213
C	0.235657	-3.950874	0.179465
C	-3.699527	-2.107826	2.555956
C	-4.116726	-2.385000	1.226969
C	-0.399054	-3.394307	2.488946
C	-2.609386	-2.902536	3.084845
C	-1.155541	-4.144712	-0.142548
C	-3.409065	-3.350096	0.391959
C	-1.792391	-3.749647	2.227810
C	-2.188718	-3.977498	0.846529
Y	-0.498067	2.071644	0.536493
Y	-1.644009	-1.411392	1.290942
Y	-0.217415	-0.496130	-1.741725
N	-0.649839	0.033056	0.196379
C	4.486410	-0.528240	0.195070
C	5.252770	0.463669	1.064052
O	5.235757	0.464948	2.276487
O	5.887822	1.336442	0.263136
C	5.318287	-1.575770	-0.500772
O	4.878476	-2.372276	-1.304905
O	6.597382	-1.492376	-0.086584
C	7.499414	-2.496265	-0.667328
H	7.275502	-2.580596	-1.739974
H	8.494537	-2.059026	-0.518271
C	6.509081	2.472377	0.955059
H	7.031288	2.095914	1.845899
H	7.229745	2.856155	0.222399
C	5.448610	3.493851	1.309035
H	4.776225	3.091237	2.079857
H	5.928810	4.406174	1.698253
H	4.858871	3.753970	0.415775
H	8.076944	-4.537754	-0.340422
C	7.338228	-3.818877	0.047991
H	7.502588	-3.690430	1.128676
H	6.329806	-4.221735	-0.124543

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C	-0.162425	4.125758	-1.144154
C	-0.113916	3.719269	-2.538916
C	-1.327151	3.757145	-0.380199
C	1.079269	4.200220	-0.410815
C	-1.213654	2.946893	-3.095932
C	1.124282	3.108837	-3.027663
C	-2.351778	2.863369	-0.926302
C	-2.283402	2.411917	-2.280097
C	2.321522	3.760578	-0.978247
C	-1.218396	3.448571	1.023799
C	1.152627	3.975323	1.007664
C	2.336942	3.122047	-2.259407
C	-0.654294	1.857058	-3.841652
C	0.008297	3.572122	1.741062
C	0.769040	1.923056	-3.791953
C	-2.777454	1.988631	0.105910
C	3.166603	3.305693	0.090113

C	2.460753	3.458820	1.343145	C	-1.858474	-2.067888	2.035271
C	-2.124314	2.375109	1.309410	C	-0.517372	-2.882289	-2.561446
C	-2.353758	0.965487	-2.506118	C	0.922929	-2.928094	-2.819681
C	-1.315033	0.634686	-3.480874	C	4.189966	-1.959864	-0.505710
C	3.231899	2.040204	-2.435305	C	1.904900	-1.410163	3.561204
C	0.235582	2.732039	2.878099	C	0.497535	-1.733290	3.562066
C	1.540437	0.717648	-3.719963	C	3.470262	-2.451942	-1.649882
C	4.074459	2.230666	-0.090809	C	-1.554726	-3.446930	-0.382543
C	-3.246414	0.598346	-0.188803	C	3.647027	-2.030880	1.911594
C	2.727264	2.645746	2.511855	C	-0.801148	-3.848373	-1.528709
C	-1.886691	1.489221	2.399657	C	-0.885136	-3.096467	2.000840
C	2.842111	0.860756	-3.171166	C	2.549238	-2.399253	2.731778
C	-2.715850	0.019437	-1.488658	C	3.762171	-2.689196	0.649248
C	4.120465	1.625890	-1.383203	C	0.293742	-2.922012	2.787218
C	1.558193	2.301373	3.305723	C	1.490539	-3.907739	-1.897513
C	-0.710973	1.707102	3.192495	C	2.696035	-3.578865	-1.227002
C	-0.599508	-0.588182	-3.397227	C	-0.803070	-3.865524	0.793465
C	0.863498	-0.582348	-3.618877	C	0.419480	-4.470804	-1.104808
C	4.365621	1.417097	1.068277	C	1.567772	-3.352333	2.284751
C	3.775191	1.630736	2.387450	C	2.822116	-3.699910	0.218712
C	-3.098541	-0.324876	1.090964	C	0.463138	-4.451081	0.346858
C	-2.387383	0.183290	2.298812	C	1.680264	-4.047418	1.028776
C	4.339398	0.223304	-1.526807	Y	-0.172753	1.490746	-1.332800
C	3.534080	-0.247606	-2.624448	Y	0.610618	-2.043043	-0.428279
C	1.401503	0.970228	3.900524	Y	1.753641	0.646057	1.412843
C	-0.012620	0.626577	3.804708	N	0.447128	-0.014445	-0.031747
C	-2.248698	-1.326256	-1.591901	C	-4.462828	0.027026	0.533263
C	-1.231695	-1.651428	-2.622671	C	-5.305408	1.016336	1.301737
C	4.603072	0.015349	0.888445	O	-4.880271	1.731009	2.184545
C	3.616054	0.293198	2.999233	O	-6.561742	1.000076	0.816576
C	-1.684015	-0.900207	2.867409	C	-5.243047	-1.150825	-0.035350
C	1.636256	-1.729679	-3.193291	O	-5.686444	-2.030490	0.673485
C	-2.582244	-1.681624	0.871489	O	-5.348008	-1.064801	-1.371958
C	4.580816	-0.600497	-0.407588	C	-5.966593	-2.229835	-2.018833
C	2.403300	-0.062558	3.732004	H	-6.827163	-2.546886	-1.413528
C	2.984744	-1.548065	-2.654310	H	-6.301996	-1.839280	-2.987546
C	-0.476571	-0.708667	3.609698	C	-7.501423	1.894878	1.505992
C	-2.319293	-2.223848	-0.398427	H	-6.998532	2.857144	1.676297
C	4.137992	-0.682204	2.050487	H	-8.316800	2.013204	0.781503

C	-7.966338	1.262241	2.798595
H	-7.122875	1.165051	3.497276
H	-8.737415	1.897981	3.261825
H	-8.395010	0.267660	2.602915
H	-5.398457	-4.188948	-2.699092
C	-4.944218	-3.337436	-2.166965
H	-4.075976	-2.983854	-2.743817
H	-4.609766	-3.679406	-1.176143

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C	-3.780916	0.472089	0.737060
C	-3.905934	-0.941306	-0.943277
C	-3.163844	-0.190847	1.849736
C	-3.109187	1.644767	0.254426
C	-3.362963	-2.204792	-0.490740
C	-3.095246	-0.445160	-2.036210
C	-2.711974	-1.592521	1.904921
C	-2.747197	-2.518971	0.806283
C	-2.669022	1.914259	-1.110520
C	-2.288086	0.575329	2.697814
C	-2.312042	2.426777	1.144324
C	-2.565514	0.914627	-2.171611
C	-2.438683	-2.614667	-1.496087
C	-1.909548	1.918566	2.404441
C	-2.238681	-1.567038	-2.435996
C	-1.566921	-1.621639	2.791107
C	-1.674152	2.965746	-0.996756
C	-1.474515	3.308922	0.391536
C	-1.380881	-0.307592	3.342189
C	-1.495063	-3.245882	0.517078
C	-1.317443	-3.273113	-0.920571
C	-1.430479	1.040065	-3.028707
C	-0.679932	2.428588	2.933260
C	-0.961535	-1.414984	-3.042159
C	-0.591882	3.097870	-1.900418
C	-0.421082	-2.458769	2.579462
C	-0.257414	3.877200	0.929129
C	-0.128991	0.159260	3.811082
C	-0.673990	-0.106792	-3.495688
C	-0.336089	-3.235837	1.359259
C	-0.501551	2.135519	-2.939441
C	0.121746	3.441058	2.264446
C	0.191909	1.547651	3.646386
C	-0.049266	-3.211928	-1.535634
C	0.134861	-2.322899	-2.694661
C	0.624822	3.690360	-1.396645
C	0.807482	4.133242	-0.021039
C	0.780982	-2.053683	3.208135
C	0.930450	-0.769201	3.832751
C	0.769673	1.690191	-3.409823
C	0.661255	0.294847	-3.728706
C	1.527479	3.180822	2.611567
C	1.539442	1.985338	3.447557
C	0.955463	-3.548573	0.766166
C	1.075554	-3.607142	-0.704270
C	1.885245	3.241332	-1.897848
C	2.220342	3.904199	0.330811
C	2.286994	-0.351670	3.690963
C	1.477466	-1.952955	-3.080297
C	2.048760	-2.454830	2.716964
C	1.974209	2.222834	-2.900718
C	2.595633	3.384497	1.642697
C	1.745305	-0.603859	-3.573448
C	2.602860	1.016757	3.435149
C	2.170648	-3.242438	1.541654
C	2.859159	3.345888	-0.850726
C	3.001608	-1.413991	3.042461
C	2.359774	-3.545421	-1.322149
C	2.574920	-2.688162	-2.492505
C	3.113176	1.381149	-2.909148
C	3.656152	2.403236	1.657686
C	3.699468	1.286491	2.578020
C	3.019706	0.002325	-3.309107
C	3.447851	-3.181095	0.882057
C	3.948586	2.406472	-0.810576
C	3.550527	-3.483800	-0.513925
C	4.106601	-1.145924	2.203350
C	4.371959	1.981406	0.474871

C	4.117064	1.491075	-1.892592
C	4.458134	0.224807	1.985059
C	3.893964	-2.091552	-2.338979
C	4.057186	-0.716043	-2.636029
C	4.383293	-2.095545	1.159527
C	4.489154	-2.588777	-1.121034
C	4.896382	0.660899	0.689063
C	4.705034	0.187606	-1.700875
C	4.980554	-1.682563	-0.103630
C	5.092081	-0.265803	-0.389521
Y	-1.369481	-0.650188	-0.157040
Y	2.464279	-1.189429	-0.421987
Y	1.022418	1.739950	0.634581
N	0.673913	-0.193138	-0.006504
C	-4.845274	-0.127675	-0.128620
C	-5.841084	-1.037317	0.624859
O	-5.709105	-1.399095	1.772128
O	-6.821290	-1.380646	-0.223454
C	-5.594800	0.954883	-0.935595
O	-5.630076	1.013280	-2.143014
O	-6.144067	1.817772	-0.063839
C	-6.647987	3.062369	-0.665093
H	-7.218878	2.806716	-1.568525
H	-7.312176	3.469374	0.107069
C	-7.776868	-2.369147	0.304635
H	-8.037977	-2.078194	1.331707
H	-8.644342	-2.260110	-0.357674
C	-7.169138	-3.752146	0.241992
H	-6.301114	-3.816702	0.914143
H	-7.916820	-4.495807	0.561128
H	-6.854941	-3.983949	-0.786920
H	-5.849531	4.952564	-1.314143
C	-5.478072	3.975528	-0.965521
H	-4.872994	4.127883	-0.057863
H	-4.845556	3.539029	-1.752788

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C	-0.197422	-4.237305	0.973632
C	-1.580967	-4.264900	1.415496
C	0.061422	-4.206274	-0.447133
C	0.761692	-3.562762	1.797063
C	-2.643500	-4.258407	0.429017
C	-1.993490	-3.362843	2.490166
C	-1.019603	-4.032674	-1.395318
C	-2.369681	-4.003200	-0.967673
C	0.356646	-2.788340	2.939723
C	1.198351	-3.495948	-0.983977
C	1.938518	-2.940037	1.248580
C	-1.026975	-2.606292	3.245230
C	-3.642535	-3.322902	0.847795
C	2.153204	-2.861658	-0.154719
C	-3.254585	-2.741147	2.096597
C	-0.573377	-3.157667	-2.434803
C	1.289518	-1.713310	3.095075
C	2.290751	-1.823658	2.084198
C	0.826808	-2.885803	-2.220439
C	-3.213662	-2.906850	-1.415166
C	-3.993937	-2.470965	-0.258206
C	-1.420431	-1.334822	3.728121
C	2.948396	-1.755739	-0.658127
C	-3.509423	-1.346529	2.344940
C	0.905714	-0.438436	3.569399
C	-1.441853	-2.159814	-2.979180
C	3.082165	-0.731994	1.606974
C	1.449156	-1.688326	-2.672343
C	-2.658263	-0.722443	3.296467
C	-2.768686	-1.959099	-2.403237
C	-0.463613	-0.279977	3.933107
C	3.672324	-0.933413	0.299850
C	2.575506	-1.116721	-1.932501
C	-4.269294	-1.091071	-0.054117
C	-4.125972	-0.511607	1.297287
C	1.629390	0.695399	3.062785
C	2.705746	0.603492	2.081523
C	-0.790886	-1.067983	-3.586886
C	0.627231	-0.841519	-3.458345
C	-1.125745	0.959801	3.716529
C	-2.478066	0.684142	3.313797

C	3.562632	0.940002	-0.925735
C	2.806962	0.335069	-2.015537
C	-3.369105	-0.641936	-2.399971
C	-4.184952	-0.239806	-1.237724
C	0.959070	1.941937	2.907490
C	2.651354	1.862843	1.274491
C	0.839359	0.563666	-3.518591
C	-4.053324	0.932184	1.432968
C	-1.437772	0.183354	-3.734935
C	-0.431995	2.082442	3.213395
C	2.934061	2.000732	-0.162169
C	-3.190584	1.535763	2.441996
C	1.854838	1.164057	-2.737330
C	-2.733538	0.412881	-3.199563
C	1.555269	2.655966	1.826101
C	-0.425580	1.209421	-3.740708
C	-4.478424	1.133885	-1.038064
C	-4.391021	1.739301	0.287137
C	-1.193319	3.035675	2.494877
C	2.030917	2.822298	-0.907522
C	1.591614	2.470317	-2.233633
C	-2.578546	2.811043	2.177177
C	-3.066509	1.785990	-2.959128
C	0.749047	3.560862	1.057324
C	-4.058065	2.119746	-1.991504
C	-0.687846	2.505089	-3.235009
C	1.027615	3.653619	-0.326988
C	-0.602840	3.808822	1.448846
C	0.344387	3.135718	-2.477654
C	-3.879591	3.092699	0.102804
C	-2.875620	3.557367	0.991168
C	-2.051852	2.828897	-2.918596
C	-3.677584	3.319056	-1.310591
C	0.006184	3.901446	-1.304744
C	-1.636181	4.138405	0.489982
C	-2.400954	3.756497	-1.842854
C	-1.353092	4.173488	-0.930270
Y	-1.540417	-1.955836	0.348719
Y	-1.931332	1.605515	-0.547634
Y	1.270036	0.110898	0.025875
N	-0.799169	-0.027306	0.074353
C	4.601966	0.077778	-0.286491
C	5.485010	0.779234	0.771900
O	5.791305	0.274943	1.829517
O	5.853075	1.983356	0.310293
C	6.564894	2.824158	1.286193
H	7.303378	2.200470	1.808875
H	7.066366	3.572068	0.659972
C	5.563475	3.441518	2.238344
H	5.065124	2.657157	2.827465
H	6.083544	4.123948	2.929836
H	7.549058	-1.711532	-2.367215
H	4.806499	4.012481	1.679293
C	5.554841	-0.539742	-1.347408
O	5.720297	-0.076466	-2.453537
O	6.131271	-1.631452	-0.825421
C	6.945695	-2.409785	-1.770442
H	7.588121	-3.013322	-1.117654
C	6.033581	-3.255370	-2.632203
H	5.401444	-3.897310	-1.999628
H	5.394642	-2.609216	-3.252726
H	6.637126	-3.894452	-3.296360

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C	0.319414	-4.132953	-1.351233
C	-0.851261	-3.710672	-2.110248
C	1.625485	-3.806315	-1.872766
C	0.212503	-4.178887	0.081640
C	-0.662536	-2.971719	-3.348678
C	-1.968737	-3.090689	-1.404256
C	1.767979	-2.928842	-3.021863
C	0.632968	-2.453320	-3.722726
C	-0.946911	-3.689592	0.766247
C	2.736206	-3.529640	-0.989732
C	1.347689	-3.974263	0.948304
C	-2.013376	-3.045810	0.045608
C	-1.574018	-1.866639	-3.346362
C	2.615676	-3.617358	0.429502

C	-2.368578	-1.901605	-2.155233	C	4.532017	0.664488	1.029304
C	2.877503	-2.058703	-2.789221	C	2.260647	2.151817	-2.783141
C	-0.534232	-3.221966	2.051091	C	0.585374	0.757879	3.895457
C	0.892935	-3.417281	2.197567	C	4.037941	1.993903	-1.024160
C	3.526396	-2.489189	-1.579236	C	-0.514216	2.871876	-2.554583
C	0.515305	-1.021385	-3.964359	C	-1.539051	2.951679	-1.521240
C	-0.876912	-0.660564	-3.694769	C	-1.533605	2.062504	2.490199
C	-2.661269	-1.967116	0.657522	C	3.127228	1.414565	2.933334
C	3.443232	-2.774335	1.264514	C	3.948882	1.716551	1.781968
C	-2.735660	-0.673970	-1.518305	C	-2.043375	2.540335	1.230676
C	-1.169967	-2.118354	2.658982	C	1.882101	3.399782	-2.182445
C	2.823163	-0.666639	-3.134324	C	0.779251	2.088160	3.401366
C	1.718415	-2.601755	3.058692	C	0.519033	3.823205	-2.221204
C	4.260027	-1.583992	-0.775767	C	3.474901	3.050077	-0.273528
C	-3.257856	-0.825650	-0.134047	C	2.085175	2.417126	2.962778
C	1.580240	-0.103480	-3.648986	C	-0.318065	2.758396	2.770325
C	-2.231477	-1.492813	1.931005	C	3.445619	2.901486	1.149191
C	3.080872	-2.326826	2.601846	C	-1.082053	3.944262	-0.554966
C	4.256666	-1.770360	0.648558	C	-1.217618	3.641529	0.819079
C	-1.197742	0.573894	-3.061781	C	2.437713	3.829386	-0.902880
C	-2.215962	0.587526	-1.985795	C	0.191662	4.481070	-0.993173
C	-0.384157	-1.312772	3.540276	C	2.302499	3.356273	1.893025
C	1.035574	-1.545407	3.780932	C	-0.105539	3.755419	1.743269
C	3.707475	0.178666	-2.423208	C	1.365278	4.447996	-0.130098
C	4.435546	-0.271844	-1.268173	C	1.223823	4.070947	1.266104
C	-2.502439	-0.117844	2.069942	Y	0.025052	-1.450002	-1.443741
C	-3.151015	0.396268	0.823650	Y	0.565334	2.056927	-0.377766
C	3.698357	-0.996428	2.798271	Y	1.641738	-0.652387	1.500998
C	4.398568	-0.673071	1.559237	N	0.446230	0.014252	-0.033919
C	1.232903	1.278604	-3.374548	C	-4.520177	-0.111223	0.346629
C	-0.184841	1.623720	-3.155893	C	-5.429739	-0.816004	1.315222
C	-0.645179	0.082621	3.631372	O	-5.051921	-1.493765	2.249397
C	1.650884	-0.230836	3.991588	O	-6.717540	-0.589960	0.971472
C	4.603770	0.836595	-0.384985	C	-5.193841	0.802041	-0.663559
C	-2.288306	1.775800	-1.114339	O	-5.301402	0.557672	-1.848312
C	3.446501	1.561920	-2.272628	O	-5.584410	1.929344	-0.039479
C	-1.691742	0.697012	2.866962	C	-6.102059	2.981162	-0.921396
C	2.972078	0.081246	3.472454	H	-6.755595	2.518174	-1.673981
C	-2.619989	1.658317	0.271623	H	-6.686674	3.619196	-0.247141

C	-4.946672	3.725515	-1.556983
H	-4.252518	4.083540	-0.780613
H	-4.406170	3.066152	-2.251152
H	-5.327586	4.593362	-2.119212
C	-7.707379	-1.265050	1.818227
H	-7.392889	-1.162565	2.866376
H	-8.627514	-0.694571	1.639444
C	-7.843248	-2.715987	1.412441
H	-8.095663	-2.791075	0.343725
H	-6.902667	-3.251499	1.606163
H	-8.646095	-3.187966	2.000825

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C	-2.564864	2.505452	1.024269
C	-3.415998	1.690813	0.178258
C	-2.217085	2.005398	2.325742
C	-1.630042	3.408031	0.429160
C	-4.030222	0.497684	0.776454
C	-3.019151	1.513330	-1.233025
C	-2.464049	0.610097	2.628326
C	-3.238405	-0.216583	1.782317
C	-1.376821	3.381155	-0.977506
C	-0.966647	2.361831	2.953327
C	-0.425178	3.821482	1.093063
C	-1.988645	2.376369	-1.800414
C	-3.726281	-0.799851	-0.738372
C	-0.057754	3.283241	2.352979
C	-3.052386	0.101716	-1.649806
C	-1.350868	0.102418	3.352192
C	-0.022186	3.815235	-1.183637
C	0.579224	4.113761	0.098520
C	-0.468186	1.202186	3.629357
C	-2.670142	-1.512089	1.385110
C	-2.849229	-1.753687	-0.063675
C	-1.187117	1.864114	-2.849034
C	1.354908	3.146900	2.605574
C	-1.993063	-0.452486	-2.447647
C	0.763287	3.300295	-2.241550
C	-0.861313	-1.216728	3.105819
C	2.002294	4.035344	0.352695
C	0.920047	0.995839	3.801580
C	-1.203542	0.462466	-3.177478
C	-1.457084	-2.015098	2.034705
C	0.147008	2.346146	-3.100636
C	2.399034	3.578968	1.684060
C	1.825206	2.006496	3.336068
C	-1.789679	-2.333882	-0.822169
C	-1.440010	-1.772964	-2.137704
C	2.182054	3.219469	-2.019684
C	2.822676	3.606195	-0.769835
C	0.491338	-1.425384	3.468278
C	1.369522	-0.342019	3.824809
C	0.905937	1.269633	-3.648721
C	0.068285	0.102473	-3.683832
C	3.538284	2.654296	1.864836
C	3.140730	1.681445	2.876963
C	-0.618509	-2.970908	1.328642
C	-0.845214	-3.177400	-0.110081
C	2.925851	2.148197	-2.604367
C	3.970285	2.704707	-0.583518
C	2.691493	-0.685722	3.414653
C	-0.200994	-2.175354	-2.774373
C	1.267387	-2.445231	2.873760
C	2.294073	1.149237	-3.413208
C	4.319455	2.183374	0.727036
C	0.580012	-1.206832	-3.536500
C	3.570636	0.304480	2.884299
C	0.729845	-3.264348	1.848544
C	4.011460	1.816941	-1.733641
C	2.648932	-2.014974	2.871226
C	0.143430	-3.823189	-0.906232
C	0.496658	-3.314558	-2.232481
C	2.844223	-0.157728	-3.426917
C	4.760396	0.806085	0.763459
C	4.452272	-0.096559	1.847876
C	2.013068	-1.324146	-3.570217
C	1.704515	-3.906576	1.009338
C	4.489241	0.463844	-1.681174

C	1.349597	-4.327360	-0.307072
C	3.538752	-2.417715	1.850489
C	4.913780	-0.012872	-0.416135
C	3.962471	-0.496499	-2.599323
C	4.456678	-1.441502	1.348909
C	1.937992	-3.489727	-2.388148
C	2.688355	-2.420984	-2.944481
C	3.091078	-3.454759	0.959313
C	2.457485	-4.119264	-1.193309
C	4.766661	-1.397645	-0.053464
C	3.876175	-1.901985	-2.275925
C	3.542291	-3.525047	-0.428928
C	4.267019	-2.387228	-0.972123
Y	-1.317535	0.261463	0.216036
Y	1.692508	-1.802293	-0.533242
Y	1.921963	1.553963	0.361229
N	0.718371	-0.084052	0.088406
C	-4.949584	-0.317922	-0.055400
C	-5.905118	0.480405	-0.961464
O	-5.884558	0.459303	-2.171655
O	-6.745675	1.173721	-0.175779
C	-5.729877	-1.394521	0.721505
O	-5.818451	-1.446273	1.927878
O	-6.279987	-2.237882	-0.167883
C	-7.011254	-3.367848	0.425462
H	-7.619559	-2.985504	1.257181
H	-7.654054	-3.712756	-0.393767
C	-6.034617	-4.429954	0.879864
H	-5.387160	-4.732956	0.042941
H	-5.415666	-4.047728	1.704553
H	-6.589861	-5.312508	1.235708
C	-7.677121	2.052830	-0.899112
H	-8.075337	1.498695	-1.760738
H	-8.469688	2.243520	-0.165124
C	-6.961496	3.317447	-1.320040
H	-6.510231	3.807367	-0.443864
H	-6.176560	3.081837	-2.053431
H	-7.680803	4.011227	-1.783736

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C	-2.029721	-3.321300	-0.185068
C	-3.128349	-2.343800	-0.068557
C	-1.361008	-3.485993	-1.447394
C	-1.216391	-3.614339	0.962277
C	-3.500006	-1.585743	-1.268872
C	-3.177924	-1.518357	1.150166
C	-1.610879	-2.557150	-2.520604
C	-2.588497	-1.563844	-2.391294
C	-1.333626	-2.852490	2.163949
C	0.033451	-3.855518	-1.540526
C	0.154800	-4.049278	0.863963
C	-2.219933	-1.738675	2.215079
C	-3.907400	-0.212556	-1.086186
C	0.813498	-4.148314	-0.387118
C	-3.639849	-0.133743	0.946695
C	-0.390773	-2.273215	-3.190796
C	-0.057332	-2.831898	2.819013
C	0.882347	-3.594497	2.029772
C	0.613105	-3.137990	-2.640357
C	-2.261436	-0.196862	-2.725808
C	-2.977788	0.659072	-1.772420
C	-1.798579	-0.623006	2.978978
C	2.236006	-3.875578	-0.402019
C	-2.737303	0.956332	1.282111
C	0.363786	-1.709744	3.574548
C	-0.075533	-0.940542	-3.603597
C	2.311048	-3.354625	2.045903
C	1.973975	-2.754805	-2.629520
C	-2.016337	0.713010	2.475229
C	-0.984577	0.147124	-3.272323
C	-0.542331	-0.613282	3.673776
C	3.028841	-3.564540	0.785172
C	2.790351	-3.172945	-1.525311
C	-2.259706	1.749419	-1.165824
C	-2.213768	1.974685	0.326484
C	1.770941	-1.441134	3.604067
C	2.740324	-2.241415	2.874925
C	1.296702	-0.652218	-3.752551

C	2.317266	-1.549558	-3.287150
C	-0.050529	0.727134	3.673629
C	-0.956444	1.532134	2.904977
C	4.082596	-2.618792	0.352343
C	3.900281	-2.388499	-1.074811
C	-0.492492	1.481859	-3.033695
C	-1.162162	2.294294	-1.997864
C	2.240238	-0.090758	3.658950
C	3.803843	-1.327719	2.450300
C	3.436242	-0.766366	-2.875747
C	-1.191991	2.889933	0.858986
C	1.782768	0.674150	-3.658786
C	1.331541	1.012150	3.666274
C	4.457334	-1.472205	1.171189
C	-0.559477	2.657703	2.155158
C	4.208084	-1.140634	-1.738879
C	0.916843	1.757679	-3.354499
C	3.479221	-0.007933	2.953186
C	3.135218	0.614215	-3.153500
C	-0.479483	3.431657	-1.488591
C	-0.468798	3.731820	-0.060701
C	1.731797	2.233103	3.063905
C	4.796033	-0.242361	0.493556
C	4.734566	-0.093880	-0.938851
C	0.791529	3.096028	2.394557
C	1.554473	2.920724	-2.815532
C	3.837320	1.200601	2.273890
C	0.798499	3.830345	-2.019187
C	3.668493	1.657228	-2.362073
C	4.547216	1.061561	1.055344
C	2.999145	2.351894	2.411567
C	4.486503	1.285689	-1.249421
C	0.849149	4.291421	0.248389
C	1.514087	3.851010	1.420375
C	2.905531	2.876966	-2.269292
C	1.625943	4.347658	-0.970561
C	4.392851	2.014880	-0.013594
C	2.885652	3.352795	1.375516
C	2.940970	3.726243	-1.078013
C	3.583606	3.200831	0.116505
Y	-1.333415	-0.590060	-0.346465
Y	1.338439	1.914919	-0.405897
Y	1.968078	-1.384066	0.585038
N	0.665107	-0.039302	-0.253218
C	-4.786230	0.159561	0.043306
C	-5.226278	1.633658	0.066642
O	-5.204026	2.374801	-0.890477
O	-5.597834	1.939940	1.321523
C	-5.995164	-0.785688	0.200417
O	-6.005331	-1.774396	0.897958
O	-6.991607	-0.331578	-0.575270
C	-8.197399	-1.176252	-0.592094
H	-8.412697	-1.485472	0.440296
H	-8.976092	-0.496343	-0.959079
C	-5.829087	3.371415	1.566238
H	-6.426222	3.774973	0.736701
H	-6.408653	3.380979	2.497286
C	-4.497822	4.079254	1.706809
H	-3.957837	4.066585	0.748775
H	-4.665508	5.128117	1.999934
H	-3.884349	3.588475	2.478992
H	-8.918609	-2.945570	-1.568485
C	-7.986688	-2.361300	-1.506768
H	-7.714516	-2.020167	-2.516992
H	-7.191710	-3.009579	-1.110665

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C	2.762819	0.659964	2.987144
C	2.718438	1.990644	2.475967
C	3.505451	2.373168	1.339523
C	4.348163	1.422724	0.663701
C	4.403362	0.100338	1.200571
C	3.664526	-0.257818	2.373739
C	3.358643	-1.656130	2.307735
C	2.109488	-2.171058	2.811466
C	1.229870	-1.253264	3.442308

C	1.580687	0.131349	3.581007	C	3.346200	2.165752	-2.671311
C	0.374870	0.895502	3.615956	C	3.678265	0.770094	-2.771744
C	0.308039	2.181036	2.990395	C	2.732441	-0.130881	-3.303258
C	1.489750	2.719812	2.430173	C	2.684665	-1.483940	-2.844246
C	1.450043	3.490886	1.215069	C	1.314648	-1.919647	-2.961009
C	2.734350	3.346952	0.594202	C	0.780097	-2.933057	-2.115059
C	4.489831	-1.061687	0.348607	C	1.691523	-3.633756	-1.255879
C	3.915381	-2.155717	1.072256	C	1.209797	-4.174332	-0.000176
C	-0.204872	-1.345279	3.295818	C	-0.084431	-3.787481	0.511446
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C	-0.962324	3.176702	1.060140	C	-2.223033	1.016564	-1.623132
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C	-0.351199	1.831470	-2.732156	O	-5.396852	-1.600919	-1.190548
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C      -3.440969    0.181790   -0.928146
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C	5.079600000	4.813100000	-0.187800000
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C	4.171244	-0.982427	-1.484913
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C	-7.948472	0.981187	2.907128
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O	-5.307510	-0.332551	-2.090169
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C	4.112354	0.942811	1.711594
C	3.889379	-0.413205	2.093946
C	2.810710	-0.769223	2.963886
C	2.412332	-2.113841	2.664381
C	1.033957	-2.525492	2.756821
C	0.091927	-1.558123	3.215335
C	-1.242208	-1.478931	2.671271
C	-1.664372	-0.115806	2.770341
C	1.400412	3.306187	1.645193
C	2.791480	3.054857	1.407667
C	4.109965	-1.505214	1.175067
C	3.254362	-2.577924	1.583837
C	2.770097	-3.517662	0.642109
C	1.471736	-4.107147	0.861329
C	0.565006	-3.533321	1.837814
C	-0.708207	-3.312290	1.162934
C	-1.615993	-2.262040	1.539652
C	-2.445823	-1.646470	0.528835

C	-3.185277	-0.468131	0.900498
C	-2.646787	0.415362	1.896744
C	-2.550206	1.828377	1.535439
C	-1.334205	2.541490	1.921507
C	-0.866230	3.306845	0.785031
C	0.520915	3.645541	0.574289
C	1.034334	3.651993	-0.787793
C	2.458166	3.458225	-0.987936
C	3.360901	3.265092	0.129970
C	4.441925	2.404120	-0.290176
C	4.730459	1.179187	0.432302
C	4.755258	0.089137	-0.543216
C	4.392092	-1.271532	-0.207296
C	3.702237	-2.073282	-1.209545
C	2.904888	-3.198235	-0.763788
C	1.646238	-3.563008	-1.413270
C	0.794836	-4.158352	-0.408385
C	-0.550237	-3.673566	-0.222769
C	-1.134684	-2.838493	-1.209887
C	-2.106557	-1.836573	-0.868329
C	-1.990360	-0.775717	-1.884263
C	-2.391603	0.618667	-1.755534
C	-3.273141	1.076380	-0.714489
C	-2.816292	2.160392	0.134623
C	-1.745091	3.013493	-0.307793
C	-1.169228	2.806401	-1.580843
C	0.192924	3.165679	-1.838016
C	0.690613	2.238884	-2.826470
C	2.071879	1.918382	-2.927122
C	2.980371	2.673624	-2.105617
C	4.216238	2.067714	-1.669445
C	4.418087	0.652190	-1.828111
C	3.568856	-0.075554	-2.690815
C	3.253166	-1.441092	-2.412145
C	1.929978	-1.681760	-2.937413
C	1.074686	-2.674214	-2.388261
C	-0.337136	-2.380264	-2.317061
C	-0.855462	-1.110600	-2.715676
C	-1.466207	1.586342	-2.287365
C	-0.306826	1.239601	-3.042557
C	2.413298	0.564214	-3.270145
C	1.400501	-0.443289	-3.413475
C	0.021886	-0.122334	-3.261453
N	0.888960	0.049507	0.070226
Sc	1.059821	-1.913406	0.197996
Sc	2.498826	1.108422	-0.344996
Sc	-0.928784	0.808712	0.166352
C	-5.267441	-4.385451	-0.521143
H	-5.615377	-5.249401	-1.107584
H	-4.174779	-4.453873	-0.405856
H	-5.733833	-4.418793	0.474521
C	-7.510190	3.465790	-0.434710
H	-8.358004	4.029017	-0.016865
H	-6.702903	4.171306	-0.680615
H	-7.836885	2.963245	-1.356989
C	-4.198955	0.116007	-0.039777
C	-4.879248	-0.864347	-1.023894
C	-5.348988	0.808885	0.738490
O	-5.134745	-0.580743	-2.172682
O	-5.145016	-2.012783	-0.390222
O	-5.910947	1.738492	-0.042891
O	-5.676217	0.503406	1.863304
C	-7.034585	2.454269	0.577123
C	-5.629752	-3.108351	-1.239018
H	-5.141099	-3.021817	-2.220154
H	-6.714566	-2.975031	-1.362988
H	-6.663717	2.916527	1.503551
H	-7.802722	1.710383	0.834704

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C	2.381122	0.266384	3.167209
C	2.073939	-1.122976	3.208642
C	0.724441	-1.573951	3.368058
C	-0.356760	-0.633078	3.423995
C	-0.042286	0.750601	3.416820
C	1.314242	1.194015	3.346702
C	1.331914	2.473693	2.700686
C	2.414963	2.859243	1.832840

C	3.487570	1.930243	1.680414	C	-1.903098	-2.863671	0.032359
C	3.494177	0.679228	2.378805	C	-2.621105	-2.232947	1.124860
C	4.236588	-0.269453	1.602903	C	-3.177756	-0.860899	1.111071
C	3.856850	-1.660755	1.561897	C	-3.068907	-0.147171	-0.463583
C	2.765817	-2.063420	2.378293	C	-2.546074	1.222562	-0.512283
C	1.814183	-3.061586	1.941742	C	-1.879623	1.348127	-1.772304
C	0.594418	-2.796705	2.622590	C	-0.949168	2.394086	-2.028196
C	-0.882671	1.707605	2.742181	C	-0.807651	3.395381	-1.009488
C	-0.037129	2.807000	2.379055	C	0.452645	4.095895	-0.872407
C	4.152894	1.742902	0.413307	C	1.620316	3.605331	-1.559973
C	4.679300	0.411317	0.409900	C	1.465757	2.677411	-2.614452
C	4.837020	-0.300711	-0.800976	C	2.464836	1.688706	-2.867395
C	4.690965	-1.735672	-0.791588	C	1.790552	0.536736	-3.419366
C	4.080275	-2.400691	0.345386	C	2.311953	-0.781049	-3.280316
C	3.009908	-3.254067	-0.169700	C	1.373509	-1.857371	-3.092841
C	1.812461	-3.548770	0.594888	C	-0.030422	-1.599553	-2.961343
C	0.546927	-3.669249	-0.118369	C	-2.349173	-0.929223	-1.486478
C	-0.680789	-3.453500	0.610615	C	-1.697977	0.038817	-2.323184
C	-0.632423	-3.088767	1.995031	C	0.167551	2.101828	-2.877558
C	-1.789410	-2.302742	2.286047	C	0.382108	0.774641	-3.369191
C	-1.630250	-0.999807	2.877530	C	-0.531097	-0.277238	-3.069581
C	-2.436653	-0.058345	2.119230	N	0.879400	-0.017643	0.034044
C	-2.005857	1.307425	1.933408	Sc	2.518294	-0.904454	-0.598340
C	-2.167240	1.977724	0.630596	Sc	0.790853	1.948609	0.032094
C	-1.320931	3.132517	0.330311	Sc	-0.741484	-0.948416	0.634198
C	-0.332004	3.624266	1.263756	C	-4.339550	-0.427675	0.290648
C	0.766052	4.210647	0.525665	C	-7.419225	-2.359769	-0.456649
C	2.127090	3.736095	0.725202	C	-7.696370	-2.123670	-1.924056
C	2.669782	3.392210	-0.591861	H	-6.975943	-3.348800	-0.275420
C	3.658991	2.346811	-0.786352	H	-8.310102	-2.219611	0.167615
C	3.594728	1.542632	-1.998615	H	-8.453663	-2.843606	-2.272455
C	4.201140	0.225759	-1.988858	H	-8.078737	-1.103819	-2.081781
C	3.625962	-0.908252	-2.709715	H	-6.778464	-2.266993	-2.512214
C	3.973511	-2.110300	-1.978194	C	-5.198454	-1.554656	-0.255793
C	2.948434	-3.051504	-1.601366	O	-4.740662	-2.501995	-0.858317
C	1.678496	-2.959853	-2.214493	O	-6.486714	-1.340020	0.052707
C	0.491688	-3.328173	-1.504241	C	-6.138090	2.798121	0.067630
C	-0.589712	-2.532674	-2.026852	C	-6.392791	3.513570	-1.235420
C	-1.770722	-2.224594	-1.265623	H	-5.439970	3.343230	0.720448

H	-7.058342	2.586754	0.631974
H	-6.847683	4.494407	-1.031212
H	-5.447074	3.667570	-1.775997
H	-7.076076	2.932272	-1.871941
O	-5.515436	1.513500	-0.273483
C	-5.078936	0.814155	0.784276
O	-5.201190	1.108536	1.952920

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C	1.608970	-1.548654	-3.045115
C	0.888343	-0.433795	-3.547293
C	-0.535448	-0.339939	-3.393744
C	-1.288388	-1.330105	-2.673928
C	-0.555326	-2.466518	-2.220441
C	0.856020	-2.593669	-2.442787
C	1.418916	-3.379867	-1.381028
C	2.733443	-3.104193	-0.857447
C	3.478388	-2.062712	-1.482974
C	2.947494	-1.337641	-2.597933
C	3.524447	-0.026626	-2.599684
C	2.762271	1.121585	-3.020250
C	1.442075	0.888175	-3.498032
C	0.369313	1.811333	-3.228575
C	-0.836576	1.054725	-3.251760
C	-0.862680	-3.111069	-0.974842
C	0.335182	-3.742712	-0.500762
C	4.321471	-1.170120	-0.721970
C	4.406553	0.051621	-1.458436
C	4.602225	1.280548	-0.790657
C	4.036402	2.478818	-1.354564
C	3.022886	2.390478	-2.386007
C	1.896364	3.216011	-1.955960
C	0.532513	2.902274	-2.319539
C	-0.513567	3.163913	-1.345967
C	-1.752018	2.453114	-1.465198
C	-1.920256	1.438586	-2.460545
C	-2.878837	0.475188	-1.987528
C	-2.483618	-0.934177	-1.930466
C	-2.704891	-1.537515	-0.603819
C	-1.805321	-2.549789	-0.070974
C	-1.482214	-2.538200	1.346619
C	-0.300040	-3.232673	1.804390
C	0.561132	-3.941482	0.881389
C	1.917968	-3.883409	1.375549
C	2.979470	-3.347899	0.542356
C	3.667195	-2.315594	1.319289
C	4.308612	-1.170244	0.708567
C	4.271667	0.103648	1.413856
C	4.435005	1.318503	0.644175
C	3.720836	2.551959	0.965626
C	3.525672	3.275650	-0.273892
C	2.212690	3.738142	-0.643638
C	1.195139	3.758773	0.341236
C	-0.171011	3.541920	-0.014728
C	-0.832553	2.936631	1.123085
C	-2.018120	2.128620	0.989855
C	-2.622915	2.117537	-0.334828
C	-3.489910	1.064544	-0.819187
C	-3.394469	-0.675722	0.343861
C	-2.637640	-0.346240	1.507258
C	-1.814629	-1.358745	2.082013
C	-0.906497	-0.725159	2.986626
C	0.326035	-1.348317	3.339010
C	0.546397	-2.689330	2.862970
C	1.896680	-3.140511	2.606236
C	2.974359	-2.189619	2.579133
C	2.777770	-0.903439	3.128786
C	3.458737	0.226645	2.586474
C	2.602829	1.372587	2.789761
C	2.664869	2.513260	1.942288
C	1.427431	3.187278	1.644537
C	0.170604	2.678953	2.113005
C	-2.103474	0.967162	1.879631
C	-1.030309	0.687606	2.822950
C	1.456657	-0.493873	3.543377
C	1.354405	0.917363	3.321217
C	0.118623	1.519087	2.932524
N	0.798276	0.003575	-0.043284

Sc	2.199609	1.342366	-0.419197
Sc	1.322624	-1.695789	0.816935
Sc	-1.135889	0.289193	-0.372778
C	-4.487588	0.239324	-0.095700
C	-6.635266	-2.293022	-1.803016
C	-6.518655	-3.779445	-1.577759
H	-7.619226	-1.890208	-1.522382
H	-6.410295	-1.997394	-2.837937
H	-7.248148	-4.303643	-2.213104
H	-5.508111	-4.127959	-1.837567
H	-6.722103	-4.026154	-0.525415
C	-5.546805	-0.335426	-1.057864
O	-6.196762	0.377977	-1.790942
O	-5.634894	-1.661157	-0.931018
C	-5.365872	2.671601	2.599090
C	-4.483139	3.868939	2.856170
H	-5.282540	1.902673	3.380526
H	-6.424582	2.936232	2.464135
H	-4.810171	4.375912	3.776772
H	-3.436204	3.553280	2.981156
H	-4.542464	4.580208	2.018903
O	-4.894912	2.085582	1.337174
C	-5.243315	0.817305	1.114914
O	-6.012275	0.140518	1.762839