Electronic Supplementary Information for

Thermodynamically driven Self-assembly of Pyridinearene to Hexameric Capsules

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A. Lützen	Project administration, funding acquisition
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1 Synthesis

Compound **1** was synthesized according to the reported procedure.[1] The ruthenium guest **G** was synthetized according to previously reported method.[2] In short, a solution of excess NH_4PF_6 (3.3 g, 20 mmols) in H_2O (30 ml) was added to a stirred solution of tris-2,2'-bipyridine ruthenium (II) chloride hexahydrate [$(bpy)_3RuCl_2 \cdot 6\ H_2O$] (1 g, 1.3 mmols) in water (30 ml). The formed precipitate was separated with the help of celite, and dried in vacuum to give tris-2,2'-bipyridine ruthenium (II) hexafluorophosphate hydrate [$(bpy)_3Ru(PF_6)_2 \cdot 3H_2O$] (0.9 g, 74 %).

2 Mass spectrometry

2.1 ESI-Q-TOF Mass spectrometry

Mass spectrometric experiments were performed with ABSciex QSTAR Elite ESI-Q-TOF mass spectrometer, equipped with an API 200 TurboIonSpray ESI Source from AB Sciex. Nitrogen was used as drying and nebulization gas. The parameters were optimized to get the maximum abundance of ions under study. The measurements and data handling was done with Analyst® QS 2.0 software.

Stock solution of host **1** was prepared with 5 mM concentration in $CHCl_3$. From $Ru^{II}(bpy)_3 \bullet 2PF_6 \bullet 3H_2O$ 1 mM stock was prepared in MeCN. Samples for host measurements were prepared with 20 µM host concentration in acetone. Samples to measure host and guest were prepared with 60 µM host concentration and 6:1 host:guest ratio in 1:1 mixture of acetone and DCM.

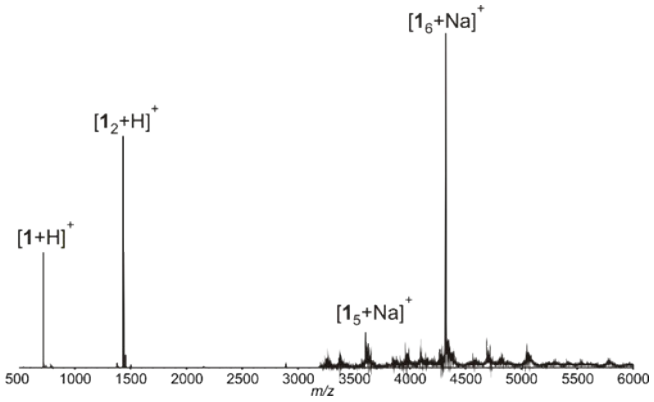


Figure S1. (+)ESI MS spectrum of **1** (20 µM in acetone).

2.2 Ion mobility mass spectrometry

Ion mobility mass spectrometry experiments were performed with Waters Synapt G2 and Agilent 6560 Ion mobility Q-TOF mass spectrometers. All CCS values were obtained using nitrogen or helium as drift gas and using stepped field- methods. Samples were prepared with 20 or 60 µM concentration and 6:1 host:guest ratio in 1:1 mixture of acetone and DCM.

Modified Waters Synapt G2 was equipped with a linear drift cell, which was filled with ~2 Torr nitrogen or helium (298K). Samples were ionized with a nanoESI ion source. In-house pulled capillary tips were used with inserted platinum wire for nanoESI. For experiments in N_2, parameters were optimized as follows: Capillary voltage 1 kV, Cone 60 V and source temperature 30 ºC. For stepped field experiment, drift voltage was varied from 225 to 300 V with 15V increments. For experiments in helium, following parameters were used: Capillary voltage 1.66 kV, Cone 180 V and source temperature 30 ºC. In stepped field experiment drift voltage was varied from 140 to 240 V with 20 V increments. Data was analyzed using MassLynx v4.1 (Waters Corporation, USA) and Microsoft Excel 2016 (Microsoft, USA).

Agilent 6560 IM Q-TOF was equipped with ESI ion source and samples were injected from syringe pump with 5 µl/min flowrate. The drift tube entrance and exit voltages were set as 1674V and 224V, respectively. As a trap filling time 20 000 µs and trap release time 150 µs were used. Gas temperature of 275 ºC, drying gas flow 5 l/min, nebulizer pressure 10 psi and capillary voltage of 5000V were set as source parameters. Before introduction of samples, ES tuning mix (Agilent technologies) was measured as a reference for CCS values and to ensure stabile conditions for CCS determination.[3,4] For stepped-field measurements, the drift tube entrance voltage was varied from 1074 V to 1674 V with 100 V increments. Data was analyzed using MassHunter IM-MS Browser (Version B08.00, Agilent Technologies, USA).

Theoretical $^{DTM}CCS_{N2}$ values were calculated with IMoS.[5] Theoretical $^{DTM}CCS_{N2}$ values were obtained using the trajectory method with diffuse scattering in nitrogen gas. Coordinates for calculations were obtained from DFT-calculated structures optimized at the RI-PBE-D3/def2-SVP level of theory (for DFT calculations see section 4). The number of rotations was 3 with 300000 gas molecules per rotations. Calculations were carried out using experimental parameters (gas, temperature and pressure).

3 NMR

Samples for ^{1}H NMR were prepared with 20 mM concentration in $CDCl_3$. Spectra were measured in 298K and calibrated using chloroform solvent signal at 7.26 ppm. Diffusion-ordered NMR spectroscopy (DOSY) measurements were performed on a Bruker Avance 400 MHz spectrometer equipped with a Great 1/10 pulsed gradient unit and a direct probe at 298 K. A LED29 pulse sequence (ledbpgp2s) was used for the diffusion experiments with a sine-shape pulsed gradient duration δ (P30) of 1.0−1.2 ms incremented from 0.68 to 32.4 G cm^{-1} in 16 steps. The pulsed gradient separation Δ (D20) was 100 ms, the spoil gradient (P19) was set to 600−800 µs, and the eddy current delay (D21) was 5 ms. The reported diffusion coefficients were obtained using the T1/T2 relaxation module in TopSpin 3.2 software. The signals at 7.10 and 4.28 ppm (d and d`) gave a diffusion coefficient of $0.411\times10^{-5}$ cm$^2$s$^{-1}$. The signals at 7.22 and 4.36 ppm (h and h`) gave a diffusion coefficient of 0.287×10^{-5} cm^{2}s^{-1}.

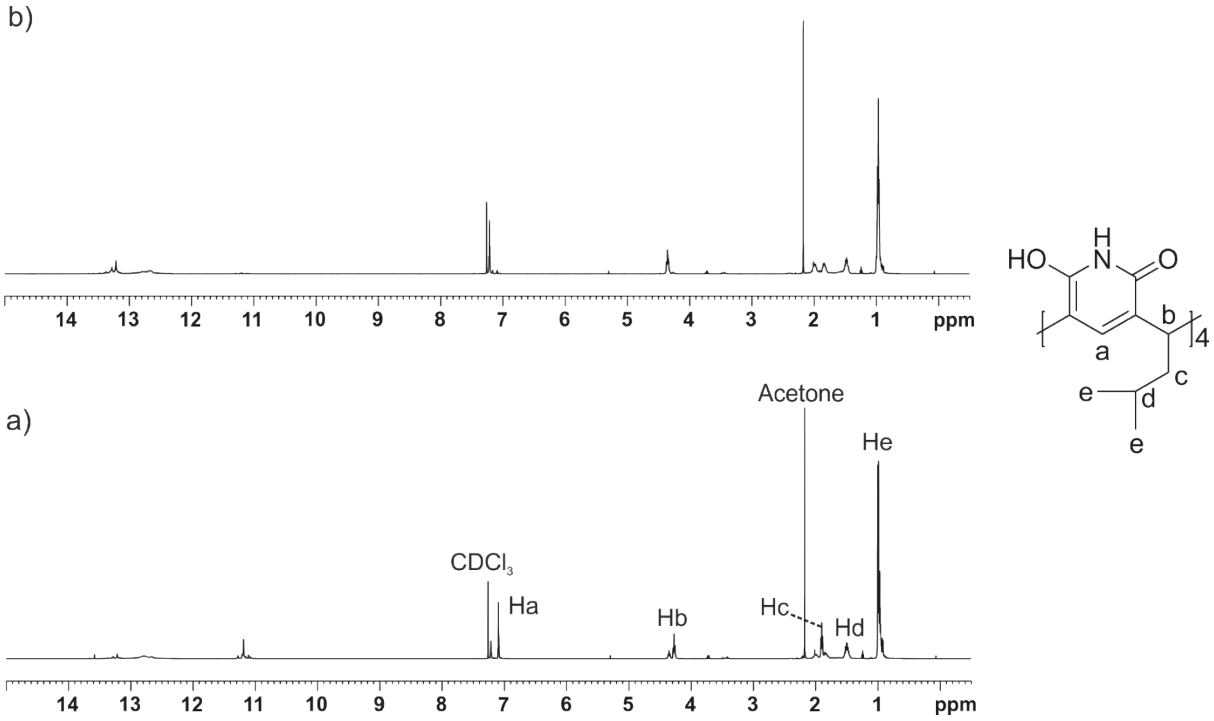
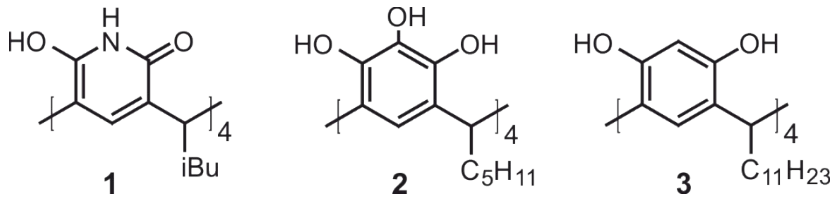


Figure S2. ^{1}H NMR spectrum of 20 mM **1** in $CDCl_3$ measured after a) 2 hours from sample preparation and b) measured after 7 days from sample preparation.

To confirm that these species correspond to dimer and hexamer, the following control experiments were performed (in $CDCl_3$, 298K) with compounds **2** and **3** (in Scheme S1), which are known to form hexameric hydrogen bonded capsules in chloroform solution: a) **1**+**2** (1:1 ratio, both 20 mM) and b) **1**+**3** (1:1 ratio, both 20 mM). ^{1}H and DOSY NMR were measured with the same parameters as mentioned above. Observed diffusion coefficients (in Table S1) for **2** and **3** are well in line with signal set h/h` and thus confirm it as hexamer. Calculated diameters also support d and d` to correspond a dimeric capsule[1] and h and h` to hexameric capsule.



Scheme S1. Structures of compounds used in the NMR control experiments.

Table S1. Diffusion coefficients (*D*) of compounds 1, 2 and 3 (in CDCl3 at 298K) and their thermodynamic radii (r) and diameters (d)

Compound	*D* (×10^{-5}cm^{2}s^{-1})	*r* (*d*) in nm
1 (species d and d`)	0.411±0.01	0.978 (1.956)
1 (species h and h`)	0.287±0.03	1.401 (2.802)
2	0.271±0.02	1.481 (2.962)
3	0.202±0.03	1.986 (3.972)

With the diffusion coefficient known, and assuming a spherical molecule, the hydrodynamic radius *r* for the molecular species was calculated using the Stokes−Einstein equation $r = k_bT/6\pi\eta D$

where k_b is the Boltzmann constant, *T* is the temperature, η is the viscosity of the medium, and *D* is the diffusion coefficient of the particle in the given medium.

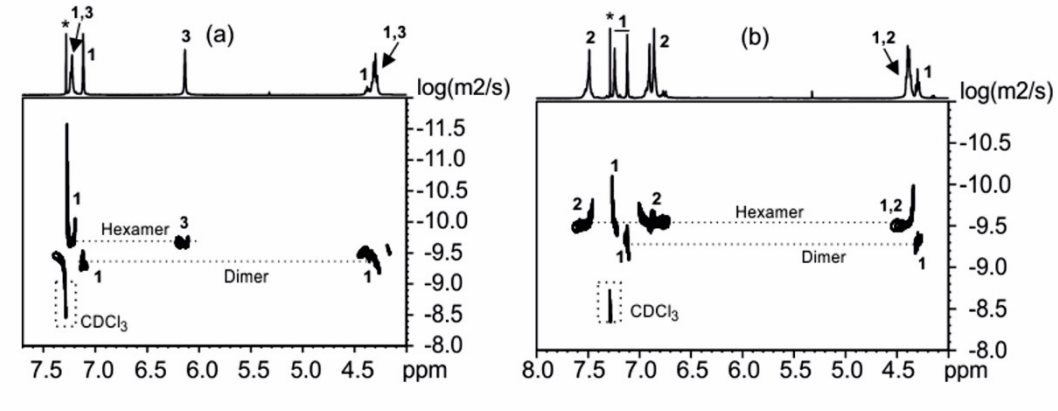


Figure S3. 2D DOSY NMR spectra (20 mM, $CDCl_3$, 298 K) measured within a few hours of sample preparation observed from a) **1**+**3** (1:1) and b) **1**+**2** (1:1)

4 X-Ray crystallography

The experimental and refinement details for $\mathbf{1}_6$·are shown below. Single-crystal X-ray data for $\mathbf{1}_6$·was measured using a Rigaku SuperNova dual-source Oxford diffractometer equipped with an Atlas detector using mirror-monochromated Cu-*K*α (λ = 1.54184 Å) radiation. The data collection and reduction for $\mathbf{1}_6$ were performed using the program *CrysAlisPro* [6] and Gaussian face index absorption correction method was applied.[6] The structure was solved with direct methods (*SHELXS*)[7] and refined by full-matrix least squares on F^2 using the *OLEX2* software,[8] which utilizes the *SHELXL*-2015 module.[7]

X-Ray Experimental details

Crystal data for $\mathbf{1}_6$: CCDC-1899745, $C_{122}H_{158}Cl_6N_{12}O_{24}$, M = 2389.29, colourless block, 0.21 x 0.14 x 0.09 mm^3, monoclinic, space group I2, a = 23.7456(11) Å, b = 29.0274(9) Å, c = 27.4514(14) Å, α = 90°, β = 101.549(4)°, γ = 90°, V = 18538.4(14) $Å^3$, Z = 4, Dc = 0.856 g/cm^3, F000 = 5072, μ= 1.249 mm^{-1} , T = 120.0(1) K, θ_{max} = 66.49°, 52848 total reflections, 19960 with Io > 2σ(Io), R_{int} = 0.0721, 30370 data, 835 parameters, 323 restraints, GooF = 1.789, R = 0.2056 and wR= 0.4494 [Io > 2σ(Io)], R = 0.2432 and wR= 0.5139 (all reflections), 2.382 <dΔρ < -0.891 e/$Å^3$.

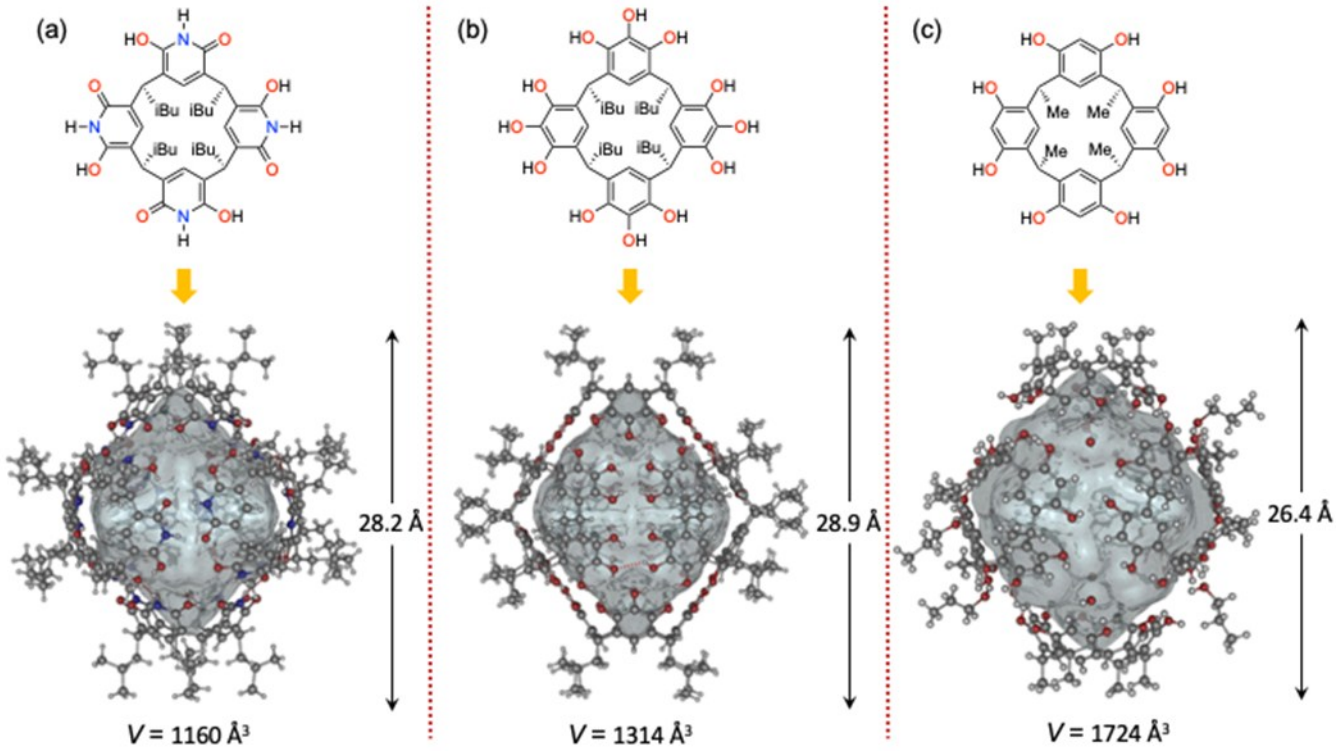


Figure S4. Comparison of cavity volumes in hexameric capsules of (a) $\mathbf{1}_6$ (b) $(pyrogallerene)_6$ (CCDC Code: CANQAJ) [9] and (c) $(C\text{-}methylresorcinarene)_6$ (CCDC Code: JEZPEM). [10]

5 DFT calculations

The geometries of **1**, $\mathbf{G}^{2+}$, $\mathbf{1}_2$, $\mathbf{1}_6$ and $[\mathbf{1}_6+\mathbf{G}]^{2+}$ were optimized at the RI-PBE-D3/def2-SVP[11-19] level of theory without symmetry constraints. The starting geometries of $\mathbf{1}_2$, $\mathbf{1}_6$ and $[\mathbf{1}_6+\mathbf{G}]^{2+}$ were constructed from the minimum structures of **1** and $\mathbf{G}^{2+}$ as well as using the crystal structure of $\mathbf{1}_6$ as a guideline. The minimum energy structure of **1** was obtained utilizing a previously attained conformational sampling procedure.[20] To evaluate the interaction energies of studied systems additional single-point energy calculations were carried out for the optimized structures at the higher level of theory, namely RI-PBE-D3/def2-TZVP level.[11-19] Frequency analysis were carried out for **1**, $\mathbf{G}^{2+}$ and $\mathbf{1}_2$ at the RI-PBE-D3/def2-SVP level to ensure that they correspond to the real minima on the potential energy hypersurface. Due to the size of systems $\mathbf{1}_6$ and $[\mathbf{1}_6+\mathbf{G}]^{2+}$ no frequency analyses were carried out for them. The resolution of identity (RI) approximation with the auxiliary SVP/J or TZVP/J Coulomb fitting basis set was used to speed up calculations.[11-13] The core electrons of Ru were treated using effective core potentials basis set.[18] Dispersion interaction was taken into account in calculations using the DFT-D3 method in combination with the damping function.[16-17] All calculations were carried out Turbomole 7.3 program package.[21]

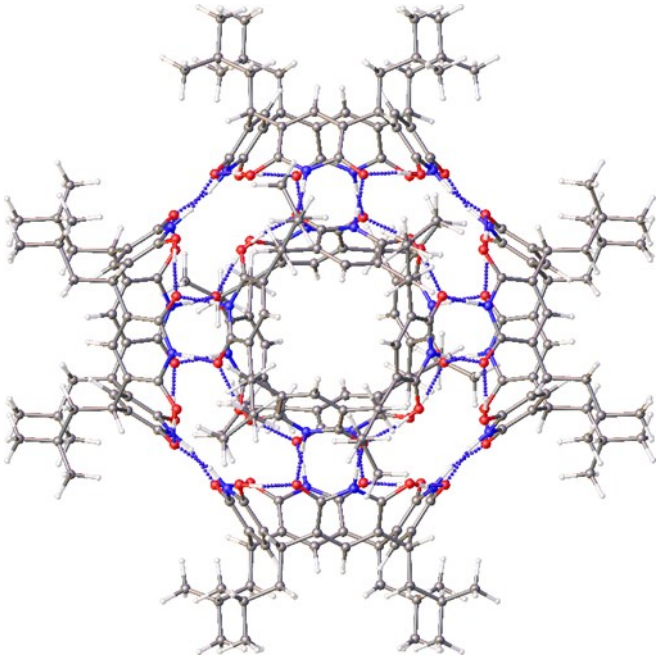


Figure S5. Optimized structure of $\mathbf{1}_6$ at the RI-PBE-D3/def2-SVP level. The hydrogen bonds are highlighted with dashed blue line. Color code: H = white; C = grey; N = blue; O = red.

References

[1] A. Kiesilä, L. Kivijärvi, N. K. Beyeh, J. O. Moilanen, M. Groessl, T. Rothe, S. Götz, F. Topić, K. Rissanen, A. Lützen and E. Kalenius, *Angew. Chem. Int. Ed*., 2017, **56**, 10942.

[2] N. K. Beyeh, M. Kogej, A. Åhman, K. Rissanen and C. A. Schalley, *Angew. Chem. Int. Ed*., 2006, **45**, 5214.

[3] S. M. Stow, T. J. Causon, X. Zheng, R. T. Kurulugama, T. Mairinger, J. C. May, E. E. Rennie, E. S. Baker, R. D. Smith, J. A. McLean, S. Hann, J. C. Fjeldsted, *Anal. Chem*. 2017, **89**, 9048-9055

[4] V. Gabelica *et al*. *Mass Spectrom. Rev*., 2019, DOI: org/10.1002/mas.21585.

[5] C. Larriba, C. J. Hogan Jr., *J. Comput. Phys*. 2013, **251**, 344; C. Larriba and C. J. Hogan Jr., *J. Phys. Chem. A*, 2013, **117,** 1887.

[6] Rigaku Oxford Diffraction, 2017, CrysAlisPro Software system, version 38.46, Rigaku Corporation, Oxford, UK

[7] G. M. Sheldrick, *Acta Crystallogr. Sect. C*, 2015, **71**, 3.

[8] O. V Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339.

[9] T. Gerkensmeier, W. Iwanek, C. Agena, R. Fröhlich, S. Kotila, C. Näther and J. Mattay, *Eur. J. Org. Chem*, 1999, **9**, 2257.

[10] R. M. Payne and C. L. Oliver, *CrystEngComm*, 2018, ***20***, 1919.

[11] K. Eichkorn, O. Treutler, H. Öhm, M. Häser and R. Ahlrichs, *Chem. Phys. Lett.* 1995, **242**, 652.

[12] K. Eichkorn, F. Weigend, O. Treutler and R. Ahlrichs, *Theor. Chem. Accounts Theory, Comput. Model. (Theoretica Chim. Acta)* 1997, **97**, 119.

[13] K. Eichkorn, O. Treutler, H. Öhm and M. Häser, R. Ahlrichs, *Chem. Phys. Lett.* 1995, **240**, 283.

[14] J. P. Perdew and Y. Wang, *Phys. Rev. B,* 1992, **45**, 13244.

[15] J. J. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.* 1996, **77**, 3865.

[16] S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104.

[17] S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.,* 2011, **32**, 1456.

[18] D. Andrae, U. Haeussermann, M. Dolg, H. Stoll and H. Preuss, *Theor. Chim. Acta,* 1990, **77**, 123.

[19] F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.,* 2005, **7**, 3297.

[20] A. Kiesilä, J. O. Moilanen, A. Kruve, C. A. Schalley, P. Barran and E. Kalenius. *unpublished results*

[21] TURBOMOLE V7.3 2018, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com.

XYZ Coordinates

1 monomer

E (RI-PBE-D3/def2-SVP) = -2372.157906517 au

Number of negative frequencies = 0

N	0.02277	-3.98548	-2.91300
C	1.24461	-3.64210	-2.38344
C	1.26725	-2.99044	-1.13567
C	0.01982	-2.69562	-0.54316
C	-1.21108	-3.00649	-1.11659
C	-1.22467	-3.66534	-2.39079
C	-2.55906	-2.59328	-0.54770
C	-2.61256	-2.58730	0.98935
C	-3.98383	-2.23196	1.59402
C	-3.89559	-2.19884	3.12449
C	2.60076	-2.54915	-0.54663
C	2.63318	-2.56374	0.99098
C	3.99648	-2.21288	1.61643
C	3.88620	-2.18732	3.14564
O	2.27870	-3.97371	-3.12541
O	-2.25254	-3.96432	-3.07468
C	-2.98745	-1.26719	-1.16541
C	-3.71182	-1.24495	-2.37072
N	-4.07806	-0.02267	-2.88532
C	-3.73879	1.22492	-2.37354
C	-3.00488	1.20935	-1.14243
C	-2.64517	-0.02079	-0.60030
O	-4.08505	-2.28677	-3.08155
O	-4.07955	2.25871	-3.02823
C	-2.60081	2.54943	-0.54518
C	-2.63319	2.56365	0.99244
C	-3.99640	2.21249	1.61791
C	-3.88599	2.18667	3.14711
C	-1.26736	2.99092	-1.13424
C	-1.24479	3.64239	-2.38212
N	-0.02299	3.98544	-2.91196
C	1.22450	3.66560	-2.38968
C	1.21099	3.00680	-1.11546
C	-0.01987	2.69601	-0.54189
O	-2.27892	3.97423	-3.12396
O	2.25235	3.96503	-3.07340
C	2.55901	2.59347	-0.54677
C	2.61264	2.58678	0.99027
C	3.98408	2.23145	1.59454
C	3.89604	2.19712	3.12499
C	2.98746	1.26769	-1.16510
C	3.71217	1.24602	-2.37022
N	4.07839	0.02397	-2.88540
C	3.73853	-1.22386	-2.37458
C	3.00471	-1.20886	-1.14341
C	2.64485	0.02102	-0.60080
O	4.08553	2.28820	-3.08047
O	4.07862	-2.25730	-3.03019
C	-5.09496	-3.17496	1.11732
C	-5.11376	3.15448	1.15367
C	5.09483	3.17520	1.11844
C	5.11365	-3.15496	1.15191
H	-3.28125	-3.35678	-0.90529

H	-3.35446	3.28217	-0.90219
H	3.28113	3.35716	-0.90408
H	3.35440	-3.28177	-0.90392
H	0.02387	-2.17795	0.42820
H	2.06263	0.02523	0.33420
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H	-2.06352	-0.02546	0.33505
H	-2.30155	-3.59325	1.34766
H	-1.85707	-1.88232	1.40087
H	-4.24608	-1.20531	1.25146
H	-4.85919	-4.23026	1.37357
H	-5.24823	-3.11961	0.02078
H	-6.06204	-2.92274	1.59763
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H	-3.61822	3.18851	3.54581
H	-3.10673	1.47267	3.48668
H	-4.84457	1.88542	3.61625
H	2.30143	3.59248	1.34910
H	1.85737	1.88141	1.40151
H	4.24664	1.20515	1.25116
H	4.85885	4.23019	1.37578
H	5.24781	3.12095	0.02181
H	6.06211	2.92277	1.59823
H	4.86100	1.89215	3.57841
H	3.12103	1.48192	3.47173
H	3.63509	3.19691	3.53319
H	1.87311	-1.86282	1.40084
H	2.31917	-3.57390	1.33489
H	4.26359	-1.18492	1.28206
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H	3.10710	-1.47323	3.48540
H	4.84488	-1.88632	3.61475
H	3.61828	-3.18918	3.54419
H	3.36358	3.07579	-3.00319
H	3.10464	-3.30672	-3.00241
H	-4.57277	-0.02535	-3.78352
H	-0.02614	4.43265	-3.83474
H	4.57344	0.02710	-3.78341
H	0.02585	-4.43319	-3.83554
H	-3.36337	-3.07461	-3.00423
H	-3.10516	3.30770	-3.00065

G^{2+} guest

E (RI-PBE-D3/def2-SVP) = -1578.047537058 au

Number of negative frequencies = 0

Ru	0.00000	0.00008	-0.00000
N	0.79117	1.58635	-1.04382
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C	0.95358	3.99530	-1.19474

C	1.81132	3.88584	-2.29440
C	2.15280	2.60558	-2.75762
C	1.62556	1.48681	-2.10769
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N	0.97807	-1.47837	-1.04370
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C	2.22786	-1.80977	-0.57897
C	0.47460	-2.15126	-2.10748
C	-1.62556	1.48681	2.10769
C	2.68104	-1.02482	0.57937
C	2.10049	0.66491	2.10730
C	-2.22786	-1.80977	0.57897
C	-0.47460	-2.15126	2.10748
C	-0.95358	3.99530	1.19474
C	-3.93665	-1.17182	-1.19486
C	-3.33296	0.56209	-2.75730
H	-1.33832	1.38302	-2.44047
C	2.98278	-2.82396	-1.19418
C	1.17976	-3.16742	-2.75726
H	-0.52819	-1.84994	-2.44086
C	-2.15280	2.60558	2.75762
H	-1.86617	0.46770	2.44099
C	3.93665	-1.17182	1.19486
C	3.33296	0.56209	2.75730
H	1.33832	1.38302	2.44047
C	-2.98278	-2.82396	1.19418
C	-1.17976	-3.16742	2.75726
H	0.52819	-1.84994	2.44086
C	-1.81132	3.88584	2.29440
H	-0.67406	4.98555	0.81125
C	-4.27084	-0.37401	-2.29431
H	-4.65433	-1.90922	-0.81155
H	-3.54864	1.21258	-3.61658
C	2.45910	-3.51206	-2.29383
H	3.97999	-3.07724	-0.81050
H	0.72440	-3.67927	-3.61672
H	-2.82386	2.46713	3.61700
C	4.27084	-0.37401	2.29431
H	4.65433	-1.90922	0.81155
H	3.54864	1.21258	3.61658
C	-2.45910	-3.51206	2.29383
H	-3.97999	-3.07724	0.81050
H	-0.72440	-3.67927	3.61672
H	-2.20895	4.78739	2.78236
H	-5.25041	-0.48041	-2.78229
H	3.04094	-4.30738	-2.78163
H	5.25041	-0.48041	2.78229
H	-3.04094	-4.30738	2.78163

1$_2$ dimer

E (RI-PBE-D3/def2-SVP) = -1578.047537058 au

Number of negative frequencies = 0

N	-0.94568	1.47987	-3.90551
C	-2.04678	2.04612	-3.32099
C	-1.91169	3.26397	-2.63133
C	-0.62372	3.83678	-2.60509
C	0.49685	3.25763	-3.20183
C	0.34016	1.98516	-3.84506
C	1.90243	3.83417	-3.10147
C	1.94867	5.37191	-3.11078
C	3.36391	5.97903	-3.07253
C	3.28249	7.50983	-3.03876
C	-3.11535	3.83181	-1.89259
C	-3.16241	5.36990	-1.88124
C	-4.40816	5.98083	-1.21235
C	-4.30623	7.51078	-1.20117
O	-3.16659	1.36756	-3.48213
O	1.29073	1.28077	-4.33996
C	2.62243	3.22454	-1.90559
C	3.36790	2.04406	-2.05820
N	3.96599	1.48150	-0.96104
C	3.89661	1.97665	0.32961
C	3.20050	3.21800	0.49991
C	2.56145	3.77042	-0.60870
O	3.56476	1.40318	-3.19540
O	4.42749	1.29079	1.27426
C	3.11533	3.83180	1.89257
C	3.16240	5.36989	1.88120
C	4.40809	5.98081	1.21220
C	4.30621	7.51076	1.20107
C	1.91166	3.26398	2.63134
C	2.04675	2.04613	3.32100
N	0.94566	1.47989	3.90553
C	-0.34017	1.98519	3.84510
C	-0.49687	3.25765	3.20187
C	0.62371	3.83680	2.60512
O	3.16656	1.36756	3.48212
O	-1.29073	1.28078	4.34003
C	-1.90245	3.83420	3.10147
C	-1.94866	5.37194	3.11078
C	-3.36390	5.97908	3.07266
C	-3.28247	7.50988	3.03884
C	-2.62244	3.22459	1.90558
C	-3.36787	2.04409	2.05820
N	-3.96595	1.48151	0.96104
C	-3.89659	1.97665	-0.32961
C	-3.20052	3.21803	-0.49991
C	-2.56150	3.77048	0.60869
O	-3.56470	1.40320	3.19539
O	-4.42744	1.29077	-1.27426
C	4.24345	5.48943	-4.22937
C	5.71290	5.51152	1.86671
C	-4.24334	5.48951	4.22958
C	-5.71291	5.51160	-1.86701
H	2.43797	3.48216	-4.00726
H	4.01143	3.47767	2.44316
H	-2.43801	3.48220	4.00726
H	-4.01146	3.47767	-2.44317
H	-0.49525	4.79485	-2.07859
H	-1.98773	4.69987	0.46716
H	0.49523	4.79488	2.07863
H	1.98763	4.69977	-0.46717

H	1.41887	5.72730	-4.02181
H	1.37066	5.78319	-2.25419
H	3.84489	5.64856	-2.12405
H	3.78034	5.72799	-5.21099
H	4.41255	4.39444	-4.19202
H	5.23922	5.97650	-4.20290
H	4.28972	7.96591	-2.95385
H	2.67868	7.86616	-2.17808
H	2.81212	7.90581	-3.96405
H	2.25965	5.78096	1.37826
H	3.09953	5.72326	2.93396
H	4.42195	5.63832	0.15280
H	6.59061	5.99456	1.39158
H	5.85430	4.41542	1.77992
H	5.73215	5.77085	2.94711
H	4.28588	7.91785	2.23458
H	3.38292	7.85315	0.68863
H	5.16994	7.96910	0.67799
H	-1.41878	5.72734	4.02177
H	-1.37072	5.78321	2.25414
H	-3.84497	5.64860	2.12423
H	-3.78013	5.72810	5.21116
H	-4.41244	4.39453	4.19228
H	-5.23911	5.97658	4.20320
H	-4.28970	7.96597	2.95403
H	-2.67874	7.86618	2.17809
H	-2.81199	7.90588	3.96408
H	-2.25971	5.78097	-1.37822
H	-3.09945	5.72326	-2.93399
H	-4.42215	5.63832	-0.15296
H	-5.73204	5.77097	-2.94741
H	-6.59066	5.99465	-1.39196
H	-5.85435	4.41551	-1.78028
H	-3.38299	7.85314	-0.68860
H	-5.17001	7.96914	-0.67818
H	-4.28576	7.91790	-2.23466
H	-2.69714	1.42672	3.76833
H	-3.77360	1.42410	-2.63872
H	4.37036	0.52047	-1.09297
H	1.07477	0.50558	4.28221
H	-4.37026	0.52046	1.09299
H	-1.07481	0.50559	-4.28222
H	2.69717	1.42668	-3.76829
H	3.77360	1.42412	2.63873
N	0.94556	-1.47986	-3.90549
C	2.04667	-2.04609	-3.32098
C	1.91160	-3.26394	-2.63132
C	0.62364	-3.83676	-2.60504
C	-0.49694	-3.25762	-3.20177
C	-0.34026	-1.98516	-3.84501
C	-1.90252	-3.83417	-3.10139
C	-1.94874	-5.37190	-3.11068
C	-3.36398	-5.97904	-3.07263
C	-3.28255	-7.50983	-3.03863
C	3.11529	-3.83180	-1.89261
C	3.16233	-5.36988	-1.88124
C	4.40813	-5.98081	-1.21247
C	4.30615	-7.51075	-1.20116
O	3.16648	-1.36754	-3.48214
O	-1.29085	-1.28078	-4.33991
C	-2.62250	-3.22453	-1.90551
C	-3.36796	-2.04404	-2.05810

N	-3.96605	-1.48151	-0.96092
C	-3.89661	-1.97666	0.32972
C	-3.20052	-3.21802	0.50001
C	-2.56150	-3.77043	-0.60862
O	-3.56482	-1.40315	-3.19529
O	-4.42744	-1.29079	1.27440
C	-3.11529	-3.83181	1.89267
C	-3.16235	-5.36989	1.88131
C	-4.40811	-5.98081	1.21242
C	-4.30618	-7.51076	1.20120
C	-1.91160	-3.26396	2.63139
C	-2.04669	-2.04608	3.32101
N	-0.94558	-1.47983	3.90551
C	0.34024	-1.98514	3.84503
C	0.49693	-3.25762	3.20186
C	-0.62366	-3.83681	2.60518
O	-3.16649	-1.36753	3.48212
O	1.29084	-1.28072	4.33988
C	1.90251	-3.83417	3.10145
C	1.94873	-5.37190	3.11076
C	3.36397	-5.97904	3.07256
C	3.28254	-7.50984	3.03870
C	2.62248	-3.22454	1.90556
C	3.36793	-2.04404	2.05816
N	3.96600	-1.48148	0.96099
C	3.89659	-1.97664	-0.32965
C	3.20052	-3.21801	-0.49995
C	2.56152	-3.77045	0.60868
O	3.56476	-1.40316	3.19536
O	4.42743	-1.29077	-1.27433
C	-4.24330	-5.48961	-4.22970
C	-5.71285	-5.51161	1.86712
C	4.24345	-5.48950	4.22946
C	5.71282	-5.51169	-1.86733
H	-2.43807	-3.48216	-4.00718
H	-4.01137	-3.47768	2.44329
H	2.43808	-3.48216	4.00723
H	4.01138	-3.47767	-2.44324
H	0.49518	-4.79480	-2.07847
H	1.98779	-4.69987	0.46718
H	-0.49522	-4.79495	2.07879
H	-1.98773	-4.69981	-0.46712
H	-1.41881	-5.72731	-4.02163
H	-1.37086	-5.78317	-2.25400
H	-3.84516	-5.64844	-2.12429
H	-3.77998	-5.72830	-5.21120
H	-4.41241	-4.39462	-4.19254
H	-5.23906	-5.97668	-4.20337
H	-4.28978	-7.96591	-2.95387
H	-2.67892	-7.86603	-2.17777
H	-2.81197	-7.90594	-3.96377
H	-2.25966	-5.78096	1.37827
H	-3.09938	-5.72327	2.93405
H	-4.42211	-5.63827	0.15305
H	-6.59060	-5.99464	1.39207
H	-5.85429	-4.41551	1.78042
H	-5.73196	-5.77100	2.94751
H	-4.28570	-7.91791	2.23468
H	-3.38294	-7.85310	0.68861
H	-5.16997	-7.96911	0.67821
H	1.41891	-5.72730	4.02177
H	1.37075	-5.78318	2.25415

H	3.84501	-5.64852	2.12412
H	3.78029	-5.72812	5.21105
H	4.41255	-4.39451	4.19219
H	5.23922	-5.97657	4.20302
H	4.28977	-7.96592	2.95386
H	2.67880	-7.86611	2.17796
H	2.81208	-7.90586	3.96394
H	2.25968	-5.78094	-1.37812
H	3.09926	-5.72326	-2.93398
H	4.42228	-5.63821	-0.15311
H	5.73180	-5.77113	-2.94771
H	6.59061	-5.99475	-1.39236
H	5.85432	-4.41559	-1.78069
H	3.38296	-7.85303	-0.68844
H	5.16998	-7.96911	-0.67827
H	4.28551	-7.91794	-2.23462
H	2.69714	-1.42666	3.76827
H	3.77355	-1.42409	-2.63874
H	-4.37047	-0.52050	-1.09283
H	-1.07464	-0.50552	4.28219
H	4.37039	-0.52046	1.09288
H	1.07466	-0.50559	-4.28226
H	-2.69722	-1.42666	-3.76820
H	-3.77359	-1.42411	2.63873

1$_6$ hexamer

E (RI-PBE-D3/def2-SVP) = -1578.047537058 au

C	1.1305	-6.4359	-6.0185
C	0.8473	-5.2742	-6.7306
C	-0.3270	-4.5381	-6.3802
N	-1.1401	-5.0873	-5.4078
C	-0.8527	-6.2156	-4.6882
C	0.3081	-6.9476	-4.9961
C	1.7412	-4.7228	-7.8294
O	-0.6518	-3.4128	-6.9048
O	-1.7337	-6.5225	-3.7488
C	0.6465	-8.2266	-4.2438
C	1.5258	-7.9014	-3.0495
C	0.8678	-7.4928	-1.8462
N	1.6752	-7.1988	-0.7655
C	3.0413	-7.1376	-0.7968
C	3.7165	-7.5086	-1.9753
C	2.9188	-7.8933	-3.0724
O	-0.4037	-7.3802	-1.7184
O	3.6009	-6.7337	0.3328
C	5.2325	-7.4102	-2.0387
C	5.6391	-6.0041	-2.4487
C	5.8383	-5.0310	-1.4206
N	6.2443	-3.7734	-1.8222
C	6.3676	-3.3653	-3.1227
C	6.1576	-4.2963	-4.1558
C	5.7880	-5.6000	-3.7721
O	5.6535	-5.2595	-0.1712
O	6.6961	-2.0927	-3.2831
C	6.3197	-3.8922	-5.6142
C	4.9872	-3.4180	-6.1662
C	4.6369	-2.0487	-5.9423
N	3.4217	-1.6279	-6.4446
C	2.4806	-2.4414	-7.0137
C	2.7877	-3.7989	-7.2268

C	4.0555	-4.2404	-6.7963
O	5.3706	-1.2084	-5.3081
O	1.3455	-1.8368	-7.3266
O	-3.7024	-4.1140	-5.3961
C	-4.0503	-3.0287	-5.9863
C	-5.4065	-2.6074	-6.1499
C	-5.6422	-1.3631	-6.7267
C	-4.6225	-0.5099	-7.1912
C	-3.2988	-0.9599	-7.0387
N	-3.0729	-2.1949	-6.4936
C	-6.5101	-3.5226	-5.6449
C	-6.8314	-3.1908	-4.1963
C	-6.0832	-3.7847	-3.1619
N	-6.3640	-3.4554	-1.8642
C	-7.2609	-2.4838	-1.4672
C	-8.0535	-1.8802	-2.4943
C	-7.8119	-2.2521	-3.8152
O	-2.2103	-0.2939	-7.3913
C	-4.9188	0.8420	-7.8244
C	-9.0404	-0.8077	-2.0688
C	-8.3344	0.5384	-1.9885
C	-7.7532	0.9764	-0.7850
N	-7.1553	2.2068	-0.7424
C	-6.9909	3.0468	-1.8264
C	-7.5908	2.6370	-3.0575
C	-8.2222	1.3975	-3.0989
O	-7.3305	-2.1748	-0.2236
O	-5.1106	-4.6704	-3.3081
C	-7.4646	3.5579	-4.2603
O	-6.3140	4.1278	-1.6833
O	-7.7345	0.3034	0.3551
C	-4.9943	1.9079	-6.7458
C	-3.7605	2.4957	-6.3211
N	-3.8388	3.4640	-5.3401
C	-4.9743	3.8025	-4.6566
C	-6.1998	3.2211	-5.0341
C	-6.1634	2.2876	-6.0903
O	-2.6083	2.1763	-6.7859
O	-4.7914	4.6842	-3.6864
O	0.4274	-7.3590	1.6677
C	-0.8452	-7.4562	1.7975
C	-1.5057	-7.8448	3.0058
C	-2.8984	-7.8203	3.0308
C	-3.6933	-7.4376	1.9310
C	-3.0159	-7.0855	0.7478
N	-1.6505	-7.1638	0.7148
C	-0.6284	-8.1663	4.2026
O	-3.5733	-6.6848	-0.3837
C	-5.2083	-7.3253	1.9952
C	-0.2853	-6.8831	4.9457
C	0.8737	-6.1533	4.6261
N	1.1625	-5.0177	5.3335
C	0.3537	-4.4611	6.3053
C	-0.8175	-5.1958	6.6689
C	-1.1031	-6.3636	5.9680
C	-1.7043	-4.6355	7.7690
C	-2.7483	-3.7079	7.1675
C	-2.4383	-2.3509	6.9550
N	-3.3777	-1.5353	6.3860
C	-4.5938	-1.9538	5.8838
C	-4.9480	-3.3216	6.1097
C	-4.0177	-4.1464	6.7384

O	0.6803	-3.3312	6.8179
O	1.7526	-6.4678	3.6872
C	-6.2827	-3.7919	5.5594
C	-6.1205	-4.2006	4.1024
C	-6.3207	-3.2705	3.0666
N	-6.1908	-3.6814	1.7675
C	-5.7887	-4.9419	1.3705
C	-5.6040	-5.9150	2.4013
C	-5.7575	-5.5075	3.7230
O	-5.3244	-1.1129	5.2475
O	-1.3018	-1.7492	7.2682
O	-5.5956	-5.1720	0.1231
O	-6.6454	-1.9964	3.2219
O	3.7309	-4.0503	5.3039
C	4.0923	-2.9947	5.9378
C	5.4535	-2.6138	6.1609
C	5.7006	-1.3958	6.7908
C	4.6847	-0.5183	7.2218
C	3.3553	-0.9306	7.0091
N	3.1208	-2.1524	6.4404
C	6.5300	-3.5311	5.6087
C	6.7990	-3.1886	4.1503
C	6.0969	-3.8352	3.1172
N	6.3887	-3.5243	1.8166
C	7.2756	-2.5446	1.4150
C	8.0195	-1.8865	2.4430
C	7.7440	-2.2174	3.7665
O	2.2646	-0.2493	7.3222
C	4.9623	0.8498	7.8242
C	9.0348	-0.8321	2.0331
C	8.3630	0.5305	1.9699
C	7.7045	0.9307	0.7914
N	7.0757	2.1450	0.7603
C	6.9273	2.9912	1.8412
C	7.6096	2.6246	3.0446
C	8.2980	1.4137	3.0671
O	7.3810	-2.2702	0.1656
O	5.1582	-4.7551	3.2774
C	7.4522	3.5483	4.2392
O	6.1951	4.0367	1.7135
O	7.6338	0.2444	-0.3382
C	4.9942	1.8994	6.7253
C	3.7701	2.5490	6.3744
N	3.8400	3.5277	5.4022
C	4.9613	3.8425	4.6831
C	6.1751	3.2024	4.9914
C	6.1423	2.2344	6.0137
O	2.6328	2.2681	6.8987
O	4.7874	4.7593	3.7440
O	3.2236	1.0752	-6.8207
C	4.0396	1.9226	-6.3086
C	4.0908	3.3041	-6.6722
C	4.9603	4.1348	-5.9720
C	5.8196	3.6859	-4.9503
C	5.7665	2.3173	-4.6306
N	4.9263	1.5000	-5.3373
C	3.1619	3.7924	-7.7719
C	1.8371	4.2336	-7.1697
C	0.8165	3.2873	-6.9565
N	-0.3590	3.6939	-6.3871
C	-0.6038	4.9567	-5.8854
C	0.4042	5.9467	-6.1121

C	1.5831	5.5526	-6.7411
O	6.4784	1.7130	-3.6921
C	6.7602	4.6242	-4.2078
C	0.1453	7.3380	-5.5619
C	0.5809	7.4016	-4.1050
C	-0.3246	7.1104	-3.0689
N	0.0969	7.2025	-1.7700
C	1.3900	7.4834	-1.3735
C	2.3249	7.8096	-2.4046
C	1.8946	7.7395	-3.7261
O	-1.6971	5.1697	-5.2489
O	0.8628	2.0021	-7.2691
C	3.7445	8.1711	-1.9989
O	1.6863	7.4305	-0.1262
O	-1.5907	6.7555	-3.2238
C	6.0440	5.2233	-3.0106
C	6.0380	4.4570	-1.8022
N	5.3827	5.0084	-0.7193
C	4.6325	6.1519	-0.7520
C	4.5984	6.9147	-1.9351
C	5.3268	6.4175	-3.0352
O	6.5901	3.3062	-1.6727
O	4.0074	6.4345	0.3798
O	1.7169	5.2614	5.3914
C	0.6031	5.0209	5.9821
C	-0.4389	5.9855	6.1467
C	-1.6343	5.5682	6.7242
C	-1.8643	4.2587	7.1884
C	-0.8135	3.3365	7.0350
N	0.3689	3.7576	6.4891
C	-0.1977	7.3987	5.6416
O	-0.8466	2.0608	7.3875
C	-3.1830	3.8402	7.8226
C	-4.1449	3.3728	6.7449
C	-4.0383	2.0103	6.3205
N	-4.9168	1.5942	5.3401
C	-5.7775	2.4086	4.6568
C	-5.8858	3.7608	5.0341
C	-5.0582	4.1958	6.0896
O	-3.1860	1.1716	6.7852
O	-6.4503	1.8095	3.6870
C	-6.8095	4.6881	4.2603
C	-6.0750	5.2572	3.0573
C	-6.1309	4.5326	1.8264
N	-5.4855	5.0942	0.7421
C	-4.7182	6.2268	0.7842
C	-4.6286	6.9493	1.9877
C	-5.3165	6.4232	3.0984
O	-6.7295	3.4062	1.6835
O	-4.1262	6.5466	-0.3561
C	-3.8153	8.2334	2.0672
C	-2.3929	7.9145	2.4921
C	-1.4745	7.5296	1.4645
N	-0.1846	7.2382	1.8610
C	0.2416	7.1596	3.1584
C	-0.6462	7.5111	4.1932
C	-1.9495	7.8913	3.8127
O	-1.7775	7.4355	0.2211
O	1.4949	6.7597	3.3041
H	6.0897	-4.5494	5.6210
H	2.1233	-2.5064	6.4345
H	6.7466	-1.0949	6.9543

H	4.0839	1.0944	8.4564
H	2.9744	4.1182	5.2482
H	7.0837	1.7242	6.2717
H	9.3321	-1.0803	0.9934
H	5.9496	-4.1176	1.0569
H	8.3053	-1.7014	4.5613
H	7.3072	4.5632	3.8151
H	6.7226	2.4892	-0.1759
H	8.8138	1.1231	3.9951
H	-7.6193	4.0493	3.8514
H	-5.6499	4.6442	-0.2025
H	-5.2596	6.9758	4.0494
H	-3.7368	8.6256	1.0324
H	0.5414	7.1224	1.0994
H	-2.6568	8.1765	4.6064
H	-2.9692	2.9444	8.4411
H	-4.9648	0.5558	5.1421
H	-5.1340	5.2475	6.4055
H	0.9028	7.5394	5.6375
H	1.1880	3.0865	6.5111
H	-2.4444	6.3057	6.8382
H	2.9371	2.9057	-8.3996
H	5.0018	0.4567	-5.1732
H	4.9904	5.2029	-6.2389
H	7.5715	3.9955	-3.7866
H	5.5188	4.5390	0.2188
H	5.3192	7.0033	-3.9670
H	-0.9571	7.4625	-5.5712
H	-1.1630	3.0065	-6.3800
H	2.3655	6.3090	-6.9060
H	3.6783	8.5540	-0.9597
H	-0.6333	7.1125	-1.0086
H	2.6171	7.9745	-4.5235
H	-6.0819	-4.5461	-5.6411
H	-2.0825	-2.5694	-6.5163
H	-6.6856	-1.0293	-6.8400
H	-4.0358	1.1047	-8.4426
H	-2.9633	4.0243	-5.1421
H	-7.1124	1.8281	-6.4064
H	-9.3409	-1.0722	-1.0341
H	-5.9008	-4.0265	-1.1029
H	-8.4125	-1.7816	-4.6086
H	-7.3158	4.5783	-3.8510
H	-6.8471	2.5735	0.2023
H	-8.6728	1.0726	-4.0500
H	-1.0483	-3.9981	8.3970
H	2.1040	-4.5621	5.1694
H	-2.0132	-6.9234	6.2348
H	0.3215	-8.5544	3.7808
H	-1.1762	-7.0466	-0.2233
H	-3.4095	-8.1064	3.9628
H	-6.9410	-2.8990	5.5690
H	-3.1836	-0.4955	6.3793
H	-4.2821	-5.2023	6.9024
H	-5.5733	-7.4590	0.9560
H	-6.4778	-3.0038	1.0062
H	-5.6000	-6.2511	4.5201
H	5.5961	-7.5439	-0.9990
H	6.5393	-3.0968	-1.0625
H	5.6209	-6.3439	-4.5669
H	6.9817	-3.0019	-5.6266
H	3.2299	-0.5870	-6.4382

H	4.3177	-5.2968	-6.9602
H	-0.3050	-8.6078	-3.8191
H	1.2009	-7.0648	0.1709
H	3.4278	-8.1953	-4.0004
H	1.0911	-4.0843	-8.4624
H	-2.0840	-4.6323	-5.2538
H	2.0427	-6.9968	-6.2759
H	-5.4753	4.5608	-2.9229
H	-2.3649	0.7218	-7.2767
H	-4.6082	-4.5450	-4.2012
H	-7.6921	-0.7119	0.1679
H	7.6574	-0.7739	-0.1698
H	5.4236	4.5769	2.9499
H	2.4236	0.7698	7.2802
H	4.6321	-4.5782	4.1489
H	4.4950	-6.2460	0.1642
H	-1.2577	-6.9821	-2.9547
H	0.5419	-2.4837	-7.2852
H	6.2793	-1.7252	-4.1542
H	6.6515	2.3599	-2.9049
H	1.8256	1.6317	-7.2171
H	-1.7036	6.2120	-4.0956
H	3.1269	6.9474	0.2109
H	-0.5001	-2.3982	7.2155
H	-6.2309	-1.6274	4.0938
H	-4.4575	-6.1787	-0.2145
H	1.2782	-6.9403	2.8998
H	-6.6852	2.4634	2.9234
H	-1.8039	1.6876	7.2741
H	1.6376	6.2616	4.1970
H	-3.2255	7.0174	-0.1694
C	-1.2020	-9.2585	5.1222
H	-1.3966	-10.1611	4.5020
H	-2.1959	-8.9530	5.5169
C	-2.2954	-5.7234	8.6827
H	-2.9233	-5.2242	9.4534
H	-2.9920	-6.3750	8.1108
C	-5.8741	-8.4124	2.8570
H	-5.5314	-9.4043	2.4880
H	-5.5164	-8.3483	3.9081
C	-6.9647	-4.8738	6.4149
H	-7.0645	-4.4796	7.4502
H	-6.3116	-5.7698	6.5031
C	4.3535	9.2909	-2.8609
H	5.3842	9.4890	-2.4925
H	4.4759	8.9490	-3.9121
C	7.4188	5.6672	-5.1277
H	8.1041	6.2864	-4.5079
H	6.6571	6.3757	-5.5212
C	3.8089	4.8478	-8.6859
H	3.0622	5.1430	-9.4558
H	4.0266	5.7763	-8.1138
C	0.7419	8.4690	-6.4177
H	0.3509	8.3582	-7.4530
H	1.8444	8.3510	-6.5054
C	-4.4927	9.3210	2.9194
H	-4.5318	9.0113	3.9869
H	-3.8453	10.2252	2.8989
C	-0.7933	8.4792	6.5612
H	-0.5661	9.4740	6.1185
H	-1.9030	8.4084	6.5759
C	-7.4752	5.7691	5.1297

H	-7.9898	5.2637	5.9765
H	-6.7049	6.4204	5.5980
C	-3.7663	4.9143	8.7574
H	-4.7084	4.5147	9.1933
H	-4.0689	5.8132	8.1766
C	2.3291	-5.8179	-8.7366
H	2.9619	-5.3257	-9.5077
H	3.0202	-6.4709	-8.1597
C	6.9977	-4.9793	-6.4664
H	7.0997	-4.5883	-7.5028
H	6.3411	-5.8728	-6.5523
C	5.8906	-8.5044	-2.8973
H	5.5408	-9.4929	-2.5261
H	5.5341	-8.4403	-3.9488
C	1.2147	-9.3270	-5.1569
H	1.4066	-10.2266	-4.5314
H	2.2091	-9.0277	-5.5550
C	8.6893	3.6053	5.1524
H	9.5643	3.8892	4.5270
H	8.9271	2.5940	5.5495
C	10.3114	-0.8558	2.8917
H	10.9934	-0.0595	2.5200
H	10.0779	-0.5784	3.9430
C	7.8105	-3.5752	6.4609
H	7.5227	-3.8587	7.4973
H	8.2564	-2.5600	6.5467
C	6.2037	0.8876	8.7326
H	6.0912	0.0951	9.5051
H	7.1149	0.6126	8.1574
C	-6.1405	0.8116	-8.7592
H	-6.2654	1.8279	-9.1937
H	-7.0703	0.6233	-8.1788
C	-8.7335	3.5946	-5.1297
H	-8.5527	4.2929	-5.9765
H	-8.9129	2.6020	-5.5979
C	-7.7436	-3.5468	-6.5645
H	-8.4905	-4.2428	-6.1228
H	-8.2386	-2.5510	-6.5773
C	-10.3209	-0.7638	-2.9210
H	-10.7809	-1.7763	-2.9010
H	-10.0721	-0.5747	-3.9883
C	-2.8290	5.3661	9.8931
C	-2.3643	4.1963	10.7690
C	-3.4996	6.4619	10.7300
H	-1.9233	5.8115	9.4226
H	-1.7685	3.4566	10.1973
H	-1.7290	4.5549	11.6042
H	-3.2315	3.6621	11.2136
H	-3.7991	7.3269	10.1020
H	-4.4147	6.0793	11.2306
H	-2.8193	6.8402	11.5200
C	-0.2893	8.4401	8.0164
C	-0.9902	9.5199	8.8493
C	1.2364	8.5616	8.1116
H	-0.5737	7.4512	8.4418
H	-2.0940	9.4066	8.8153
H	-0.6807	9.4739	9.9132
H	-0.7466	10.5365	8.4729
H	1.7553	7.7191	7.6116
H	1.5910	9.5042	7.6415
H	1.5677	8.5710	9.1699
C	-5.9171	9.7023	2.4743

C	-5.9704	10.1618	1.0123
C	-6.5017	10.7609	3.4169
H	-6.5505	8.7905	2.5611
H	-5.6676	9.3591	0.3102
H	-6.9972	10.4731	0.7322
H	-5.2992	11.0312	0.8429
H	-6.5005	10.4120	4.4707
H	-5.9129	11.7022	3.3756
H	-7.5484	11.0088	3.1466
C	-8.4793	6.6701	4.3858
C	-9.0368	7.7381	5.3342
C	-9.6052	5.8687	3.7210
H	-7.9215	7.1965	3.5787
H	-8.2243	8.3461	5.7842
H	-9.7210	8.4317	4.8043
H	-9.6082	7.2748	6.1669
H	-9.2232	5.1747	2.9456
H	-10.1611	5.2654	4.4708
H	-10.3343	6.5438	3.2287
C	8.5747	4.5768	6.3421
C	8.2621	6.0112	5.8990
C	9.8451	4.5185	7.1986
H	7.7273	4.2309	6.9764
H	7.2821	6.0863	5.3863
H	8.2306	6.6968	6.7700
H	9.0394	6.3914	5.2017
H	10.0490	3.4865	7.5535
H	10.7327	4.8549	6.6212
H	9.7604	5.1701	8.0920
C	6.4601	2.2410	9.4223
C	7.7453	2.1759	10.2560
C	5.2670	2.7034	10.2675
H	6.6174	2.9991	8.6221
H	8.6175	1.8812	9.6358
H	7.9777	3.1573	10.7174
H	7.6524	1.4331	11.0770
H	4.3587	2.8693	9.6538
H	5.0160	1.9522	11.0471
H	5.4941	3.6579	10.7843
C	8.8982	-4.5392	5.9509
C	8.3862	-5.9776	5.8086
C	10.1341	-4.4706	6.8559
H	9.2052	-4.1922	4.9383
H	7.5725	-6.0598	5.0602
H	9.2002	-6.6575	5.4848
H	7.9961	-6.3597	6.7766
H	10.5285	-3.4353	6.9273
H	9.8944	-4.8089	7.8866
H	10.9512	-5.1155	6.4735
C	11.0579	-2.2033	2.9041
C	12.2753	-2.1264	3.8331
C	11.4555	-2.6660	1.4971
H	10.3636	-2.9660	3.3237
H	11.9828	-1.8327	4.8629
H	12.7964	-3.1032	3.8980
H	13.0106	-1.3778	3.4680
H	10.5731	-2.8394	0.8488
H	12.0998	-1.9113	0.9969
H	12.0252	-3.6165	1.5391
C	8.3762	-5.4397	-5.9561
C	9.3661	-4.2773	-5.8133
C	8.9347	-6.5444	-6.8610

H	8.2288	-5.8791	-4.9436
H	9.0304	-3.5316	-5.0649
H	10.3617	-4.6426	-5.4894
H	9.5024	-3.7484	-6.7812
H	8.2352	-7.4034	-6.9328
H	9.1083	-6.1676	-7.8917
H	9.9016	-6.9299	-6.4783
C	7.4309	-8.4786	-2.9089
C	7.9725	-9.5713	-3.8382
C	8.0294	-8.5928	-1.5016
H	7.7453	-7.4960	-3.3278
H	7.5727	-9.4637	-4.8682
H	9.0791	-9.5353	-3.9023
H	7.6905	-10.5823	-3.4739
H	7.7385	-7.7421	-0.8531
H	7.6968	-9.5282	-1.0021
H	9.1374	-8.6119	-1.5428
C	0.3149	-9.7138	-6.3458
C	-1.0829	-10.1610	-5.9010
C	1.0002	-10.7844	-7.2031
H	0.1895	-8.8070	-6.9798
H	-1.6378	-9.3502	-5.3875
H	-1.6933	-10.4767	-6.7713
H	-1.0222	-11.0244	-5.2038
H	1.9949	-10.4442	-7.5595
H	1.1542	-11.7211	-6.6258
H	0.3924	-11.0375	-8.0956
C	1.2850	-6.7146	-9.4285
C	1.9835	-7.8007	-10.2553
C	0.2956	-5.9111	-10.2812
H	0.7012	-7.2250	-8.6295
H	2.6680	-8.4106	-9.6294
H	1.2492	-8.4901	-10.7194
H	2.5876	-7.3539	-11.0739
H	-0.3014	-5.2023	-9.6728
H	0.8272	-5.3236	-11.0605
H	-0.4183	-6.5835	-10.7988
C	-7.4575	-3.9607	-8.0205
C	-8.7444	-3.8990	-8.8517
C	-6.7930	-5.3393	-8.1183
H	-6.7475	-3.2159	-8.4460
H	-9.2043	-2.8893	-8.8146
H	-8.5496	-4.1403	-9.9165
H	-9.4983	-4.6237	-8.4762
H	-5.8029	-5.3630	-7.6203
H	-7.4271	-6.1214	-7.6478
H	-6.6362	-5.6289	-9.1772
C	-6.0627	-0.2242	-9.8966
C	-4.8172	-0.0399	-10.7721
C	-7.3469	-0.1901	-10.7336
H	-5.9954	-1.2320	-9.4277
H	-3.8787	-0.1872	-10.2007
H	-4.8101	-0.7677	-11.6087
H	-4.7882	0.9791	-11.2147
H	-8.2458	-0.3650	-10.1060
H	-7.4736	0.7948	-11.2319
H	-7.3340	-0.9666	-11.5253
C	-11.3628	0.2796	-2.4755
C	-11.7876	0.0957	-1.0136
C	-12.5719	0.2576	-3.4182
H	-10.8893	1.2838	-2.5620
H	-10.9410	0.2341	-0.3115

H	-12.5703	0.8296	-0.7334
H	-12.2056	-0.9201	-0.8447
H	-12.2688	0.4313	-4.4720
H	-13.0931	-0.7227	-3.3775
H	-13.3095	1.0404	-3.1477
C	-10.0156	4.0144	-4.3858
C	-11.2195	3.9629	-5.3339
C	-9.8841	5.3904	-3.7217
H	-10.1927	3.2685	-3.5783
H	-11.3402	2.9550	-5.7833
H	-12.1621	4.2091	-4.8039
H	-11.1040	4.6889	-6.1671
H	-9.0914	5.4068	-2.9467
H	-9.6400	6.1731	-4.4719
H	-10.8329	5.6845	-3.2287
C	8.1973	5.0825	-6.3212
C	9.2890	4.0988	-5.8830
C	8.7732	6.2123	-7.1832
H	7.4720	4.5182	-6.9501
H	8.8700	3.2120	-5.3663
H	9.8627	3.7290	-6.7570
H	10.0097	4.5852	-5.1909
H	7.9773	6.9022	-7.5338
H	9.5106	6.8155	-6.6115
H	9.2903	5.8132	-8.0795
C	5.1071	4.3949	-9.3804
C	5.6917	5.5428	-10.2121
C	4.9079	3.1334	-10.2293
H	5.8445	4.1492	-8.5832
H	5.8763	6.4429	-9.5892
H	6.6555	5.2538	-10.6785
H	4.9991	5.8379	-11.0292
H	4.5969	2.2625	-9.6179
H	4.1309	3.2955	-11.0072
H	5.8468	2.8528	-10.7484
C	3.5533	10.6072	-2.8728
C	4.2201	11.6243	-3.8065
C	3.3545	11.1847	-1.4662
H	2.5451	10.3817	-3.2879
H	4.3264	11.2225	-4.8359
H	3.6299	12.5610	-3.8711
H	5.2362	11.8926	-3.4457
H	2.7695	10.5056	-0.8139
H	4.3316	11.3713	-0.9705
H	2.8111	12.1505	-1.5077
C	0.4471	9.8930	-5.9100
C	-1.0555	10.1652	-5.7699
C	1.1232	10.9294	-6.8155
H	0.8996	9.9879	-4.8969
H	-1.5328	9.5012	-5.0215
H	-1.2403	11.2100	-5.4474
H	-1.5797	10.0162	-6.7385
H	2.2176	10.7567	-6.8841
H	0.7127	10.8876	-7.8471
H	0.9691	11.9598	-6.4354
C	-1.2547	-6.6230	9.3760
C	-1.9574	-7.7017	10.2089
C	-0.2592	-5.8214	10.2234
H	-0.6753	-7.1400	8.5781
H	-2.6472	-8.3100	9.5873
H	-1.2259	-8.3937	10.6738
H	-2.5566	-7.2482	11.0273

H	0.3401	-5.1181	9.6110
H	-0.7859	-5.2282	11.0017
H	0.4525	-6.4955	10.7418
C	-0.3051	-9.6414	6.3145
C	1.0918	-10.0956	5.8742
C	-0.9950	-10.7050	7.1769
H	-0.1776	-8.7315	6.9436
H	1.6500	-9.2894	5.3570
H	1.6999	-10.4084	6.7471
H	1.0294	-10.9626	5.1817
H	-1.9896	-10.3600	7.5293
H	-1.1503	-11.6447	6.6049
H	-0.3897	-10.9543	8.0721
C	-7.4141	-8.3763	2.8696
C	-7.9622	-9.4628	3.8023
C	-8.0143	-8.4906	1.4631
H	-7.7219	-7.3905	3.2859
H	-7.5604	-9.3554	4.8316
H	-9.0684	-9.4189	3.8676
H	-7.6877	-10.4767	3.4402
H	-7.7184	-7.6437	0.8118
H	-7.6882	-9.4296	0.9660
H	-9.1224	-8.5023	1.5050
C	-8.3453	-5.3300	5.9065
C	-9.3311	-4.1641	5.7634
C	-8.9068	-6.4316	6.8133
H	-8.2005	-5.7711	4.8944
H	-8.9934	-3.4205	5.0138
H	-10.3284	-4.5262	5.4409
H	-9.4644	-3.6336	6.7309
H	-8.2105	-7.2933	6.8848
H	-9.0774	-6.0531	7.8438
H	-9.8757	-6.8137	6.4323

[1$_2$**+G]**$^{2+}$ hexamer with guest

E (RI-PBE-D3/def2-SVP) = -1578.047537058 au

C	1.13392	-6.44291	-6.00818
C	0.84845	-5.27709	-6.71155
C	-0.32976	-4.54942	-6.35727
N	-1.14956	-5.11561	-5.40007
C	-0.86062	-6.25237	-4.69609
C	0.30888	-6.96844	-4.99254
C	1.73715	-4.72016	-7.81267
O	-0.65576	-3.41550	-6.86205
O	-1.75345	-6.57947	-3.76583
C	0.65560	-8.24739	-4.24345
C	1.51921	-7.91197	-3.03918
C	0.85799	-7.50958	-1.84048
N	1.65441	-7.23032	-0.74877
C	3.01993	-7.14353	-0.77466
C	3.70391	-7.49935	-1.95122
C	2.91407	-7.89558	-3.05008
O	-0.41762	-7.37606	-1.71445
O	3.56372	-6.71898	0.35650
C	5.21893	-7.38351	-2.01482
C	5.60314	-5.97191	-2.42871
C	5.76202	-4.98629	-1.40795
N	6.16708	-3.72970	-1.80896
C	6.32700	-3.33570	-3.10903
C	6.14098	-4.27152	-4.14028

C	5.77820	-5.57685	-3.75202
O	5.54275	-5.19767	-0.15881
O	6.65444	-2.05889	-3.26893
C	6.31365	-3.87640	-5.60106
C	4.98023	-3.40075	-6.15364
C	4.61811	-2.04011	-5.92360
N	3.40135	-1.61940	-6.41750
C	2.46246	-2.43452	-6.98893
C	2.77729	-3.79003	-7.20813
C	4.04984	-4.22475	-6.78770
O	5.33706	-1.19452	-5.26752
O	1.32371	-1.83263	-7.28892
O	-3.69152	-4.11732	-5.35217
C	-4.04502	-3.03382	-5.95423
C	-5.39817	-2.61793	-6.12549
C	-5.62843	-1.37199	-6.70547
C	-4.60663	-0.51525	-7.15561
C	-3.28302	-0.96163	-6.98867
N	-3.06183	-2.19808	-6.44379
C	-6.50971	-3.52769	-5.62431
C	-6.81552	-3.19457	-4.17139
C	-6.05708	-3.77977	-3.14182
N	-6.30583	-3.42878	-1.84395
C	-7.19719	-2.45455	-1.44455
C	-8.01402	-1.86970	-2.46143
C	-7.79434	-2.25627	-3.78223
O	-2.18929	-0.29405	-7.31837
C	-4.90103	0.83430	-7.79439
C	-9.01062	-0.80741	-2.03188
C	-8.31209	0.54309	-1.95888
C	-7.72008	0.98754	-0.76451
N	-7.13174	2.22310	-0.73352
C	-6.97046	3.05054	-1.82612
C	-7.58386	2.64238	-3.04642
C	-8.21941	1.40257	-3.07111
O	-7.23692	-2.12863	-0.20162
O	-5.08793	-4.67400	-3.29452
C	-7.47549	3.55642	-4.25739
O	-6.26880	4.12264	-1.68695
O	-7.66716	0.31762	0.37777
C	-4.98271	1.90180	-6.71745
C	-3.75580	2.50471	-6.29519
N	-3.84668	3.49556	-5.33713
C	-4.98999	3.83665	-4.66873
C	-6.20488	3.22881	-5.02678
C	-6.15644	2.27921	-6.06985
O	-2.59661	2.18064	-6.73916
O	-4.82284	4.74754	-3.71536
O	0.44601	-7.37050	1.67953
C	-0.83175	-7.47425	1.80861
C	-1.49787	-7.85519	3.01193
C	-2.89215	-7.82184	3.02334
C	-3.67751	-7.42502	1.92158
C	-2.98970	-7.07946	0.74419
N	-1.62550	-7.18480	0.71778
C	-0.63841	-8.18688	4.22017
O	-3.52887	-6.65035	-0.38737
C	-5.19222	-7.30581	1.98131
C	-0.28932	-6.90161	4.95725
C	0.87569	-6.18452	4.64511
N	1.16087	-5.03535	5.33033
C	0.34416	-4.46068	6.28538

C	-0.82664	-5.19101	6.65800
C	-1.11050	-6.36716	5.97112
C	-1.70932	-4.62696	7.76023
C	-2.75662	-3.70419	7.15687
C	-2.44946	-2.34829	6.93111
N	-3.39660	-1.53835	6.36601
C	-4.61691	-1.96418	5.88457
C	-4.96940	-3.32737	6.11825
C	-4.03013	-4.14579	6.74623
O	0.66724	-3.31795	6.77180
O	1.76736	-6.52206	3.71814
C	-6.30356	-3.81195	5.57460
C	-6.13403	-4.20472	4.11283
C	-6.32950	-3.26930	3.08358
N	-6.15634	-3.65610	1.78248
C	-5.73535	-4.90779	1.38001
C	-5.57919	-5.89642	2.39884
C	-5.76068	-5.50663	3.72242
O	-5.34655	-1.12205	5.23687
O	-1.31034	-1.74115	7.21937
O	-5.50040	-5.11267	0.13350
O	-6.67668	-1.99777	3.24875
O	3.70259	-4.02876	5.26294
C	4.07583	-2.98319	5.91858
C	5.43539	-2.61665	6.14800
C	5.68422	-1.39902	6.78207
C	4.67176	-0.51411	7.20279
C	3.34030	-0.91877	6.98373
N	3.10340	-2.13949	6.41260
C	6.51385	-3.53370	5.59516
C	6.76955	-3.18649	4.13434
C	6.05129	-3.81470	3.10313
N	6.31238	-3.47903	1.80307
C	7.19876	-2.50057	1.40201
C	7.97378	-1.87110	2.42266
C	7.71930	-2.22035	3.74597
O	2.24996	-0.23302	7.28359
C	4.95776	0.85152	7.80749
C	9.00485	-0.83329	2.00873
C	8.34858	0.53715	1.94561
C	7.69863	0.95246	0.76925
N	7.09189	2.17883	0.74385
C	6.93612	3.00789	1.83586
C	7.61489	2.63552	3.03446
C	8.29739	1.41890	3.04481
O	7.27197	-2.20472	0.15290
O	5.10864	-4.73602	3.26297
C	7.47419	3.55062	4.23921
O	6.18346	4.04646	1.71015
O	7.60229	0.26967	-0.36213
C	4.99675	1.89964	6.70651
C	3.77796	2.55686	6.35204
N	3.85921	3.55011	5.39516
C	4.98851	3.86777	4.69153
C	6.19290	3.21209	4.98802
C	6.14950	2.23468	6.00349
O	2.63270	2.27266	6.85652
O	4.82608	4.80494	3.76159
O	3.20460	1.08003	-6.77483
C	4.03340	1.93065	-6.28860
C	4.08124	3.30968	-6.66122
C	4.95869	4.14304	-5.97478

C	5.83238	3.69855	-4.96138
C	5.79306	2.33111	-4.64915
N	4.93950	1.51016	-5.33390
C	3.15155	3.79263	-7.76325
C	1.82927	4.23939	-7.15961
C	0.80792	3.29629	-6.93330
N	-0.36669	3.71268	-6.36826
C	-0.60708	4.98275	-5.88720
C	0.39817	5.96867	-6.12097
C	1.57611	5.56336	-6.74913
O	6.53116	1.72707	-3.72252
C	6.77182	4.64303	-4.22487
C	0.15225	7.36660	-5.57718
C	0.57770	7.41546	-4.11555
C	-0.33007	7.11730	-3.08616
N	0.09194	7.15974	-1.78517
C	1.38671	7.42005	-1.38299
C	2.32085	7.77916	-2.40193
C	1.89217	7.74217	-3.72540
O	-1.70116	5.19465	-5.23978
O	0.85067	2.00605	-7.22096
C	3.73518	8.14780	-1.98450
O	1.68196	7.31825	-0.13662
O	-1.60519	6.78341	-3.25107
C	6.05583	5.22174	-3.01618
C	6.05939	4.45448	-1.81280
N	5.41267	4.99748	-0.72163
C	4.63988	6.12665	-0.74766
C	4.59494	6.89505	-1.92507
C	5.33039	6.41288	-3.02724
O	6.60818	3.29589	-1.68399
O	3.99947	6.37951	0.38426
O	1.72513	5.25422	5.34792
C	0.61005	5.01923	5.95020
C	-0.42605	5.98374	6.12207
C	-1.62029	5.56080	6.70234
C	-1.85209	4.24760	7.15231
C	-0.80431	3.32388	6.98473
N	0.37710	3.74992	6.43943
C	-0.19332	7.40122	5.62104
O	-0.83615	2.04287	7.31422
C	-3.16802	3.82851	7.79169
C	-4.13399	3.36555	6.71526
C	-4.04334	2.00148	6.29305
N	-4.94720	1.58510	5.33517
C	-5.81419	2.40491	4.66701
C	-5.89487	3.76094	5.02522
C	-5.04777	4.19353	6.06800
O	-3.18341	1.15919	6.73688
O	-6.51976	1.80490	3.71370
C	-6.81365	4.69781	4.25592
C	-6.07613	5.24827	3.04487
C	-6.12389	4.51322	1.82447
N	-5.48800	5.06640	0.73172
C	-4.71151	6.19330	0.76259
C	-4.62160	6.92789	1.95710
C	-5.31932	6.41801	3.06956
O	-6.70242	3.36995	1.68538
O	-4.10532	6.48242	-0.37992
C	-3.80072	8.20771	2.02990
C	-2.38247	7.87526	2.45905
C	-1.46815	7.45975	1.44187

N	-0.17870	7.17456	1.84080
C	0.25021	7.13491	3.13849
C	-0.63524	7.49969	4.16832
C	-1.93729	7.87853	3.77966
O	-1.77086	7.33108	0.19910
O	1.50916	6.74233	3.29076
H	6.08221	-4.55549	5.61322
H	2.10624	-2.49941	6.41274
H	6.73037	-1.10624	6.95678
H	4.08205	1.10280	8.44051
H	2.99891	4.15471	5.25957
H	7.08749	1.72040	6.26402
H	9.29860	-1.08777	0.96961
H	5.86873	-4.07150	1.04294
H	8.30443	-1.72689	4.53718
H	7.34687	4.57363	3.82964
H	6.79871	2.55802	-0.20536
H	8.81671	1.12115	3.96793
H	-7.63940	4.07269	3.85834
H	-5.69757	4.64225	-0.22088
H	-5.26973	6.98562	4.01151
H	-3.71960	8.59533	0.99357
H	0.54769	7.05557	1.07780
H	-2.64056	8.18891	4.56681
H	-2.95238	2.93191	8.40832
H	-5.01773	0.54312	5.16215
H	-5.11183	5.24633	6.38154
H	0.90501	7.55745	5.62857
H	1.20326	3.08519	6.47076
H	-2.42696	6.29897	6.83059
H	2.92555	2.90309	-8.38652
H	5.02435	0.46499	-5.18476
H	4.98712	5.20909	-6.24828
H	7.59921	4.02486	-3.82007
H	5.60291	4.56045	0.22676
H	5.32045	7.00783	-3.95273
H	-0.94719	7.51265	-5.59943
H	-1.17742	3.02973	-6.36434
H	2.35763	6.31701	-6.92798
H	3.66050	8.52492	-0.94381
H	-0.63982	7.06618	-1.02330
H	2.61462	7.99945	-4.51517
H	-6.09635	-4.55719	-5.63226
H	-2.07342	-2.58194	-6.47555
H	-6.67080	-1.04163	-6.83335
H	-4.01651	1.09574	-8.41074
H	-2.97942	4.07746	-5.16431
H	-7.10036	1.80861	-6.38342
H	-9.30575	-1.07161	-0.99557
H	-5.83968	-3.99870	-1.08119
H	-8.41459	-1.80189	-4.56920
H	-7.34662	4.58397	-3.85970
H	-6.86846	2.61620	0.21908
H	-8.68700	1.07644	-4.01286
H	-1.05154	-3.98708	8.38373
H	2.10874	-4.58685	5.18112
H	-2.01978	-6.92446	6.24457
H	0.31034	-8.59439	3.81484
H	-1.15216	-7.13083	-0.23076
H	-3.41229	-8.11086	3.94882
H	-6.97897	-2.93224	5.59725
H	-3.20973	-0.49494	6.36221

H	-4.29298	-5.19924	6.92479
H	-5.55641	-7.42947	0.94067
H	-6.44121	-2.97550	1.02073
H	-5.62243	-6.26111	4.51204
H	5.58635	-7.51104	-0.97578
H	6.45906	-3.04956	-1.04882
H	5.64251	-6.33010	-4.54329
H	6.98281	-2.99178	-5.61915
H	3.21469	-0.57585	-6.41712
H	4.31914	-5.27717	-6.96259
H	-0.29415	-8.64769	-3.83328
H	1.17986	-7.16595	0.20064
H	3.43102	-8.19685	-3.97341
H	1.08219	-4.08723	-8.44610
H	-2.10293	-4.67210	-5.26440
H	2.04795	-6.99886	-6.26842
H	-5.50143	4.61136	-2.94936
H	-2.35226	0.72173	-7.23171
H	-4.61647	-4.56796	-4.21128
H	-7.63475	-0.70243	0.18563
H	7.61232	-0.75435	-0.18594
H	5.46714	4.62545	2.97328
H	2.41910	0.78518	7.25832
H	4.61470	-4.57832	4.16060
H	4.45600	-6.21653	0.18010
H	-1.27750	-7.04492	-2.97750
H	0.52610	-2.48780	-7.26374
H	6.27015	-1.70969	-4.16614
H	6.71612	2.37850	-2.94379
H	1.81566	1.63896	-7.18674
H	-1.71827	6.27271	-4.14639
H	3.11440	6.89174	0.20691
H	-0.51039	-2.39385	7.18462
H	-6.29002	-1.64497	4.14384
H	-4.41501	-6.13998	-0.20986
H	1.29497	-7.00696	2.93914
H	-6.74141	2.46081	2.94795
H	-1.79763	1.67662	7.22825
H	1.65319	6.28076	4.20742
H	-3.20528	6.96359	-0.18800
C	-1.23964	-9.26483	5.13921
H	-1.44314	-10.16645	4.52105
H	-2.23197	-8.94116	5.52305
C	-2.29557	-5.71226	8.68063
H	-2.92613	-5.21011	9.44667
H	-2.98885	-6.37110	8.11300
C	-5.86537	-8.39742	2.83219
H	-5.51810	-9.38632	2.46069
H	-5.51696	-8.33909	3.88666
C	-6.96388	-4.91289	6.42270
H	-7.06123	-4.53061	7.46230
H	-6.29788	-5.80044	6.49731
C	4.34467	9.27624	-2.83530
H	5.37507	9.46887	-2.46418
H	4.46760	8.94551	-3.88991
C	7.40439	5.70269	-5.14417
H	8.08398	6.32948	-4.52630
H	6.62779	6.40044	-5.52731
C	3.79898	4.84230	-8.68396
H	3.04904	5.13739	-9.45019
H	4.02349	5.77206	-8.11658
C	0.77631	8.48840	-6.42537

H	0.39579	8.38226	-7.46475
H	1.87777	8.35417	-6.50066
C	-4.47087	9.30403	2.87656
H	-4.51826	8.99777	3.94465
H	-3.81304	10.20028	2.85680
C	-0.80915	8.47563	6.53435
H	-0.59146	9.47152	6.09004
H	-1.91799	8.39138	6.54209
C	-7.45381	5.79415	5.12577
H	-7.96339	5.29974	5.98156
H	-6.66927	6.43744	5.58118
C	-3.74798	4.90076	8.73123
H	-4.69058	4.50063	9.16465
H	-4.04935	5.80285	8.15472
C	2.33194	-5.81196	-8.71967
H	2.96534	-5.31509	-9.48682
H	3.02372	-6.46373	-8.14214
C	6.98674	-4.97189	-6.44636
H	7.08589	-4.58848	-7.48538
H	6.32802	-5.86457	-6.52435
C	5.88920	-8.47191	-2.87161
H	5.54433	-9.46229	-2.50179
H	5.53686	-8.41061	-3.92461
C	1.24995	-9.33548	-5.15532
H	1.45070	-10.23323	-4.53063
H	2.24279	-9.01915	-5.54392
C	8.71366	3.57840	5.15111
H	9.59178	3.85282	4.52654
H	8.93510	2.56004	5.53928
C	10.28276	-0.87058	2.86518
H	10.96857	-0.07730	2.49509
H	10.05394	-0.59573	3.91817
C	7.79914	-3.56884	6.44046
H	7.51665	-3.84595	7.47958
H	8.24304	-2.55209	6.51799
C	6.20025	0.88156	8.71506
H	6.08573	0.08481	9.48230
H	7.11062	0.60769	8.13796
C	-6.11943	0.80147	-8.73410
H	-6.24366	1.81812	-9.16701
H	-7.05153	0.61144	-8.15787
C	-8.74491	3.56317	-5.12739
H	-8.57114	4.25155	-5.98319
H	-8.91008	2.56215	-5.58267
C	-7.74831	-3.53071	-6.53736
H	-8.50222	-4.21680	-6.09294
H	-8.22922	-2.52804	-6.54488
C	-10.29522	-0.77448	-2.87843
H	-10.74320	-1.79197	-2.85841
H	-10.05362	-0.58068	-3.94654
Ru	-0.02560	0.01539	-0.00210
N	-0.96629	1.55914	-0.98188
C	-2.21890	1.88538	-0.52091
C	-2.90197	3.01011	-1.01419
C	-2.29348	3.83174	-1.96922
C	-1.01754	3.48064	-2.43849
C	-0.39229	2.34058	-1.92880
H	-3.90639	3.25522	-0.64728
H	-2.80911	4.72759	-2.34071
H	-0.51177	4.08588	-3.20176
H	0.60462	2.02803	-2.27100
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C	-2.74168	0.98110	0.51434
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C	2.70684	0.96754	-0.45035
C	2.17410	-0.74538	-1.96879
C	-2.22386	-0.82713	1.92426
C	2.18327	1.83717	0.61463
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C	0.51298	-2.82740	0.44782
C	1.73082	-1.51002	1.96601
C	-4.05764	1.01087	1.00657
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C	-2.45259	-2.53246	-2.56353
H	-2.03592	-0.40225	-2.32444
C	4.03272	0.99023	-0.91454
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H	1.39590	-1.41278	-2.36588
C	-3.52410	-0.85484	2.43324
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C	0.96848	3.39128	2.55855
H	-0.66941	1.96715	2.31820
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C	2.40788	-2.62921	2.45709
H	1.92062	-0.50235	2.36257
C	-4.46576	0.07414	1.96229
H	-4.77169	1.75791	0.63836
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H	-3.22342	-2.38156	-3.33051
C	4.43774	0.09899	-1.91440
H	4.75527	1.69706	-0.48981
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H	-3.79593	-1.59438	3.19737
C	2.25844	3.73574	2.12504
H	3.88955	3.17673	0.81996
H	0.45218	3.98431	3.32469
C	2.12891	-3.89301	1.91308
H	0.90309	-4.96657	0.48866
H	3.14394	-2.51694	3.26392
H	-5.49957	0.07311	2.33325
H	-2.60805	-4.71346	-2.53090
H	5.47852	0.09068	-2.26626
H	2.78116	4.61412	2.52754
H	2.65541	-4.79062	2.26552
C	-2.81059	5.34392	9.87065
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H	-1.90268	5.79117	9.40533
H	-1.75276	3.42929	10.17104
H	-1.72039	4.52165	11.58121
H	-3.22120	3.63383	11.18071
H	-3.77920	7.30553	10.08772
H	-4.39836	6.05250	11.20823
H	-2.80349	6.80895	11.50413
C	-0.31320	8.44799	7.99293
C	-1.03376	9.52341	8.81474
C	1.21024	8.59050	8.09689

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H	-0.73187	9.48521	9.88062
H	-0.79837	10.54084	8.43678
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H	1.55554	9.53483	7.62425
H	1.53292	8.61219	9.15708
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H	-6.94728	10.48992	0.67681
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H	-5.86306	11.70046	3.32599
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C	-8.45763	6.70307	4.39061
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H	-7.90793	7.21718	3.56957
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C	8.32976	5.98595	5.91697
C	9.88978	4.45451	7.19985
H	7.76628	4.20673	6.98390
H	7.34837	6.08686	5.41048
H	8.31610	6.66450	6.79330
H	9.11172	6.35753	5.22060
H	10.07786	3.41658	7.54527
H	10.78065	4.78224	6.62337
H	9.81822	5.09915	8.09873
C	6.45959	2.22970	9.41454
C	7.74837	2.15459	10.24195
C	5.27039	2.68399	10.26977
H	6.61526	2.99555	8.62091
H	8.61832	1.86594	9.61596
H	7.98271	3.13087	10.71173
H	7.65821	1.40486	11.05631
H	4.35780	2.85873	9.66435
H	5.02376	1.92616	11.04389
H	5.50157	3.63232	10.79500
C	8.88619	-4.53516	5.93241
C	8.37781	-5.97692	5.81123
C	10.12707	-4.45113	6.82922
H	9.18649	-4.19902	4.91373
H	7.56047	-6.07452	5.06807
H	9.19261	-6.65707	5.49174
H	7.99685	-6.34888	6.78639
H	10.51907	-3.41426	6.88655
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H	10.94331	-5.09754	6.44893
C	11.02225	-2.22242	2.86850
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H	10.53692	-2.84763	0.80717
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C	8.36691	-5.43032	-5.93785
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C	8.91553	-6.54588	-6.83542
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H	8.21378	-7.40384	-6.89430
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H	9.08480	-9.48525	-3.86356
H	7.70025	-10.53890	-3.44379
H	7.72868	-7.70648	-0.81304
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C	0.36580	-9.73380	-6.35250
C	-1.02804	-10.20501	-5.92003
C	1.07716	-10.79223	-7.20382
H	0.23173	-8.82859	-6.98769
H	-1.60517	-9.40506	-5.41321
H	-1.62325	-10.53185	-6.79607
H	-0.95923	-11.06807	-5.22374
H	2.07021	-10.43702	-7.54971
H	1.23814	-11.72773	-6.62736
H	0.48252	-11.05211	-8.10246
C	1.29382	-6.71022	-9.41926
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C	0.30735	-5.90720	-10.27598
H	0.70723	-7.22672	-8.62571
H	2.68663	-8.39941	-9.61815
H	1.27429	-8.48083	-10.71518
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H	0.84164	-5.31591	-11.05016
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C	-7.47694	-3.94642	-7.99607
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H	-5.96877	-1.24156	-9.40944
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C	-11.34756	0.25524	-2.42480
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C	5.09073	4.38127	-9.38592
C	5.67183	5.52592	-10.22456
C	4.87927	3.11906	-10.23089
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H	5.86493	6.42709	-9.60598
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H	4.97472	5.82060	-11.03734
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H	4.09715	3.28278	-11.00285
H	5.81232	2.83609	-10.75814
C	3.54745	10.59478	-2.83202
C	4.21605	11.61653	-3.75950
C	3.35798	11.16076	-1.41937
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C	0.49518	9.91725	-5.92238
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H	0.93699	10.00900	-4.90388
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C	-1.25121	-6.60106	9.38292
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H	-1.21979	-8.36068	10.69354
H	-2.55714	-7.22083	11.03310
H	0.33731	-5.08544	9.61682
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H	0.44669	-6.45438	10.75655
C	-0.35972	-9.65799	6.34122
C	1.03232	-10.13998	5.91491
C	-1.07796	-10.70579	7.19988
H	-0.22179	-8.74843	6.96931
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H	1.62445	-10.46275	6.79455
H	0.96010	-11.00828	5.22551
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H	-0.48638	-10.96123	8.10180
C	-7.40584	-8.36474	2.82962
C	-7.95707	-9.45457	3.75679
C	-7.99147	-8.48216	1.41717
H	-7.72232	-7.38069	3.24429
H	-7.56696	-9.34603	4.79023
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H	-7.67523	-10.46670	3.39683
H	-7.69693	-7.63374	0.76654
H	-7.65724	-9.41987	0.92383
H	-9.09926	-8.50040	1.44950
C	-8.34268	-5.38191	5.92014
C	-9.34617	-4.22832	5.80155
C	-8.87876	-6.50185	6.81982
H	-8.20222	-5.80985	4.90130
H	-9.03057	-3.47018	5.05625
H	-10.34107	-4.60173	5.48637
H	-9.47787	-3.71226	6.77661
H	-8.16990	-7.35414	6.87595
H	-9.04677	-6.13749	7.85537
H	-9.84478	-6.89356	6.44289