Supporting information for

adj-Dicarbachlorin, the first free base carbaporphyrinoid system with an

internal methylene unit.

Timothy D. Lash,* Deyaa I. AbuSalim and Gregory M. Ferrence

Department of Chemistry, Illinois State University, Normal, Illinois 61790-4160, USA

E-mail: tdlash@ilstu.edu

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Experimental Procedures

Melting points are uncorrected. NMR spectra were recorded using a 400 or 500 MHz NMR spectrometer and were run at 300 K. ¹H NMR values are reported as chemical shifts δ , relative integral, multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad peak) and coupling constant (*J*). Chemical shifts are reported in parts per million (ppm) relative to CDCl₃ (¹H residual CHCl₃ δ 7.26, ¹³C CDCl₃ triplet δ 77.23) and coupling constants were taken directly from the spectra. NMR assignments were made with the aid of ¹H-¹H COSY, HSQC, DEPT-135 and nOe difference proton NMR spectroscopy. 2D experiments were performed using standard software. High-resolution mass spectra (HRMS) were carried out using a double focusing magnetic sector instrument.



Dicarbachlorin 14. A mixture of dipyrrylmethane dialdehyde 9^{S1} (400 mg, 1.40 mmol) and dicyclopentadienylmethane 13^{S2} (700 mg, 4.16 mmol) in 1% w/v KOH-methanol (380 mL) was stirred under reflux in a foil covered round bottom flask under a nitrogen atmosphere for 4 days. The solution was concentrated under reduced pressure, diluted with water and extracted several times with dichloromethane. The combined extracts were dried over sodium sulfate, filtered and the solvent removed on a rotary evaporator. The residue was run through a grade 3 alumina column, eluting with dichloromethane. The colored fractions were evaporated and further purified on grade 2 alumina, eluting with 70% dichloromethane-30% hexanes. The red product fraction was evaporated under reduced pressure to give the dicarbachlorin (27-40 mg, 0.068-0.10 mmol, 5-7%) as a brown solid. A sample was recrystallized from hexanes to give maroon or purple microcrystals, mp 211-212 °C, dec; UV-vis (1% Et₃N-CHCl₃) λ_{max} (log ε) 398 (5.08), 418 (sh, 4.83), 501 (4.14), 533 (4.17), 564 (sh, 3.31), 619 (3.50), 683 nm (3.72); UV-vis (0.05% TFA-CH₂Cl₂) λ_{max} (log ε) 396 (sh, 4.85), 419 (5.45), 539 (3.96), 579 (4.30), 606 (4.10), 662 nm (3.69); ¹H NMR (500 MHz, CDCl₃): δ -6.68 (2H, s, 22-CH₂), -4.03 (1H, s, 21-H), 1.72 (3H, t, *J*

= 7.7 Hz, 17-CH₂CH₃), 1.76 (3H, t, J = 7.7 Hz, 13-CH₂CH₃), 3.27 (3H, s, 18-CH₃), 3.42 (3H, s, 12-CH₃), 3.81 (2H, q, J = 7.7 Hz, 17-CH₂), 3.89 (2H, q, J = 7.7 Hz, 13-CH₂), 4.53-4.56 (2H, m, 2-CH₂), 4.57-4.60 (2H, m, 3-CH₂), 9.07 (1H, s, 20-H), 9.47 (1H, d, J = 3.8 Hz, 7-H), 9.51 (1H, s, 5-H), 9.52 (1H, s, 15-H), 9.68 (1H, d, J = 3.8 Hz, 8-H), 9.97 (1H, s, 10-H); ¹³C NMR (125 MHz, CDCl₃): δ 11.5 (12-CH₃), 11.7 (18-CH₃), 17.7 (CH₂CH₃), 17.8 (CH₂CH₃), 19.7 (13-CH₂), 19.9 (17-CH₂), 32.9 (22-CH₂), 34.6 (2-CH₂), 36.2 (3-CH₂), 100.6 (15-CH), 105.7 (20-CH), 106.8 (10-CH), 114.6 (5-CH), 130.7, 132.2 (21-CH), 133.9, 135.5 (7-CH), 138.2 (8-CH), 138.9, 143.6, 146.4, 151.8, 152.8; ¹H NMR (500 MHz, TFA-CDCl₃, cation **14**H⁺): δ -7.42 (2H, s, 22-CH2), -5.53 (1H, s, 21-H), -4.19 (1H, br s), -4.04 (1H, br s) (2 x NH), 1.70 (3H, t, J = 7.7 Hz), 1.74 (3H, t, J = 7.7 Hz) (2 x CH₂CH₃), 3.43 (3H, s, 18-CH₃), 3.55 (3H, s, 12-CH₃), 4.03-4.77 (4H, 2 overlapping quartets, 2 x CH₂CH₃), 4.74-4.77 (2H, m, 2-CH₂), 4.79-4.82 (2H, m, 3-CH₂), 9.52 (1H, s, 20-H), 10.02 (1H, d, J = 4.1 Hz, 7-H), 10.06 (1H, s, 5-H), 10.15 (1H, s, 15-H), 10.24 (1H, d, J = 4.1 Hz, 8-H), 10.51 (1H, s, 10-H); ¹³C NMR (125 MHz, TFA-CDCl₃, cation 14H⁺): δ 11.4 (12-CH₃), 11.5 (18-CH₃), 16.7 (CH₂CH₃), 17.0 (CH₂CH₃), 20.0 (CH₂CH₃), 20.2 (CH₂CH₃), 30.9 (22-CH₂), 36.0 (2-CH₂), 37.0 (3-CH₂), 99.3 (15-CH), 104.6 (20-CH), 108.9 (10-CH), 118.2 (5-CH), 132.1 (21-CH), 132.8, 133.0, 133.6, 133.8, 139.1, 140.8 (7-CH), 142.2, 142.8, 143.5 (8-CH), 145.17, 145.25, 149.0, 158.6, 158.7; HR MS (ESI⁺) calcd for $C_{28}H_{30}N_2 + H$ 395.2482, found 395.2474.

Computational Studies. All calculations in this study were performed using the Gaussian 09 Suite of programs.^{S3} The geometries of the porphyrinoid systems were optimized using B3LYP with a 6-311++G** basis set. Frequency calculations at the same level of theory were used and confirmed all the stationary points were minima. In addition, electronic single point energies were calculated using M06-2X and B3LYP-D functionals, in both cases with a 6-311++G** basis set. Gaussview running on an OS X platform was used to visualize the 3D conformations of the optimized structures. Two types of NMR calculations were used in this study. The first involved using the GIAO method^{S4} to obtain NICS values and the second calculated using CGST in order to obtain AICD plots.^{S5} NICS(0) was calculated at the mean position of all the heavy atoms that make up the porphyrinoid core. NICS(a), NICS(b), NICS(c) and NICS(d) values were obtained by applying the same method to the mean position of the heavy atoms that comprise the individual rings of each macrocycle. In addition, NICS(1)_{zz}, NICS(1a)_{zz}, NICS(1b)_{zz}, NICS(1c)_{zz} and NICS(1d)_{zz} were obtained by applying the same method to ghost atoms placed 1 Å above

each of the corresponding NICS(0) points and extracting the zz contribution of the magnetic tensor.^{S6,S7} AICD plots for all the compounds were plotted using Gaussview at three different isosurface values and can be found in Figures S22-S27.

Crystallographic experimental details for *adj*-dibenzodicarbaporphyrin 7. X-ray quality crystals of 7 (C₃₆H₃₂N₂) were suspended in mineral oil at ambient temperature and a suitable crystal was selected. A mineral oil coated black plate thereby obtained of approximate dimensions 0.116 mm x 0.065 mm x 0.021 mm was mounted on a 50 µm MicroMesh MiTeGen Micromount and transferred to a Bruker AXS SMART APEX CCD X-ray diffractometer. The X-ray diffraction data were collected at 100(2) K using Mo-K_{α} ($\lambda = 0.71073$ Å) radiation. A total of 2232 frames were collected. The total exposure time was 74.40 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm.^{S8} The integration of the twinned data yielded a total of 9949 reflections to a maximum θ angle of 26.022° (0.81 Å resolution), of which 9949 were independent (completeness = 99.8%, R_{sig} = 12.39%; twinning software merges reflections while integrating thereby making total and independent reflections equal) and 5143 (51.69%) were observed with $F_o^2 > 2\sigma(F_o^2)$. The final triclinic cell constants of a = 7.9415(4) Å, b = 15.4054(7) Å, c = 21.5716(9) Å, $\alpha = 102.614(3)^{\circ}$, $\beta = 95.363(3)^\circ$, $\gamma = 97.396(3)^\circ$, volume = 2533.8(2) Å³, are based upon the refinement of the XYZ-centroids of 5840 reflections above 20 $\sigma(I)$ with 5.34° < 2 θ < 44.94°. Limiting indicies were as follows: $-9 \le h \le 9$, $-19 \le k \le 18$, $0 \le l \le 26$. Data were corrected for absorption effects using the multi-scan method (TWINABS).⁵⁸ The ratio of minimum to maximum apparent transmission was 0.93 with minimum and maximum TWINABS generated transmission coefficients of 0.70 and 0.75. Solution and data analysis were performed using the WinGX software package.^{S9} The structure was solved and refined in the space group P-1 (no. 2) with Z =4, $Z' = 2.^{S10}$ The solution was achieved by charge-flipping methods using the program SUPERFLIP^{S11} and the refinement was completed using the program SHELXL-2014/7.^{S12} The data was refined as a 2-component twin with the final twin occupancy (BASF) converging to 0.13379. All non-H atoms were refined anisotropically. With the exception of the internal C-H and N-H hydrogen atoms, which were freely refined, all H atoms were included in the refinement in the riding-model approximation (C--H = 0.95, 0.98, and 0.99 Å for Ar--H, CH₃, and CH₂; $U_{iso}(H) = 1.2U_{eq}(C)$ except for methyl groups, where $U_{iso}(H) = 1.5U_{eq}(C)$). Full-matrix least-squares refinement on F^2 led to convergence, $(\Delta/\sigma)_{max} = 0.000$, $(\Delta/\sigma)_{mean} = 0.000$, with $R_1 =$

0.0727 and $wR_2 = 0.194$ for 5143 data with $F_o^2 > 2\sigma(F_o^2)$ using 0 restraints and 700 parameters. A final difference Fourier synthesis showed features in the range of $\Delta \rho_{max} = 0.413 \text{ e}^{-}/\text{Å}^3$ to $\Delta \rho_{min} = -0.641 \text{ e}^{-}/\text{Å}^3$. All residual electron density away was within accepted norms and was deemed of no chemical significance. Molecular diagrams were generated using ORTEP-3.^{S13} CCDC-1417823 contains the supplementary crystallographic data for this structure. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via https://summary.ccdc.cam.ac.uk/structure-summary?ccdc=1417823.

Crystallographic experimental details for dicarbachlorin 14. X-ray quality crystals of 14 (C₂₈H₃₀N₂) were suspended in mineral oil at ambient temperature and a suitable crystal was selected. A mineral oil coated red needle thereby obtained of approximate dimensions 0.085 mm x 0.200 mm x 0.395 mm was mounted on a 50 µm MicroMesh MiTeGen Micromount and transferred to a Bruker AXS SMART APEX CCD X-ray diffractometer. The X-ray diffraction data were collected at 100(2) K using Mo-K_a ($\lambda = 0.71073$ Å) radiation. A total of 3672 frames were collected. The total exposure time was 10.20 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm.^{S8} The integration of the data using a triclinic unit cell yielded a total of 71618 reflections to a maximum θ angle of 28.784° (0.74 Å resolution), of which 11056 were independent (average redundancy 6.478, completeness = 99.6%, R_{int} = 4.88%, R_{sig} = 3.24%) and 7944 (71.85%) were observed with $F_o^2 > 2\sigma(F_o^2)$. The final cell constants of a = 9.6391(4) Å, b = 11.5516(4) Å, c = 19.4951(7) Å, $\alpha = 80.562(2)^{\circ}$, $\beta =$ $85.708(3)^\circ$, $\gamma = 85.426(2)^\circ$, volume = 2130.30(14) Å³, are based upon the refinement of the XYZ-centroids of 9947 reflections above 20 $\sigma(I)$ with 4.44° < 2 θ < 57.4°. Limiting indicies were as follows: $-13 \le h \le 13$, $-15 \le k \le 15$, $-26 \le l \le 26$. Data were corrected for absorption effects using the multi-scan method (SADABS).⁵⁸ The ratio of minimum to maximum apparent transmission was 0.927 with minimum and maximum SADABS generated transmission coefficients of 0.6914 and 0.7458. Solution and data analysis were performed using the WinGX software package.^{S9} The structure was solved and refined in the space group P-1 (no. 2) with Z =4, $Z' = 2.^{S10}$ The solution was achieved by charge-flipping methods using the program SUPERFLIP^{S11} and the refinement was completed using the program SHELXL-2014/7.^{S12} All non-H atoms were refined anisotropically. One of the two crystallographically independent main residues is well ordered with the exception of the H atoms attached to C18a, which were

modeled as an idealized, two position, disordered methyl group. The other main residue showed disorder in about half of the atoms. The free variable corresponding to the disorder occupancy converged to 0.83617. Equal U_{ii} constraints were applied to corresponding pairs of major and minor component non-hydrogen atoms. The internal C-H and N-H hydrogen atoms of the wellordered residue were freely refined. Most other H atoms were identifiable in the difference Fourier; however, all other H atoms were included in the refinement in the riding-model approximation (C--H = 0.95, 0.98, and 0.99 Å for Ar--H, CH₃, and CH₂; $U_{iso}(H) = 1.2U_{eq}(C)$ except for methyl groups, where $U_{iso}(H) = 1.5U_{eq}(C)$). The internal N-H hydrogen atom of the disordered residue was not identified in the difference Fourier and assigned to N54/N54B based on the observed location of the N-H hydrogen atom in the well-ordered residue corresponding to N54 in the higher part of the disordered residue. Full-matrix least-squares refinement on F^2 led to convergence, $(\Delta/\sigma)_{\text{max}} = 0.000$, $(\Delta/\sigma)_{\text{mean}} = 0.000$, with $R_1 = 0.0550$ and $wR_2 = 0.1484$ for 7944 data with $F_o^2 > 2\sigma(F_o^2)$ using 0 restraints and 600 parameters. A final difference Fourier synthesis showed features in the range of $\Delta \rho_{max} = 0.497 \text{ e}^{-1}/\text{Å}^3$ to $\Delta \rho_{min} = -0.367 \text{ e}^{-1}/\text{Å}^3$. All residual electron density away was within accepted norms and was deemed of no chemical significance. Molecular diagrams were generated using ORTEP-3.^{S13} CCDC-1417925 contains the supplementary crystallographic data for this structure. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via https://summary.ccdc.cam.ac.uk/structuresummary?ccdc=1417925.

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Figure S1. Color POV-Ray rendered space-filling drawing of dibenzodicarbaporphyrin 7.



Figure S2. Color POV-Ray rendered space-filling drawing of dicarbachlorin 14.

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Table S1. Summary of framework bond distances (Å) of compounds **7** and **14**. Each contains two crystallographically independent molecules, but only MOLE 1 values are provided for **14** since the disorder present in MOLE 2 lowers the bond precision significantly.



	7 (MOLE 1)	7 (MOLE 2)	14 (MOLE 1)
C2-C2a	1.385(5)	1.386(5)	
C2a-C2b	1.388(5)	1.392(5)	
C2b-C3b	1.391(5)	1.397(5)	
C3b-C3a	1.382(5)	1.384(5)	
C3a-C3	1.391(4)	1.384(5)	
C7-C7a	1.390(5)	1.385(5)	
C7a-C7b	1.382(5)	1.387(5)	
C7b-C8b	1.390(5)	1.384(5)	
C8b-C8a	1.384(5)	1.391(5)	
C8a-C8	1.388(5)	1.378(5)	
C21-C1	1.383(5)	1.395(5)	1.488(2)
C1-C2	1.477(5)	1.475(5)	1.427(2)
C2-C3	1.411(5)	1.423(5)	1.395(2)
C3-C4	1.474(5)	1.461(5)	1.426(2)
C4-C21	1.411(5)	1.407(5)	1.491(2)
C4-C5	1.393(5)	1.405(5)	1.385(2)
C5-C6	1.405(5)	1.391(5)	1.407(2)
C6-C22	1.410(5)	1.410(5)	1.399(2)
C6-C7	1.462(5)	1.470(5)	1.505(2)
C7-C8	1.413(5)	1.414(5)	1.534(2)
C8-C9	1.474(5)	1.480(5)	1.509(2)
C9-C22	1.403(5)	1.388(5)	1.405(2)
C9-C10	1.400(5)	1.408(5)	1.379(2)
C10-C11	1.397(5)	1.388(5)	1.416(2)
C11-N23	1.381(5)	1.383(5)	1.354(2)
C11-C12	1.428(5)	1.441(5)	1.466(2)
C12-C13	1.378(5)	1.369(5)	1.357(2)
C13-C14	1.428(5)	1.429(5)	1.496(2)
C14-N23	1.391(4)	1.392(4)	1.3807(19)
C14-C15	1.387(5)	1.393(5)	1.387(2)
C15-C16	1.391(5)	1.389(5)	1.399(2)
C16-N24	1.392(4)	1.386(4)	1.3751(18)
C16-C17	1.412(5)	1.420(5)	1.427(2)
C17-C18	1.384(5)	1.378(5)	1.387(2)
C18-C19	1.430(5)	1.433(5)	1.422(2)
C19-N24	1.384(5)	1.381(5)	1.3788(19)
C19-C20	1.389(5)	1.397(5)	1.413(2)
C20-C1	1.409(5)	1.400(5)	1.374(2)

Orange – more aromatic (1.38-1.41), green – single bond limit (\geq 1.46), blue – more single bond like (1.42-1.45), purple more double bond like (\leq 1.37).



Figure S3. UV-vis spectrum of dicarbachlorin 14 in 1% Et₃N-CHCl₃.



Figure S4. UV-vis spectrum of dicarbachlorin cation 14H⁺ in 0.05% TFA-CHCl₃.



Figure S5. UV-vis spectrum of dicarbachlorin cation **14**H⁺ in 1% TFA-CHCl₃.



Figure S6. UV-vis spectrum of dicarbachlorin cation **14**H⁺ in 10% TFA-CHCl₃.



Figure S7. 500 MHz proton NMR spectrum of dicarbachlorin 14 in CDCl₃.



Figure S8. ¹H-¹H COSY NMR spectrum of dicarbachlorin **14** in CDCl₃.



Figure S9. HSQC NMR spectrum of dicarbachlorin 14 in CDCl₃.



Figure S10. Selected nOe difference proton NMR spectra for dicarbachlorin 14 in CDCl₃.



Figure S11. DEPT-135 NMR spectrum of dicarbachlorin 14 in CDCl₃.



Figure S12. 125 MHz carbon-13 NMR spectrum of dicarbachlorin 14 in CDCl₃.



Figure S13. 500 MHz proton NMR spectrum of dicarbachlorin cation 14H⁺ in TFA-CDCl₃.



Figure S14. ¹H-¹H COSY NMR spectrum of dicarbachlorin cation **14**H⁺ in TFA-CDCl₃.



Figure S15. HSQC NMR spectrum of dicarbachlorin cation $14H^+$ in TFA-CDCl₃.



Figure S16. DEPT-135 NMR spectrum of dicarbachlorin cation $14H^+$ in TFA-CDCl₃.



Figure S17. 125 MHz carbon-13 NMR spectrum of dicarbachlorin cation 14H⁺ in TFA-CDCl₃.



Scheme S18. 500 MHz proton NMR spectrum of crude dicarbaporphyrin **15** in CDCl₃. This compound was only observed for a single experiment and eluted from the alumina column as an impure reddish-pink fraction prior to the dicarbachlorin fraction.



Figure S19. ESI mass spectrum for dicarbachlorin 14.



	16	16'	16"	16 H⁺
ΔG	-958.5782270	-958.5776600	-958.5668770	-958.9682020
B3LYP	-958.8725587	-958.8719694	-958.8609677	-959.2762669
M06-2X	-958.4611496	-958.4602386	-958.4501835	-958.8583110
B3LYP-D	-958.9165650	-958.9161657	-958.9054148	-958.8583110

Table S2. Calculated energies in hartrees for dicarbachlorins.

Molecule	Dihedral	Dihedral	Dihedral	Dihedral	Mean Absolute
	ab	da	bc	cd	Dihedral
16	0.00	0.00	0.00	0.00	0.00
16'	5.66	-7.62	1.77	0.95	4.00
16"	20.04	-15.14	-15.59	9.25	15.01
16 H⁺	-6.75	15.47	4.33	-12.45	9.75

Table S3. Dihedral angles (deg.) between the four 5-membered rings in each macrocycle.

Molecule	а	b	С	d
16	0.00	0.00	0.00	0.00
16'	11.78	3.03	2.48	3.66
16"	15.16	19.24	6.47	7.51
16 H⁺	13.68	3.78	10.33	12.91

Table S4. Angles (deg.) between the plane of each of the 5-membered rings and the overall plane of the macrocyle.

	Calculated	X-ray Minimum	Difference (kcal/mol)
ΔG	-1264.664743	-1264.662322	1.52
B3LYP	-1265.024166	-1265.020334	2.40
M06-2X	-1264.499772	-1264.49443	3.35
B3LYP-D	-1265.080558	-1265.076418	2.60



Table S5. Comparison of the energies in hartrees for the calculated minimum of unsubstituted *adj*-dibenzodicarbaporphyrin with the local minimum derived from the X-ray structure of **7**. These results demonstrate that the observed structure is 2.40-3.35 kcal/mol higher in energy than the conformational minimum (ΔG 1.52 kcal/mol) and this result is attributed to conformational changes due to crystal packing forces.



Figure S20. Calculated 3D geometry (arial and side on views) of dicarbachlorin **16**.



Figure S21. Calculated bond lengths for dicarbachlorin 16.

AICD plots for selected structures (isosurface values of 0.05, 0.06 and 0.07):



Figure S22. AICD plots for dicarbachlorin 16.



Figure S23. AICD plots for dicarbachlorin 16'.



Figure S24. AICD plots for dicarbachlorin 16".



Figure S25. AICD plots for dicarbachlorin $16H^+$.



Figure S26. AICD plots of *opp*-dibenzodicarbaporphyrin.



Figure S27. AICD plots of *adj*-dibenzodicarbaporphyrin.

Cartesian Coordinates:

16:

	X	Y	Z
С	-4.283589	-1.006942	0.000024
С	-4.402995	0.369906	0.000007
С	-3.093998	0.920771	-0.000003
Ν	-2.220839	-0.141429	0.000005
С	-2.900711	-1.342329	0.000023
С	0.964551	-4.176361	-0.000025
С	-0.419879	-4.275922	-0.000006
С	-1.015059	-2.987108	0.000013
С	0.114939	-1.993507	0.000005
С	1.376018	-2.816617	-0.00002
С	-2.349619	-2.646438	0.00003
С	4.308156	1.136359	0.000087
С	4.440366	-0.414445	-0.000024
С	3.006461	-0.931195	-0.000023
С	2.146429	0.15438	-0.000026
С	2.808339	1.391979	0.000016
С	2.662568	-2.304331	-0.000027
С	-1.076334	4.189075	-0.000025
С	0.277508	4.271779	-0.000014
С	0.782864	2.900538	-0.000004
Ν	-0.242739	2.016777	-0.00001
С	-1.395528	2.769161	-0.000023
С	-2.693129	2.266771	-0.000018
С	2.180071	2.623842	0.000017
Η	-5.083088	-1.73238	0.000035
Η	-5.314227	0.948494	0.000003
Η	-1.224513	0.039354	0.000006
Η	1.645113	-5.018904	-0.000042
Η	-0.973972	-5.20655	-0.000004
Η	0.072808	-1.348457	0.884072
Η	0.072777	-1.348445	-0.884052
Η	-3.082543	-3.447446	0.000047
Η	4.784404	1.583525	-0.877593

Η	4.784262	1.583366	0.877929
Η	4.986118	-0.776585	0.877253
Η	4.986035	-0.776448	-0.877412
Η	1.077385	0.138987	-0.000059
Η	3.480857	-3.020795	-0.000029
Η	-1.796838	4.994776	-0.000032
Η	0.890784	5.162034	-0.000012
Η	-3.497502	2.994149	-0.000022
Η	2.812621	3.507681	0.000045

16':

	Χ	Y	Ζ
С	4.235695	-1.229629	0.085412
С	4.423137	0.11755	0.058611
С	3.09739	0.709318	0.017911
Ν	2.134095	-0.265304	0.016916
С	2.797115	-1.449017	0.055325
С	-1.165354	-4.133577	-0.040662
С	0.212736	-4.294439	0.017869
С	0.864063	-3.032748	0.002216
С	-0.212297	-1.993353	-0.09582
С	-1.509487	-2.755807	-0.096677
С	2.209412	-2.744152	0.059954
С	-4.218303	1.330339	0.172527
С	-4.436574	-0.210076	0.167264
С	-3.052672	-0.801716	-0.065953
С	-2.147011	0.240259	-0.194081
С	-2.716799	1.511031	-0.012872
С	-2.774712	-2.188067	-0.085856
С	1.317017	4.119054	-0.053664
С	-0.052965	4.270389	-0.04161
С	-0.65633	2.976527	-0.019325
Ν	0.384067	2.076505	-0.019368
С	1.60399	2.726313	-0.032646
С	2.844328	2.08396	-0.011783
С	-2.048999	2.722467	0.018552
Η	4.987844	-2.005367	0.118618

Η	5.356835	0.662069	0.06746
Η	-1.884473	-4.943586	-0.029401
Η	0.722608	-5.248207	0.080435
Η	-0.069938	-1.408991	-1.009059
Η	-0.147971	-1.285097	0.733333
Η	2.905815	-3.576697	0.113095
Η	-4.559943	1.785079	1.106452
Η	-4.769297	1.819992	-0.636487
Η	-5.13316	-0.523943	-0.616635
Н	-4.855401	-0.5606	1.115848
Н	-1.117297	0.101776	-0.447849
Η	-3.623942	-2.865217	-0.029023
Н	2.062557	4.899532	-0.073224
Н	-0.609205	5.195494	-0.052977
Н	0.368589	1.066254	0.050852
Η	3.708899	2.739094	-0.014338
Н	-2.649936	3.62225	0.111926

16":

	X	Y	Z
С	-4.370892	0.486925	0.357589
С	-4.283074	-0.89104	0.336002
С	-2.92499	-1.255465	0.1142
Ν	-2.217818	-0.063977	0.047861
С	-3.071878	1.027894	0.158207
С	0.401	4.2512	-0.465638
С	-0.954844	4.189093	-0.44295
С	-1.355088	2.829767	-0.045013
С	-0.158677	2.1082	0.179682
С	0.945611	2.93631	-0.085511
С	-2.669965	2.366727	0.046987
С	4.360182	-0.559152	0.421464
С	4.315335	0.994439	0.34194
С	2.8536	1.328535	0.067393
С	2.159619	0.125486	-0.113141
С	2.9443	-1.00933	0.079912
С	2.318275	2.613294	-0.02376
С	-0.545443	-4.242073	-0.375077
С	0.831068	-4.187971	-0.381827

С	1.240184	-2.845358	-0.138533
Ν	0.065379	-2.107215	-0.018722
С	-1.052874	-2.934857	-0.121977
С	-2.385949	-2.541827	-0.011824
С	2.544068	-2.345408	-0.027082
Η	-5.259206	1.078686	0.520138
Η	-5.087881	-1.59713	0.47517
Η	-1.329725	0.03298	-0.421739
Η	1.004198	5.102368	-0.752666
Η	-1.645486	4.978217	-0.708602
Η	-0.101018	1.161466	0.684269
Η	-3.475174	3.092306	-0.011299
Η	4.645049	-0.89783	1.42254
Η	5.087418	-0.989903	-0.273654
Η	4.955096	1.376534	-0.46044
Η	4.663567	1.457798	1.269011
Η	1.149141	0.101357	-0.479913
Η	3.019111	3.445139	-0.051048
Η	-1.163827	-5.109405	-0.551268
Η	1.512472	-5.005133	-0.565468
Η	0.047494	-1.246837	0.50562
Η	-3.109695	-3.348063	-0.031085
Η	3.318135	-3.106551	0.000214

16H⁺:

	X	Y	Z
С	-4.35347	-0.541301	0.346471
С	-4.291972	0.838486	0.369743
С	-2.953395	1.230897	0.105038
Ν	-2.229224	0.057929	-0.052677
С	-3.058228	-1.047832	0.061419
С	0.483406	-4.25625	-0.170344
С	-0.903454	-4.209164	-0.161974
С	-1.360425	-2.865805	-0.146
С	-0.13127	-1.995567	-0.196667
С	1.034716	-2.947724	-0.163736
С	-2.654381	-2.399819	-0.035232
С	4.370692	0.6243	0.366051
С	4.318055	-0.927644	0.335427

С	2.871467	-1.265919	0.016433
С	2.165646	-0.077766	-0.139995
С	2.94628	1.066438	0.081756
С	2.369772	-2.585301	-0.071248
С	-0.601354	4.244084	-0.311393
С	0.77185	4.203008	-0.317987
С	1.190708	2.860087	-0.078838
Ν	0.031101	2.104964	0.034899
С	-1.095309	2.928565	-0.068175
С	-2.422683	2.526234	0.025493
С	2.511042	2.388897	0.028293
H	-5.220997	-1.15491	0.535481
Η	-5.100051	1.521251	0.583757
Н	-1.357187	0.036213	-0.552897
Н	1.070316	-5.165609	-0.157881
Н	-1.550939	-5.076438	-0.142124
H	-0.098112	-1.303893	0.649173
Η	-0.109867	-1.416806	-1.128568
Η	-3.457867	-3.125939	0.029502
H	5.056781	1.02662	-0.384889
Η	4.710785	1.001252	1.334155
Н	4.618746	-1.363409	1.2924
H	4.986387	-1.348208	-0.421718
Η	1.151397	-0.017962	-0.479309
Н	3.093729	-3.392334	0.001217
Η	-1.227064	5.10559	-0.489874
Η	1.445991	5.026231	-0.499189
H	-3.151437	3.328322	0.035731
H	3.26324	3.16943	0.078765
H	0.016865	1.264934	0.593502