Supporting Information

Modeling Kinetics and Thermodynamics of Guest Encapsulation into [M₄L₆]¹²⁻ Supramolecular Organometallic Cage

Gantulga Norjmaa, a Pietro Vidossich, b Jean-Didier Maréchal a* and Gregori Ujaque a*

a Departament de Química and Centro de Innovación en Química Avanzada (ORFEO-CINQA), Universitat Autònoma de Barcelona, Cerdanyola del Valles, 08193 Barcelona, Catalonia, Spain
b Laboratory of Molecular Modeling and Drug Discovery, Istituto Italiano di Tecnologia, Via Morego 30, 16163, Genova, Italy

Contents:
1. Behavior of the metallocage 1 in solution .................................................. S2
2. Correlations for binding energies ................................................................. S3
3. Snapshots of the APR simulations .............................................................. S5
4. Analysis of the encapsulation process ....................................................... S6
5. APR simulation detail and setup ................................................................. S8
6. Force field parameters and charges derived in implicit water solvent and in gas phase ................................................................. S10
7. Cartesian coordinates of the metallocage and NEt₄⁺ encapsulated in the metallocage optimized at DFT level ........................................ S26
1. Behavior of the metallocage 1 in solution

Figure S1. Optimized geometries of (a) metallocage, 1, and (b) NEt₄⁺ encapsulated in the metallocage with implicit solvent. In both cases, 11 K⁺ ions (purple spheres) were added explicitly in order to neutralize the system.

Figure S2. The number of K⁺ < 11 Å from the center of mass of the metallocage 1 during classical molecular dynamic simulation.
Figure S3. Cavity volume of the $2 \subset 1$ system in water solvent.

2. Correlations for binding energies

Figure S4. Plot of the computed vs experimental binding Gibbs energies.
Figure S5. Correlation between binding Gibbs energy and the cavity volume of the metallocage of the host-guest complexes.

\[ y = 0.048x - 20.343 \]
\[ R^2 = 0.309 \]

Figure S6. Correlation between binding Gibbs energy and the guest volume of the metallocage of the host-guest complexes.

\[ y = 0.031x - 328.04 \]
\[ R^2 = 0.001 \]
Table S1. Evaluation of the average number of water molecules inside the cavity along with the substrate, $V_{cavity}$ and packing coefficients for the guests+solvent encapsulated system.

| Host-guest complexes | $V_{guest}$ | 200ns of classical plain MDs | H2O inside | V cavity | PC % |
|----------------------|-------------|-----------------------------|------------|----------|------|
| 2 in 1 | $[\text{Et}_4\text{N}]^+$ | 142.2 | 2 | 324 | 56% |
| 3 in 1 | $[\text{Me}_4\text{N}]^+$ | 78.61 | 4 | 279 | 56% |
| 4 in 1 | $[\text{Et}_4\text{P}]^+$ | 154.6 | 2 | 306 | 63% |
| 5 in 1 | $[\text{5spiro}]^+$ | 122.4 | 3 | 297 | 61% |
| 6 in 1 | $[\text{Pr}_4\text{N}]^+$ | 204 | 0 | 456 | 45% |
| 7 in 1 | $[\text{Me}_2\text{Pr}_2\text{N}]^+$ | 141.3 | 2 | 325 | 55% |

3. Snapshots of the APR simulations

Figure S7. MD snapshots from APR simulations of 2 $\subset$ 1.
4. Analysis of the encapsulation process

(a) COM distance: 6.6 Å (ion-pair intermediate)
(b) 3.9 Å (before TS for encapsulation)
(c) COM distance: 3.3 Å (TS region)
(d) 3.1 Å (after TS for encapsulation)

Figure S8. Encapsulation event of 2 into the metallocage 1 in water solvent. K⁺ counter ions are in purple sphere and explicit solvent water molecules are in white surface.
Figure S9. Cavity volumes and packing coefficients of the metallocage during the encapsulation process.

Figure S10. Snapshot of the most populated structure of the encapsulated state of 6 < 1 complex from APR simulations for binding free energy calculations.
Table S2. Comparison of calculated ΔΔG.

| Guest relative to NEt₄⁺ | APR | Experiment | FEP | Full QM |
|-------------------------|-----|------------|-----|---------|
|                         | ΔΔG | ΔΔG        | ΔΔG | ΔΔE     |
| NMe₄⁺                   | 5.13 ± 0.99 | 2.87 ± 0.01 | 6.30 ± 0.05 | 15.9 |
| PEt₄⁺                   | -2.04 ± 0.84 | -0.64 ± 0.04 | -0.27 ± 0.01 | -1.6 |
| NPr₃⁺                   | 5.66 ± 0.92 | 3.46 ± 0.04 | 5.07 ± 0.10 | -0.3 |
| NMe₂Pr₂⁺                | 0.42 ± 1.12 | 1.41 ± 0.04 | 3.19 ± 0.11 | 4.9 |

Figure S11. Calculated ESP centers (yellow dots) obtained from QM ESP calculation.

5. APR simulation detail and setup

MD simulations in each APR window:
1. Minimizing 50000 cycles,
2. Running 1ps NVT at 10 K,
3. Heating the system from 10 K to 298.15 K in 100 ps,
4. Equilibrating the system under constant pressure, 50 NPT cycle,
5. NPT Production from 2.5 ns to 25 ns depending on the standard error of the mean (SEM) of the restraint forces, the SEM threshold is 0.100.

The cutoff for non-bonding interactions: 9 Å
The approach employed for computing the electrostatic forces and potential: The Particle Mesh Ewald (PME) method
The type of thermostat: Langevin
The type of barostat: Monte Carlo
The time step: 4 fs (hydrogen mass repartitioning was used)
Figure S12. Schematic representation of the APR simulations in this study.

Table S3. Comparison between calculated binding Gibbs energies of the NEt₄⁺ in the metallocage obtained using atomic charges derived with implicit solvent and without implicit solvent.

|                         | Atomic charges of [Ga₄L₆]¹²⁻ and NEt₄⁺ |
|-------------------------|----------------------------------------|
|                         | Geometry optimization in               | charge derivation in |
|                         | implicit solvent                      | implicit solvent     |
|                         | implicit solvent                      | vacuum               |
| Calculated ∆Gᵦ.bind     | -6.3 ± 0.6                             | 2.7 ± 0.5            |
| Experimental ∆Gᵦ.bind    | -6.2 ± 0.01                            |                       |

Figure S13. The number of K⁺ in less than 5 Å from the center of mass of the metallocage during 400 ns classical molecular dynamic simulation of the metallocage.
**Figure S14.** The number of $\text{K}^+$ in less than 5 Å from the center of mass of the metallocage (a) during umbrella sampling simulations and (b) during the APR simulations.

6. Force field parameters and charges derived in implicit water solvent

**BOND**

| Bond     | BONDI-M4 | CHARGED | Source        | created by         |
|----------|----------|---------|---------------|--------------------|
| A1-M4    | 52.7     | 1.9974  | SOURCE4_SOURCE5 | 17 0.0088          |
| A2-M4    | 24.6     | 2.0712  | Created by Seminario method using MCPB.py |                    |
| A3-M4    | 46.8     | 2.0187  | Created by Seminario method using MCPB.py |                    |
| A4-M4    | 46.9     | 2.0131  | Created by Seminario method using MCPB.py |                    |
| A5-M4    | 40.9     | 2.0296  | Created by Seminario method using MCPB.py |                    |
| A6-M4    | 60.4     | 1.9850  | Created by Seminario method using MCPB.py |                    |
| Y1-M1    | 50.2     | 2.0040  | Created by Seminario method using MCPB.py |                    |
| Y2-M1    | 44.0     | 2.0236  | Created by Seminario method using MCPB.py |                    |
| Y3-M1    | 43.7     | 2.0256  | Created by Seminario method using MCPB.py |                    |
| Y4-M1    | 57.5     | 1.9869  | Created by Seminario method using MCPB.py |                    |
| Y5-M1    | 51.3     | 1.9990  | Created by Seminario method using MCPB.py |                    |
| Y6-M1    | 31.0     | 2.0520  | Created by Seminario method using MCPB.py |                    |
| Y7-M2    | 28.2     | 2.0631  | Created by Seminario method using MCPB.py |                    |
| Y8-M2    | 57.5     | 1.9891  | Created by Seminario method using MCPB.py |                    |
| Y9-M2    | 28.2     | 2.0633  | Created by Seminario method using MCPB.py |                    |
| Z1-M2    | 60.6     | 1.9835  | Created by Seminario method using MCPB.py |                    |
| Z2-M2    | 48.2     | 2.0048  | Created by Seminario method using MCPB.py |                    |
| Z3-M2    | 52.8     | 2.0065  | Created by Seminario method using MCPB.py |                    |
| Z4-M3    | 22.2     | 2.0778  | Created by Seminario method using MCPB.py |                    |
| Z5-M3    | 51.0     | 2.0026  | Created by Seminario method using MCPB.py |                    |
| Z6-M3    | 46.7     | 2.0180  | Created by Seminario method using MCPB.py |                    |
| Z7-M3    | 41.7     | 2.0263  | Created by Seminario method using MCPB.py |                    |
| Z8-M3    | 65.9     | 1.9725  | Created by Seminario method using MCPB.py |                    |
| Z9-M3    | 41.5     | 2.0321  | Created by Seminario method using MCPB.py |                    |
| ca-A1    | 598.1    | 1.2358  | SOURCE4_SOURCE5 | 17 0.0088          |

**ANGL**

| ANGL     | ANGULARI A-M2 | CHARGED | Source        | created by         |
|----------|---------------|---------|---------------|--------------------|
| A1-M4-A2 | 85.30         | 81.38   | Created by Seminario method using MCPB.py |                    |
| A1-M4-A3 | 33.20         | 95.49   | Created by Seminario method using MCPB.py |                    |
A1-M4-A4  60.35    89.89    Created by Seminario method using MCPB.py
A1-M4-A5  65.00    170.39   Created by Seminario method using MCPB.py
A1-M4-A6  46.37    94.74    Created by Seminario method using MCPB.py
A2-M4-A3  46.08    83.68    Created by Seminario method using MCPB.py
A2-M4-A4  85.81    161.51   Created by Seminario method using MCPB.py
A2-M4-A5  46.96    90.09    Created by Seminario method using MCPB.py
A2-M4-A6  49.11    95.05    Created by Seminario method using MCPB.py
A3-M4-A4  74.59    80.95    Created by Seminario method using MCPB.py
A3-M4-A5  48.24    87.89    Created by Seminario method using MCPB.py
A3-M4-A6  55.36    169.38   Created by Seminario method using MCPB.py
A4-M4-A5  51.64    99.53    Created by Seminario method using MCPB.py
A4-M4-A6  68.53    101.93   Created by Seminario method using MCPB.py
A5-M4-A6  70.35    81.56    Created by Seminario method using MCPB.py
Y1-M1-Y2  20.08    170.54   Created by Seminario method using MCPB.py
Y1-M1-Y3  67.84    96.08    Created by Seminario method using MCPB.py
Y1-M1-Y4  39.55    95.47    Created by Seminario method using MCPB.py
Y1-M1-Y5  32.02    98.02    Created by Seminario method using MCPB.py
Y1-M1-Y6  45.05    90.73    Created by Seminario method using MCPB.py
Y2-M1-Y3  32.10    93.97    Created by Seminario method using MCPB.py
Y2-M1-Y4  42.68    172.17   Created by Seminario method using MCPB.py
Y2-M1-Y5  26.10    86.04    Created by Seminario method using MCPB.py
Y3-M1-Y4  73.41    82.43    Created by Seminario method using MCPB.py
Y3-M1-Y5  78.09    80.16    Created by Seminario method using MCPB.py
Y3-M1-Y6  42.67    82.80    Created by Seminario method using MCPB.py
Y4-M1-Y5  37.28    94.82    Created by Seminario method using MCPB.py
Y4-M1-Y6  21.45    85.86    Created by Seminario method using MCPB.py
Y7-M2-Z1  62.05    169.59   Created by Seminario method using MCPB.py
Y7-M2-Z2  42.08    92.21    Created by Seminario method using MCPB.py
Y7-M2-Z3  35.35    97.42    Created by Seminario method using MCPB.py
Y8-M2-Z1  31.38    97.96    Created by Seminario method using MCPB.py
Y8-M2-Z2  37.98    85.86    Created by Seminario method using MCPB.py
Z1-M2-Z2  52.17    92.21    Created by Seminario method using MCPB.py
Z1-M2-Z3  27.43    97.42    Created by Seminario method using MCPB.py
Z2-M2-Z3  72.57    82.22    Created by Seminario method using MCPB.py
Z4-M3-Z5  78.09    80.16    Created by Seminario method using MCPB.py
Z4-M3-Z6  42.67    82.80    Created by Seminario method using MCPB.py
Z4-M3-Z7  78.68    160.54   Created by Seminario method using MCPB.py
Z4-M3-Z8  36.45    98.03    Created by Seminario method using MCPB.py
Z4-M3-Z9  47.53    97.04    Created by Seminario method using MCPB.py
| Reaction | Energy | Reaction Energy | Source(s) | Charge(s) |
|----------|--------|----------------|-----------|-----------|
| Z5-M3-Z6 | 37.52  | 95.08          | Source4   | 35        | 1.2620    |
| Z5-M3-Z7 | 55.98  | 90.12          | Source4   | 35        | 1.2620    |
| Z5-M3-Z8 | 63.21  | 94.85          | Source4   | 35        | 1.2620    |
| Z5-M3-Z9 | 36.09  | 175.87         | Source4   | 35        | 1.2620    |
| Z6-M3-Z7 | 76.87  | 99.57          | Source4   | 35        | 1.2620    |
| Z6-M3-Z8 | 47.46  | 170.03         | Source4   | 35        | 1.2620    |
| Z6-M3-Z9 | 45.11  | 87.55          | Source4   | 35        | 1.2620    |
| Z7-M3-Z8 | 35.88  | 93.43          | Source4   | 35        | 1.2620    |
| Z7-M3-Z9 | 33.09  | 93.43          | Source4   | 35        | 1.2620    |
| Z8-M3-Z9 | 74.00  | 82.49          | Source4   | 35        | 1.2620    |

Charges:

1 C1 3.8930 3.0180 0.2580 ca 1 BOX -0.118210
2 H1 4.4740 2.6430 1.0920 ha 1 BOX 0.097843
3 C2 2.3130 3.8290 -1.9420 ca 1 BOX 0.014595
4 C3 3.7300 2.2060 -0.8420 ca 1 BOX -0.204358
5 H2 4.1880 1.2260 -0.8590 ha 1 BOX 0.157942
6 C4 2.9470 2.5980 -1.9450 ca 1 BOX -0.138191
7 H3 2.8030 1.9140 -2.7660 ha 1 BOX 0.146863
8 C5 3.3310 4.3250 0.2700 ca 1 BOX 0.051206
9 C6 2.5510 4.7550 -0.8610 ca 1 BOX 0.051206
10 C7 3.5440 5.2520 1.3540 ca 1 BOX 0.014595
|   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|
| 59 | C40 | 9.1010 | 2.0680 | -1.7650 | ca | 1 BOX | -0.254700 |
| 60 | H20 | 9.8030 | 2.3980 | -2.5270 | ha | 1 BOX | 0.154515 |
| 61 | C41 | 8.1170 | 1.1450 | -2.0820 | ca | 1 BOX | -0.200037 |
| 62 | H21 | 8.0410 | 0.7340 | -3.0840 | ha | 1 BOX | -0.071397 |
| 63 | C42 | 2.1280 | -7.2340 | -2.0180 | c | 1 BOX | 0.423034 |
| 64 | C43 | 1.0720 | -7.8760 | -2.8450 | ca | 1 BOX | -0.254700 |
| 65 | C44 | 0.9870 | -9.2920 | -2.8130 | ca | 1 BOX | -0.071397 |
| 66 | H22 | 1.5870 | -9.8290 | -2.0860 | ha | 1 BOX | 0.123842 |
| 67 | C45 | 0.1840 | -9.9740 | -3.7100 | ca | 1 BOX | 0.222567 |
| 68 | H23 | 0.1210 | -11.0590 | -3.6720 | ha | 1 BOX | 0.154515 |
| 69 | C46 | -0.5270 | -9.2710 | -4.7050 | ca | 1 BOX | -0.191262 |
| 70 | H24 | -1.1160 | -9.8040 | -5.4480 | ha | 1 BOX | 0.119344 |
| 71 | C47 | -0.4700 | -7.8810 | -4.7690 | ca | 1 BOX | 0.222567 |
| 72 | H25 | 0.1720 | 2.3030 | -0.9230 | ha | 1 BOX | 0.157942 |
| 73 | C48 | 0.4430 | 0.5060 | -2.0730 | ca | 1 BOX | 0.157942 |
| 74 | H26 | 1.4030 | 0.2880 | -1.6310 | ha | 1 BOX | 0.146863 |
| 75 | C49 | -1.4910 | 1.9650 | -2.2170 | ca | 1 BOX | -0.118210 |
| 76 | H27 | -2.0100 | 2.8610 | -1.8960 | ha | 1 BOX | 0.097843 |
| 77 | C50 | -0.0730 | -0.3370 | -3.0410 | ca | 1 BOX | 0.014595 |
| 78 | C51 | -2.0900 | 1.0880 | -3.1630 | ca | 1 BOX | 0.051206 |
| 79 | C52 | -1.3950 | -0.1040 | -3.5690 | ca | 1 BOX | 0.051206 |
| 80 | C53 | -3.3850 | 1.3570 | -3.7220 | ca | 1 BOX | 0.014595 |
| 81 | C54 | -2.0450 | 1.0880 | -3.1630 | ca | 1 BOX | 0.051206 |
| 82 | C55 | -2.0900 | 1.0880 | -3.1630 | ca | 1 BOX | 0.051206 |
| 83 | C56 | -3.3850 | 1.3570 | -3.7220 | ca | 1 BOX | 0.014595 |
| 84 | C57 | -4.9780 | 0.6380 | -4.9540 | ha | 1 BOX | 0.146863 |
| 85 | C58 | -3.3240 | -0.7580 | -4.9010 | ca | 1 BOX | -0.204358 |
| 86 | H30 | -3.8130 | -1.4690 | -5.5600 | ha | 1 BOX | 0.157942 |
| 87 | C59 | -5.2980 | 2.8640 | -3.2160 | c | 1 BOX | 0.423034 |
| 88 | C60 | -5.6550 | 4.2950 | -3.0180 | ca | 1 BOX | -0.071397 |
| 89 | C61 | -7.0300 | 4.6000 | -2.8500 | ca | 1 BOX | -0.200037 |
| 90 | H32 | -7.4510 | 5.9020 | -2.6470 | ca | 1 BOX | -0.254700 |
| 91 | C62 | -8.5080 | 6.1220 | -2.5200 | ha | 1 BOX | 0.154515 |
| 92 | C63 | -6.5110 | 6.9510 | -2.6070 | ca | 1 BOX | -0.191262 |
| 93 | H33 | -6.8300 | 7.9790 | -2.4520 | ha | 1 BOX | 0.119344 |
| 94 | C64 | -5.1520 | 6.6940 | -2.7670 | ca | 1 BOX | 0.222567 |
| 95 | C65 | -4.7020 | 5.3420 | -2.9660 | ca | 1 BOX | 0.064252 |
| 96 | H34 | -2.0190 | -1.4860 | -3.7480 | c | 1 BOX | 0.423034 |
| 97 | C66 | 2.4980 | -2.6570 | -4.5380 | ca | 1 BOX | -0.071397 |
| 98 | C67 | 1.6310 | -3.5540 | -5.2010 | ca | 1 BOX | 0.064252 |
| 99 | C68 | 3.8980 | -2.8610 | -4.6290 | ca | 1 BOX | -0.200037 |
| 100 | C69 | 4.5550 | -2.1690 | -4.1160 | ha | 1 BOX | 0.123842 |
| 101 | C70 | 4.4110 | -3.9400 | -5.3270 | ca | 1 BOX | -0.254700 |
| 102 | C71 | 5.4860 | -4.0960 | -5.3710 | ha | 1 BOX | 0.154515 |
| 103 | C72 | 2.1680 | -4.6820 | -5.9100 | ca | 1 BOX | 0.222567 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 107 C72 | -3.5490 | -4.8590 | -5.9600 ca | 1 BOX | -0.191262 |
| 108 H36 | 3.9470 | -5.7190 | -6.4930 ha | 1 BOX | 0.119344 |
| 109 C73 | -1.5300 | -2.4660 | -0.4230 ca | 1 BOX | -0.204358 |
| 110 H37 | -0.7970 | -1.7590 | -0.7930 ha | 1 BOX | 0.157942 |
| 111 C74 | -1.5700 | -2.7800 | 0.9540 ca | 1 BOX | -0.204358 |
| 112 H38 | -0.7970 | -1.7590 | -0.7930 ha | 1 BOX | 0.157942 |
| 113 C75 | -1.5700 | -2.7800 | 0.9540 ca | 1 BOX | -0.138191 |
| 114 H39 | -0.7970 | -1.7590 | -0.7930 ha | 1 BOX | 0.157942 |
| 115 C76 | -2.4240 | -3.0450 | -1.2950 ca | 1 BOX | -0.118210 |
| 116 C77 | -2.5340 | -3.6340 | 1.4510 ca | 1 BOX | 0.014595 |
| 117 C78 | -3.4320 | -3.9280 | -0.8190 ca | 1 BOX | 0.051206 |
| 118 C79 | -3.5220 | -4.2010 | 0.5870 ca | 1 BOX | 0.051206 |
| 119 C80 | -4.4010 | -4.5200 | -1.6960 ca | 1 BOX | 0.014595 |
| 120 H40 | -4.7040 | -5.1360 | 2.1460 ha | 1 BOX | 0.097843 |
| 121 C81 | -5.4510 | -5.2580 | -1.1810 ca | 1 BOX | -0.138191 |
| 122 H41 | -6.1810 | -5.6910 | -1.8550 ha | 1 BOX | 0.146863 |
| 123 C82 | -5.5560 | -5.4680 | 0.2110 ca | 1 BOX | -0.204358 |
| 124 H42 | -6.3980 | -6.0350 | 0.5980 ha | 1 BOX | 0.157942 |
| 125 C83 | -5.1070 | -4.1980 | -4.0690 c | 1 BOX | 0.423034 |
| 126 C84 | -4.5450 | -4.1500 | -5.4480 ca | 1 BOX | -0.071397 |
| 127 C85 | -3.1800 | -4.3930 | -5.7370 ca | 1 BOX | 0.064252 |
| 128 C86 | -5.4330 | -3.8610 | -6.5130 ca | 1 BOX | -0.200037 |
| 129 H43 | -6.4730 | -3.6630 | -6.2780 ha | 1 BOX | 0.123842 |
| 130 C87 | -4.9830 | -3.8320 | -7.8220 ca | 1 BOX | -0.254700 |
| 131 H44 | -5.6710 | -3.6000 | -8.6310 ha | 1 BOX | 0.154515 |
| 132 C88 | -3.6340 | -4.1180 | -8.1190 ca | 1 BOX | -0.191262 |
| 133 H45 | -3.2800 | -4.1180 | -9.1470 ha | 1 BOX | 0.119344 |
| 134 C89 | -2.7320 | -4.4140 | -7.1000 ca | 1 BOX | 0.222567 |
| 135 C90 | -2.3630 | -5.0150 | 3.5050 c | 1 BOX | 0.423034 |
| 136 C91 | -2.4660 | -4.9600 | 4.9930 ca | 1 BOX | -0.071397 |
| 137 C92 | -2.2120 | -6.1350 | 5.7430 ca | 1 BOX | -0.200037 |
| 138 H46 | -1.9000 | -7.0310 | 5.2170 ha | 1 BOX | 0.123842 |
| 139 C93 | -2.8500 | -3.7890 | 5.6820 ca | 1 BOX | 0.064252 |
| 140 C94 | -2.3670 | -6.1390 | 7.1200 ca | 1 BOX | -0.254700 |
| 141 H47 | -2.1630 | -7.0440 | 7.6870 ha | 1 BOX | 0.154515 |
| 142 C95 | -2.8130 | -4.9840 | 7.8010 ca | 1 BOX | -0.191262 |
| 143 H48 | -2.9680 | -5.0030 | 8.8770 ha | 1 BOX | 0.119344 |
| 144 C96 | -3.0770 | -3.8100 | 7.1000 ca | 1 BOX | 0.222567 |
| 145 C97 | -0.5890 | 2.5330 | 1.5940 ca | 1 BOX | -0.138191 |
| 146 H49 | 0.4240 | 2.9050 | 1.6950 ha | 1 BOX | 0.146863 |
| 147 C98 | -0.8790 | 1.1770 | 1.8630 ca | 1 BOX | -0.204358 |
| 148 H50 | -0.0710 | 0.5130 | 2.1410 ha | 1 BOX | 0.157942 |
| 149 C99 | -1.5820 | 3.3740 | 1.1390 ca | 1 BOX | 0.014595 |
| 150 C100 | -2.1650 | 0.6960 | 1.7760 ca | 1 BOX | -0.118210 |
| 151 H51 | -2.3710 | -0.3430 | 2.0090 ha | 1 BOX | 0.097843 |
| 152 C101 | -2.9190 | 2.8880 | 0.9380 ca | 1 BOX | 0.051206 |
| 153 C102 | -3.2180 | 1.5380 | 1.3230 ca | 1 BOX | 0.051206 |
| 154 C103 | -3.9420 | 3.6870 | 0.3590 ca | 1 BOX | -0.118210 |
| ID  | Lat.   | Long.  | Area  | Type  | Box   | Notes |
|-----|--------|--------|-------|-------|-------|-------|
| H52 | -3.7340| 4.7030 | 0.0470| ha    | 1 BOX | 0.097843 |
| C104| -4.5700| 7.0690 | 0.9740| ca    | 1 BOX | -0.071397 |
| C105| -5.2050| 3.1670 | 0.1710| ca    | 1 BOX | -0.204358 |
| H53 | -5.9760| 3.7760 | -0.2910| ha    | 1 BOX | 0.157942 |
| C106| -5.5310| 1.8680 | 0.6080| ca    | 1 BOX | -0.138191 |
| H54 | -6.5450| 1.5030 | 0.5050| ha    | 1 BOX | 0.146863 |
| C107| -0.7900| 5.7000 | 1.5690| c     | 1 BOX | 0.423034 |
| C108| -0.8490| 7.0690 | 1.0740| c     | 1 BOX | 0.014595 |
| C109| -1.2030| 7.3180 | -0.3020| ca    | 1 BOX | 0.064252 |
| C110| -0.2280| 8.1360 | 1.6630| ca    | 1 BOX | -0.200037 |
| H55 | 0.1800 | 7.9470 | 2.6510| ha    | 1 BOX | 0.123842 |
| C111| -0.0960| 9.3800 | 1.0650| ca    | 1 BOX | 0.154515 |
| H56 | 0.3810 | 10.1950| 1.6040| ha    | 1 BOX | 0.146863 |
| C112| -1.1620| 8.5640 | -0.9680| ca   | 1 BOX | 0.222567 |
| C113| -0.5290| 9.5870 | -0.2630| ca   | 1 BOX | -0.191262 |
| H57 | -0.3750| 10.5460| -0.7520| ha  | 1 BOX | 0.119344 |
| C114| -5.9080| -1.0050| 1.4750| c    | 1 BOX | 0.423034 |
| C115| -6.3130| -1.9910| 2.5110| ca  | 1 BOX | -0.071397 |
| C116| -7.1910| -3.0280| 2.1090| ca  | 1 BOX | -0.200037 |
| H58 | -7.5040| -3.0620| 1.0710| ha | 1 BOX | 0.157942 |
| C117| -5.8910| -1.9200| 3.8620| ca | 1 BOX | 0.014595 |
| C118| -7.6110| -3.9940| 3.0050| ca | 1 BOX | -0.254700 |
| H59 | -8.2740| -4.7920| 2.6800| ha | 1 BOX | 0.154515 |
| C119| -6.3190| -2.9410| 4.7820| ca | 1 BOX | 0.222567 |
| C120| -7.1660| -3.9560| 4.3420| ca | 1 BOX | -0.191262 |
| H60 | -7.4780| -4.7160| 5.0550| ca | 1 BOX | 0.119344 |
| C121| 1.6320 | -2.5640| 3.8390| ca | 1 BOX | -0.138191 |
| C122| 1.9770 | -3.5650| 3.6270| ha | 1 BOX | 0.146863 |
| C123| 0.3040 | -2.3490| 4.2570| ca | 1 BOX | -0.204358 |
| H62 | -0.3660| -3.1970| 4.3330| ha | 1 BOX | 0.157942 |
| C124| -6.3190| -2.9410| 4.7820| ca | 1 BOX | 0.222567 |
| C125| -7.1660| -3.9560| 4.3420| ca | 1 BOX | -0.191262 |
| H63 | -7.4780| -4.7160| 5.0550| ca | 1 BOX | 0.119344 |
| C126| 1.6320 | -2.5640| 3.8390| ca | 1 BOX | -0.138191 |
| C127| 1.9770 | -3.5650| 3.6270| ha | 1 BOX | 0.146863 |
| C128| 0.3040 | -2.3490| 4.2570| ca | 1 BOX | -0.204358 |
| H64 | -3.8330| 0.8870 | 3.2610| ha | 1 BOX | 0.097843 |
| C129| 0.2720 | 1.3700 | 4.8030| ca | 1 BOX | 0.014595 |
| C130| 2.3770 | 2.2510 | 3.9880| ca | 1 BOX | -0.204358 |
| H65 | 2.9920 | 3.1120 | 3.7620| ca | 1 BOX | 0.157942 |
| C131| 1.1060 | 2.4510 | 4.5600| ca | 1 BOX | -0.138191 |
| C132| 0.7680 | 3.4530 | 4.7760| ha | 1 BOX | 0.146863 |
| C133| -1.8470| 2.5980 | 5.3410| c  | 1 BOX | 0.423034 |
| C134| -3.1790| 2.3900 | 5.9790| ca | 1 BOX | -0.071397 |
| C135| -3.6840| 1.1230 | 6.3480| ca | 1 BOX | 0.064252 |
| C136| -4.9840| 1.0140 | 6.9460| ca | 1 BOX | 0.222567 |
| C137| -5.7310| 2.1660 | 7.1750| ca | 1 BOX | -0.191262 |
| C138| -6.7130| 2.0720 | 7.6320| ha | 1 BOX | 0.119344 |
|    |     |     |     |     |    |     |
|----|-----|-----|-----|-----|----|-----|
| 203 | C136 | -5.2210 | 3.4290 | 6.8120 | ca | 1 BOX | -0.254700 |
| 204 | H68  | -5.8170 | 4.3190 | 6.9960 | ha | 1 BOX | 0.154515  |
| 205 | C137 | -3.9740 | 3.5380 | 6.2190 | ca | 1 BOX | -0.071397 |
| 206 | H69  | -3.5810 | 4.5070 | 5.9310 | ha | 1 BOX | 0.064252  |
| 207 | C138 | 4.4880  | -2.7010 | 2.7840 | c  | 1 BOX | 0.423034  |
| 208 | C139 | 5.9510  | -2.5280 | 2.5800 | ca | 1 BOX | -0.071397 |
| 210 | C140 | 6.6670  | -1.3590 | 2.9350 | ca | 1 BOX | 0.064252  |
| 211 | C141 | 8.0490  | -1.2430 | 2.5610 | ca | 1 BOX | 0.222567  |
| 212 | H70  | 9.7290  | -2.1870 | 1.6320 | ha | 1 BOX | 0.119344  |
| 213 | C143 | 7.9740  | -3.4750 | 1.5980 | ca | 1 BOX | -0.254700 |
| 214 | H71  | 8.4790  | -4.2890 | 1.0860 | ha | 1 BOX | 0.154515  |
| 215 | C144 | 6.6320  | -3.5820 | 1.9200 | ca | 1 BOX | -0.200037 |
| 216 | H72  | 6.0690  | -4.4690 | 1.6500 | ha | 1 BOX | 0.123842  |
| 217 | N1   | 1.4180  | 4.2450  | -2.9410 | n  | 1 BOX | -0.205011 |
| 218 | H73  | 0.7560  | 4.9860  | -2.6950 | hn | 1 BOX | 0.188275  |
| 219 | N2   | 4.3200  | 4.8210  | 2.4450  | n  | 1 BOX | -0.205011 |
| 220 | H74  | 4.8710  | 3.9670  | 2.3360  | hn | 1 BOX | 0.188275  |
| 221 | N3   | 2.2370  | -5.8690 | -2.1040 | n  | 1 BOX | -0.205011 |
| 222 | H75  | 1.5330  | -5.4150 | -2.6960 | hn | 1 BOX | 0.188275  |
| 224 | N6   | 5.4810  | -0.8660 | -0.4360 | n  | 1 BOX | -0.205011 |
| 225 | H76  | 5.5990  | -0.3600 | 0.4500  | hn | 1 BOX | 0.188275  |
| 226 | N5   | -4.8940 | -0.1540 | 1.8290  | n  | 1 BOX | -0.205011 |
| 227 | N9   | -4.5550 | -0.2820 | 2.7880  | hn | 1 BOX | 0.188275  |
| 228 | N2   | -1.3170 | 4.7130  | 0.7820  | n  | 1 BOX | -0.205011 |
| 229 | N7   | -1.7540 | 5.0610  | -0.0780 | hn | 1 BOX | 0.188275  |
| 230 | N4   | 2.6010  | -3.8410 | 2.8530  | n  | 1 BOX | -0.205011 |
| 231 | N8   | -2.7710 | -3.0310 | 3.4580  | hn | 1 BOX | 0.188275  |
| 232 | H80  | -4.1850 | -4.3700 | -3.0770 | n  | 1 BOX | -0.205011 |
| 233 | N9   | -3.2170 | -4.4320 | -3.4110 | hn | 1 BOX | 0.188275  |
| 234 | H81  | 0.6620  | -1.4300 | -3.5350 | n  | 1 BOX | -0.205011 |
| 235 | N10  | 0.1550  | -2.1840 | -4.0030 | hn | 1 BOX | 0.188275  |
| 236 | H82  | -1.0110 | 1.5090  | 5.3550  | n  | 1 BOX | -0.205011 |
| 237 | N11  | -1.4680 | 0.6640  | 5.7030  | hn | 1 BOX | 0.188275  |
| 238 | H83  | -3.9740 | 2.6070  | -3.4470 | n  | 1 BOX | -0.205011 |
| 239 | N12  | -3.3650 | 3.4270  | -3.3650 | hn | 1 BOX | 0.188275  |
| 240 | H84  | 3.8580  | -1.6450 | 3.3870  | n  | 1 BOX | -0.205011 |
| 241 | O1   | 4.4950  | -0.8730 | 3.6090  | hn | 1 BOX | 0.188275  |
| 242 | O2   | 1.2880  | -5.5260 | -6.4790 | Y1 | 1 BOX | -0.594030 |
| 243 | O3   | 0.3000  | -3.4420 | -5.2040 | Y2 | 1 BOX | 0.406087  |
| 244 | O4   | -2.2530 | -4.6310 | -4.8090 | Y3 | 1 BOX | 0.406087  |
| 245 | O5   | -1.4410 | -4.7230 | -7.3240 | Y4 | 1 BOX | -0.594030 |
| 246 | O6   | -1.0670 | -7.1610 | -5.7340 | Y5 | 1 BOX | -0.594030 |
| 247 | O7   | 0.1920  | -5.8350 | -3.8120 | Y6 | 1 BOX | 0.406087  |
| 248 | O8   | -0.6210 | 5.9270  | -3.2440 | Y7 | 1 BOX | 0.406087  |
| 249 | O9   | -2.2570 | 7.1910  | -4.8650 | Y8 | 1 BOX | -0.594030 |
| 250 | O10  | -3.3900 | 5.1640  | -3.0940 | Y9 | 1 BOX | 0.406087  |
| 251 | O11  | -4.2220 | 7.6640  | -2.7360 | Z1 | 1 BOX | -0.594030 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|251| O11| -1.5740| 8.6700| -2.2480 Z2| 1 BOX| -0.594030|
|252| O12| -2.1350| 6.4310| -0.9720 Z3| 1 BOX| -0.406087|
|253| O13| 6.1400| -0.2970| 3.5600 Z4| 1 BOX| -0.406087|
|254| O14| 8.6560| -0.0760| 2.8330 Z5| 1 BOX| -0.594030|
|255| O15| 6.4230| 0.9550| 1.1750 Z6| 1 BOX| -0.594030|
|256| O16| 8.6560| -0.0760| 2.8330 Z5| 1 BOX| -0.594030|
|257| O17| 7.8170| 1.9630| 4.7590 Z7| 1 BOX| -0.594030|
|258| O18| 5.8060| 2.7470| 3.2380 Z9| 1 BOX| -0.406087|
|259| O19| -5.8760| -2.8610| 6.0460 A1| 1 BOX| -0.594030|
|260| O20| -5.1110| -0.9610| 4.3590 A2| 1 BOX| -0.406087|
|261| O21| -3.0730| -2.6240| 5.0850 A3| 1 BOX| -0.406087|
|262| O22| -3.5530| -2.6780| 7.6570 A4| 1 BOX| -0.594030|
|263| O23| -3.0360| -0.0290| 6.1610 A5| 1 BOX| -0.406087|
|264| O24| -5.4160| -0.2270| 7.2440 A6| 1 BOX| -0.594030|
|265| O25| -6.4410| -0.9680| 0.3480 o| 1 BOX| -0.610825|
|266| O26| -6.3290| -4.0870| -3.8410 o| 1 BOX| -0.610825|
|267| O27| -6.1560| 1.9580| -3.1790 o| 1 BOX| -0.610825|
|268| O28| 1.7580| 2.6910| -4.6070 o| 1 BOX| -0.610825|
|269| O29| 2.8090| -0.6200| -3.3260 o| 1 BOX| -0.610825|
|270| O30| 6.0570| -0.7120| -2.6540 o| 1 BOX| -0.610825|
|271| O31| 3.6860| 6.3030| 4.0900 o| 1 BOX| -0.610825|
|272| O32| 3.8870| -3.7280| 2.4100 o| 1 BOX| -0.610825|
|273| O33| -2.0900| -6.0690| 2.8920 o| 1 BOX| -0.610825|
|274| O34| -0.2710| 5.4760| 2.6810 o| 1 BOX| -0.610825|
|275| O35| 2.9150| -7.9070| -1.3200 o| 1 BOX| -0.610825|
|276| O36| -1.5200| 3.6980| 4.8580 o| 1 BOX| -0.610825|
|277| GA1| -0.5120| -5.2420| -5.6460 M1| 1 BOX| 0.689487|
|278| GA2| -2.3770| 6.9510| -2.8940 M2| 1 BOX| 0.689487|
|279| GA3| 7.2580| 1.3520| 2.9680 M3| 1 BOX| 0.689487|
|280| GA4| -4.3730| -1.5550| 6.2010 M4| 1 BOX| 0.689487|

Force field parameters and charges derived in gas phase

BOND

A1-M4 45.0 2.0010 Created by Seminario method using MCPB.py
A2-M4 15.0 2.0988 Created by Seminario method using MCPB.py
A3-M4 14.2 2.0806 Created by Seminario method using MCPB.py
A4-M4 46.6 1.9992 Created by Seminario method using MCPB.py
A5-M4 5.6 2.1491 Created by Seminario method using MCPB.py
A6-M4 44.8 2.0010 Created by Seminario method using MCPB.py
Y1-M1 48.3 1.9980 Created by Seminario method using MCPB.py
Y2-M1 15.5 2.0804 Created by Seminario method using MCPB.py
Y3-M1 8.0 2.1338 Created by Seminario method using MCPB.py
Y4-M1 52.3 1.9895 Created by Seminario method using MCPB.py
Y5-M1 48.9 1.9969 Created by Seminario method using MCPB.py
Y6-M1 4.5 2.1585 Created by Seminario method using MCPB.py
Y7-M2 6.3 2.1486 Created by Seminario method using MCPB.py
Y8-M2 44.0 2.0037 Created by Seminario method using MCPB.py
Y9-M2  8.9  2.1328 Created by Seminario method using MCPB.py
Z1-M2  48.7  1.9918 Created by Seminario method using MCPB.py
Z2-M2  45.8  1.9987 Created by Seminario method using MCPB.py
Z3-M2  21.8  2.0441 Created by Seminario method using MCPB.py
Z4-M3  48.7  1.9918 Created by Seminario method using MCPB.py
Z5-M3  45.8  1.9987 Created by Seminario method using MCPB.py
Z6-M3  10.8  2.1242 Created by Seminario method using MCPB.py
Z7-M3  46.8  1.9995 Created by Seminario method using MCPB.py
Z8-M3  47.2  2.0009 Created by Seminario method using MCPB.py
Z9-M3  12.0  2.1180 Created by Seminario method using MCPB.py
ca-A1  598.1  1.2358 SOURCE4_SOURCE5  17  0.0088

ANGL
A1-M4-A2  116.15  80.77 Created by Seminario method using MCPB.py
A1-M4-A3  54.66  92.38 Created by Seminario method using MCPB.py
A1-M4-A4  70.38  93.10 Created by Seminario method using MCPB.py
A1-M4-A5  89.64  168.75 Created by Seminario method using MCPB.py
A1-M4-A6  88.89  89.31 Created by Seminario method using MCPB.py
A2-M4-A3  61.57  96.81 Created by Seminario method using MCPB.py
A2-M4-A4  94.45  173.51 Created by Seminario method using MCPB.py
A2-M4-A5  64.27  96.62 Created by Seminario method using MCPB.py
A2-M4-A6  51.98  90.64 Created by Seminario method using MCPB.py
A3-M4-A4  121.35  81.23 Created by Seminario method using MCPB.py
A3-M4-A5  54.76  98.80 Created by Seminario method using MCPB.py
A3-M4-A6  94.73  172.53 Created by Seminario method using MCPB.py
A4-M4-A5  54.79  89.81 Created by Seminario method using MCPB.py
A4-M4-A6  79.77  91.42 Created by Seminario method using MCPB.py
A5-M4-A6  93.71  79.75 Created by Seminario method using MCPB.py
Y1-M1-Y2  121.57  81.57 Created by Seminario method using MCPB.py
Y1-M1-Y3  55.98  172.02 Created by Seminario method using MCPB.py
Y1-M1-Y4  72.22  91.77 Created by Seminario method using MCPB.py
Y1-M1-Y5  92.58  90.83 Created by Seminario method using MCPB.py
Y1-M1-Y6  59.44  87.47 Created by Seminario method using MCPB.py
Y2-M1-Y3  74.43  96.62 Created by Seminario method using MCPB.py
Y2-M1-Y4  54.16  91.28 Created by Seminario method using MCPB.py
Y2-M1-Y5  108.94  172.51 Created by Seminario method using MCPB.py
Y2-M1-Y6  51.72  97.32 Created by Seminario method using MCPB.py
Y3-M1-Y4  98.87  80.29 Created by Seminario method using MCPB.py
Y3-M1-Y5  65.73  88.55 Created by Seminario method using MCPB.py
Y3-M1-Y6  63.72  100.23 Created by Seminario method using MCPB.py
Y4-M1-Y5  84.37  91.69 Created by Seminario method using MCPB.py
Y4-M1-Y6  65.36  171.16 Created by Seminario method using MCPB.py
Y5-M1-Y6  90.80  79.51 Created by Seminario method using MCPB.py
Y7-M2-Y8  95.16  79.46 Created by Seminario method using MCPB.py
Y7-M2-Y9  63.48  100.54 Created by Seminario method using MCPB.py
Y7-M2-Z1  69.27  170.18 Created by Seminario method using MCPB.py
Y7-M2-Z2  42.20  86.63 Created by Seminario method using MCPB.py
Y7-M2-Z3  66.25  92.87 Created by Seminario method using MCPB.py
| Edge     | X1  | X2  | Created by Seminario method using MCPB.py |
|----------|-----|-----|------------------------------------------|
| Y8-M2-Y9 | 64.08 | 90.03 |                                          |
| Y8-M2-Z1 | 86.64 | 90.75 |                                          |
| Y8-M2-Z2 | 93.78 | 91.84 |                                          |
| Y8-M2-Z3 | 117.75 | 170.78 |                                     |
| Y9-M2-Z1 | 100.54 | 80.09 |                                          |
| Y9-M2-Z2 | 56.04 | 172.81 |                                          |
| Y9-M2-Z3 | 76.68 | 96.46 |                                          |
| Z1-M2-Z2 | 68.34 | 92.94 |                                          |
| Z1-M2-Z3 | 63.23 | 96.80 |                                          |
| Z2-M2-Z3 | 122.74 | 82.53 |                                          |
| Z4-M3-Z5 | 112.58 | 80.39 |                                          |
| Z4-M3-Z6 | 58.53 | 96.35 |                                          |
| Z4-M3-Z7 | 106.35 | 169.34 |                                     |
| Z4-M3-Z8 | 57.07 | 92.68 |                                          |
| Z6-M3-Z7 | 105.38 | 80.02 |                                          |
| Z6-M3-Z8 | 91.88 | 170.96 |                                         |
| Z6-M3-Z9 | 68.21 | 98.96 |                                          |
| Z7-M3-Z8 | 86.91 | 91.00 |                                          |
| Z7-M3-Z9 | 60.35 | 91.62 |                                          |
| Z8-M3-Z9 | 109.04 | 80.02 |                                          |
| ca-A1-M4 | 55.32 | 111.39 |                                         |
| ca-A2-M4 | 48.52 | 108.72 |                                         |
| ca-A3-M4 | 46.98 | 110.68 |                                         |
| ca-A4-M4 | 57.93 | 112.89 |                                         |
| ca-A5-M4 | 59.65 | 109.91 |                                         |
| ca-A6-M4 | 58.83 | 110.22 |                                         |
| ca-A1-M1 | 58.91 | 112.57 |                                         |
| ca-A2-M1 | 50.12 | 110.10 |                                         |
| ca-A3-M1 | 57.90 | 108.64 |                                         |
| ca-A4-M1 | 55.51 | 112.84 |                                         |
| ca-A5-M1 | 52.71 | 112.72 |                                         |
| ca-Y2-M1 | 59.39 | 108.02 |                                         |
| ca-Y7-M2 | 54.62 | 108.65 |                                         |
| ca-Y8-M2 | 52.19 | 112.76 |                                         |
| ca-Y9-M2 | 55.63 | 108.73 |                                         |
| ca-Z1-M2 | 54.74 | 112.58 |                                         |
| ca-Z2-M2 | 59.83 | 111.73 |                                         |
| ca-Z3-M2 | 54.80 | 110.70 |                                         |
| ca-Z4-M3 | 49.78 | 110.53 |                                         |
| ca-Z5-M3 | 57.76 | 113.47 |                                         |
| ca-Z6-M3 | 53.64 | 108.88 |                                         |
| ca-Z7-M3 | 55.87 | 112.13 |                                         |
| ca-Z8-M3 | 55.77 | 112.04 |                                         |
Charges:

|   |   |   |   |   |
|---|---|---|---|---|
| 1 C1 | 5.3900 | 5.8910 | -1.6280 ca | 1 BOX | -0.143496 |
| 2 H1 | 6.2160 | 5.4540 | -1.0780 ha | 1 BOX | 0.139616 |
| 3 C2 | 3.1970 | 7.0220 | -3.0500 ca | 1 BOX | 0.393566 |
| 4 C3 | 5.5500 | 6.3950 | -2.8970 ca | 1 BOX | -0.195908 |
| 5 H2 | 6.5290 | 6.3550 | -3.3770 ha | 1 BOX | 0.135251 |
| 6 C4 | 4.4690 | 6.9560 | -3.6060 ca | 1 BOX | -0.181359 |
| 7 H3 | 4.6230 | 7.3590 | -4.5970 ha | 1 BOX | 0.114661 |
| 8 C5 | 4.1110 | 5.9140 | -1.0180 ca | 1 BOX | 0.001430 |
| 9 C6 | 2.9840 | 6.4760 | -1.7280 ca | 1 BOX | 0.001430 |
| 10 C7 | 3.9270 | 5.3870 | 0.3040 ca | 1 BOX | 0.393566 |
| 11 C8 | 1.7120 | 6.4750 | -1.0910 ca | 1 BOX | -0.143496 |
| 12 H4 | 0.8500 | 6.9220 | -1.5780 ha | 1 BOX | 0.139616 |
| 13 C9 | 2.6640 | 5.3780 | 0.8580 ca | 1 BOX | -0.181359 |
| 14 H5 | 2.5310 | 4.9760 | 1.8590 ha | 1 BOX | 0.114661 |
| 15 C10 | 1.5560 | 5.9220 | 0.1640 ca | 1 BOX | -0.195908 |
| 16 H6 | 0.5800 | 5.9320 | 0.6420 ha | 1 BOX | 0.135251 |
| 17 C11 | 5.8870 | 5.8030 | 1.7010 c | 1 BOX | 0.807075 |
| 18 C12 | 6.8720 | 5.2730 | 2.6950 ca | 1 BOX | -0.153938 |
| 19 C13 | 7.1600 | 3.9040 | 2.9570 ca | 1 BOX | 0.213805 |
| 20 C14 | 7.5330 | 6.2900 | 3.4490 ca | 1 BOX | -0.301874 |
| 21 H7 | 7.2760 | 7.3170 | 3.2080 ha | 1 BOX | 0.116258 |
| 22 C15 | 8.1360 | 3.5930 | 4.0060 ca | 1 BOX | 0.263385 |
| 23 C16 | 8.7410 | 4.6290 | 4.7210 ca | 1 BOX | -0.230920 |
| 24 H8 | 9.4560 | 4.3520 | 5.4980 ha | 1 BOX | 0.042985 |
| 25 C17 | 8.4410 | 5.9810 | 4.4410 ca | 1 BOX | -0.198917 |
| 26 H9 | 8.9250 | 6.7800 | 5.0140 ha | 1 BOX | 0.028481 |
| 27 C18 | 2.2510 | 8.5880 | -4.7380 c | 1 BOX | 0.807075 |
| 28 C19 | 1.0290 | 8.9840 | -5.4920 ca | 1 BOX | -0.153938 |
| 29 C20 | 1.2530 | 9.9470 | -6.5240 ca | 1 BOX | -0.301874 |
| 30 H10 | 2.2760 | 10.2860 | -6.6630 ha | 1 BOX | 0.116258 |
| 31 C21 | -0.2860 | 8.4890 | -5.2650 ca | 1 BOX | 0.213805 |
| 32 C22 | 0.2200 | 10.4180 | -7.3070 ca | 1 BOX | -0.198917 |
| 33 H11 | 0.4180 | 11.1460 | -8.1010 ha | 1 BOX | 0.028481 |
| 34 C23 | -1.3800 | 9.0300 | -6.0800 ca | 1 BOX | 0.263385 |
| 35 C24 | -1.1000 | 9.9600 | -7.0830 ca | 1 BOX | -0.230920 |
| 36 H12 | -1.9390 | 10.3270 | -7.6770 ha | 1 BOX | 0.042985 |
| 37 C25 | 4.7310 | -6.3050 | -2.4680 ca | 1 BOX | 0.393566 |
| 38 C26 | 6.6540 | -4.8240 | -0.9630 ca | 1 BOX | -0.143496 |
| 39 H13 | 7.3780 | -4.2560 | -0.3930 ha | 1 BOX | 0.139616 |
| 40 C27 | 6.7000 | -6.1950 | -1.0270 ca | 1 BOX | -0.195908 |
| 41 H14 | 7.4800 | -6.7360 | -0.4890 ha | 1 BOX | 0.135251 |
| 42 C28 | 5.7610 | -6.9340 | -1.7740 ca | 1 BOX | -0.181359 |
| 43 H15 | 5.8360 | -8.0080 | -1.8270 ha | 1 BOX | 0.114661 |
|   |   |   |   |   |
|---|---|---|---|---|
| 44 | C29 | 5.6210 | -4.1260 | -1.6380 ca | 1 BOX | 0.001430 |
| 45 | C30 | 4.6240 | -4.8610 | -2.3850 ca | 1 BOX | 0.001430 |
| 46 | C31 | 5.5510 | -2.6920 | -1.5660 ca | 1 BOX | 0.393566 |
| 47 | C32 | 3.5680 | -4.1310 | -2.9950 ca | 1 BOX | -0.143496 |
| 48 | H16 | 2.8110 | -4.6380 | -3.5890 ha | 1 BOX | 0.139616 |
| 49 | C33 | 4.4780 | -2.0410 | -2.1420 ca | 1 BOX | -0.181359 |
| 50 | H17 | 4.4200 | -0.9580 | -2.0780 ha | 1 BOX | 0.114661 |
| 51 | C34 | 3.4890 | -2.7620 | -2.8490 ca | 1 BOX | -0.195908 |
| 52 | H18 | 2.6680 | -2.2210 | -3.3120 ha | 1 BOX | 0.135251 |
| 53 | C35 | 7.8480 | -1.8350 | -1.4530 c | 1 BOX | 0.807075 |
| 54 | C36 | 8.7710 | -0.7960 | -0.9050 ca | 1 BOX | -0.153938 |
| 55 | C37 | 8.5140 | 0.0700 | 0.1950 ca | 1 BOX | 0.213805 |
| 56 | C38 | 9.5410 | 1.0520 | 0.5560 ca | 1 BOX | 0.263385 |
| 57 | C39 | 10.7250 | 1.1200 | -0.1820 ca | 1 BOX | -0.230920 |
| 58 | H19 | 11.4600 | 1.8700 | 0.1160 ha | 1 BOX | 0.042985 |
| 59 | C40 | 10.9580 | 0.2480 | -1.2690 ca | 1 BOX | -0.198917 |
| 60 | H20 | 11.8920 | 0.3190 | -1.8370 ha | 1 BOX | 0.028481 |
| 61 | C41 | 10.0050 | -0.6870 | -1.6160 ca | 1 BOX | -0.301874 |
| 62 | H21 | 10.1490 | -1.3680 | -2.4490 ha | 1 BOX | 0.116258 |
| 63 | C42 | 3.9320 | -8.3740 | -3.6240 c | 1 BOX | 0.807075 |
| 64 | C43 | 2.7660 | -9.0530 | -4.2560 ca | 1 BOX | -0.153938 |
| 65 | C44 | 2.9440 | -10.4620 | -4.4270 ca | 1 BOX | -0.301874 |
| 66 | H22 | 3.8830 | -10.8820 | -4.0800 ha | 1 BOX | 0.116258 |
| 67 | C45 | 1.9700 | -11.2500 | -5.0000 ca | 1 BOX | -0.198917 |
| 68 | H23 | 2.1230 | -12.3310 | -5.1020 ha | 1 BOX | 0.028481 |
| 69 | C46 | 0.7680 | -10.6620 | -5.4560 ca | 1 BOX | -0.230920 |
| 70 | H24 | -0.0150 | -11.2560 | -5.9290 ha | 1 BOX | 0.042985 |
| 71 | C47 | 0.5460 | -9.2890 | -5.3320 ca | 1 BOX | 0.263385 |
| 72 | C48 | 1.5530 | -8.4390 | -4.6830 ca | 1 BOX | 0.213805 |
| 73 | C49 | -1.7160 | 0.5070 | -4.1680 ca | 1 BOX | -0.195908 |
| 74 | H25 | -1.7510 | 0.5920 | -3.0850 ha | 1 BOX | 0.135251 |
| 75 | C50 | -1.1060 | -0.6270 | -4.7480 ca | 1 BOX | -0.181359 |
| 76 | H26 | -0.6680 | -1.3910 | -4.1110 ha | 1 BOX | 0.114661 |
| 77 | C51 | -2.2480 | 1.5090 | -4.9500 ca | 1 BOX | -0.143496 |
| 78 | H27 | -2.7110 | 2.3750 | -4.4870 ha | 1 BOX | 0.139616 |
| 79 | C52 | -1.0380 | -0.7810 | -6.1210 ca | 1 BOX | 0.393566 |
| 80 | C53 | -2.2170 | 1.4050 | -6.3660 ca | 1 BOX | 0.001430 |
| 81 | C54 | -1.6270 | 0.2280 | -6.9670 ca | 1 BOX | 0.001430 |
| 82 | C55 | -2.7990 | 2.4160 | -7.2160 ca | 1 BOX | 0.393566 |
| 83 | C56 | -1.6920 | 0.0740 | -8.3770 ca | 1 BOX | -0.143496 |
| 84 | H28 | -1.2880 | -0.8220 | -8.8260 ha | 1 BOX | 0.139616 |
| 85 | C57 | -2.7840 | 2.2330 | -8.5890 ca | 1 BOX | -0.181359 |
| 86 | H29 | -3.2310 | 2.9910 | -9.2190 ha | 1 BOX | 0.114661 |
| 87 | C58 | -2.2540 | 1.0570 | -9.1580 ca | 1 BOX | -0.195908 |
| 88 | H30 | -2.2890 | 0.9310 | -10.2410 ha | 1 BOX | 0.135251 |
| 89 | C59 | -4.6510 | 4.0480 | -7.1250 ca | 1 BOX | 0.807075 |
| 90 | C60 | -5.2380 | 5.2310 | -6.4360 ca | 1 BOX | -0.153938 |
| 91 | C61 | -6.5800 | 5.5270 | -6.8250 ca | 1 BOX | -0.301874 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 92 H31 | -7.0340 | 4.8680 | -7.5590 ha | 1 BOX | 0.116258 |
| 93 C62 | -7.2690 | 6.5910 | -6.2840 ca | 1 BOX | -0.198917 |
| 94 H32 | -8.3040 | 6.7880 | -6.5850 ha | 1 BOX | 0.028481 |
| 95 C63 | -6.6410 | 7.4260 | -5.3330 ca | 1 BOX | -0.230920 |
| 96 H33 | -7.1600 | 8.2780 | -4.9240 ca | 1 BOX | 0.263385 |
| 97 C64 | -5.3270 | 7.1930 | -7.7400 ca | 1 BOX | -0.230920 |
| 98 C65 | -4.5860 | 6.0530 | -5.4740 ca | 1 BOX | 0.213805 |
| 99 C66 | 5.0820 | -1.9980 | -7.5680 c | 1 BOX | 0.807075 |
| 100 C67 | 1.0830 | -3.3420 | -9.1520 ca | 1 BOX | -0.153938 |
| 101 C68 | 0.3870 | -4.5810 | -9.3460 ca | 1 BOX | 0.213805 |
| 102 C69 | 1.9030 | -2.3460 | -9.860 ca | 1 BOX | -0.301874 |
| 103 H34 | 0.3140 | -4.4460 | -10.600 ha | 1 BOX | 0.028481 |
| 104 C70 | 2.2120 | -3.460 | -10.320 ca | 1 BOX | 0.135251 |
| 105 C71 | 2.4290 | -5.7300 | -9.1280 ca | 1 BOX | -0.143496 |
| 106 C72 | 2.4910 | -6.680 | -9.5520 ca | 1 BOX | 0.195908 |
| 107 C73 | -3.3720 | -6.0070 | 1.5160 ca | 1 BOX | 0.001430 |
| 108 C74 | -3.3060 | -6.9500 | 0.1000 ca | 1 BOX | 0.001430 |
| 109 C75 | -4.3360 | -7.2160 | 1.9750 ca | 1 BOX | 0.139616 |
| 110 C76 | -4.5610 | -7.3260 | 3.0260 ha | 1 BOX | 0.139616 |
| 111 C77 | -4.5130 | -8.9380 | 1.4660 ca | 1 BOX | 0.135251 |
| 112 C78 | -3.4910 | -8.3460 | 1.4660 ca | 1 BOX | 0.139616 |
| 113 C79 | -3.3720 | -8.9500 | 0.7940 ca | 1 BOX | 0.139616 |
| 114 C80 | -3.4360 | -7.1150 | -4.5550 ca | 1 BOX | -0.153938 |
| 115 C81 | -4.2920 | -8.1250 | -0.2750 ca | 1 BOX | -0.181359 |
| 116 C82 | -4.5130 | -9.3800 | -0.9560 ha | 1 BOX | 0.114661 |
| 117 C83 | -4.5880 | -8.2450 | 1.0970 ca | 1 BOX | 0.195908 |
| 118 C84 | -5.0240 | -9.1750 | 1.4660 ca | 1 BOX | 0.135251 |
| 119 C85 | -6.0700 | -7.2220 | -3.0920 c | 1 BOX | 0.807075 |
| 120 C86 | -6.4350 | -7.1150 | -4.5550 ca | 1 BOX | 0.153938 |
| 121 C87 | -6.3090 | -8.170 | -5.1780 ca | 1 BOX | 0.213805 |
| 122 C88 | -6.4920 | -7.3880 | -5.3630 ca | 1 BOX | -0.301874 |
| 123 C89 | -6.4190 | -7.5990 | -4.8400 ha | 1 BOX | 0.116258 |
| 124 C90 | -6.4250 | -7.3850 | -6.7390 ca | 1 BOX | -0.198917 |
| 125 C91 | -6.3220 | -7.5800 | -7.3360 ha | 1 BOX | 0.028481 |
| 126 C92 | -4.1940 | -7.1250 | -7.3810 ca | 1 BOX | -0.230920 |
| 127 C93 | -4.1030 | -7.1270 | -8.4680 ha | 1 BOX | 0.028481 |
| 128 C94 | -3.0390 | -6.8600 | -6.6430 ca | 1 BOX | 0.263385 |
| 129 C95 | -3.2750 | -5.9070 | 4.7000 c | 1 BOX | 0.807075 |
| 130 C96 | -3.6290 | -5.7090 | 6.1400 ca | 1 BOX | -0.153938 |
| 131 C97 | -3.4250 | -6.8580 | 6.9590 ca | 1 BOX | -0.301874 |
| 132 C98 | -3.0030 | -7.7340 | 6.4760 ha | 1 BOX | 0.116258 |
| 133 C99 | -4.1500 | -4.5200 | 6.7160 ca | 1 BOX | 0.213805 |
| 140 | C94 | -3.7570 | -6.8540 | 8.2980 ca | 1 BOX | -0.198917  |
|-----|-----|---------|---------|----------|-------|------------|
| 141 | H47 | -3.5940 | -7.7480 | 8.9090 ha | 1 BOX | 0.028481   |
| 142 | C95 | -4.3050 | -5.6910 | 8.8840 ca | 1 BOX | -0.230920  |
| 143 | H48 | -4.5810 | -5.6600 | 9.9400 ha | 1 BOX | 0.042985   |
| 144 | C96 | -4.5120 | -4.5320 | 8.1310 ca | 1 BOX | 0.263385   |
| 145 | H49 | -3.3160 | 2.9650 | 0.0420 ca | 1 BOX | -0.181359  |
| 146 | C97 | -2.7140 | 2.9960 | -0.8630 ha | 1 BOX | 0.114661   |
| 147 | C98 | -3.7980 | 1.7290 | 0.5280 ca | 1 BOX | -0.195908  |
| 148 | H50 | -3.5690 | 0.8200 | -0.0230 ha | 1 BOX | 0.135251   |
| 149 | C99 | -3.5810 | 4.1480 | 0.7070 ca | 1 BOX | 0.393566   |
| 150 | H51 | -4.5390 | 1.6600 | 1.6870 ca | 1 BOX | -0.143496  |
| 151 | C100| -4.3820 | 4.1130 | 1.9070 ca | 1 BOX | 0.001430   |
| 152 | C101| -4.8530 | 2.8430 | -1.2970 ca | 1 BOX | 0.213805   |
| 153 | H52 | -4.4390 | 6.2550 | 2.0000 ha | 1 BOX | 0.139616   |
| 154 | C102| -5.6720 | 2.8120 | 3.5900 ca | 1 BOX | -0.153938  |
| 155 | H53 | -5.5640 | 5.2360 | 3.7060 ca | 1 BOX | 0.042985   |
| 156 | C103| -6.0030 | 3.9970 | 4.2180 ca | 1 BOX | -0.143496  |
| 157 | H54 | -2.3380 | 6.2970 | -0.8000 c | 1 BOX | 0.116258   |
| 158 | C104| -2.0630 | 7.5810 | 0.0860 ca | 1 BOX | -0.153938  |
| 159 | C105| -2.2690 | 7.8160 | -1.2970 ca | 1 BOX | 0.213805   |
| 160 | H55 | -1.4770 | 9.9250 | 0.4320 ca | 1 BOX | -0.198917  |
| 161 | C106| -1.4610 | 8.4100 | 1.9720 ha | 1 BOX | 0.116258   |
| 162 | H56 | -1.4100 | 10.7320 | 1.0910 ha | 1 BOX | 0.028481   |
| 163 | C107| -2.3380 | 6.2970 | -0.8000 c | 1 BOX | 0.807075   |
| 164 | C108| -2.0630 | 7.5810 | 0.0860 ca | 1 BOX | -0.153938  |
| 165 | C109| -2.2690 | 7.8160 | -1.2970 ca | 1 BOX | 0.213805   |
| 166 | H57 | -1.6180 | 11.1930 | -1.3460 ha | 1 BOX | 0.042985   |
| 167 | C110| -7.5770 | 1.4160 | 4.2540 c | 1 BOX | 0.042985   |
| 168 | C111| -8.0540 | 0.1280 | 4.8380 ca | 1 BOX | -0.153938  |
| 169 | C112| -9.4540 | -0.1030 | 4.6930 ca | 1 BOX | -0.198917  |
| 170 | H58 | -10.0230 | -0.6520 | 4.1600 ha | 1 BOX | 0.116258   |
| 171 | C113| -7.2500 | -0.8230 | 5.5240 ca | 1 BOX | 0.213805   |
| 172 | H59 | -11.1250 | -1.4050 | 5.0630 ha | 1 BOX | 0.028481   |
| 173 | C114| -7.9050 | -2.0030 | 6.0930 ca | 1 BOX | 0.263385   |
| 174 | C115| -9.2770 | -2.1870 | 5.9060 ca | 1 BOX | -0.230920  |
| 175 | H60 | -9.7250 | -3.0860 | 6.3310 ha | 1 BOX | 0.042985   |
| 176 | C116| -2.0810 | -0.2520 | 4.7760 ca | 1 BOX | -0.181359  |
| 177 | H61 | 2.5270 | -0.2700 | 3.7850 ha | 1 BOX | 0.114661   |
| 178 | C117| 0.6840 | -0.1090 | 4.9160 ca | 1 BOX | -0.195908  |
| 179 | H62 | 0.0730 | 0.0010 | 4.0240 ha | 1 BOX | 0.135251   |
| 180 | C118| 2.9020 | -0.3880 | 5.8830 ca | 1 BOX | 0.393566   |
| 181 | C119| 0.0840 | -0.1270 | 6.1570 ca | 1 BOX | -0.143496  |
| 182 | H63 | -0.9930 | -0.0220 | 6.2370 ha | 1 BOX | 0.139616   |
| Number | Element | X-Coordinate | Y-Coordinate | Z-Coordinate | Box | Factor |
|--------|---------|--------------|--------------|--------------|-----|--------|
| 236   | H82    | -1.7630      | -0.6020      | 8.1640       | 1 BOX | 0.582649 |
| 237   | N11    | -3.4310      | 3.5660       | -6.6690      | 1 BOX | -0.990800 |
| 238   | H83    | -3.0020      | 4.1050       | -5.9140      | 1 BOX | 0.582649 |
| 239   | N12    | 4.3060       | -0.4970      | 5.6790       | 1 BOX | -0.990800 |
| 240   | H84    | 4.7220       | 0.0020       | 4.8870       | 1 BOX | 0.582649 |
| 241   | O1     | 0.9590       | -6.9500      | -7.4200      | 1 BOX | -0.496622 |
| 242   | O2     | 0.0840       | -4.7240      | -6.2440      | 1 BOX | -0.547732 |
| 243   | O3     | -1.9760      | -6.5240      | -4.5560      | 1 BOX | -0.547732 |
| 244   | O4     | -1.8810      | -6.6380      | -7.2130      | 1 BOX | -0.496622 |
| 245   | O5     | -0.5440      | -8.7150      | -5.7690      | 1 BOX | -0.496622 |
| 246   | O6     | 1.2550       | -7.1660      | -4.5680      | 1 BOX | -0.547732 |
| 247   | O7     | -0.6170      | 7.5890       | -4.3720      | 1 BOX | -0.547732 |
| 248   | O8     | -2.5920      | 8.6020       | -5.8300      | 1 BOX | -0.496622 |
| 249   | O9     | -3.3580      | 5.8920       | -5.0350      | 1 BOX | -0.547732 |
| 250   | O10    | -4.7130      | 7.9530       | -4.0510      | 1 BOX | -0.496622 |
| 251   | O11    | -2.4000      | 9.3890       | -3.0700      | 1 BOX | -0.496622 |
| 252   | O12    | -2.6020      | 6.8840       | -2.1790      | 1 BOX | -0.547732 |
| 253   | O13    | 6.4560       | 0.0940       | 3.9400       | 1 BOX | -0.547732 |
| 254   | O14    | 9.0230       | -0.3070      | 3.3770       | 1 BOX | -0.496622 |
| 255   | O15    | 7.4270       | 0.0710       | 0.9370       | 1 BOX | -0.547732 |
| 256   | O16    | 9.2960       | 1.8440       | 1.5710       | 1 BOX | -0.496622 |
| 257   | O17    | 8.3970       | 2.3290       | 4.2360       | 1 BOX | -0.496622 |
| 258   | O18    | 6.6350       | 2.8700       | 2.3330       | 1 BOX | -0.547732 |
| 259   | O19    | -7.1590      | -2.8510      | 6.7590       | 1 BOX | -0.496622 |
| 260   | O20    | -5.9500      | -0.7250      | 5.7190       | 1 BOX | -0.547732 |
| 261   | O21    | -4.3440      | -3.3830      | 6.0730       | 1 BOX | -0.547732 |
| 262   | O22    | -5.0260      | -3.4370      | 8.6400       | 1 BOX | -0.496622 |
| 263   | O23    | -3.7450      | -0.8830      | 7.9980       | 1 BOX | -0.547732 |
| 264   | O24    | -6.3390      | -0.8920      | 8.6040       | 1 BOX | -0.496622 |
| 265   | O25    | -8.3780      | 2.2950       | 3.8920       | 1 BOX | -0.677284 |
| 266   | O26    | -5.6970      | -7.6490      | -2.6700      | 1 BOX | -0.677284 |
| 267   | O27    | -5.2490      | 3.4930       | -8.0640      | 1 BOX | -0.677284 |
| 268   | O28    | 3.3480       | 9.1330       | -4.9780      | 1 BOX | -0.677284 |
| 269   | O29    | 1.0130       | -0.9550      | -8.0770      | 1 BOX | -0.677284 |
| 270   | O30    | 8.1900       | -2.5840      | -2.3820      | 1 BOX | -0.677284 |
| 271   | O31    | 5.7900       | 7.0190       | 1.4680       | 1 BOX | -0.677284 |
| 272   | O32    | 4.6440       | -2.3520      | 6.9790       | 1 BOX | -0.677284 |
| 273   | O33    | -2.6600      | -6.9110      | 4.3150       | 1 BOX | -0.677284 |
| 274   | O34    | -1.9610      | 6.0990       | 1.9610       | 1 BOX | -0.677284 |
| 275   | O35    | 4.9990       | -8.9980      | -3.4520      | 1 BOX | -0.677284 |
| 276   | O36    | -1.0720      | 1.1190       | 10.7330      | 1 BOX | -0.677284 |
| 277   | GA1    | -0.3600      | -6.7330      | -5.9340      | 1 BOX | 0.839067 |
| 278   | GA2    | -2.7400      | 7.6830       | -4.0560      | 1 BOX | 0.839067 |
| 279   | GA3    | 7.8150       | 1.1550       | 2.7230       | 1 BOX | 0.839067 |
| 280   | GA4    | -5.4000      | -2.0400      | 7.2610       | 1 BOX | 0.839067 |

# 7. Cartesian coordinates:
#

NEt₄⁺ encapsulated in the metallocage (neutral complex with K⁺ counter ions)

320 atoms

C  0.406481  -1.268382  5.839094
H  0.611211  -2.330805  5.909344
C  -0.047501  1.520207  5.754510
C  1.376728  -0.378129  6.241795
H  2.326579  -0.747956  6.610860
C  1.167531  1.013803  6.184148
H  1.958909  1.689095  6.472151
C  -0.850929  -0.795243  5.370779
C  -1.100607  0.622364  5.348816
C  -1.889832  -1.691491  4.921930
C  -2.375670  1.088263  4.917917
H  -2.591570  2.145947  4.820643
C  -3.115972  -1.189486  4.513678
H  -3.886081  -1.864779  4.170136
C  -3.351605  0.197293  4.528126
H  -4.312547  0.569790  4.199452
C  -2.477027  -4.117589  5.019310
C  -1.854838  -5.471412  5.080822
C  -0.465907  -7.10929  4.973289
C  -2.729199  -6.570065  5.270999
H  -3.792177  -6.373238  5.352619
C  0.032932  -7.053651  5.072062
C  -0.859702  -8.107188  5.253972
H  -0.465870  -9.119021  5.317781
C  -2.242299  -7.863490  5.353119
H  -2.925968  -8.695840  5.496646
C  0.314788  3.931634  6.348405
C  -0.312273  5.278287  6.197419
C  0.386051  6.376228  6.756244
H  1.346721  7.191956  7.223835
C  -1.560471  5.508101  5.574332
C  -0.142887  7.655659  6.705351
H  0.409106  8.489953  7.129278
C  -2.117851  6.827695  5.555534
C  -1.397012  7.883073  6.111101
H  -1.823752  8.882605  6.074524
C  4.566316  -1.527685  -1.234412
C  3.851782  -2.803329  1.181439
H  3.511152  -3.319321  2.073198
C  3.841747  -3.488669  -0.014361
H  3.552886  -4.532099  -0.030485
C  4.208597  -2.866050  -1.223669
H  4.203644  -3.430571  -2.144284
C  4.226149  -1.429160   1.220288
C  4.537532  -0.760240  -0.012729
C  4.305498  -0.680733   2.450226
C  4.815221   0.635681   0.014623
H   4.958386   1.203738  -0.896905
C  4.617374   0.667103   2.432550
H   4.646881   1.225633   3.356414
C  4.852596   1.320696   1.209388
H   5.041421   2.385227   1.205217
C  4.675673  -1.124259   4.873431
C  4.385609  -2.110878   5.955653
C  3.660264  -3.308249   5.757195
C  3.455762  -4.212932   6.849873
C  3.951536  -3.881909   8.109619
H   3.780655  -4.569510   8.934622
C  4.656739  -2.680813   8.307628
H   5.030487  -2.436169   9.298055
C  4.876575  -1.813287   7.250267
H   5.420110  -0.886493   7.395892
C   5.627834  -1.410786  -3.496720
C   6.184313  -0.419816  -4.462639
C   6.548110  -0.899326  -5.744393
H   6.457532  -1.961372  -5.943792
C   6.981150  -0.027855  -6.730647
H   7.246789  -0.406974  -7.713647
C   7.060686   1.352710  -6.472822
H   7.376438   2.046649  -7.248435
C   6.736705   1.860343  -5.214352
C   6.326487   0.956646  -4.180436
C   1.747809   5.788289   3.215660
H   1.548750   6.199388   4.200961
C   3.082980   5.508049   2.852603
H   3.886850   5.727237   3.539740
C   0.705909   5.590397   2.336431
H  -0.299400   5.864602   2.637808
C   3.368747   4.984707   1.601325
C   0.953633   5.026728   1.053382
C   2.295831   4.659757   0.695034
C  -0.094060   4.781881   0.100137
C   2.525897   3.978337  -0.530039
H  -3.512402   3.632731  -0.809444
C   0.170321   4.088502  -1.064602
H  -0.654849   3.823078  -1.710493
C   1.479052   3.678233  -1.370231
H   1.666504   3.103624  -2.264492
C  -2.273222   5.816409  -0.470166
C  -3.520491   6.348117   0.138035
C  -4.408884   7.069339  -0.697683
| Atoms | x         | y         | z         |
|-------|-----------|-----------|-----------|
| H     | -4.12695  | 7.238904  | -1.731192 |
| C     | -5.620556 | 7.531651  | -0.212548 |
| H     | -6.293698 | 8.083233  | -0.863316 |
| C     | -5.995535 | 7.279466  | 1.121626  |
| H     | -6.955404 | 7.620235  | 1.503042  |
| C     | -5.143956 | 6.587369  | 1.979562  |
| C     | -3.870358 | 6.137174  | 1.492064  |
| C     | -5.871634 | 4.804020  | 1.780423  |
| C     | -7.068230 | 4.610973  | 0.906885  |
| C     | -7.006835 | 4.154361  | -0.431694 |
| C     | -8.324873 | 4.952390  | 1.457864  |
| H     | -8.357473 | 5.295565  | 2.486250  |
| C     | -9.484412 | 4.878690  | 0.701068  |
| H     | 10.440087 | 5.152342  | 1.139262  |
| C     | 8.204307  | 4.117532  | -1.217318 |
| C     | 9.426629  | 4.467376  | -0.642761 |
| H     | 10.324857 | 4.419438  | -1.253970 |
| C     | 3.125559  | -1.413111 | -6.056834 |
| H     | 4.126024  | -1.564961 | -6.445791 |
| C     | 2.185876  | -2.461233 | -6.152419 |
| H     | 2.462023  | -3.393884 | -6.628453 |
| C     | 2.784877  | -0.195822 | -5.507354 |
| C     | 3.518808  | 0.601893  | -5.461522 |
| C     | 0.897744  | -2.289875 | -5.681487 |
| C     | 1.483003  | 0.003239  | -4.973256 |
| C     | 0.515143  | -1.061594 | -5.041038 |
| C     | 1.083697  | 1.239534  | -4.366866 |
| C     | -0.777849 | -0.869243 | -4.475078 |
| H     | -1.528395 | -1.648131 | -4.527978 |
| C     | -0.153478 | 1.354639  | -3.759455 |
| H     | -0.413092 | 2.271816  | -3.250838 |
| C     | -1.085147 | 0.301054  | -3.815144 |
| H     | -2.047890 | 0.423187  | -3.337722 |
| C     | 1.552237  | 3.603063  | -4.827946 |
| C     | 2.527546  | 4.706062  | -4.698729 |
| C     | 3.783727  | 4.556128  | -4.063907 |
| C     | 2.179220  | 5.963185  | -5.257330 |
| H     | 1.214897  | 6.066682  | -5.743527 |
| C     | 3.061763  | 7.027547  | -5.202575 |
| H     | 2.787721  | 7.985875  | -5.635287 |
| C     | 4.327410  | 6.874975  | -4.599512 |
| H     | 5.028284  | 7.706001  | -4.564732 |
| C     | 4.704877  | 5.658869  | -4.038047 |
| C     | 0.029707  | -4.626481 | -5.739983 |
| C     | -1.219945 | -5.399821 | -5.976537 |
| C     | -1.094988 | -6.768605 | -6.333650 |
| H     | -0.100272 | -7.187162 | -6.464170 |
| C     | -2.505751 | -4.825250 | -5.876115 |
| Atoms | X     | Y     | Z     |
|-------|-------|-------|-------|
| C     | -1.41797 | -5.083468 | 0.036929 |
| C     | -2.448831 | -4.525389 | -0.794358 |
| C     | -3.066674 | -5.608943 | 1.736004 |
| H     | -0.985136 | -6.027000 | 1.954284 |
| C     | -3.814576 | -4.628480 | -0.351465 |
| C     | -3.017353 | -6.000009 | 2.716277 |
| C     | -4.102544 | -5.134506 | 0.903879 |
| C     | -5.130393 | -5.196669 | 1.235277 |
| C     | -6.883907 | -3.420256 | -2.201530 |
| C     | -6.335269 | -3.218244 | -3.486564 |
| C     | -7.204067 | -2.922616 | -4.593150 |
| C     | -8.575252 | -2.801861 | -4.372355 |
| H     | -9.220211 | -2.567785 | -5.216077 |
| C     | -9.117432 | -2.999960 | -3.087747 |
| H     | -10.191722 | -2.931586 | -2.940033 |
| C     | -8.288160 | -3.307896 | -2.019840 |
| C     | -8.709012 | -3.537158 | -1.044241 |
| C     | -1.878824 | -6.515728 | -0.145781 |
| C     | 2.902389 | -6.985946 | 0.822658 |
| C     | 2.981914 | -6.503090 | 2.148977 |
| C     | 3.999139 | -7.008953 | 3.025586 |
| C     | 4.910150 | -7.953066 | 2.555096 |
| C     | 5.675556 | -8.326107 | 3.232570 |
| C     | 4.832424 | -8.417796 | 1.226523 |
| C     | 5.547948 | -9.155275 | 0.873705 |
| C     | 3.846276 | -7.942982 | 0.377918 |
| C     | 3.778704 | -8.299245 | -0.644330 |
| N     | -0.312486 | 2.901692 | 5.686234 |
| H     | -1.089585 | 3.208818 | 5.101975 |
| N     | -1.603051 | -3.065034 | 4.905561 |
| H     | -0.624953 | -3.352675 | 4.828219 |
| N     | 4.985321 | -0.870880 | -2.403650 |
| H     | 5.050815 | 0.145082 | -2.372121 |
| N     | 4.071314 | -1.364457 | 3.659375 |
| H     | 3.450498 | -2.174927 | 3.652525 |
| N     | -4.370374 | 1.311533 | -4.282917 |
| H     | -4.623626 | 0.323428 | -4.364679 |
| N     | -5.236179 | 1.618732 | 1.816125 |
| H     | -4.749883 | 2.462153 | 2.136456 |
| N     | -0.093611 | -3.272141 | -5.864143 |
| H     | -1.065658 | -2.958892 | -5.908246 |
| N     | 1.948950 | 2.361029 | -4.420311 |
| H     | 2.910436 | 2.292334 | -4.072109 |
| N     | 4.671443 | 4.787347 | 1.119439 |
| H     | 4.764336 | 4.539060 | 0.134359 |
| N     | -4.823239 | -4.260007 | -1.261739 |
H  -4.571355  -4.225313  -2.250987
N  -1.392649   5.232946   0.395478
H  -1.711223   5.217970   1.368185
O   8.081733   3.695781  -2.489222
O   5.886666   3.737408  -1.039143
O   4.188162   3.423459  -3.489991
O   5.904294   5.452463  -3.464488
O   6.785609   3.163100  -4.916400
O   6.103946   1.488329  -2.964065
O  -2.303576   4.536608   5.011114
O  -3.322343   6.981387   4.987891
O  -3.074752   5.515754   2.370872
O  -5.453703   6.310976   3.255139
O  -5.174050   4.853726   5.726690
O  -4.601914   3.474703   3.551213
O   2.158514  -5.860399   2.658055
O   4.032070  -6.507303   4.276616
O   3.164801  -3.682078   4.564792
O   2.787139  -5.346909   6.597397
O   1.359985  -7.232486   4.977427
O   0.442517  -4.742204   4.788689
O  -4.434714  -2.512157  -7.634841
O  -4.223094  -1.102095  -5.387325
O  -2.715404  -3.559432  -5.512275
O  -4.850682  -4.992249  -6.173812
O  -5.029615  -3.305130  -3.745549
O  -6.637920  -2.771108  -5.796695
O  -3.170640   2.919755  -5.414408
O   0.404638   3.788471  -5.314498
O  -2.042625   5.914213  -1.696834
O   1.323385   3.763634   7.054435
O   5.974337   5.002825   3.003361
O   5.442927  -0.165604   5.061182
O  -3.710195  -3.964169   5.097444
O   1.864859  -6.916356  -1.331518
O   1.109660  -5.192195  -5.463863
O  -7.006158   0.248647   2.283124
O   5.718763  -2.634622  -3.689077
O  -6.479270  -3.515872   0.152628
Ga   6.136105   3.510434  -3.033566
Ga  -3.963446   5.286090   4.134215
Ga   2.287192  -5.488418   4.658551
Ga  -4.640538  -3.041445  -5.689978
N   0.144874   0.116862   1.135170
C  -1.171678   0.579038   1.751749
H  -1.910496  -0.179820   1.498485
H -1.018033  0.552475  2.826977
C  0.621690  1.123594  1.891001
H  1.620858  1.339286  2.158391
H  0.709209  1.350787  1.762808
H -0.342624  2.690029  0.729912
H -1.268080  2.195796  2.164179
H  0.204822  3.152349  2.343840
C -1.663408  1.953697  1.327106
H -1.910276  2.011019  0.264345
H -0.956394  2.746427  1.569958
H -2.572702  2.154745  1.897747
C  1.219058  1.196620  1.258829
H  0.924982  1.992734  0.578133
H  2.137708  0.752251  0.880100
C  1.445407  1.740895  2.661419
H  2.239416  2.490067  2.591230
H  1.777592  0.974818  3.363711
H  0.562390  2.233980  3.070855
C -0.085734  -0.180300  -0.347296
H -0.924917  -0.876847  -0.396346
H -0.407731  0.761636  -0.794560
C  1.117938  -0.733198  -1.097664
H  0.786087  -0.970426  -2.112281
H  1.505747  -1.653967  -0.655630
H  1.930605  -0.007154  -1.174923
K -0.691760  1.983946  -7.135697
K  5.784811  -4.516742  3.633564
K -5.915299  7.481917  5.659444
K -7.754018  -0.973639  0.080290
K  0.337959  -7.086737  -3.452386
K -3.462615  3.447851  7.336373
K -1.865627  4.896617  -4.108136
K  8.376182  5.304391  -4.693153
K -6.555179  -4.161499  -8.142938
K  7.989871  1.066682  -1.053439
K  3.436381  -7.989809  6.480901

Metallo cage (with 11 K⁺ counter ions)

291 atoms

C  0.523963  -1.204699  5.989125
H  0.672772  -2.273763  6.076401
C  0.167263  1.593481  5.890522
C  1.403247  -0.358779  6.625055
H  2.237149  -0.770254  7.183266
C  1.239352  1.039833  6.571880

S33
|  |  |  |  |
|---|---|---|---|
| H  | 1.937533 | 1.683877 | 7.085455 |
| C  | -0.561466 | -0.681043 | 5.235544 |
| C  | -0.748383 | 0.742799  | 5.168881 |
| C  | -1.501564 | -1.539001 | 4.559028 |
| C  | -1.848931 | 1.252190  | 4.419165 |
| H  | -2.001155 | 2.318429  | 4.286974 |
| C  | -2.567762 | -1.002042 | 3.860920 |
| H  | -3.259663 | -1.657596 | 3.347479 |
| C  | -2.732565 | 0.395824  | 3.796420 |
| H  | -3.554750 | 0.809522  | 3.227160 |
| C  | -2.226234 | -3.893367 | 4.904011 |
| C  | -1.683351 | -5.220509 | 5.318469 |
| C  | -0.303348 | -5.492682 | 5.445679 |
| C  | -2.608530 | -6.247788 | 5.625502 |
| H  | -3.667687 | -6.032025 | 5.534075 |
| C  | 0.145461  | -6.790925 | 5.856763 |
| C  | -0.795313 | -7.774267 | 6.148731 |
| H  | -0.449646 | -8.757812 | 6.458414 |
| C  | -2.172640 | -7.497825 | 6.034897 |
| H  | -2.894501 | -8.276121 | 6.267063 |
| C  | 0.251321  | 3.900896  | 6.869169 |
| C  | -0.363427 | 5.254133  | 6.735681 |
| C  | 0.149816  | 6.269934  | 7.579783 |
| H  | 0.990939  | 6.030221  | 8.220867 |
| C  | -1.456273 | 5.552276  | 5.887179 |
| C  | -0.407597 | 7.537043  | 7.589921 |
| H  | 0.003503  | 8.308898  | 8.234839 |
| C  | -2.047405 | 6.857296  | 5.929380 |
| C  | -1.512121 | 7.830471  | 6.769758 |
| H  | -1.966590 | 8.818594  | 6.777674 |
| C  | 4.159223  | -2.130566 | -1.562370 |
| C  | 3.880386  | -3.128007 | 1.064197 |
| H  | 3.743620  | -3.521857 | 2.064354 |
| C  | 4.670211  | -3.781817 | 0.144052 |
| H  | 5.185768  | -4.697956 | 0.413566 |
| C  | 4.844447  | -3.266377 | -1.156908 |
| H  | 5.549067  | -3.740026 | -1.829940 |
| C  | 3.193492  | -1.939672 | 0.695186 |
| C  | 3.259176  | -1.466984 | -0.658089 |
| H  | 2.481102  | -1.146665 | 1.651496 |
| C  | 2.501142  | 0.316543  | -1.027793 |
| H  | 2.521065  | 0.032008  | -2.053167 |
| C  | 1.752803  | -0.047585 | 1.263535 |
| H  | 1.219130  | 0.525405  | 2.011944 |
| C  | 1.746115  | 0.359252  | -0.092006 |
| H  | 1.174221  | 1.234064  | -0.381125 |
| C  | 3.778412  | 1.007588  | 3.687460 |
| C  | 4.068551  | -1.662661 | 4.992112 |
H  7.765454  4.063135  2.991680
C  9.147979  3.656289  1.388577
H 10.029827  3.883485  1.981462
C  8.186255  2.980897  -0.741860
C  9.301585  3.278766  0.039288
H 10.290548  3.210174  -0.408090
C  2.875667  -0.233847 -5.953124
H  3.796167  -0.193811 -6.525063
C  2.032704  -1.357232 -6.083896
H  2.304870  -2.160913 -6.756624
C  2.553532  0.796952  -5.096805
H  3.231927  1.632579 -4.970620
C  0.848549  -1.438989 -5.370766
C  1.344619  0.745982  -4.345813
C  0.457831  -0.377203 -4.485515
C  0.983729  1.789961  -3.403682
C  -0.752821  -0.392426 -3.733748
H  -1.459597  -1.206326 -3.840506
C  -0.160991  1.706241  -2.673120
H  -0.369967  2.471863  -1.929536
C  -1.038986  0.612590 -2.836943
H  -1.938830  0.563645  -2.239606
C  1.841793  3.950341  -4.160062
C  3.066561  4.770538  -4.231879
C  4.306230  4.287245  -3.751886
C  2.987318  6.086247  -4.751021
H  2.031966  6.445892  -5.120160
C  4.104912  6.904529  -4.749397
H  4.038603  7.917541  -5.137049
C  5.333554  6.441759  -4.229856
C  6.203665  7.094399  -4.208915
C  5.453715  5.147702  -3.726833
C  0.346621  -3.861355  -5.522298
C  -0.768401  -4.831818  -5.652395
C  -0.450137  -6.171835  -5.984287
H  0.594615  -6.452060  -6.072235
C  -2.124005  -4.455462  -5.522805
C  -1.455819  -7.092347  -6.231073
H  -1.205313  -8.117544  -6.490359
C  -2.809379  -6.703025  -6.171510
H  -3.601336  -7.415660  -6.390978
C  -3.159632  -5.396487  -5.837286
C  -4.547006  -0.098884  0.615534
H  -4.542218  -0.658897  1.546008
C  -4.229054  -0.742972  -0.599001
H  -3.968174  -1.793622  -0.591628
C  -4.860083  1.248660  0.632634
C  -4.231525  -0.044093 -1.786284
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | -3.991023  | -0.569990  | -2.703083  |
| C    | -4.800376  | 2.029004   | -0.568037  |
| C    | -4.492390  | 1.354997   | -1.800426  |
| C    | -5.033187  | 3.431682   | -0.573996  |
| H    | -5.261167  | 3.950902   | 0.350899   |
| C    | -4.447952  | 2.130627   | -3.007465  |
| C    | -4.979051  | 4.139442   | -1.755613  |
| H    | -5.172187  | 5.205958   | -1.754087  |
| C    | -4.699311  | 3.490583   | -2.977620  |
| H    | -4.721027  | 4.048769   | -3.907932  |
| C    | -6.164012  | 1.410336   | 2.716366   |
| C    | -6.342171  | 2.181607   | 3.972590   |
| C    | -5.469449  | 3.220286   | 4.369616   |
| C    | -7.450151  | 1.859108   | 4.791708   |
| H    | -8.108780  | 1.056323   | 4.478126   |
| C    | -7.699102  | 2.557940   | 5.961901   |
| H    | -8.556367  | 2.302975   | 6.578599   |
| C    | -5.743154  | 3.950084   | 5.575314   |
| C    | -6.847358  | 3.608281   | 6.355675   |
| H    | -7.034463  | 4.165173   | 7.271345   |
| C    | -3.432032  | 1.841378   | -5.264668  |
| C    | -3.434713  | 0.918786   | -6.430322  |
| C    | -3.033602  | 1.432516   | -7.692161  |
| H    | -2.829991  | 2.496775   | -7.782968  |
| C    | -3.834720  | -0.432747  | -6.331846  |
| C    | -3.014061  | 0.616585   | -8.813794  |
| H    | -2.720729  | 1.024360   | -9.777326  |
| C    | -3.834149  | -1.267859  | -7.503366  |
| C    | -3.402597  | -0.734159  | -8.717479  |
| H    | -3.96598  | -1.374665  | -9.596243  |
| C    | 0.503925   | -3.973106  | -1.195642  |
| H    | 1.540396   | -3.787848  | -1.448048  |
| C    | -0.526890  | -3.437849  | -1.991199  |
| H    | -0.264936  | -2.877704  | -2.879800  |
| C    | 0.208888   | -4.710660  | -0.064876  |
| C    | -1.849611  | -3.621114  | -1.650215  |
| H    | -2.616617  | -3.193016  | -2.285019  |
| C    | -1.150539  | -4.849734  | 0.376211   |
| C    | -2.195702  | -4.318792  | -0.458203  |
| C    | -1.490202  | -5.481317  | 1.604197   |
| H    | -0.716899  | -5.888177  | 2.246824   |
| C    | -3.562097  | -4.523071  | -0.052543  |
| C    | -2.807783  | -5.576666  | 1.994521   |
| H    | -3.056613  | -6.045948  | 2.940273   |
| C    | -3.849792  | -5.113613  | 1.165280   |
| H    | -4.879855  | -5.255919  | 1.463863   |
| C    | -5.851698  | -3.763113  | -0.716836  |
| C    | -6.700113  | -3.527399  | -1.917538  |
|   | O    | O    | O    | O    | O    | O    | O    | O    | O    | O    | O    | O    | O    | K    | K    | K    | K    | K    | K    | K    | K    | K    | K    | K    | K    |
|---|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
|   | -2.025081 | 4.660270 | 5.056220 |
|   | -3.115037 | 7.078732 | 5.146424 |
|   | -2.981589 | 5.733883 | 2.435230 |
|   | -5.329712 | 6.370036 | 3.513813 |
|   | -4.869700 | 4.919492 | 5.908488 |
|   | -4.375257 | 3.576906 | 3.692791 |
|   | 2.019855  | -5.999207 | 3.105318 |
|   | 4.068048  | -6.636351 | 4.667926 |
|   | 3.168673  | -3.780642 | 4.280445 |
|   | 3.319436  | -4.808303 | 6.715982 |
|   | 1.476437  | -6.987696 | 5.920620 |
|   | 0.654602  | -4.596230 | 5.187694 |
|   | -4.253829 | -2.527958 | -7.357774 |
|   | -4.242576 | -0.993867 | -5.193828 |
|   | -2.513035 | -3.235514 | -5.145063 |
|   | -4.428874 | -4.956526 | -5.794141 |
|   | -4.854017 | -3.210136 | -3.439941 |
|   | -6.480789 | -2.934088 | -5.526152 |
|   | -2.756688 | 2.900046  | -5.264805 |
|   | 0.806142  | 4.206490  | -4.833126 |
|   | -2.256503 | 6.459770  | -1.663181 |
|   | 1.006450  | 3.623945  | 7.816277 |
|   | 5.269223  | 3.893108  | 3.058647 |
|   | 4.491978  | -0.090956 | 3.225640 |
|   | -3.449640 | -3.675820 | 4.830085 |
|   | 2.447365  | -6.150915 | -1.100214 |
|   | 1.540425  | -4.226690 | -5.459753 |
|   | -6.862808 | 0.406283  | 2.458898 |
|   | 4.974684  | -3.255813 | -4.138487 |
|   | -6.301077 | -3.599882 | 0.439671 |
| Ga| 6.395811  | 2.638300  | -2.863208 |
| Ga| -3.731632 | 5.400681  | 4.256511 |
| Ga| 2.424364  | -5.478458 | 5.013199 |
| Ga| -4.475557 | -2.978726 | -5.386465 |
| K | -0.184935 | 2.391535  | -6.700787 |
| K | 5.951587  | -4.563916 | 4.017920 |
| K | -5.710014 | 7.509713  | 5.922948 |
| K | -7.681219 | -1.179292 | 0.559498 |
| K | 3.030881  | -5.153012 | -3.505377 |
| K | -3.327431 | 2.830499  | 6.918142 |
| K | -1.618697 | 4.759244  | -3.593188 |
| K | 9.074107  | 4.157802  | -4.141220 |
| K | -6.152892 | -4.377734 | -7.839305 |
| K | 5.545565  | 0.423264  | 0.674284 |
| K | 3.823899  | -7.417848 | 7.262625 |