Supporting information

Shape and size directed self-selection in organic cage formation

Koushik Acharyya and Partha Sarathi Mukherjee*

Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India. Fax: 91-80-2360-1552; Tel; 91-80-2293-3352

E-mail: psm@ipc.iisc.ernet.in

Materials and methods: All chemicals and solvents were purchased from commercially available sources and were used without further purification. Aldehyde **C** was synthesized following the reported procedure.[1] NMR spectra for the characterization of the products were recorded on a Bruker 400 MHz spectrometer. In ^{1}H NMR spectra chemical shift (δ) values are reported in ppm relative to the TMS (0.00 ppm), as an internal standard in $CDCl_3$. Bruker ALPHA FTIR spectrometer was used for recording IR spectra. High resolution mass spectra were recorded on a Q-TOF instrument by electrospray ionization (ESI) technique.

Aldehyde A: In a 100 mL flame dried double-neck round bottom flask 500 mg of 4-bromobenzaldehyde (2.70×10^{-3} mol) and 920 mg (6.14×10^{-3} mol) of 3-formylphenylboronic acid were taken in 50 mL THF and onto that 20 mL aqueous solution of 700 mg (5.10×10^{-3} mol) K_2CO_3 was added. The resulting solution mixture was stirred under nitrogen atmosphere at room temperature for 10 minutes followed by addition of 80 mg (6.92×10^{-5} mol) of $Pd(PPh_3)_4$ and heated to 80 °C for 48h. After completion of the reaction THF was completely removed and the aqueous part was extracted with dichloromethane (50 mL × 3). Organic part was then dried over sodium sulphate and completely removed. The resulting solid mass was purified by silica

gel column chromatography in dichloromethane to get white powder. Isolated yield: 90 % (510 mg, 2.43× 10^{-3} mol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 7.66 (t, 1H), 7.78 (d, 2H), 7.92 (t, 2H), 7.99 (d, 2H), 8.15 (s, 1H), 10.08 (s, 1H), 10.10 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 128.3, 128.6, 130.3, 130.4, 130.9, 133.6, 136.2, 137.5, 141.2, 146.0, 192.2, 192.4.

Aldehyde B: Aldehyde **B** was prepared as pale yellow solid from 402 mg (2.00 × 10^{-3} mol) of 5-bromosalicylaldehyde and 440 mg (2.93× 10^{-3} mol) of 3-formylphenylboronic acid, following the same synthetic protocol employed for aldehyde **A**. Isolated yield: 65 % (293 mg, 1.30× 10^{-3} mol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 7.14 (d, 1 H), 7.73 (dd, 2H), 7.82 (m, 1H), 7.84 (s, 1H), 7.96 (d, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.1, 121.3, 127.5, 130.9, 132.2, 132.8, 135.7, 136.2, 145.6, 162.3, 192.2, 196.9.

Cage $A_3X_2^{II}$: In a 8 mL glass vial 4 mL chloroform solution of 2.9 mg (2.00 × 10^{-5} mol) of amine **X** was added drop-wise slowly to the stirring solution of 6.3 mg (3.00 × 10^{-5} mol) of aldehyde **A** in 3 mL chloroform. The resulting solution mixture was kept for stirring at room temperature for an additional 24 h. After completion of the reaction, solvent was reduced in volume and the product was predicated out as white solid by adding *n*-pentane. Isolated yield = 92 % (7.5 mg, 9.21 × 10^{-6} mol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 2.78-2.88 (m, 12H), 3.48-3.68 (m,12H), 6.70 (br, 2H), 6.76 (d, 4H), 6.95 (d, 2H), 7.00 (s, 1H), 7.09 (d, 4H), 7.43 (d, 2H), 7.51-7.60 (m, 4H), 7.61 (s, 2H), 7.80 (d, 2H), 7.93 (d,1H), 7.93 (d, 3H), 8.13 (d, 2H), 8.21 (d,1H) ; ^{13}C NMR (100 MHz, $CDCl_3$): 56.1, 56.3, 56.8, 57.1, 59.6, 60.1, 60.3, 60.6, 125.4, 125.6, 126.5, 126.7, 128.5, 128.8, 129.0, 129.5, 129.7, 129.9, 130.2, 135.7, 135.9, 137.9 (two peaks), 140.3, 140.4, 141.4, 161.1, 161.3, 161.8, 162.4; ESI-HRMS ($CHCl_3$/CH_3CN, 1:1), m/z $[M+H]^+$ 815.4729 (calculated 815.4549); FTIR (cm^{-1}) ν: 2890, 2820, 2802, 1641, 1606, 1441, 1329, 1287, 1064, 1034, 910, 833, 793, 692.

Cage $B_3X_2^{II}$: This cage was synthesized as yellow solid, from 6.8 mg (3.00×10^{-5} mol) of aldehyde **B** and 2.9 mg (2.00×10^{-5} mol) of amine **X** following the same procedure as employed for the cage **$A_3X_2^{II}$.** Obtained solid sample was re-dissolved in chloroform and crystallized by slow vapor diffusion of n-pentane to get pure cage **$B_3X_2^{II}$**. Isolated yield = 75 % (6.5 mg, 7.50×10^{-6} mol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 2.80-2.89 (m, 12H), 3.51-3.69 (m, 12H), 6.68- 6.72 (m, 5H), 6.95 (d, 2H), 7.05-7.07 (m, 6H), 7.13 (d, 2H), 7.33 (d, 2H), 7.51 (s, 1H), 7.59(s, 2H), 7.64 (dd, 2H), 7.72 (dd, 1H), 7.89 (s, 2H), 7.98 (br, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$): 55.8, 56.2 (two peaks), 56.8, 57.9, 58.1, 59.5, 60.0, 118.2, 118.5, 119.0, 125.5, 125.7, 128.2, 128.7,129.8, 129.9, 130.0, 130.7, 131.0,134.2, 134.3, 140.8, 141.0, 161.8, 162.1, 162.3, 162.6, 165.5, 165.6. ESI-HRMS ($CHCl_3/CH_3CN$, 1:1), m/z $[M+H]^+$ 863.4617 (calculated 863.4397), $[M+2H]^{2+}$ 432. 2354 (calculated 432.2237); FTIR (cm^{-1}) ν: 2943, 2884, 2808, 1635, 1594, 1482, 1435, 1264, 1164, 1069, 1028, 916, 814.

Cage C_3X_2(I and II): This cage was synthesized as yellow solid following the same procedure as employed for the cage **$A_3X_2^{II}$**, from 4.9 mg (3.00×10^{-5} mol) of aldehyde **C** and 2.9 mg (2.00×10^{-5} mol) of amine **X**. Isolated yield = 84 % (5.6 mg, 8.40×10^{-6} mol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 2.32 (s, 9H), 2.89-3.00 (m, 12H), 3.17-3.31(m, 6H), 3.74-3.80 (m, 6H), 5.17-5.22 (m, 3H), 7.31(s, 2H), 7.51 (s, 3H), 7.63 (d, 1H), 7.94-7.98 (m, 3H), 14.95-15.12 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 16.1, 16.2, 16.3, 56.2, 56.3, 56.4, 56.8, 57.0, 57.6, 60.2, 60.5, 116.8, 116.9, 125.6, 126.4, 127.1, 128.4, 128.7, 130.0, 130.7, 132.5, 132.7, 132.8, 133.1, 161.1, 161.5 (two peaks), 164.7, 165.6, 166.0, 166.2, 166.3. ESI-HRMS ($CHCl_3/CH_3CN$, 1:1), m/z $[M+H]^+$ 677.4089 (calculated 677.3928); FTIR (cm^{-1}) ν: 2920, 2837, 2802, 1611, 1435, 1364, 1270, 1151,1075, 1026, 916, 875, 740.

X-ray crystal data collection and structure solution: X-ray data of $\mathbf{A_3X_2^{II}}$, $\mathbf{B_3X_2^{II}}$, $\mathbf{B_3X^{I}}$ and $\mathbf{C_3X^{I}}$ were collected on a Bruker SMART APEX CCD diffractometer using the SMART/SAINT software,[2] equipped with a low temperature device. All the diffraction quality crystals were mounted on a loop coated with traces of viscous oil. The intensity data of all the compounds were collected at 100(2) K, by using graphite monochromatic Mo-Kα radiation (0.7107 Å). The structures were solved by direct methods and refined by full-matrix least squares on F^2 employing the SHELX-97[3] incorporated in WinGX.[4] Empirical absorption corrections were applied with SADABS.[5] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed by using the riding models and refined isotropically. Disordered solvent molecules in the crystal structure of $\mathbf{B_3X^{I}}$ were treated by using the SQUEEZE program in PLATON.[6] Crystallographic data and refinement parameters are provided in the table S1.

Computational methodology: Full geometry optimizations were carried out using Gaussian 09 package.[7] The hybrid B3LYP functional has been used in all calculations as implemented in Gaussian 09 package, mixing the exact Hartree-Fock-type exchange with Becke's expression for the exchange functional[8] and that proposed by Lee-Yang-Parr for the correlation contribution.[9] The 6-31G basis set was used for all calculations. Frequency calculations carried on the optimized structures confirmed the absence of any imaginary frequencies.

Table S1. Crystallographic data and refinement parameters**.**

Compound	$\mathbf{A_3X_2^{II}}$	$\mathbf{B_3X_2^{II}}$	$\mathbf{B_3X^{I}}$	$\mathbf{C_3X^{I}}$
Empirical formula	$C_{55}H_{55}Cl_3N_8$	$C_{56}H_{56}Cl_6N_8O_3$	$C_{48}H_{42}N_4O_6$	$C_{33}H_{36}N_4O_6$
Fw	934.42	1101.79	770.86	584.66
T (K)	100 (2)	100 (2)	100 (2)	100 (2)
Crystal system	triclinic	monoclinic	trigonal	monoclinic
Space group	$P\bar{1}$	$P2_1/c$	$P\bar{3}c1$	$P2_1/n$
a/Å	10.6574(14)	17.6515(12)	13.5006(14)	7.2035(9)
b/Å	14.7322(19)	27.3690(18)	13.5006(14)	18.776(2)
c/Å	17.013(2)	11.1516(8)	29.691(3)	21.734(3)
α/deg	66.539(4)	90	90	90
β/deg	80.163(4)	102.653(2)	90	91.764(4)
γ/deg	80.329(4)	90	120	90
V/Å^3	2399.5(5)	5256.6(6)	4686.6(12)	2938.1(6)
Z	2	4	4	4
ρ_{calcd} (g cm^{-3})	1.293	1.392	1.092	1.322
μ (Mo Kα) (mm^{-1})	0.238	0.381	0.073	0.092
λ/Å	0.71073	0.71073	0.71073	0.71073
F (000)	984.0	2296.0	1624.0	1240.0
Unique reflns.	8428	9243	2756	5167
GOF (F^2)	1.102	1.048	1.292	1.099
R_1[a]	0.0662	0.0552	0.1320	0.0981
wR_2[b]	0.1956	0.1279	0.3269	0.2848

[a] $R_1 = \Sigma \big| |F_o| - |F_c| \big| / \Sigma |F_o|$, [b] $wR_2 = [\Sigma\{w(F_o^2 - F_c^2)^2\}/\Sigma\{w(F_o^2)^2\}]^{1/2}$.

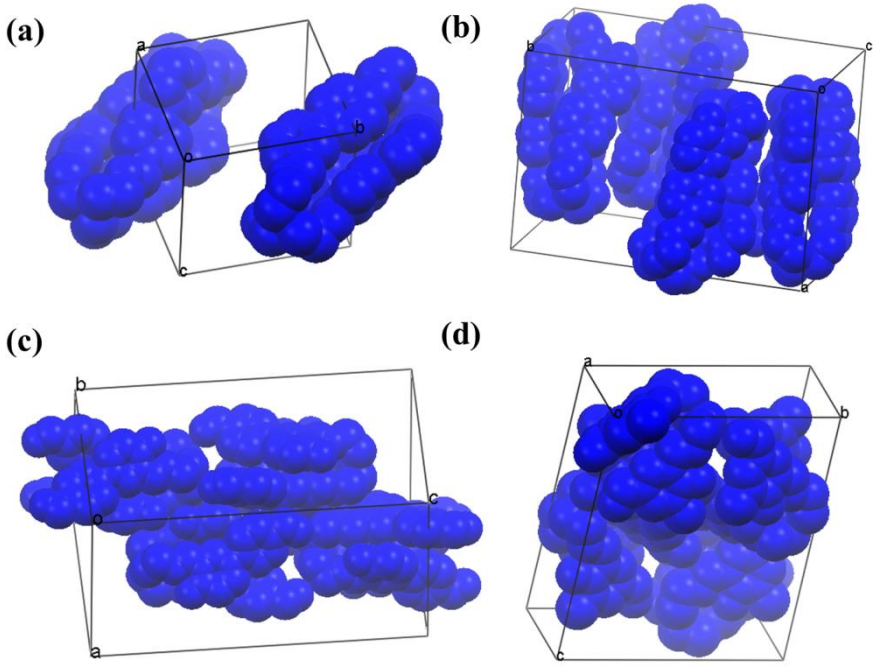

Fig. S1: Unit cell packing diagrams of (a) $\mathbf{A_3X_2^{II}}$ (b) $\mathbf{B_3X_2^{II}}$ (c) $\mathbf{B_3X^{I}}$ and (d) $\mathbf{C_3X^{I}}$.

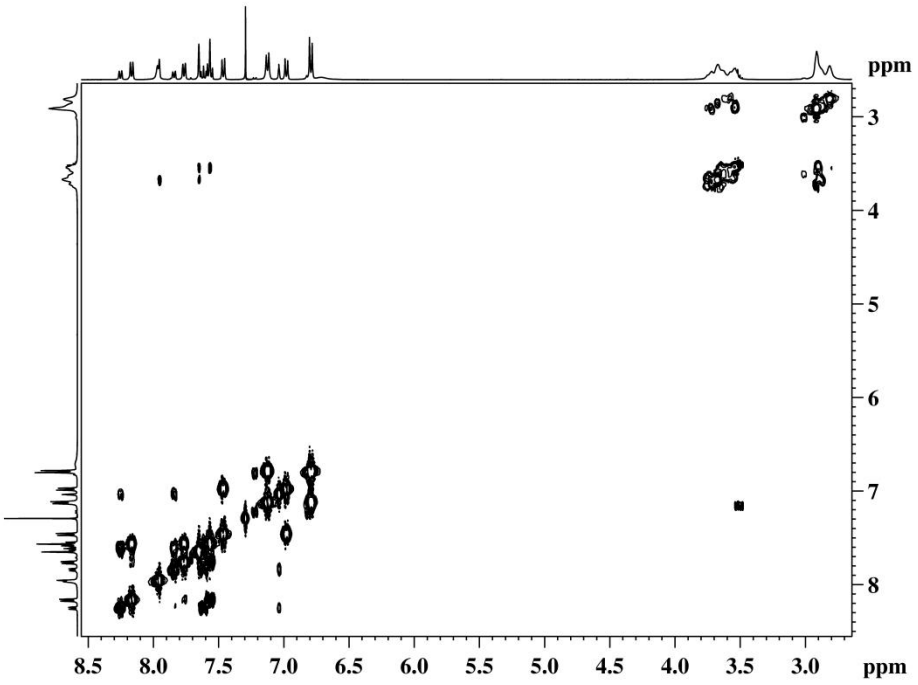

Fig. S4: ^{1}H- ^{1}H COSY spectrum of cage $\mathbf{A_3X_2^{II}}$ recorded in $CDCl_3$.

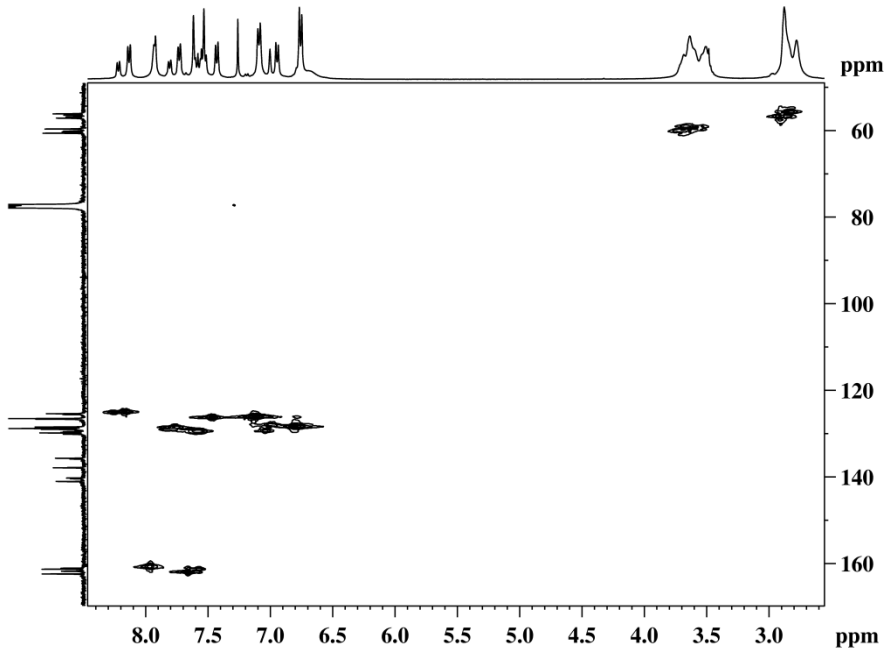

Fig. S5: ^{1}H- ^{13}C HMQC spectrum of cage $\mathbf{A_3X_2^{II}}$ recorded in $CDCl_3$.

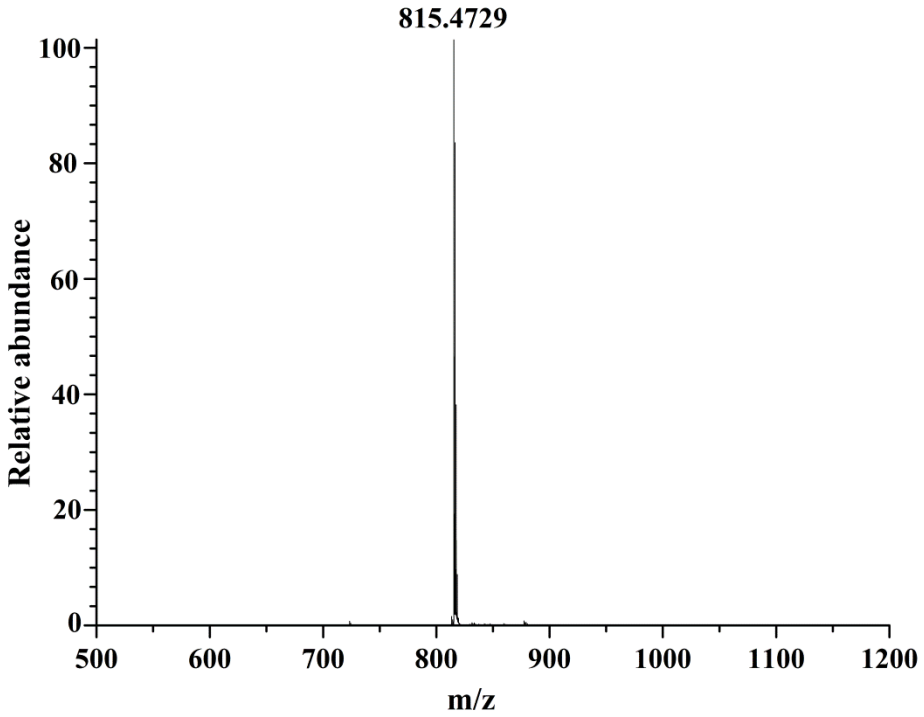

Fig. S6: ESI-HRMS spectrum of cage $\mathbf{A_3X_2^{II}}$ recorded in $CHCl_3$-MeCN (1:1, v/v).

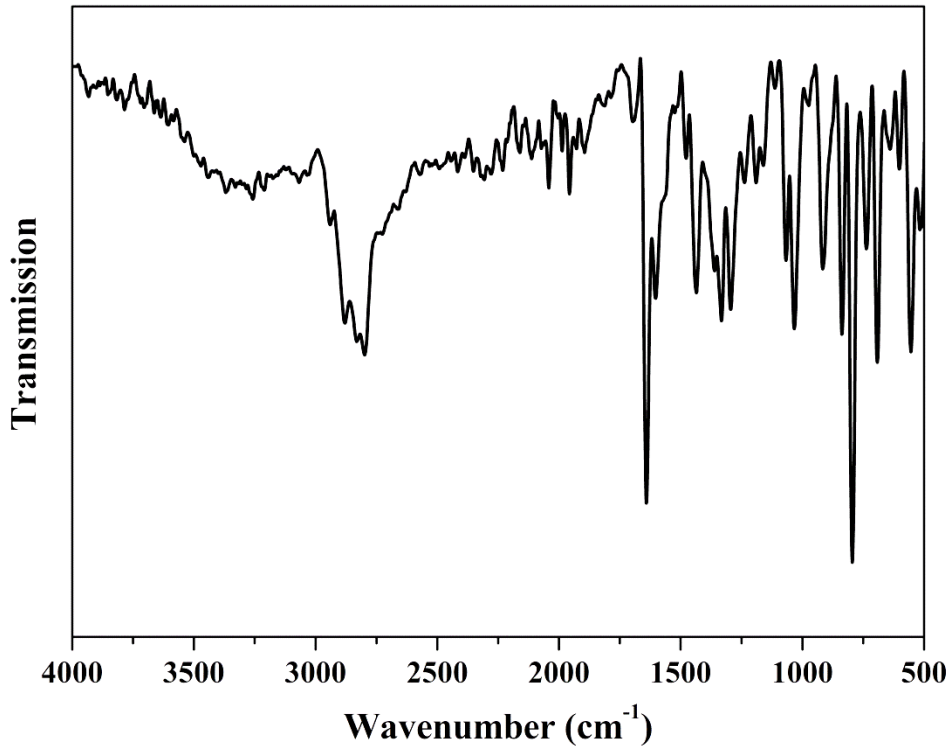

Fig. S7: FTIR spectrum of cage $\mathbf{A_3X_2^{II}}$.

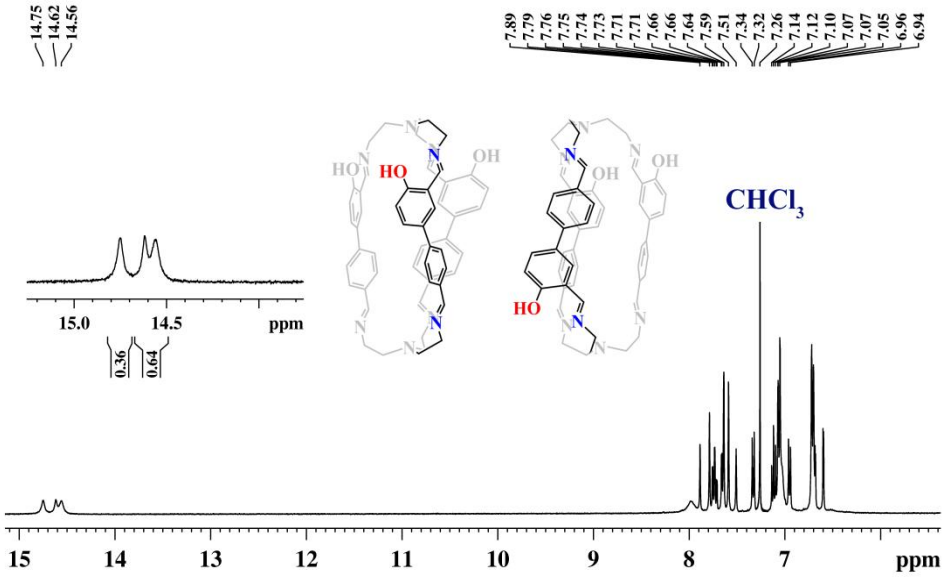

Fig. S8: Partial ^{1}H NMR spectrum of as synthesized cage $\mathbf{B_3X_2}$ (I and II) recorded in $CDCl_3$.

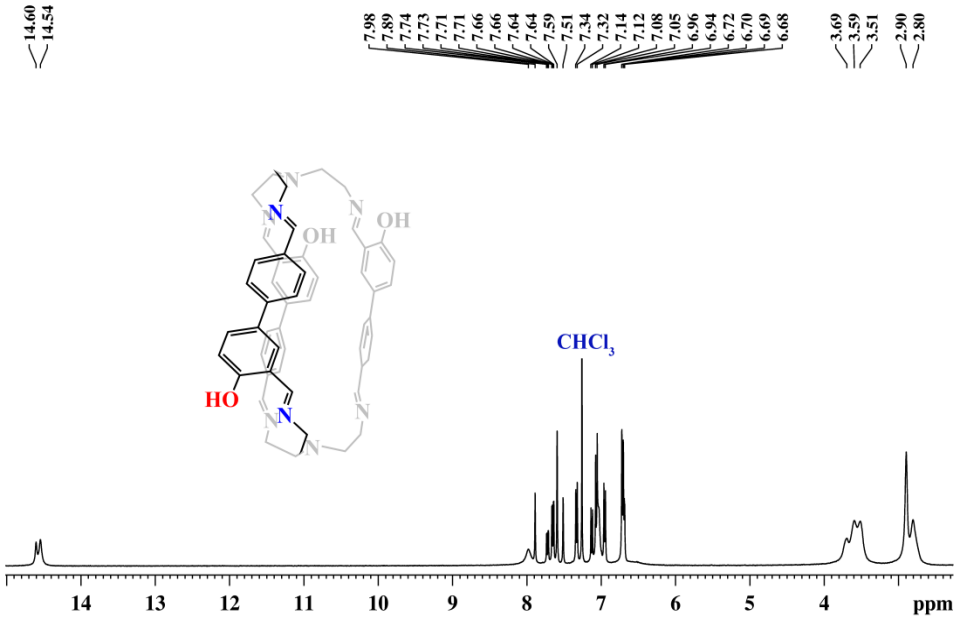

Fig. S9: ^{1}H NMR spectrum of cage (single crystals) $\mathbf{B_3X_2^{II}}$ recorded in $CDCl_3$.

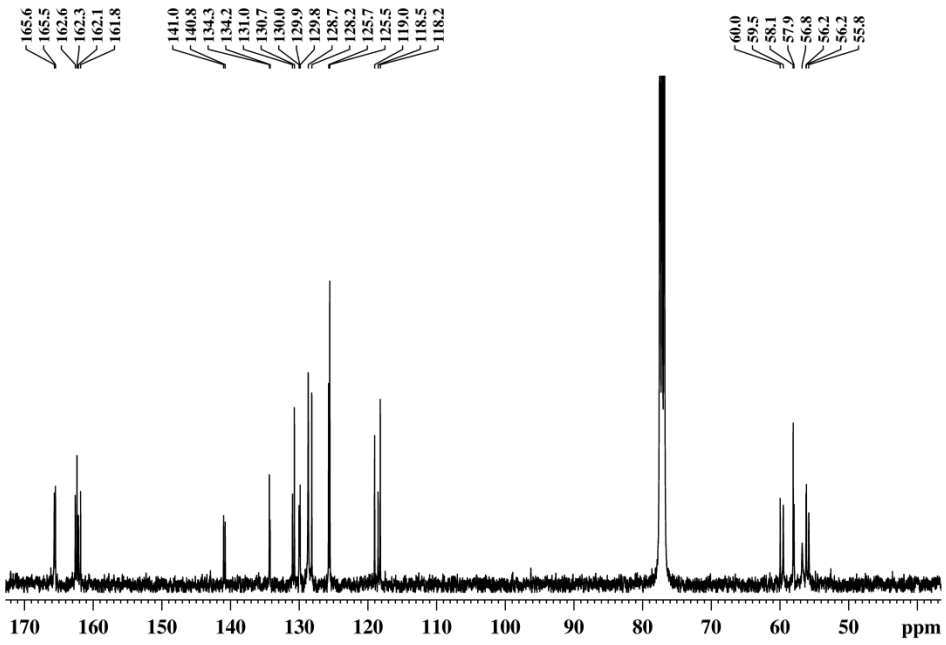

Fig. S10: ^{13}C NMR spectrum of cage (single crystals) $\mathbf{B_3X_2^{II}}$ recorded in $CDCl_3$.

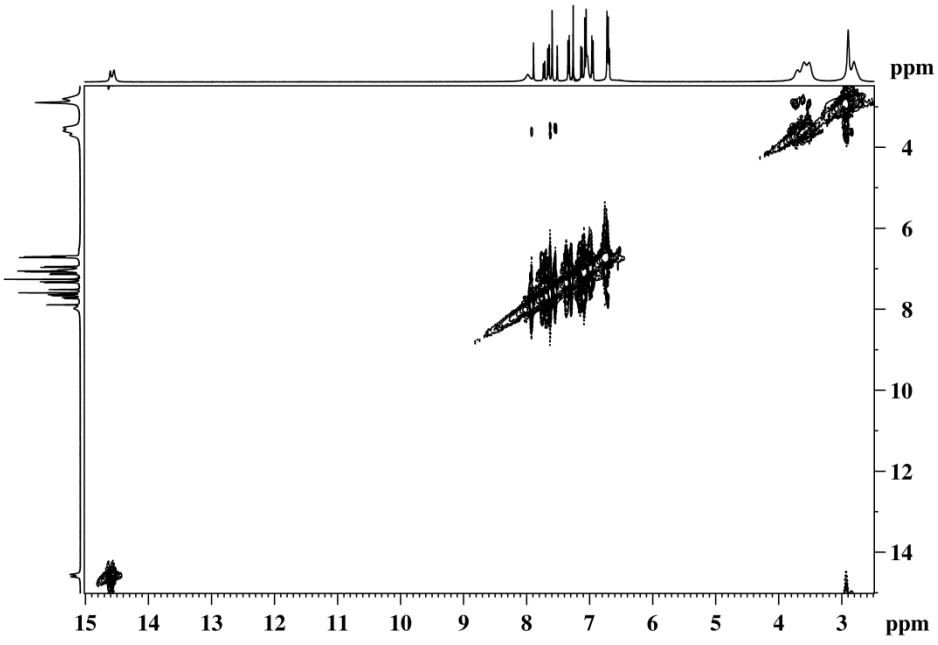

Fig. S11: ^{1}H- ^{1}H COSY spectrum of cage (single crystals) $\mathbf{B_3X_2^{II}}$ recorded in $CDCl_3$.

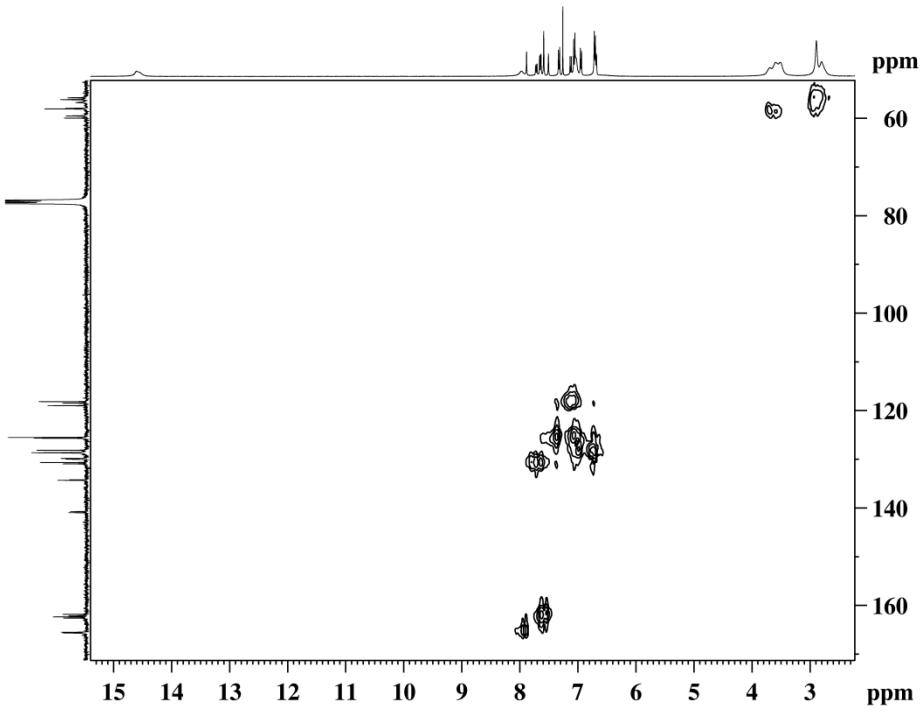

Fig. S12: ^{1}H- ^{13}C HMQC spectrum of cage (single crystals) $\mathbf{B_3X_2^{II}}$ recorded in $CDCl_3$.

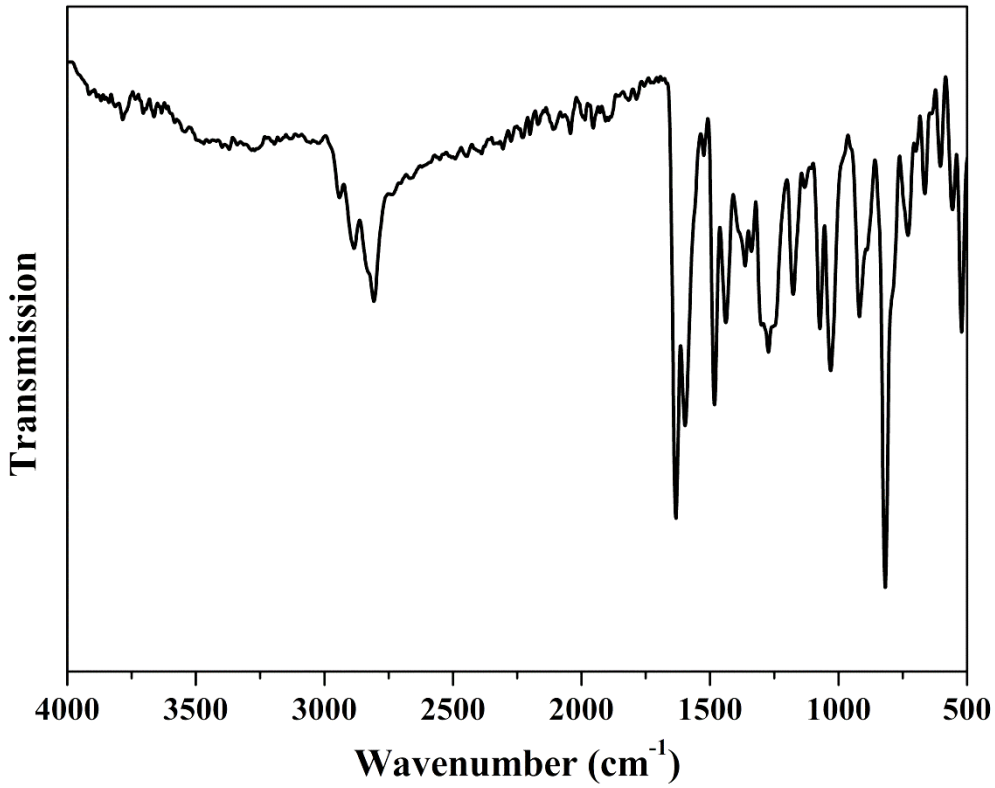

Fig. S13: FTIR spectrum of cage (single crystals) $\mathbf{B_3X_2^{II}}$.

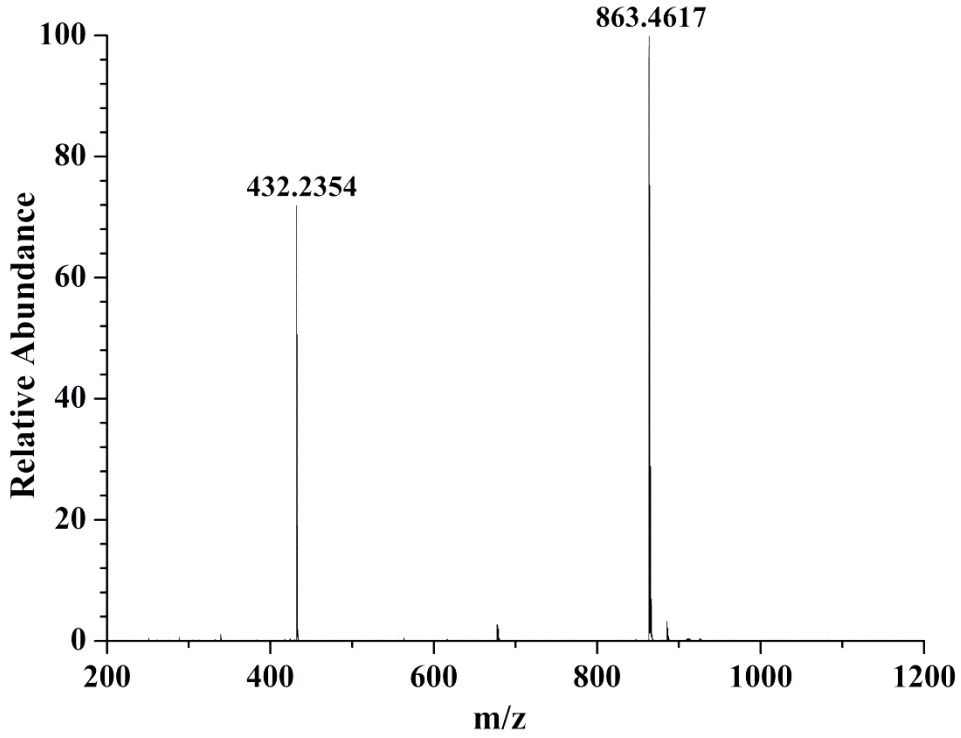

Fig. S14: ESI-HRMS spectrum of cage $\mathbf{B_3X_2^{II}}$ (single crystals) recorded in $CHCl_3$-MeCN (1:1, v/v).

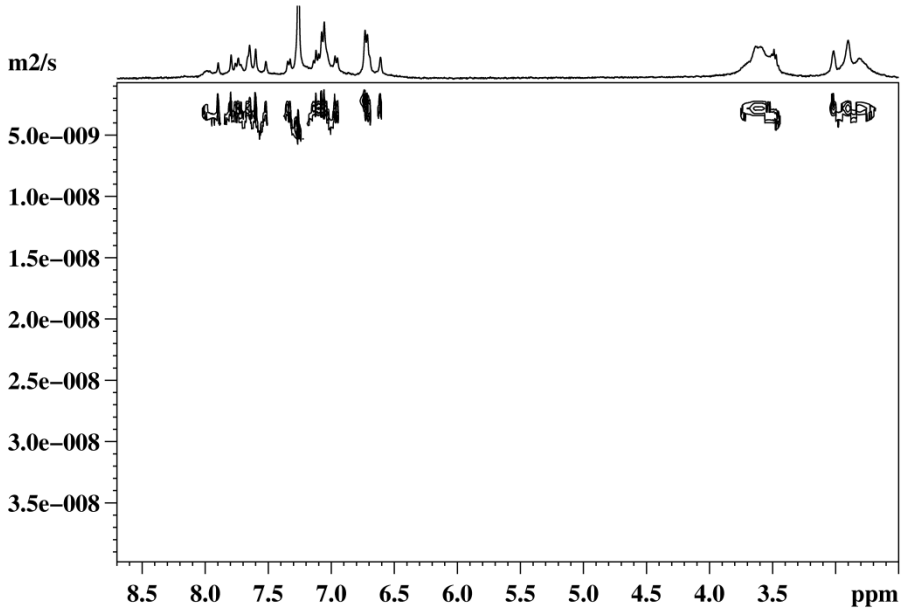

Fig. S15: ^{1}H DOSY spectrum of cage $\mathbf{B_3X_2}$ (I and II) recorded in $CDCl_3$.

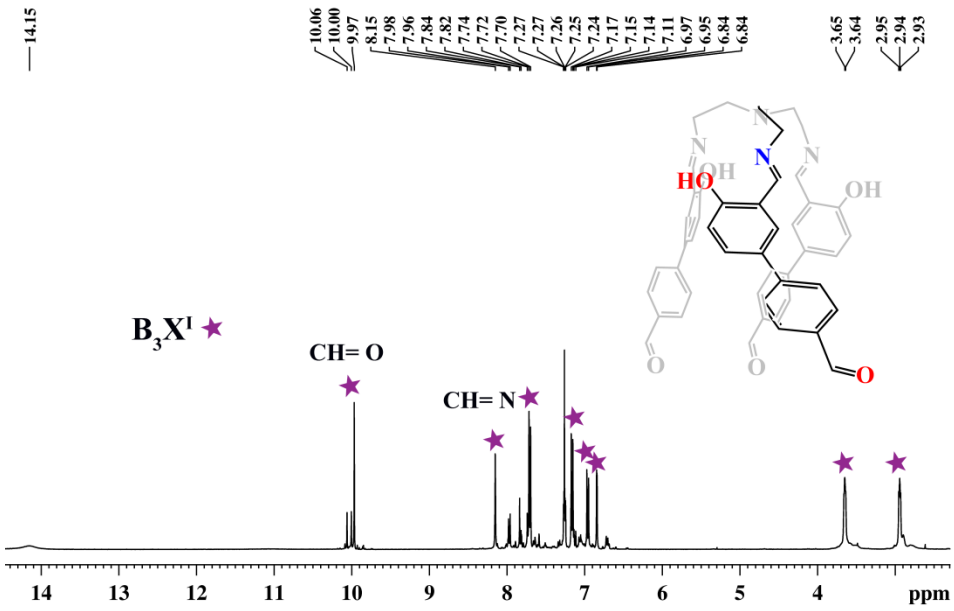

Fig. S16: ^{1}H NMR spectrum of $\mathbf{B_3X^I}$ (crude) recorded in $CDCl_3$.

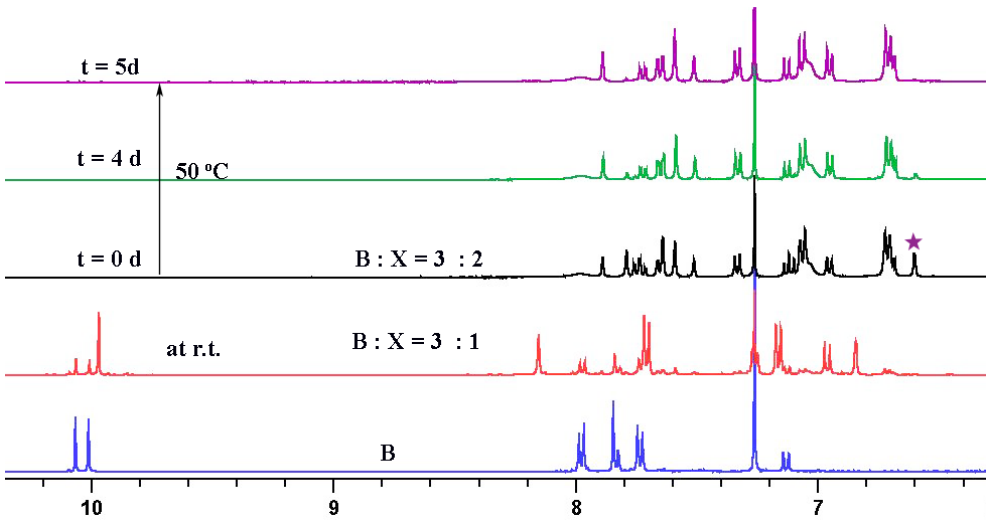

Fig. S17: Time dependent ^{1}H NMR spectra recorded in $CDCl_3$ during formation of isomeric cages $\mathbf{B_3X_2^I}$ and $\mathbf{B_3X_2^{II}}$ in a step wise fashion followed by selective formation of cage $\mathbf{B_3X_2^{II}}$ upon heating.

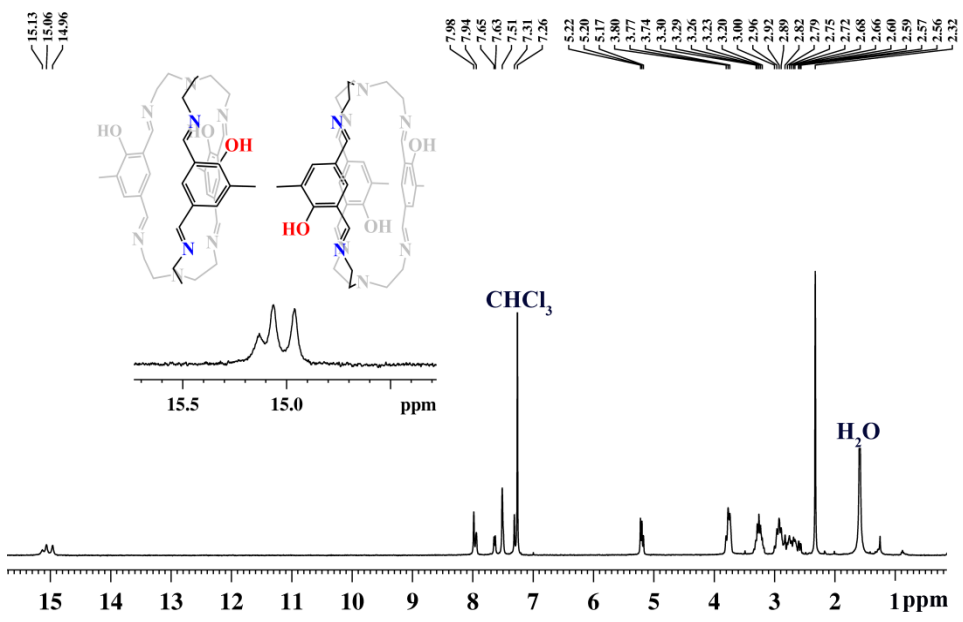

Fig. S18: ^{1}H NMR spectrum of cage C_3X_2 (I and II) recorded in $CDCl_3$.

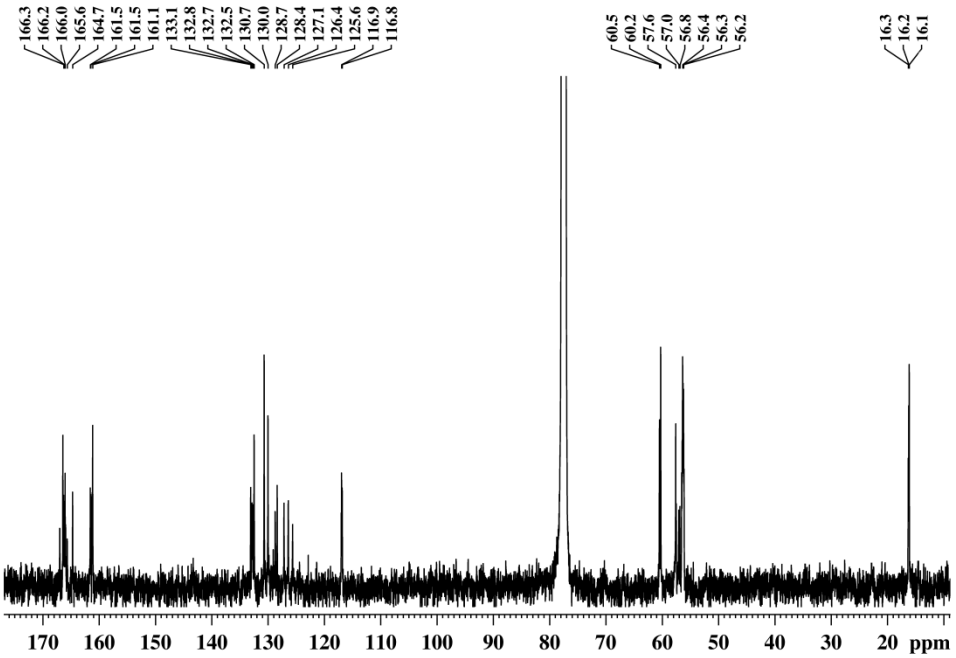

Fig. S19: ^{13}C NMR spectrum of cage $\mathbf{C_3X_2}$ (I and II) recorded in $CDCl_3$.

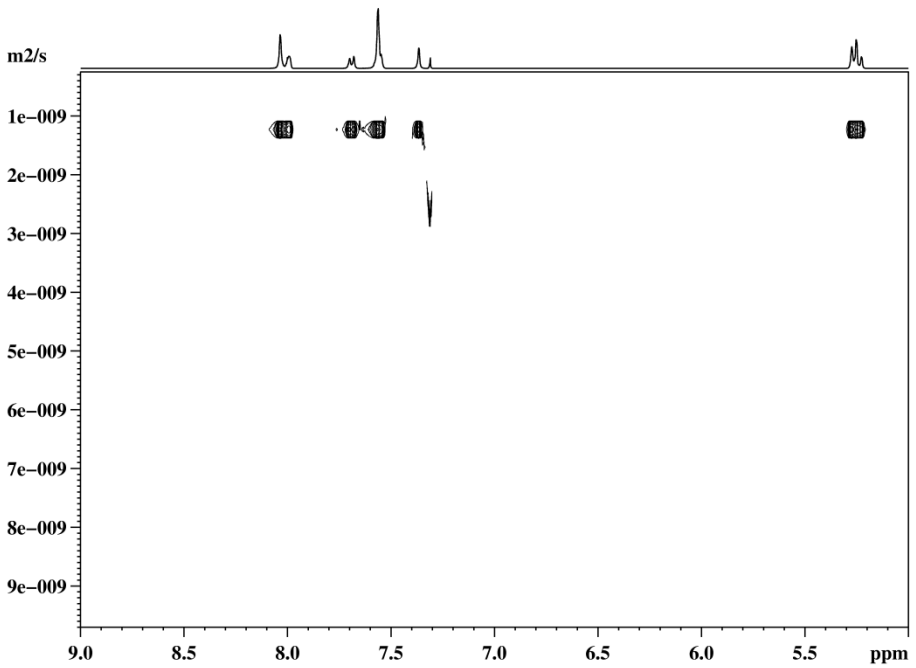

Fig. S20: ^{1}H DOSY spectrum of cage $\mathbf{C_3X_2}$ (I and II) recorded in $CDCl_3$.

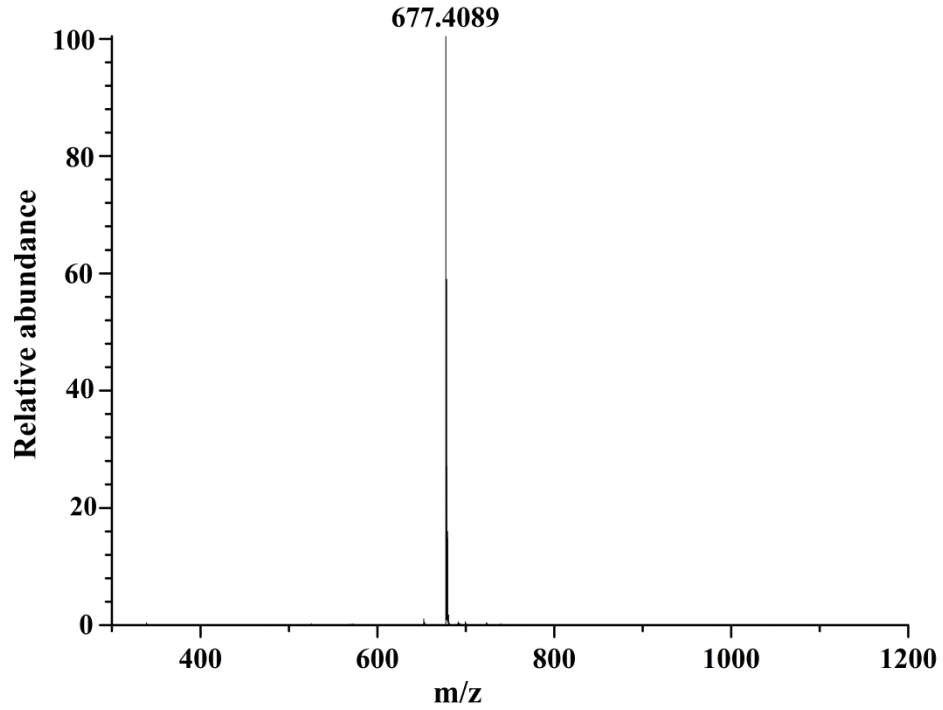

Fig. S21: ESI-HRMS spectrum of cage $\mathbf{C_3X_2}$ (I and II) recorded in $CHCl_3$-MeCN (1:1, v/v).

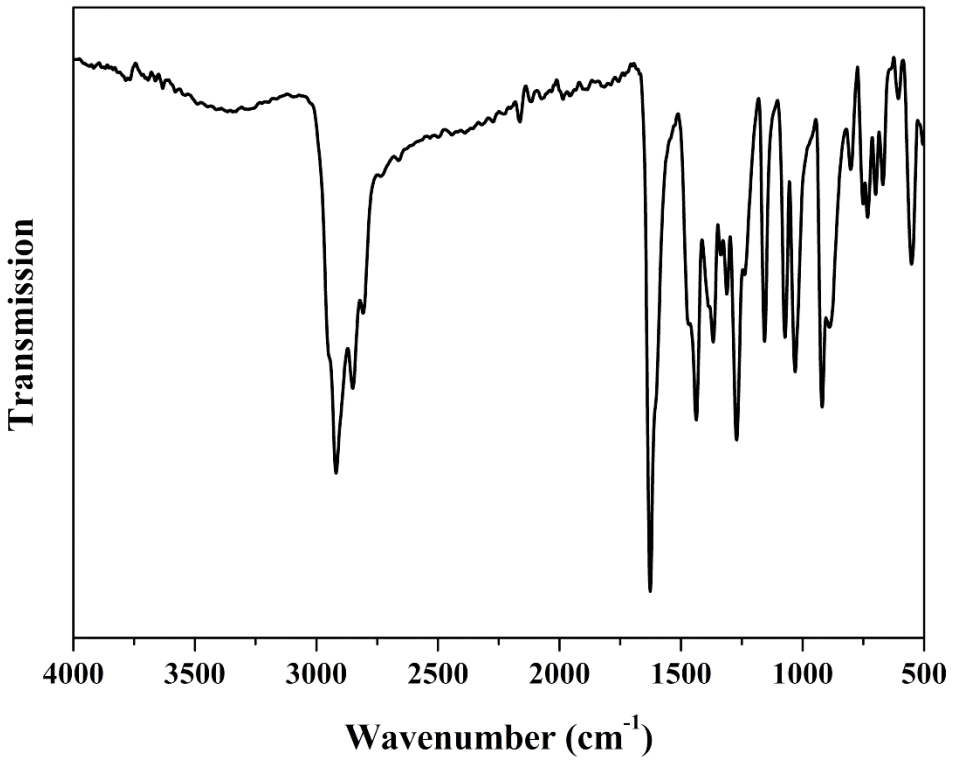

Fig. S22: FTIR spectrum of cage $\mathbf{C_3X_2^{II}}$.

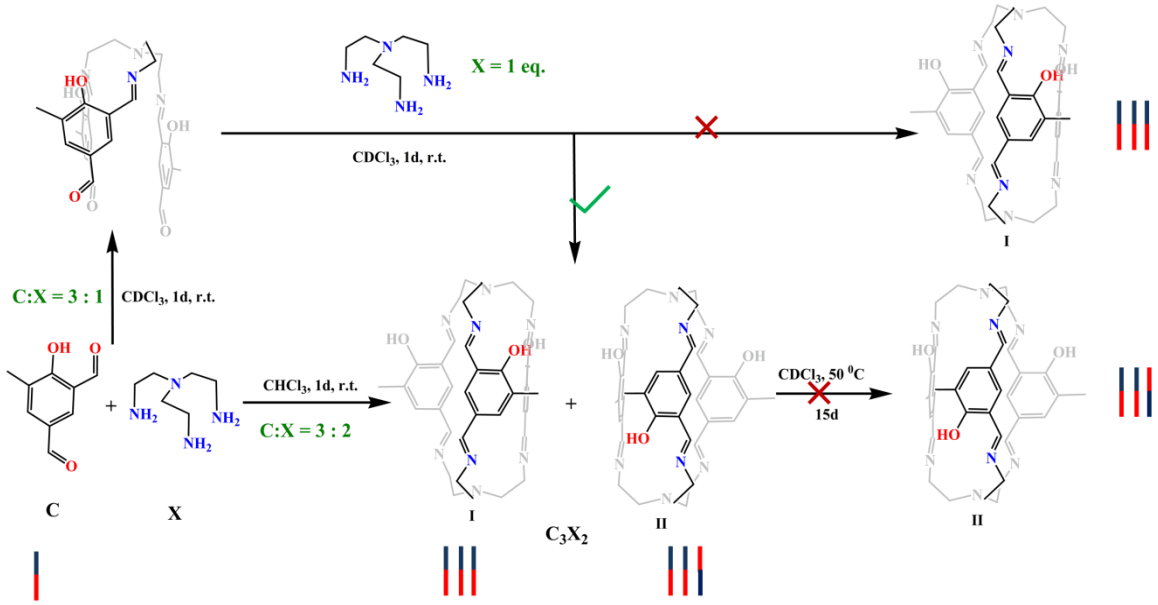

Fig. S23: Schematic representation of different chemical transformations monitored during self-selection experiment of $\mathbf{C_3X_2}$.

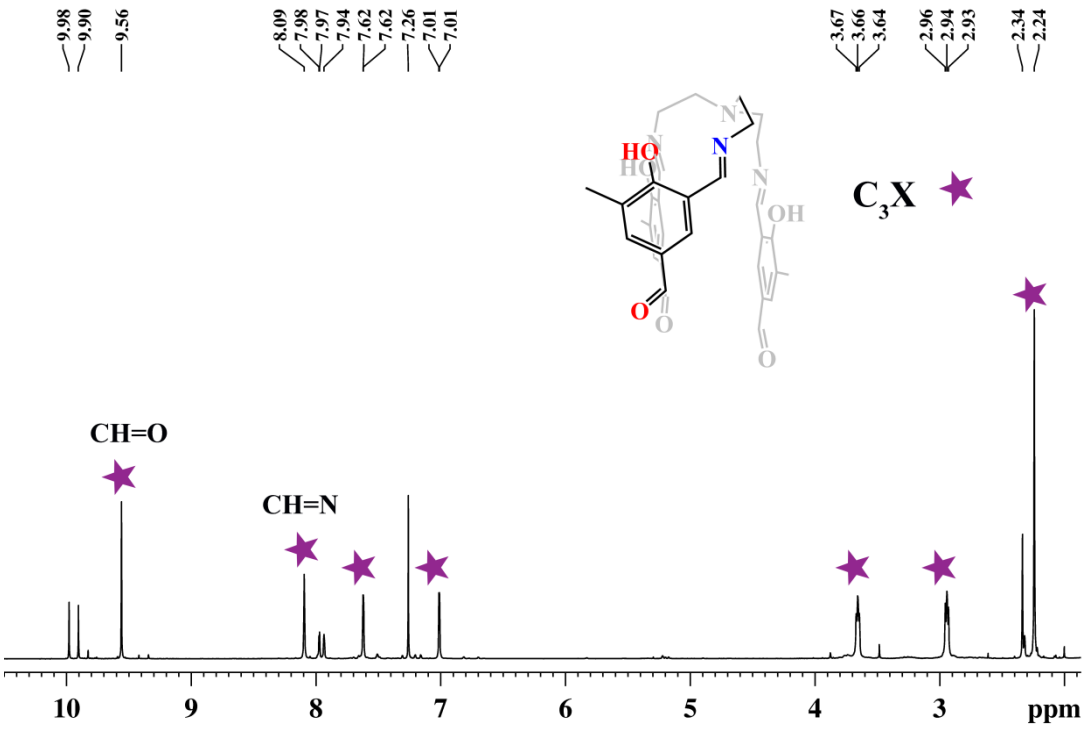

Fig. S24: ^{1}H NMR spectrum of $\mathbf{C_3X^I}$ (crude) recorded in $CDCl_3$.

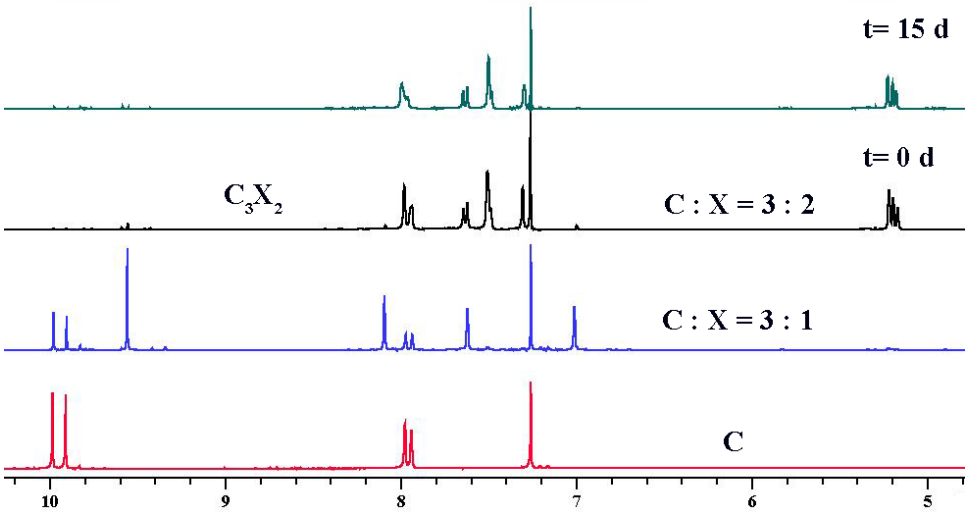

Fig. S25: Time dependent ^{1}H NMR spectra recorded in $CDCl_3$ during formation of isomeric cages $\mathbf{C_3X_2^I}$ and $\mathbf{C_3X_2^{II}}$ in a step wise fashion.

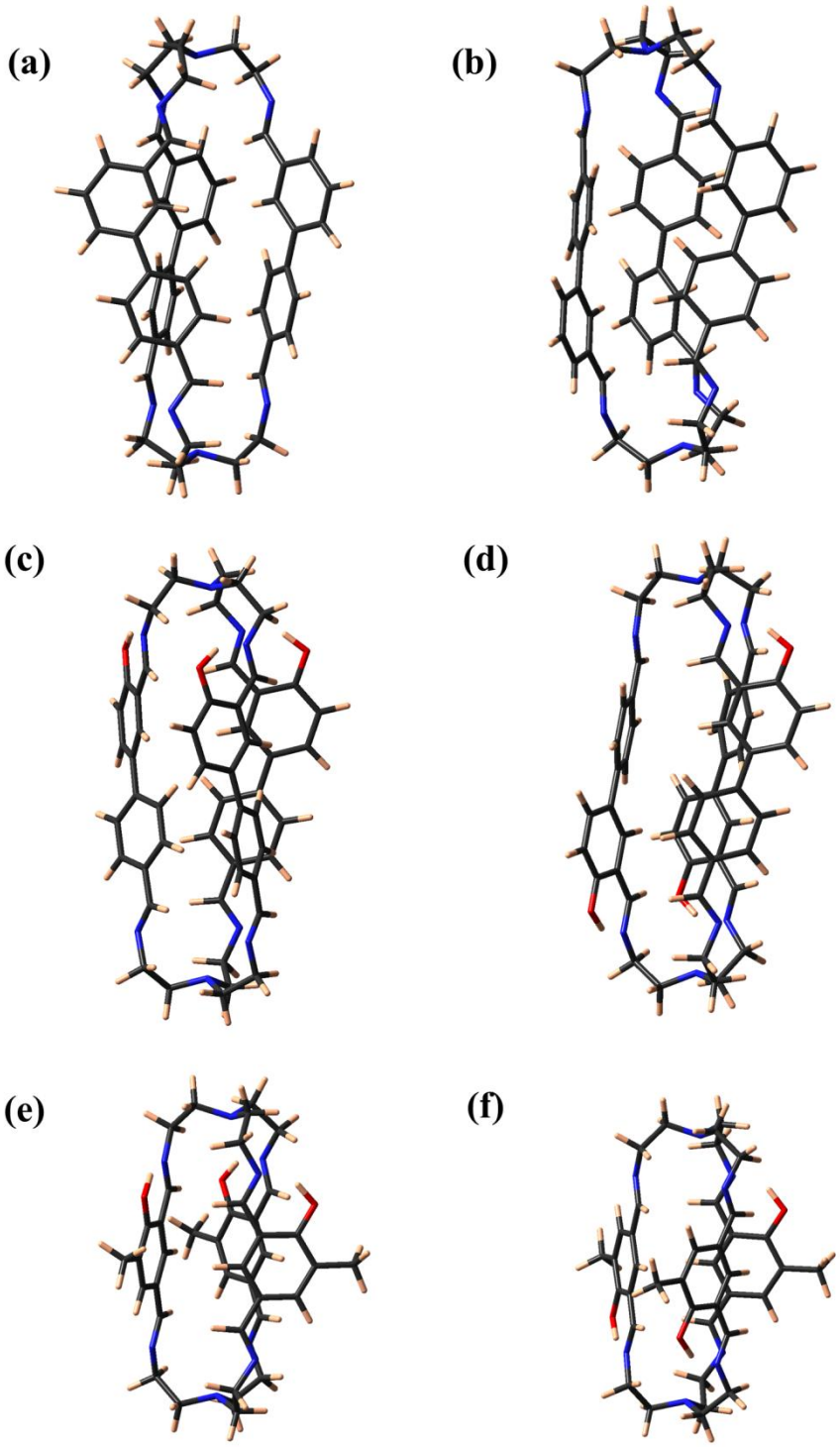

Fig. S26: DFT optimized structures of cage (a) $\mathbf{A_3X_2^I}$, (b) $\mathbf{A_3X_2^{II}}$, (c) $\mathbf{B_3X_2^I}$, (d) $\mathbf{B_3X_2^{II}}$, (e) $\mathbf{C_3X_2^I}$ and (f) $\mathbf{C_3X_2^{II}}$.

$A_3X_2^I$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-5.635716	-2.463522	-0.811565
2	7	0	-5.540201	0.572659	2.509686
3	7	0	-7.319090	0.284838	-0.091427
4	6	0	-1.971922	-2.617769	-0.926130
5	1	0	-1.788290	-2.113460	0.017611
6	7	0	7.395788	0.085340	-0.004336
7	7	0	5.696686	0.890774	2.546548
8	7	0	5.600070	-2.485621	-0.517717
9	6	0	0.513883	-2.964802	-1.206345
10	7	0	-5.488114	2.274596	-1.704517
11	6	0	1.608725	-2.984472	-2.102498
12	1	0	1.429063	-3.081576	-3.167807
13	6	0	2.920047	-2.854023	-1.650963
14	1	0	3.752914	-2.875745	-2.345512
15	6	0	-4.401881	-2.339595	-0.472567
16	1	0	-4.106012	-1.953780	0.513183
17	6	0	2.995874	0.086753	3.423538
18	1	0	3.817091	-0.234035	4.055291
19	6	0	-2.499881	-3.850898	-3.367650
20	1	0	-2.696662	-4.339823	-4.316712
21	6	0	-1.180279	-3.724572	-2.918418
22	1	0	-0.377875	-4.143650	-3.515416
23	7	0	5.756027	1.858535	-2.057223
24	6	0	-3.560129	-3.380764	-2.594915
25	6	0	0.800267	-2.816038	0.165688
26	1	0	-0.003975	-2.828022	0.892059
27	6	0	-7.682188	-1.106344	-0.418848
28	1	0	-7.686937	-1.223291	-1.507032
29	1	0	-8.704989	-1.339906	-0.065884
30	6	0	-0.790272	-0.321137	3.139673
31	6	0	2.208820	1.349149	1.518806
32	1	0	2.407221	1.985212	0.663443
33	6	0	3.278149	0.911361	2.316575
34	6	0	4.557052	-2.515289	0.234787
35	1	0	4.638760	-2.427002	1.328107
36	6	0	-3.463396	-1.177048	3.547091
37	6	0	-0.695520	3.075900	-1.383103
38	6	0	-3.299860	-2.766479	-1.355129
39	6	0	-7.683947	0.697513	1.278025
40	1	0	-7.898311	-0.195793	1.873670
41	1	0	-8.606549	1.305835	1.272012
42	6	0	-0.888011	-3.098389	-1.689811
43	6	0	-6.580636	1.478689	2.005597
44	1	0	-6.173720	2.264432	1.349166
45	1	0	-7.032177	1.966064	2.882062
46	6	0	-1.881018	0.449381	2.688331
47	1	0	-1.701333	1.400706	2.197631
48	6	0	4.639313	1.336210	1.964633

49	1	0	4.703186	2.072969	1.151360
50	6	0	0.607939	0.118306	2.886524
51	6	0	2.110670	-2.667330	0.616970
52	1	0	2.299738	-2.532818	1.677485
53	6	0	-2.396508	-1.948130	4.007052
54	1	0	-2.588392	-2.884971	4.520742
55	6	0	0.902811	0.950044	1.789499
56	1	0	0.112935	1.262657	1.117403
57	6	0	-4.301134	0.876318	2.358341
58	1	0	-3.988884	1.790007	1.831584
59	6	0	-7.669312	1.264870	-1.135509
60	1	0	-7.817320	2.241842	-0.664457
61	1	0	-8.622418	0.996536	-1.628720
62	6	0	-3.127702	2.746690	-1.475353
63	6	0	-1.074554	-1.532471	3.802107
64	1	0	-0.260942	-2.164757	4.141379
65	6	0	0.683010	2.611668	-1.696101
66	6	0	-1.825165	2.349768	-1.811122
67	1	0	-1.695704	1.466076	-2.428245
68	6	0	4.700650	1.149589	-2.252897
69	1	0	4.767321	0.087041	-2.526297
70	6	0	-6.698499	-2.145234	0.152179
71	1	0	-6.301938	-1.794814	1.117758
72	1	0	-7.244349	-3.082310	0.325869
73	6	0	7.860625	1.139310	-0.934274
74	1	0	8.933716	1.001390	-1.179628
75	1	0	7.770183	2.106745	-0.432799
76	6	0	6.998625	1.415565	2.116613
77	1	0	7.548307	1.708340	3.019869
78	1	0	6.892282	2.313404	1.486020
79	6	0	-3.207552	0.032989	2.872936
80	6	0	3.191384	-2.676363	-0.280620
81	6	0	-0.915361	4.231061	-0.605257
82	6	0	-4.270244	1.934596	-1.928512
83	1	0	-4.015576	1.012959	-2.472968
84	6	0	-3.319056	3.913412	-0.710277
85	6	0	1.684474	-0.292430	3.707079
86	1	0	1.489016	-0.896398	4.587430
87	6	0	0.949146	1.248415	-1.933269
88	6	0	3.338877	1.681564	-2.107827
89	6	0	3.081945	3.052249	-1.908621
90	6	0	-6.586970	1.442984	-2.208789
91	1	0	-6.240088	0.464032	-2.578267
92	1	0	-7.036441	1.981877	-3.055565
93	6	0	7.778287	-1.270078	-0.459863
94	1	0	8.842703	-1.477160	-0.226173
95	1	0	7.678386	-1.312994	-1.547250
96	6	0	6.921277	-2.403891	0.116994
97	1	0	7.440799	-3.346855	-0.104327
98	1	0	6.845559	-2.323256	1.214085
99	6	0	7.067952	1.230217	-2.248203
100	1	0	7.639073	1.870222	-2.932896
101	1	0	6.983107	0.236999	-2.718587
102	6	0	2.249800	0.795552	-2.146044

103	1	0	2.427191	-0.263751	-2.295287
104	6	0	7.829433	0.347728	1.387219
105	1	0	8.897204	0.644603	1.415888
106	1	0	7.741973	-0.579164	1.960301
107	6	0	-2.212981	4.646065	-0.282250
108	1	0	-2.354486	5.540080	0.316954
109	6	0	1.778811	3.506447	-1.717152
110	1	0	1.605098	4.569725	-1.590413
111	1	0	3.918523	3.742227	-1.906242
112	1	0	-0.069783	4.794617	-0.226611
113	1	0	0.144118	0.523043	-1.903428
114	1	0	-4.590399	-3.492515	-2.912027
115	1	0	-4.492144	-1.483376	3.696329
116	1	0	-4.331105	4.217463	-0.469916

$A_3X_2^{II}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	6.084503	2.249684	0.072439
2	7	0	5.295435	-1.805923	2.002263
3	7	0	7.288542	-0.699842	-0.256153
4	6	0	2.461107	2.789988	-0.120360
5	1	0	2.170205	2.135415	0.696756
6	7	0	-7.299105	0.579154	-0.255181
7	7	0	-5.833355	-0.498832	2.277273
8	7	0	-5.109069	2.916478	-0.519246
9	6	0	0.023442	3.255127	-0.573002
10	7	0	5.227465	-1.372193	-2.541530
11	6	0	-0.940047	3.200215	-1.606379
12	1	0	-0.614879	3.258055	-2.640270
13	6	0	-2.295912	3.057435	-1.322532
14	1	0	-3.033402	3.028146	-2.117019
15	6	0	4.834248	2.205466	0.365149
16	1	0	4.455044	1.623890	1.217632
17	6	0	-3.041874	-0.066813	3.074890
18	1	0	-3.775759	0.633561	3.458450
19	6	0	3.233213	4.407318	-2.259348
20	1	0	3.527537	5.047908	-3.084751
21	6	0	1.875715	4.251502	-1.954851
22	1	0	1.129748	4.783192	-2.536211
23	7	0	-5.963835	-1.684234	-2.082922
24	6	0	4.206322	3.751276	-1.507182
25	6	0	-0.426839	3.140785	0.756028
26	1	0	0.287254	3.196516	1.570868
27	6	0	7.926089	0.600062	0.019729
28	1	0	8.104918	1.115739	-0.928951
29	1	0	8.911556	0.463631	0.503651
30	6	0	0.713086	-0.712363	3.219729
31	6	0	-2.535628	-2.024279	1.749589
32	1	0	-2.859540	-2.839561	1.110297
33	6	0	-3.483702	-1.109702	2.238594

34	6	0	-4.165902	2.876231	0.354114
35	1	0	-4.385820	2.816533	1.430440
36	6	0	3.466234	-0.549188	3.867535
37	6	0	0.467356	-0.880355	-1.705536
38	1	0	-0.322810	-0.209611	-1.387210
39	6	0	3.824015	2.931430	-0.427493
40	6	0	7.466434	-1.699637	0.813983
41	1	0	7.734072	-1.183404	1.741318
42	1	0	8.300583	-2.385136	0.575748
43	6	0	1.466274	3.435654	-0.882007
44	6	0	6.203975	-2.525405	1.100179
45	1	0	5.718202	-2.821896	0.156817
46	1	0	6.506984	-3.441016	1.628086
47	6	0	1.699264	-1.183366	2.329922
48	1	0	1.403447	-1.597000	1.370793
49	6	0	-4.894778	-1.277624	1.869198
50	1	0	-5.107517	-2.130961	1.209188
51	6	0	-0.730747	-0.845647	2.891986
52	6	0	-1.784159	2.993823	1.040143
53	1	0	-2.112059	2.917622	2.072116
54	6	0	2.503717	-0.053803	4.746368
55	1	0	2.808955	0.383130	5.692137
56	6	0	-1.186512	-1.898006	2.074095
57	1	0	-0.484127	-2.635413	1.702927
58	6	0	4.043007	-1.730415	1.724019
59	1	0	3.628206	-2.151816	0.797056
60	6	0	7.518985	-1.226159	-1.614404
61	1	0	7.415437	-2.315661	-1.589051
62	1	0	8.547943	-1.007905	-1.956613
63	6	0	2.830013	-1.233632	-2.183658
64	6	0	1.141205	-0.142728	4.435234
65	1	0	0.406904	0.200903	5.156200
66	6	0	-1.489589	-4.073498	-1.484056
67	1	0	-0.671541	-4.751709	-1.264761
68	6	0	1.765441	-0.388297	-1.826811
69	1	0	1.960605	0.660484	-1.631604
70	6	0	-4.725480	-1.380906	-2.240047
71	1	0	-4.416807	-0.384858	-2.590076
72	6	0	7.065239	1.531174	0.892790
73	1	0	6.597760	0.959040	1.709981
74	1	0	7.723592	2.289566	1.338176
75	6	0	-7.890212	-0.376783	-1.217871
76	1	0	-8.867817	-0.005094	-1.586139
77	1	0	-8.083033	-1.321025	-0.701541
78	6	0	-7.211052	-0.788509	1.865259
79	1	0	-7.800952	-0.947772	2.778133
80	1	0	-7.276783	-1.710423	1.263349
81	6	0	3.065029	-1.126519	2.647156
82	6	0	-2.739771	2.956520	0.009959
83	6	0	0.179413	-2.235646	-1.963185
84	6	0	4.180709	-0.665241	-2.299337
85	1	0	4.243981	0.423988	-2.170811
86	6	0	2.554347	-2.593053	-2.430149
87	1	0	3.372529	-3.243596	-2.718854

88	6	0	-1.691568	0.063520	3.389569
89	1	0	-1.369929	0.892966	4.011325
90	6	0	-1.213544	-2.742356	-1.853870
91	6	0	-3.630749	-2.328311	-1.972614
92	6	0	-3.881394	-3.664410	-1.604686
93	6	0	6.525380	-0.696467	-2.660817
94	1	0	6.437003	0.399112	-2.575797
95	1	0	6.922964	-0.929477	-3.657771
96	6	0	-7.420055	1.972978	-0.735764
97	1	0	-8.466446	2.331005	-0.636810
98	1	0	-7.179305	1.989551	-1.802502
99	6	0	-6.497467	2.985419	-0.047867
100	1	0	-6.868011	3.985419	-0.315027
101	1	0	-6.561817	2.901664	1.049414
102	6	0	-6.991984	-0.694744	-2.422725
103	1	0	-7.622837	-1.144506	-3.201005
104	1	0	-6.557396	0.228650	-2.839598
105	6	0	-2.305917	-1.889198	-2.103170
106	1	0	-2.126027	-0.865031	-2.414436
107	6	0	-7.833265	0.394744	1.111709
108	1	0	-8.934917	0.271212	1.095763
109	1	0	-7.623097	1.294380	1.694847
110	6	0	1.252606	-3.080146	-2.328784
111	1	0	1.057381	-4.121308	-2.564736
112	6	0	-2.810542	-4.526764	-1.367289
113	1	0	-2.999041	-5.557389	-1.082858
114	1	0	4.523104	-0.519557	4.105938
115	1	0	-4.909436	-3.997108	-1.518663
116	1	0	5.262060	3.852735	-1.729753

$B_3X_2^I$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.605327	-3.142015	-2.815147
2	1	0	-5.221725	-2.880442	-2.033151
3	8	0	-4.669852	-1.058786	3.728877
4	1	0	-5.267069	-0.340675	3.297743
5	7	0	-5.343423	-2.369086	-0.491710
6	7	0	-5.355544	0.991212	2.355203
7	7	0	-7.149764	0.222158	-0.079364
8	6	0	-1.680409	-2.558248	-0.634316
9	1	0	-1.484021	-2.163374	0.356914
10	7	0	7.670853	0.050836	0.084998
11	7	0	5.893949	0.946879	2.572211
12	7	0	5.903190	-2.548317	-0.371041
13	6	0	0.792903	-2.929496	-0.981936
14	7	0	-5.137683	1.752361	-1.940447
15	6	0	1.880341	-3.053575	-1.880286
16	1	0	1.695655	-3.203129	-2.938134
17	6	0	3.200738	-2.957865	-1.446928
18	1	0	4.023098	-3.053046	-2.147988

19	6	0	-4.099052	-2.266973	-0.136609
20	1	0	-3.822451	-1.958189	0.877054
21	6	0	3.143697	0.290267	3.423769
22	1	0	3.936784	-0.015311	4.097703
23	6	0	-2.271729	-3.506666	-3.193516
24	1	0	-2.516089	-3.881801	-4.180200
25	6	0	-0.959004	-3.466939	-2.739867
26	1	0	-0.181514	-3.839905	-3.396277
27	7	0	6.127607	1.780058	-2.074349
28	6	0	-3.320762	-3.084989	-2.362998
29	6	0	1.106461	-2.734206	0.379806
30	1	0	0.316642	-2.668190	1.118114
31	6	0	-7.505740	-1.207341	-0.105347
32	1	0	-7.688751	-1.506523	-1.143591
33	1	0	-8.446490	-1.385689	0.445253
34	6	0	-0.649891	0.024049	3.084379
35	6	0	2.450481	1.445680	1.418075
36	1	0	2.693115	2.012212	0.525758
37	6	0	3.483785	1.026671	2.271952
38	6	0	4.870501	-2.552067	0.396801
39	1	0	4.969200	-2.430123	1.485653
40	6	0	-3.369711	-0.693501	3.520835
41	6	0	-0.395218	2.766599	-1.683487
42	6	0	-3.021737	-2.615382	-1.053076
43	6	0	-7.523287	0.935543	1.155030
44	1	0	-7.805421	0.195536	1.912355
45	1	0	-8.410627	1.572517	0.989361
46	6	0	-0.619576	-2.983502	-1.449928
47	6	0	-6.413171	1.812143	1.755105
48	1	0	-6.003204	2.502276	1.004970
49	1	0	-6.861490	2.416170	2.557162
50	6	0	-1.696270	0.799585	2.562427
51	1	0	-1.473493	1.701004	2.000375
52	6	0	4.866419	1.390675	1.937155
53	1	0	4.974379	2.085743	1.092316
54	6	0	0.770299	0.377659	2.828596
55	6	0	2.425698	-2.619752	0.811958
56	1	0	2.629337	-2.436217	1.862460
57	6	0	-2.334927	-1.477889	4.051381
58	1	0	-2.598741	-2.360112	4.622473
59	6	0	1.124414	1.114876	1.681964
60	1	0	0.362845	1.407861	0.969348
61	6	0	-4.103461	1.272546	2.164295
62	1	0	-3.802972	2.124157	1.544398
63	6	0	-7.401194	0.952106	-1.333073
64	1	0	-7.572827	2.007547	-1.094406
65	1	0	-8.319147	0.585136	-1.827206
66	6	0	-2.807842	2.304397	-1.782483
67	6	0	-1.006671	-1.125527	3.832696
68	1	0	-0.225815	-1.763755	4.232325
69	6	0	1.010337	2.356060	-1.936973
70	6	0	-1.476475	1.966274	-2.081576
71	1	0	-1.297641	1.056716	-2.646287
72	6	0	5.099910	1.035225	-2.284829

73	1	0	5.208393	-0.034807	-2.512701
74	6	0	-6.429686	-2.142461	0.467761
75	1	0	-6.047636	-1.762237	1.424707
76	1	0	-6.897075	-3.119067	0.658084
77	6	0	8.180306	1.094902	-0.833984
78	1	0	9.264924	0.955412	-1.022193
79	1	0	8.064077	2.067547	-0.348660
80	6	0	7.220692	1.428706	2.166679
81	1	0	7.749339	1.732818	3.078649
82	1	0	7.152634	2.313106	1.512503
83	6	0	-3.047195	0.461678	2.754571
84	6	0	3.496342	-2.712942	-0.092717
85	6	0	-0.695698	3.953250	-0.968450
86	6	0	-3.903724	1.428297	-2.173735
87	1	0	-3.644308	0.481561	-2.661913
88	6	0	-3.073206	3.509378	-1.072909
89	6	0	1.812141	-0.017684	3.700391
90	1	0	1.574497	-0.549346	4.616435
91	6	0	1.343697	0.995546	-2.092632
92	6	0	3.717338	1.524611	-2.215001
93	6	0	3.395746	2.890799	-2.095956
94	6	0	-6.251307	0.887888	-2.348966
95	1	0	-5.919252	-0.148975	-2.503184
96	1	0	-6.629924	1.264761	-3.310669
97	6	0	8.071877	-1.308224	-0.344450
98	1	0	9.138247	-1.497338	-0.102318
99	1	0	7.977676	-1.369118	-1.431452
100	6	0	7.231759	-2.449035	0.244923
101	1	0	7.760801	-3.385555	0.019430
102	1	0	7.169253	-2.368817	1.342910
103	6	0	7.458714	1.172188	-2.189107
104	1	0	8.058260	1.817939	-2.843060
105	1	0	7.414461	0.176808	-2.660666
106	6	0	2.667667	0.592176	-2.243634
107	1	0	2.894912	-0.464010	-2.329976
108	6	0	8.052238	0.327246	1.489586
109	1	0	9.125337	0.598425	1.557338
110	1	0	7.918032	-0.586103	2.074711
111	6	0	-2.003322	4.322684	-0.672482
112	1	0	-2.223306	5.230510	-0.123353
113	6	0	2.067672	3.296215	-1.972271
114	1	0	1.846187	4.356411	-1.907154
115	1	0	4.200979	3.617263	-2.100625
116	8	0	-4.352047	3.872012	-0.756909
117	1	0	-4.982606	3.172677	-1.176817
118	1	0	0.114488	4.581609	-0.615342
119	1	0	0.572077	0.235815	-2.041933

$B_3X_2^{II}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	5.289197	0.394744	3.883412
2	1	0	5.914563	0.012427	3.159784
3	8	0	4.671204	-3.386218	-1.660759
4	1	0	5.245537	-2.620554	-2.035029
5	7	0	6.059350	-0.844082	1.785066
6	7	0	5.291118	-1.098976	-2.635771
7	8	0	-5.523868	3.782838	-1.510596
8	1	0	-6.079092	3.256857	-0.820511
9	7	0	7.254508	0.511236	-0.807727
10	6	0	2.413024	-1.110183	2.122049
11	1	0	2.218038	-1.641555	1.195790
12	7	0	-7.447590	-0.644076	0.462035
13	7	0	-5.940850	-1.547690	-2.119439
14	7	0	-5.148232	-1.850656	2.230651
15	6	0	-0.046725	-1.168643	2.662007
16	7	0	5.136105	2.794260	-0.355453
17	6	0	-1.151472	-0.450385	3.178438
18	1	0	-0.980499	0.416371	3.808400
19	6	0	-2.461811	-0.821678	2.885808
20	1	0	-3.300708	-0.277826	3.306933
21	6	0	4.827658	-1.158439	1.522688
22	1	0	4.574432	-1.766978	0.648521
23	6	0	-3.176734	-2.519505	-2.348070
24	1	0	-3.957988	-3.264973	-2.449040
25	6	0	2.969056	0.330459	4.452435
26	1	0	3.204231	0.875319	5.359068
27	6	0	1.667635	-0.058467	4.155845
28	1	0	0.881025	0.178596	4.864064
29	7	0	-6.079755	2.276037	0.471214
30	6	0	4.020785	-0.002229	3.584333
31	6	0	-0.322801	-2.273115	1.831023
32	1	0	0.491853	-2.869431	1.436979
33	6	0	7.938287	-0.118995	0.337164
34	1	0	8.065387	0.627536	1.127196
35	1	0	8.952872	-0.461675	0.059295
36	6	0	0.621080	-2.311173	-2.086127
37	6	0	-2.532925	-0.199548	-2.137537
38	1	0	-2.800059	0.848421	-2.057595
39	6	0	-3.547910	-1.165595	-2.237057
40	6	0	-4.085102	-2.355487	1.710445
41	1	0	-4.142029	-3.183954	0.988612
42	6	0	3.360451	-3.031067	-1.813312
43	6	0	0.460248	2.774265	0.950531
44	1	0	-0.247686	2.715696	1.769921
45	6	0	3.742184	-0.750048	2.404984
46	6	0	7.518012	-0.164297	-2.091644
47	1	0	7.765936	-1.211896	-1.891768
48	1	0	8.395098	0.276492	-2.603773
49	6	0	1.350874	-0.778351	2.976984
50	6	0	6.323853	-0.145738	-3.053270
51	1	0	5.912497	0.869888	-3.147906
52	1	0	6.681095	-0.457629	-4.045255
53	6	0	1.642303	-1.417968	-2.439166
54	1	0	1.390453	-0.440848	-2.838713

55	6	0	-4.949136	-0.731540	-2.185833
56	1	0	-5.104031	0.357275	-2.188991
57	6	0	-0.808812	-1.923898	-2.182238
58	6	0	-1.632232	-2.628543	1.516272
59	1	0	-1.816477	-3.475634	0.862451
60	6	0	2.350808	-3.937285	-1.457956
61	1	0	2.641616	-4.908943	-1.076590
62	6	0	-1.191622	-0.571046	-2.092425
63	1	0	-0.441583	0.196692	-1.939768
64	6	0	4.033403	-0.788926	-2.682006
65	1	0	3.704191	0.206634	-3.001605
66	6	0	7.420924	1.976885	-0.879362
67	1	0	7.154901	2.303938	-1.889009
68	1	0	8.477723	2.266215	-0.715118
69	6	0	2.773469	2.730786	0.187734
70	6	0	1.012726	-3.580911	-1.593746
71	1	0	0.251668	-4.292541	-1.292228
72	6	0	-1.883205	4.065781	-1.692815
73	1	0	-1.147174	4.604383	-2.280034
74	6	0	1.819708	2.612735	1.213842
75	1	0	2.149187	2.405414	2.227596
76	6	0	-4.813066	2.098979	0.691201
77	1	0	-4.464165	1.464347	1.513361
78	6	0	7.157836	-1.304352	0.930785
79	1	0	6.791417	-1.963730	0.130641
80	1	0	7.840563	-1.887493	1.562536
81	6	0	-8.016462	0.710645	0.594625
82	1	0	-8.999613	0.682608	1.105542
83	1	0	-8.192957	1.118520	-0.405165
84	6	0	-7.298217	-0.999880	-2.038031
85	1	0	-7.887503	-1.444730	-2.850356
86	1	0	-7.315164	0.094858	-2.175218
87	6	0	3.002516	-1.746273	-2.308644
88	6	0	-2.724520	-1.915199	2.038481
89	6	0	-0.002748	3.042635	-0.353273
90	6	0	4.201073	2.612764	0.510384
91	1	0	4.430172	2.380149	1.560614
92	6	0	2.321684	2.996238	-1.119328
93	1	0	3.057068	3.091243	-1.910994
94	6	0	-1.833131	-2.887155	-2.334533
95	1	0	-1.572056	-3.933420	-2.457927
96	6	0	-1.448837	3.226812	-0.635483
97	6	0	-3.808143	2.755449	-0.134111
98	6	0	-4.209472	3.596782	-1.211906
99	6	0	6.532986	2.755948	0.095300
100	1	0	6.628141	2.359708	1.119895
101	1	0	6.895958	3.793987	0.112363
102	6	0	-7.544892	-1.419756	1.717156
103	1	0	-8.530492	-1.920318	1.796177
104	1	0	-7.475131	-0.727397	2.560785
105	6	0	-6.442500	-2.464533	1.899521
106	1	0	-6.729634	-3.093905	2.755147
107	1	0	-6.372241	-3.124535	1.019220
108	6	0	-7.094565	1.685944	1.348056

109	1	0	-7.706390	2.512872	1.730867
110	1	0	-6.628465	1.184074	2.207915
111	6	0	-2.435590	2.585843	0.127857
112	1	0	-2.146355	1.906828	0.924684
113	6	0	-7.966040	-1.384341	-0.708204
114	1	0	-9.062387	-1.257533	-0.805506
115	1	0	-7.781387	-2.450632	-0.549534
116	6	0	0.962469	3.139175	-1.383784
117	1	0	0.638422	3.319529	-2.403728
118	6	0	-3.229990	4.245471	-1.980783
119	1	0	-3.555980	4.893688	-2.785350

$C_3X_2^I$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.007625	-1.335180	5.079968
2	6	0	-0.013626	5.067281	-1.396107
3	6	0	-0.002017	-3.744868	-3.690935
4	8	0	2.282357	-0.312581	3.811550
5	8	0	2.288418	-3.151174	-2.173767
6	7	0	3.425212	-2.492040	0.006796
7	6	0	-2.700761	-2.355560	0.354987
8	6	0	1.032556	-2.506258	-0.206425
9	6	0	1.026442	1.078527	2.278066
10	7	0	-3.830607	1.094400	2.353293
11	7	0	-3.824416	-2.585835	-0.227100
12	6	0	-1.410899	1.020281	2.372644
13	6	0	-1.404799	-2.557936	-0.304163
14	6	0	-0.105664	-0.356343	3.937220
15	6	0	-1.320377	-3.030618	-1.635976
16	6	0	1.085963	-2.968591	-1.550030
17	7	0	-5.618125	-0.002606	0.000217
18	6	0	-0.229144	0.808781	-2.196808
19	6	0	-0.223115	-2.303124	0.394818
20	6	0	2.254865	0.672208	-2.237581
21	6	0	-1.411751	1.540121	-2.068135
22	6	0	2.260396	-2.271634	0.537755
23	7	0	-3.831102	1.485475	-2.128359
24	6	0	1.025771	1.432382	-2.069611
25	6	0	-5.068599	-2.405652	0.528119
26	6	0	-2.707277	0.866799	-2.221712
27	6	0	4.653607	-2.303066	0.782859
28	6	0	-0.109599	3.587039	-1.666784
29	6	0	1.079926	0.140172	3.344973
30	6	0	-0.229265	1.501768	1.805293
31	6	0	1.077177	2.826879	-1.796497
32	6	0	-0.099772	-3.236494	-2.274749
33	6	0	-5.075784	1.656446	1.820037
34	7	0	5.292887	0.003765	0.000536
35	7	0	3.419065	1.243357	-2.161509
36	6	0	-2.707011	1.491385	1.869256
37	7	0	3.419370	1.255218	2.157528

38	6	0	-1.329155	2.929669	-1.810064
39	6	0	-1.326323	0.096848	3.442389
40	6	0	2.254243	1.607048	1.703728
41	6	0	-6.010194	-1.415462	-0.171937
42	6	0	-6.013974	0.553659	1.309285
43	6	0	-5.075683	0.741474	-2.347024
44	6	0	4.648298	0.478496	-2.387091
45	6	0	-6.014088	0.851851	-1.136851
46	6	0	5.661948	-1.423240	0.030336
47	6	0	5.658222	0.692357	-1.250675
48	6	0	5.658020	0.744031	1.222084
49	6	0	4.646996	1.834008	1.605281
50	1	0	0.561193	-0.909238	5.914850
51	1	0	-1.001357	-1.614529	5.441594
52	1	0	0.523332	-2.246654	4.780080
53	1	0	0.551487	5.575897	-2.186042
54	1	0	0.520201	5.267599	-0.459309
55	1	0	-1.008070	5.518258	-1.333005
56	1	0	0.530708	-3.034108	-4.334134
57	1	0	-0.995894	-3.918612	-4.113237
58	1	0	0.564811	-4.682346	-3.734021
59	1	0	-4.881132	-2.089172	1.567644
60	1	0	-5.572248	-3.381513	0.562633
61	1	0	4.434813	-1.883997	1.776070
62	1	0	5.109184	-3.291902	0.931295
63	1	0	-5.997047	-1.653809	-1.239448
64	1	0	-7.045492	-1.588089	0.183906
65	1	0	-7.049866	0.946417	1.278576
66	1	0	-6.001130	-0.252036	2.049037
67	1	0	-5.581934	1.200164	-3.207524
68	1	0	-4.889149	-0.316924	-2.594109
69	1	0	-6.001565	1.895673	-0.809961
70	1	0	-7.049820	0.628179	-1.461646
71	1	0	6.664404	-1.571314	0.475310
72	1	0	5.719124	-1.789041	-0.999945
73	1	0	5.714052	1.767664	-1.052646
74	1	0	6.660501	0.382710	-1.603440
75	1	0	6.659649	1.205491	1.129424
76	1	0	5.715022	0.035236	2.054486
77	1	0	5.100863	2.459788	2.386213
78	1	0	4.427069	2.481957	0.744074
79	1	0	-0.268098	-1.939412	1.417692
80	1	0	-2.249192	-3.239916	-2.156750
81	1	0	-2.255130	-0.252332	3.881764
82	1	0	-0.274008	2.211060	0.983400
83	1	0	-0.272529	-0.258911	-2.393424
84	1	0	2.166422	-0.399222	-2.445243
85	1	0	2.170423	-1.913938	1.568725
86	1	0	2.164185	2.323693	0.880712
87	1	0	-2.659918	2.220134	1.047630
88	1	0	-2.659673	-0.211019	-2.432134
89	1	0	-2.653782	-1.999749	1.394010
90	1	0	4.430699	-0.591615	-2.519832
91	1	0	5.101990	0.844372	-3.318624

92	1	0	3.031490	-2.973917	-1.476403
93	1	0	3.025505	0.204492	3.311939
94	1	0	-5.581670	2.170426	2.648940
95	1	0	-4.890095	2.401330	1.028444
96	8	0	2.278519	3.459556	-1.639463
97	1	0	3.022587	2.767457	-1.832530
98	1	0	-2.258826	3.483868	-1.731064

$C_3X_2^{II}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.217557	0.982419	-5.157934
2	6	0	-0.417770	-4.968937	1.781531
3	6	0	0.230768	4.008068	3.434595
4	8	0	2.446230	-0.044015	-3.785758
5	8	0	2.529322	3.209220	2.034858
6	8	0	-2.677088	-3.304552	1.829677
7	7	0	3.695572	2.328240	-0.050338
8	6	0	-2.413924	2.450678	-0.587138
9	6	0	1.302055	2.462947	0.086722
10	6	0	1.112753	-1.270266	-2.180648
11	7	0	-3.736869	-1.090330	-2.333428
12	7	0	-3.547931	2.749140	-0.055923
13	6	0	-1.318151	-1.125559	-2.320912
14	6	0	-1.132074	2.635816	0.101926
15	6	0	0.063659	0.089920	-3.952339
16	6	0	-1.062940	3.201649	1.398252
17	6	0	1.340492	3.024074	1.393065
18	7	0	-5.507053	0.293568	-0.141124
19	6	0	-0.132482	-0.662301	2.213861
20	6	0	0.056248	2.274666	-0.537574
21	6	0	2.340619	-0.764176	2.336090
22	6	0	-1.395119	-1.270146	2.099616
23	6	0	2.538300	2.115818	-0.598596
24	7	0	-3.784912	-1.031169	2.127878
25	6	0	1.038480	-1.424149	2.190452
26	6	0	-4.769312	2.593433	-0.854237
27	6	0	-2.612868	-0.475782	2.168934
28	6	0	4.935888	2.024863	-0.768006
29	6	0	-0.295187	-3.473053	1.923064
30	6	0	1.219986	-0.411970	-3.308586
31	6	0	-0.164829	-1.612519	-1.702415
32	6	0	0.933240	-2.829556	2.048143
33	6	0	0.147356	3.398368	2.058315
34	6	0	-5.014641	-1.554826	-1.786238
35	7	0	5.403349	-0.283087	0.124221
36	7	0	3.458365	-1.402784	2.298620
37	6	0	-2.639090	-1.508626	-1.808772
38	7	0	3.494170	-1.545377	-2.013629
39	6	0	-1.470418	-2.682492	1.951288
40	6	0	-1.181031	-0.279881	-3.448272

41	6	0	2.309547	-1.806937	-1.551549
42	6	0	-5.811371	1.738425	-0.121811
43	6	0	-5.912272	-0.372481	-1.395258
44	6	0	-5.003146	-0.228609	2.266553
45	6	0	4.707831	-0.665971	2.516141
46	6	0	-5.950244	-0.415073	1.071645
47	6	0	5.858197	1.116426	0.058460
48	6	0	5.720409	-0.955159	1.400840
49	6	0	5.741518	-1.080638	-1.067039
50	6	0	4.686190	-2.143204	-1.404577
51	1	0	0.773829	0.474190	-5.954388
52	1	0	-0.758623	1.281190	-5.550600
53	1	0	0.787849	1.886871	-4.914515
54	1	0	0.567282	-5.444775	1.779356
55	1	0	-0.939444	-5.238951	0.855657
56	1	0	-1.009012	-5.393945	2.601242
57	1	0	0.721421	3.328495	4.141531
58	1	0	-0.765261	4.250233	3.816532
59	1	0	0.832349	4.924668	3.422860
60	1	0	-4.562753	2.174956	-1.853159
61	1	0	-5.196379	3.596316	-0.994975
62	1	0	4.725295	1.576474	-1.750241
63	1	0	5.459648	2.975009	-0.940686
64	1	0	-5.838941	2.078189	0.917972
65	1	0	-6.812053	1.939268	-0.551381
66	1	0	-6.963454	-0.718097	-1.341450
67	1	0	-5.857784	0.357917	-2.207685
68	1	0	-5.521645	-0.573852	3.171175
69	1	0	-4.760761	0.835520	2.402379
70	1	0	-6.005144	-1.485661	0.850893
71	1	0	-6.968395	-0.101075	1.376079
72	1	0	6.885374	1.190627	-0.349058
73	1	0	5.893985	1.516523	1.076617
74	1	0	5.720604	-2.036731	1.234719
75	1	0	6.734584	-0.683771	1.751238
76	1	0	6.723807	-1.578932	-0.954427
77	1	0	5.827477	-0.408857	-1.927247
78	1	0	5.119889	-2.836422	-2.138572
79	1	0	4.422661	-2.720907	-0.506735
80	1	0	0.022745	1.840241	-1.532941
81	1	0	-1.994034	3.496652	1.871741
82	1	0	-2.088424	0.075141	-3.926014
83	1	0	-0.247448	-2.262898	-0.835934
84	1	0	1.851388	-3.408503	2.053030
85	1	0	-0.074454	0.417332	2.321608
86	1	0	2.307969	0.323277	2.494365
87	1	0	2.460086	1.682393	-1.601322
88	1	0	2.172823	-2.449591	-0.676017
89	1	0	-2.637064	-2.189959	-0.945404
90	1	0	-2.503789	0.608657	2.270942
91	1	0	-2.347849	2.045045	-1.606769
92	1	0	4.541427	0.419804	2.617158
93	1	0	5.139557	-1.022837	3.461984
94	1	0	3.283633	2.931682	1.383859

95	1	0	3.160585	-0.556349	-3.241068
96	1	0	-3.413535	-2.583889	1.929380
97	1	0	-5.526812	-2.116011	-2.580013
98	1	0	-4.879094	-2.238818	-0.931433

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