SUPPORTING INFORMATION

Guest-Induced Self-Assembly of Macrocyclic Boronic Ester Containing Diarylethene Units: Enhancement of Photoresponsivity

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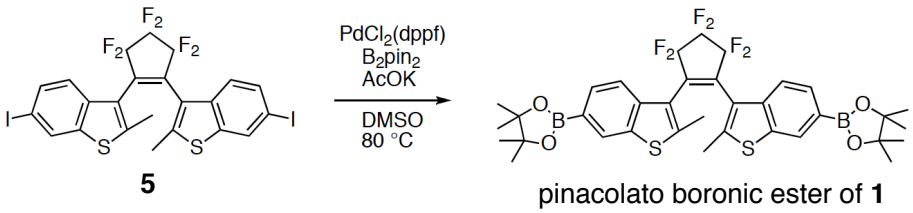
Contents

• Materials and instrumentations

^{1}H and ^{13}C NMR spectra were recorded on a Bruker DRX-500, a JEOL ECX-400, a JEOL AL-400, a JEOL Lambda-400 (400 MHz for ^{1}H NMR and 100 MHz for ^{13}C), a JEOL AL-300 or a JEOL Lambda-300 (300 MHz for ^{1}H and 75 MHz for ^{13}C) spectrometer in $CDCl_3$ [using residual $CHCl_3$ (for ^{1}H, δ_H = 7.26) and $CDCl_3$ (for ^{13}C, δ_C = 77.0) as internal standard], or CD_2Cl_2 [using residual CH_2Cl_2 (for ^{1}H, δ_H = 5.32) and CD_2Cl_2 (for ^{13}C, δ_C = 54.0) as internal standard]. ^{11}B NMR spectra were recorded on a JEOL ECX-400 (127 MHz) spectrometer using BF_3•OEt_2 (for ^{11}B, δ_B = 0.00) as external standard. IR spectra were recorded on an FT/IR-460 plus (JASCO Co., Ltd.). 500 W high-pressure Hg lamp, BA-H500 (USHIO Co. Ltd.) or 500 W super high-pressure Hg lamp, BA-H502 (USHIO Co. Ltd.) was used for photoirradiation. UV-vis spectra were recorded using a JASCO V-650 or a JASCO V-565 spectrometer of MCPD-2000 (Otsuka Electronic Co.). Silica Gel 60N (Kanto Chemical Co., Inc.) was used for silica gel flash column chromatography. Elemental analyses were performed on a Perkin-Elmer 2400 or vario MICRO cube instrument. Low-resolution mass analyses (FAB^+) were performed on a JEOL JMS-700 mass spectrometer. Diodide **5** was prepared according to the literature procedure (K. Matsuda, M. Irie, *Chem. Eur. J.,* 2001, **7**, 3466 – 3473.).

• Synthesis and physical data of pinacolato boronic ester of 1

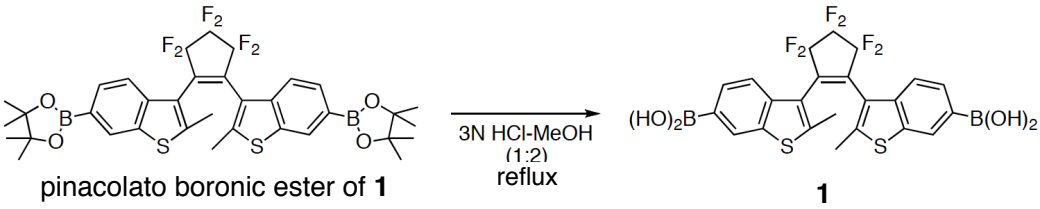


5

To a DMSO solution of **5** (2.1 g, 2.9 mmol) was added $PdCl_2$(dppf) (0.24 g 0.33 mmol), B_2pin_2 (1.6 g, 6.3 mmol) and AcOK (2.3 g, 23 mmol). After the mixture was heated at 80 ºC for 13 h, the reaction mixture was quenched with pH 7 phosphate buffer and filtered through a pad of Celite. The organic materials were extracted with diethyl ether four times, and the combined extracts were washed with brine, and dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by silica gel column chromatography (hexane : dichloromethane = 2 :1) to give pinacolato boronic ester of **1** (1.1 g, 52 %).

Physical data of pinacolato boronic ester of **1**: White solid; ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.13 (s, 2H, antiparallel), 8.07 (s, 2H, parallel), 7.73 (d, *J* = 8.0 Hz, 2H, antiparallel), 7.62 (d, *J* = 8.0 Hz, 2H, antiparallel), 7.56 (brs, 4H, parallel), 2.51 (s, 6H, parallel), 2.26 (s, 6H, antiparallel), 1.34 (s, 24H, antiparallel), 1.31 (s, 24H, parallel); parallel : antiparallel = 43 : 57; ^{13}C NMR (100 MHz, CD_2Cl_2): δ 145.6, 145.3, 141.8-143.1 (m), 141.0, 138.5, 138.4, 130.8, 130.7, 129.5, 129.3, 125.7, 122.0, 121.9, 121.8, 119.9, 119.7, 109.2-119.9 (m), 84.6, 84.6, 25.3, 25.2, 25.2, 15.9, 15.8; ^{11}B NMR (127 MHz): δ 29.9; IR (KBr, cm^{-1}): 1146,1354, 1386, 1600, 2979; m.p.: 156-157 ºC; E.A. Calcd. for $C_{35}H_{36}B_2F_6O_4S_2$: C, 58.35; H, 5.04; S, 8.90. Found: C, 58.50; H, 4.94; S, 8.66.

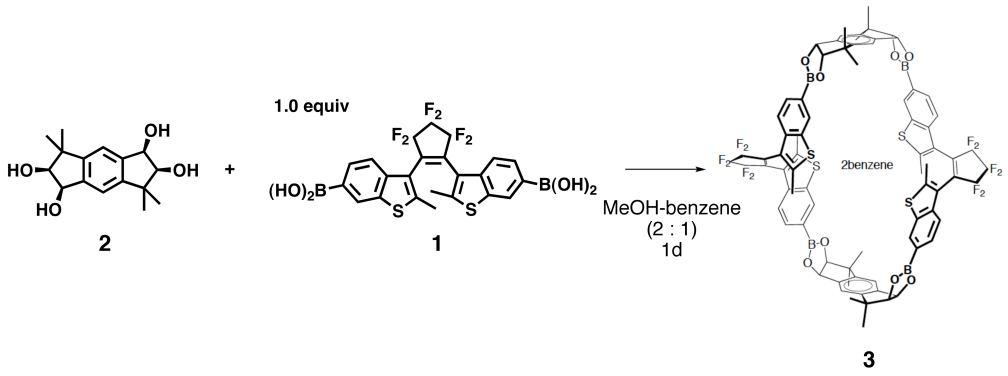
• Synthesis and physical data of 1



After a methanol (95 mL) and 3N HCl (47 mL) solution of pinacolato boronic ester of **1** (0.86 g, 1.2 mmol) was refluxed for 9 d, the hot reaction mixture was filtered and then water (95 mL) was added. After the mixture was stored at 0 ºC overnight, **1** (0.55 g, 82%) was obtained by filtration.

Physical data of **1**: White solid; ^{1}H NMR (400 MHz, acetone-d_6): δ 8.28 (s, 2H, antiparallel), 8.19 (s, 2H, parallel), 7.93 (d, J = 8.8 Hz, 2H, antiparallel), 7.76 (d, J = 8.0 Hz, 2H, parallel), 7.70 (d, J = 8.8 Hz, 2H, antiparallel), 7.68 (d, J = 8.0 Hz, 2H, parallel), 7.25 (brs, 4H, antiparallel), 7.18 (brs, 4H, parallel), 2.59 (s, 6 H, parallel), 2.35 (s, 6H, antiparallel); parallel : antiparallel = 41 : 59; ^{13}C NMR (100 MHz, acetone-d_6): δ 145.4, 145.4, 142.5-143.6 (m), 140.8, 138.9, 138.9, 131.4, 131.3, 129.4, 129.2, 122.2, 120.1, 120.0, 109.7-120.3 (m), 15.8; ^{11}B NMR (127 MHz): δ 28.7; IR (KBr, cm^{-1}): 1147, 1341, 1598, 3424; m.p.: 285-286 ºC; E.A. Calcd. for $C_{23}H_{16}B_2F_6O_4S_2$: C, 49.67; H, 2.90; S, 11.53. Found: C, 49.69; H, 3.02; S, 11.69.

• Self-assembly of 3•2benzene



Di(boronic acid) **1** (65.0 mg, 0.12 mmol) was added to a methanol (6.0 mL) and benzene (3.0 mL) solution of tetrol **2** (31.0 mg, 0.11 mmol). The reaction mixture became homogeneous in a moment, and in a few seconds precipitation started to occur. After the mixture was stirred at room temperature for 1 day, **3**•2benzene (76.0 mg, 81%) was obtained as a white powder by filtration.

Physical data of **3**•2benzene: White solid; ^{1}H NMR (400 MHz, $CDCl_3$, major isomer): δ 7.97 (s, 4H), 7.78 (d, J = 8.2 Hz, 4H), 7.62 (d, J = 8.2 Hz, 4H), 7.36 (s, 12H, benzene), 7.27 (s, 4H), 5.87 (d, J = 5.4 Hz, 4H), 4.78 (d, J = 5.4 Hz, 4H), 2.10 (s, 12H), 1.47 (s, 12 H), 1.26 (s, 12H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.8, 149.0, 144.7, 144.5, 142.1, 142.3-141.7 (m), 141.7, 140.6, 140.4, 137.8, 137.6, 130.4, 130.0, 128.8, 128.4, 128.3, 123.9, 121.6, 121.4, 120.9, 119.7, 118.9, 118.8, 118.9-111.1 (m), 91.5, 90.0, 83.7, 82.5, 47.0, 46.3, 30.9, 30.8, 24.6, 22.2, 15.2, 15.1; ^{11}B NMR (127 MHz): δ 31.3; FAB-MS: m/z Calcd for $C_{78}H_{60}B_4F_{12}O_8S_4$ [M-2•benzene]$^+$ 1524, Found 1524. IR (KBr, cm^{-1}): 2958, 1600, 1359, 1271, 1097; m.p.: 319 ºC; E.A. Calcd. for $C_{90}H_{72}B_4F_{12}O_8S_4$: C, 64.30; H, 4.32; S, 7.63. Found: C, 64.35; H, 4.28; S, 7.79;

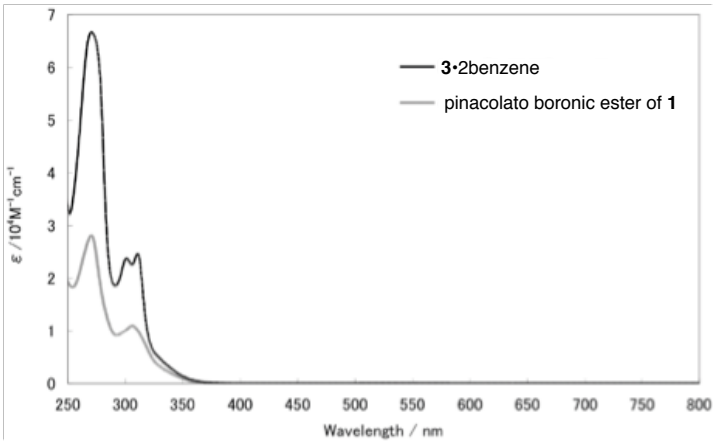
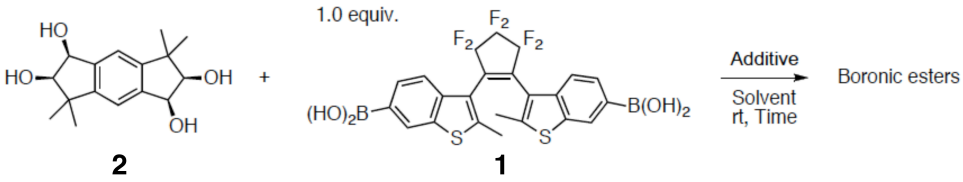
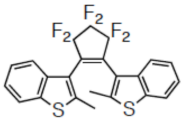


Fig. S1. UV-vis spectrum of **3**•2benzene and pinacolato boronic ester of **1**.

Table S1. Template-induced selective formation of macrocyclic boronic ester **3**•2benzene.



Entry	Solvent, Additive	time	precipitate
1	MeOH-toluene (2:1)	10 min	Oligomer
2		1 d	Oligomer
3	MeOH-benzene (2:1)	10 min	Oligomer
4		1 d	**3 · 2 benzene** 81%
5	MeOH with 12 eq. naphthalene	1 d	Oligomer
6	MeOH with 3.0 eq. triphenylene	1 d	Oligomer
7	MeOH-nitrobenzene (2:1)	1 d	Oligomer
8	MeOH-C_6F_6 (2:1)	1 d	Oligomer
9	MeOH with 5.0 eq. 1,2,4,5-tetracyanobenzene	1 d	Oligomer
10	MeOH with 50 eq. DDQ	1 d	Oligomer
11	MeOH-anisole (2:1)	1 d	Oligomer
12	MeOH with 50 eq. 1,4-dimethoxybenzene	1 d	Oligomer
13	MeOH with 50 eq. 	1 d	Oligomer

• X-ray crystal structure of 3•6toluene

Single crystals of **3**•6toluene suitable for X-ray single crystal diffraction were prepared from a toluene solution of **3** by slow solvent evaporation over several days. The single crystal X-ray diffraction data were recorded on a Rigaku R-AXIS RAPID (IP area detector system) at 173K using Mo*K*α radiation. The structure was solved by direct methods using SIR2004 (M.C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G.L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori, R. Spagna, *J. Appl. Cryst.*, 2005, **38**, 381) and refined by full-matrix least squares using SHELXL-97 (G.M. Sheldrick, *Acta Cryst.* A, 2008, **64**,112).

Crystal structure of **3**•6toluene: $C_{78}H_{60}B_4F_{12}O_8S_4$ $(C_7H_8)_6$, M_r = 2077.54, Orthorhombic, a = 17.2237(16) Å, b = 28.777(2) Å, c = 22.1354(19) Å, V = 10971.2(16) Å3, D_{calc} = 1.258 g cm^{-3}, T = 173 K, no. of unique reflections = 10023, R_{int} = 0.0956, no. of parameters = 581, no. of restraints = 17, R_1 = 0.1806, wR_2 = 0.5125, S = 1.808 for 81396 reflections, max/min. residual density 1.069/-0.623 eÅ^{-3}. CCDC reference number 825696.

Table S2. Crystal data and structure refinement for **3**•6toluene

Identification code	new
Empirical formula	C_{120} H_{60} B_4 F_{12} O_8 S_4
Formula weight	2077.54
Temperature	173(2) K
Wavelength	0.71075 Å
Crystal system	Orthorhombic
Space group	*P b c n*
Unit cell dimensions	*a* = 17.2237(16) Å
	b = 28.777(2) Å
	c = 22.1354(19) Å
Volume	10971.2(16) Å^3
Z	4
Density (calculated)	1.258 g cm^{-3}
Absorption coefficient	0.163 mm^{-1}
F(000)	4336
Crystal size	0.20 x 0.10 x 0.05 mm^3
Theta range for data collection	3.00 to 25.35°.
Index ranges	-20<=h<=20, -34<=k<=34, -26<=l<=23
Reflections collected	81396
Independent reflections	10023 [R(int) = 0.0956]
Completeness to theta = 25.35°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9919 and 0.9681

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10023 / 21 / 581
Goodness-of-fit on F^2	1.802
Final R indices [I>2sigma(I)]	R1 = 0.1806, wR2 = 0.4902
R indices (all data)	R1 = 0.2206, wR2 = 0.5125
Largest diff. peak and hole	1.069 and -0.623 e.Å^{-3}

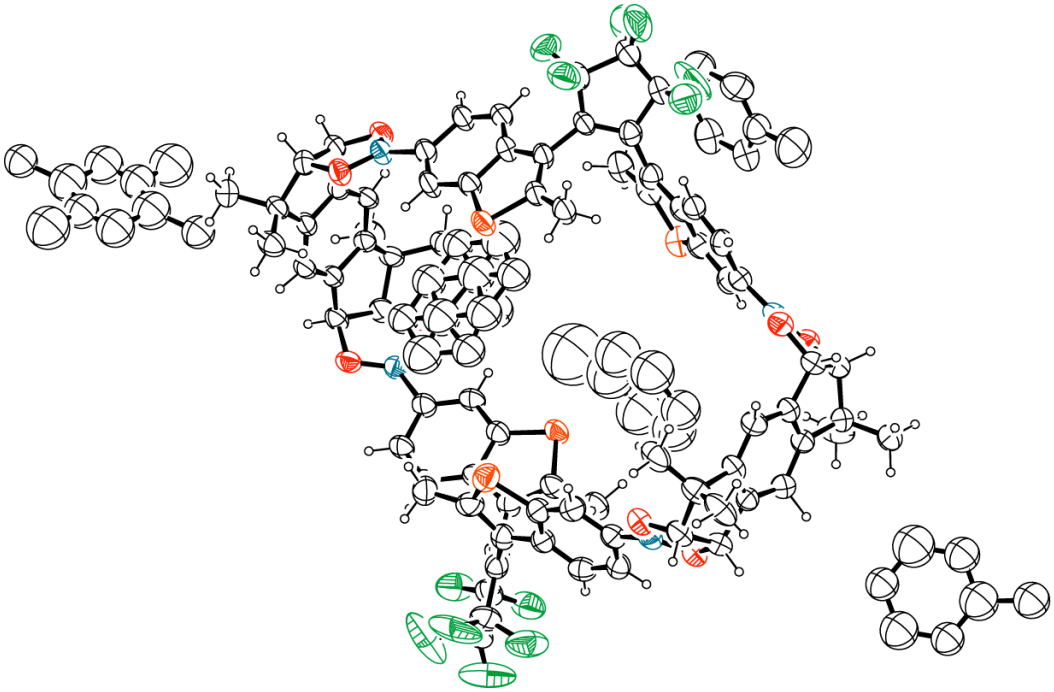


Fig. S2. ORTEP drawing (30 % probability ellipsoids) of **3**•6toluene

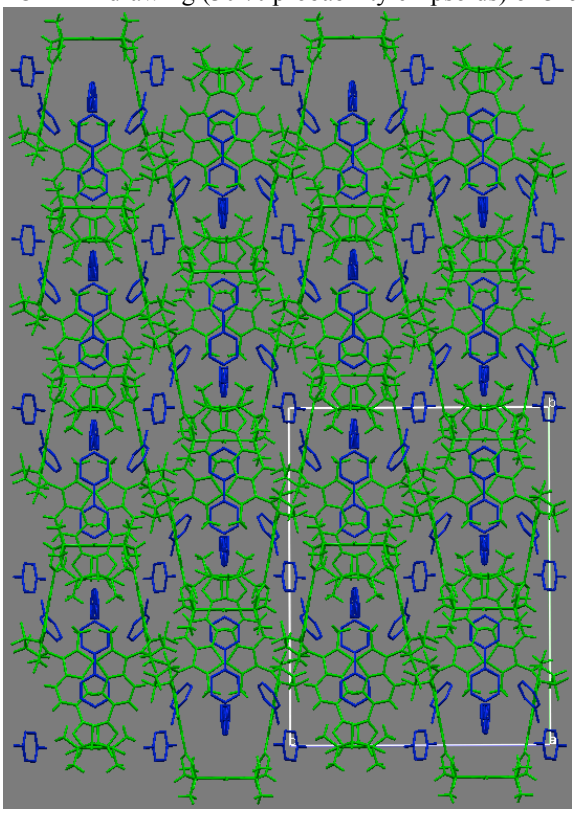


Fig. S3. Packing view of **3**•6toluene along with *a*-xis.

• X-ray crystal structure of 3•3benzene•0.5*n*-hexane

Single crystals of **3**•3benzene•0.5*n*-hexane suitable for X-ray single crystal diffraction were obtained by slow diffusion of *n*-hexane vapor into a solution of **3** in benzene over several days. The single crystal X-ray diffraction data were recorded in a similar manner as described above.

Crystal structure of **3**•3benzene•0.5*n*-hexane: $C_{78}H_{60}B_4F_{12}O_8S_4$, $(C_6H_6)_3$, $(C_6H_{14})_{0.5}$, M_r = 1802.15, Monoclinic, a = 15.3200(16) Å, b = 36.839(4) Å, c = 17.4290(18) Å, β = 102.972(3) °, V = 9585.4(18) Å^3, D_{calc} = 1.249 g cm^{-3}, T = 173 K, no. of unique reflections = 16747, R_{int} = 0.1357, no. of parameters = 1096, no. of restraints = 92, R_1 = 0.2113, wR_2 = 0.5270, S = 1.615 for 61621 reflections, max/min. residual density 0.816/-0.480 eÅ^{-3}. CCDC reference number 847902.

Table S3. Crystal data and structure refinement for **3**•3benzene•0.5*n*-hexane

Identification code	shelx
Empirical formula	$C_{99}H_{85}B_4F_{12}O_8S_4$
Formula weight	1802.15
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P\,2_1/n$
Unit cell dimensions	a = 15.3200(16) Å
	b = 36.839(4) Å β= 102.972(3)°.
	c = 17.4290(18) Å
Volume	9585.4(18) Å^3
Z	4
Density (calculated)	1.249 Mg/m^3
Absorption coefficient	0.176 mm^{-1}
F(000)	3740
Crystal size	0.35 x 0.30 x 0.10 mm^3
Theta range for data collection	2.98 to 25.03°.
Index ranges	-17<=h<=18, -43<=k<=43, -20<=l<=20
Reflections collected	61621
Independent reflections	16747 [R(int) = 0.1357]
Completeness to theta = 25.03°	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9826 and 0.9409
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16747 / 92 / 1096
Goodness-of-fit on F^2	1.615
Final R indices [I>2sigma(I)]	R1 = 0.2113, wR2 = 0.4961
R indices (all data)	R1 = 0.2835, wR2 = 0.5270
Extinction coefficient	0.070(7)
Largest diff. peak and hole	0.816 and -0.480 e.Å^{-3}

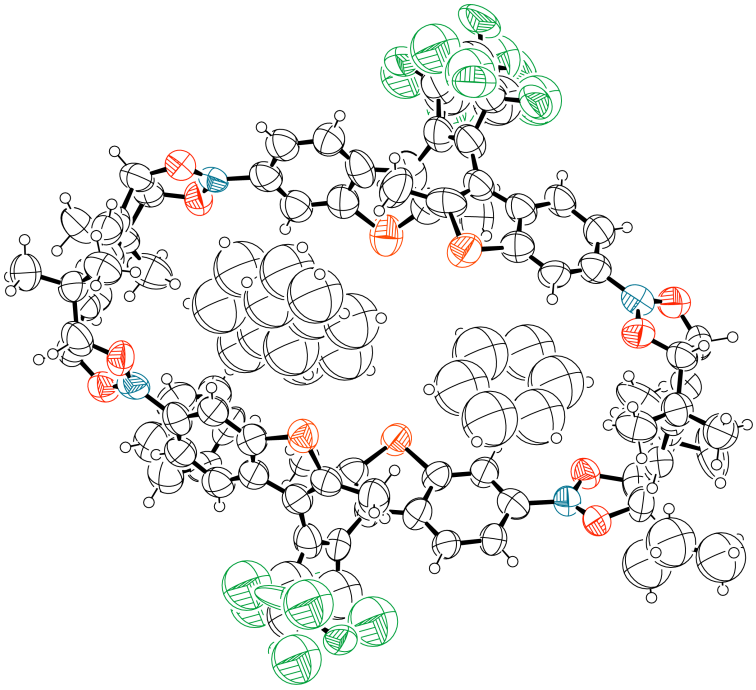


Fig. S4. ORTEP drawing (50 % probability ellipsoids) of **3**•3benzene•0.5*n*-hexane

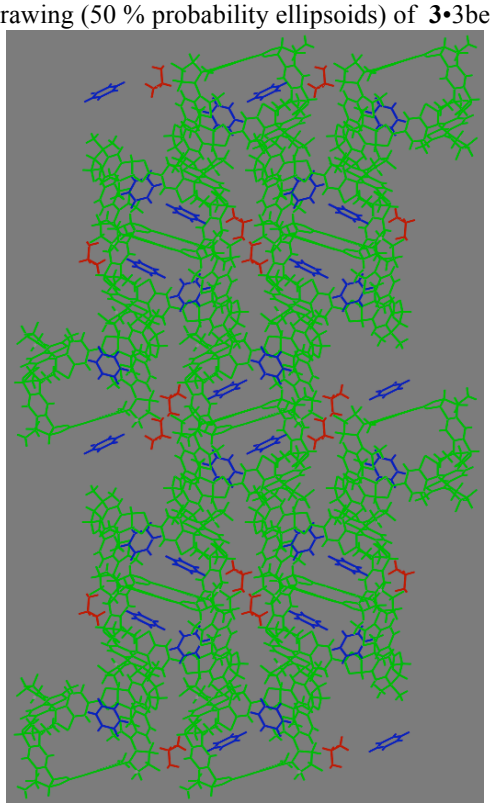


Fig. S5. Packing view of **3**•3benzene•0.5*n*-hexane along with *a*-axis.

• Photoisomerization of 3•2benzene (NMR study)

3•2benzene (4.2 mg, 0.0025 mmol) was placed into a quartz NMR tube and then CD_2Cl_2 (0.5 mL) was added. After the mixture was degassed by freeze-dry technique, this sample solution was irradiated at 313 nm using a 500 W high-pressure Hg lamp (Eikosha Co.) combined with a bandpass filter (313 ± 2 nm, Asahi Spectra Co.) at room temperature. The change of the reaction mixture was observed by ^{1}H NMR. Upon irradiation of the photostationary state mixture with visible light (546 nm),

the ^{1}H NMR spectrum completely returned to the initial state (open-open form, OO). It suggested that photostationary mixture contained only closed-closed form (CC), and closed-open (CO) form and did not contain any decomposition product caused by deformation of boronic ester.

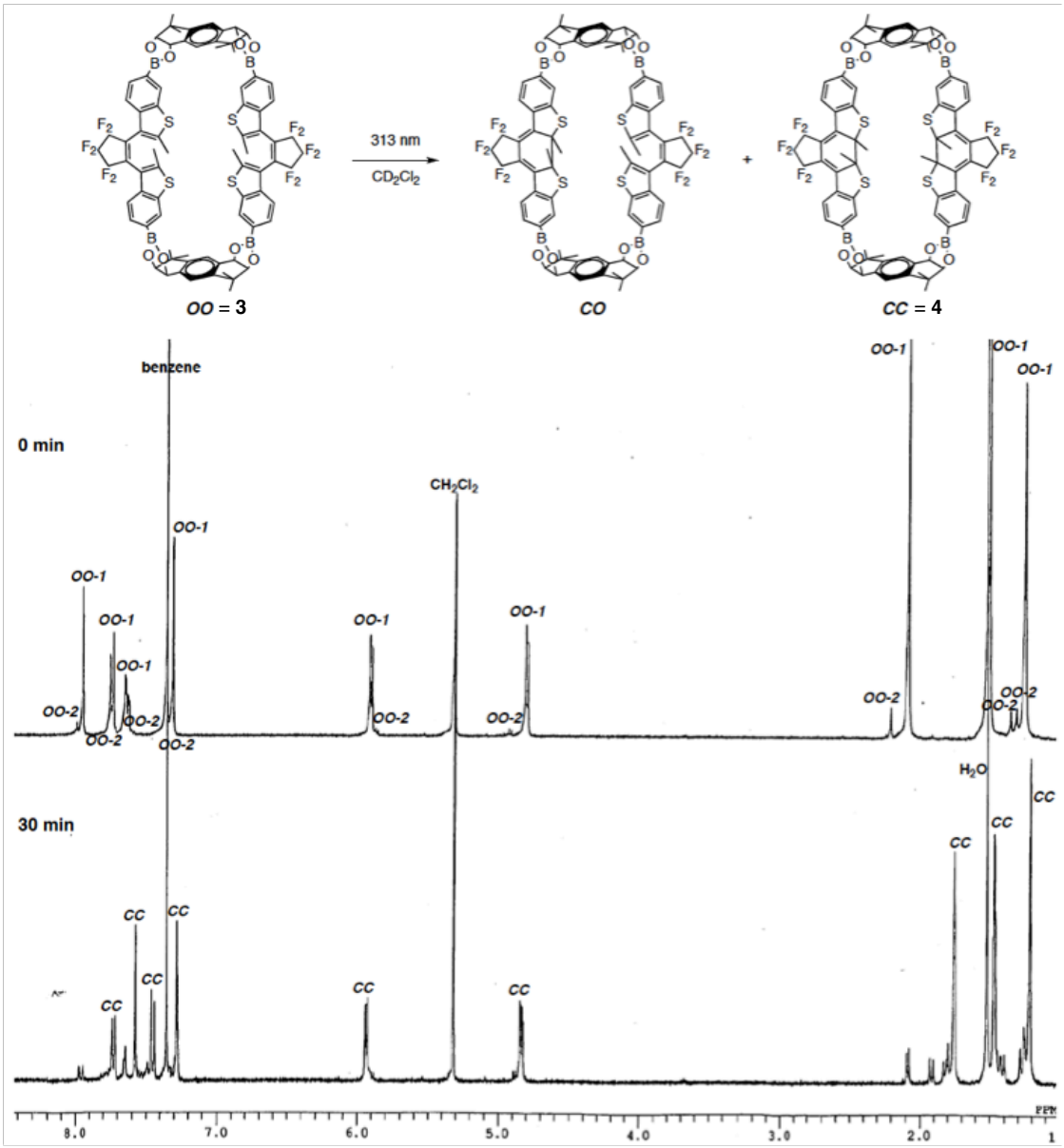


Fig. S6. ^{1}H NMR spectral change of **3** under photoirradiation.

• Photoisomerization of 3•2benzene (UV-vis measurement)

A dichloromethane solution (4 mL) containing **3**•2benzene (0.11 mM) was placed into a quartz cuvette (d = 1 cm) and bubbled with argon filled with a dichloromethane vapor for 15 min, and then the cuvette was sealed with a rubber septum (Aldrich Z553921). The sample solution was kept at 25 ± 1 °C using temperature control unit (TAITEC LabBath LB-21 JR) and irradiated at 313 nm using a 500 W high-pressure Hg lamp (Eikosha Co.) combined with a bandpass filter (313 ± 2 nm, Asahi Spectra Co.). The absorption spectrum completely returned to its initial state with several clear isosbestic points, when it was irradiated at 509 nm using a bandpass filter (509 ± 2 nm, Asahi Spectra Co.). UV/vis absorption spectral change of the irradiated solution was observed using MCPD-2000. Initial reaction rate of photocyclization or photocycloreversion was

calculated from the time dependent plots of the yield of closed-form or open-form diarylethene unit, which was calculated using molar extinction coefficients (2.15×10^4) at 550 nm of closed-form **4**. The incident light intensity into the solution was also determined using a $K_3Fe(C_2O_4)_3$ actinometer (K. C. Kurien, *J. Chem. Soc. B* 1971, 2081–2082.). Quantum yield for photocyclization or photocycloreversion was examined at three incident light intensities, 9.94×10^{-11}, 1.51×10^{-10}, 2.85×10^{-10} einstein s^{-1} for photocyclization, or 5.92×10^{-11}, 1.10×10^{-10}, 4.26×10^{-10} einstein s^{-1} for photocycloreversion, using neutral density filters (Asahi Spectra Co.), for high accuracy of measurement. Initial rate method gave the quantum yield 0.67 (Φ_{313}) for photocyclization and 0.64 (Φ_{509}) for photocycloreversion.

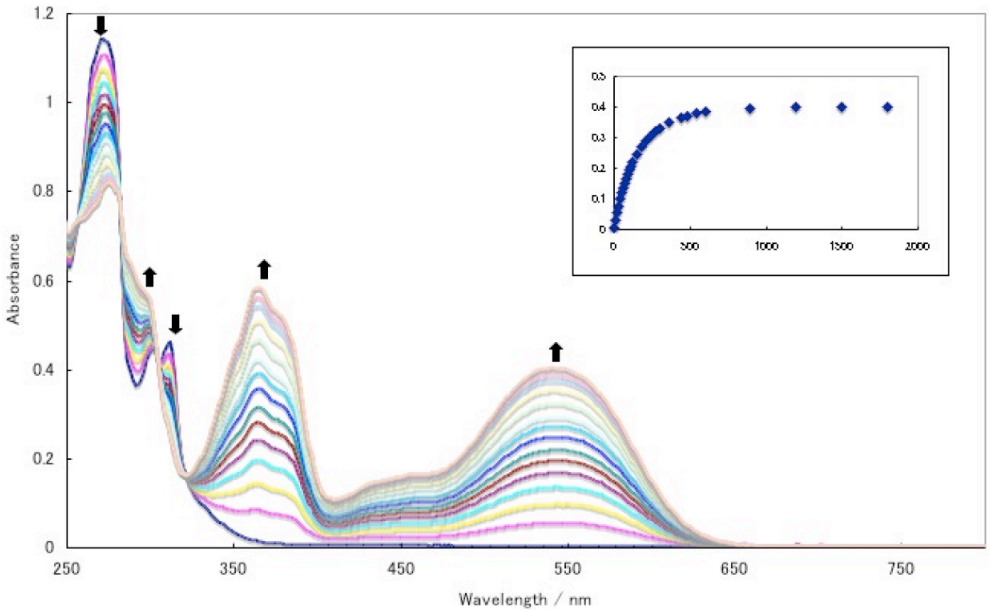


Fig. S7. UV/vis absorption spectral changes of **3** (2.0×10^{-5} M) in CH_2Cl_2 upon the UV light irradiation (313 nm). Isosbestic points are observed at 256, 282, 305, and 321 nm. The inset shows time-dependent absorption change at 550 nm.

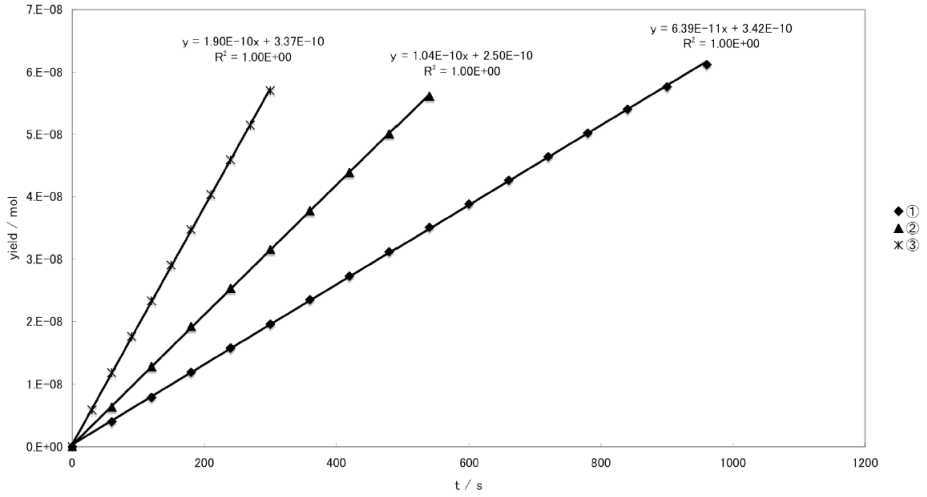


Fig. S8. The time dependent plots of the yield of closed-ring form of **3** at three light intensities (9.94×10^{-11}, 1.51×10^{-10}, 2.85×10^{-10} einstein s^{-1}).

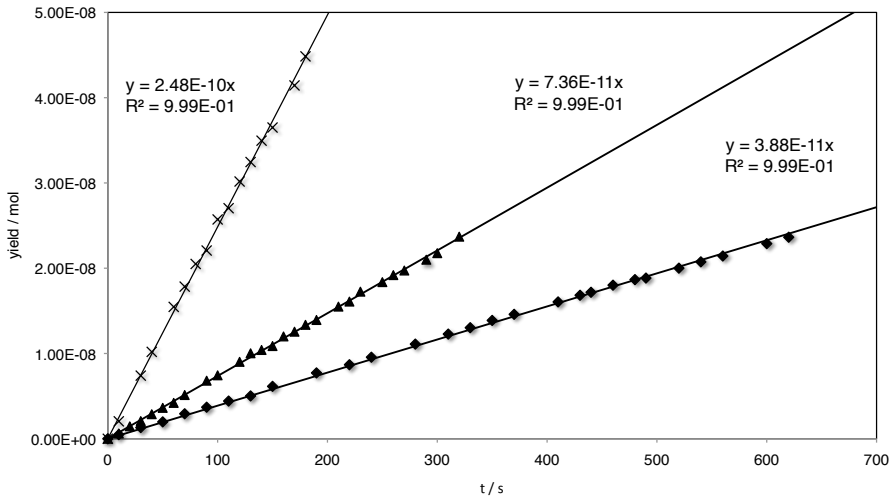


Fig. S9. The time dependent plots of the yield of open-ring form of **3** at three light intensities (5.92×10^{-11}, 1.10×10^{-10}, 4.26×10^{-10} einstein s^{-1}).

The same procedure was employed in the case of pinacolato boronic ester of **1** .

•Photoisomerization of pinacolato boronic ester of 1 (NMR study)

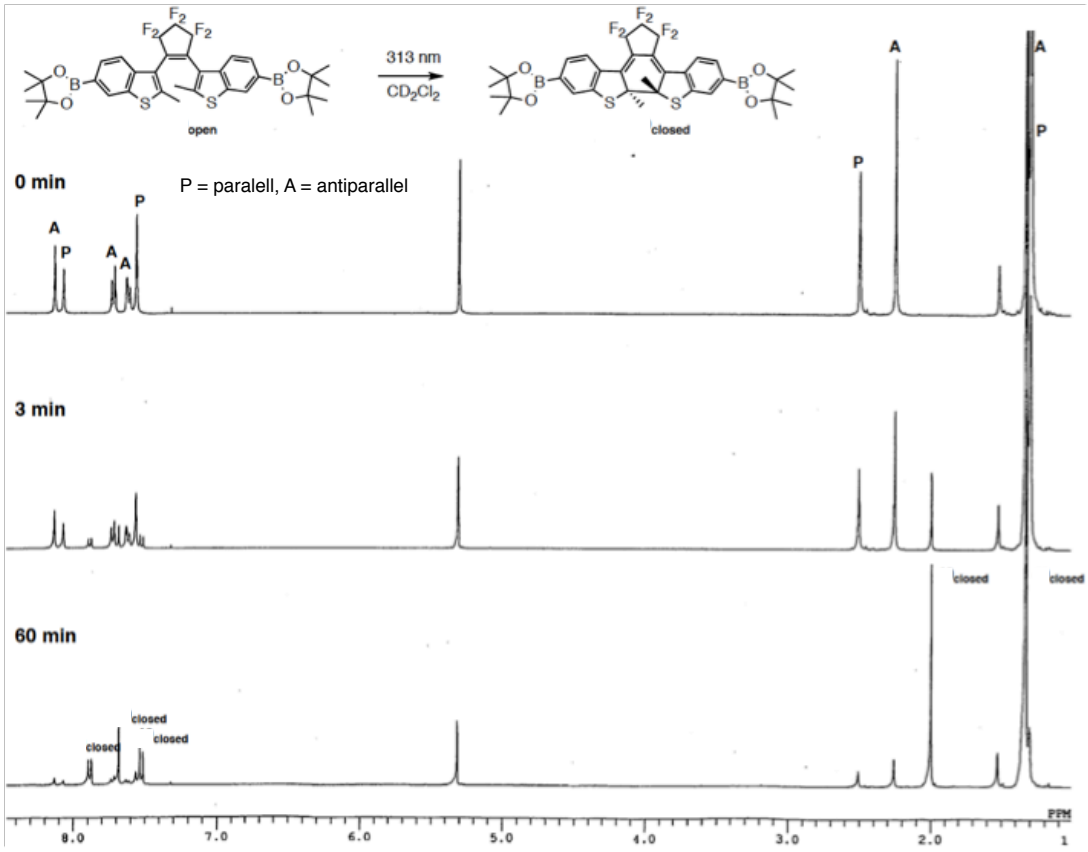


Fig. S10. ^{1}H NMR spectral change of pinacolato boronic ester of **1** under photoirradiation.

•Photoisomerization of pinacolato boronic ester of 1 (UV-vis measurement)

A dichloromethane solution (4 mL) containing **1** (0.23 mM) was placed into a quartz cuvette (d = 1 cm) and bubbled with argon filled with a dichloromethane vapor for 15 min, and then the cuvette was sealed with a rubber septum (Aldrich Z553921). The sample solution was kept at 25 ± 1 °C using temperature control unit (TAITEC LabBath LB-21 JR) and irradiated at 313

nm using a 500 W high-pressure Hg lamp (Eikosha Co.) combined with a bandpass filter (313 ± 2 nm, Asahi Spectra Co.). The absorption spectrum returned to its initial state with several clear isosbestic points, when it was irradiated at 509 nm using a bandpass filter (509 ± 2 nm, Asahi Spectra Co.). UV/vis absorption spectral change of the irradiated solution was observed using MCPD-2000. Initial reaction rate of photocyclization or photocycloreversion was calculated from the time dependent plots of the yield of closed-form or open-form diarylethene unit, which was calculated using molar extinction coefficients (1.23×10^4) at 550 nm of closed-form **1**. The incident light intensity into the solution was also determined using a $K_3Fe(C_2O_4)_3$ actinometer (K. C. Kurien, *J. Chem. Soc. B* 1971, 2081–2082.). Quantum yield for photocyclization or photocycloreversion was examined at three incident light intensities, 9.94×10^{-11}, 1.51×10^{-10}, 2.85×10^{-10} einstein s^{-1} for photocyclization, or 5.92×10^{-11}, 1.10×10^{-10}, 4.26×10^{-10} einstein s^{-1} for photocycloreversion, using neutral density filters (Asahi Spectra Co.), for high accuracy of measurement. Initial rate method gave the quantum yield 0.30 (Φ_{313}) for photocyclization and 0.27 (Φ_{509}) for photocycloreversion.

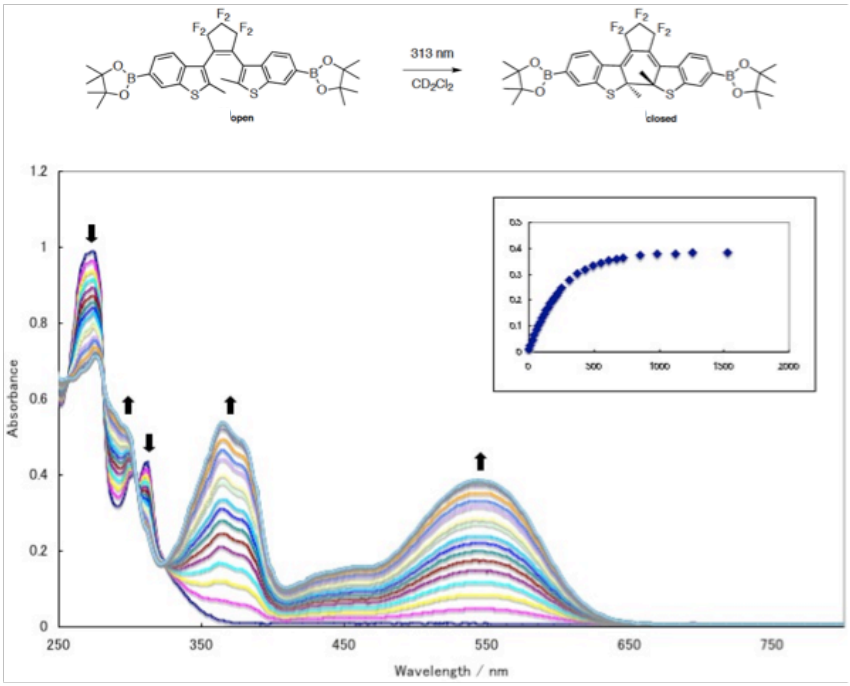


Fig. S11. UV/vis absorption spectral changes of pinacolato boronic ester of **1** (6.0×10^{-5} M) in CH_2Cl_2 upon the UV light irradiation (313 nm). Isosbestic points are observed at 256, 281, 305, and 324 nm. The inset shows time-dependent absorption change at 550 nm.

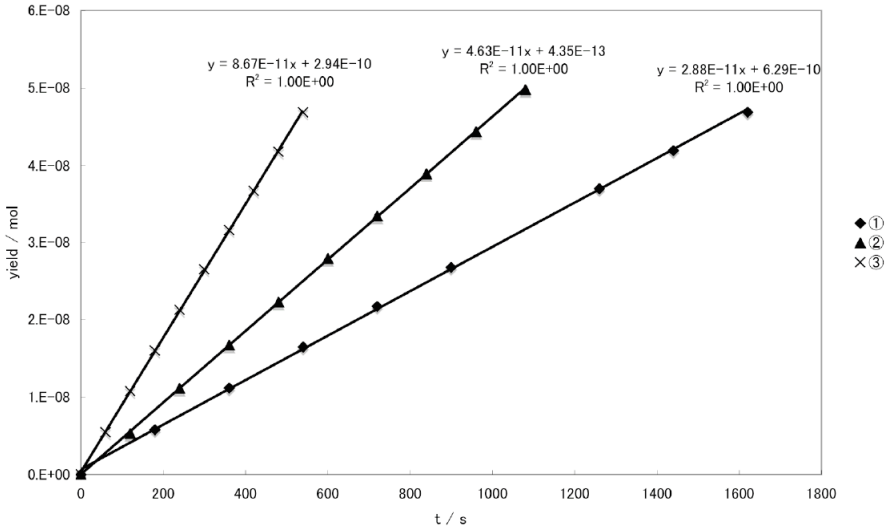


Fig. S12. The time dependent plots of the yield of closed-form of pinacolato boronic ester of **1** at three light intensities (9.94×10^{-11}, 1.51×10^{-10}, 2.85×10^{-10} einstein s^{-1}).

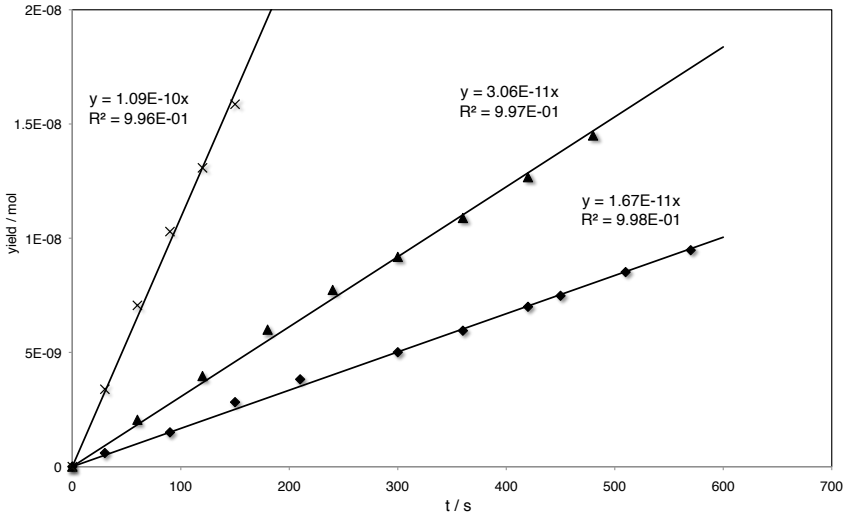


Fig. S13. The time dependent plots of the yield of open-form of pinacolato boronic ester of **1** at three light intensities (5.92×10^{-11}, 1.10×10^{-10}, 4.26×10^{-10} einstein s^{-1}).

• Isolation of 4

A dichloromethane (0.95 mL) solution of **3**•2benzene (64.8 mg, 0.039 mmol) was placed into a quartz cuvette (d = 1 cm) and bubbled with argon filled with a dichloromethane vapor for 15 min, and then the cuvette was sealed with a rubber septum (Aldrich Z553921). The sample solution was irradiated at 313 nm using a 500 W super high-pressure Hg lamp at room temperature for 3 h, and stored for 12 h in the dark. Filtration of the precipitates followed by heating at 80 °C for 8 h in vacuo gave **4** (44.3 mg, 75%) as deep purple solid.

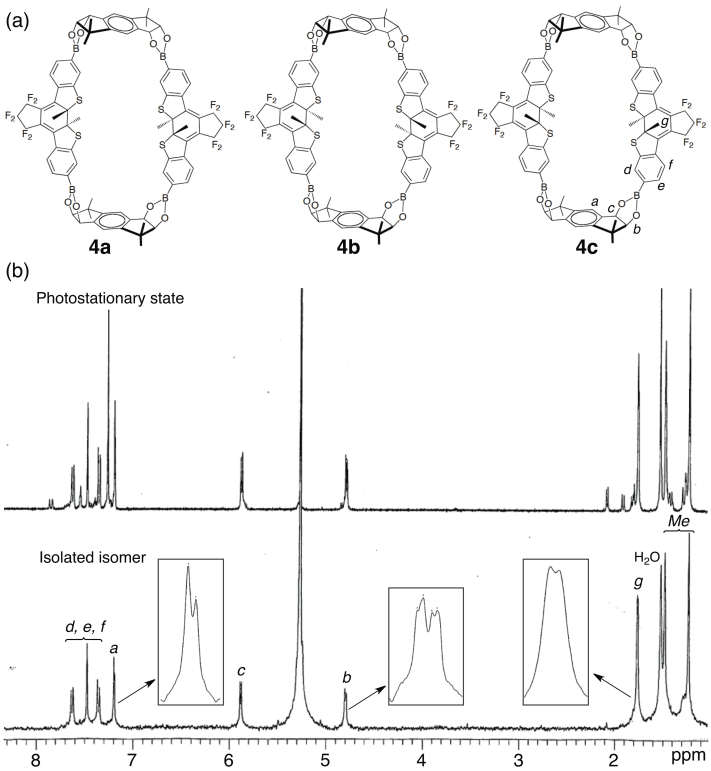


Fig. S14. (a) Possible diastereomers of closed-ring form of macrocyclic boronic esters **4**. (b) ^{1}H NMR spectra (400 MHz, CD_2Cl_2) of photostationary state (top) and isolated closed-form **4** (bottom).

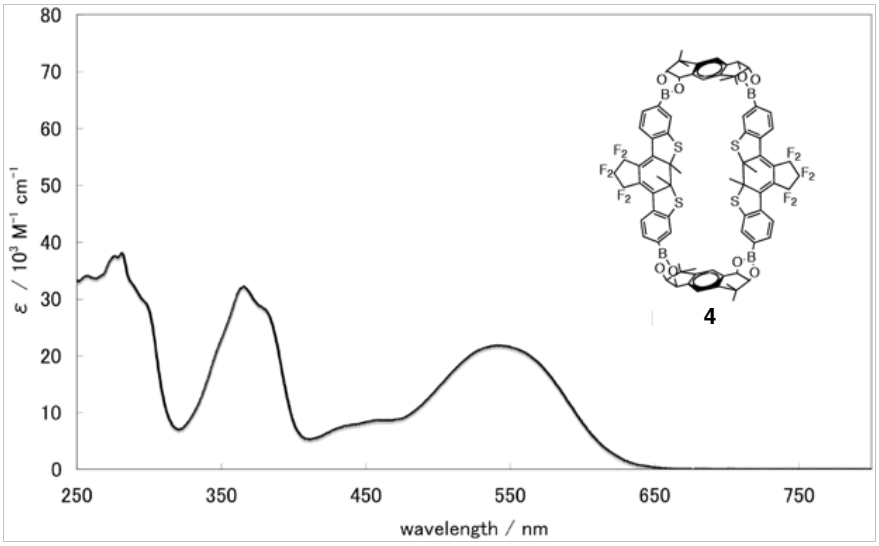


Fig. S15. UV spectrum of **4**.

• Isolation of closed-form of pinacolato boronic ester of 1

Closed-form of pinacolato boronic ester of **1** was isolated by HPLC under following condition.

ULTRON VX-SIL (250 mm × 20 mm)

flow rate 10 ml/ min, *n*-hexane : dichloromethane = 60 : 40, 254 nm, r.t., retention time 17-22 min.

Physical data of closed-form of pinacolato boronic ester of **1**: Deep purple solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.34 (s, 24H), 1.99 (s, 6H), 7.55 (d, J = 8.3 Hz, 2H), 7.69 (s, 2H), 7.88 (d, J = 8.3 Hz, 2H).

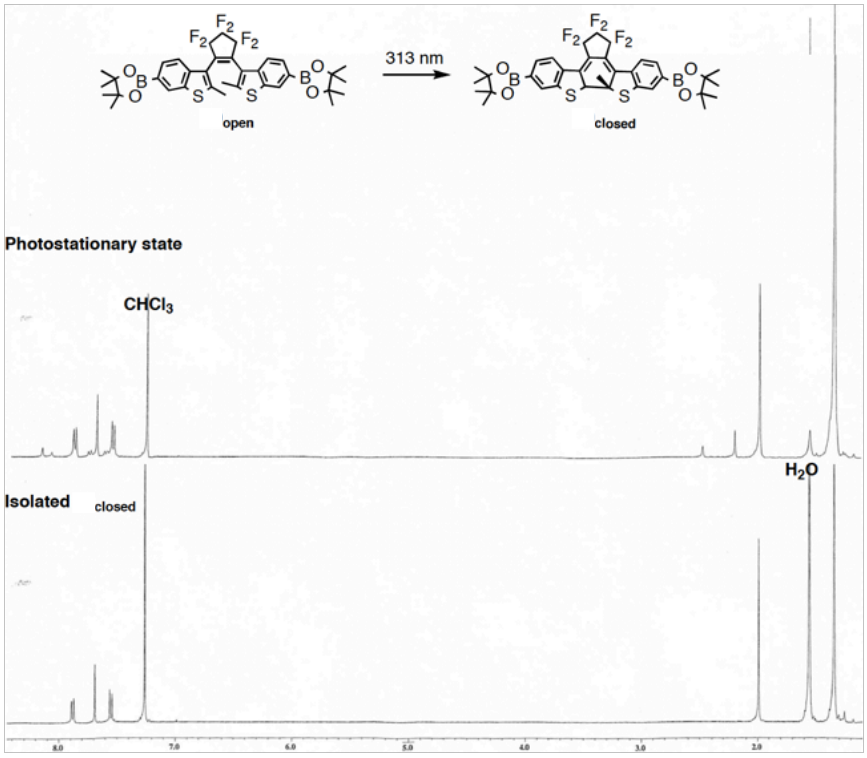


Fig. S16. ^{1}H NMR spectra of photostationary state and isolated closed-form of pinacolato boronic ester of **1**.

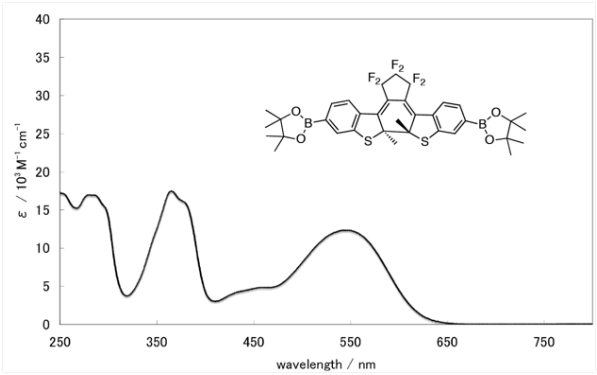
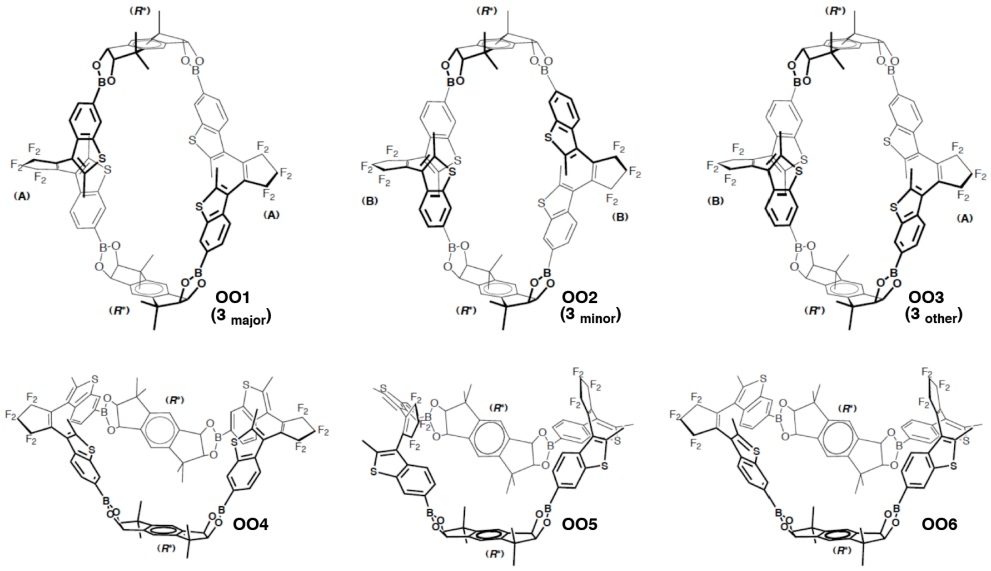


Fig. S17. UV spectrum of closed-form of pinacolato boronic ester of **1**.

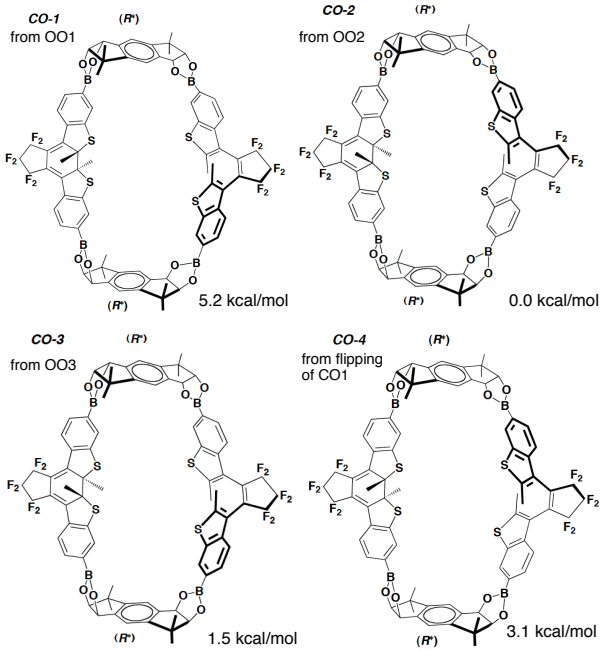
• Structures and relative energies of isomers of 3, open-closed ring form and closed ring form of the macrocyclic boronic esters

Possible six structures of *homo*-**3** are shown below.



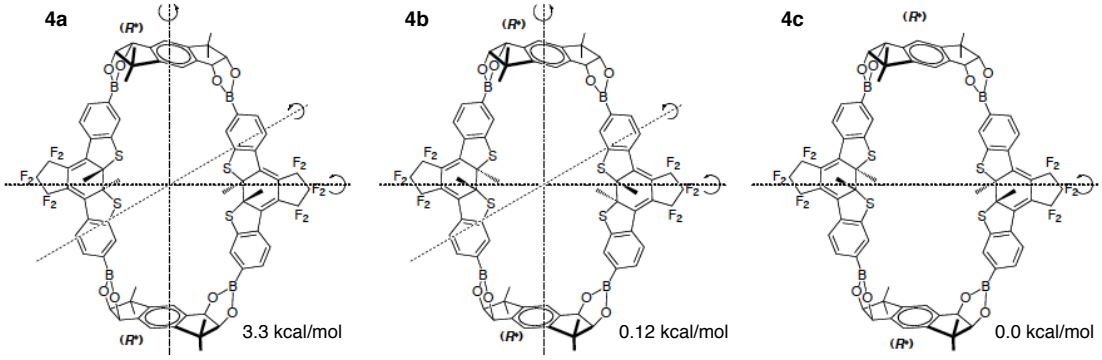
6 possible *homo* isomers of **3**.

Three structures of open-closed ring form (**CO1**~**CO3**) of macrocyclic boronic esters derived from **OO1**~**OO3** respectively and one additional open-closed form (**CO-4**) derived from **CO-1** by flipping the open ring moiety with the relative energies are shown below.



When one of the diarylethene unit of $\mathbf{3}_{major}$ (**OO1**) cyclized, **CO1** was generated and **CO4** is a rotational isomer of the remaining diarylethene unit of **CO1**. From the DFT calculation, **CO4** is more stable than **CO1** by 2.1 kcal/mol and it supports the conformational change from **CO1** to **CO4**, which will give **4c**.

Possible three structures of closed-ring form of macrocyclic boronic esters with the relative energies are shown below. Without further conformational change, **CO1** will give **4a**, **CO2** will give **4b** and both **CO3** and **CO4** will give 4c.



Using molecular mechanics force field (MMFF) from CONFLEX program,[S1] conformational analysis of all isomers was conducted. Optimizations of all structures were performed with DFT calculation at the B3LYP/6-31G** level (Gaussian 09).[S2] All of the geometries were characterized to be minima with no imaginary frequencies by vibrational analysis. Total energies were corrected with zero-point energies.

(S1) (a) Goto, H.; Osawa, E. *J. Am. Chem. Soc.* **1989**, *111*, 8950 – 8951. (b) Goto, H.; Osawa, E. *J. Chem. Soc., Perkin Trans.* **1993**, *2*, 187 – 198. (c) Goto, H.; Ohta, K.; Kamakura, T.; Obata, S.; Nakayama, N.; Matsumoto, T.; Osawa, E. CONFLEX, Conflex, Corp.: Tokyo. JAPAN, 2004.

(S2) Frisch, M. J.; et al. Gaussian 09, Revision B.01; Gaussian, Inc.: Wallingford. CT, 2009.

• Cartesian coordinates of all optimized geometries and total energies

OO1 E = –6499.827537 (au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.842889	-3.08391	-2.935862
2	16	0	-1.08835	-3.130582	3.06062
3	16	0	-0.842895	3.083949	-2.935957
4	16	0	1.088347	3.130534	3.06053
5	9	0	0.300257	-7.810692	-2.364855
6	9	0	1.651772	-8.130565	-0.663697
7	9	0	-1.786095	-8.566978	-1.041131
8	9	0	-0.261185	-9.77075	-0.000683
9	9	0	-0.141281	-8.07377	2.002633
10	9	0	-2.236062	-7.827489	1.397557
11	9	0	-1.65181	8.130514	-0.663693
12	9	0	-0.30028	7.810737	-2.364857
13	9	0	0.261099	9.770747	-0.000633
14	9	0	1.786051	8.567042	-1.0411
15	9	0	0.141216	8.073707	2.002635
16	9	0	2.236013	7.827514	1.397581

17	8	0	6.676882	1.894317	2.994194
18	8	0	7.436472	3.08118	1.176435
19	8	0	6.520252	-2.326683	-2.957185
20	8	0	7.193972	-3.57504	-1.146506
21	8	0	-6.676873	-1.894335	2.994211
22	8	0	-7.436451	-3.081182	1.176436
23	8	0	-6.520252	2.326704	-2.957171
24	8	0	-7.193949	3.575047	-1.146473
25	6	0	8.085537	1.596606	2.921318
26	1	0	8.5756	2.096768	3.764258
27	6	0	8.486705	2.16193	1.529559
28	1	0	9.434921	2.709077	1.521534
29	6	0	8.37778	-0.643373	-2.874375
30	6	0	7.948444	-2.139448	-2.88931
31	1	0	8.394685	-2.676359	-3.734017
32	6	0	8.308145	-2.734513	-1.498976
33	1	0	9.214232	-3.348938	-1.492245
34	6	0	8.39576	0.071086	2.906311
35	6	0	7.40267	0.25685	-3.646953
36	1	0	6.396906	0.201412	-3.227186
37	1	0	7.348863	-0.044685	-4.698225
38	1	0	7.736857	1.29903	-3.616849
39	6	0	9.794281	-0.527422	-3.483926
40	1	0	10.172311	0.494181	-3.380171
41	1	0	9.781077	-0.777681	-4.550449
42	1	0	10.505387	-1.194392	-2.984725
43	6	0	9.795498	-0.158646	3.522418
44	1	0	10.560303	0.450114	3.028171
45	1	0	10.091316	-1.20694	3.418169
46	1	0	9.797098	0.090001	4.589433
47	6	0	7.348238	-0.74952	3.673077
48	1	0	7.312474	-0.444586	4.724127
49	1	0	7.599548	-1.814729	3.644188
50	1	0	6.352218	-0.614986	3.247958
51	6	0	0.408278	-7.680962	-1.020251
52	6	0	-0.661583	-8.51619	-0.278396
53	6	0	-0.954363	-7.671227	0.979141
54	6	0	-8.085527	-1.596621	2.921328
55	1	0	-8.575596	-2.096788	3.764262
56	6	0	-8.486687	-2.161937	1.529562
57	1	0	-9.434902	-2.709085	1.52153
58	6	0	-8.377779	0.643397	-2.874352

59	6	0	-7.948443	2.139471	-2.889282
60	1	0	-8.394692	2.676389	-3.73398
61	6	0	-8.308128	2.734527	-1.498939
62	1	0	-9.214213	3.348957	-1.492197
63	6	0	-8.395745	-0.071101	2.906329
64	6	0	-7.402675	-0.256821	-3.646944
65	1	0	-6.396908	-0.201386	-3.227183
66	1	0	-7.348875	0.044721	-4.698214
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68	6	0	-9.794285	0.52745	-3.483895
69	1	0	-10.172315	-0.494153	-3.380144
70	1	0	-9.781088	0.777716	-4.550416
71	1	0	-10.505387	1.194418	-2.984685
72	6	0	-9.795484	0.158631	3.522435
73	1	0	-10.56029	-0.450123	3.028184
74	1	0	-10.091298	1.206926	3.418192
75	1	0	-9.797086	-0.090022	4.589449
76	6	0	-7.348222	0.749497	3.673102
77	1	0	-7.312461	0.444557	4.72415
78	1	0	-7.599529	1.814707	3.644219
79	1	0	-6.352202	0.614962	3.247983
80	6	0	-0.4083	7.680966	-1.020257
81	6	0	0.661534	8.516204	-0.278375
82	6	0	0.954325	7.671218	0.979143
83	5	0	6.371185	2.801728	2.004123
84	5	0	6.150156	-3.212515	-1.969397
85	5	0	-6.37117	-2.801737	2.004134
86	5	0	-6.150142	3.212524	-1.969378
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89	6	0	-8.428923	0.234	1.410167
90	6	0	-8.490719	-0.903821	-0.751411
91	6	0	-8.428435	0.340996	-1.378339
92	6	0	-8.40037	1.480281	0.783175
93	1	0	-8.492618	-1.828155	-1.322281
94	1	0	-8.332731	2.402213	1.354002
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99	6	0	-3.577829	-5.150062	0.740497
100	6	0	-2.617104	-3.57447	2.317119

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103	1	0	-3.480345	-6.000136	0.073559
104	6	0	-0.236056	-4.392197	2.186435
105	6	0	-1.071706	-5.11074	1.370913
106	6	0	0.15562	-6.260929	-0.551004
107	6	0	-0.620091	-6.255167	0.555916
108	6	0	1.235396	-4.576592	2.405641
109	1	0	1.520781	-5.610257	2.196907
110	1	0	1.51321	-4.350642	3.439012
111	1	0	1.823857	-3.925165	1.750193
112	6	0	-0.093966	-4.306156	-2.092466
113	6	0	0.692756	-5.118279	-1.316857
114	6	0	4.710149	-3.759846	-1.785924
115	6	0	2.102601	-4.782426	-1.387835
116	6	0	3.625486	-3.173718	-2.449762
117	6	0	4.470018	-4.858528	-0.926003
118	6	0	3.198941	-5.375419	-0.732479
119	6	0	2.341739	-3.676096	-2.237951
120	1	0	3.787627	-2.331858	-3.116185
121	1	0	5.312132	-5.31033	-0.410667
122	1	0	3.045494	-6.23592	-0.091254
123	6	0	-1.577072	-4.365277	-2.301144
124	1	0	-1.841221	-4.112991	-3.332128
125	1	0	-2.104411	-3.668748	-1.640164
126	1	0	-1.950189	-5.370447	-2.092179
127	6	0	8.406478	-1.514055	-0.610677
128	6	0	8.495812	0.937172	0.642478
129	6	0	8.428446	-0.340982	-1.37836
130	6	0	8.400391	-1.480282	0.783146
131	6	0	8.428941	-0.234006	1.410147
132	6	0	8.490733	0.90383	-0.751423
133	1	0	8.332754	-2.402218	1.353968
134	1	0	8.492628	1.828168	-1.322287
135	6	0	4.975684	3.454865	1.823889
136	6	0	2.451216	4.667024	1.433343
137	6	0	4.807588	4.541609	0.931464
138	6	0	3.861069	2.978316	2.524663
139	6	0	2.617111	3.57444	2.31706
140	6	0	3.577858	5.150071	0.740493
141	1	0	5.673632	4.908844	0.38937
142	1	0	3.969182	2.148168	3.216215

143	1	0	3.480384	6.000159	0.07357
144	6	0	1.071722	5.110721	1.370857
145	6	0	0.236056	4.392139	2.186328
146	6	0	-1.23541	4.576495	2.405474
147	1	0	-1.823829	3.925076	1.749977
148	1	0	-1.520808	5.610161	2.196758
149	1	0	-1.513266	4.350507	3.438824
150	6	0	0.620107	6.255157	0.555873
151	6	0	-0.155598	6.260928	-0.551052
152	6	0	-0.692735	5.118288	-1.316917
153	6	0	0.093972	4.306196	-2.092576
154	6	0	-4.710132	3.759854	-1.785921
155	6	0	-2.102578	4.782428	-1.387868
156	6	0	-3.625483	3.17374	-2.449794
157	6	0	-4.469984	4.85852	-0.925984
158	6	0	-3.198904	5.375409	-0.732478
159	6	0	-2.341732	3.676116	-2.238002
160	1	0	-3.787636	2.331893	-3.11623
161	1	0	-5.312089	5.310312	-0.410623
162	1	0	-3.045443	6.235901	-0.091242
163	6	0	1.577068	4.365348	-2.301315
164	1	0	1.841177	4.113088	-3.332316
165	1	0	2.104445	3.668813	-1.640372
166	1	0	1.950176	5.37052	-2.092345

OO2 E = –6499.823034 (au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.606912	-1.820092	1.456882
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3	16	0	0.606867	1.81994	1.456867
4	16	0	-3.656381	5.7141	1.407092
5	9	0	-1.548323	-5.462524	-2.924704
6	9	0	-1.356112	-3.296454	-3.246926
7	9	0	-0.054181	-5.467967	-5.031448
8	9	0	0.940115	-3.582272	-4.480821
9	9	0	2.725313	-5.325219	-3.720109
10	9	0	1.220761	-6.810819	-3.150465
11	9	0	1.356215	3.296566	-3.246858
12	9	0	1.54851	5.462563	-2.924218

13	9	0	-0.939841	3.582719	-4.48101
14	9	0	0.05463	5.468454	-5.031185
15	9	0	-2.72503	5.325679	-3.720254
16	9	0	-1.220451	6.811045	-3.150117
17	8	0	-8.246	1.787925	-1.336907
18	8	0	-8.35632	2.554163	0.828061
19	8	0	-5.712083	-3.103439	3.501454
20	8	0	-6.721934	-4.156289	1.723956
21	8	0	8.245962	-1.788033	-1.336905
22	8	0	8.356279	-2.554219	0.828081
23	8	0	5.712039	3.103411	3.501398
24	8	0	6.721857	4.15623	1.723863
25	6	0	-9.500101	1.288378	-0.838236
26	1	0	-10.303314	1.825564	-1.354838
27	6	0	-9.418498	1.588325	0.687632
28	1	0	-10.329676	2.022731	1.111067
29	6	0	-7.706364	-1.807735	4.266207
30	6	0	-7.103101	-3.184828	3.865717
31	1	0	-7.195908	-3.916754	4.676021
32	6	0	-7.785053	-3.618144	2.536428
33	1	0	-8.551135	-4.391416	2.650821
34	6	0	-9.650671	-0.253948	-1.000366
35	6	0	-6.674947	-0.880178	4.924359
36	1	0	-5.84067	-0.675269	4.251582
37	1	0	-6.272378	-1.334407	5.835739
38	1	0	-7.138502	0.071213	5.205091
39	6	0	-8.888756	-2.045805	5.234795
40	1	0	-9.40934	-1.105512	5.440171
41	1	0	-8.534706	-2.453263	6.188288
42	1	0	-9.622088	-2.74339	4.81602
43	6	0	-11.152698	-0.594362	-1.142638
44	1	0	-11.741939	-0.175209	-0.319863
45	1	0	-11.301491	-1.678424	-1.135671
46	1	0	-11.552782	-0.202877	-2.084483
47	6	0	-8.877255	-0.79812	-2.210285
48	1	0	-9.239158	-0.341814	-3.137422
49	1	0	-9.014993	-1.880786	-2.297371
50	1	0	-7.80968	-0.589084	-2.125432
51	6	0	-0.659333	-4.415364	-2.941743
52	6	0	0.417164	-4.741144	-4.001147
53	6	0	1.490803	-5.47071	-3.17231
54	6	0	9.500058	-1.288466	-0.838244

55	1	0	10.303276	-1.825657	-1.354835
56	6	0	9.418457	-1.588384	0.687631
57	1	0	10.329636	-2.022781	1.111073
58	6	0	7.706339	1.80774	4.266152
59	6	0	7.103062	3.18482	3.865639
60	1	0	7.195873	3.916765	4.675927
61	6	0	7.784992	3.618112	2.536332
62	1	0	8.551069	4.391394	2.650697
63	6	0	9.650615	0.253858	-1.000405
64	6	0	6.674937	0.88019	4.924337
65	1	0	5.840656	0.675257	4.251572
66	1	0	6.272373	1.334437	5.835709
67	1	0	7.138504	-0.071189	5.205087
68	6	0	8.888742	2.04584	5.234721
69	1	0	9.409336	1.105557	5.440109
70	1	0	8.5347	2.453315	6.18821
71	1	0	9.622062	2.743423	4.815922
72	6	0	11.152639	0.594281	-1.14269
73	1	0	11.741887	0.17515	-0.319909
74	1	0	11.301422	1.678345	-1.135746
75	1	0	11.552723	0.202781	-2.084528
76	6	0	8.87719	0.798	-2.210331
77	1	0	9.239094	0.34168	-3.137461
78	1	0	9.014918	1.880666	-2.297437
79	1	0	7.809617	0.588955	-2.125471
80	6	0	0.659456	4.415463	-2.941581
81	6	0	-0.416886	4.74148	-4.001069
82	6	0	-1.49059	5.470961	-3.172243
83	5	0	-7.64773	2.541664	-0.353207
84	5	0	-5.54208	-3.710254	2.276687
85	5	0	7.647692	-2.54175	-0.353189
86	5	0	5.542014	3.710198	2.276621
87	6	0	9.049369	-0.252985	1.294284
88	6	0	8.317584	2.316352	1.975671
89	6	0	8.604662	-0.010417	2.593652
90	6	0	9.131494	0.770397	0.339471
91	6	0	8.768392	2.074881	0.678347
92	6	0	8.230028	1.290934	2.928599
93	1	0	8.518259	-0.826005	3.306173
94	1	0	8.795054	2.878244	-0.052488
95	6	0	4.164808	3.807754	1.56725
96	6	0	1.715975	3.788453	0.125034

97	6	0	3.141558	2.929075	1.939761
98	6	0	3.931593	4.692008	0.488831
99	6	0	2.731443	4.708124	-0.207616
100	6	0	1.952674	2.915241	1.213651
101	1	0	3.289887	2.242658	2.767842
102	1	0	4.720855	5.376513	0.192293
103	1	0	2.590459	5.402824	-1.024659
104	6	0	0.410941	3.552907	-0.486845
105	6	0	-0.269735	2.512848	0.106309
106	6	0	-1.575426	1.885573	-0.271001
107	1	0	-1.533237	0.799624	-0.147273
108	1	0	-1.82339	2.103018	-1.310898
109	1	0	-2.396951	2.257992	0.349416
110	6	0	-0.126011	4.289511	-1.646998
111	6	0	-1.346577	4.871021	-1.78797
112	6	0	-2.23608	5.757401	0.376079
113	6	0	-2.408434	5.033952	-0.777315
114	6	0	-1.032375	6.531628	0.819307
115	1	0	-0.455224	5.977103	1.567956
116	1	0	-1.319567	7.489474	1.263563
117	1	0	-0.375741	6.73261	-0.029644
118	6	0	-6.289509	3.266568	-0.548885
119	6	0	-3.723978	4.420225	-0.872924
120	6	0	-5.516817	3.037333	-1.712453
121	6	0	-5.772128	4.103727	0.447449
122	6	0	-4.51121	4.675735	0.274713
123	6	0	-4.257568	3.590236	-1.878482
124	1	0	-5.919985	2.392948	-2.487619
125	1	0	-6.343845	4.286881	1.352282
126	1	0	-3.683254	3.38554	-2.774411
127	6	0	-8.31764	-2.316392	1.975744
128	6	0	-9.04941	0.252937	1.294309
129	6	0	-8.768456	-2.074944	0.678419
130	6	0	-8.230066	-1.290954	2.92865
131	6	0	-8.604694	0.010392	2.593679
132	6	0	-9.131548	-0.770464	0.339518
133	1	0	-8.795128	-2.878323	-0.0524
134	1	0	-8.51828	0.825995	3.306183
135	6	0	-4.164886	-3.807834	1.567296
136	6	0	-1.716074	-3.788568	0.125025
137	6	0	-3.141615	-2.929174	1.939788
138	6	0	-3.931698	-4.692098	0.488881

139	6	0	-2.731561	-4.708234	-0.207587
140	6	0	-1.952742	-2.91536	1.213657
141	1	0	-3.289915	-2.242757	2.767874
142	1	0	-4.720973	-5.376599	0.192364
143	1	0	-2.590603	-5.402955	-1.024613
144	6	0	0.269684	-2.513032	0.10634
145	6	0	-0.411038	-3.553028	-0.486868
146	6	0	1.575434	-1.885846	-0.270918
147	1	0	1.533324	-0.799897	-0.147169
148	1	0	1.82341	-2.103291	-1.310812
149	1	0	2.396914	-2.258342	0.349513
150	6	0	1.346564	-4.871033	-1.787953
151	6	0	0.125964	-4.289585	-1.647034
152	6	0	6.289466	-3.266651	-0.548848
153	6	0	3.723925	-4.420271	-0.872861
154	6	0	5.516818	-3.037502	-1.712463
155	6	0	5.772047	-4.103727	0.447536
156	6	0	4.511123	-4.675724	0.274811
157	6	0	4.257565	-3.590397	-1.878485
158	1	0	5.920026	-2.393197	-2.487676
159	1	0	6.343739	-4.286826	1.352395
160	1	0	3.683282	-3.385786	-2.774457
161	6	0	2.235981	-5.757377	0.376157
162	6	0	2.40837	-5.033958	-0.777249
163	6	0	1.03226	-6.531583	0.819377
164	1	0	1.319434	-7.489417	1.263671
165	1	0	0.375648	-6.732588	-0.029585
166	1	0	0.455092	-5.977031	1.567993

OO3 E = –6499.824029 (au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.54634	-5.579806	1.976457
2	16	0	-0.62812	-1.520691	1.229331
3	16	0	-2.039692	1.66569	-2.941522
4	16	0	0.39465	3.4177	2.585269
5	9	0	2.375528	-6.34638	-3.040006
6	9	0	0.815961	-7.560763	-2.094611
7	9	0	0.66433	-4.724111	-4.140863
8	9	0	-0.468707	-6.611725	-4.19447

9	9	0	-1.88778	-5.97686	-2.127069
10	9	0	-1.523807	-3.969663	-2.941412
11	9	0	-3.116885	6.68888	-2.611576
12	9	0	-1.136997	6.650226	-3.552791
13	9	0	-2.323737	8.138072	-0.623204
14	9	0	-0.964088	8.885468	-2.187129
15	9	0	-0.055912	7.751507	0.568873
16	9	0	1.019774	7.453622	-1.322232
17	8	0	6.026925	3.152701	2.934578
18	8	0	6.786546	3.892259	0.89417
19	8	0	8.026241	-2.396533	-1.730888
20	8	0	8.341829	-2.917857	0.486351
21	8	0	-5.624854	-2.302085	3.856852
22	8	0	-6.575823	-3.947634	2.561828
23	8	0	-7.636045	0.643163	-2.133535
24	8	0	-8.109196	2.10419	-0.42188
25	6	0	7.460394	3.147239	3.057572
26	1	0	7.735366	3.942508	3.759472
27	6	0	7.945464	3.403125	1.599743
28	1	0	8.732324	4.159954	1.517039
29	6	0	9.428619	-0.326805	-1.745824
30	6	0	9.31551	-1.844303	-1.408514
31	1	0	10.073867	-2.43038	-1.93936
32	6	0	9.381237	-1.980247	0.141868
33	1	0	10.330912	-2.371375	0.520447
34	6	0	8.038024	1.772372	3.508499
35	6	0	8.531671	0.084178	-2.922564
36	1	0	7.481341	-0.12185	-2.710597
37	1	0	8.808204	-0.46341	-3.82943
38	1	0	8.642878	1.152911	-3.132815
39	6	0	10.904075	0.001823	-2.073284
40	1	0	11.037449	1.080861	-2.196791
41	1	0	11.214014	-0.487299	-3.003384
42	1	0	11.578774	-0.324117	-1.274281
43	6	0	9.321465	2.018348	4.335278
44	1	0	10.037361	2.644457	3.791871
45	1	0	9.819041	1.070615	4.562444
46	1	0	9.084504	2.513576	5.283429
47	6	0	7.034976	0.954155	4.335303
48	1	0	6.745467	1.49726	5.240722
49	1	0	7.480376	0.003194	4.645186
50	1	0	6.129693	0.743837	3.763486

51	6	0	1.159842	-6.282719	-2.438208
52	6	0	0.092585	-5.696793	-3.38237
53	6	0	-0.913686	-5.051006	-2.401791
54	6	0	-7.011015	-2.334462	4.255738
55	1	0	-7.064359	-2.771583	5.259264
56	6	0	-7.662009	-3.201321	3.142309
57	1	0	-8.417799	-3.909239	3.49618
58	6	0	-9.187253	-1.186523	-1.421746
59	6	0	-8.984738	0.323147	-1.734756
60	1	0	-9.658478	0.66576	-2.5283
61	6	0	-9.136021	1.09404	-0.394037
62	1	0	-10.102026	1.591657	-0.262584
63	6	0	-7.687529	-0.935219	4.19656
64	6	0	-8.298637	-2.091366	-2.287255
65	1	0	-7.240786	-1.8768	-2.127572
66	1	0	-8.518306	-1.945222	-3.349968
67	1	0	-8.479933	-3.145366	-2.053196
68	6	0	-10.675051	-1.546293	-1.64342
69	1	0	-10.871769	-2.571198	-1.314485
70	1	0	-10.939614	-1.473678	-2.704173
71	1	0	-11.341769	-0.885547	-1.078897
72	6	0	-8.900226	-0.927829	5.156178
73	1	0	-9.586838	-1.755367	4.948531
74	1	0	-9.464971	0.003124	5.048272
75	1	0	-8.573125	-1.007532	6.198825
76	6	0	-6.724311	0.201338	4.566901
77	1	0	-6.349501	0.072478	5.587795
78	1	0	-7.235536	1.168557	4.521737
79	1	0	-5.867157	0.229103	3.892184
80	6	0	-1.785938	6.617702	-2.350157
81	6	0	-1.320279	7.799873	-1.475169
82	6	0	-0.153361	7.193966	-0.661397
83	5	0	5.693609	3.654353	1.69597
84	5	0	7.521508	-3.024204	-0.614833
85	5	0	-5.424115	-3.265771	2.89333
86	5	0	-7.201245	1.711678	-1.382201
87	6	0	-8.192113	-2.1652	2.172913
88	6	0	-8.853071	0.031991	0.647306
89	6	0	-8.165559	-0.885972	2.746853
90	6	0	-8.535683	-2.364013	0.836558
91	6	0	-8.851376	-1.244314	0.066606
92	6	0	-8.516353	0.229843	1.986294

93	1	0	-8.494085	-3.358495	0.401508
94	1	0	-8.472775	1.234069	2.398293
95	6	0	-4.073729	-3.501363	2.166903
96	6	0	-1.753729	-3.792786	0.56282
97	6	0	-3.075416	-2.520934	2.202358
98	6	0	-3.876283	-4.638739	1.34905
99	6	0	-2.737766	-4.801554	0.575238
100	6	0	-1.944116	-2.667398	1.400536
101	1	0	-3.201974	-1.639102	2.823132
102	1	0	-4.650407	-5.399505	1.31693
103	1	0	-2.623104	-5.681304	-0.044899
104	6	0	0.168932	-2.533051	0.040594
105	6	0	-0.519546	-3.698129	-0.203904
106	6	0	1.109113	-5.371893	-1.228394
107	6	0	-0.069372	-4.701556	-1.188197
108	6	0	1.428486	-2.025059	-0.590123
109	1	0	2.297987	-2.189703	0.054778
110	1	0	1.358874	-0.951062	-0.786878
111	1	0	1.618543	-2.533329	-1.536766
112	6	0	2.074374	-5.794693	1.043767
113	6	0	2.207889	-5.346404	-0.245857
114	6	0	6.139322	-3.726608	-0.590808
115	6	0	3.529233	-4.814083	-0.53112
116	6	0	5.655447	-4.307212	0.58821
117	6	0	5.310266	-3.720031	-1.737888
118	6	0	4.029603	-4.247003	-1.719562
119	6	0	4.369053	-4.846213	0.607002
120	1	0	6.273298	-4.315201	1.481045
121	1	0	5.689609	-3.273422	-2.651861
122	1	0	3.413608	-4.225051	-2.611198
123	6	0	0.874329	-6.41152	1.695186
124	1	0	1.159209	-7.252499	2.33451
125	1	0	0.178844	-6.779355	0.93791
126	1	0	0.340479	-5.684866	2.318081
127	6	0	9.061301	-0.588567	0.637329
128	6	0	8.383946	2.038777	1.119172
129	6	0	9.036974	0.328164	-0.423027
130	6	0	8.7474	-0.211631	1.942204
131	6	0	8.40148	1.119348	2.177535
132	6	0	8.699999	1.661611	-0.186065
133	1	0	8.744056	-0.947805	2.741327
134	1	0	8.652568	2.386475	-0.994052

135	6	0	4.229666	3.95725	1.278002
136	6	0	1.566401	4.625993	0.574746
137	6	0	3.936902	4.697734	0.108313
138	6	0	3.167628	3.531947	2.085598
139	6	0	1.860594	3.853959	1.724556
140	6	0	2.638384	5.036309	-0.242545
141	1	0	4.758442	5.022236	-0.523289
142	1	0	3.367558	2.963282	2.988706
143	1	0	2.44746	5.628205	-1.129724
144	6	0	0.137867	4.854117	0.424692
145	6	0	-0.603822	4.272413	1.424231
146	6	0	-2.084996	4.315592	1.645569
147	1	0	-2.581372	3.440859	1.212223
148	1	0	-2.516214	5.204167	1.179749
149	1	0	-2.322962	4.341401	2.712789
150	6	0	-0.469296	5.710219	-0.612325
151	6	0	-1.386667	5.39066	-1.555965
152	6	0	-1.908637	4.064287	-1.935773
153	6	0	-1.130887	3.113385	-2.547059
154	6	0	-5.821166	2.399677	-1.563596
155	6	0	-3.289373	3.648399	-1.76807
156	6	0	-4.762805	1.726782	-2.185686
157	6	0	-5.595311	3.702075	-1.055589
158	6	0	-4.365196	4.329596	-1.165897
159	6	0	-3.51303	2.342625	-2.265368
160	1	0	-4.912587	0.727701	-2.583683
161	1	0	-6.415281	4.222287	-0.569722
162	1	0	-4.227567	5.339856	-0.795881
163	6	0	0.323941	3.192195	-2.902218
164	1	0	0.544269	2.615636	-3.804778
165	1	0	0.954815	2.805185	-2.094075
166	1	0	0.613141	4.230171	-3.083876

CO1 E = –6499.796179 (au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.299173	-1.824096	-2.938899
2	16	0	-0.863577	-2.38761	2.7967
3	9	0	2.032672	-6.816141	-2.015335
4	9	0	-0.076259	-6.836368	-2.609644

5	9	0	1.530783	-7.765172	0.36023
6	9	0	-0.00416	-8.793983	-0.838597
7	9	0	-0.602287	-7.112403	1.706641
8	9	0	-1.874996	-7.167159	-0.082639
9	8	0	-6.530365	-1.717759	3.291013
10	8	0	-7.355636	-3.184874	1.724109
11	8	0	-7.26297	1.588651	-2.799185
12	8	0	-7.96825	3.070745	-1.188558
13	8	0	6.569	1.502446	3.338363
14	8	0	7.520022	3.132406	2.024115
15	8	0	7.02241	-1.268596	-2.922358
16	8	0	7.651433	-2.874605	-1.401281
17	6	0	-7.963811	-1.603731	3.397534
18	1	0	-8.266236	-2.056797	4.348323
19	6	0	-8.465722	-2.369045	2.140082
20	1	0	-9.324062	-3.023737	2.321337
21	6	0	-9.085592	-0.09625	-2.512535
22	6	0	-8.693404	1.393439	-2.709754
23	1	0	-9.14755	1.822462	-3.609883
24	6	0	-9.047146	2.134933	-1.393447
25	1	0	-9.987109	2.694259	-1.419262
26	6	0	-8.47567	-0.137446	3.275268
27	6	0	-8.155594	-1.055501	-3.26838
28	1	0	-7.121426	-0.946699	-2.937779
29	1	0	-8.190278	-0.857996	-4.344948
30	1	0	-8.465053	-2.093983	-3.112486
31	6	0	-10.543753	-0.294569	-2.988772
32	1	0	-10.886685	-1.306223	-2.751649
33	1	0	-10.623037	-0.155391	-4.072628
34	1	0	-11.229494	0.407389	-2.502414
35	6	0	-9.815757	-0.013913	4.037035
36	1	0	-10.541895	-0.763445	3.704371
37	1	0	-10.260652	0.971851	3.87028
38	1	0	-9.664445	-0.13947	5.114832
39	6	0	-7.468974	0.884775	3.822126
40	1	0	-7.276514	0.706112	4.885142
41	1	0	-7.861729	1.90188	3.722551
42	1	0	-6.517529	0.825289	3.291236
43	6	0	7.996021	1.346485	3.518599
44	1	0	8.24895	1.709281	4.521106
45	6	0	8.570419	2.202658	2.359332
46	1	0	9.468687	2.774464	2.610776

47	6	0	8.915397	0.315949	-2.497536
48	6	0	8.455233	-1.136941	-2.81362
49	1	0	8.898171	-1.50759	-3.744907
50	6	0	8.782408	-1.999953	-1.563552
51	1	0	9.682807	-2.61499	-1.6584
52	6	0	8.477058	-0.112059	3.287643
53	6	0	7.998267	1.373844	-3.127297
54	1	0	6.973011	1.272824	-2.767709
55	1	0	7.986843	1.274563	-4.21773
56	1	0	8.353923	2.381714	-2.889968
57	6	0	10.362441	0.501979	-3.010851
58	1	0	10.755642	1.474221	-2.698532
59	1	0	10.397262	0.458264	-4.105037
60	1	0	11.034923	-0.267293	-2.616257
61	6	0	9.823715	-0.313561	4.020878
62	1	0	10.561959	0.441504	3.730666
63	1	0	10.244266	-1.294306	3.779192
64	1	0	9.688663	-0.260408	5.106846
65	6	0	7.458433	-1.152366	3.773791
66	1	0	7.280301	-1.044404	4.848894
67	1	0	7.83222	-2.166676	3.600673
68	1	0	6.502887	-1.040453	3.258971
69	6	0	0.770539	-6.619723	-1.557634
70	6	0	0.426284	-7.591375	-0.414062
71	6	0	-0.637734	-6.807911	0.387491
72	5	0	-6.235607	-2.674845	2.345068
73	5	0	-6.91207	2.594878	-1.931835
74	5	0	6.356798	2.573142	2.503055
75	5	0	6.618211	-2.315185	-2.123427
76	6	0	8.773799	1.179137	1.260097
77	6	0	8.855023	-0.97757	-0.450252
78	6	0	8.691064	-0.122783	1.775951
79	6	0	8.88013	1.421837	-0.108989
80	6	0	8.897373	0.323592	-0.970182
81	6	0	8.754739	-1.220795	0.918937
82	1	0	8.879361	2.440181	-0.48699
83	1	0	8.661651	-2.237537	1.289746
84	6	0	-9.016236	1.022439	-0.364794
85	6	0	-8.743951	-1.263783	1.146291
86	6	0	-9.005202	-0.231456	-0.993822
87	6	0	-8.874622	1.152738	1.016233
88	6	0	-8.716806	-0.010158	1.772329

89	6	0	-8.888634	-1.394712	-0.234343
90	1	0	-8.826911	2.137548	1.472121
91	1	0	-8.847841	-2.37529	-0.699879
92	6	0	-4.799918	-3.13737	1.982677
93	6	0	-2.208802	-4.014908	1.244059
94	6	0	-4.60865	-4.150058	1.012739
95	6	0	-3.67295	-2.555155	2.575949
96	6	0	-2.401446	-2.989373	2.201107
97	6	0	-3.346827	-4.588091	0.643968
98	1	0	-5.482283	-4.594343	0.545846
99	1	0	-3.793661	-1.769852	3.31617
100	1	0	-3.234041	-5.373484	-0.092679
101	6	0	-0.798804	-4.288838	1.012867
102	6	0	0.028927	-3.49757	1.771921
103	6	0	1.524826	-3.493462	1.842462
104	1	0	1.949025	-2.677246	1.247429
105	1	0	1.931076	-4.430074	1.456576
106	1	0	1.8699	-3.368881	2.873239
107	6	0	-0.301062	-5.35073	0.116829
108	6	0	0.524975	-5.2491	-0.953472
109	6	0	1.085633	-4.044423	-1.592773
110	6	0	0.321229	-3.094455	-2.222909
111	6	0	5.15611	-2.820097	-2.002094
112	6	0	2.510566	-3.768577	-1.667171
113	6	0	4.086849	-2.106789	-2.557666
114	6	0	4.88009	-4.004308	-1.276166
115	6	0	3.590707	-4.48209	-1.112401
116	6	0	2.784742	-2.575267	-2.37608
117	1	0	4.273424	-1.192155	-3.112496
118	1	0	5.709463	-4.550871	-0.838019
119	1	0	3.411819	-5.404048	-0.570383
120	6	0	-1.168625	-3.039635	-2.368534
121	1	0	-1.456365	-2.723525	-3.375661
122	1	0	-1.611402	-2.331704	-1.658998
123	1	0	-1.60589	-4.022293	-2.180419
124	6	0	-5.45561	3.115168	-1.733833
125	6	0	-2.831553	4.034236	-1.175532
126	6	0	-5.177347	4.488565	-1.585318
127	6	0	-4.404211	2.199022	-1.588823
128	6	0	-3.125843	2.652058	-1.268799
129	6	0	-3.891642	4.948575	-1.335083
130	1	0	-5.986016	5.208098	-1.66948

131	1	0	-4.594423	1.133874	-1.679464
132	1	0	-3.714772	6.01073	-1.247787
133	6	0	-1.444244	4.292605	-0.822377
134	6	0	-0.582613	3.011353	-0.801888
135	16	0	-1.778693	1.582085	-0.865709
136	6	0	-0.771649	5.441275	-0.524848
137	6	0	4.951753	3.086474	2.065217
138	6	0	2.473616	4.015285	1.06066
139	6	0	4.691842	4.463739	1.919366
140	6	0	3.94587	2.171495	1.719466
141	6	0	2.740555	2.631094	1.193482
142	6	0	3.469071	4.929059	1.453808
143	1	0	5.46263	5.181226	2.183567
144	1	0	4.119723	1.105507	1.829852
145	1	0	3.292668	5.993297	1.388806
146	6	0	0.268079	3.023767	0.490894
147	16	0	1.446539	1.5787	0.600361
148	6	0	1.159612	4.279052	0.493266
149	6	0	0.587404	5.420654	0.020043
150	6	0	1.148712	6.816915	0.044913
151	6	0	-1.212029	6.87215	-0.671952
152	6	0	0.113282	7.679169	-0.726352
153	9	0	-0.01399	8.917152	-0.212223
154	9	0	0.503583	7.777299	-2.021522
155	9	0	2.375945	6.932194	-0.538145
156	9	0	1.270953	7.303731	1.319511
157	9	0	-1.941491	7.128616	-1.794473
158	9	0	-1.954563	7.303684	0.394469
159	6	0	0.254702	2.966234	-2.105076
160	1	0	0.831509	2.04187	-2.163046
161	1	0	0.943634	3.812627	-2.157086
162	1	0	-0.417368	3.01183	-2.964559
163	6	0	-0.577192	3.04215	1.790862
164	1	0	-1.189548	2.142683	1.866727
165	1	0	-1.232204	3.917284	1.816273
166	1	0	0.090189	3.084734	2.654001

CO2 E = –6499.804413 (au)

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

1	16	0	-0.814361	1.650974	-1.036758
2	16	0	3.189629	5.686498	-1.711433
3	9	0	-1.269825	3.52283	3.566245
4	9	0	-1.661549	5.619389	3.039917
5	9	0	1.06607	4.095973	4.583746
6	9	0	-0.008328	5.973347	4.998038
7	9	0	2.678595	5.826986	3.497703
8	9	0	1.050743	7.163679	2.895917
9	8	0	8.234111	2.412566	1.080665
10	8	0	8.129961	2.885054	-1.1668
11	8	0	6.074694	-3.46868	-3.181009
12	8	0	7.131056	-3.9947	-1.20855
13	8	0	-8.436705	-2.025282	1.242113
14	8	0	-8.333776	-2.612939	-0.97771
15	8	0	-5.821325	3.093091	-3.345824
16	8	0	-6.871517	4.073098	-1.550522
17	6	0	9.493758	1.957986	0.556443
18	1	0	10.27563	2.621673	0.942126
19	6	0	9.292432	2.050432	-0.985772
20	1	0	10.127549	2.512694	-1.521645
21	6	0	7.858042	-1.937242	-4.043213
22	6	0	7.476853	-3.341939	-3.480027
23	1	0	7.739356	-4.13764	-4.185506
24	6	0	8.159674	-3.486565	-2.085614
25	1	0	8.995911	-4.192518	-2.066168
26	6	0	9.793358	0.467981	0.899006
27	6	0	6.684749	-1.247872	-4.755288
28	1	0	5.841163	-1.098368	-4.079504
29	1	0	6.33801	-1.85012	-5.601171
30	1	0	6.995559	-0.273401	-5.14574
31	6	0	9.041515	-2.100421	-5.025736
32	1	0	9.411658	-1.121533	-5.345439
33	1	0	8.73175	-2.654395	-5.91884
34	1	0	9.878773	-2.635147	-4.564305
35	6	0	11.325344	0.277637	0.99388
36	1	0	11.833487	0.633668	0.091188
37	1	0	11.573402	-0.781127	1.115603
38	1	0	11.731678	0.822653	1.853014
39	6	0	9.13133	0.018719	2.209899
40	1	0	9.495022	0.616451	3.051925
41	1	0	9.369496	-1.029375	2.418876
42	1	0	8.046501	0.1265	2.162968

43	6	0	-9.659777	-1.51456	0.678796
44	1	0	-10.489262	-2.082693	1.112994
45	6	0	-9.475258	-1.736768	-0.853985
46	1	0	-10.325817	-2.218765	-1.345909
47	6	0	-7.799779	1.859252	-4.23097
48	6	0	-7.200841	3.207974	-3.744373
49	1	0	-7.264391	3.982595	-4.516956
50	6	0	-7.915652	3.576756	-2.412815
51	1	0	-8.679343	4.354996	-2.507065
52	6	0	-9.840562	0.01998	0.906714
53	6	0	-6.761782	0.970072	-4.930361
54	1	0	-5.929058	0.735218	-4.265564
55	1	0	-6.357681	1.471763	-5.815757
56	1	0	-7.220044	0.032466	-5.261625
57	6	0	-8.971339	2.153554	-5.197273
58	1	0	-9.488455	1.226739	-5.463522
59	1	0	-8.606312	2.616043	-6.120985
60	1	0	-9.710309	2.825118	-4.747171
61	6	0	-11.35221	0.329656	1.012915
62	1	0	-11.904884	-0.058345	0.15045
63	1	0	-11.520212	1.410143	1.053233
64	1	0	-11.777041	-0.113964	1.92019
65	6	0	-9.117898	0.51861	2.166627
66	1	0	-9.501705	0.012867	3.058446
67	1	0	-9.27915	1.593388	2.298971
68	1	0	-8.044254	0.332674	2.109813
69	6	0	-0.690775	4.650409	3.092674
70	6	0	0.435172	5.160371	4.021232
71	6	0	1.400909	5.849603	3.037478
72	5	0	7.504954	2.973717	0.057334
73	5	0	5.935326	-3.868843	-1.873431
74	5	0	-7.717057	-2.645289	0.249976
75	5	0	-5.679347	3.645493	-2.092681
76	6	0	-9.158315	-0.361892	-1.388862
77	6	0	-8.457889	2.246867	-1.929373
78	6	0	-8.69422	-0.05032	-2.66619
79	6	0	-9.288382	0.611353	-0.38935
80	6	0	-8.937878	1.936856	-0.656863
81	6	0	-8.338721	1.27104	-2.930575
82	1	0	-8.575973	-0.829396	-3.414135
83	1	0	-8.994085	2.703433	0.110899
84	6	0	-4.316697	3.725553	-1.352415

85	6	0	-1.877129	3.763547	0.096913
86	6	0	-3.323091	2.780745	-1.633976
87	6	0	-4.065742	4.690502	-0.349751
88	6	0	-2.867398	4.734285	0.347669
89	6	0	-2.138218	2.792978	-0.899978
90	1	0	-3.487201	2.030861	-2.401843
91	1	0	-4.83532	5.421716	-0.120443
92	1	0	-2.705481	5.493087	1.102129
93	6	0	-0.569471	3.571986	0.711869
94	6	0	0.091708	2.470998	0.220279
95	6	0	1.405972	1.886468	0.637194
96	1	0	1.341252	0.796108	0.706177
97	1	0	1.70895	2.270061	1.612475
98	1	0	2.200611	2.127823	-0.07633
99	6	0	0.003049	4.440538	1.758711
100	6	0	1.191228	5.096696	1.739445
101	6	0	1.857142	5.782615	-0.572893
102	6	0	2.158087	5.194568	0.630024
103	6	0	0.58581	6.457967	-0.988517
104	1	0	-0.043755	5.78994	-1.587073
105	1	0	0.789732	7.350083	-1.588109
106	1	0	0.011635	6.761844	-0.110645
107	6	0	6.107835	3.613218	0.270651
108	6	0	3.504777	4.649032	0.675969
109	6	0	5.439299	3.46999	1.510208
110	6	0	5.463544	4.29938	-0.766071
111	6	0	4.184934	4.815668	-0.553875
112	6	0	4.162341	3.964969	1.71726
113	1	0	5.942195	2.94379	2.315731
114	1	0	5.954728	4.415432	-1.727569
115	1	0	3.671944	3.83309	2.674707
116	6	0	8.554478	-2.075243	-1.722012
117	6	0	9.032597	0.619441	-1.401135
118	6	0	9.023084	-1.625199	-0.488143
119	6	0	8.331119	-1.198853	-2.792693
120	6	0	8.572109	0.167529	-2.637694
121	6	0	9.261873	-0.259684	-0.332986
122	1	0	9.167089	-2.32231	0.332714
123	1	0	8.381526	0.871249	-3.443255
124	6	0	4.55022	-4.11615	-1.209987
125	6	0	2.026228	-4.408144	0.033815
126	6	0	3.376233	-4.048169	-1.977325

127	6	0	4.441126	-4.341515	0.176797
128	6	0	3.205703	-4.480507	0.797515
129	6	0	2.136928	-4.200994	-1.36357
130	1	0	3.44049	-3.861693	-3.044772
131	1	0	5.345063	-4.381976	0.776299
132	1	0	3.157182	-4.617979	1.868907
133	16	0	0.582015	-4.139509	-2.212214
134	6	0	0.639988	-4.475606	0.476789
135	6	0	-0.321078	-3.923197	-0.590045
136	6	0	-6.305766	-3.260699	0.476564
137	6	0	-3.658309	-4.189579	0.879106
138	6	0	-5.82253	-3.553812	1.767911
139	6	0	-5.449023	-3.443131	-0.618638
140	6	0	-4.140396	-3.874023	-0.414886
141	6	0	-4.530933	-4.019298	1.97308
142	1	0	-6.473336	-3.401477	2.623205
143	1	0	-5.798249	-3.208857	-1.619331
144	1	0	-4.195433	-4.234597	2.977325
145	16	0	-2.935808	-3.988504	-1.702412
146	6	0	-2.248567	-4.548559	0.881616
147	6	0	-1.661269	-4.695046	-0.538002
148	6	0	0.079477	-4.84948	1.658796
149	6	0	-1.363557	-4.772657	1.894948
150	6	0	0.778164	-5.269917	2.924299
151	6	0	-0.362934	-5.72398	3.870423
152	6	0	-1.623654	-4.974192	3.363612
153	9	0	1.447386	-4.228124	3.51254
154	9	0	-0.095934	-5.477676	5.166455
155	9	0	-0.560896	-7.056242	3.704741
156	9	0	1.682006	-6.27394	2.754511
157	9	0	-1.744953	-3.793583	4.045065
158	9	0	-2.734338	-5.712148	3.643953
159	6	0	-0.474409	-2.402117	-0.329247
160	1	0	-0.931539	-2.2203	0.647507
161	1	0	-1.091622	-1.934357	-1.096306
162	1	0	0.512051	-1.93381	-0.341322
163	6	0	-1.530128	-6.20508	-0.855001
164	1	0	-1.190143	-6.359607	-1.880056
165	1	0	-2.504345	-6.684008	-0.735841
166	1	0	-0.820404	-6.685465	-0.177134

CO3 E = –6499.801948 (au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.262073	6.211769	-1.926032
2	16	0	1.396982	1.990077	-0.885394
3	8	0	7.388824	4.027048	0.528411
4	8	0	6.896546	3.58548	-1.671617
5	8	0	7.410351	-3.048098	-2.769107
6	8	0	8.323584	-2.852339	-0.669927
7	8	0	-7.601308	-3.74002	0.62679
8	8	0	-7.144676	-3.670873	-1.624578
9	8	0	-7.067206	3.328751	-2.943098
10	8	0	-8.003832	3.10076	-0.856887
11	6	0	8.665959	3.766557	-0.072032
12	1	0	9.274819	4.670119	0.03297
13	6	0	8.329132	3.414017	-1.557436
14	1	0	8.803596	4.069621	-2.294529
15	6	0	8.768217	-1.254842	-3.828197
16	6	0	8.746873	-2.577264	-3.005589
17	1	0	9.301318	-3.375456	-3.510952
18	6	0	9.276601	-2.245823	-1.574232
19	1	0	10.264437	-2.658906	-1.349261
20	6	0	9.392683	2.525841	0.555085
21	6	0	7.567916	-1.125781	-4.776716
22	1	0	6.624386	-1.131915	-4.228838
23	1	0	7.549894	-1.953929	-5.492456
24	1	0	7.632812	-0.19463	-5.349045
25	6	0	10.082936	-1.197	-4.641978
26	1	0	10.185785	-0.225832	-5.135547
27	1	0	10.095035	-1.974248	-5.414118
28	1	0	10.960866	-1.336282	-4.002068
29	6	0	10.904974	2.833074	0.657358
30	1	0	11.318412	3.141305	-0.309059
31	1	0	11.457797	1.947729	0.986292
32	1	0	11.087906	3.635865	1.380281
33	6	0	8.846807	2.158546	1.943688
34	1	0	8.973497	2.991072	2.642404
35	1	0	9.389033	1.29738	2.347683
36	1	0	7.784417	1.912363	1.906434
37	6	0	-8.871804	-3.462136	0.014351
38	1	0	-9.520147	-4.32712	0.189915

39	6	0	-8.518216	-3.241459	-1.490614
40	1	0	-9.121861	-3.835908	-2.18372
41	6	0	-8.275527	1.368198	-3.931777
42	6	0	-8.356162	2.747931	-3.195479
43	1	0	-8.937503	3.469254	-3.779145
44	6	0	-8.940261	2.487937	-1.76966
45	1	0	-9.920609	2.944195	-1.598473
46	6	0	-9.529459	-2.147959	0.541299
47	6	0	-6.944443	1.169943	-4.673111
48	1	0	-6.095363	1.218034	-3.989406
49	1	0	-6.806413	1.942649	-5.435799
50	1	0	-6.931253	0.19758	-5.176259
51	6	0	-9.449085	1.268881	-4.93394
52	1	0	-9.48978	0.272124	-5.383807
53	1	0	-9.332047	2.001063	-5.74057
54	1	0	-10.412026	1.44979	-4.444179
55	6	0	-11.065262	-2.331262	0.556274
56	1	0	-11.44217	-2.651932	-0.420961
57	1	0	-11.561851	-1.389454	0.808726
58	1	0	-11.35952	-3.080452	1.29963
59	6	0	-9.040444	-1.763144	1.945772
60	1	0	-9.277913	-2.550823	2.667736
61	1	0	-9.532409	-0.844348	2.281002
62	1	0	-7.96097	-1.605055	1.962613
63	5	0	6.405909	3.868713	-0.419979
64	5	0	7.219844	-3.189476	-1.415564
65	5	0	-6.652585	-3.871656	-0.357727
66	5	0	-6.912561	3.505728	-1.587473
67	6	0	-8.66336	-1.752305	-1.694484
68	6	0	-8.943553	0.987173	-1.626078
69	6	0	-8.338531	-1.020259	-2.836875
70	6	0	-9.152384	-1.133692	-0.535259
71	6	0	-9.287246	0.254022	-0.49042
72	6	0	-8.492279	0.366917	-2.798843
73	1	0	-7.960766	-1.523204	-3.72303
74	1	0	-9.633696	0.759847	0.406729
75	6	0	-5.610419	4.06931	-0.958101
76	6	0	-3.166328	4.93409	0.178282
77	6	0	-4.715422	4.824882	-1.725429
78	6	0	-5.273665	3.772906	0.383925
79	6	0	-4.073493	4.177849	0.946082
80	6	0	-3.521664	5.262228	-1.151576

81	1	0	-4.948044	5.056064	-2.760596
82	1	0	-5.970985	3.19292	0.980751
83	1	0	-3.834632	3.920622	1.97141
84	6	0	-1.837751	5.417716	0.518873
85	6	0	-1.24505	6.122731	-0.49814
86	6	0	0.098693	6.785291	-0.514462
87	1	0	0.83816	6.177339	-1.047544
88	1	0	0.460617	6.936678	0.504549
89	1	0	0.05151	7.760807	-1.007867
90	6	0	0.224547	2.671332	0.227399
91	6	0	0.759731	3.667698	1.008561
92	6	0	4.894006	3.935071	-0.066091
93	6	0	2.176857	3.886744	0.748278
94	6	0	4.415862	4.76991	0.970267
95	6	0	3.989169	3.082405	-0.708992
96	6	0	2.660871	3.048452	-0.284589
97	6	0	3.084847	4.774093	1.359121
98	1	0	5.114825	5.426577	1.479791
99	1	0	4.328847	2.431804	-1.50932
100	1	0	2.752577	5.432407	2.151146
101	6	0	9.207124	-0.736875	-1.499948
102	6	0	8.69855	1.961257	-1.703171
103	6	0	9.416642	0.066518	-0.378728
104	6	0	8.807789	-0.195887	-2.73102
105	6	0	8.532779	1.166555	-2.837286
106	6	0	9.172261	1.437051	-0.493312
107	1	0	9.733705	-0.374058	0.562582
108	1	0	8.172151	1.599943	-3.766137
109	6	0	5.846242	-3.619786	-0.825584
110	6	0	3.279593	-4.191785	0.216741
111	6	0	4.743694	-3.730102	-1.688539
112	6	0	5.645688	-3.805139	0.556455
113	6	0	4.388654	-4.090216	1.077121
114	6	0	3.482417	-4.005739	-1.172313
115	1	0	4.878256	-3.574983	-2.754197
116	1	0	6.488648	-3.699355	1.232247
117	1	0	4.26324	-4.199197	2.145649
118	16	0	2.006582	-4.128988	-2.145464
119	6	0	1.878646	-4.424873	0.543734
120	6	0	0.953055	-3.996449	-0.606665
121	6	0	-5.164696	-4.198485	-0.042098
122	6	0	-2.447469	-4.706572	0.58805

123	6	0	-4.757087	-4.46576	1.280855
124	6	0	-4.194359	-4.189146	-1.054306
125	6	0	-2.85817	-4.426125	-0.739083
126	6	0	-3.429527	-4.716468	1.59845
127	1	0	-5.501641	-4.468783	2.070509
128	1	0	-4.484869	-3.974363	-2.078115
129	1	0	-3.155963	-4.915591	2.624319
130	16	0	-1.54269	-4.337429	-1.915527
131	6	0	-1.004645	-4.857022	0.711625
132	6	0	-0.291745	-4.912662	-0.655688
133	6	0	1.271788	-4.863977	1.678761
134	6	0	-0.184084	-4.972177	1.795177
135	6	0	1.91563	-5.197969	2.997902
136	6	0	0.769343	-5.79313	3.855088
137	6	0	-0.533642	-5.215774	3.239709
138	9	0	2.404496	-4.084032	3.629775
139	9	0	0.894928	-5.509475	5.164773
140	9	0	0.759889	-7.140173	3.692758
141	9	0	2.946124	-6.082433	2.903707
142	9	0	-0.868604	-4.065428	3.899721
143	9	0	-1.553008	-6.099936	3.434515
144	6	0	0.610248	-2.499927	-0.384525
145	1	0	0.047212	-2.370369	0.544582
146	1	0	0.016602	-2.110821	-1.212061
147	1	0	1.532689	-1.920656	-0.311637
148	6	0	0.02957	-6.396604	-0.96275
149	1	0	0.455207	-6.505355	-1.961024
150	1	0	-0.891276	-6.981436	-0.910874
151	1	0	0.739678	-6.799234	-0.235902
152	6	0	-1.658141	5.726812	3.104302
153	6	0	0.317984	4.396686	3.48297
154	6	0	-0.983969	4.854417	4.180904
155	9	0	-1.236608	7.02115	3.234973
156	9	0	-3.00916	5.733307	3.242891
157	9	0	-0.765845	5.504009	5.339472
158	9	0	-1.767771	3.770663	4.42237
159	9	0	1.305249	5.292224	3.808728
160	9	0	0.721042	3.176718	3.908536
161	6	0	-1.164623	5.134554	1.800192
162	6	0	-0.032955	4.41415	2.005761
163	6	0	-1.156913	2.093348	0.240751
164	1	0	-1.120838	1.00051	0.191998

165	1	0	-1.750358	2.444827	-0.609739
166	1	0	-1.685003	2.375661	1.152523

CO4 E = –6499.799526 (au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.420692	-4.762946	3.170733
2	16	0	-1.044175	-1.601668	0.969333
3	9	0	1.109244	-8.181747	-0.155863
4	9	0	2.71582	-7.233348	-1.301139
5	9	0	0.063291	-8.063805	-2.586879
6	9	0	1.054452	-6.143942	-3.009884
7	9	0	-1.604671	-7.00214	-0.92628
8	9	0	-1.331847	-5.312051	-2.303971
9	8	0	-6.382526	-2.192829	3.246695
10	8	0	-7.05478	-3.895182	1.85336
11	8	0	-7.46081	0.879488	-2.906481
12	8	0	-8.436845	2.21257	-1.306971
13	8	0	6.934792	4.420599	1.317077
14	8	0	7.081949	3.797731	-0.890017
15	8	0	8.073762	-3.076384	-1.238547
16	8	0	8.342706	-2.656339	1.004791
17	6	0	-7.816875	-2.273148	3.410519
18	1	0	-8.017241	-2.717142	4.392192
19	6	0	-8.237446	-3.158695	2.20896
20	1	0	-9.038069	-3.872582	2.426783
21	6	0	-8.923647	-1.132158	-2.560382
22	6	0	-8.821774	0.402658	-2.80235
23	1	0	-9.349922	0.7039	-3.713715
24	6	0	-9.327566	1.100581	-1.510051
25	1	0	-10.349816	1.486608	-1.572889
26	6	0	-8.534241	-0.905028	3.239302
27	6	0	-7.778011	-1.909206	-3.225048
28	1	0	-6.80728	-1.583197	-2.848098
29	1	0	-7.789192	-1.759559	-4.309782
30	1	0	-7.882031	-2.982619	-3.037272
31	6	0	-10.282017	-1.630894	-3.106084
32	1	0	-10.433646	-2.682686	-2.845337
33	1	0	-10.319418	-1.543546	-4.197522
34	1	0	-11.120913	-1.063704	-2.688464

35	6	0	-9.884354	-0.952993	3.992239
36	1	0	-10.491825	-1.810852	3.684379
37	1	0	-10.465573	-0.048578	3.788182
38	1	0	-9.726487	-1.016645	5.074559
39	6	0	-7.691024	0.270031	3.754375
40	1	0	-7.481567	0.154918	4.823062
41	1	0	-8.226322	1.215767	3.621629
42	1	0	-6.737399	0.332486	3.227631
43	6	0	8.316563	4.073803	1.141934
44	1	0	8.910573	4.969459	1.349329
45	6	0	8.41064	3.604405	-0.345966
46	1	0	9.10398	4.192009	-0.956259
47	6	0	9.506814	-1.200164	-2.038944
48	6	0	9.370581	-2.47015	-1.144454
49	1	0	10.115466	-3.2273	-1.412629
50	6	0	9.452996	-2.008418	0.34456
51	1	0	10.371366	-2.309445	0.8584
52	6	0	8.774671	2.879483	2.050128
53	6	0	8.568091	-1.228316	-3.254173
54	1	0	7.522666	-1.287915	-2.947597
55	1	0	8.784282	-2.092853	-3.889808
56	1	0	8.703513	-0.327136	-3.861027
57	6	0	10.97358	-1.081984	-2.515992
58	1	0	11.130163	-0.137962	-3.046769
59	1	0	11.226387	-1.901309	-3.198129
60	1	0	11.674705	-1.108129	-1.6748
61	6	0	10.174286	3.195278	2.626029
62	1	0	10.889069	3.438726	1.832548
63	1	0	10.5701	2.335355	3.175098
64	1	0	10.125554	4.045104	3.31595
65	6	0	7.794692	2.602408	3.20158
66	1	0	7.701054	3.47863	3.850078
67	1	0	8.155491	1.768704	3.812663
68	1	0	6.799222	2.352	2.830892
69	6	0	1.440601	-7.062987	-0.870186
70	6	0	0.461594	-6.897761	-2.045416
71	6	0	-0.692222	-6.094668	-1.404248
72	5	0	-5.992843	-3.18807	2.378513
73	5	0	-7.310243	1.946901	-2.053377
74	5	0	6.272038	4.230499	0.128512
75	5	0	7.533461	-3.180052	0.022749
76	6	0	8.769078	2.144216	-0.269019

77	6	0	9.264519	-0.510388	0.276098
78	6	0	8.882655	1.720571	1.061608
79	6	0	8.940043	1.265647	-1.338845
80	6	0	9.204148	-0.073743	-1.05549
81	6	0	9.119659	0.373682	1.344883
82	1	0	8.854551	1.620937	-2.362226
83	1	0	9.175996	0.013011	2.368399
84	6	0	-9.142447	0.038401	-0.449138
85	6	0	-8.606255	-2.136052	1.152561
86	6	0	-8.906923	-1.213222	-1.034248
87	6	0	-9.072898	0.231893	0.930031
88	6	0	-8.771728	-0.869093	1.731036
89	6	0	-8.663741	-2.326617	-0.227743
90	1	0	-9.188695	1.226673	1.350755
91	1	0	-8.460648	-3.304713	-0.654434
92	6	0	-4.530981	-3.488989	1.947732
93	6	0	-1.975946	-4.047123	0.846402
94	6	0	-4.172757	-4.789778	1.523737
95	6	0	-3.577776	-2.469109	1.850396
96	6	0	-2.332006	-2.749928	1.287153
97	6	0	-2.918732	-5.080601	1.010904
98	1	0	-4.909175	-5.584645	1.594403
99	1	0	-3.820612	-1.460877	2.172686
100	1	0	-2.680807	-6.089872	0.703996
101	6	0	-0.64081	-4.081108	0.261348
102	6	0	-0.040572	-2.843147	0.2435
103	6	0	1.276197	-2.431135	-0.338649
104	1	0	1.612492	-3.154059	-1.083521
105	1	0	2.053848	-2.361538	0.429264
106	1	0	1.19876	-1.453464	-0.823485
107	6	0	-0.012523	-5.289974	-0.306392
108	6	0	2.220267	-5.368357	0.939162
109	6	0	2.018063	-5.358257	2.295824
110	6	0	6.134418	-3.808413	0.25693
111	6	0	3.538237	-4.889973	0.55634
112	6	0	5.591665	-3.964094	1.538362
113	6	0	5.36179	-4.200524	-0.862839
114	6	0	4.087891	-4.724463	-0.729329
115	6	0	4.310597	-4.50197	1.676215
116	1	0	6.161728	-3.659653	2.411124
117	1	0	5.78487	-4.076154	-1.854592
118	1	0	3.519228	-5.013651	-1.605468

119	6	0	0.800908	-5.782176	3.059082
120	1	0	1.071284	-6.358712	3.948931
121	1	0	0.157256	-6.402986	2.432388
122	1	0	0.215471	-4.916225	3.388482
123	6	0	-6.002905	2.770321	-1.866188
124	6	0	-3.632902	4.210898	-1.290275
125	6	0	-6.009355	3.870422	-0.983732
126	6	0	-4.793205	2.402875	-2.473624
127	6	0	-3.625353	3.104483	-2.175196
128	6	0	-4.855587	4.584221	-0.699015
129	1	0	-6.940875	4.152974	-0.5043
130	1	0	-4.762542	1.551691	-3.146989
131	1	0	-4.900708	5.416503	-0.012161
132	6	0	-2.303653	4.741461	-1.034737
133	6	0	-1.225317	4.136703	-1.958242
134	16	0	-2.023498	2.660683	-2.779795
135	6	0	-1.85318	5.667897	-0.141235
136	6	0	4.740908	4.482766	-0.000915
137	6	0	1.950118	4.907546	-0.107824
138	6	0	4.096734	5.340059	0.913525
139	6	0	3.968138	3.824707	-0.971703
140	6	0	2.589991	4.02349	-1.009579
141	6	0	2.727488	5.564096	0.861935
142	1	0	4.68597	5.826179	1.68451
143	1	0	4.444054	3.146181	-1.673004
144	1	0	2.261231	6.216328	1.587355
145	6	0	0.004813	3.746351	-1.101164
146	16	0	1.477259	3.215671	-2.132144
147	6	0	0.509157	4.963924	-0.310247
148	6	0	-0.427402	5.841926	0.136094
149	6	0	-0.227103	7.025936	1.044835
150	6	0	-2.631409	6.644775	0.699595
151	6	0	-1.598083	7.747314	1.053755
152	9	0	-1.863809	8.351055	2.227124
153	9	0	-1.606176	8.677357	0.065902
154	9	0	0.756619	7.876249	0.645289
155	9	0	0.07248	6.644785	2.328558
156	9	0	-3.695849	7.212764	0.065522
157	9	0	-3.104938	6.088157	1.856854
158	6	0	-0.914547	5.174739	-3.0645
159	1	0	-0.226384	4.763544	-3.804134
160	1	0	-0.467013	6.075384	-2.636341

161	1	0	-1.84268	5.452389	-3.568669
162	6	0	-0.294664	2.627178	-0.070612
163	1	0	-0.57611	1.699667	-0.569653
164	1	0	-1.111055	2.928148	0.592867
165	1	0	0.593487	2.445695	0.537955
166	6	0	1.211702	-5.814131	-0.039193

4a E = –6499.782045 (au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.497128	-3.337202	-2.759382
2	16	0	-2.058374	-3.504459	-2.239477
3	16	0	-2.058351	3.504452	2.239467
4	16	0	1.497147	3.337204	2.759379
5	9	0	2.621881	-7.800586	0.468217
6	9	0	2.023995	-6.517403	2.147058
7	9	0	0.41521	-9.086832	0.423289
8	9	0	0.580842	-8.648028	2.573667
9	9	0	-1.206969	-6.787932	2.460901
10	9	0	-1.898236	-8.059149	0.810677
11	9	0	-1.898221	8.059148	-0.810678
12	9	0	-1.206949	6.787936	-2.460903
13	9	0	0.415223	9.086837	-0.423288
14	9	0	0.580857	8.648036	-2.573666
15	9	0	2.621895	7.800601	-0.468214
16	9	0	2.024018	6.517418	-2.147059
17	8	0	7.113929	2.245073	2.911183
18	8	0	7.87067	3.390269	1.066008
19	8	0	7.113917	-2.245085	-2.911184
20	8	0	7.870655	-3.390293	-1.066017
21	8	0	-7.718341	-4.001258	1.07076
22	8	0	-7.695144	-3.202735	-1.083565
23	8	0	-7.718323	4.001272	-1.070759
24	8	0	-7.695126	3.202748	1.083566
25	6	0	8.528656	1.959729	2.850944
26	1	0	9.0076	2.490355	3.681182
27	6	0	8.927459	2.490407	1.44548
28	1	0	9.870811	3.045566	1.425128
29	6	0	8.861954	-0.438618	-2.879839
30	6	0	8.528647	-1.959748	-2.85094

31	1	0	9.007589	-2.490376	-3.681179
32	6	0	8.927442	-2.490434	-1.445477
33	1	0	9.870773	-3.045581	-1.425128
34	6	0	8.861954	0.438597	2.879843
35	6	0	7.815938	0.378212	-3.653132
36	1	0	6.823028	0.267159	-3.213155
37	1	0	7.763984	0.050307	-4.696509
38	1	0	8.081369	1.440284	-3.650897
39	6	0	10.256064	-0.247951	-3.52131
40	1	0	10.569165	0.798044	-3.450016
41	1	0	10.238462	-0.525065	-4.581046
42	1	0	11.018509	-0.854971	-3.021231
43	6	0	10.256065	0.247922	3.521309
44	1	0	11.018511	0.854937	3.021226
45	1	0	10.56916	-0.798075	3.450014
46	1	0	10.238468	0.525036	4.581045
47	6	0	7.815936	-0.378226	3.653141
48	1	0	7.763986	-0.050317	4.696517
49	1	0	8.081364	-1.440299	3.65091
50	1	0	6.823026	-0.267172	3.214167
51	6	0	1.573538	-7.109603	0.99817
52	6	0	0.432332	-8.099183	1.353599
53	6	0	-0.869567	-7.268973	1.221148
54	6	0	-9.009419	-3.400262	0.906909
55	1	0	-9.761051	-4.183974	1.044636
56	6	0	-8.984645	-2.819767	-0.544879
57	1	0	-9.753567	-3.233195	-1.205195
58	6	0	-9.258287	2.207862	-1.894932
59	6	0	-9.009404	3.400281	-0.906905
60	1	0	-9.761033	4.183996	-1.04463
61	6	0	-8.98463	2.819786	0.544883
62	1	0	-9.753548	3.233218	1.205201
63	6	0	-9.258295	-2.207842	1.894936
64	6	0	-8.276873	2.202649	-3.078098
65	1	0	-7.241578	2.122824	-2.742389
66	1	0	-8.370213	3.122368	-3.663291
67	1	0	-8.491783	1.35885	-3.74179
68	6	0	-10.70813	2.291011	-2.426255
69	1	0	-10.948833	1.412972	-3.033448
70	1	0	-10.840089	3.181949	-3.050139
71	1	0	-11.433684	2.33598	-1.606914
72	6	0	-10.708138	-2.290984	2.426261

73	1	0	-11.433693	-2.335949	1.606922
74	1	0	-10.948836	-1.412943	3.033456
75	1	0	-10.8401	-3.181921	3.050146
76	6	0	-8.276879	-2.202633	3.078101
77	1	0	-8.370223	-3.122351	3.663294
78	1	0	-8.491784	-1.358833	3.741793
79	1	0	-7.241584	-2.122814	2.74239
80	6	0	-0.869549	7.268975	-1.22115
81	6	0	0.432348	8.099189	-1.353599
82	6	0	1.573556	7.109612	-0.99817
83	5	0	6.806707	3.120884	1.896896
84	5	0	6.806689	-3.120901	-1.896903
85	5	0	-6.996066	-3.835002	-0.08665
86	5	0	-6.996047	3.835012	0.08665
87	6	0	-9.082479	-1.327147	-0.366038
88	6	0	-9.082471	1.327167	0.366042
89	6	0	-9.123134	-0.9845	0.992421
90	6	0	-9.101367	-0.358759	-1.369913
91	6	0	-9.123131	0.98452	-0.992417
92	6	0	-9.101363	0.358779	1.369917
93	1	0	-9.092695	-0.651273	-2.41653
94	1	0	-9.092688	0.651292	2.416534
95	6	0	-5.512986	-4.297389	-0.182487
96	6	0	-2.784805	-5.03179	-0.159726
97	6	0	-4.63812	-3.773305	-1.147952
98	6	0	-5.003619	-5.189143	0.782986
99	6	0	-3.666662	-5.561773	0.798138
100	6	0	-3.291548	-4.129528	-1.126416
101	1	0	-5.007946	-3.070964	-1.888615
102	1	0	-5.67128	-5.575034	1.546588
103	1	0	-3.303779	-6.227081	1.569182
104	6	0	5.408276	-3.761017	-1.662639
105	6	0	2.886067	-4.913332	-1.086138
106	6	0	4.265845	-3.331954	-2.354141
107	6	0	5.268964	-4.769263	-0.686567
108	6	0	4.039678	-5.344084	-0.402612
109	6	0	3.022316	-3.885739	-2.051816
110	1	0	4.348154	-2.549548	-3.102431
111	1	0	6.147555	-5.096873	-0.140376
112	1	0	3.97355	-6.114416	0.351494
113	6	0	8.953266	-1.242888	-0.591524
114	6	0	8.953281	1.242864	0.591528

115	6	0	8.919107	-0.093066	-1.392695
116	6	0	8.941467	-1.170595	0.801002
117	6	0	8.919103	0.093043	1.392698
118	6	0	8.941488	1.170571	-0.800998
119	1	0	8.910129	-2.078251	1.397273
120	1	0	8.910165	2.078228	-1.397269
121	6	0	5.408294	3.761002	1.66263
122	6	0	2.886088	4.913326	1.086129
123	6	0	5.268984	4.769245	0.686554
124	6	0	4.265863	3.331946	2.354134
125	6	0	3.022335	3.885734	2.051809
126	6	0	4.0397	5.34407	0.402599
127	1	0	6.147576	5.096849	0.14036
128	1	0	4.34817	2.549542	3.102427
129	1	0	3.973575	6.114399	-0.35151
130	6	0	-5.512965	4.297394	0.182485
131	6	0	-2.784784	5.031791	0.159722
132	6	0	-4.638099	3.773305	1.147947
133	6	0	-5.003599	5.189151	-0.782986
134	6	0	-3.666641	5.561778	-0.798139
135	6	0	-3.291526	4.129526	1.126409
136	1	0	-5.007924	3.070962	1.888607
137	1	0	-5.671261	5.575046	-1.546585
138	1	0	-3.303758	6.22709	-1.569181
139	6	0	0.928584	-6.130064	0.053914
140	6	0	1.503756	-5.306991	-0.868663
141	6	0	-0.519149	-6.163601	0.26076
142	6	0	-1.348632	-5.234444	-0.28433
143	6	0	0.528734	-4.673711	-1.8833
144	6	0	-0.693287	-4.116816	-1.111647
145	6	0	-0.33037	-2.973001	-0.129611
146	1	0	0.415531	-3.312673	0.595074
147	1	0	-1.223773	-2.662882	0.415855
148	1	0	0.069585	-2.112313	-0.665825
149	6	0	0.168754	-5.75143	-2.935091
150	1	0	-0.449321	-5.331029	-3.729457
151	1	0	-0.375642	-6.578466	-2.472374
152	1	0	1.086619	-6.143115	-3.37873
153	6	0	-1.348611	5.234445	0.284325
154	6	0	-0.693264	4.116815	1.111638
155	6	0	-0.519129	6.163604	-0.260763
156	6	0	0.928605	6.130068	-0.053918

157	6	0	1.503778	5.306991	0.868656
158	6	0	0.528756	4.673712	1.883293
159	6	0	0.168773	5.751433	2.935081
160	1	0	-0.449302	5.331033	3.729447
161	1	0	-0.375624	6.578467	2.472361
162	1	0	1.086637	6.14312	3.37872
163	6	0	-0.330344	2.973005	0.129599
164	1	0	-1.223746	2.662886	-0.41587
165	1	0	0.069611	2.112315	0.66581
166	1	0	0.415558	3.31268	-0.595083

4b E = –6499.787110 (au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.327932	-4.2053	-1.809742
2	16	0	1.214244	-4.208297	-2.19635
3	16	0	2.327907	4.205122	-1.80981
4	16	0	-1.214165	4.207781	-2.196374
5	9	0	-1.368203	-4.150651	3.975553
6	9	0	-2.226871	-6.111574	3.485764
7	9	0	0.334534	-5.765699	5.113669
8	9	0	0.011521	-7.330143	3.599793
9	9	0	2.236235	-6.406702	2.746854
10	9	0	1.871261	-4.398567	3.552486
11	9	0	2.226833	6.112051	3.485412
12	9	0	1.368245	4.151194	3.975607
13	9	0	-0.011552	7.330584	3.599373
14	9	0	-0.334601	5.766304	5.113407
15	9	0	-2.236219	6.407071	2.746363
16	9	0	-1.871379	4.399062	3.552373
17	8	0	-6.687965	3.387857	-2.987243
18	8	0	-7.697757	3.664868	-0.941347
19	8	0	-8.146848	-3.033668	1.029245
20	8	0	-7.852515	-3.202006	-1.243902
21	8	0	6.68793	-3.387965	-2.98716
22	8	0	7.697734	-3.664873	-0.941252
23	8	0	8.146879	3.033655	1.029175
24	8	0	7.852568	3.201867	-1.243979
25	6	0	-8.081192	3.136506	-3.239203
26	1	0	-8.456731	3.945171	-3.875441

27	6	0	-8.710545	3.114032	-1.811558
28	1	0	-9.612315	3.72538	-1.707286
29	6	0	-9.833288	-1.188021	0.925326
30	6	0	-9.408709	-2.622601	0.475801
31	1	0	-10.157352	-3.366688	0.767381
32	6	0	-9.140502	-2.572962	-1.061575
33	1	0	-9.870311	-3.12498	-1.662158
34	6	0	-8.337764	1.740266	-3.88439
35	6	0	-9.189997	-0.77189	2.256897
36	1	0	-8.100729	-0.778708	2.192355
37	1	0	-9.484717	-1.455172	3.059682
38	1	0	-9.515946	0.234367	2.539636
39	6	0	-11.374026	-1.142186	1.052875
40	1	0	-11.713502	-0.120803	1.25
41	1	0	-11.713912	-1.778172	1.877723
42	1	0	-11.86478	-1.481259	0.134117
43	6	0	-9.586663	1.834399	-4.792312
44	1	0	-10.449814	2.237203	-4.251438
45	1	0	-9.864713	0.844133	-5.165723
46	1	0	-9.391657	2.480407	-5.655489
47	6	0	-7.139323	1.237368	-4.702853
48	1	0	-6.908624	1.931578	-5.517235
49	1	0	-7.364647	0.263652	-5.150001
50	1	0	-6.247382	1.136563	-4.08245
51	6	0	-1.152577	-5.301488	3.267709
52	6	0	0.129169	-5.993773	3.803152
53	6	0	1.277031	-5.454702	2.911785
54	6	0	8.081157	-3.136617	-3.239141
55	1	0	8.456674	-3.945291	-3.875377
56	6	0	8.710543	-3.114117	-1.811511
57	1	0	9.61227	-3.72552	-1.70722
58	6	0	9.833285	1.187954	0.92532
59	6	0	9.408732	2.622541	0.475769
60	1	0	10.157402	3.366597	0.76736
61	6	0	9.140574	2.572873	-1.06162
62	1	0	9.870376	3.124915	-1.662191
63	6	0	8.337748	-1.740395	-3.884361
64	6	0	9.189913	0.771857	2.25686
65	1	0	8.100648	0.778595	2.192218
66	1	0	9.48451	1.45521	3.059627
67	1	0	9.515892	-0.234362	2.539704
68	6	0	11.374019	1.142129	1.052937

69	1	0	11.713504	0.120742	1.250016
70	1	0	11.713861	1.778072	1.877838
71	1	0	11.864799	1.481274	0.134221
72	6	0	9.586648	-1.834581	-4.792284
73	1	0	10.449797	-2.237368	-4.251394
74	1	0	9.864709	-0.844336	-5.165741
75	1	0	9.391633	-2.480631	-5.655428
76	6	0	7.139328	-1.237492	-4.702852
77	1	0	6.908636	-1.931733	-5.517208
78	1	0	7.364684	-0.2638	-5.150039
79	1	0	6.247381	-1.136637	-4.082469
80	6	0	1.152563	5.301886	3.267537
81	6	0	-0.129209	5.994242	3.802866
82	6	0	-1.277062	5.455059	2.911536
83	5	0	-6.526792	3.704781	-1.659653
84	5	0	-7.296397	-3.362865	0.001945
85	5	0	6.526768	-3.704843	-1.659544
86	5	0	7.296425	3.362775	0.001828
87	6	0	8.939758	-1.64659	-1.534927
88	6	0	9.08568	1.099727	-1.3839
89	6	0	8.657884	-0.873049	-2.669873
90	6	0	9.319171	-1.065791	-0.324989
91	6	0	9.3967	0.326246	-0.257224
92	6	0	8.724098	0.518546	-2.599249
93	1	0	9.522181	-1.68668	0.543229
94	1	0	8.477855	1.140725	-3.455365
95	6	0	5.136867	-4.030149	-1.04244
96	6	0	2.583981	-4.454976	0.098178
97	6	0	3.991517	-4.010634	-1.854686
98	6	0	4.985287	-4.27037	0.337573
99	6	0	3.734971	-4.478411	0.907172
100	6	0	2.737644	-4.222086	-1.29065
101	1	0	4.089026	-3.812091	-2.917333
102	1	0	5.865397	-4.268749	0.972913
103	1	0	3.651151	-4.628822	1.974615
104	6	0	-5.833905	-3.834905	0.243192
105	6	0	-3.138838	-4.568051	0.726761
106	6	0	-4.917897	-3.887133	-0.817301
107	6	0	-5.383802	-4.154156	1.540465
108	6	0	-4.067461	-4.519045	1.7856
109	6	0	-3.589555	-4.228677	-0.573033
110	1	0	-5.241037	-3.631912	-1.821795

111	1	0	-6.084019	-4.105329	2.368306
112	1	0	-3.759692	-4.757089	2.793317
113	6	0	-9.085589	-1.09982	-1.383864
114	6	0	-8.939716	1.646498	-1.534939
115	6	0	-9.396647	-0.326325	-0.257207
116	6	0	-8.724046	-0.518654	-2.599227
117	6	0	-8.657854	0.872945	-2.669877
118	6	0	-9.319144	1.065712	-0.324998
119	1	0	-8.477822	-1.140842	-3.455342
120	1	0	-9.522182	1.68662	0.543201
121	6	0	-5.136858	4.03012	-1.042623
122	6	0	-2.583992	4.454938	0.098068
123	6	0	-4.985325	4.270522	0.337356
124	6	0	-3.991462	4.010406	-1.854803
125	6	0	-2.737612	4.221853	-1.29074
126	6	0	-3.735008	4.478564	0.90699
127	1	0	-5.865452	4.269109	0.972672
128	1	0	-4.088897	3.811717	-2.917431
129	1	0	-3.651235	4.629102	1.974419
130	6	0	5.833919	3.8348	0.243024
131	6	0	3.138848	4.567977	0.726685
132	6	0	4.917848	3.886939	-0.81741
133	6	0	5.383876	4.154171	1.540297
134	6	0	4.06754	4.519082	1.785459
135	6	0	3.58953	4.228526	-0.573109
136	1	0	5.240919	3.631583	-1.821895
137	1	0	6.084125	4.105427	2.368112
138	1	0	3.759821	4.757166	2.793184
139	6	0	-0.850781	-5.039716	1.815974
140	6	0	-1.708466	-4.83138	0.77597
141	6	0	0.602219	-5.033292	1.633658
142	6	0	1.186513	-4.599473	0.484443
143	6	0	-1.0634	-4.896233	-0.624452
144	6	0	0.241941	-4.066203	-0.605685
145	6	0	1.708475	4.831331	0.775897
146	6	0	1.063382	4.896054	-0.624508
147	6	0	0.850775	5.039832	1.815857
148	6	0	-0.602224	5.033416	1.633503
149	6	0	-1.186516	4.599422	0.484359
150	6	0	-0.241927	4.065971	-0.605648
151	6	0	0.85534	6.388022	-0.985439
152	1	0	1.810624	6.912271	-0.912504

153	1	0	0.146368	6.858811	-0.29989
154	1	0	0.477467	6.4943	-2.003146
155	6	0	-0.012873	2.559278	-0.317264
156	1	0	0.5887	2.099963	-1.101936
157	1	0	-0.977083	2.049263	-0.270259
158	1	0	0.496566	2.424188	0.641228
159	6	0	0.012914	-2.559452	-0.317605
160	1	0	0.977133	-2.049449	-0.270623
161	1	0	-0.496611	-2.424149	0.640808
162	1	0	-0.58857	-2.10028	-1.102433
163	6	0	-0.855445	-6.38822	-0.985352
164	1	0	-0.146552	-6.859052	-0.299757
165	1	0	-0.477525	-6.494528	-2.003037
166	1	0	-1.810771	-6.912396	-0.912474

4c E = –6499.787294 (au)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.348974	4.191827	-2.21927
2	16	0	2.190082	4.243978	-1.803821
3	16	0	1.387347	-4.284051	-2.237207
4	16	0	-2.143286	-4.156576	-1.759972
5	9	0	-2.445251	6.366677	2.717221
6	9	0	-2.055347	4.36379	3.52436
7	9	0	-0.242131	7.324138	3.588732
8	9	0	-0.553287	5.753995	5.099192
9	9	0	1.183215	4.165867	3.974011
10	9	0	2.016084	6.14003	3.49289
11	9	0	1.872335	-4.195159	3.603848
12	9	0	2.484627	-6.196515	2.939432
13	9	0	0.416988	-5.714128	5.141236
14	9	0	0.293375	-7.301366	3.621862
15	9	0	-1.395555	-4.290909	3.980945
16	9	0	-2.027362	-6.28259	3.31042
17	8	0	-8.011983	-3.123151	1.080981
18	8	0	-7.717414	-3.34381	-1.187741
19	8	0	-6.795871	3.22765	-3.041858
20	8	0	-7.827858	3.507984	-1.007509
21	8	0	8.009796	3.16969	1.074741

22	8	0	7.727113	3.350917	-1.199059
23	8	0	6.810844	-3.277483	-3.020455
24	8	0	7.832257	-3.545573	-0.978892
25	6	0	-9.295795	-2.796447	0.521554
26	1	0	-10.002089	-3.572904	0.833974
27	6	0	-9.0323	-2.769933	-1.017038
28	1	0	-9.737352	-3.367184	-1.603692
29	6	0	-8.388754	1.516695	-3.92158
30	6	0	-8.17935	2.930843	-3.298832
31	1	0	-8.574245	3.717032	-3.951303
32	6	0	-8.817706	2.912888	-1.875076
33	1	0	-9.738348	3.497949	-1.786432
34	6	0	-9.796064	-1.376353	0.935886
35	6	0	-7.172017	1.039619	-4.728197
36	1	0	-6.279312	0.979308	-4.103689
37	1	0	-6.961937	1.727004	-5.553879
38	1	0	-7.363571	0.051485	-5.159161
39	6	0	-9.637099	1.556267	-4.834359
40	1	0	-9.88241	0.551829	-5.192447
41	1	0	-9.459518	2.194259	-5.707192
42	1	0	-10.5144	1.940212	-4.302597
43	6	0	-11.338395	-1.406074	1.048069
44	1	0	-11.802443	-1.787613	0.132112
45	1	0	-11.73065	-0.399385	1.221618
46	1	0	-11.653983	-2.041979	1.882596
47	6	0	-9.189064	-0.900061	2.264216
48	1	0	-9.456567	-1.580701	3.078705
49	1	0	-9.570156	0.09337	2.521998
50	1	0	-8.100344	-0.851469	2.209813
51	6	0	-1.472606	5.42979	2.889357
52	6	0	-0.340664	5.985982	3.790519
53	6	0	0.956004	5.313958	3.26528
54	6	0	9.2865	2.798641	0.526564
55	1	0	10.011697	3.560801	0.830469
56	6	0	9.030774	2.756913	-1.013051
57	1	0	9.748936	3.336113	-1.60207
58	6	0	8.38959	-1.546039	-3.891175
59	6	0	8.192112	-2.960999	-3.26673
60	1	0	8.602801	-3.743285	-3.914162
61	6	0	8.81834	-2.932928	-1.83805
62	1	0	9.747496	-3.503487	-1.743027
63	6	0	9.750005	1.372453	0.965067

64	6	0	7.169771	-1.081678	-4.700745
65	1	0	6.275354	-1.030079	-4.077867
66	1	0	6.968286	-1.771623	-5.526414
67	1	0	7.352242	-0.091796	-5.131581
68	6	0	9.63997	-1.575335	-4.801435
69	1	0	9.876592	-0.569299	-5.160845
70	1	0	9.470063	-2.216514	-5.67344
71	1	0	10.519735	-1.950174	-4.267237
72	6	0	11.289499	1.373417	1.112884
73	1	0	11.781475	1.737432	0.204376
74	1	0	11.658386	0.361189	1.304423
75	1	0	11.598194	2.011057	1.948638
76	6	0	9.102676	0.920471	2.283098
77	1	0	9.365582	1.602442	3.097925
78	1	0	9.456054	-0.07869	2.557727
79	1	0	8.014639	0.894382	2.204191
80	6	0	1.431576	-5.331798	2.983066
81	6	0	0.287751	-5.959834	3.824171
82	6	0	-1.017855	-5.373019	3.228449
83	5	0	-7.148223	-3.436516	0.059575
84	5	0	-6.652913	3.567943	-1.718029
85	5	0	7.158806	3.487523	0.044227
86	5	0	6.665557	-3.630341	-1.700153
87	6	0	9.023457	1.286572	-1.351358
88	6	0	8.981325	-1.46109	-1.538313
89	6	0	9.35483	0.51086	-0.232126
90	6	0	8.688568	0.70811	-2.575556
91	6	0	8.673892	-0.683898	-2.664099
92	6	0	9.33109	-0.882202	-0.318574
93	1	0	8.424373	1.331911	-3.425128
94	1	0	9.553674	-1.506604	0.542328
95	6	0	5.684894	3.927083	0.277136
96	6	0	2.97411	4.613531	0.740116
97	6	0	4.776927	3.966795	-0.790818
98	6	0	5.218536	4.23359	1.571726
99	6	0	3.894224	4.575722	1.806789
100	6	0	3.441028	4.284973	-0.55674
101	1	0	5.112999	3.720784	-1.793358
102	1	0	5.912577	4.193983	2.40525
103	1	0	3.573752	4.805129	2.812555
104	6	0	-5.275672	3.932352	-1.094252
105	6	0	-2.740545	4.410374	0.064908

106	6	0	-4.124273	3.9366	-1.898171
107	6	0	-5.139348	4.178046	0.286396