Supporting Information

Stereoisomerism in nanohoops with heterogeneous biaryl linkages of *E/Z*- and *R/S*-geometries

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General

All the reactions were preformed in N_2 atmosphere expect otherwise noted. Flash silica gel column chromatography was performed on silica gel 60N (spherical and neutral gel, 40-50 μm, Kanto). GPC was performed on Japan Analytical Industry LC-9104 with JAIGEL 1H, 2H and 2.5H polystyrene columns with eluent of $CHCl_3$. Columns for HPLC are specified in the corresponding sections. Proton (^{1}H) and carbon (^{13}C) NMR spectra were recorded on a JEOL JNM-ECA II 600

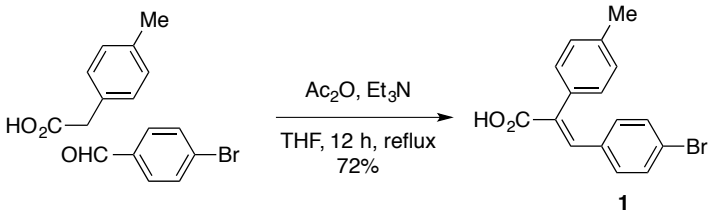
(^{1}H: 600 MHz; ^{13}C: 150 MHz) spectrometer. DEPT spectra were recorded for the assignment of CH, and CH_3. Chemical shift values were given in ppm relative to internal chloroform (^{1}H NMR: δ 7.26, ^{13}C NMR: δ 77.16), 1,1,2,2,-tetrachloroethane (^{1}H NMR: δ 5.91, ^{13}C NMR: δ 74.08), DMSO (^{1}H NMR: δ 2.50, ^{13}C NMR: δ 39.51) and toluene (^{1}H NMR: δ 2.08). High-resolution MALDI TOF MS analyses were performed on a Bruker Daltonics solariX 9.4T instrument using tetracyanoquinodimethane as the matrix. CD spectroscopy was performed on a JASCO J-1500 circular dichroism spectrometer.

Materials

Acetic anhydride, triethylamine, *p*-bromobenzaldehyde, cesium fluoride, iodine, triphenylphosphine, potassium acetate and copper(II) bromide were purchased from Wako. 1,3-Diiodo-5,5-dimethylhydantoin, *p*-tolylacetic acid, $PdCl_2(dppf)•CH_2Cl_2$, bis(pinacolato)diboron and *n*-butyllithium in hexane were purchased from TCI. Nitrobenzene, *o*-dichlorobenzene and cyclohexane were purchased from Kanto. 1,4-Dioxane was purchased from Nacalai. Anhydrous 1,2-dichloroethane was purchased from Aldrich. $PtCl_2(cod)$ was synthesized as reported in literature.[1] Anhydrous THF (stabilizer free, Kanto) was purified by a solvent purification system (GlassContour) equipped with columns of activated alumina and supported copper catalyst (Q-5).[2] Other solvents were distilled and dried over 4-Å molecular sieves.

Synthesis

Compound **1**

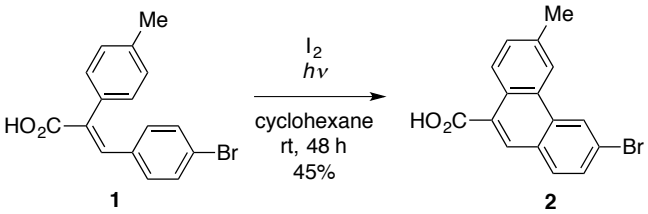


A mixture of *p*-bromobenzaldehyde (12.4 g, 66.6 mmol), *p*-tolylacetic acid (10.0 g, 66.6 mmol), triethylamine (33.6 g, 333 mmol) and acetic anhydride (67.6 g, 666 mmol) was refluxed in THF (320 mL) for 12 h. After removal of volatile materials in vacuo, the residue was dissolved in 20% aqueous potassium hydroxide (500 mL). Dropwise addition of conc. hydrochloric acid (250 mL) afforded crude materials as precipitates. The precipitates were filtered, dried in air and recrystallized from ethanol to afford compound **1** in 72% yield (15.3 g, 48.0 mmol). ^{1}H NMR (600

(1) McDermott, J. X.; White, J. F.; Whitesides, G. M. Thermal decomposition of bis(phosphine)platinum(II) metallocycles. *J. Am. Chem. Soc.* **1976**, *98*, 6521-6528.
(2) Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. Safe and convenient procedure for solvent purification. *Organometallics* **1996**, *15*, 1518-1520.

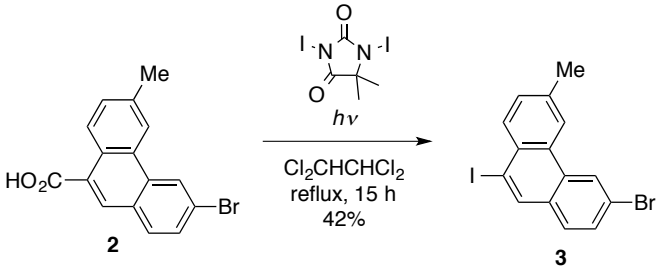
MHz, $CDCl_3$) δ 2.39 (s, 3H), 6.95 (d, J = 8.6 Hz, 2H), 7.10 (d, J = 8.2 Hz, 2H), 7.19 (d, J = 8.2 Hz, 2H), 7.31 (d, J = 8.6 Hz, 2H), 7.83 (s, 1H) ppm, ^{13}C NMR (150 MHz, $CDCl_3$) δ 21.5 (CH_3), 124.4, 129.6 (CH), 129.9 (CH), 131.5, 131.8 (CH), 132.3, 132.4 (CH), 133.2, 138.4, 142.3 (CH), 163.5 ppm. HRMS calcd for $C_{16}H_{13}BrO_2$ $[M]^+$ 316.0093, found 316.0093.

Compound **2**



A mixture of compound **1** (10.0 g, 31.6 mmol) and iodine (200 mg, 1.58 mmol) in cyclohexane (2.2 L) was irradiated with 400 W Hg-lamp at room temperature for 48 h under air. Precipitates formed during the reaction was obtained by filtration and washed with hot ethyl acetate (500 mL) to afford analytically pure compound **2** in 45% yield (4.48 g, 14.2 mmol). ^{1}H NMR (600 MHz, DMSO-d_6) δ 2.60 (s, 3H), 7.59 (d, J = 8.3 Hz, 1H), 7.83 (d, J = 8.3 Hz, 1H), 8.09 (d, J = 8.3 Hz, 1H), 8.43 (s, 1H), 8.74 (m, 2H) 9.07 (s, 1H) ppm, ^{13}C NMR (150 MHz, DMSO-d_6) δ 21.1 (CH_3), 122.6 (CH), 123.1, 125.4 (CH), 126.0 (CH), 126.6, 127.4, 128.6, 129.2, 129.5 (CH), 129.6 (CH), 130.0 (CH), 131.7 (CH), 132.5, 136.9, 168.4 ppm. HRMS calcd for $C_{16}H_{11}BrO_2$ $[M]^+$ 313.9937, found 313.9937.

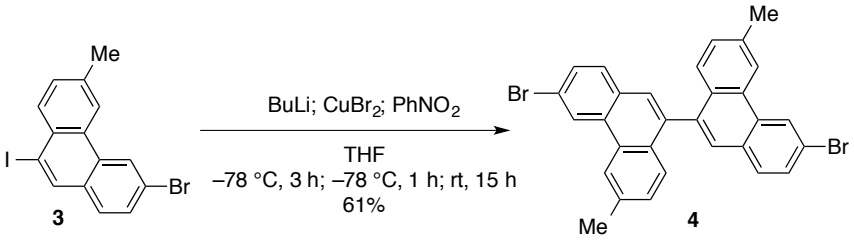
Compound **3**



A mixture of compound **2** (1.50 g, 4.76 mmol) and 1,3-diiodo-5,5-dimethylhydantoin (2.71 g, 7.14 mmol) in dichloroethane (160 mL) was irradiated with 100 W tungsten-lamp under reflux conditions for 15 h. The crude mixture was washed with saturated aqueous $Na_2S_2O_3$ and brine and purified by silica gel column chromatography and subsequent GPC to afford compound **3** in 42% yield (794 mg, 2.0 mmol). ^{1}H NMR (600 MHz, $CDCl_3$) δ 2.65 (s, 3H), 7.52 (dd, J = 1.4 Hz, 8.6 Hz, 1H), 7.62 (d, J = 8.6 Hz, 1H), 7.67 (dd, J =1.4 Hz, 8.6 Hz, 1H), 8.10 (d, J = 8.6 Hz, 1H), 8.31 (m, 2H) 8.77 (d, J =1.4 Hz, 1H) ppm, ^{13}C NMR (150 MHz, $CDCl_3$) δ 21.9 (CH_3), 99.2, 121.4, 122.7

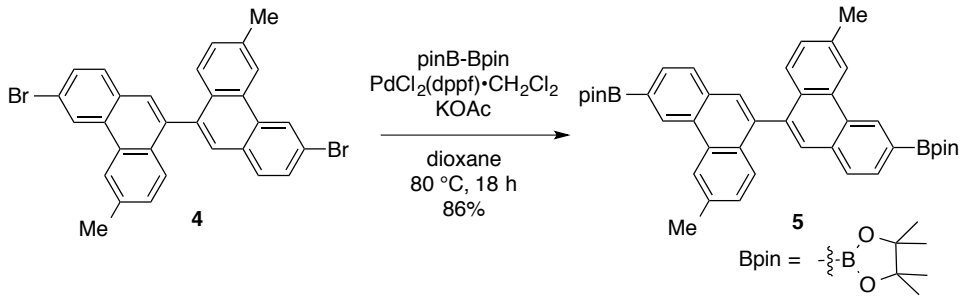
(CH), 125.7 (CH), 129.1 (CH), 129.5, 130.3 (2 CH), 130.5, 131.6, 131.7, 133.3 (CH), 137.0 (CH), 138.0 ppm. HRMS calcd for $C_{15}H_{10}BrI$ $[M]^+$ 395.9005, found 395.9005.

Compound **4**



To a solution of compound **3** (650 mg, 1.64 mmol) in THF (33 mL) was added *n*-butyllithium (1.54 M; 1.2 mL, 1.80 mmol) dropwise at –78 °C. After 3 h, $CuBr_2$ (366 mg, 1.64 mmol) was added, and the mixture was stirred for 1 h at –78 °C. Nitrobenzene (0.84 mL, 8.20 mmol) was added to the mixture. The mixture was warmed to room temperature and stirred for 15 h. After addition of water (20 mL), the crude mixture was diluted with $CHCl_3$ (200 mL) and washed with brine. Purification with silica gel column chromatography afforded compound **4** in 61% yield (270 mg, 0.50 mmol). For kinetic analysis of the racemization, enantiomers were separated by HPLC using Daicel Chiralpack AD column (20 ϕ × 250 mm) with 50% MeOH in $CHCl_3$ as eluent. ^{1}H NMR (600 MHz, $C_2D_2Cl_4$) δ 2.53 (s, 6H), 7.16 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.3 Hz, 2H), 7.66 (m, 4H), 7.70 (d, *J* = 8.3 Hz, 2H), 8.42 (s, 2H) 8.83 (s, 2H) ppm, ^{13}C NMR (150 MHz, $C_2D_2Cl_4$) δ 22.2 (CH_3), 121.0, 122.7 (CH), 125.6 (CH), 127.0 (CH), 127.6 (CH), 129.33 (CH), 129.37, 130.2 (CH), 130.3, 130.4 (1 CH, 2 carbons), 131.5, 137.2, 137.5 ppm. HRMS calcd for $C_{30}H_{20}Br_2$ $[M]^+$ 539.9906, found 539.9905.

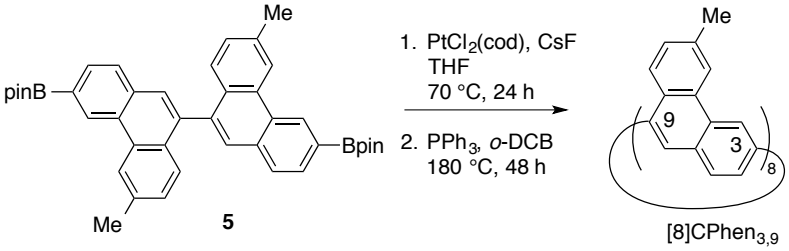
Compound **5**



A mixture of compound **4** (222 mg, 0.41 mmol), $PdCl_2(dppf)•CH_2Cl_2$ (67 mg, 0.08 mmol), bis(pinacolato)diboron (313 mg, 1.23 mmol) and potassium acetate (201 mg, 2.05 mmol) in 1,4-dioxane (20.5 mL) was stirred at 80 °C for 18 h. After addition of water (200 mL), the crude mixture was diluted with $CHCl_3$ (200 mL) and washed with brine. Purification with silica gel column chromatography afforded compound **5** in 86% yield (224 mg, 0.35 mmol). ^{1}H NMR (600

MHz, $CDCl_3$) δ 1.46 (s, 24H) 2.61 (s, 6H), 7.20 (d, *J* = 7.3 Hz, 2H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.76 (s, 2H), 7.87 (d, *J* = 8.2 Hz, 2H), 8.02 (d, *J* = 7.3 Hz, 2H), 8.74 (s, 2H) 9.25 (s, 2H) ppm, ^{13}C NMR (150 MHz, $CDCl_3$) δ 22.1 (CH_3), 25.1 (CH_3), 84.2, 123.0 (CH), 127.5 (2 CH), 128.0 (CH), 128.5 (CH), 129.4, 130.17 (CH), 130.24, 130.8, 132.2 (CH), 134.0, 136.6, 138.6 ppm. HRMS calcd for $C_{42}H_{44}B_2O_4$ $[M]^+$ 633.3456, found 633.3457.

[8]CPhen$_{3,9}$



A mixture of compound **5** (97 mg, 0.153 mmol), $PtCl_2$(cod) (57 mg, 0.153 mmol) and CsF (139 mg, 0.917 mmol) in THF (7.7 mL) was refluxed for 24 h. After addition of water (20 mL), the precipitates were obtained by filtration and washed with MeOH (20 mL). The crude Pt-complex was dissolved in *o*-DCB (7.7 mL), and PPh_3 (401 mg, 1.53 mmol) was added. The mixture was stirred at 180 °C for 48 h. After addition of MeOH (50 mL), precipitates were collected and washed with MeOH. The crude material was dissolved in $CHCl_3$ (100 mL) and filtered through a pad of silica gel (5 g). The filtrate was purified by GPC. Contaminants of plasticizers were removed by washing the solid material with 1:1 CH_2Cl_2/*n*-hexane (200 mL) to afford [8]CPhen$_{3,9}$ in 5% yield (2.9 mg, 1.9 μmol). The purity of the product was confirmed by analytical HPLC using two different columns (Cosmosil BuckyPrep: 4.6ϕ, 250 mm and Cosmosil πNAP: 4.6ϕ, 250 mm). For kinetic analysis of the racemization, enantiomers were separated by HPLC using Cosmosil Cholester (50ϕ, 250+250 mm) with 30% MeOH in $CHCl_3$ as eluent. ^1H NMR (600 MHz, toluene-d_8) δ 2.50 (s, 24H), 7.32 (d, *J* = 8.9 Hz, 8H), 7.37 (d, *J* = 8.9 Hz, 8H), 7.41 (s, 8H), 7.46 (d, *J* = 8.9 Hz, 8H), 8.57 (d, *J* = 8.9 Hz, 8H), 8.59 (s, 8H), 9.05 (s, 8H) ppm, ^{13}C NMR (150 MHz, $C_2D_2Cl_4$) δ 22.3 (CH_3), 120.6 (CH), 123.6 (CH), 127.4 (CH), 128.3 (CH), 128.8 (CH), 128.9 (CH), 129.0 (CH), 129.7, 130.8, 130.9, 132.6, 136.9, 137.1, 139.0 ppm. HRMS calcd for $C_{120}H_{80}$ $[M]^+$ 1520.6255, found 1520.6253.

Crystallographic analysis

A single crystal (ca. 0.10 × 0.07 × 0.01 mm^3) suitable for X-ray analysis was obtained from slow diffusion of pentane into *o*-DCB solution of [8]CPhen$_{3,9}$. A single crystal was mounted on a thin polymer tip with cryoprotectant oil and frozen at –178 °C via flash-cooling. The diffraction analysis of a single crystal with a synchrotron X-ray source was conducted at –178 °C at the beamline

PF-AR NE3A at the KEK Photon Factory using a diffractometer equipped with a Dectris PILATUS 2M-F PAD detector. The collected diffraction data were processed with the CrysAlisPro software program.[3] The structures were solved by direct method using the SHELXT software program[4] and refined by full-matrix least-squares on F^2 using the SHELX program suite[5] running on the Yadokari-XG 2009 software program.[6] In the refinements, [8]CPhen$_{3,9}$ molecules were restrained by SIMU and DFIX, pentane molecules were restrained by SIMU, DFIX and DANG, and *o*-DCB molecules were restrained by SIMU, DFIX, DANG, FLAT, ISOR and AFIX 66. The non-hydrogen atoms were analyzed anisotropically, and hydrogen atoms were input at calculated positions and refined with a riding model.

Stereoisomers

Stereoisomers of [8]CPhen$_{3,9}$ were counted as follows. All the possible combinations of alternate *E/Z* and *R/S* linkages in the hoop were listed as shown in Table S1. The strings of the letters were examined, and the overlapping strings were removed from counting.

Table S1. Possible combinations of biaryl geometries for counting of [8]CPhen$_{3,9}$ stereoisomers[a,b]

	x,*R*,*x*,*R*,*x*,*R*,*x*,*R*	*x*,*R*,*x*,*R*,*x*,*R*,*x*,*S*	*x*,*R*,*x*,*S*,*x*,*R*,*x*,*S*	*x*,*R*,*x*,*R*,*x*,*S*,*x*,*S*	*x*,*R*,*x*,*S*,*x*,*S*,*x*,*S*	*x*,*S*,*x*,*S*,*x*,*S*,*x*,*S*
E,*y*,*E*,*y*,*E*,*y*,*E*,*y*	*E*,*R*,*E*,*R*,*E*,*R*,*E*,*R** (*E*,*R*,*E*,*R*,*E*,*R*,*E*,*R*) (*E*,*R*,*E*,*R*,*E*,*R*,*E*,*R*) (*E*,*R*,*E*,*R*,*E*,*R*,*E*,*R*)	*E*,*R*,*E*,*R*,*E*,*R*,*E*,*S** (*E*,*R*,*E*,*R*,*E*,*R*,*E*,*S*) (*E*,*R*,*E*,*R*,*E*,*R*,*E*,*S*) (*E*,*R*,*E*,*R*,*E*,*R*,*E*,*S*)	*E*,*R*,*E*,*S*,*E*,*R*,*E*,*S* (*E*,*R*,*E*,*S*,*E*,*R*,*E*,*S*) (*E*,*R*,*E*,*S*,*E*,*R*,*E*,*S*) (*E*,*R*,*E*,*S*,*E*,*R*,*E*,*S*)	*E*,*R*,*E*,*R*,*E*,*S*,*E*,*S* (*E*,*R*,*E*,*R*,*E*,*S*,*E*,*S*) (*E*,*R*,*E*,*R*,*E*,*S*,*E*,*S*) (*E*,*R*,*E*,*R*,*E*,*S*,*E*,*S*)	*E*,*R*,*E*,*S*,*E*,*S*,*E*,*S** (*E*,*R*,*E*,*S*,*E*,*S*,*E*,*S*) (*E*,*R*,*E*,*S*,*E*,*S*,*E*,*S*) (*E*,*R*,*E*,*S*,*E*,*S*,*E*,*S*)	*E*,*S*,*E*,*S*,*E*,*S*,*E*,*S** (*E*,*S*,*E*,*S*,*E*,*S*,*E*,*S*) (*E*,*S*,*E*,*S*,*E*,*S*,*E*,*S*) (*E*,*S*,*E*,*S*,*E*,*S*,*E*,*S*)
E,*y*,*E*,*y*,*E*,*y*,*Z*,*y*	*E*,*R*,*E*,*R*,*E*,*R*,*Z*,*R** (*E*,*R*,*E*,*R*,*Z*,*R*,*E*,*R*) (*E*,*R*,*Z*,*R*,*E*,*R*,*E*,*R*) (*Z*,*R*,*E*,*R*,*E*,*R*,*E*,*R*)	*E*,*R*,*E*,*R*,*E*,*R*,*Z*,*S** *E*,*R*,*E*,*R*,*Z*,*R*,*E*,*S** (*E*,*R*,*Z*,*R*,*E*,*R*,*E*,*S*) (*Z*,*R*,*E*,*R*,*E*,*R*,*E*,*S*)	*E*,*R*,*E*,*S*,*E*,*R*,*Z*,*S* (*E*,*R*,*E*,*S*,*Z*,*R*,*E*,*S*) (*E*,*R*,*Z*,*S*,*E*,*R*,*E*,*S*) (*Z*,*R*,*E*,*S*,*E*,*R*,*E*,*S*)	*E*,*R*,*E*,*R*,*E*,*S*,*Z*,*S** *E*,*R*,*E*,*R*,*Z*,*S*,*E*,*S* *E*,*R*,*Z*,*R*,*E*,*S*,*E*,*S** (*Z*,*R*,*E*,*R*,*E*,*S*,*E*,*S*)	*E*,*R*,*E*,*S*,*E*,*S*,*Z*,*S** (*E*,*R*,*E*,*S*,*Z*,*S*,*E*,*S*) *E*,*R*,*Z*,*S*,*E*,*S*,*E*,*S** (*Z*,*R*,*E*,*S*,*E*,*S*,*E*,*S*)	*E*,*S*,*E*,*S*,*E*,*S*,*Z*,*S** (*E*,*S*,*E*,*S*,*Z*,*S*,*E*,*S*) (*E*,*S*,*Z*,*S*,*E*,*S*,*E*,*S*) (*Z*,*S*,*E*,*S*,*E*,*S*,*E*,*S*)
E,*y*,*Z*,*y*,*E*,*y*,*Z*,*y*	*E*,*R*,*Z*,*R*,*E*,*R*,*Z*,*R** (*Z*,*R*,*E*,*R*,*Z*,*R*,*E*,*R*) (*E*,*R*,*Z*,*R*,*E*,*R*,*Z*,*R*) (*Z*,*R*,*E*,*R*,*Z*,*R*,*E*,*R*)	*E*,*R*,*Z*,*R*,*E*,*R*,*Z*,*S** (*Z*,*R*,*E*,*R*,*Z*,*R*,*E*,*S*) (*E*,*R*,*Z*,*R*,*E*,*R*,*Z*,*S*) (*Z*,*R*,*E*,*R*,*Z*,*R*,*E*,*S*)	*E*,*R*,*Z*,*S*,*E*,*R*,*Z*,*S* (*Z*,*R*,*E*,*S*,*Z*,*R*,*E*,*S*) (*E*,*R*,*Z*,*S*,*E*,*R*,*Z*,*S*) (*Z*,*R*,*E*,*S*,*Z*,*R*,*E*,*S*)	*E*,*R*,*Z*,*R*,*E*,*S*,*Z*,*S* *Z*,*R*,*E*,*R*,*Z*,*S*,*E*,*S* (*E*,*R*,*Z*,*R*,*E*,*S*,*Z*,*S*) (*Z*,*R*,*E*,*R*,*Z*,*S*,*E*,*S*)	*E*,*R*,*Z*,*S*,*E*,*S*,*Z*,*S** (*Z*,*R*,*E*,*S*,*Z*,*S*,*E*,*S*) (*E*,*R*,*Z*,*S*,*E*,*S*,*Z*,*S*) (*Z*,*R*,*E*,*S*,*Z*,*S*,*E*,*S*)	*E*,*S*,*Z*,*S*,*E*,*S*,*Z*,*S** (*Z*,*S*,*E*,*S*,*Z*,*S*,*E*,*S*) (*E*,*S*,*Z*,*S*,*E*,*S*,*Z*,*S*) (*Z*,*S*,*E*,*S*,*Z*,*S*,*E*,*S*)
E,*y*,*E*,*y*,*Z*,*y*,*Z*,*y*	*E*,*R*,*E*,*R*,*Z*,*R*,*Z*,*R** (*E*,*R*,*Z*,*R*,*Z*,*R*,*E*,*R*) (*Z*,*R*,*Z*,*R*,*E*,*R*,*E*,*R*) (*Z*,*R*,*E*,*R*,*Z*,*R*,*Z*,*R*)	*E*,*R*,*E*,*R*,*Z*,*R*,*Z*,*S** *E*,*R*,*Z*,*R*,*Z*,*R*,*E*,*S** (*Z*,*R*,*Z*,*R*,*E*,*R*,*E*,*S*) *Z*,*R*,*E*,*R*,*E*,*R*,*Z*,*S**	*E*,*R*,*E*,*S*,*Z*,*R*,*Z*,*S** *E*,*R*,*Z*,*S*,*Z*,*R*,*E*,*S** (*Z*,*R*,*Z*,*S*,*E*,*R*,*E*,*S*) (*Z*,*R*,*E*,*S*,*E*,*R*,*Z*,*S*)	*E*,*R*,*E*,*R*,*Z*,*S*,*Z*,*S** *E*,*R*,*Z*,*R*,*Z*,*S*,*E*,*S** (*Z*,*R*,*Z*,*R*,*E*,*S*,*E*,*S*) (*Z*,*R*,*E*,*R*,*E*,*S*,*Z*,*S*)	*E*,*R*,*E*,*S*,*Z*,*S*,*Z*,*S** *E*,*R*,*Z*,*S*,*Z*,*S*,*E*,*S** *Z*,*R*,*Z*,*S*,*E*,*S*,*E*,*S** (*Z*,*R*,*E*,*S*,*E*,*S*,*Z*,*S*)	*E*,*S*,*E*,*S*,*Z*,*S*,*Z*,*S** (*E*,*S*,*Z*,*S*,*Z*,*S*,*E*,*S*) (*Z*,*S*,*Z*,*S*,*E*,*S*,*E*,*S*) (*Z*,*S*,*E*,*S*,*E*,*S*,*Z*,*S*)
E,*y*,*Z*,*y*,*Z*,*y*,*Z*,*y*	*E*,*R*,*Z*,*R*,*Z*,*R*,*Z*,*R** (*Z*,*R*,*Z*,*R*,*Z*,*R*,*E*,*R*) (*Z*,*R*,*Z*,*R*,*E*,*R*,*Z*,*R*) (*Z*,*R*,*E*,*R*,*Z*,*R*,*Z*,*R*)	*E*,*R*,*Z*,*R*,*Z*,*R*,*Z*,*S** (*Z*,*R*,*Z*,*R*,*Z*,*R*,*E*,*S*) *Z*,*R*,*Z*,*R*,*E*,*R*,*Z*,*S** (*Z*,*R*,*E*,*R*,*Z*,*R*,*Z*,*S*)	*E*,*R*,*Z*,*S*,*Z*,*R*,*Z*,*S* (*Z*,*R*,*Z*,*S*,*Z*,*R*,*E*,*S*) (*Z*,*R*,*Z*,*S*,*E*,*R*,*Z*,*S*) (*Z*,*R*,*E*,*S*,*Z*,*R*,*Z*,*S*)	*E*,*R*,*Z*,*R*,*Z*,*S*,*Z*,*S* *Z*,*R*,*Z*,*R*,*Z*,*S*,*E*,*S** (*Z*,*R*,*Z*,*R*,*E*,*S*,*E*,*S*) *Z*,*R*,*E*,*R*,*Z*,*S*,*Z*,*S**	*E*,*R*,*Z*,*S*,*Z*,*S*,*Z*,*S** *Z*,*R*,*Z*,*S*,*Z*,*S*,*E*,*S** (*Z*,*R*,*Z*,*S*,*E*,*S*,*E*,*S*) (*Z*,*R*,*E*,*S*,*Z*,*S*,*Z*,*S*)	*E*,*S*,*Z*,*S*,*Z*,*S*,*Z*,*S** (*Z*,*S*,*Z*,*S*,*Z*,*S*,*E*,*S*) (*Z*,*S*,*Z*,*S*,*E*,*S*,*Z*,*S*) (*Z*,*S*,*E*,*S*,*Z*,*S*,*Z*,*S*)
Z,*y*,*Z*,*y*,*Z*,*y*,*Z*,*y*	*Z*,*R*,*Z*,*R*,*Z*,*R*,*Z*,*R** (*Z*,*R*,*Z*,*R*,*Z*,*R*,*Z*,*R*) (*Z*,*R*,*Z*,*R*,*Z*,*R*,*Z*,*R*) (*Z*,*R*,*Z*,*R*,*Z*,*R*,*Z*,*R*)	*Z*,*R*,*Z*,*R*,*Z*,*R*,*Z*,*S** (*Z*,*R*,*Z*,*R*,*Z*,*R*,*Z*,*S*) (*Z*,*R*,*Z*,*R*,*Z*,*R*,*Z*,*S*) (*Z*,*R*,*Z*,*R*,*Z*,*R*,*Z*,*S*)	*Z*,*R*,*Z*,*S*,*Z*,*R*,*Z*,*S* (*Z*,*R*,*Z*,*S*,*Z*,*R*,*Z*,*S*) (*Z*,*R*,*Z*,*S*,*Z*,*R*,*Z*,*S*) (*Z*,*R*,*Z*,*S*,*Z*,*R*,*Z*,*S*)	*Z*,*R*,*Z*,*R*,*Z*,*S*,*Z*,*S* (*Z*,*R*,*Z*,*R*,*Z*,*S*,*Z*,*S*) (*Z*,*R*,*Z*,*R*,*Z*,*S*,*Z*,*S*) (*Z*,*R*,*Z*,*R*,*Z*,*S*,*Z*,*S*)	*Z*,*R*,*Z*,*S*,*Z*,*S*,*Z*,*S** (*Z*,*R*,*Z*,*S*,*Z*,*S*,*Z*,*S*) (*Z*,*R*,*Z*,*S*,*Z*,*S*,*Z*,*S*) (*Z*,*R*,*Z*,*S*,*Z*,*S*,*Z*,*S*)	*Z*,*S*,*Z*,*S*,*Z*,*S*,*Z*,*S** (*Z*,*S*,*Z*,*S*,*Z*,*S*,*Z*,*S*) (*Z*,*S*,*Z*,*S*,*Z*,*S*,*Z*,*S*) (*Z*,*S*,*Z*,*S*,*Z*,*S*,*Z*,*S*)

a. Combinations in a parenthesis ( ) indicate the presence of an identical geometry in the same frame and should be removed from the count. *b*. Combinations with an asterisk * indicate the presence of enantiomeric pair.

(3) CrysAlisPro 1.171.38.43, Rigaku OD, **2015**.
(4) Sheldrick, G. M. Crystal structure refinement with SHELXL. *Acta Crystallogr. A* **2015**, *71*, 3-8.
(5) Sheldrick, G. M. A short history of SHELX. *Acta Crystallogr. A* **2008**, *64*, 112-122.
(6) Kabuto, C.; Akine, S.; Nemoto, T.; Kwon, E. Release of software (Yadokari-XG 2009) for crystal structure analyses. *J. Cryst. Soc. Jpn.* **2009**, *51*, 218-224.

Theoretical calculations

The Gaussian 09 program suite was used.[7] Calculations were performed either at the semiempirical PM6 method[8] or at the DFT method using the B3LYP functional, the gradient correction of the exchange functional by Becke[9,10] and the correlation functional by Lee, Yang and Parr.[11] The 6-31G(d,p) split valence plus polarization basis set was used.[12,13,14,15,16] Analysis of rotational barriers for binaphthyl was performed by a relaxed potential energy surface scan method. Spectra calculations were performed by time-dependent DFT (TD DFT) for the first 30 singlet-singlet transitions with an additional keyword of IOP(9/40=2) to output information on smaller contributions to each electronic transition. Note that, although the spectral analysis with the B3LYP functional yields an excellent consistence in the ordering of states with the experimental results, it tends to underestimate the excitation energy to afford slightly red-shifted theoretical spectra.[17]

NMR analyses

Assignments of ^{1}H resonances of [8]CPhen$_{3,9}$

Three singlets (H^4/H^5/H^{10}) and four doublets (H^8/H^7/H^2/H^1) were assigned as follows. NOE correlations with a methyl resonance in a NOESY spectrum established the H^5 (singlet) and H^7 (doublet) resonances (Fig. S1). A NOE correlation with the H^5 resonance located the H^4 (singlet)

(7) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E., Jr.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09 (Revision B.01); Gaussian, Inc.: Wallingford, CT, 2010.

(8) Stewart, J. J. P. Optimization of parameters for semiempirical methods V: Modification of NDDO approximations and application to 70 elements. *J. Mol. Model.* **2007**, *13*, 1173-1213.

(9) Beck, A. D. Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A* **1988***, 38***,** 3098-3100.

(10) Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98***,** 5648-5652.

(11) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **1988***, 37***,** 785-789.

(12) Ditchfield, R.; Hehre, W. J.; Pople, J. A. Self-consistent molecularorbital methods. IX. An extended Gaussian-type basis for molecular-orbital studies of organic molecules. *J. Chem. Phys.* **1971**, *54***,** 724-728.

(13) Hehre, W. J.; Ditchfield, R.: Pople, J. A. Self-consistent molecular orbital methods. XII. Further extensions of Gaussian-type basis sets for use in molecular orbital studies of organic molecules. *J. Chem. Phys.* **1972,** *56***,** 2257-2261.

(14) Hariharan, P. C.; Pople, J. A. Accuracy of AH_n equilibrium geometries by single determinant molecular orbital theory. *Mol. Phys.* **1974**, *27***,** 209-214.

(15) Gordon, M. S. The isomers of silacyclopropane. *Chem. Phys. Lett.* **1980**, *76***,** 163-168.

(16) Hariharan, P. C.; Pople, J. A. The influence of polarization functions on molecular orbital hydrogenation energies. *Theor. Chem. Acc.* **1973**, *28,* 213-222.

(17) Bauernschmitt, R.; Ahlrichs, R. Treatment of electronic excitations within the adiabatic approximation of time dependent density functional theory. *Chem. Phys. Lett.* **1996**, *256***,** 454-464.

resonance. One remaining singlet was thus assigned as a H^{10} (singlet) resonance. A coupling correlation with the H^7 resonance allowed the assignment of the H^8 (doublet) resonance (Fig. S2). Thus, two remaining doublets originated from H^2 and H^1 resonances, and the NOE correlation with the H^4 resonance established the H^2 resonance at the *E*-biaryl linkage.

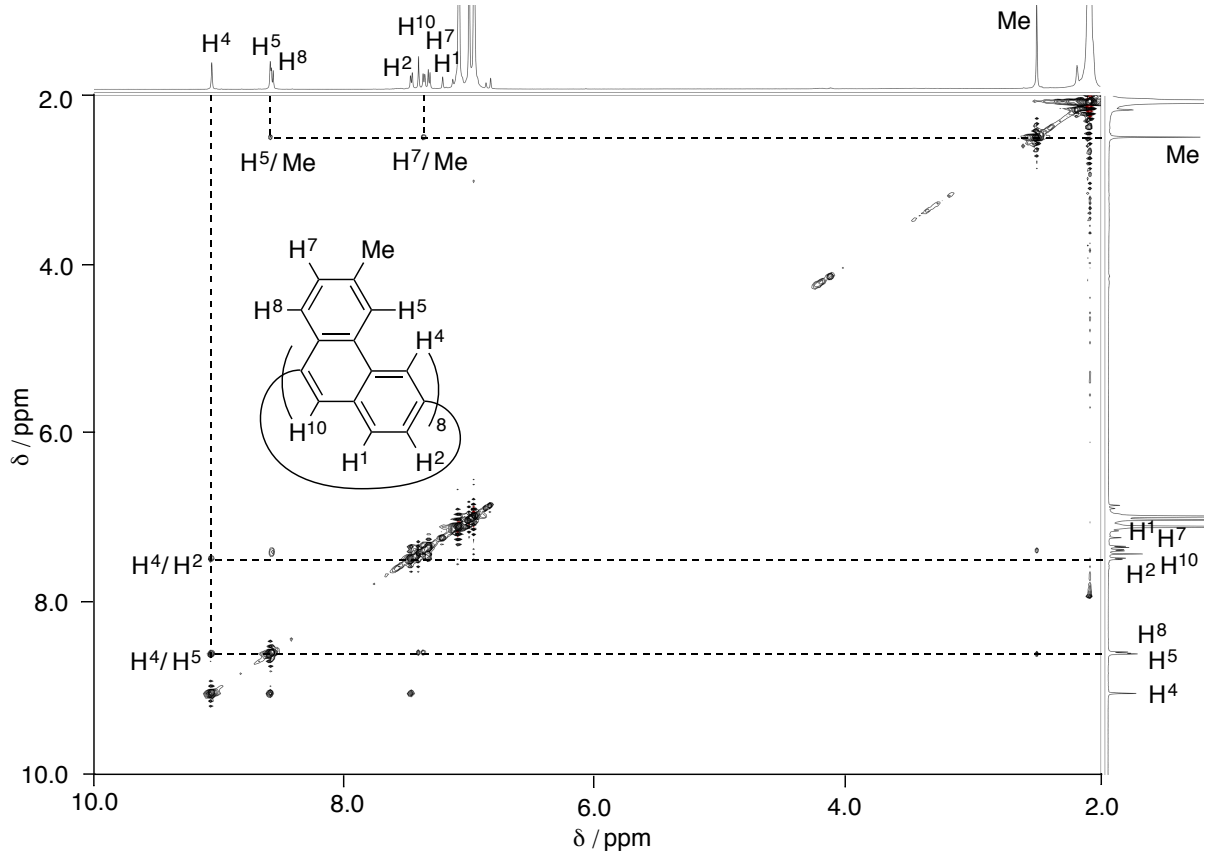


Fig. S1. NOESY spectrum of [8]CPhen$_{3,9}$ in toluene-d_8 (25 °C, 600 MHz).

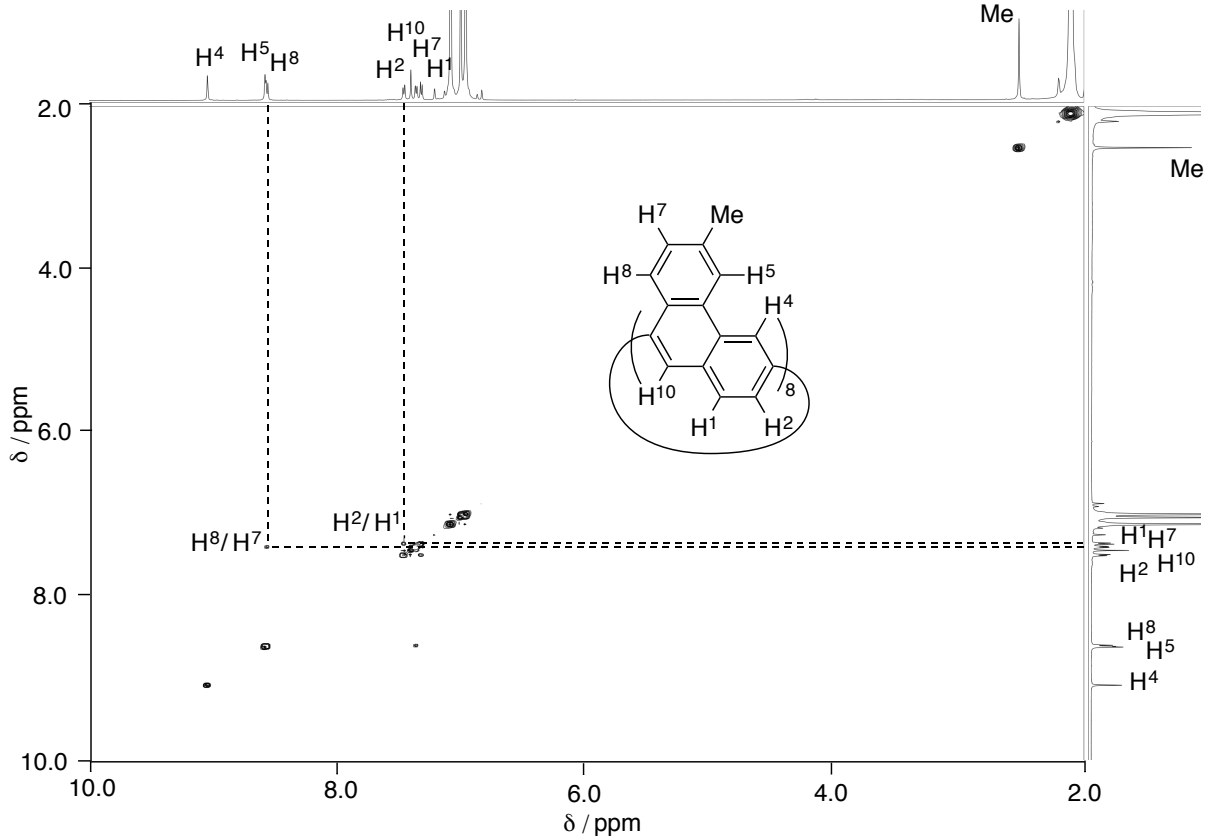


Fig. S2. COSY spectrum of [8]CPhen$_{3,9}$ in toluene-d_8 (25 °C, 600 MHz).

VT NMR analyses

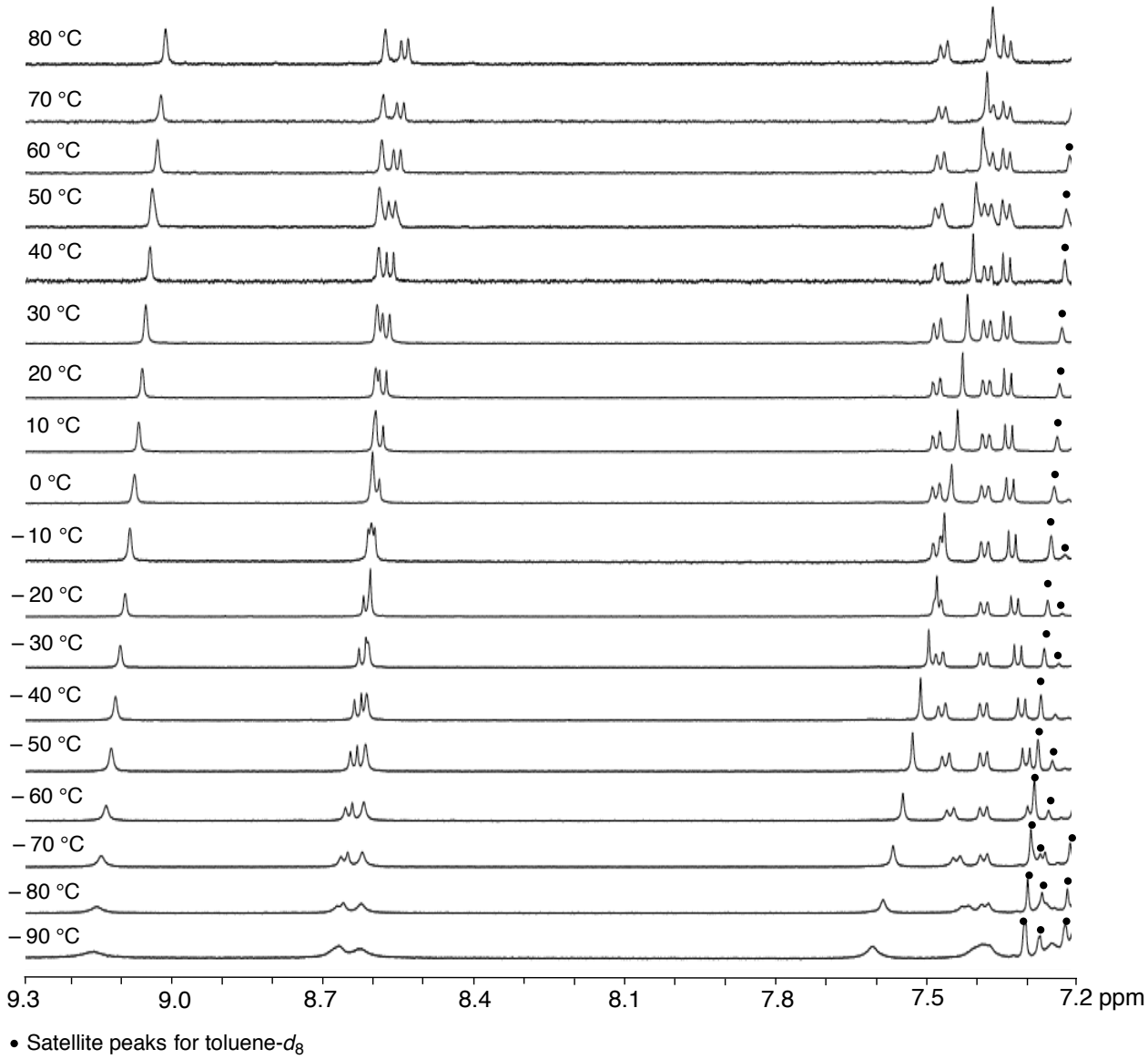


Fig. S3. VT-NMR analysis of [8]CPhen$_{3,9}$ in toluene-d_8 (600 MHz). Black dots show the satellite resonances of toluene.

Separation of enantiomers

Enantiomers of [8]CPhen$_{3,9}$ were separated on a recycling, preparative scale HPLC (Fig. S4). The compound was slowly oxidized in solution, and the specimen for the present chromatogram contained oxidized compounds (*m/z* = 1552: [8]CPhen$_{3,9}$+2O). After the separation, analytical HPLC was performed to confirm the separation (Fig. S5).

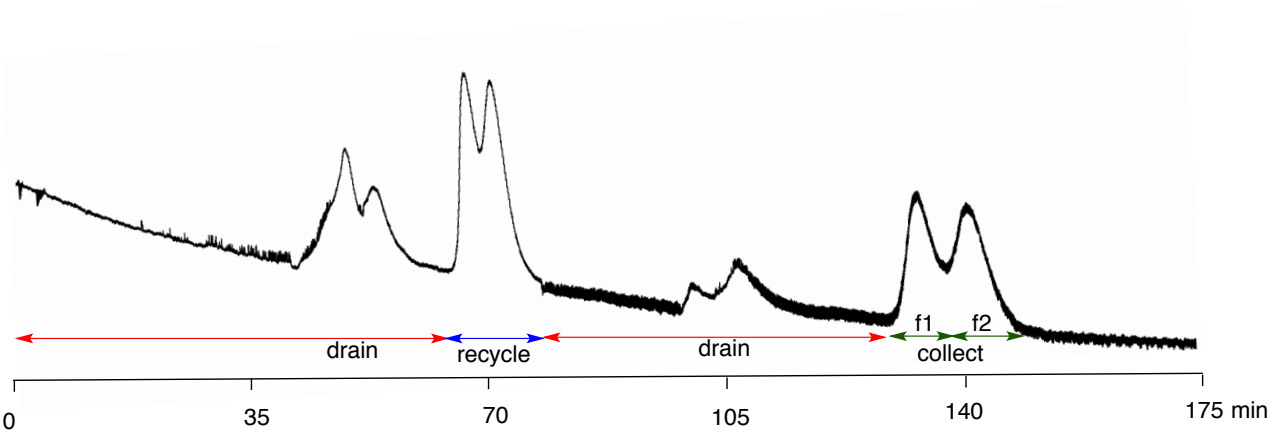


Fig. S4. Separation of enantiomers of [8]CPhen$_{3,9}$. Column = COSMOSIL Cholester (50ϕ, 250+250 mm), eluent = 30% MeOH/$CHCl_3$, flow rate = 14.0 mL/min, detector = UV-vis (280 nm).

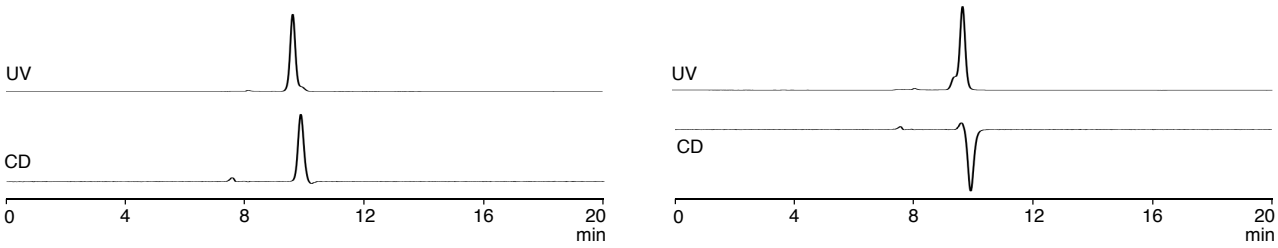


Fig. S5. Analysis of separated enantiomers of [8]CPhen$_{3,9}$. Column = COSMOSIL Cholester (4.6ϕ, 250+250+250 mm), eluent = 30% MeOH/$CHCl_3$, flow rate = 1.0 mL/min, detector = UV-vis (280 nm) and CD (379 nm), temperature = 40 °C.

VT CD analyses

VT CD analyses of (–)-**4**

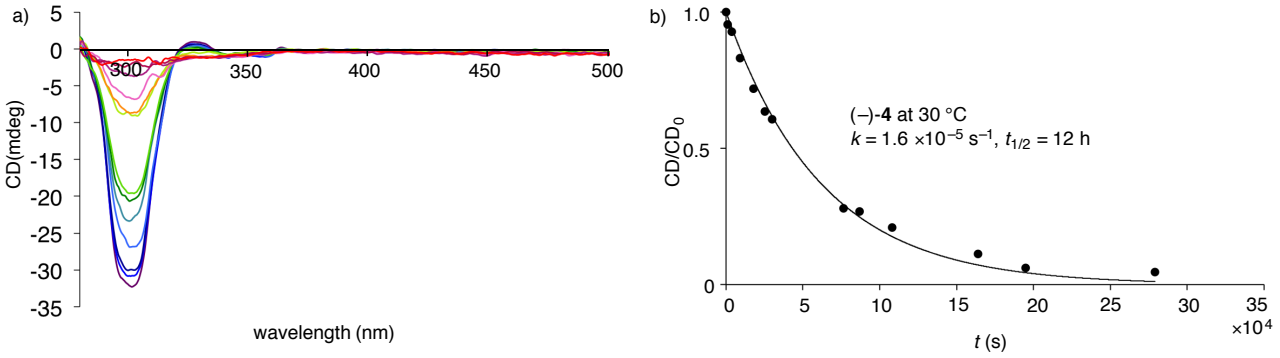


Fig. S6. Racemization kinetics of (–)-**4** at 30 °C. (a) VT CD spectra. (b) Decay of the CD signal at 302 nm. The coefficient of determination (R^2) was 0.994199021 and confirmed the sufficient goodness of fit for the analysis.

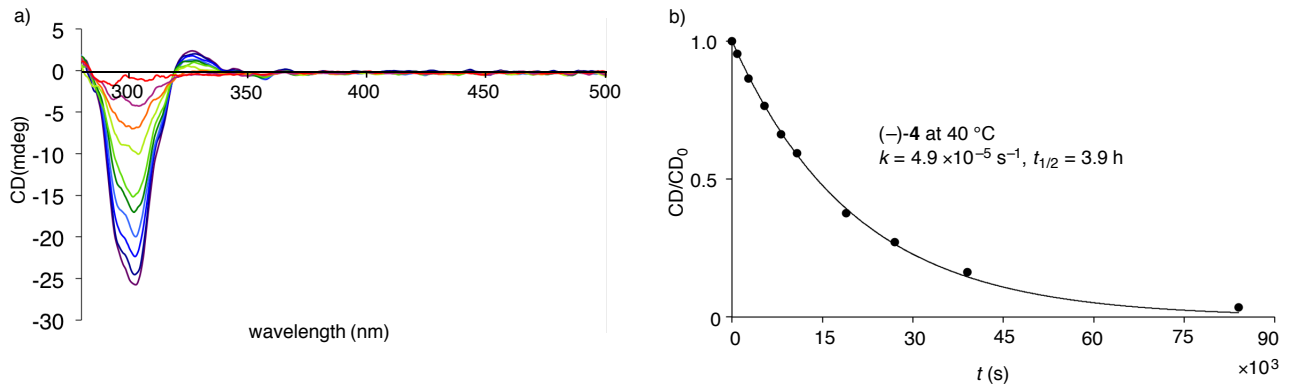


Fig. S7. Racemization kinetics of (–)-**4** at 40 °C. (a) VT CD spectra. (b) Decay of the CD signal at 302 nm. The coefficient of determination (R^2) was 0.998794998 and confirmed the sufficient goodness of fit for the analysis.

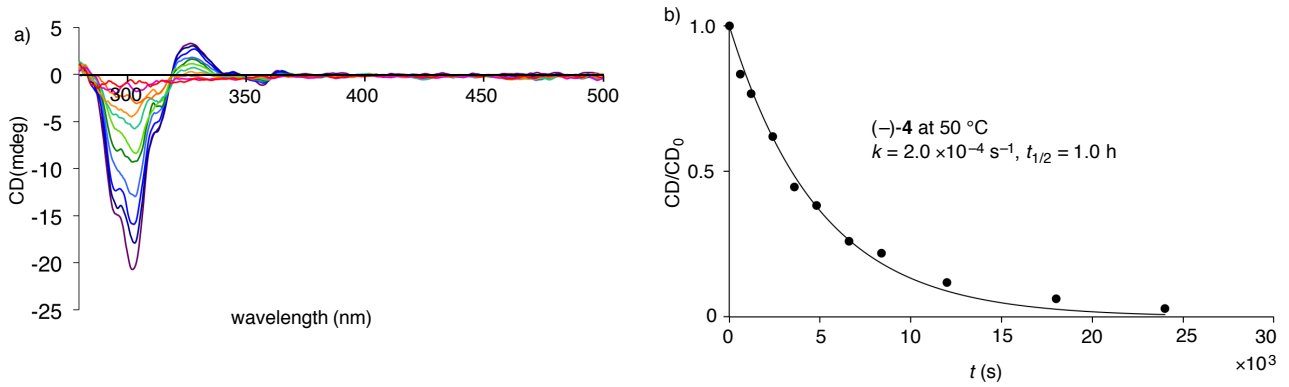


Fig. S8. Racemization kinetics of (–)-**4** at 50 °C. (a) VT CD spectra. (b) Decay of the CD signal at 302 nm. The coefficient of determination (R^2) was 0.99263868 and confirmed the sufficient goodness of fit for the analysis.

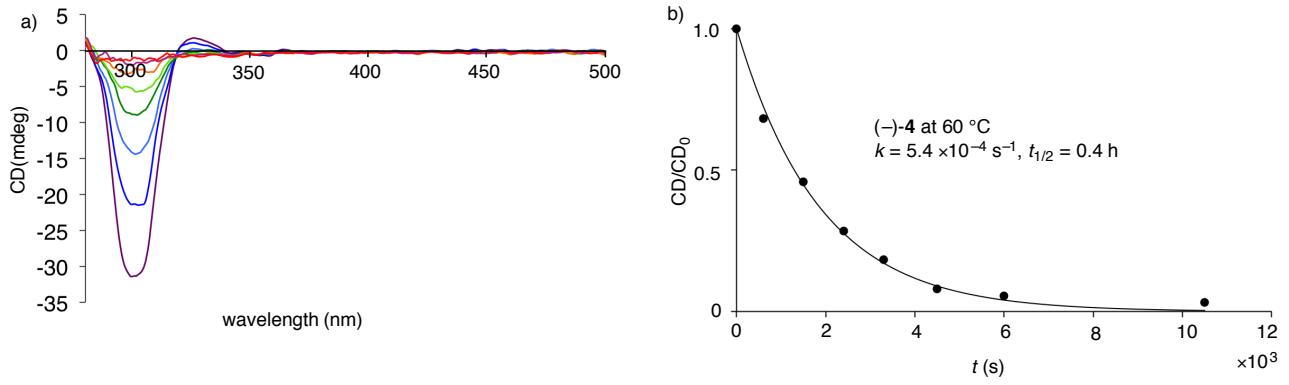


Fig. S9. Racemization kinetics of (–)-**4** at 60 °C. (a) VT CD spectra. (b) Decay of the CD signal at 302 nm. The coefficient of determination (R^2) was 0.99605121 and confirmed the sufficient goodness of fit for the analysis.

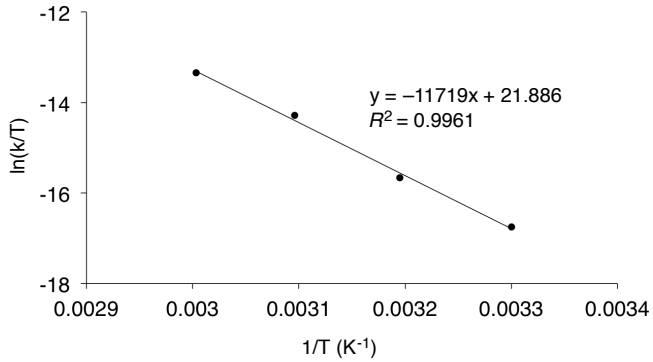


Fig. S10. Eyring plot for racemization of (–)-**4** to reveal the activation energy with $\Delta H^{\ddagger}$ = +23 kcal/mol, $\Delta S^{\ddagger}$ = –3.7 cal/mol•K and $\Delta G^{\ddagger}$ = +24 kcal/mol at 25 °C.

VT CD analyses of (*E,S,E,S,E,S,E,S*)-[8]CPhen$_{3,9}$

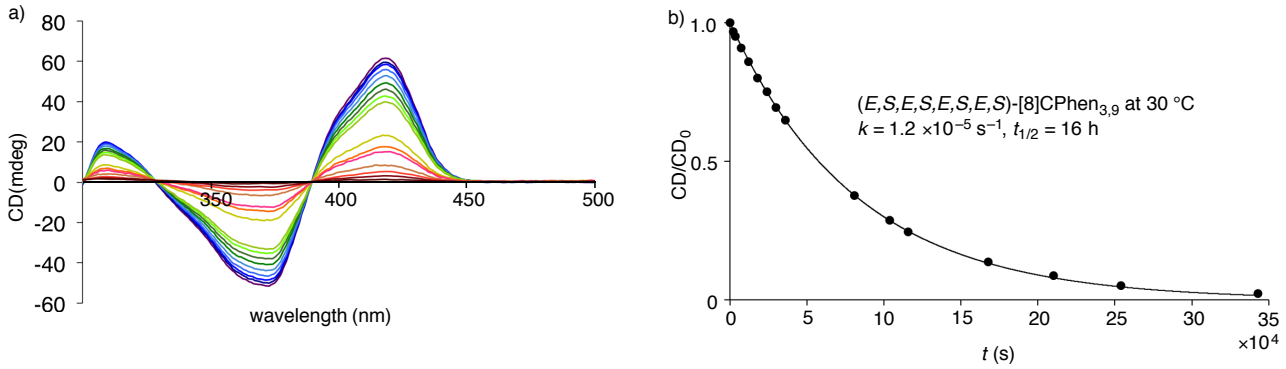


Fig. S11. Racemization kinetics of (*E,S,E,S,E,S,E,S*)-[8]CPhen$_{3,9}$ at 30 °C. (a) VT CD spectra. (b) Decay of the CD signal at 419 nm. The coefficient of determination (R^2) was 0.999784569 and confirmed the sufficient goodness of fit for the analysis.

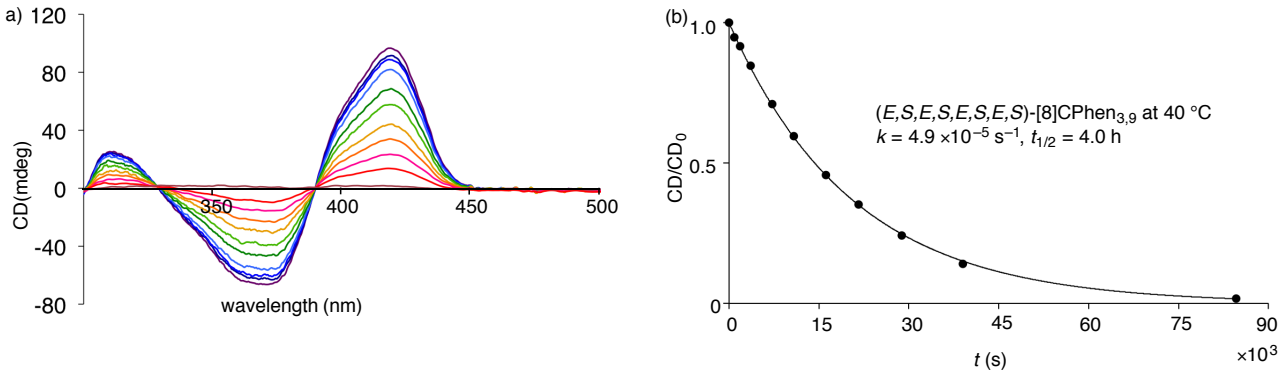


Fig. S12. Racemization kinetics of (*E,S,E,S,E,S,E,S*)-[8]CPhen$_{3,9}$ at 40 °C. (a) VT CD spectra. (b) Decay of the CD signal at 419 nm. The coefficient of determination (R^2) was 0.99971099 and confirmed the sufficient goodness of fit for the analysis.

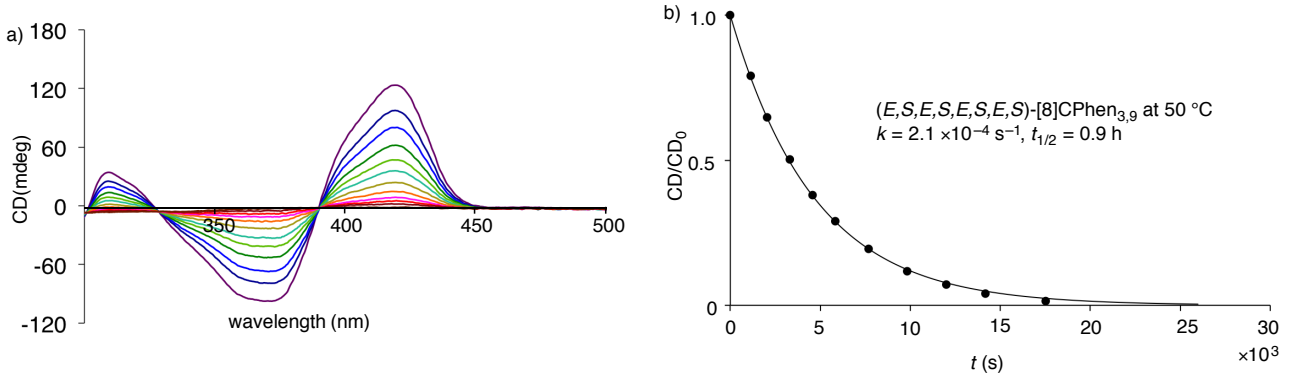


Fig. S13. Racemization kinetics of (*E,S,E,S,E,S,E,S*)-[8]CPhen$_{3,9}$ at 50 °C. (a) VT CD spectra. (b) Decay of the CD signal at 419 nm. The coefficient of determination (R^2) was 0.999539945 and confirmed the sufficient goodness of fit for the analysis.

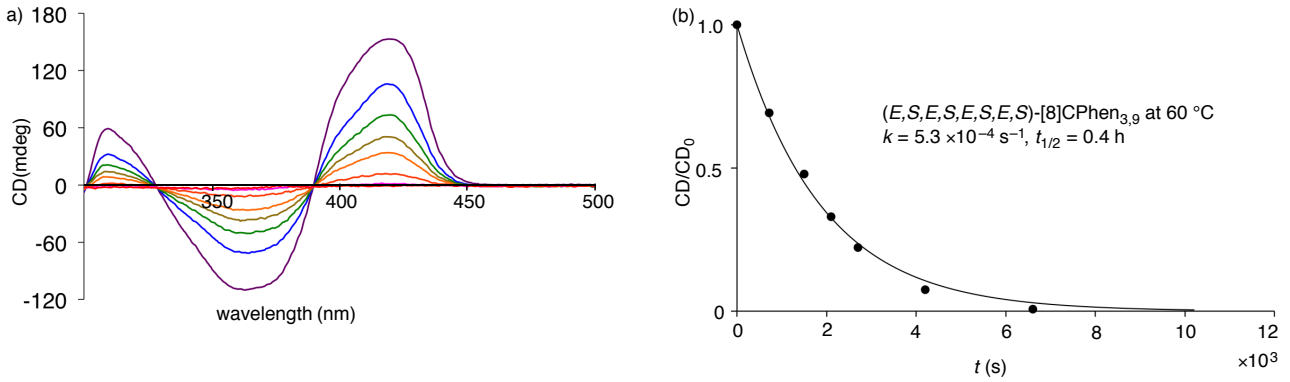


Fig. S14. Racemization kinetics of (*E,S,E,S,E,S,E,S*)-[8]CPhen$_{3,9}$ at 60 °C. (a) VT CD spectra. (b) Decay of the CD signal at 419 nm. The coefficient of determination (R^2) was 0.996916068 and confirmed the sufficient goodness of fit for the analysis.

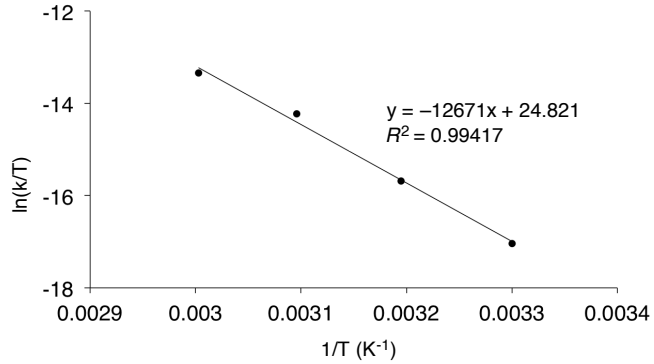


Fig. S15. Eyring plot for racemization of (*E,S,E,S,E,S,E,S*)-[8]CPhen$_{3,9}$ to reveal the activation energy with $\Delta H^{\ddagger}$ = +25 kcal/mol, $\Delta S^{\ddagger}$ = +2.1 cal/mol•K and $\Delta G^{\ddagger}$ = +24 kcal/mol at 25 °C.

Isomerization profile

As shown in a scheme below, there appears two *E/Z*-paths for the conversion from (*E,y*^{1},*E,y*^{2},*E,y*^{3},*E,y*^{4})-isomer to (*Z,y*^{1},*Z,y*^{2},*Z,y*^{3},*Z,y*^{4})-isomer under the condition of single-linkage

rotation. One path (top path) is shown in Fig. 9, and the other (bottom path) is shown in Fig. S16.

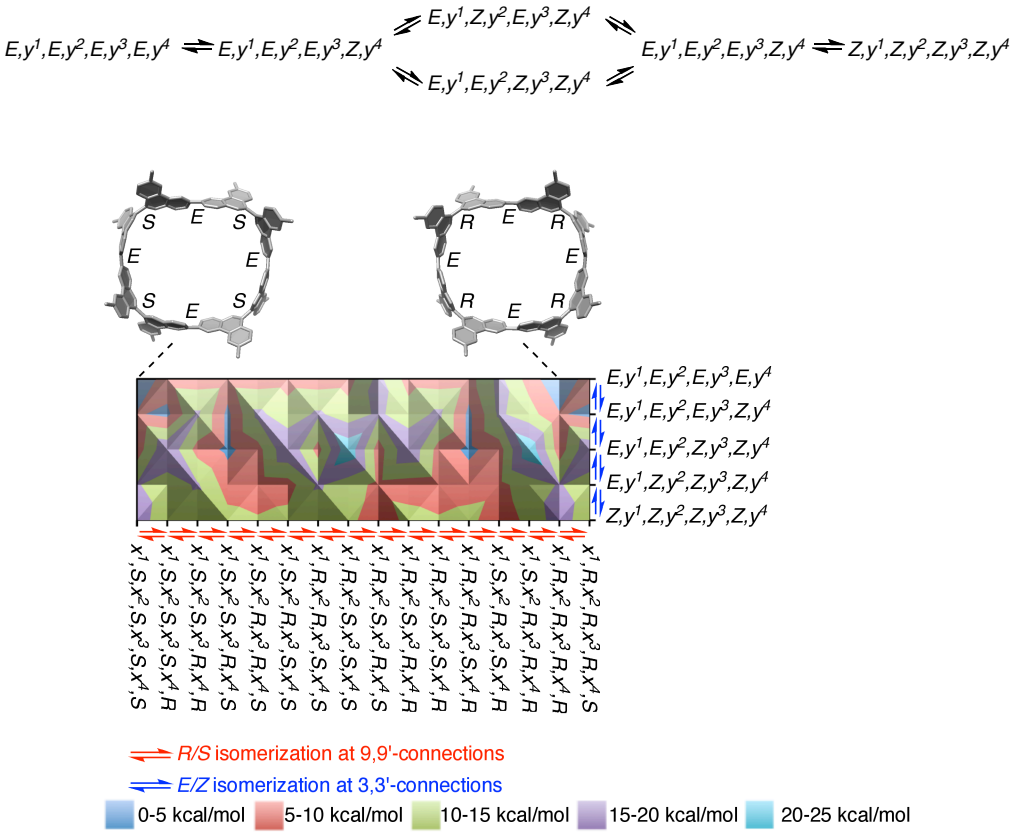


Fig. S16. Isomerization profile of [8]CPhen$_{3,9}$. Adjacent isomers are interconvertible through a single-linkage rotation. All the stereoisomers expect for (E,y^1,Z,y^2,E,y^3,Z,y^4)-isomers are mapped. See Fig. 9 for a profile involving (E,y^1,Z,y^2,E,y^3,Z,y^4)-isomers.

Supplementary data

HPLC chromatogram

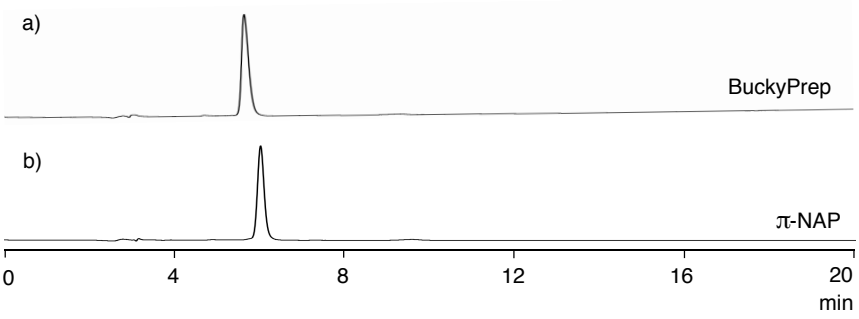


Fig. S17. Chromatogram confirming the purity of [8]CPhen$_{3,9}$. (a) Column = COSMOSIL BuckyPrep (4.6ϕ, 250 mm), eluent = 70% CHCl3/MeOH, flow rate = 1.0 mL/min, detector = UV-vis (280 nm), temperature = 40 °C. (b) Column = COSMOSIL π-NAP (4.6ϕ, 250 mm), eluent = 60% CHCl3/MeOH, flow rate = 1.0 mL/min, detector = UV-vis (280 nm), temperature = 40 °C.

NMR spectra

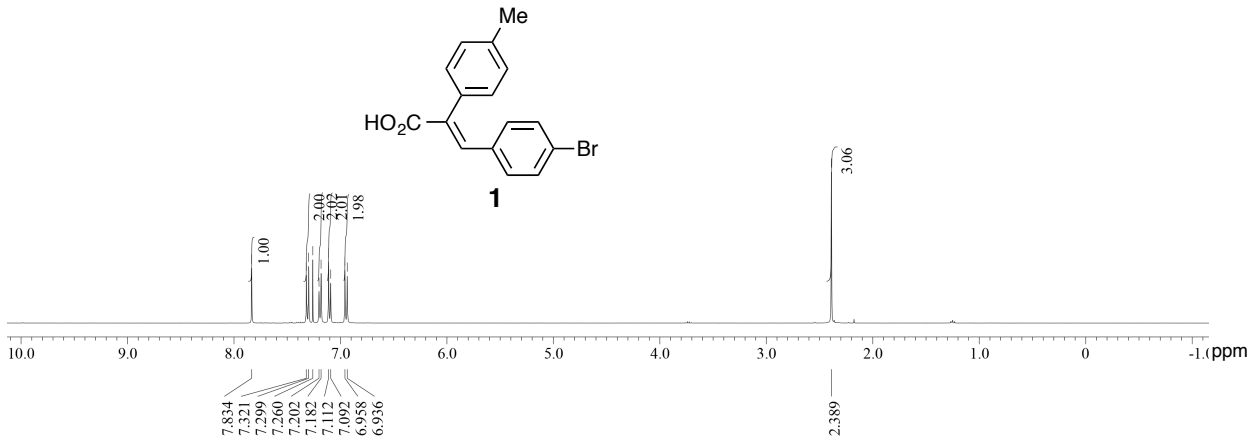


Fig. S18. ^{1}H NMR spectrum of **1** in $CDCl_3$ (25 °C, 600 MHz)

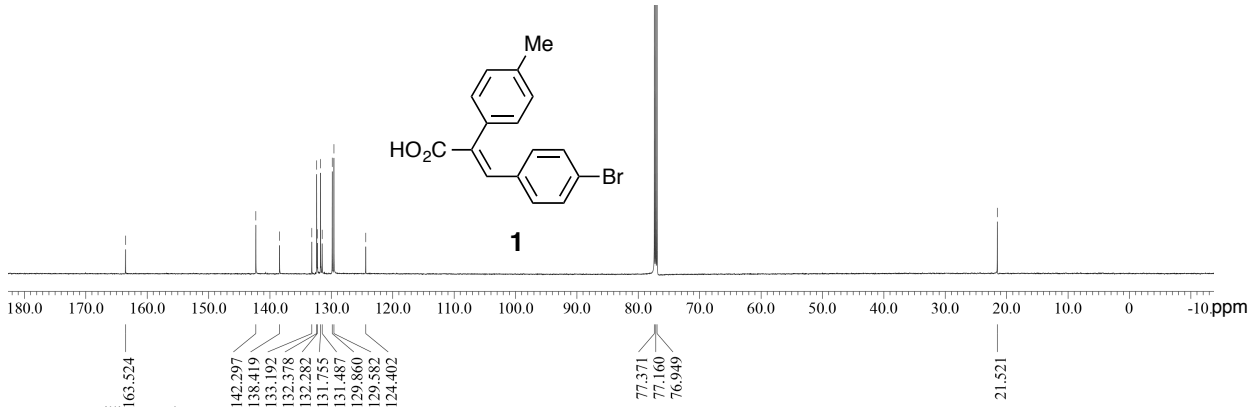


Fig. S19. ^{13}C NMR spectrum of **1** in $CDCl_3$ (25 °C, 150 MHz)

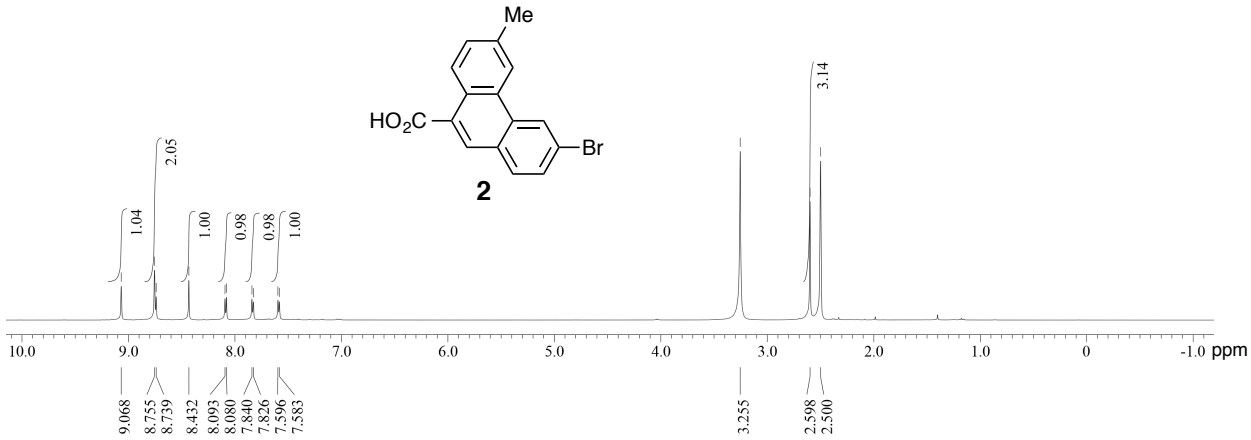


Fig. S20. ^{1}H NMR spectrum of **2** in DMSO-d_6 (25 °C, 600 MHz)

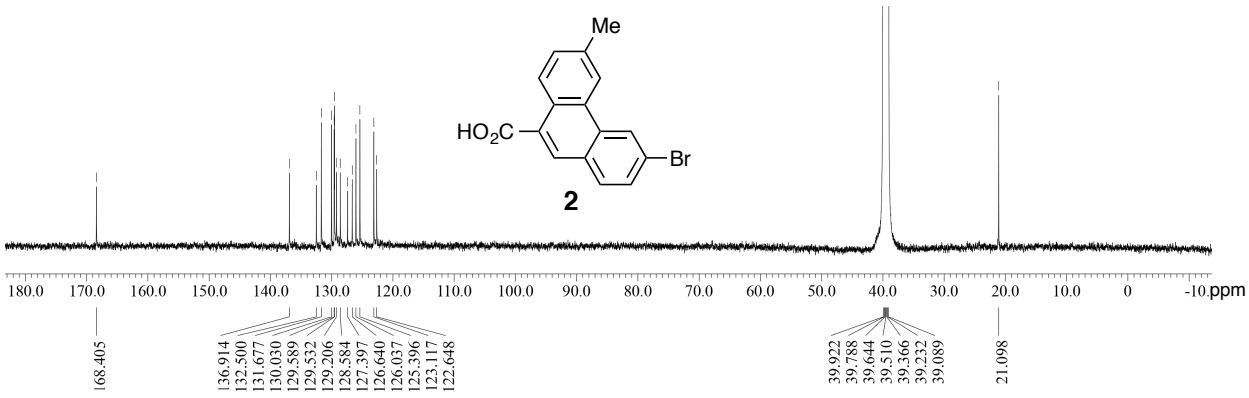


Fig. S21. ^{13}C NMR spectrum of **2** in DMSO-d_6 (25 °C, 150 MHz)

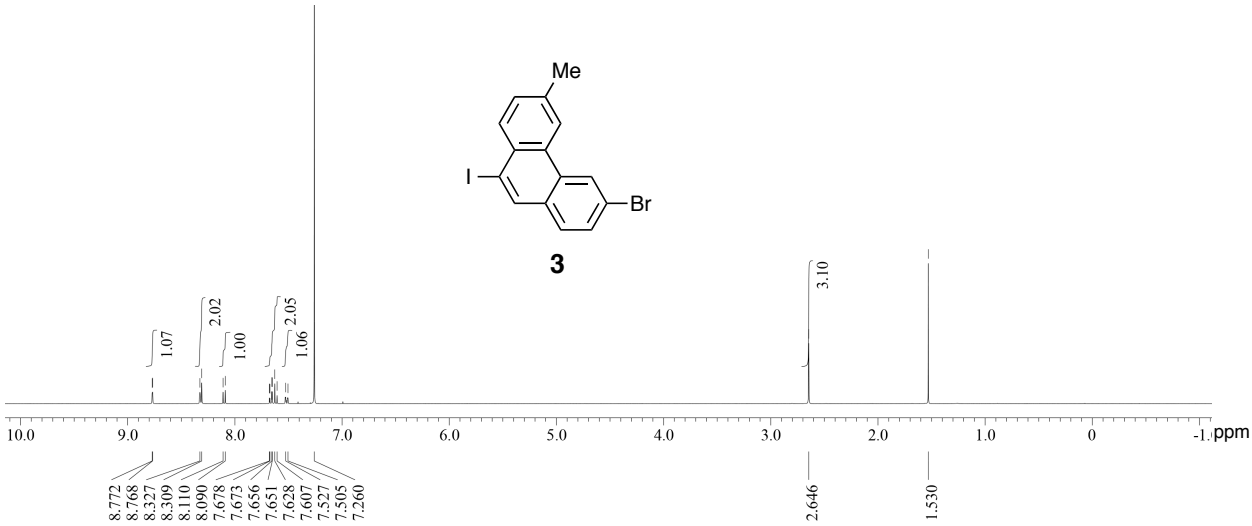


Fig. S22. ^{1}H NMR spectrum of **3** in $CDCl_3$ (25 °C, 600 MHz)

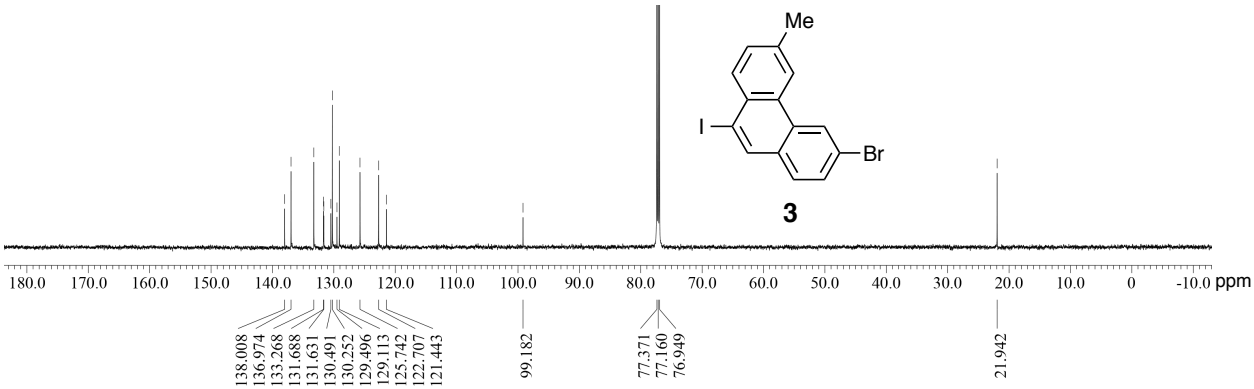


Fig. S23. ^{13}C NMR spectrum of **3** in $CDCl_3$ (25 °C, 150 MHz)

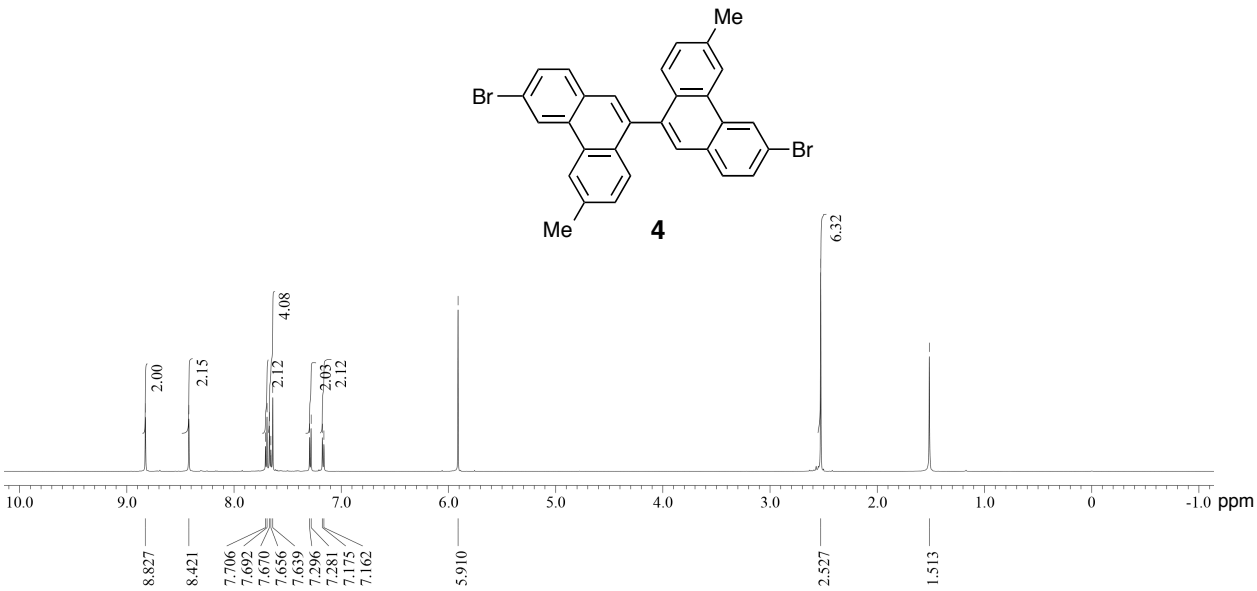


Fig. S24. ^{1}H NMR spectrum of **4** in $C_2D_2Cl_4$ (25 °C, 600 MHz)

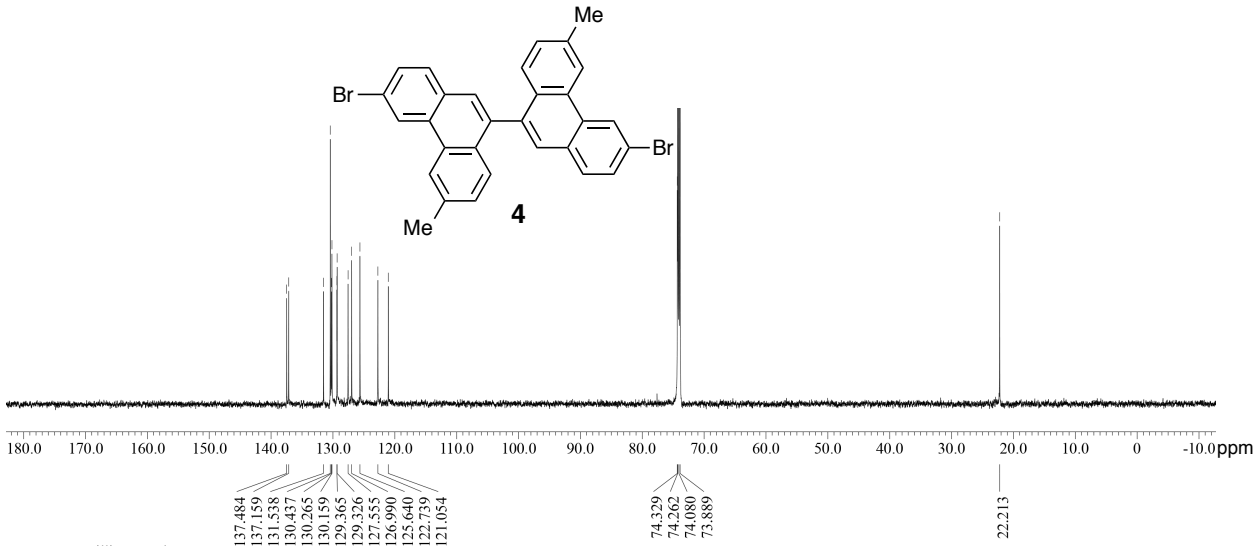


Fig. S25. ^{13}C NMR spectrum of **4** in $C_2D_2Cl_4$ (25 °C, 150 MHz)

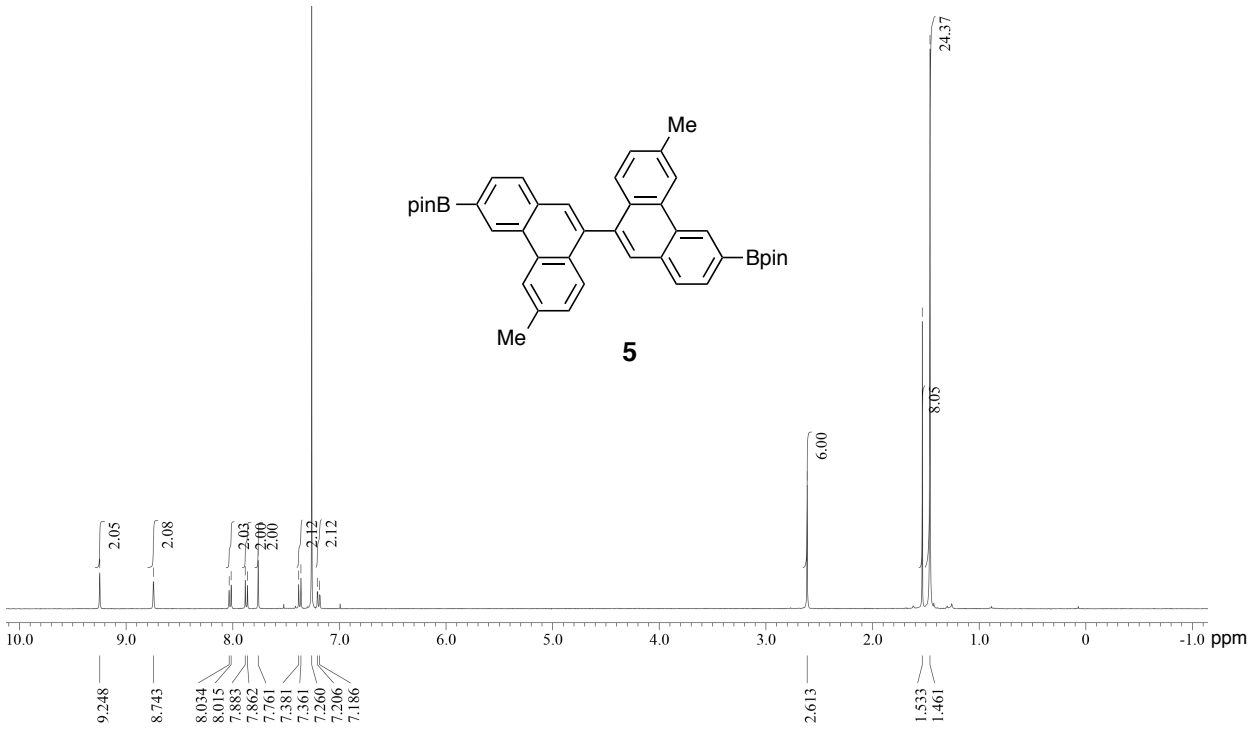


Fig. S26. ^{1}H NMR spectrum of **5** in $CDCl_3$ (25 °C, 600 MHz)

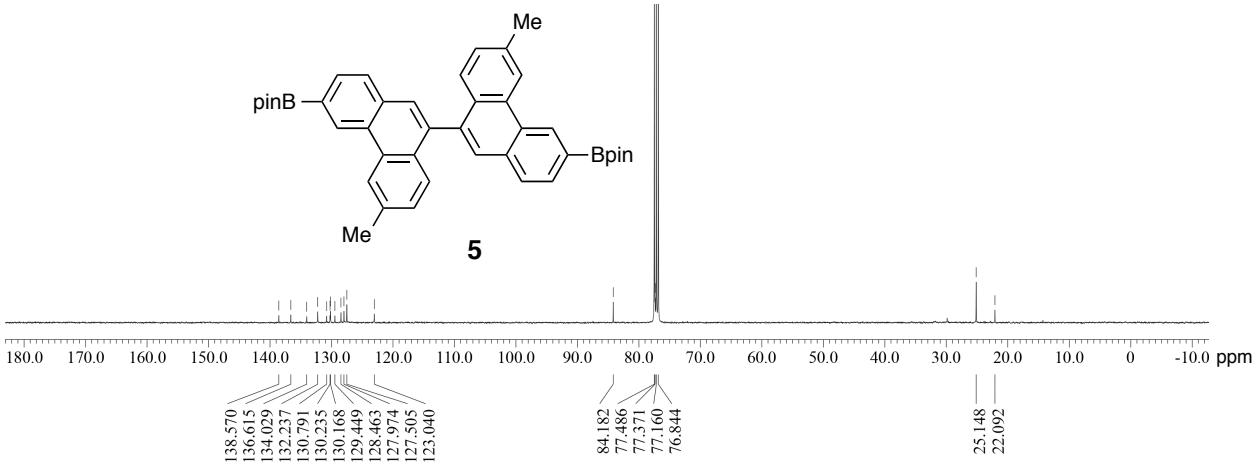


Fig. S27. ^{13}C NMR spectrum of **5** in $CDCl_3$ (25 °C, 150 MHz)

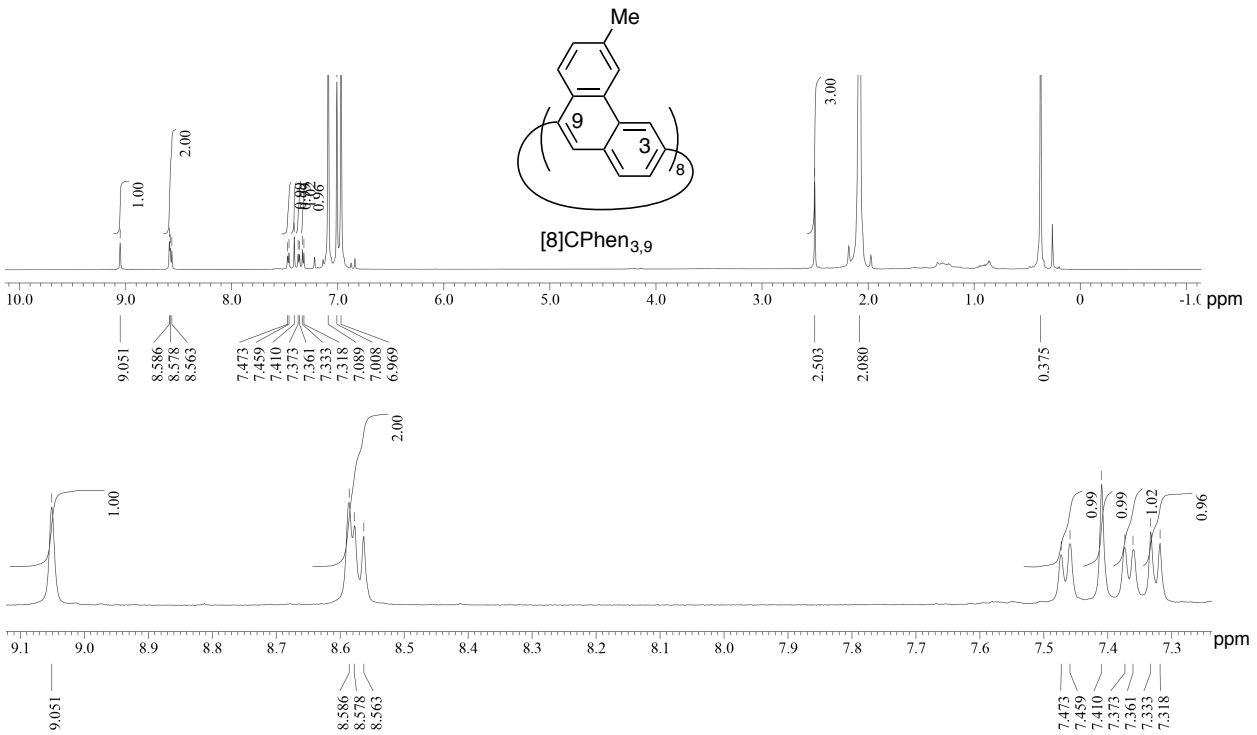


Fig. S28. ^{1}H NMR spectrum of [8]CPhen$_{3,9}$ in toluene-d_8 (25 °C, 600 MHz). Spectrum expanded for the aromatic region is shown below.

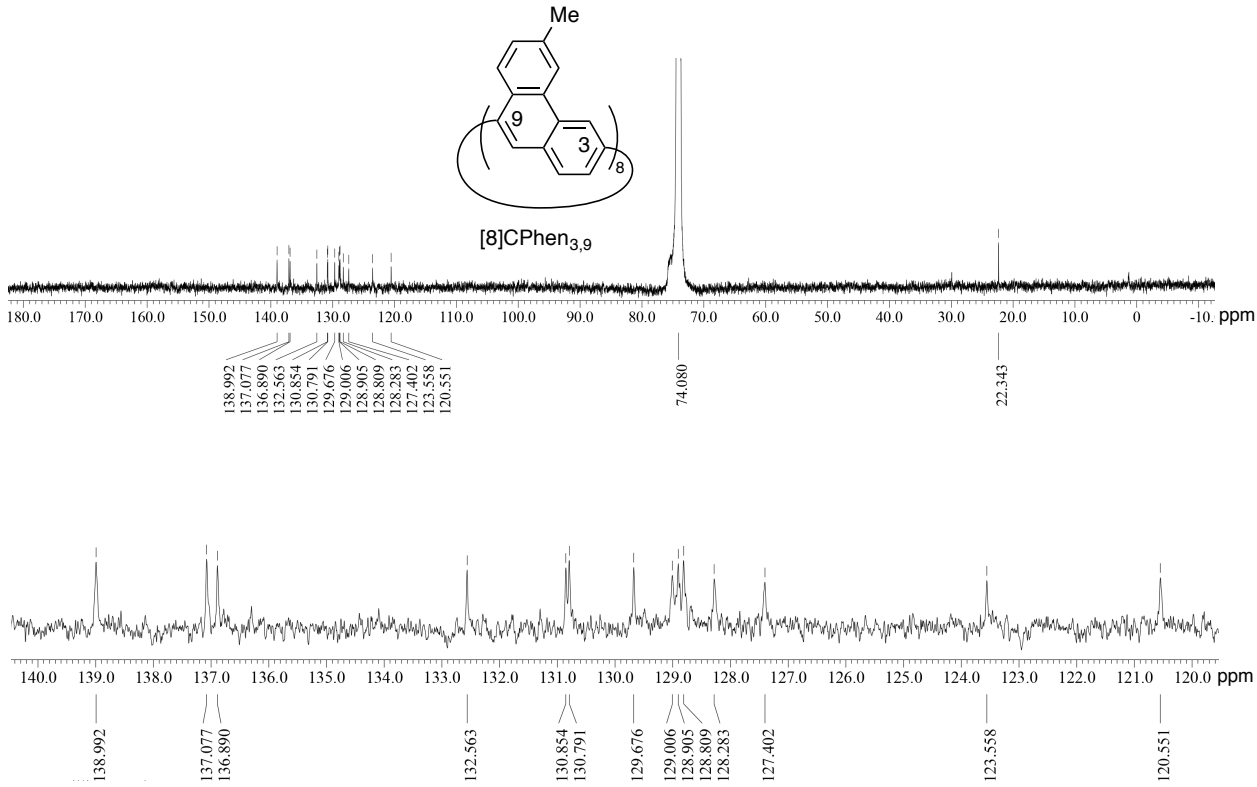


Fig. S29. ^{13}C NMR spectrum of [8]CPhen$_{3,9}$ in $C_2D_2Cl_4$ (25 °C, 150 MHz). Spectrum expanded for the aromatic region is shown below.

Crytallographic data

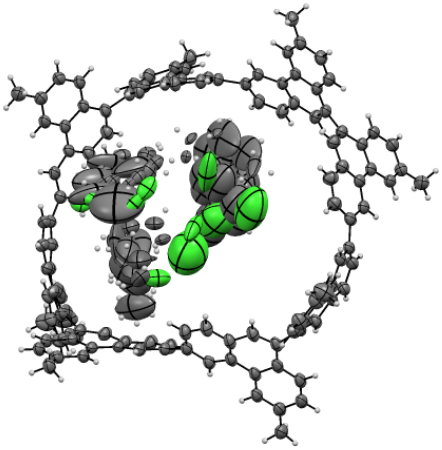


Fig. S30. ORTEP diagram of [8]CPhen$_{3,9}$ (50% probability level).

Table S2. Crystal data and structure refinement for [8]CPhen$_{3,9}$

Data deposition	CCDC 1497765
Empirical formula	$C_{152}H_{136}Cl_4$
Formula weight	2104.40
Temperature	95(2) K
Wavelength	0.85000 Å
Crystal system	Monoclinic
Space group	*P*2/*c*
Crystal color	yellow
Unit cell dimensions	a = 10.0764(2) Å α = 90°
	b = 18.3514(5) Å β = 94.5927(18)°
	c = 33.4402(6) Å γ = 90°
Volume	6163.8(2) Å^3
Z	2
Density (calculated)	1.134 Mg/m^3
Absorption coefficient	0.232 mm^{-1}
F(000)	2232
Crystal size	0.10 × 0.07 × 0.01 mm^3
Theta range for data collection	2.425 to 29.614°
Index ranges	–11<=*h*<=11, –19<=*k*<=19, –38<=*l*<=38
Reflections collected	30868
Independent reflections	9591 [*R*(int) = 0.0340]
Completeness to theta = 33.723 °	94.2 %

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.87864
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9591 / 1332 / 1168
Goodness-of-fit on F^2	1.603
Final R indices [$I>2\sigma(I)$]	$R_1 = 0.0810$, $wR_2 = 0.2151$
R indices (all data)	$R_1 = 0.1055$, $wR_2 = 0.2288$
Extinction coefficient	n/a
Largest diff. peak and hole	0.559 and - 0.297 e•Å^{-3}

Cartesian coordinates

Table S3. Cartesian coordinate of *E,R,E,R,E,R,E,R* (1)

SCF Done: E(RB3LYP) = -4621.35469074 A.U. after 9 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	10.450177	0.374766	3.336486
2	6	0	9.963123	-0.263770	2.214705
3	6	0	9.198868	0.427139	1.244354
4	6	0	8.936945	1.815959	1.450124
5	6	0	9.453945	2.435639	2.610518
6	6	0	10.200379	1.747465	3.554355
7	6	0	8.713983	-0.233326	0.044978
8	6	0	8.142884	2.548023	0.471715
9	6	0	7.879138	1.921391	-0.778262
10	6	0	8.183373	0.537643	-0.958118
11	6	0	7.155312	2.633393	-1.763075
12	6	0	6.587448	3.855369	-1.481339
13	6	0	6.717454	4.435245	-0.192946
14	6	0	7.544150	3.799486	0.733050
15	6	0	10.750424	2.437129	4.779081
16	6	0	10.107997	-2.696235	-3.335907
17	6	0	9.774192	-1.964167	-2.215051
18	6	0	8.872990	-2.466036	-1.245970
19	6	0	8.307279	-3.761184	-1.451882
20	6	0	8.673877	-4.481195	-2.611610
21	6	0	9.557432	-3.978154	-3.554077
22	6	0	8.546369	-1.713419	-0.047138
23	6	0	7.369112	-4.297081	-0.473929
24	6	0	7.251323	-3.627329	0.775927
25	6	0	7.856473	-2.346236	0.955737
26	6	0	6.386321	-4.159747	1.760290
27	6	0	5.560748	-5.224703	1.478352
28	6	0	5.559079	-5.819540	0.190245
29	6	0	6.506691	-5.383680	-0.735610
30	6	0	9.941048	-4.774059	-4.777897
31	6	0	-10.109356	2.698140	-3.334225
32	6	0	-9.775137	1.965515	-2.213865
33	6	0	-8.873182	2.466661	-1.245077
34	6	0	-8.307415	3.761820	-1.450631
35	6	0	-8.674594	4.482518	-2.609794
36	6	0	-9.558592	3.980062	-3.552115
37	6	0	-8.546130	1.713403	-0.046769
38	6	0	-7.368814	4.297210	-0.472847
39	6	0	-7.250593	3.626932	0.776658
40	6	0	-7.855721	2.345773	0.956120
41	6	0	-6.385186	4.158965	1.760874
42	6	0	-5.559717	5.224003	1.479054
43	6	0	-5.558489	5.819400	0.191197
44	6	0	-6.506391	5.383790	-0.734456
45	6	0	-9.942227	4.776340	-4.775687
46	6	0	-10.452983	-0.376509	3.334257
47	6	0	-9.965043	0.262543	2.213137
48	6	0	-9.199618	-0.427788	1.243269
49	6	0	-8.937818	-1.816681	1.448684
50	6	0	-9.455787	-2.436923	2.608378

51	6	0	-10.203075	-1.749219	3.551893
52	6	0	-8.713751	0.233228	0.044570
53	6	0	-8.142983	-2.548329	0.470622
54	6	0	-7.878436	-1.921265	-0.778963
55	6	0	-8.182532	-0.537442	-0.958517
56	6	0	-7.154006	-2.632958	-1.763547
57	6	0	-6.586358	-3.855023	-1.481840
58	6	0	-6.717140	-4.435295	-0.193699
59	6	0	-7.544370	-3.799828	0.731968
60	6	0	-10.754182	-2.439388	4.775871
61	6	0	-2.693600	-10.107439	-3.333532
62	6	0	-1.962190	-9.772137	-2.212714
63	6	0	-2.465001	-8.870361	-1.244641
64	6	0	-3.760345	-8.305458	-1.451650
65	6	0	-4.479761	-8.673765	-2.611270
66	6	0	-3.975814	-9.557880	-3.552718
67	6	0	-1.713169	-8.542526	-0.045689
68	6	0	-4.297287	-7.366881	-0.474575
69	6	0	-3.628258	-7.247914	0.775565
70	6	0	-2.346867	-7.852135	0.956405
71	6	0	-4.161853	-6.382862	1.759227
72	6	0	-5.227269	-5.558279	1.476356
73	6	0	-5.821279	-5.557488	0.187893
74	6	0	-5.384184	-6.505133	-0.737339
75	6	0	-4.770942	-9.942987	-4.776568
76	6	0	0.373726	-10.444197	3.340180
77	6	0	-0.264363	-9.957800	2.217819
78	6	0	0.426917	-9.194119	1.247246
79	6	0	1.815789	-8.932549	1.453207
80	6	0	2.435043	-9.449016	2.614090
81	6	0	1.746361	-10.194419	3.558398
82	6	0	-0.233043	-8.709794	0.047354
83	6	0	2.548348	-8.139325	0.474501
84	6	0	1.922159	-7.876103	-0.775813
85	6	0	0.538386	-8.180041	-0.955898
86	6	0	2.634699	-7.153171	-1.760876
87	6	0	3.856813	-6.585662	-1.479146
88	6	0	4.436278	-6.715050	-0.190501
89	6	0	3.799964	-7.540921	0.735835
90	6	0	2.435369	-10.742980	4.784188
91	6	0	2.694276	10.106239	-3.334465
92	6	0	1.962969	9.771747	-2.213357
93	6	0	2.465557	8.870179	-1.244974
94	6	0	3.760815	8.305080	-1.451792
95	6	0	4.480172	8.672595	-2.611665
96	6	0	3.976290	9.556223	-3.553560
97	6	0	1.713614	8.542769	-0.045961
98	6	0	4.297614	7.366776	-0.474490
99	6	0	3.628480	7.248183	0.775609
100	6	0	2.347167	7.852597	0.956229
101	6	0	4.161912	6.383217	1.759470
102	6	0	5.227281	5.558426	1.476806
103	6	0	5.821468	5.557430	0.188399
104	6	0	5.384503	6.504961	-0.737013
105	6	0	4.771258	9.940489	-4.777789
106	6	0	-0.373106	10.445414	3.339217
107	6	0	0.264926	9.958633	2.217024
108	6	0	-0.426404	9.194665	1.246729
109	6	0	-1.815192	8.932998	1.452947

110	6	0	-2.434415	9.449882	2.613639
111	6	0	-1.745771	10.195847	3.557502
112	6	0	0.233516	8.710058	0.046925
113	6	0	-2.547789	8.139409	0.474583
114	6	0	-1.921749	7.876048	-0.775759
115	6	0	-0.537999	8.180035	-0.956071
116	6	0	-2.634476	7.153014	-1.760625
117	6	0	-3.856574	6.585538	-1.478658
118	6	0	-4.435761	6.714871	-0.189886
119	6	0	-3.799267	7.540887	0.736227
120	6	0	-2.434929	10.745674	4.782620
121	1	0	6.980831	2.162260	-2.726788
122	1	0	5.952493	4.332852	-2.220199
123	1	0	7.668033	4.250152	1.711519
124	1	0	7.835831	0.062028	-1.870328
125	1	0	10.180368	-1.314454	2.055314
126	1	0	11.045894	-0.181509	4.055987
127	1	0	9.288417	3.498133	2.758554
128	1	0	10.492494	3.499416	4.791290
129	1	0	10.358190	1.986467	5.698425
130	1	0	11.842651	2.356126	4.825098
131	1	0	4.835008	-5.548611	2.216851
132	1	0	6.527090	-5.850099	-1.714393
133	1	0	6.320559	-3.661328	2.723858
134	1	0	7.622637	-1.804497	1.867339
135	1	0	8.274447	-5.479473	-2.760285
136	1	0	10.220901	-0.988644	-2.055623
137	1	0	10.814522	-2.287961	-4.054349
138	1	0	9.456725	-5.754163	-4.787833
139	1	0	9.655873	-4.250076	-5.697826
140	1	0	11.024413	-4.934433	-4.825167
141	1	0	-6.319047	3.660157	2.724213
142	1	0	-4.833644	5.547463	2.217411
143	1	0	-6.527106	5.850487	-1.713095
144	1	0	-7.621509	1.803602	1.867357
145	1	0	-10.222273	0.990190	-2.054452
146	1	0	-10.816566	2.290434	-4.052324
147	1	0	-8.275170	5.480844	-2.758143
148	1	0	-9.462324	5.758633	-4.782432
149	1	0	-9.651758	4.255332	-5.695681
150	1	0	-11.026145	4.931780	-4.826049
151	1	0	-5.950850	-4.332230	-2.220396
152	1	0	-7.668847	-4.250787	1.710221
153	1	0	-6.978857	-2.161484	-2.726970
154	1	0	-7.834388	-0.061565	-1.870353
155	1	0	-9.290493	-3.499516	2.755946
156	1	0	-10.182521	1.313187	2.053886
157	1	0	-11.049605	0.179344	4.053337
158	1	0	-11.845875	-2.352829	4.824369
159	1	0	-10.501703	-3.503022	4.784734
160	1	0	-10.357737	-1.993268	5.695625
161	1	0	-3.664003	-6.316268	2.723034
162	1	0	-5.552114	-4.832413	2.214328
163	1	0	-5.849931	-6.526210	-1.716405
164	1	0	-1.805759	-7.617499	1.868170
165	1	0	-0.986675	-10.218494	-2.052255
166	1	0	-2.284723	-10.814633	-4.050973
167	1	0	-5.478303	-8.275292	-2.760595
168	1	0	-4.247071	-9.657590	-5.696517

169	1	0	-4.930115	-11.026508	-4.823358
170	1	0	-5.751569	-9.459690	-4.787060
171	1	0	4.334905	-5.951583	-2.218363
172	1	0	4.250477	-7.664676	1.714372
173	1	0	2.163960	-6.979214	-2.724875
174	1	0	0.063204	-7.833155	-1.868580
175	1	0	3.497598	-9.283957	2.762128
176	1	0	-1.314947	-10.175250	2.058138
177	1	0	-0.182842	-11.039514	4.059790
178	1	0	3.500456	-10.496564	4.790001
179	1	0	1.993133	-10.338877	5.702520
180	1	0	2.342565	-11.833829	4.838764
181	1	0	3.664000	6.316871	2.723260
182	1	0	5.552045	4.832708	2.214959
183	1	0	5.850308	6.525858	-1.716064
184	1	0	1.806018	7.618215	1.868025
185	1	0	0.987501	10.218269	-2.053122
186	1	0	2.285415	10.813021	-4.052320
187	1	0	5.478564	8.273701	-2.760950
188	1	0	5.752593	9.458658	-4.787140
189	1	0	4.248060	9.652848	-5.697412
190	1	0	4.928802	11.024199	-4.826350
191	1	0	-4.334717	5.951364	-2.217766
192	1	0	-4.249605	7.664837	1.714815
193	1	0	-2.163916	6.978962	-2.724696
194	1	0	-0.062956	7.832970	-1.868749
195	1	0	-3.496900	9.284564	2.761946
196	1	0	1.315534	10.175928	2.057300
197	1	0	0.183539	11.040829	4.058681
198	1	0	-3.497424	10.488583	4.794748
199	1	0	-1.984522	10.352506	5.701692
200	1	0	-2.353037	11.837803	4.829304

Table S4. Cartesian coordinate of *E,R,E,R,E,R,Z,S* (2)

SCF Done: E(RB3LYP) = -4621.34869885 A.U. after 7 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.661842	-6.562677	3.497200
2	6	0	-1.123379	-7.123961	2.358214
3	6	0	-1.903013	-7.336015	1.193828
4	6	0	-3.254336	-6.879434	1.206821
5	6	0	-3.778792	-6.330122	2.399685
6	6	0	-3.017398	-6.172604	3.545522
7	6	0	-1.363946	-7.957533	-0.009099
8	6	0	-4.040087	-6.933272	-0.016391
9	6	0	-3.533014	-7.664582	-1.124609
10	6	0	-2.197748	-8.180727	-1.074003
11	6	0	-4.304209	-7.721636	-2.311527
12	6	0	-5.448952	-6.965468	-2.457337
13	6	0	-5.886909	-6.112364	-1.412410
14	6	0	-5.208279	-6.164640	-0.197406
15	6	0	-3.603956	-5.598060	4.811662
16	6	0	1.198129	-10.772711	2.267331
17	6	0	0.398039	-9.963362	1.487695
18	6	0	0.951501	-8.954607	0.664576
19	6	0	2.369591	-8.783362	0.653814

20	6	0	3.155954	-9.631385	1.466446
21	6	0	2.602487	-10.618209	2.268076
22	6	0	0.114134	-8.120203	-0.175666
23	6	0	2.961073	-7.752940	-0.191174
24	6	0	2.131153	-7.138589	-1.169902
25	6	0	0.716476	-7.337832	-1.124768
26	6	0	2.697527	-6.204763	-2.066432
27	6	0	3.995741	-5.774661	-1.911286
28	6	0	4.790627	-6.249354	-0.836416
29	6	0	4.280799	-7.271491	-0.036665
30	6	0	3.466747	-11.519868	3.115746
31	6	0	-1.013174	9.487626	4.093617
32	6	0	-0.328520	9.199006	2.931206
33	6	0	-0.951672	8.525266	1.853710
34	6	0	-2.322213	8.147263	1.991578
35	6	0	-2.990372	8.461600	3.197013
36	6	0	-2.367496	9.118615	4.246674
37	6	0	-0.242864	8.248474	0.616242
38	6	0	-2.988133	7.450061	0.898661
39	6	0	-2.324654	7.389500	-0.358648
40	6	0	-0.960474	7.799050	-0.463136
41	6	0	-2.975888	6.767455	-1.449431
42	6	0	-4.174289	6.111276	-1.280352
43	6	0	-4.788370	6.042388	-0.003400
44	6	0	-4.211894	6.760843	1.043598
45	6	0	-3.108825	9.450897	5.518773
46	6	0	2.113970	10.261513	-2.515278
47	6	0	1.406182	9.726970	-1.458461
48	6	0	1.977040	8.755038	-0.602433
49	6	0	3.318179	8.333972	-0.854423
50	6	0	4.011549	8.904863	-1.945811
51	6	0	3.439972	9.853931	-2.778936
52	6	0	1.246931	8.213244	0.530923
53	6	0	3.928619	7.330783	0.008291
54	6	0	3.263344	6.997335	1.221058
55	6	0	1.930519	7.457695	1.449713
56	6	0	3.867889	6.070321	2.102218
57	6	0	5.007871	5.387453	1.741296
58	6	0	5.605539	5.597072	0.471873
59	6	0	5.090198	6.607701	-0.339000
60	6	0	4.207787	10.455087	-3.930992
61	6	0	10.824135	0.595574	2.954490
62	6	0	10.349197	0.025097	1.791103
63	6	0	9.476336	0.726658	0.926160
64	6	0	9.095809	2.057009	1.280905
65	6	0	9.601787	2.607141	2.480340
66	6	0	10.452192	1.906966	3.322181
67	6	0	8.995110	0.139586	-0.313542
68	6	0	8.201857	2.805483	0.406259
69	6	0	7.958264	2.286987	-0.895871
70	6	0	8.367545	0.957910	-1.219533
71	6	0	7.150396	3.027415	-1.789956
72	6	0	6.486529	4.158961	-1.373264
73	6	0	6.594938	4.610004	-0.032505
74	6	0	7.497223	3.960476	0.809989
75	6	0	10.988262	2.524206	4.591008
76	6	0	10.142655	-1.887505	-4.063902
77	6	0	9.922588	-1.300810	-2.834045
78	6	0	9.132591	-1.932733	-1.844892

79	6	0	8.564122	-3.206737	-2.145669
80	6	0	8.809236	-3.776066	-3.415462
81	6	0	9.582163	-3.144700	-4.377932
82	6	0	8.917299	-1.333062	-0.537101
83	6	0	7.747317	-3.878736	-1.144307
84	6	0	7.792687	-3.389480	0.190765
85	6	0	8.383977	-2.115504	0.457139
86	6	0	7.072146	-4.076763	1.195849
87	6	0	6.205442	-5.098135	0.873267
88	6	0	6.010157	-5.478322	-0.478976
89	6	0	6.836236	-4.912110	-1.449145
90	6	0	9.840027	-3.780454	-5.722425
91	6	0	-10.658454	-1.571124	2.428683
92	6	0	-10.195963	-0.775405	1.400493
93	6	0	-9.426857	-1.311176	0.340201
94	6	0	-9.133929	-2.708458	0.354850
95	6	0	-9.624076	-3.491470	1.424409
96	6	0	-10.376728	-2.954493	2.457396
97	6	0	-8.968266	-0.485242	-0.764389
98	6	0	-8.338163	-3.284147	-0.721182
99	6	0	-8.120861	-2.496363	-1.885938
100	6	0	-8.450630	-1.106083	-1.873340
101	6	0	-7.411384	-3.060868	-2.971844
102	6	0	-6.801622	-4.290655	-2.857499
103	6	0	-6.865837	-5.018525	-1.641784
104	6	0	-7.691462	-4.535282	-0.627472
105	6	0	-10.900930	-3.816091	3.580459
106	6	0	-10.359221	2.427165	-3.772726
107	6	0	-10.029702	1.545889	-2.763561
108	6	0	-9.137254	1.908862	-1.726831
109	6	0	-8.579249	3.223745	-1.741818
110	6	0	-8.941069	4.098195	-2.791762
111	6	0	-9.813290	3.728998	-3.803935
112	6	0	-8.811215	0.994018	-0.646305
113	6	0	-7.656176	3.624038	-0.687352
114	6	0	-7.539877	2.781886	0.453588
115	6	0	-8.130838	1.481966	0.440796
116	6	0	-6.694603	3.178313	1.516206
117	6	0	-5.888990	4.289191	1.405801
118	6	0	-5.886464	5.066741	0.219235
119	6	0	-6.810831	4.751317	-0.776228
120	6	0	-10.191515	4.688282	-4.906169
121	1	0	-3.944839	-8.326891	-3.139892
122	1	0	-5.995339	-6.989608	-3.395572
123	1	0	-5.509149	-5.479060	0.585376
124	1	0	-1.802981	-8.664163	-1.963798
125	1	0	-0.081648	-7.415959	2.359489
126	1	0	-1.033594	-6.424758	4.373771
127	1	0	-4.822270	-6.033509	2.428315
128	1	0	-3.566639	-6.323642	5.632909
129	1	0	-3.046417	-4.713875	5.141631
130	1	0	-4.647629	-5.303630	4.672820
131	1	0	4.381493	-4.986001	-2.548772
132	1	0	4.894553	-7.653189	0.772665
133	1	0	2.066469	-5.766540	-2.835093
134	1	0	0.100227	-6.734054	-1.784527
135	1	0	4.236730	-9.532007	1.440353
136	1	0	-0.678703	-10.100637	1.488440
137	1	0	0.745225	-11.547259	2.881248

138	1	0	4.529411	-11.304730	2.975632
139	1	0	3.302459	-12.575334	2.869862
140	1	0	3.238791	-11.401536	4.181744
141	1	0	-2.476159	6.747111	-2.414310
142	1	0	-4.605779	5.560829	-2.109864
143	1	0	-4.690149	6.730108	2.016318
144	1	0	-0.449170	7.606181	-1.401474
145	1	0	0.706007	9.506731	2.824642
146	1	0	-0.508826	10.018426	4.897307
147	1	0	-4.040638	8.207559	3.299762
148	1	0	-2.648637	8.962350	6.385808
149	1	0	-3.096899	10.528968	5.716744
150	1	0	-4.153003	9.130709	5.470231
151	1	0	5.395942	4.610068	2.391269
152	1	0	5.558120	6.788804	-1.300388
153	1	0	3.371796	5.841480	3.041724
154	1	0	1.405168	7.063573	2.314508
155	1	0	5.041997	8.614699	-2.125193
156	1	0	0.394968	10.065654	-1.260815
157	1	0	1.650972	11.016808	-3.145503
158	1	0	5.225676	10.059871	-3.984465
159	1	0	3.716318	10.245321	-4.888404
160	1	0	4.275105	11.545348	-3.839287
161	1	0	6.992356	2.642445	-2.793960
162	1	0	5.794127	4.652648	-2.047041
163	1	0	7.602290	4.314714	1.829751
164	1	0	8.019490	0.545228	-2.161161
165	1	0	10.660898	-0.976811	1.516009
166	1	0	11.504539	0.034109	3.589985
167	1	0	9.342584	3.628546	2.741351
168	1	0	10.702006	1.935725	5.470611
169	1	0	12.083546	2.569569	4.580302
170	1	0	10.612670	3.541096	4.732550
171	1	0	5.583274	-5.540232	1.644906
172	1	0	6.707731	-5.216555	-2.482459
173	1	0	7.141081	-3.726431	2.222340
174	1	0	8.239511	-1.696830	1.448289
175	1	0	8.406817	-4.759750	-3.637725
176	1	0	10.375797	-0.342179	-2.605426
177	1	0	10.767420	-1.382294	-4.796326
178	1	0	9.363836	-4.761414	-5.799905
179	1	0	9.455362	-3.155908	-6.537367
180	1	0	10.913350	-3.912843	-5.901435
181	1	0	-7.280447	-2.470894	-3.875161
182	1	0	-6.179264	-4.658724	-3.666763
183	1	0	-7.767740	-5.104380	0.292761
184	1	0	-8.125511	-0.507169	-2.718728
185	1	0	-10.438151	0.281766	1.386379
186	1	0	-11.260247	-1.131296	3.220172
187	1	0	-9.434222	-4.560328	1.424449
188	1	0	-10.504150	-3.490773	4.549481
189	1	0	-11.993551	-3.760407	3.648524
190	1	0	-10.627201	-4.865500	3.442538
191	1	0	-5.179798	4.517573	2.194544
192	1	0	-6.829183	5.356523	-1.675856
193	1	0	-6.629997	2.545195	2.397189
194	1	0	-7.897186	0.817230	1.266870
195	1	0	-8.546707	5.109514	-2.794905
196	1	0	-10.473135	0.556197	-2.746005

197	1	0	-11.058627	2.121343	-4.546881
198	1	0	-9.695844	5.655021	-4.784303
199	1	0	-9.915356	4.291490	-5.890194
200	1	0	-11.273115	4.865864	-4.926028

Table S5. Cartesian coordinate of *E,R,E,R,Z,S,Z,R* (3)

SCF Done: E(RB3LYP) = -4621.34868696 A.U. after 5 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-10.234820	-2.449127	-2.677030
2	6	0	-9.778223	-1.460546	-1.830169
3	6	0	-8.928330	-1.757666	-0.738054
4	6	0	-8.540282	-3.116731	-0.528229
5	6	0	-9.032235	-4.101470	-1.414979
6	6	0	-9.866950	-3.798207	-2.479364
7	6	0	-8.480116	-0.724232	0.177248
8	6	0	-7.642357	-3.444147	0.572686
9	6	0	-7.385185	-2.437376	1.545130
10	6	0	-7.830784	-1.099376	1.324732
11	6	0	-6.540000	-2.739628	2.636879
12	6	0	-5.867573	-3.937817	2.702607
13	6	0	-6.013253	-4.914198	1.682068
14	6	0	-6.946780	-4.669137	0.674409
15	6	0	-10.387272	-4.872727	-3.402911
16	6	0	-10.233895	2.452012	2.677374
17	6	0	-9.777661	1.463279	1.830497
18	6	0	-8.927756	1.760121	0.738314
19	6	0	-8.539304	3.119065	0.528439
20	6	0	-9.030904	4.103968	1.415202
21	6	0	-9.865659	3.800982	2.479635
22	6	0	-8.479893	0.726530	-0.176982
23	6	0	-7.641320	3.446183	-0.572515
24	6	0	-7.384482	2.439307	-1.544939
25	6	0	-7.830485	1.101452	-1.324496
26	6	0	-6.539237	2.741266	-2.636723
27	6	0	-5.866454	3.939251	-2.702511
28	6	0	-6.011826	4.915717	-1.682009
29	6	0	-6.945393	4.670970	-0.674311
30	6	0	-10.385865	4.875718	3.402995
31	6	0	10.302232	-1.422378	-3.448440
32	6	0	9.941199	-0.779571	-2.281754
33	6	0	9.110904	-1.403253	-1.320499
34	6	0	8.651716	-2.729594	-1.582016
35	6	0	9.041071	-3.355496	-2.787676
36	6	0	9.851689	-2.731813	-3.723587
37	6	0	8.751461	-0.743134	-0.075554
38	6	0	7.800633	-3.398589	-0.606943
39	6	0	7.688180	-2.819981	0.687899
40	6	0	8.171572	-1.494983	0.915920
41	6	0	6.933375	-3.493384	1.676916
42	6	0	6.190448	-4.610083	1.363494
43	6	0	6.158358	-5.105626	0.035127
44	6	0	7.011605	-4.530209	-0.905555
45	6	0	10.263125	-3.428069	-4.998024
46	6	0	10.302510	1.419545	3.448733
47	6	0	9.941345	0.776824	2.282040

48	6	0	9.111251	1.400721	1.320750
49	6	0	8.652428	2.727195	1.582228
50	6	0	9.041907	3.353003	2.787896
51	6	0	9.852313	2.729106	3.723848
52	6	0	8.751667	0.740685	0.075797
53	6	0	7.801578	3.396420	0.607106
54	6	0	7.689020	2.817827	-0.687733
55	6	0	8.172047	1.492688	-0.915715
56	6	0	6.934454	3.491429	-1.676793
57	6	0	6.191833	4.608348	-1.363421
58	6	0	6.159828	5.103924	-0.035067
59	6	0	7.012869	4.528274	0.905664
60	6	0	10.263877	3.425255	4.998302
61	6	0	1.840149	10.797849	-2.789208
62	6	0	1.019846	10.181587	-1.866184
63	6	0	1.497458	9.151367	-1.021797
64	6	0	2.869031	8.766642	-1.134475
65	6	0	3.677119	9.418443	-2.093430
66	6	0	3.193343	10.418604	-2.922549
67	6	0	0.642673	8.513676	-0.032213
68	6	0	3.400905	7.729314	-0.259498
69	6	0	2.602523	7.319371	0.844114
70	6	0	1.234509	7.719790	0.918630
71	6	0	3.127093	6.381342	1.763161
72	6	0	4.334275	5.762227	1.531111
73	6	0	5.074480	6.041364	0.353689
74	6	0	4.621984	7.057010	-0.487744
75	6	0	4.082848	11.106074	-3.929650
76	6	0	-2.099273	9.067177	3.376948
77	6	0	-1.275346	9.048972	2.269799
78	6	0	-1.701339	8.494991	1.039223
79	6	0	-3.023133	7.963585	0.960625
80	6	0	-3.837258	7.996043	2.115193
81	6	0	-3.403305	8.529648	3.318751
82	6	0	-0.844491	8.486305	-0.137812
83	6	0	-3.504546	7.423122	-0.303065
84	6	0	-2.744928	7.691070	-1.474542
85	6	0	-1.417871	8.207768	-1.354606
86	6	0	-3.257996	7.273956	-2.725733
87	6	0	-4.387619	6.490533	-2.805345
88	6	0	-5.049764	6.047062	-1.630157
89	6	0	-4.626133	6.574312	-0.409574
90	6	0	-4.296333	8.560038	4.535148
91	6	0	-2.101824	-9.066202	-3.377291
92	6	0	-1.277902	-9.048350	-2.270136
93	6	0	-1.703760	-8.494408	-1.039492
94	6	0	-3.025408	-7.962647	-0.960840
95	6	0	-3.839532	-7.994748	-2.115422
96	6	0	-3.405719	-8.528339	-3.319034
97	6	0	-0.846914	-8.486068	0.137540
98	6	0	-3.506671	-7.422175	0.302902
99	6	0	-2.747118	-7.690428	1.474354
100	6	0	-1.420208	-8.207482	1.354364
101	6	0	-3.260064	-7.273280	2.725584
102	6	0	-4.389469	-6.489553	2.805271
103	6	0	-5.051506	-6.045808	1.630124
104	6	0	-4.628034	-6.573079	0.409497
105	6	0	-4.298799	-8.558493	-4.535398
106	6	0	1.837042	-10.798577	2.788773

107	6	0	1.016917	-10.181992	1.865806
108	6	0	1.494827	-9.151821	1.021530
109	6	0	2.866501	-8.767478	1.134270
110	6	0	3.674393	-9.419585	2.093182
111	6	0	3.190325	-10.419683	2.922207
112	6	0	0.640246	-8.513837	0.031961
113	6	0	3.398685	-7.730249	0.259363
114	6	0	2.600445	-7.320019	-0.844243
115	6	0	1.232320	-7.720052	-0.918816
116	6	0	3.125298	-6.382084	-1.763226
117	6	0	4.332652	-5.763326	-1.531114
118	6	0	5.072750	-6.042738	-0.353690
119	6	0	4.619947	-7.058298	0.487680
120	6	0	4.079524	-11.107206	3.929541
121	1	0	-6.363795	-1.975900	3.389718
122	1	0	-5.151193	-4.096396	3.500691
123	1	0	-7.089218	-5.420254	-0.094239
124	1	0	-7.506076	-0.338076	2.028065
125	1	0	-10.084288	-0.431621	-1.986076
126	1	0	-10.897376	-2.189996	-3.499154
127	1	0	-8.771415	-5.141431	-1.245441
128	1	0	-10.076434	-4.691338	-4.438554
129	1	0	-10.023529	-5.862045	-3.112771
130	1	0	-11.483061	-4.904234	-3.399908
131	1	0	-5.150044	4.097592	-3.500616
132	1	0	-7.087585	5.422160	0.094311
133	1	0	-6.363282	1.977457	-3.389537
134	1	0	-7.506037	0.340035	-2.027822
135	1	0	-8.769750	5.143844	1.245652
136	1	0	-10.083988	0.434442	1.986471
137	1	0	-10.896438	2.193092	3.499575
138	1	0	-10.077943	4.692645	4.439197
139	1	0	-10.019335	5.864539	3.114671
140	1	0	-11.481587	4.909604	3.397355
141	1	0	6.879543	-3.066825	2.675060
142	1	0	5.541364	-5.053318	2.111902
143	1	0	7.006153	-4.921802	-1.917247
144	1	0	7.917297	-1.027849	1.862229
145	1	0	10.313148	0.219151	-2.079939
146	1	0	10.954261	-0.920493	-4.159078
147	1	0	8.722996	-4.375931	-2.977107
148	1	0	9.899461	-2.888595	-5.880619
149	1	0	11.354182	-3.485354	-5.086429
150	1	0	9.869237	-4.446845	-5.043589
151	1	0	5.542906	5.051751	-2.111866
152	1	0	7.007494	4.919892	1.917347
153	1	0	6.880540	3.064871	-2.674932
154	1	0	7.917687	1.025616	-1.862032
155	1	0	8.724110	4.373529	2.977305
156	1	0	10.313030	-0.222000	2.080246
157	1	0	10.954377	0.917493	4.159402
158	1	0	9.870441	4.444212	5.043748
159	1	0	9.899836	2.886001	5.880878
160	1	0	11.354945	3.482050	5.086866
161	1	0	2.525024	6.096738	2.622033
162	1	0	4.675631	4.979340	2.200456
163	1	0	5.197774	7.285563	-1.378424
164	1	0	0.621420	7.249284	1.680350
165	1	0	-0.011218	10.502540	-1.765105

166	1	0	1.443717	11.595880	-3.412128
167	1	0	4.727059	9.152134	-2.164483
168	1	0	3.705131	10.971682	-4.950096
169	1	0	4.131207	12.185914	-3.747110
170	1	0	5.103125	10.714814	-3.896679
171	1	0	-4.745910	6.171237	-3.778375
172	1	0	-5.100595	6.226745	0.500783
173	1	0	-2.715636	7.539281	-3.629478
174	1	0	-0.805910	8.220565	-2.251002
175	1	0	-4.854447	7.622154	2.051504
176	1	0	-0.283683	9.483767	2.330992
177	1	0	-1.745468	9.514415	4.302605
178	1	0	-5.289218	8.159546	4.313780
179	1	0	-3.871832	7.967183	5.354061
180	1	0	-4.421880	9.581477	4.912363
181	1	0	-2.717766	-7.538827	3.629301
182	1	0	-4.747664	-6.170243	3.778332
183	1	0	-5.102416	-6.225311	-0.500826
184	1	0	-0.808238	-8.220533	2.250751
185	1	0	-0.286350	-9.483392	-2.331373
186	1	0	-1.748121	-9.513397	-4.303009
187	1	0	-4.856614	-7.620574	-2.051709
188	1	0	-3.873414	-7.967065	-5.354877
189	1	0	-4.425903	-9.580102	-4.911645
190	1	0	-5.291079	-8.156310	-4.314386
191	1	0	4.674249	-4.980501	-2.200410
192	1	0	5.195644	-7.287056	1.378367
193	1	0	2.523328	-6.097263	-2.622094
194	1	0	0.619378	-7.249331	-1.680521
195	1	0	4.724412	-9.153590	2.164250
196	1	0	-0.014221	-10.502680	1.764644
197	1	0	1.440401	-11.596605	3.411565
198	1	0	5.100868	-10.718975	3.893895
199	1	0	3.703936	-10.969070	4.950291
200	1	0	4.124398	-12.187633	3.749713

Table S6. Cartesian coordinate of *E,R,E,R,E,R,Z,R* (4)

SCF Done: E(RB3LYP) = -4621.34592255 A.U. after 6 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-10.787116	2.506245	-3.099380
2	6	0	-10.274779	1.586704	-2.206615
3	6	0	-9.275327	1.942398	-1.270452
4	6	0	-8.805526	3.291345	-1.261581
5	6	0	-9.352407	4.203910	-2.191568
6	6	0	-10.327415	3.840981	-3.108095
7	6	0	-8.751154	0.984424	-0.309731
8	6	0	-7.784287	3.690060	-0.301022
9	6	0	-7.496184	2.798375	0.769138
10	6	0	-7.991720	1.459785	0.730716
11	6	0	-6.568200	3.192539	1.760971
12	6	0	-5.837621	4.351454	1.625842
13	6	0	-5.993590	5.175721	0.481929
14	6	0	-7.006217	4.861777	-0.424618
15	6	0	-10.903440	4.839797	-4.082238
16	6	0	-9.656891	-2.022400	2.795934

17	6	0	-9.530693	-1.106276	1.771219
18	6	0	-8.890461	-1.441736	0.554893
19	6	0	-8.378390	-2.764972	0.403570
20	6	0	-8.521878	-3.674881	1.474958
21	6	0	-9.145866	-3.331963	2.664601
22	6	0	-8.772327	-0.488915	-0.538523
23	6	0	-7.727868	-3.141724	-0.843594
24	6	0	-7.888921	-2.281066	-1.963961
25	6	0	-8.411946	-0.964312	-1.775803
26	6	0	-7.337425	-2.670428	-3.208226
27	6	0	-6.510327	-3.766986	-3.303116
28	6	0	-6.178925	-4.525776	-2.150512
29	6	0	-6.851883	-4.242465	-0.962504
30	6	0	-9.298621	-4.326487	3.789659
31	6	0	11.076155	0.913170	2.491171
32	6	0	10.493191	0.211423	1.455752
33	6	0	9.465825	0.776621	0.663513
34	6	0	9.048808	2.113279	0.949914
35	6	0	9.667741	2.798880	2.019886
36	6	0	10.664577	2.228559	2.796159
37	6	0	8.863909	0.048202	-0.442251
38	6	0	8.014717	2.737099	0.133337
39	6	0	7.631172	2.079215	-1.068198
40	6	0	8.063549	0.741743	-1.315563
41	6	0	6.695048	2.701427	-1.926324
42	6	0	6.060459	3.865568	-1.556957
43	6	0	6.320605	4.461356	-0.296330
44	6	0	7.326220	3.914858	0.499927
45	6	0	11.313643	2.988424	3.927392
46	6	0	9.572444	-2.170464	-4.185553
47	6	0	9.504314	-1.510264	-2.975507
48	6	0	8.940874	-2.121187	-1.830009
49	6	0	8.450671	-3.455844	-1.950087
50	6	0	8.531865	-4.098868	-3.205896
51	6	0	9.077031	-3.485438	-4.323044
52	6	0	8.882184	-1.439509	-0.545190
53	6	0	7.896294	-4.122574	-0.780632
54	6	0	8.119850	-3.530227	0.491971
55	6	0	8.601058	-2.186931	0.572586
56	6	0	7.689171	-4.224618	1.648267
57	6	0	6.922509	-5.363495	1.547865
58	6	0	6.509794	-5.851703	0.279729
59	6	0	7.066261	-5.261649	-0.855181
60	6	0	9.162572	-4.197989	-5.650815
61	6	0	-0.066151	-6.816928	3.734999
62	6	0	-0.339506	-7.263702	2.459058
63	6	0	0.695093	-7.530009	1.528099
64	6	0	2.036067	-7.252263	1.925214
65	6	0	2.280150	-6.815801	3.247925
66	6	0	1.262010	-6.602909	4.162218
67	6	0	0.431579	-8.031364	0.186081
68	6	0	3.109876	-7.375080	0.951452
69	6	0	2.841167	-8.012418	-0.289616
70	6	0	1.488712	-8.338985	-0.631085
71	6	0	3.902221	-8.159028	-1.217245
72	6	0	5.131759	-7.572031	-0.999396
73	6	0	5.364318	-6.790133	0.161793
74	6	0	4.365893	-6.763453	1.133814
75	6	0	1.548612	-6.151381	5.573294

76	6	0	-3.010840	-10.550631	1.414478
77	6	0	-1.927472	-9.826093	0.962858
78	6	0	-2.092760	-8.705412	0.115118
79	6	0	-3.416536	-8.328149	-0.270247
80	6	0	-4.500555	-9.095961	0.213237
81	6	0	-4.326175	-10.193777	1.042039
82	6	0	-0.952063	-7.960572	-0.380183
83	6	0	-3.610597	-7.176844	-1.144465
84	6	0	-2.461687	-6.623659	-1.775901
85	6	0	-1.156416	-7.034485	-1.367243
86	6	0	-2.619900	-5.559108	-2.690079
87	6	0	-3.847336	-4.969205	-2.879474
88	6	0	-4.984249	-5.408897	-2.152348
89	6	0	-4.856102	-6.536844	-1.342553
90	6	0	-5.501460	-11.005460	1.530385
91	6	0	-0.918896	9.652603	4.015988
92	6	0	-0.303881	9.340097	2.820915
93	6	0	-0.993360	8.657633	1.790491
94	6	0	-2.357539	8.297954	2.012181
95	6	0	-2.953374	8.634696	3.248762
96	6	0	-2.265403	9.299509	4.251950
97	6	0	-0.359714	8.353620	0.517901
98	6	0	-3.093845	7.598053	0.967524
99	6	0	-2.512940	7.534210	-0.329626
100	6	0	-1.149796	7.918052	-0.516300
101	6	0	-3.240738	6.924335	-1.378123
102	6	0	-4.427084	6.270254	-1.131008
103	6	0	-4.945448	6.186837	0.186772
104	6	0	-4.302292	6.904400	1.194780
105	6	0	-2.930121	9.657461	5.558953
106	6	0	1.888090	10.137822	-2.831100
107	6	0	1.224260	9.685411	-1.709142
108	6	0	1.803400	8.727450	-0.843099
109	6	0	3.108022	8.236601	-1.152834
110	6	0	3.756269	8.722557	-2.310879
111	6	0	3.175494	9.656697	-3.154513
112	6	0	1.121121	8.268861	0.356056
113	6	0	3.733775	7.257491	-0.273823
114	6	0	3.136756	7.021487	0.995961
115	6	0	1.834096	7.538713	1.273692
116	6	0	3.769956	6.134411	1.898010
117	6	0	4.869485	5.398035	1.515448
118	6	0	5.386496	5.505107	0.199406
119	6	0	4.845844	6.472069	-0.646771
120	6	0	3.894898	10.166065	-4.379694
121	1	0	-6.376394	2.522269	2.594646
122	1	0	-5.060606	4.583930	2.346594
123	1	0	-7.145680	5.501575	-1.289485
124	1	0	-7.608016	0.767254	1.472878
125	1	0	-10.655223	0.570871	-2.202391
126	1	0	-11.565315	2.203782	-3.795777
127	1	0	-9.023806	5.238334	-2.169098
128	1	0	-10.471082	5.833845	-3.940487
129	1	0	-10.715026	4.537430	-5.119192
130	1	0	-11.990146	4.926821	-3.967912
131	1	0	-6.060544	-4.021229	-4.257872
132	1	0	-6.585821	-4.799658	-0.070911
133	1	0	-7.520592	-2.048688	-4.080681
134	1	0	-8.343897	-0.278171	-2.614127

135	1	0	-8.161146	-4.691564	1.352280
136	1	0	-9.944163	-0.109953	1.885737
137	1	0	-10.168368	-1.737064	3.711905
138	1	0	-8.873522	-5.298631	3.526203
139	1	0	-8.796318	-3.976949	4.699348
140	1	0	-10.353376	-4.479286	4.046245
141	1	0	6.428418	2.206819	-2.856574
142	1	0	5.283524	4.281151	-2.190351
143	1	0	7.539550	4.380756	1.456027
144	1	0	7.618922	0.224379	-2.159458
145	1	0	10.838762	-0.790105	1.223994
146	1	0	11.872839	0.453485	3.070849
147	1	0	9.377622	3.824319	2.226073
148	1	0	10.921164	4.005854	4.004691
149	1	0	11.143727	2.490389	4.889383
150	1	0	12.399086	3.056369	3.790822
151	1	0	6.585632	-5.862529	2.450620
152	1	0	6.750014	-5.609274	-1.831972
153	1	0	7.927949	-3.813658	2.625757
154	1	0	8.579359	-1.707841	1.546438
155	1	0	8.187732	-5.124742	-3.293639
156	1	0	9.906099	-0.506749	-2.887476
157	1	0	10.026061	-1.677323	-5.041761
158	1	0	10.197827	-4.256015	-6.006411
159	1	0	8.773144	-5.217414	-5.585079
160	1	0	8.589366	-3.670006	-6.422095
161	1	0	3.717360	-8.700741	-2.141414
162	1	0	5.914198	-7.674723	-1.745002
163	1	0	4.509703	-6.136769	2.004454
164	1	0	1.293098	-8.734530	-1.624369
165	1	0	-1.369204	-7.423424	2.167246
166	1	0	-0.886452	-6.634191	4.424772
167	1	0	3.304606	-6.659100	3.569999
168	1	0	1.059466	-5.194775	5.791433
169	1	0	1.174805	-6.875310	6.306880
170	1	0	2.621075	-6.025379	5.744317
171	1	0	-3.928231	-4.096049	-3.517580
172	1	0	-5.729552	-6.891006	-0.805184
173	1	0	-1.740384	-5.161926	-3.189737
174	1	0	-0.306757	-6.490618	-1.769549
175	1	0	-5.508520	-8.838998	-0.097418
176	1	0	-0.921376	-10.117822	1.247595
177	1	0	-2.852456	-11.413605	2.056469
178	1	0	-6.447758	-10.608806	1.153003
179	1	0	-5.424380	-12.050793	1.209253
180	1	0	-5.553010	-11.011514	2.625533
181	1	0	-2.807847	6.907381	-2.374842
182	1	0	-4.917337	5.725554	-1.931344
183	1	0	-4.707885	6.861816	2.199899
184	1	0	-0.699250	7.707230	-1.481288
185	1	0	0.725553	9.636701	2.651706
186	1	0	-0.364738	10.190589	4.781188
187	1	0	-3.999114	8.393839	3.412172
188	1	0	-3.977999	9.346211	5.574511
189	1	0	-2.425464	9.177489	6.405788
190	1	0	-2.897965	10.738168	5.739542
191	1	0	5.284227	4.656365	2.190666
192	1	0	5.254287	6.569596	-1.646972
193	1	0	3.327734	5.982018	2.879031

194	1	0	1.348796	7.206790	2.186404
195	1	0	4.760830	8.378213	-2.535211
196	1	0	0.243760	10.081137	-1.467605
197	1	0	1.420848	10.885331	-3.467455
198	1	0	4.895756	9.734714	-4.465419
199	1	0	3.344251	9.918644	-5.295059
200	1	0	3.999850	11.256882	-4.355695

Table S7. Cartesian coordinate of *Z,R,Z,S,Z,R,Z,S* (5)

SCF Done: E(RB3LYP) = -4621.34463867 A.U. after 8 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.615586	-10.417127	-1.313427
2	6	0	-2.558522	-9.864557	-0.619634
3	6	0	-2.726522	-8.723749	0.200606
4	6	0	-4.032445	-8.150112	0.305586
5	6	0	-5.089099	-8.745003	-0.420445
6	6	0	-4.909304	-9.858879	-1.225899
7	6	0	-1.620528	-8.159227	0.955844
8	6	0	-4.241556	-6.979550	1.150314
9	6	0	-3.184951	-6.597480	2.022966
10	6	0	-1.900659	-7.204310	1.900344
11	6	0	-3.373864	-5.503288	2.896989
12	6	0	-4.510038	-4.732279	2.828945
13	6	0	-5.525903	-5.014696	1.878355
14	6	0	-5.395456	-6.165068	1.099247
15	6	0	-6.059879	-10.478438	-1.981329
16	1	0	-2.571267	-5.232295	3.577688
17	1	0	-4.586860	-3.844305	3.446266
18	1	0	-6.181020	-6.401376	0.389732
19	1	0	-1.092765	-6.780743	2.488153
20	1	0	-1.576190	-10.320225	-0.682444
21	1	0	-3.454558	-11.302205	-1.923961
22	1	0	-6.089827	-8.335772	-0.324046
23	1	0	-6.197146	-11.530439	-1.705624
24	1	0	-6.998898	-9.955079	-1.782268
25	1	0	-5.884679	-10.452566	-3.063401
26	6	0	1.526574	-9.007924	3.917517
27	6	0	0.543758	-8.903865	2.954106
28	6	0	0.840118	-8.471071	1.639828
29	6	0	2.193096	-8.147854	1.324800
30	6	0	3.172297	-8.261945	2.337089
31	6	0	2.868252	-8.681352	3.622909
32	6	0	-0.185951	-8.379360	0.611635
33	6	0	2.528927	-7.718600	-0.025050
34	6	0	1.561482	-7.917834	-1.048130
35	6	0	0.214033	-8.241322	-0.694844
36	6	0	1.910161	-7.599561	-2.382558
37	6	0	3.090637	-6.952224	-2.672060
38	6	0	3.978978	-6.562676	-1.635100
39	6	0	3.710810	-7.016680	-0.343912
40	6	0	3.934481	-8.807096	4.683788
41	1	0	3.318381	-6.689928	-3.700244
42	1	0	4.365393	-6.706203	0.462795
43	1	0	1.201042	-7.818850	-3.176534
44	1	0	-0.532390	-8.199184	-1.482238

45	1	0	4.207962	-8.046756	2.092504
46	1	0	-0.478279	-9.174114	3.196590
47	1	0	1.267728	-9.359093	4.913356
48	1	0	4.922898	-8.554050	4.291095
49	1	0	3.731114	-8.142359	5.531689
50	1	0	3.981993	-9.827174	5.082284
51	6	0	-1.526519	9.007492	3.917660
52	6	0	-0.543728	8.903454	2.954220
53	6	0	-0.840143	8.470765	1.639926
54	6	0	-2.193154	8.147687	1.324889
55	6	0	-3.172334	8.261801	2.337182
56	6	0	-2.868233	8.681044	3.623045
57	6	0	0.185878	8.379137	0.611687
58	6	0	-2.529048	7.718609	-0.024995
59	6	0	-1.561597	7.917857	-1.048065
60	6	0	-0.214134	8.241232	-0.694771
61	6	0	-1.910278	7.599683	-2.382510
62	6	0	-3.090782	6.952434	-2.672064
63	6	0	-3.979194	6.562937	-1.635145
64	6	0	-3.710995	7.016821	-0.343914
65	6	0	-3.934446	8.806816	4.683933
66	1	0	-1.201129	7.818958	-3.176464
67	1	0	-3.318502	6.690165	-3.700261
68	1	0	-4.365599	6.706319	0.462774
69	1	0	0.532271	8.199111	-1.482183
70	1	0	0.478339	9.173606	3.196714
71	1	0	-1.267629	9.358569	4.913521
72	1	0	-4.208029	8.046766	2.092568
73	1	0	-3.731132	8.142020	5.531800
74	1	0	-3.981889	9.826877	5.082483
75	1	0	-4.922880	8.553861	4.291223
76	6	0	3.615521	10.417841	-1.312570
77	6	0	2.558456	9.864990	-0.619007
78	6	0	2.726450	8.723870	0.200808
79	6	0	4.032391	8.150238	0.305631
80	6	0	5.089044	8.745423	-0.420164
81	6	0	4.909251	9.859590	-1.225211
82	6	0	1.620458	8.159039	0.955838
83	6	0	4.241528	6.979480	1.150098
84	6	0	3.184900	6.597148	2.022618
85	6	0	1.900590	7.203901	1.900071
86	6	0	3.373837	5.502838	2.896479
87	6	0	4.510100	4.731978	2.828434
88	6	0	5.525997	5.014640	1.877955
89	6	0	5.395498	6.165094	1.098971
90	6	0	6.059843	10.479485	-1.980337
91	1	0	4.586985	3.843926	3.445635
92	1	0	6.181112	6.401582	0.389567
93	1	0	2.571213	5.231664	3.577074
94	1	0	1.092687	6.780125	2.487723
95	1	0	6.089791	8.336227	-0.323840
96	1	0	1.576138	10.320706	-0.681630
97	1	0	3.454490	11.303149	-1.922769
98	1	0	6.998864	9.956050	-1.781483
99	1	0	5.884668	10.454092	-3.062424
100	1	0	6.197098	11.531365	-1.704166
101	6	0	9.007802	1.526318	-3.917956
102	6	0	8.903834	0.543534	-2.954487
103	6	0	8.471300	0.839995	-1.640144

104	6	0	8.148105	2.192991	-1.325143
105	6	0	8.262076	3.172142	-2.337490
106	6	0	8.681321	2.868027	-3.623356
107	6	0	8.379764	-0.185981	-0.611875
108	6	0	7.718907	2.528880	0.024735
109	6	0	7.918178	1.561455	1.047831
110	6	0	8.241682	0.214030	0.694559
111	6	0	7.599862	1.910116	2.382255
112	6	0	6.952480	3.090564	2.671740
113	6	0	6.562975	3.978903	1.634779
114	6	0	7.016924	3.710751	0.343599
115	6	0	8.807574	3.934336	-4.684098
116	1	0	7.819126	1.200979	3.176225
117	1	0	6.690037	3.318296	3.699889
118	1	0	6.706379	4.365323	-0.463094
119	1	0	8.199503	-0.532379	1.481969
120	1	0	9.173912	-0.478560	-3.196985
121	1	0	9.358812	1.267408	-4.913836
122	1	0	8.046967	4.207821	-2.092899
123	1	0	9.828621	3.983982	-5.079866
124	1	0	8.145580	3.729414	-5.533741
125	1	0	8.551441	4.922269	-4.292201
126	6	0	10.417352	-3.615402	1.313600
127	6	0	9.864941	-2.558448	0.619540
128	6	0	8.724058	-2.726480	-0.200583
129	6	0	8.150278	-4.032362	-0.305343
130	6	0	8.745002	-5.088917	0.421001
131	6	0	9.858855	-4.909055	1.226494
132	6	0	8.159641	-1.620554	-0.955986
133	6	0	6.979804	-4.241528	-1.150220
134	6	0	6.597810	-3.184964	-2.022971
135	6	0	7.204671	-1.900700	-1.900430
136	6	0	5.503677	-3.373901	-2.897055
137	6	0	4.732659	-4.510057	-2.829028
138	6	0	5.014929	-5.525872	-1.878331
139	6	0	6.165205	-5.395351	-1.099068
140	6	0	10.478015	-6.059357	1.982651
141	1	0	3.844773	-4.586871	-3.446460
142	1	0	6.401323	-6.180769	-0.389337
143	1	0	5.232778	-2.571356	-3.577852
144	1	0	6.781121	-1.092775	-2.488222
145	1	0	8.335643	-6.089620	0.324862
146	1	0	10.320837	-1.576197	0.682003
147	1	0	11.302493	-3.454335	1.924033
148	1	0	10.448213	-5.885379	3.064842
149	1	0	9.957000	-6.999111	1.780901
150	1	0	11.531176	-6.194367	1.710357
151	6	0	-9.007752	-1.526728	-3.917716
152	6	0	-8.903771	-0.543827	-2.954367
153	6	0	-8.471068	-0.840097	-1.640030
154	6	0	-8.147760	-2.193040	-1.324920
155	6	0	-8.261746	-3.172316	-2.337142
156	6	0	-8.681133	-2.868378	-3.623003
157	6	0	-8.379491	0.185979	-0.611840
158	6	0	-7.718551	-2.528811	0.024971
159	6	0	-7.917848	-1.561335	1.048007
160	6	0	-8.241378	-0.213933	0.694635
161	6	0	-7.599555	-1.909935	2.382458
162	6	0	-6.952237	-3.090408	2.672030

163	6	0	-6.562746	-3.978827	1.635125
164	6	0	-7.016652	-3.710709	0.343918
165	6	0	-8.807423	-3.934826	-4.683604
166	1	0	-7.818832	-1.200757	3.176386
167	1	0	-6.689872	-3.318110	3.700203
168	1	0	-6.706168	-4.365360	-0.462737
169	1	0	-8.199231	0.532538	1.481990
170	1	0	-9.173942	0.478214	-3.196962
171	1	0	-9.358877	-1.267961	-4.913593
172	1	0	-8.046597	-4.207961	-2.092424
173	1	0	-9.828518	-3.984622	-5.079232
174	1	0	-8.145563	-3.729946	-5.533365
175	1	0	-8.551140	-4.922685	-4.291623
176	6	0	-10.417498	3.615221	1.313384
177	6	0	-9.864897	2.558293	0.619433
178	6	0	-8.724061	2.726450	-0.200725
179	6	0	-8.150466	4.032413	-0.305574
180	6	0	-8.745392	5.088941	0.420652
181	6	0	-9.859234	4.908968	1.226140
182	6	0	-8.159490	1.620555	-0.956040
183	6	0	-6.979959	4.241680	-1.150411
184	6	0	-6.597795	3.185107	-2.023079
185	6	0	-7.204494	1.900768	-1.900468
186	6	0	-5.503647	3.374111	-2.897126
187	6	0	-4.732735	4.510343	-2.829105
188	6	0	-5.015137	5.526152	-1.878449
189	6	0	-6.165464	5.395586	-1.099269
190	6	0	-10.478605	6.059235	1.982178
191	1	0	-3.844807	4.587220	-3.446468
192	1	0	-6.401676	6.181011	-0.389584
193	1	0	-5.232630	2.571553	-3.577861
194	1	0	-6.780801	1.092861	-2.488176
195	1	0	-8.336198	6.089702	0.324436
196	1	0	-10.320606	1.575958	0.682012
197	1	0	-11.302610	3.454057	1.923832
198	1	0	-10.448817	5.885354	3.064385
199	1	0	-9.957739	6.999057	1.780369
200	1	0	-11.531779	6.194047	1.709834

Table S8. Cartesian coordinate of *Z,R,E,R,Z,S,E,S* (6)

SCF Done: E(RB3LYP) = -4621.34405630 A.U. after 6 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	9.902607	2.191287	3.041266
2	6	0	9.598722	1.318508	2.017145
3	6	0	8.845455	1.730873	0.892192
4	6	0	8.399754	3.089186	0.831895
5	6	0	8.734694	3.952325	1.900019
6	6	0	9.470538	3.534838	2.998139
7	6	0	8.556709	0.820804	-0.200896
8	6	0	7.612584	3.541608	-0.310487
9	6	0	7.497978	2.664078	-1.424457
10	6	0	7.988695	1.329013	-1.340791
11	6	0	6.760164	3.079254	-2.555308
12	6	0	6.065676	4.264848	-2.551623
13	6	0	6.081775	5.119704	-1.417510

14	6	0	6.900209	4.761967	-0.344205
15	6	0	9.818530	4.483714	4.119210
16	1	0	6.689859	2.410065	-3.408649
17	1	0	5.434998	4.504667	-3.399332
18	1	0	6.942172	5.419078	0.516846
19	1	0	7.777978	0.665390	-2.173609
20	1	0	9.955174	0.294702	2.056764
21	1	0	10.493377	1.845462	3.885896
22	1	0	8.427673	4.992344	1.853863
23	1	0	10.903236	4.550794	4.262273
24	1	0	9.443951	5.491805	3.922425
25	1	0	9.391396	4.147506	5.071455
26	6	0	10.579108	-1.739138	-3.144148
27	6	0	10.067169	-0.954898	-2.130589
28	6	0	9.157426	-1.477578	-1.180964
29	6	0	8.773636	-2.846241	-1.294392
30	6	0	9.316787	-3.619221	-2.345342
31	6	0	10.208150	-3.095962	-3.269271
32	6	0	8.635522	-0.666045	-0.092875
33	6	0	7.830492	-3.402282	-0.335063
34	6	0	7.562528	-2.660541	0.849537
35	6	0	7.980595	-1.294328	0.936353
36	6	0	6.713669	-3.225613	1.830829
37	6	0	6.022587	-4.393196	1.584772
38	6	0	6.138526	-5.047264	0.332281
39	6	0	7.088998	-4.578762	-0.572390
40	6	0	10.788769	-3.946278	-4.372879
41	1	0	5.300079	-4.756986	2.308844
42	1	0	7.193772	-5.089526	-1.523913
43	1	0	6.542570	-2.677686	2.753752
44	1	0	7.607821	-0.707625	1.770975
45	1	0	9.054200	-4.670274	-2.415356
46	1	0	10.374697	0.081554	-2.043105
47	1	0	11.288061	-1.311359	-3.848743
48	1	0	10.397351	-4.966543	-4.341486
49	1	0	10.557715	-3.528278	-5.359634
50	1	0	11.881087	-4.003664	-4.298709
51	6	0	-10.579211	1.739167	3.143982
52	6	0	-10.067244	0.954918	2.130441
53	6	0	-9.157462	1.477584	1.180850
54	6	0	-8.773659	2.846243	1.294290
55	6	0	-9.316840	3.619231	2.345215
56	6	0	-10.208247	3.095986	3.269113
57	6	0	-8.635526	0.666038	0.092784
58	6	0	-7.830474	3.402274	0.334994
59	6	0	-7.562473	2.660524	-0.849593
60	6	0	-7.980547	1.294314	-0.936417
61	6	0	-6.713582	3.225588	-1.830859
62	6	0	-6.022506	4.393172	-1.584788
63	6	0	-6.138480	5.047247	-0.332304
64	6	0	-7.088981	4.578748	0.572341
65	6	0	-10.788926	3.946328	4.372670
66	1	0	-6.542452	2.677655	-2.753773
67	1	0	-5.299975	4.756955	-2.308841
68	1	0	-7.193783	5.089517	1.523858
69	1	0	-7.607738	0.707605	-1.771019
70	1	0	-10.374781	-0.081531	2.042953
71	1	0	-11.288193	1.311394	3.848553
72	1	0	-9.054240	4.670280	2.415240

73	1	0	-11.881208	4.004040	4.298201
74	1	0	-10.558270	3.528139	5.359436
75	1	0	-10.397212	4.966487	4.341510
76	6	0	-9.902534	-2.191312	-3.041388
77	6	0	-9.598683	-1.318527	-2.017259
78	6	0	-8.845432	-1.730876	-0.892292
79	6	0	-8.399728	-3.089187	-0.831980
80	6	0	-8.734634	-3.952333	-1.900108
81	6	0	-9.470448	-3.534855	-2.998252
82	6	0	-8.556735	-0.820807	0.200816
83	6	0	-7.612605	-3.541608	0.310437
84	6	0	-7.498085	-2.664094	1.424428
85	6	0	-7.988805	-1.329029	1.340746
86	6	0	-6.760341	-3.079284	2.555317
87	6	0	-6.065829	-4.264867	2.551652
88	6	0	-6.081827	-5.119693	1.417520
89	6	0	-6.900207	-4.761949	0.344172
90	6	0	-9.818358	-4.483728	-4.119351
91	1	0	-5.435210	-4.504686	3.399406
92	1	0	-6.942107	-5.419037	-0.516899
93	1	0	-6.690105	-2.410118	3.408683
94	1	0	-7.778137	-0.665417	2.173584
95	1	0	-8.427619	-4.992353	-1.853928
96	1	0	-9.955161	-0.294731	-2.056888
97	1	0	-10.493297	-1.845495	-3.886026
98	1	0	-9.444214	-5.491932	-3.922316
99	1	0	-10.903031	-4.550427	-4.262829
100	1	0	-9.390730	-4.147781	-5.071469
101	6	0	-1.806919	-9.077598	-3.537192
102	6	0	-1.061518	-9.097474	-2.375396
103	6	0	-1.566827	-8.573950	-1.161861
104	6	0	-2.889937	-8.039051	-1.159379
105	6	0	-3.620992	-8.028663	-2.368472
106	6	0	-3.107324	-8.529188	-3.554806
107	6	0	-0.790727	-8.599119	0.071708
108	6	0	-3.463658	-7.548936	0.086348
109	6	0	-2.793709	-7.876569	1.296282
110	6	0	-1.455230	-8.374427	1.252966
111	6	0	-3.408959	-7.537302	2.523842
112	6	0	-4.548705	-6.766508	2.556822
113	6	0	-5.112962	-6.246033	1.361379
114	6	0	-4.591160	-6.702990	0.150027
115	6	0	-3.913066	-8.515339	-4.830986
116	1	0	-2.940278	-7.855073	3.451558
117	1	0	-4.989654	-6.516356	3.515469
118	1	0	-4.992301	-6.306530	-0.775616
119	1	0	-0.911957	-8.413109	2.191415
120	1	0	-0.071634	-9.540548	-2.380987
121	1	0	-1.393001	-9.503044	-4.448078
122	1	0	-4.638503	-7.650185	-2.363253
123	1	0	-3.428513	-7.901653	-5.599686
124	1	0	-4.018369	-9.523835	-5.247162
125	1	0	-4.916485	-8.113372	-4.667223
126	6	0	1.763020	-10.797201	2.949071
127	6	0	0.997855	-10.230114	1.949960
128	6	0	1.499200	-9.191008	1.130885
129	6	0	2.842363	-8.751688	1.345468
130	6	0	3.592828	-9.352132	2.381645
131	6	0	3.082218	-10.356672	3.189093

132	6	0	0.700031	-8.596666	0.068293
133	6	0	3.411736	-7.721427	0.485663
134	6	0	2.692123	-7.373077	-0.690647
135	6	0	1.342532	-7.808017	-0.853606
136	6	0	3.266036	-6.462662	-1.607111
137	6	0	4.443791	-5.814323	-1.314237
138	6	0	5.095078	-6.026195	-0.071870
139	6	0	4.595565	-7.008140	0.781857
140	6	0	3.910118	-10.985454	4.283338
141	1	0	4.828150	-5.058410	-1.991226
142	1	0	5.103879	-7.181671	1.724768
143	1	0	2.725568	-6.227207	-2.520101
144	1	0	0.778255	-7.366757	-1.668168
145	1	0	4.622079	-9.042003	2.532234
146	1	0	-0.005557	-10.599376	1.768284
147	1	0	1.350068	-11.603838	3.549771
148	1	0	4.921254	-10.570662	4.309920
149	1	0	3.455920	-10.822821	5.267987
150	1	0	3.994866	-12.069665	4.146356
151	6	0	1.806919	9.077506	3.537324
152	6	0	1.061523	9.097429	2.375527
153	6	0	1.566829	8.573933	1.161977
154	6	0	2.889931	8.039019	1.159483
155	6	0	3.620981	8.028579	2.368580
156	6	0	3.107314	8.529072	3.554928
157	6	0	0.790734	8.599154	-0.071595
158	6	0	3.463655	7.548948	-0.086260
159	6	0	2.793722	7.876647	-1.296185
160	6	0	1.455247	8.374516	-1.252858
161	6	0	3.408977	7.537430	-2.523757
162	6	0	4.548708	6.766613	-2.556763
163	6	0	5.112937	6.246067	-1.361338
164	6	0	4.591141	6.702983	-0.149969
165	6	0	3.913043	8.515149	4.831115
166	1	0	2.940312	7.855259	-3.451461
167	1	0	4.989665	6.516494	-3.515415
168	1	0	4.992273	6.306468	0.775655
169	1	0	0.911984	8.413245	-2.191311
170	1	0	0.071648	9.540520	2.381125
171	1	0	1.393007	9.502936	4.448221
172	1	0	4.638487	7.650090	2.363351
173	1	0	4.018205	9.523597	5.247441
174	1	0	3.428563	7.901285	5.599721
175	1	0	4.916517	8.113337	4.667306
176	6	0	-1.762987	10.797265	-2.948949
177	6	0	-0.997834	10.230171	-1.949835
178	6	0	-1.499180	9.191042	-1.130789
179	6	0	-2.842330	8.751706	-1.345407
180	6	0	-3.592781	9.352151	-2.381593
181	6	0	-3.082170	10.356713	-3.189013
182	6	0	-0.700021	8.596698	-0.068190
183	6	0	-3.411710	7.721431	-0.485621
184	6	0	-2.692118	7.373086	0.690705
185	6	0	-1.342533	7.808034	0.853691
186	6	0	-3.266044	6.462669	1.607156
187	6	0	-4.443790	5.814320	1.314256
188	6	0	-5.095048	6.026182	0.071875
189	6	0	-4.595522	7.008132	-0.781842
190	6	0	-3.910042	10.985464	-4.283299

191	1	0	-4.828155	5.058405	1.991239
192	1	0	-5.103819	7.181660	-1.724764
193	1	0	-2.725596	6.227219	2.520159
194	1	0	-0.778267	7.366768	1.668257
195	1	0	-4.622024	9.042007	-2.532209
196	1	0	0.005568	10.599447	-1.768126
197	1	0	-1.350042	11.603928	-3.549619
198	1	0	-4.921315	10.570991	-4.309606
199	1	0	-3.994409	12.069740	-4.146610
200	1	0	-3.456057	10.822401	-5.267978

Table S9. Cartesian coordinate of *Z,R,E,S,Z,R,E,S* (7)

SCF Done: E(RB3LYP) = -4621.34307330 A.U. after 6 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-10.982900	1.348265	-2.171428
2	6	0	-10.513998	0.634886	-1.086858
3	6	0	-9.676692	1.232081	-0.115123
4	6	0	-9.327144	2.607108	-0.276745
5	6	0	-9.823832	3.304525	-1.400793
6	6	0	-10.639511	2.706160	-2.348943
7	6	0	-9.201438	0.493901	1.044654
8	6	0	-8.473893	3.251205	0.713324
9	6	0	-8.257585	2.573740	1.945324
10	6	0	-8.630487	1.200746	2.073960
11	6	0	-7.504844	3.214056	2.957270
12	6	0	-6.853639	4.402242	2.710534
13	6	0	-6.913472	5.004758	1.427903
14	6	0	-7.777587	4.456996	0.480476
15	6	0	-11.168109	3.478233	-3.533293
16	1	0	-7.376316	2.711048	3.912061
17	1	0	-6.202229	4.825945	3.468115
18	1	0	-7.847944	4.933136	-0.491889
19	1	0	-8.291382	0.674624	2.960677
20	1	0	-10.804607	-0.402247	-0.958177
21	1	0	-11.637404	0.863250	-2.891470
22	1	0	-9.587608	4.358333	-1.511583
23	1	0	-12.264108	3.476351	-3.553357
24	1	0	-10.835449	4.519459	-3.514149
25	1	0	-10.831171	3.035993	-4.478313
26	6	0	-10.287406	-2.106036	4.448384
27	6	0	-10.083073	-1.336147	3.321159
28	6	0	-9.266036	-1.785731	2.257077
29	6	0	-8.654624	-3.070726	2.370984
30	6	0	-8.883910	-3.829443	3.540708
31	6	0	-9.682809	-3.375203	4.578828
32	6	0	-9.066970	-0.991347	1.054708
33	6	0	-7.816993	-3.563770	1.285798
34	6	0	-7.874045	-2.881577	0.038727
35	6	0	-8.501760	-1.599998	-0.038596
36	6	0	-7.139353	-3.393213	-1.056586
37	6	0	-6.256427	-4.437778	-0.891318
38	6	0	-6.055425	-5.016236	0.387693
39	6	0	-6.885048	-4.613501	1.433316
40	6	0	-9.923806	-4.211924	5.811712
41	1	0	-5.628885	-4.750186	-1.719936

42	1	0	-6.748905	-5.069195	2.408561
43	1	0	-7.215781	-2.892498	-2.018195
44	1	0	-8.367680	-1.034976	-0.955618
45	1	0	-8.447149	-4.820307	3.617905
46	1	0	-10.570984	-0.371390	3.232651
47	1	0	-10.933793	-1.737432	5.241068
48	1	0	-9.400981	-5.170367	5.754890
49	1	0	-9.579681	-3.695656	6.715627
50	1	0	-10.991276	-4.419597	5.949934
51	6	0	10.287430	2.106041	4.448308
52	6	0	10.083093	1.336158	3.321079
53	6	0	9.266054	1.785750	2.257002
54	6	0	8.654640	3.070743	2.370920
55	6	0	8.883930	3.829453	3.540649
56	6	0	9.682834	3.375207	4.578762
57	6	0	9.066979	0.991371	1.054632
58	6	0	7.817003	3.563791	1.285742
59	6	0	7.874051	2.881608	0.038665
60	6	0	8.501764	1.600027	-0.038667
61	6	0	7.139356	3.393253	-1.056641
62	6	0	6.256428	4.437815	-0.891362
63	6	0	6.055423	5.016255	0.387657
64	6	0	6.885050	4.613513	1.433274
65	6	0	9.923836	4.211920	5.811651
66	1	0	7.215782	2.892547	-2.018255
67	1	0	5.628882	4.750226	-1.719974
68	1	0	6.748906	5.069195	2.408524
69	1	0	8.367675	1.035009	-0.955690
70	1	0	10.571002	0.371402	3.232563
71	1	0	10.933820	1.737432	5.240988
72	1	0	8.447169	4.820316	3.617853
73	1	0	9.579714	3.695647	6.715564
74	1	0	10.991306	4.419592	5.949870
75	1	0	9.401011	5.170364	5.754836
76	6	0	10.982840	-1.348296	-2.171515
77	6	0	10.513959	-0.634899	-1.086948
78	6	0	9.676662	-1.232076	-0.115193
79	6	0	9.327104	-2.607104	-0.276791
80	6	0	9.823772	-3.304538	-1.400837
81	6	0	10.639440	-2.706192	-2.349007
82	6	0	9.201430	-0.493878	1.044583
83	6	0	8.473865	-3.251183	0.713300
84	6	0	8.257578	-2.573700	1.945294
85	6	0	8.630491	-1.200707	2.073907
86	6	0	7.504847	-3.213996	2.957260
87	6	0	6.853634	-4.402182	2.710552
88	6	0	6.913450	-5.004721	1.427931
89	6	0	7.777554	-4.456978	0.480483
90	6	0	11.168016	-3.478284	-3.533354
91	1	0	6.202233	-4.825873	3.468148
92	1	0	7.847897	-4.933136	-0.491875
93	1	0	7.376335	-2.710973	3.912045
94	1	0	8.291406	-0.674572	2.960623
95	1	0	9.587540	-4.358348	-1.511608
96	1	0	10.804577	0.402233	-0.958285
97	1	0	11.637337	-0.863295	-2.891573
98	1	0	10.835351	-4.519508	-3.514190
99	1	0	10.831067	-3.036055	-4.478375
100	1	0	12.264015	-3.476409	-3.553434

101	6	0	1.616390	-5.701490	-3.797368
102	6	0	1.065963	-6.381536	-2.731197
103	6	0	1.846180	-6.767480	-1.612650
104	6	0	3.213598	-6.362126	-1.584572
105	6	0	3.749149	-5.686978	-2.705848
106	6	0	2.985549	-5.359120	-3.813539
107	6	0	1.293055	-7.517719	-0.492551
108	6	0	4.005684	-6.596964	-0.386884
109	6	0	3.476883	-7.437762	0.629918
110	6	0	2.124123	-7.897714	0.529159
111	6	0	4.250569	-7.666934	1.794175
112	6	0	5.424777	-6.978306	2.018952
113	6	0	5.892434	-6.025984	1.078029
114	6	0	5.206697	-5.904451	-0.127838
115	6	0	3.584381	-4.652791	-5.005040
116	1	0	3.871304	-8.352857	2.547384
117	1	0	5.973664	-7.132924	2.943236
118	1	0	5.533640	-5.143295	-0.825895
119	1	0	1.718325	-8.476102	1.355023
120	1	0	0.013576	-6.631669	-2.755521
121	1	0	0.986785	-5.431026	-4.641471
122	1	0	4.802643	-5.426790	-2.709905
123	1	0	3.515345	-5.268939	-5.909442
124	1	0	3.057689	-3.715102	-5.216957
125	1	0	4.639049	-4.415218	-4.842256
126	6	0	-1.338417	-9.942582	-3.106045
127	6	0	-0.518629	-9.263429	-2.228887
128	6	0	-1.047167	-8.363269	-1.273862
129	6	0	-2.461374	-8.167756	-1.229032
130	6	0	-3.268545	-8.882072	-2.143651
131	6	0	-2.739146	-9.760548	-3.076639
132	6	0	-0.188241	-7.662961	-0.338310
133	6	0	-3.028367	-7.250474	-0.248043
134	6	0	-2.179744	-6.782086	0.793612
135	6	0	-0.769058	-6.997643	0.708527
136	6	0	-2.723549	-5.967900	1.812639
137	6	0	-4.019027	-5.508833	1.734806
138	6	0	-4.832588	-5.829539	0.617992
139	6	0	-4.343357	-6.737635	-0.319746
140	6	0	-3.625690	-10.520828	-4.032922
141	1	0	-4.389498	-4.810602	2.478268
142	1	0	-4.972180	-6.999742	-1.164221
143	1	0	-2.078062	-5.643031	2.624387
144	1	0	-0.136708	-6.497159	1.436089
145	1	0	-4.346891	-8.765655	-2.097006
146	1	0	0.554932	-9.421019	-2.255921
147	1	0	-0.904119	-10.635209	-3.822690
148	1	0	-4.681176	-10.282495	-3.877022
149	1	0	-3.379483	-10.286039	-5.075202
150	1	0	-3.504846	-11.603757	-3.912953
151	6	0	-1.616329	5.701144	-3.797303
152	6	0	-1.065919	6.381276	-2.731179
153	6	0	-1.846160	6.767349	-1.612691
154	6	0	-3.213582	6.362005	-1.584611
155	6	0	-3.749116	5.686766	-2.705840
156	6	0	-2.985495	5.358800	-3.813484
157	6	0	-1.293058	7.517680	-0.492634
158	6	0	-4.005690	6.596921	-0.386954
159	6	0	-3.476904	7.437771	0.629810

160	6	0	-2.124145	7.897722	0.529043
161	6	0	-4.250605	7.667001	1.794046
162	6	0	-5.424812	6.978379	2.018845
163	6	0	-5.892457	6.026010	1.077964
164	6	0	-5.206706	5.904420	-0.127890
165	6	0	-3.584306	4.652371	-5.004936
166	1	0	-3.871350	8.352964	2.547225
167	1	0	-5.973709	7.133041	2.943116
168	1	0	-5.533635	5.143225	-0.825911
169	1	0	-1.718364	8.476161	1.354880
170	1	0	-0.013526	6.631372	-2.755498
171	1	0	-0.986705	5.430586	-4.641362
172	1	0	-4.802610	5.426584	-2.709895
173	1	0	-3.515236	5.268435	-5.909393
174	1	0	-3.057623	3.714654	-5.216753
175	1	0	-4.638983	4.414830	-4.842158
176	6	0	1.338471	9.942870	-3.105818
177	6	0	0.518663	9.263625	-2.228749
178	6	0	1.047177	8.363354	-1.273814
179	6	0	2.461385	8.167852	-1.228961
180	6	0	3.268577	8.882263	-2.143488
181	6	0	2.739198	9.760831	-3.076401
182	6	0	0.188234	7.662947	-0.338349
183	6	0	3.028360	7.250503	-0.248026
184	6	0	2.179719	6.782050	0.793585
185	6	0	0.769032	6.997590	0.708473
186	6	0	2.723509	5.967816	1.812582
187	6	0	4.018994	5.508769	1.734754
188	6	0	4.832575	5.829538	0.617972
189	6	0	4.343355	6.737679	-0.319729
190	6	0	3.625764	10.521212	-4.032583
191	1	0	4.389455	4.810502	2.478187
192	1	0	4.972196	6.999841	-1.164173
193	1	0	2.078007	5.642896	2.624297
194	1	0	0.136670	6.497049	1.435986
195	1	0	4.346922	8.765853	-2.096821
196	1	0	-0.554897	9.421222	-2.255790
197	1	0	0.904189	10.635574	-3.822397
198	1	0	4.681247	10.282866	-3.876681
199	1	0	3.379584	10.286531	-5.074893
200	1	0	3.504915	11.604129	-3.912504

Table S10. Cartesian coordinate of *Z,R,Z,R,Z,S,E,S* (8)

SCF Done: E(RB3LYP) = -4621.34305687 A.U. after 14 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.828593	-10.406548	1.172415
2	6	0	-1.789141	-9.691338	0.615182
3	6	0	-2.027790	-8.592116	-0.243177
4	6	0	-3.380764	-8.225525	-0.526563
5	6	0	-4.417527	-8.985185	0.061775
6	6	0	-4.171368	-10.062426	0.899423
7	6	0	-0.934410	-7.862377	-0.852729
8	6	0	-3.651336	-7.090438	-1.402749
9	6	0	-2.558507	-6.537851	-2.126925
10	6	0	-1.224034	-6.946820	-1.828432

11	6	0	-2.792310	-5.476748	-3.028485
12	6	0	-4.031130	-4.887930	-3.119226
13	6	0	-5.109395	-5.331452	-2.309284
14	6	0	-4.912825	-6.461200	-1.513706
15	6	0	-5.299523	-10.864132	1.502003
16	1	0	-1.956364	-5.078592	-3.597347
17	1	0	-4.157476	-4.012759	-3.746257
18	1	0	-5.740155	-6.822869	-0.912771
19	1	0	-0.411872	-6.413557	-2.313571
20	1	0	-0.761656	-9.974185	0.822003
21	1	0	-2.614447	-11.252566	1.820744
22	1	0	-5.448945	-8.737923	-0.169665
23	1	0	-5.240322	-11.918511	1.207899
24	1	0	-6.274915	-10.483622	1.187276
25	1	0	-5.266138	-10.836480	2.597561
26	6	0	0.442010	-6.632453	3.111589
27	6	0	0.015238	-7.118538	1.893160
28	6	0	0.927868	-7.403644	0.847846
29	6	0	2.306551	-7.108028	1.066280
30	6	0	2.709212	-6.626933	2.333105
31	6	0	1.810701	-6.393499	3.361119
32	6	0	0.501957	-7.941796	-0.436415
33	6	0	3.251886	-7.253803	-0.030296
34	6	0	2.835018	-7.941587	-1.202239
35	6	0	1.453013	-8.282824	-1.362240
36	6	0	3.762148	-8.107018	-2.259928
37	6	0	4.988184	-7.476053	-2.237655
38	6	0	5.351368	-6.642842	-1.148365
39	6	0	4.506136	-6.607577	-0.041593
40	6	0	2.266782	-5.896732	4.711196
41	1	0	5.661081	-7.576359	-3.084029
42	1	0	4.757544	-5.940698	0.774678
43	1	0	3.465886	-8.687622	-3.129833
44	1	0	1.139499	-8.706120	-2.312902
45	1	0	3.764152	-6.450139	2.517215
46	1	0	-1.041194	-7.295742	1.737018
47	1	0	-0.286621	-6.435915	3.894253
48	1	0	3.344927	-5.716391	4.729121
49	1	0	2.035002	-6.620851	5.501309
50	1	0	1.764915	-4.959997	4.979796
51	6	0	-1.760388	8.942131	-3.227281
52	6	0	-0.944598	8.863931	-2.116693
53	6	0	-1.402923	8.307712	-0.898863
54	6	0	-2.750126	7.839549	-0.836593
55	6	0	-3.554560	7.931607	-1.994732
56	6	0	-3.088631	8.465931	-3.185951
57	6	0	-0.553660	8.236300	0.281723
58	6	0	-3.266166	7.300473	0.414198
59	6	0	-2.498860	7.508312	1.592868
60	6	0	-1.148088	7.961372	1.488968
61	6	0	-3.032863	7.093553	2.835887
62	6	0	-4.195988	6.360481	2.897855
63	6	0	-4.874137	5.972439	1.712257
64	6	0	-4.429660	6.505265	0.502163
65	6	0	-3.971714	8.560278	-4.406326
66	1	0	-2.480299	7.316875	3.744760
67	1	0	-4.571766	6.033433	3.861895
68	1	0	-4.923060	6.197143	-0.412918
69	1	0	-0.542857	7.926431	2.389098

70	1	0	0.066523	9.253177	-2.164851
71	1	0	-1.380422	9.389534	-4.142441
72	1	0	-4.588450	7.604623	-1.943303
73	1	0	-3.570117	7.963341	-5.233773
74	1	0	-4.047179	9.593177	-4.765235
75	1	0	-4.983486	8.202482	-4.197760
76	6	0	2.191859	10.327364	3.046887
77	6	0	1.361071	9.787979	2.085786
78	6	0	1.800929	8.760169	1.218194
79	6	0	3.147048	8.299123	1.346025
80	6	0	3.966692	8.872501	2.344505
81	6	0	3.518360	9.868927	3.197638
82	6	0	0.934468	8.198995	0.191943
83	6	0	3.645751	7.270728	0.442023
84	6	0	2.854690	6.947882	-0.695373
85	6	0	1.507029	7.413604	-0.777622
86	6	0	3.359599	6.033290	-1.648481
87	6	0	4.537491	5.356240	-1.424845
88	6	0	5.258943	5.544231	-0.218563
89	6	0	4.828431	6.531216	0.666228
90	6	0	4.419058	10.470760	4.248640
91	1	0	4.868117	4.597703	-2.127132
92	1	0	5.391144	6.686025	1.580993
93	1	0	2.765678	5.817050	-2.532596
94	1	0	0.887815	6.999423	-1.566605
95	1	0	4.999035	8.547742	2.427734
96	1	0	0.352062	10.169405	1.973421
97	1	0	1.825236	11.126057	3.687000
98	1	0	4.519014	11.554170	4.115157
99	1	0	5.421149	10.035043	4.215414
100	1	0	4.016928	10.309231	5.255799
101	6	0	10.750994	1.254642	-3.362585
102	6	0	10.293112	0.485299	-2.312293
103	6	0	9.365286	0.993613	-1.372515
104	6	0	8.915126	2.339368	-1.527461
105	6	0	9.403238	3.095941	-2.616848
106	6	0	10.305370	2.582984	-3.536020
107	6	0	8.894740	0.194857	-0.250871
108	6	0	7.977805	2.897615	-0.562190
109	6	0	7.759025	2.179146	0.646207
110	6	0	8.221841	0.831569	0.762131
111	6	0	6.931401	2.748215	1.642390
112	6	0	6.226873	3.907606	1.401809
113	6	0	6.301019	4.545749	0.137903
114	6	0	7.215436	4.062637	-0.796233
115	6	0	10.820711	3.416566	-4.683932
116	1	0	6.796455	2.213815	2.579100
117	1	0	5.528771	4.281253	2.144352
118	1	0	7.285727	4.561779	-1.757126
119	1	0	7.882328	0.260896	1.620897
120	1	0	10.661316	-0.527095	-2.186618
121	1	0	11.475272	0.837956	-4.058194
122	1	0	9.089019	4.129579	-2.722303
123	1	0	10.562114	2.965798	-5.649355
124	1	0	11.913099	3.503005	-4.654760
125	1	0	10.404014	4.427086	-4.664825
126	6	0	10.064229	-2.401089	3.132065
127	6	0	9.826579	-1.615284	2.022730
128	6	0	9.121412	-2.112098	0.900847

129	6	0	8.662448	-3.464689	0.935490
130	6	0	8.923461	-4.237942	2.089275
131	6	0	9.608967	-3.736365	3.184851
132	6	0	8.891713	-1.296561	-0.281321
133	6	0	7.945760	-4.010772	-0.210077
134	6	0	7.961925	-3.263199	-1.420305
135	6	0	8.435670	-1.916414	-1.417883
136	6	0	7.344897	-3.805834	-2.571164
137	6	0	6.610225	-4.967563	-2.499048
138	6	0	6.445397	-5.643864	-1.262713
139	6	0	7.169608	-5.189625	-0.160914
140	6	0	9.884253	-4.588868	4.399644
141	1	0	6.067575	-5.313875	-3.372427
142	1	0	7.068749	-5.721233	0.779287
143	1	0	7.391687	-3.248028	-3.502748
144	1	0	8.278253	-1.332528	-2.319131
145	1	0	8.605743	-5.275786	2.109485
146	1	0	10.202320	-0.598248	1.993718
147	1	0	10.621998	-1.992246	3.970999
148	1	0	9.494853	-5.602770	4.274915
149	1	0	9.423359	-4.161138	5.297890
150	1	0	10.959652	-4.664322	4.598270
151	6	0	-9.684602	-2.422875	3.018280
152	6	0	-9.539183	-1.402742	2.099645
153	6	0	-8.915422	-1.619028	0.848257
154	6	0	-8.440771	-2.929832	0.549518
155	6	0	-8.600955	-3.948681	1.514928
156	6	0	-9.209531	-3.723029	2.740059
157	6	0	-8.773006	-0.554993	-0.135775
158	6	0	-7.810999	-3.182696	-0.737920
159	6	0	-7.976333	-2.210105	-1.761837
160	6	0	-8.452756	-0.904033	-1.425072
161	6	0	-7.464773	-2.491844	-3.051233
162	6	0	-6.661753	-3.589066	-3.270276
163	6	0	-6.301855	-4.451079	-2.200531
164	6	0	-6.947929	-4.272653	-0.977421
165	6	0	-9.383407	-4.831266	3.749817
166	1	0	-7.658380	-1.789689	-3.857976
167	1	0	-6.250438	-3.760765	-4.259783
168	1	0	-6.670244	-4.907444	-0.143321
169	1	0	-8.371153	-0.132994	-2.184986
170	1	0	-9.922887	-0.414134	2.327916
171	1	0	-10.183543	-2.226688	3.964116
172	1	0	-8.267723	-4.954191	1.276318
173	1	0	-8.980710	-5.777811	3.379631
174	1	0	-10.441083	-4.987845	3.991757
175	1	0	-8.872470	-4.594952	4.690619
176	6	0	-10.677385	2.854676	-2.238625
177	6	0	-10.185418	1.798691	-1.498968
178	6	0	-9.177206	1.983329	-0.523513
179	6	0	-8.677204	3.306038	-0.306505
180	6	0	-9.206352	4.360731	-1.084489
181	6	0	-10.188053	4.164317	-2.043510
182	6	0	-8.677844	0.875632	0.274254
183	6	0	-7.648147	3.534268	0.702243
184	6	0	-7.349344	2.465033	1.591603
185	6	0	-7.877012	1.163352	1.350619
186	6	0	-6.399739	2.665227	2.618324
187	6	0	-5.681101	3.833933	2.697380

188	6	0	-5.872806	4.873246	1.749374
189	6	0	-6.888299	4.722171	0.804072
190	6	0	-10.739711	5.313106	-2.852383
191	1	0	-4.896266	3.924486	3.439856
192	1	0	-7.056876	5.523877	0.093182
193	1	0	-6.192362	1.849976	3.306296
194	1	0	-7.502616	0.355041	1.969974
195	1	0	-8.854941	5.372436	-0.907929
196	1	0	-10.589493	0.803014	-1.647678
197	1	0	-11.461817	2.679425	-2.970725
198	1	0	-10.551784	5.171354	-3.923301
199	1	0	-10.288996	6.264428	-2.557287
200	1	0	-11.825084	5.403010	-2.728271

Table S11. Cartesian coordinate of *E,R,E,R,Z,R,Z,R* (9)

SCF Done: E(RB3LYP) = -4621.34284879 A.U. after 5 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.731609	-5.421761	-3.398532
2	6	0	0.281007	-6.095647	-2.282589
3	6	0	1.178147	-6.644933	-1.332412
4	6	0	2.572359	-6.418165	-1.529596
5	6	0	2.999315	-5.743721	-2.696387
6	6	0	2.111869	-5.250630	-3.638309
7	6	0	0.728340	-7.407410	-0.173785
8	6	0	3.513381	-6.834071	-0.502246
9	6	0	3.061306	-7.689734	0.538541
10	6	0	1.661875	-7.983322	0.647401
11	6	0	3.980904	-8.080285	1.543834
12	6	0	5.244026	-7.527002	1.612273
13	6	0	5.659426	-6.563063	0.659167
14	6	0	4.810837	-6.291269	-0.410691
15	6	0	2.591592	-4.546466	-4.883679
16	6	0	-0.731180	-5.420696	3.398070
17	6	0	-0.280662	-6.094924	2.282300
18	6	0	-1.177871	-6.644483	1.332345
19	6	0	-2.572064	-6.417633	1.529555
20	6	0	-2.998934	-5.742844	2.696177
21	6	0	-2.111418	-5.249484	3.637896
22	6	0	-0.728153	-7.407311	0.173909
23	6	0	-3.513165	-6.833815	0.502384
24	6	0	-3.061168	-7.689729	-0.538232
25	6	0	-1.661749	-7.983384	-0.647091
26	6	0	-3.980839	-8.080506	-1.543368
27	6	0	-5.243983	-7.527262	-1.611833
28	6	0	-5.659337	-6.563151	-0.658888
29	6	0	-4.810641	-6.291070	0.410816
30	6	0	-2.591054	-4.544970	4.883101
31	6	0	1.528966	9.428645	-3.339668
32	6	0	0.842817	9.008063	-2.219084
33	6	0	1.453217	8.182938	-1.244286
34	6	0	2.812406	7.791768	-1.442828
35	6	0	3.482378	8.243023	-2.602791
36	6	0	2.871979	9.047693	-3.552094
37	6	0	0.744789	7.764491	-0.046636
38	6	0	3.467302	6.943960	-0.455043

39	6	0	2.811419	6.738650	0.790902
40	6	0	1.457278	7.161275	0.958685
41	6	0	3.458150	5.973026	1.789322
42	6	0	4.642170	5.320159	1.528249
43	6	0	5.241396	5.396075	0.244873
44	6	0	4.672730	6.250399	-0.698833
45	6	0	3.615210	9.523683	-4.776488
46	6	0	-1.529175	9.428596	3.339533
47	6	0	-0.843024	9.008031	2.218944
48	6	0	-1.453413	8.182896	1.244149
49	6	0	-2.812588	7.791687	1.442704
50	6	0	-3.482564	8.242926	2.602672
51	6	0	-2.872177	9.047612	3.551969
52	6	0	-0.744983	7.764470	0.046494
53	6	0	-3.467468	6.943857	0.454928
54	6	0	-2.811589	6.738556	-0.791021
55	6	0	-1.457461	7.161222	-0.958816
56	6	0	-3.458304	5.972908	-1.789432
57	6	0	-4.642304	5.320008	-1.528346
58	6	0	-5.241517	5.395911	-0.244966
59	6	0	-4.672872	6.250259	0.698731
60	6	0	-3.615411	9.523585	4.776369
61	6	0	-10.918470	1.330213	-3.368200
62	6	0	-10.509316	0.553108	-2.303766
63	6	0	-9.565094	1.026498	-1.362226
64	6	0	-9.042397	2.345329	-1.530935
65	6	0	-9.484518	3.110629	-2.633873
66	6	0	-10.404890	2.632162	-3.553656
67	6	0	-9.151161	0.220503	-0.225315
68	6	0	-8.077082	2.864470	-0.570029
69	6	0	-7.888332	2.140301	0.639839
70	6	0	-8.435692	0.828632	0.775989
71	6	0	-7.012327	2.658415	1.621918
72	6	0	-6.244460	3.772673	1.369693
73	6	0	-6.309244	4.426543	0.112612
74	6	0	-7.263133	3.993600	-0.808213
75	6	0	-10.867854	3.475710	-4.716559
76	6	0	-10.515576	-2.163891	3.229760
77	6	0	-10.232795	-1.441222	2.088279
78	6	0	-9.520666	-2.014463	1.008415
79	6	0	-9.098867	-3.372920	1.122296
80	6	0	-9.403820	-4.081185	2.306289
81	6	0	-10.099616	-3.506871	3.359136
82	6	0	-9.242177	-1.268247	-0.209073
83	6	0	-8.366146	-3.987513	0.023906
84	6	0	-8.365965	-3.319886	-1.232366
85	6	0	-8.808288	-1.962574	-1.311279
86	6	0	-7.737448	-3.942013	-2.336807
87	6	0	-6.984930	-5.084594	-2.171924
88	6	0	-6.813502	-5.654108	-0.884453
89	6	0	-7.569789	-5.143233	0.169405
90	6	0	-10.426908	-4.289593	4.607553
91	6	0	10.515601	-2.163826	-3.229625
92	6	0	10.232785	-1.441105	-2.088188
93	6	0	9.520645	-2.014301	-1.008306
94	6	0	9.098872	-3.372776	-1.122120
95	6	0	9.403861	-4.081093	-2.306076
96	6	0	10.099673	-3.506825	-3.358934
97	6	0	9.242096	-1.268020	0.209119

98	6	0	8.366130	-3.987321	-0.023719
99	6	0	8.365853	-3.319599	1.232503
100	6	0	8.808140	-1.962276	1.311345
101	6	0	7.737303	-3.941663	2.336964
102	6	0	6.984844	-5.084284	2.172139
103	6	0	6.813523	-5.653923	0.884704
104	6	0	7.569845	-5.143104	-0.169152
105	6	0	10.427099	-4.289637	-4.607259
106	6	0	10.918359	1.330486	3.368205
107	6	0	10.509213	0.553361	2.303784
108	6	0	9.565017	1.026743	1.362213
109	6	0	9.042325	2.345580	1.530890
110	6	0	9.484443	3.110906	2.633813
111	6	0	10.404798	2.632449	3.553619
112	6	0	9.151098	0.220734	0.225309
113	6	0	8.077017	2.864699	0.569965
114	6	0	7.888295	2.140520	-0.639901
115	6	0	8.435659	0.828850	-0.776024
116	6	0	7.012302	2.658626	-1.621996
117	6	0	6.244413	3.772872	-1.369782
118	6	0	6.309152	4.426735	-0.112694
119	6	0	7.263041	3.993811	0.808141
120	6	0	10.867764	3.476020	4.716506
121	1	0	3.651867	-8.775890	2.311697
122	1	0	5.908837	-7.795910	2.428047
123	1	0	5.104151	-5.517776	-1.109885
124	1	0	1.331434	-8.581130	1.492891
125	1	0	-0.784393	-6.210376	-2.130885
126	1	0	0.011571	-5.021569	-4.108116
127	1	0	4.062922	-5.620844	-2.873766
128	1	0	3.681512	-4.463373	-4.903060
129	1	0	2.279800	-5.081154	-5.788728
130	1	0	2.176349	-3.534281	-4.951968
131	1	0	-5.908842	-7.796338	-2.427513
132	1	0	-5.103924	-5.517420	1.109849
133	1	0	-3.651855	-8.776273	-2.311107
134	1	0	-1.331376	-8.581434	-1.492437
135	1	0	-4.062526	-5.619898	2.873594
136	1	0	0.784727	-6.209701	2.130564
137	1	0	-0.011085	-5.020293	4.107477
138	1	0	-3.680956	-4.461619	4.902398
139	1	0	-2.279448	-5.079565	5.788271
140	1	0	-2.175574	-3.532873	4.951228
141	1	0	2.965890	5.843281	2.749531
142	1	0	5.071260	4.663861	2.278418
143	1	0	5.141560	6.327536	-1.673816
144	1	0	0.947219	6.861432	1.869237
145	1	0	-0.182411	9.326238	-2.064531
146	1	0	1.034827	10.073440	-4.062239
147	1	0	4.524918	7.977249	-2.745790
148	1	0	4.651891	9.176595	-4.776691
149	1	0	3.140198	9.160610	-5.695609
150	1	0	3.627369	10.618208	-4.834808
151	1	0	-5.071388	4.663700	-2.278510
152	1	0	-5.141701	6.327387	1.673716
153	1	0	-2.966050	5.843176	-2.749646
154	1	0	-0.947398	6.861384	-1.869369
155	1	0	-4.525094	7.977123	2.745680
156	1	0	0.182196	9.326229	2.064384

157	1	0	-1.035045	10.073402	4.062101
158	1	0	-3.627631	10.618110	4.834666
159	1	0	-4.652072	9.176439	4.776598
160	1	0	-3.140360	9.160558	5.695487
161	1	0	-6.893872	2.115714	2.556046
162	1	0	-5.511114	4.096421	2.100957
163	1	0	-7.330735	4.504937	-1.762461
164	1	0	-8.133625	0.251320	1.644094
165	1	0	-10.929861	-0.437336	-2.166965
166	1	0	-11.656420	0.941441	-4.065587
167	1	0	-9.116639	4.124978	-2.752654
168	1	0	-10.618244	3.003271	-5.673988
169	1	0	-11.955436	3.611788	-4.702016
170	1	0	-10.406073	4.466543	-4.702723
171	1	0	-6.425281	-5.486633	-3.010643
172	1	0	-7.463919	-5.595164	1.150038
173	1	0	-7.779201	-3.453939	-3.306998
174	1	0	-8.620568	-1.430987	-2.239031
175	1	0	-9.114716	-5.124923	2.383501
176	1	0	-10.576183	-0.416008	2.001018
177	1	0	-11.078846	-1.698362	4.034786
178	1	0	-10.061371	-5.317936	4.543904
179	1	0	-9.977410	-3.828430	5.494939
180	1	0	-11.508512	-4.327942	4.781561
181	1	0	7.778988	-3.453498	3.307112
182	1	0	6.425176	-5.486277	3.010864
183	1	0	7.464061	-5.595136	-1.149746
184	1	0	8.620355	-1.430625	2.239046
185	1	0	10.576141	-0.415876	-2.000977
186	1	0	11.078865	-1.698323	-4.034670
187	1	0	9.114769	-5.124835	-2.383253
188	1	0	10.060604	-5.317664	-4.544018
189	1	0	9.978633	-3.827921	-5.494875
190	1	0	11.508791	-4.328943	-4.780532
191	1	0	5.511076	4.096606	-2.101062
192	1	0	7.330623	4.505140	1.762394
193	1	0	6.893867	2.115926	-2.556127
194	1	0	8.133612	0.251524	-1.644126
195	1	0	9.116574	4.125263	2.752558
196	1	0	10.929741	-0.437096	2.167018
197	1	0	11.656290	0.941722	4.065616
198	1	0	10.406004	4.466862	4.702637
199	1	0	10.618131	3.003611	5.673944
200	1	0	11.955348	3.612074	4.701974

Table S12. Cartesian coordinate of *E,R,E,R,E,S,E,S* (10)

SCF Done: E(RB3LYP) = -4621.34281789 A.U. after 6 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.051874	-5.247183	4.392185
2	6	0	-4.943623	-5.863121	3.162752
3	6	0	-5.808816	-5.537035	2.088672
4	6	0	-6.752702	-4.486596	2.292456
5	6	0	-6.851078	-3.894287	3.572672
6	6	0	-6.032111	-4.259423	4.627917
7	6	0	-5.738334	-6.200774	0.792995

8	6	0	-7.542082	-4.005761	1.169036
9	6	0	-7.549990	-4.761897	-0.034186
10	6	0	-6.652631	-5.869379	-0.173635
11	6	0	-8.321604	-4.293966	-1.126438
12	6	0	-8.920977	-3.051776	-1.096096
13	6	0	-8.784917	-2.214704	0.040503
14	6	0	-8.165208	-2.740173	1.171346
15	6	0	-6.168320	-3.625213	5.990404
16	1	0	-8.378969	-4.902556	-2.025317
17	1	0	-9.459162	-2.688561	-1.966667
18	1	0	-8.025809	-2.090390	2.027072
19	1	0	-6.617939	-6.380063	-1.132432
20	1	0	-4.183496	-6.619731	3.020608
21	1	0	-4.375688	-5.532857	5.194252
22	1	0	-7.607842	-3.135557	3.744113
23	1	0	-5.228154	-3.159206	6.307542
24	1	0	-6.943895	-2.854689	5.998442
25	1	0	-6.428188	-4.369724	6.752236
26	6	0	-4.667097	-10.119353	2.583038
27	6	0	-5.042803	-8.951797	1.951804
28	6	0	-4.149280	-8.250047	1.108572
29	6	0	-2.836101	-8.778288	0.914517
30	6	0	-2.487765	-9.975856	1.579855
31	6	0	-3.371368	-10.653906	2.405649
32	6	0	-4.549028	-7.032904	0.428601
33	6	0	-1.903388	-8.080981	0.037370
34	6	0	-2.417831	-7.043901	-0.789770
35	6	0	-3.734578	-6.539723	-0.556183
36	6	0	-1.562686	-6.416253	-1.723300
37	6	0	-0.214992	-6.695228	-1.745287
38	6	0	0.348410	-7.606183	-0.815459
39	6	0	-0.510569	-8.321344	0.017702
40	6	0	-2.978541	-11.940254	3.090807
41	1	0	0.441268	-6.138212	-2.405939
42	1	0	-0.082167	-9.033285	0.715547
43	1	0	-1.971976	-5.649633	-2.375882
44	1	0	-4.036630	-5.647827	-1.097260
45	1	0	-1.503066	-10.402322	1.415569
46	1	0	-6.044724	-8.557753	2.089886
47	1	0	-5.378769	-10.641898	3.217390
48	1	0	-1.949490	-12.223194	2.853791
49	1	0	-3.059421	-11.851105	4.180522
50	1	0	-3.631627	-12.767561	2.789339
51	6	0	4.335517	8.325498	4.709956
52	6	0	4.759202	7.906527	3.465039
53	6	0	3.858202	7.781234	2.381178
54	6	0	2.486319	8.107456	2.601525
55	6	0	2.088459	8.530665	3.889709
56	6	0	2.980273	8.643822	4.945166
57	6	0	4.301612	7.364569	1.059873
58	6	0	1.539069	7.997282	1.500504
59	6	0	2.059777	7.850193	0.184722
60	6	0	3.441316	7.530644	0.002909
61	6	0	1.162217	7.831779	-0.908770
62	6	0	-0.200381	7.794599	-0.706762
63	6	0	-0.733144	7.760034	0.606784
64	6	0	0.140899	7.928712	1.679521
65	6	0	2.531791	9.110301	6.308826
66	1	0	1.564763	7.759672	-1.915721

67	1	0	-0.869365	7.680527	-1.553902
68	1	0	-0.265490	7.924162	2.685410
69	1	0	3.760817	7.250544	-0.996094
70	1	0	5.807864	7.683594	3.300345
71	1	0	5.056580	8.425729	5.517444
72	1	0	1.052794	8.811341	4.054545
73	1	0	2.707342	8.340338	7.069458
74	1	0	3.082951	10.003196	6.625800
75	1	0	1.465916	9.353067	6.319305
76	6	0	7.269596	8.015911	-2.149460
77	6	0	6.432426	7.878286	-1.061033
78	6	0	6.386803	6.679935	-0.309938
79	6	0	7.240022	5.603044	-0.700475
80	6	0	8.082332	5.780587	-1.821311
81	6	0	8.113475	6.958187	-2.552335
82	6	0	5.527813	6.540340	0.854748
83	6	0	7.222119	4.360202	0.060511
84	6	0	6.556897	4.359947	1.318000
85	6	0	5.721407	5.460214	1.679486
86	6	0	6.588959	3.189670	2.111788
87	6	0	7.125792	2.018536	1.626152
88	6	0	7.655329	1.956486	0.311697
89	6	0	7.747902	3.140787	-0.419056
90	6	0	9.032630	7.125098	-3.737893
91	1	0	7.051686	1.109042	2.213282
92	1	0	8.172730	3.102414	-1.416420
93	1	0	6.107231	3.204601	3.085881
94	1	0	5.106678	5.348193	2.567044
95	1	0	8.756717	4.978696	-2.105278
96	1	0	5.805752	8.709071	-0.755109
97	1	0	7.291017	8.955578	-2.695921
98	1	0	9.642718	6.232767	-3.901178
99	1	0	8.465375	7.315748	-4.656610
100	1	0	9.710804	7.975105	-3.599642
101	6	0	9.456507	-5.236422	2.162042
102	6	0	8.628544	-5.376499	1.066883
103	6	0	8.202716	-4.256911	0.313432
104	6	0	8.658268	-2.962147	0.708851
105	6	0	9.504049	-2.858248	1.836231
106	6	0	9.908902	-3.962761	2.569849
107	6	0	7.352791	-4.401339	-0.857632
108	6	0	8.245060	-1.791187	-0.054078
109	6	0	7.625593	-2.004749	-1.316732
110	6	0	7.193052	-3.315688	-1.682451
111	6	0	7.284432	-0.886216	-2.112441
112	6	0	7.410030	0.395147	-1.624614
113	6	0	7.879600	0.623695	-0.305766
114	6	0	8.343916	-0.467816	0.427819
115	6	0	10.822830	-3.823857	3.763014
116	1	0	6.841404	-1.055224	-3.090355
117	1	0	7.051025	1.232322	-2.214235
118	1	0	8.724901	-0.295096	1.428652
119	1	0	6.580846	-3.407171	-2.574053
120	1	0	8.307402	-6.365367	0.757831
121	1	0	9.777006	-6.118984	2.710148
122	1	0	9.880350	-1.881370	2.123526
123	1	0	10.339984	-4.187691	4.677710
124	1	0	11.740424	-4.409089	3.632391
125	1	0	11.110523	-2.782284	3.928834

126	6	0	6.806334	-6.465986	-4.720441
127	6	0	7.069919	-5.935308	-3.473932
128	6	0	6.175437	-6.110675	-2.391605
129	6	0	4.982916	-6.862300	-2.615406
130	6	0	4.744953	-7.388064	-3.905282
131	6	0	5.627092	-7.204724	-4.959018
132	6	0	6.458940	-5.576707	-1.068397
133	6	0	4.049522	-7.067962	-1.516091
134	6	0	4.493735	-6.764282	-0.199049
135	6	0	5.696983	-6.015160	-0.013838
136	6	0	3.638336	-7.041358	0.893266
137	6	0	2.337274	-7.446776	0.689532
138	6	0	1.822559	-7.582207	-0.624654
139	6	0	2.704442	-7.455193	-1.696802
140	6	0	5.356856	-7.790354	-6.323687
141	1	0	1.667151	-7.558469	1.536069
142	1	0	2.318453	-7.579841	-2.703085
143	1	0	3.995595	-6.846270	1.900999
144	1	0	5.906948	-5.649581	0.986502
145	1	0	3.855657	-7.987808	-4.072817
146	1	0	7.989947	-5.385772	-3.306528
147	1	0	7.522241	-6.326072	-5.526610
148	1	0	4.414196	-8.343637	-6.343436
149	1	0	5.301829	-7.006644	-7.088375
150	1	0	6.155460	-8.477054	-6.627758
151	6	0	-6.528707	3.331984	-4.395598
152	6	0	-6.612818	3.948378	-3.164545
153	6	0	-7.314346	3.358517	-2.083570
154	6	0	-7.868732	2.059023	-2.282864
155	6	0	-7.783263	1.468033	-3.564597
156	6	0	-7.138204	2.079960	-4.626200
157	6	0	-7.450026	4.008162	-0.785913
158	6	0	-8.448302	1.347304	-1.154191
159	6	0	-8.690624	2.059639	0.051375
160	6	0	-8.199119	3.397906	0.187108
161	6	0	-9.259174	1.366412	1.148431
162	6	0	-9.422521	-0.003079	1.119342
163	6	0	-9.030723	-0.750501	-0.020359
164	6	0	-8.625684	-0.052190	-1.154963
165	6	0	-7.075335	1.437069	-5.989979
166	1	0	-9.503522	1.923145	2.049533
167	1	0	-9.805818	-0.521729	1.993153
168	1	0	-8.289787	-0.621505	-2.013504
169	1	0	-8.322509	3.891758	1.147400
170	1	0	-6.137897	4.910591	-3.026939
171	1	0	-5.990559	3.822467	-5.203037
172	1	0	-8.255219	0.505089	-3.731569
173	1	0	-7.557262	2.064849	-6.748736
174	1	0	-6.037964	1.287830	-6.311502
175	1	0	-7.571876	0.463036	-5.997784
176	6	0	-7.709979	8.064189	-2.573955
177	6	0	-7.685283	6.837556	-1.943416
178	6	0	-6.608221	6.460792	-1.106838
179	6	0	-5.534603	7.384427	-0.918543
180	6	0	-5.595188	8.630776	-1.582809
181	6	0	-6.654893	8.988028	-2.402419
182	6	0	-6.590485	5.179572	-0.427283
183	6	0	-4.422244	7.025499	-0.046993
184	6	0	-4.571117	5.878340	0.781276

185	6	0	-5.655517	4.976038	0.552980
186	6	0	-3.555758	5.560785	1.711215
187	6	0	-2.370797	6.260740	1.729284
188	6	0	-2.135266	7.304679	0.798409
189	6	0	-3.181516	7.702836	-0.032358
190	6	0	-6.701859	10.332400	-3.087100
191	1	0	-1.567766	5.946739	2.388042
192	1	0	-3.008343	8.514651	-0.731210
193	1	0	-3.693011	4.703258	2.364626
194	1	0	-5.650867	4.034756	1.094696
195	1	0	-4.799895	9.352120	-1.422501
196	1	0	-8.507549	6.141732	-2.077210
197	1	0	-8.556029	8.329472	-3.203060
198	1	0	-5.813075	10.928328	-2.863051
199	1	0	-6.765787	10.221633	-4.175925
200	1	0	-7.579947	10.908900	-2.773203

Table S13. Cartesian coordinate of *E,R,Z,S,Z,R,E,S* (11)

SCF Done: E(RB3LYP) = -4621.34254559 A.U. after 14 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-10.696057	-2.475721	-2.768311
2	6	0	-10.317529	-1.483689	-1.886871
3	6	0	-9.488560	-1.760460	-0.773722
4	6	0	-9.048977	-3.104444	-0.574976
5	6	0	-9.457023	-4.093347	-1.498512
6	6	0	-10.266262	-3.808404	-2.587429
7	6	0	-9.111693	-0.725535	0.175270
8	6	0	-8.196528	-3.419382	0.563792
9	6	0	-8.056287	-2.437112	1.583534
10	6	0	-8.523963	-1.106583	1.355585
11	6	0	-7.296793	-2.748133	2.735755
12	6	0	-6.577092	-3.919763	2.815650
13	6	0	-6.572862	-4.838835	1.735478
14	6	0	-7.433552	-4.602846	0.664432
15	6	0	-10.699038	-4.886732	-3.550830
16	1	0	-7.223265	-2.009123	3.529276
17	1	0	-5.926885	-4.094698	3.666837
18	1	0	-7.452642	-5.319572	-0.149586
19	1	0	-8.256655	-0.351100	2.088010
20	1	0	-10.673656	-0.469581	-2.032332
21	1	0	-11.345895	-2.231973	-3.605200
22	1	0	-9.154164	-5.122878	-1.334860
23	1	0	-11.791355	-4.970172	-3.590968
24	1	0	-10.299053	-5.863434	-3.265823
25	1	0	-10.358334	-4.669243	-4.570009
26	6	0	-10.696156	2.474840	2.768747
27	6	0	-10.317573	1.482835	1.887302
28	6	0	-9.488718	1.759683	0.774086
29	6	0	-9.049333	3.103722	0.575262
30	6	0	-9.457419	4.092593	1.498817
31	6	0	-10.266532	3.807574	2.587803
32	6	0	-9.111770	0.724788	-0.174902
33	6	0	-8.197009	3.418737	-0.563564
34	6	0	-8.056736	2.436474	-1.583310
35	6	0	-8.524210	1.105890	-1.355289

36	6	0	-7.297392	2.747590	-2.735607
37	6	0	-6.577835	3.919304	-2.815574
38	6	0	-6.573604	4.838370	-1.735390
39	6	0	-7.434182	4.602289	-0.664278
40	6	0	-10.699371	4.885870	3.551211
41	1	0	-5.927734	4.094319	-3.666826
42	1	0	-7.453287	5.319017	0.149740
43	1	0	-7.223849	2.008585	-3.529133
44	1	0	-8.256878	0.350422	-2.087724
45	1	0	-9.154690	5.122156	1.335121
46	1	0	-10.673564	0.468686	2.032806
47	1	0	-11.345895	2.231032	3.605695
48	1	0	-10.299421	5.862592	3.266224
49	1	0	-10.358680	4.668380	4.570393
50	1	0	-11.791693	4.969268	3.591327
51	6	0	10.653579	-0.899994	3.674371
52	6	0	10.353759	-0.444574	2.406045
53	6	0	9.521077	-1.183212	1.533170
54	6	0	8.997280	-2.429179	1.992556
55	6	0	9.321564	-2.861546	3.297822
56	6	0	10.133822	-2.124656	4.146471
57	6	0	9.218690	-0.721351	0.186272
58	6	0	8.150616	-3.219293	1.108404
59	6	0	8.129177	-2.873918	-0.271245
60	6	0	8.664797	-1.618294	-0.694144
61	6	0	7.394640	-3.683384	-1.168960
62	6	0	6.573310	-4.687586	-0.705529
63	6	0	6.436108	-4.921814	0.686410
64	6	0	7.278211	-4.233255	1.559010
65	6	0	10.476152	-2.615168	5.532249
66	1	0	7.415268	-3.442975	-2.228664
67	1	0	5.938111	-5.228411	-1.399780
68	1	0	7.193415	-4.425909	2.623552
69	1	0	8.454395	-1.308994	-1.712793
70	1	0	10.778471	0.490065	2.055497
71	1	0	11.310426	-0.315441	4.313837
72	1	0	8.951313	-3.823244	3.639417
73	1	0	10.112993	-1.921594	6.299919
74	1	0	11.560399	-2.701709	5.667863
75	1	0	10.034297	-3.595014	5.731941
76	6	0	10.653694	0.900959	-3.673930
77	6	0	10.353857	0.445524	-2.405613
78	6	0	9.521008	1.184055	-1.532810
79	6	0	8.997053	2.429932	-1.992262
80	6	0	9.321354	2.862316	-3.297515
81	6	0	10.133787	2.125526	-4.146095
82	6	0	9.218608	0.722191	-0.185903
83	6	0	8.150226	3.219950	-1.108172
84	6	0	8.128784	2.874628	0.271496
85	6	0	8.664564	1.619087	0.694460
86	6	0	7.394094	3.684020	1.169146
87	6	0	6.572628	4.688085	0.705642
88	6	0	6.435441	4.922223	-0.686305
89	6	0	7.277682	4.233751	-1.558850
90	6	0	10.476100	2.616050	-5.531873
91	1	0	5.937314	5.228836	1.399846
92	1	0	7.192888	4.426353	-2.623400
93	1	0	7.414703	3.443651	2.228859
94	1	0	8.454155	1.309791	1.713109

95	1	0	8.950979	3.823947	-3.639163
96	1	0	10.778685	-0.489044	-2.055016
97	1	0	11.310682	0.316493	-4.313330
98	1	0	10.034258	3.595907	-5.731541
99	1	0	10.112906	1.922497	-6.299548
100	1	0	11.560344	2.702565	-5.667510
101	6	0	1.770580	10.664550	1.292327
102	6	0	0.950409	9.780591	0.622354
103	6	0	1.478128	8.656831	-0.056181
104	6	0	2.890943	8.449266	-0.037334
105	6	0	3.698574	9.376135	0.660281
106	6	0	3.170192	10.474170	1.321876
107	6	0	0.619955	7.737158	-0.778433
108	6	0	3.456025	7.300603	-0.734427
109	6	0	2.612032	6.582040	-1.626592
110	6	0	1.202057	6.819739	-1.612355
111	6	0	3.157162	5.524548	-2.389377
112	6	0	4.444087	5.086346	-2.171381
113	6	0	5.245846	5.677135	-1.161299
114	6	0	4.761359	6.809104	-0.507662
115	6	0	4.056760	11.458225	2.045785
116	1	0	2.517136	5.005045	-3.097604
117	1	0	4.813152	4.211924	-2.697367
118	1	0	5.381474	7.275593	0.250751
119	1	0	0.570336	6.148368	-2.186791
120	1	0	-0.122147	9.945568	0.599734
121	1	0	1.337468	11.525112	1.796118
122	1	0	4.776332	9.245843	0.653594
123	1	0	3.794513	11.522396	3.108362
124	1	0	3.953644	12.467530	1.630450
125	1	0	5.110351	11.174580	1.977719
126	6	0	-1.169676	6.743423	3.073468
127	6	0	-0.624011	7.120049	1.864232
128	6	0	-1.411530	7.212600	0.689402
129	6	0	-2.782850	6.829761	0.776457
130	6	0	-3.313242	6.472942	2.038106
131	6	0	-2.541652	6.432164	3.187120
132	6	0	-0.861191	7.640373	-0.590420
133	6	0	-3.584907	6.757911	-0.435406
134	6	0	-3.053834	7.290416	-1.641770
135	6	0	-1.695347	7.743474	-1.672996
136	6	0	-3.836519	7.218479	-2.820245
137	6	0	-5.028969	6.524893	-2.845841
138	6	0	-5.507137	5.871508	-1.681756
139	6	0	-4.804597	6.052294	-0.493199
140	6	0	-3.134051	6.061155	4.524459
141	1	0	-5.587476	6.444487	-3.773779
142	1	0	-5.141296	5.513127	0.383880
143	1	0	-3.452776	7.671243	-3.730957
144	1	0	-1.290592	8.080574	-2.623706
145	1	0	-4.368813	6.234508	2.117530
146	1	0	0.430637	7.356431	1.815631
147	1	0	-0.534139	6.692053	3.954124
148	1	0	-4.196373	5.817209	4.439290
149	1	0	-3.035140	6.881461	5.245250
150	1	0	-2.623896	5.192883	4.957536
151	6	0	-1.169201	-6.743848	-3.073802
152	6	0	-0.623401	-7.120340	-1.864596
153	6	0	-1.410808	-7.212806	-0.689672

154	6	0	-2.782147	-6.830060	-0.776620
155	6	0	-3.312683	-6.473366	-2.038258
156	6	0	-2.541209	-6.432641	-3.187342
157	6	0	-0.860313	-7.640422	0.590125
158	6	0	-3.584100	-6.758171	0.435314
159	6	0	-3.052876	-7.290561	1.641667
160	6	0	-1.694355	-7.743508	1.672796
161	6	0	-3.835465	-7.218626	2.820207
162	6	0	-5.027975	-6.525149	2.845866
163	6	0	-5.506298	-5.871867	1.681786
164	6	0	-4.803845	-6.052652	0.493181
165	6	0	-3.133711	-6.061642	-4.524638
166	1	0	-3.451594	-7.671298	3.730912
167	1	0	-5.586413	-6.444746	3.773846
168	1	0	-5.140667	-5.513555	-0.383892
169	1	0	-1.289457	-8.080486	2.623490
170	1	0	0.431257	-7.356693	-1.816068
171	1	0	-0.533771	-6.692550	-3.954541
172	1	0	-4.368276	-6.235008	-2.117594
173	1	0	-3.033812	-6.881511	-5.245780
174	1	0	-2.624357	-5.192640	-4.957206
175	1	0	-4.196296	-5.818794	-4.439575
176	6	0	1.771574	-10.664035	-1.293250
177	6	0	0.951364	-9.780227	-0.623145
178	6	0	1.479046	-8.656566	0.055610
179	6	0	2.891840	-8.448959	0.036836
180	6	0	3.699526	-9.375696	-0.660912
181	6	0	3.171196	-10.473619	-1.322712
182	6	0	0.620840	-7.737069	0.778026
183	6	0	3.456866	-7.300408	0.734157
184	6	0	2.612849	-6.582085	1.626495
185	6	0	1.202893	-6.819842	1.612206
186	6	0	3.157956	-5.524736	2.389509
187	6	0	4.444844	-5.086416	2.171564
188	6	0	5.246602	-5.676921	1.161305
189	6	0	4.762164	-6.808778	0.507453
190	6	0	4.057805	-11.457559	-2.046727
191	1	0	4.813881	-4.212095	2.697736
192	1	0	5.382266	-7.275078	-0.251087
193	1	0	2.517932	-5.005440	3.097891
194	1	0	0.571119	-6.148660	2.186809
195	1	0	4.777279	-9.245367	-0.654155
196	1	0	-0.121191	-9.945220	-0.600584
197	1	0	1.338520	-11.524517	-1.797228
198	1	0	5.111378	-11.173829	-1.978706
199	1	0	3.795502	-11.521708	-3.109288
200	1	0	3.954809	-12.466889	-1.631419

Table S14. Cartesian coordinate of *Z,R,Z,R,E,R,Z,S* (12)

SCF Done: E(RB3LYP) = -4621.34215963 A.U. after 6 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	10.118615	3.267794	-2.836839
2	6	0	9.819943	2.226758	-1.982489
3	6	0	8.901369	2.383882	-0.917205
4	6	0	8.280412	3.659911	-0.736761

5	6	0	8.615140	4.701492	-1.632076
6	6	0	9.514253	4.533434	-2.673570
7	6	0	8.614815	1.298074	0.002518
8	6	0	7.326047	3.852075	0.349677
9	6	0	7.206967	2.816199	1.318187
10	6	0	7.867561	1.568592	1.119695
11	6	0	6.314635	2.983017	2.400813
12	6	0	5.492173	4.081357	2.477341
13	6	0	5.521663	5.087290	1.475691
14	6	0	6.471038	4.972738	0.459500
15	6	0	9.858089	5.668199	-3.607644
16	6	0	10.648561	-1.438126	2.782554
17	6	0	10.134878	-0.570978	1.839988
18	6	0	9.409134	-1.042743	0.720402
19	6	0	9.212681	-2.449583	0.585346
20	6	0	9.751319	-3.307255	1.571037
21	6	0	10.462919	-2.832841	2.662097
22	6	0	8.896207	-0.137423	-0.295179
23	6	0	8.460160	-2.958039	-0.552994
24	6	0	8.206834	-2.071064	-1.636682
25	6	0	8.439112	-0.669144	-1.474260
26	6	0	7.545670	-2.567258	-2.784615
27	6	0	7.007366	-3.835396	-2.799717
28	6	0	7.095648	-4.671599	-1.657048
29	6	0	7.882358	-4.245288	-0.588539
30	6	0	11.044411	-3.770772	3.691907
31	6	0	-11.277618	0.884102	-2.776410
32	6	0	-10.631775	0.092756	-1.847550
33	6	0	-9.641645	0.620782	-0.986309
34	6	0	-9.330704	2.010420	-1.087736
35	6	0	-10.007455	2.788311	-2.053781
36	6	0	-10.968231	2.255761	-2.899898
37	6	0	-8.965636	-0.203643	0.005852
38	6	0	-8.338866	2.590714	-0.192159
39	6	0	-7.938394	1.824486	0.937297
40	6	0	-8.256462	0.432308	0.995487
41	6	0	-7.063511	2.404880	1.885064
42	6	0	-6.475628	3.628263	1.648784
43	6	0	-6.718784	4.320900	0.435684
44	6	0	-7.690349	3.821914	-0.430415
45	6	0	-11.687930	3.112358	-3.913079
46	6	0	-9.136098	-3.182247	3.278899
47	6	0	-9.244597	-2.304614	2.218707
48	6	0	-8.652676	-2.583250	0.964453
49	6	0	-7.942523	-3.812446	0.812067
50	6	0	-7.846456	-4.683244	1.920335
51	6	0	-8.423599	-4.393808	3.147367
52	6	0	-8.778356	-1.672624	-0.164891
53	6	0	-7.348068	-4.142201	-0.476196
54	6	0	-7.748954	-3.375394	-1.604083
55	6	0	-8.453304	-2.147489	-1.412428
56	6	0	-7.266390	-3.738217	-2.883970
57	6	0	-6.288076	-4.695950	-3.023312
58	6	0	-5.725334	-5.328148	-1.883795
59	6	0	-6.318162	-5.094560	-0.643263
60	6	0	-8.317142	-5.346987	4.312828
61	6	0	-1.238404	-10.726974	1.295732
62	6	0	-0.341696	-9.884100	0.673051
63	6	0	-0.779335	-8.807171	-0.133689

64	6	0	-2.185703	-8.606514	-0.303379
65	6	0	-3.071799	-9.492287	0.351827
66	6	0	-2.630582	-10.541206	1.143806
67	6	0	0.166028	-7.937322	-0.805084
68	6	0	-2.664256	-7.516011	-1.146776
69	6	0	-1.705032	-6.824494	-1.937833
70	6	0	-0.311659	-7.053604	-1.735143
71	6	0	-2.134536	-5.815742	-2.826967
72	6	0	-3.449831	-5.420326	-2.860716
73	6	0	-4.407971	-6.006800	-1.992703
74	6	0	-4.007426	-7.071214	-1.185654
75	6	0	-3.601203	-11.477223	1.822306
76	6	0	1.743137	-6.759901	3.112932
77	6	0	1.266441	-7.222613	1.904044
78	6	0	2.104906	-7.328239	0.766859
79	6	0	3.450433	-6.868301	0.886435
80	6	0	3.909508	-6.419709	2.146198
81	6	0	3.090554	-6.366657	3.261930
82	6	0	1.631217	-7.841944	-0.510893
83	6	0	4.294531	-6.810143	-0.297516
84	6	0	3.856337	-7.463265	-1.481164
85	6	0	2.525774	-7.989291	-1.539826
86	6	0	4.678570	-7.409674	-2.633539
87	6	0	5.800658	-6.608026	-2.672247
88	6	0	6.164651	-5.824626	-1.547695
89	6	0	5.444868	-5.997017	-0.367376
90	6	0	3.607657	-5.899776	4.600546
91	6	0	0.996452	8.994679	-3.290067
92	6	0	0.238871	8.890374	-2.141058
93	6	0	0.768148	8.334297	-0.952248
94	6	0	2.127703	7.897534	-0.960146
95	6	0	2.870737	8.014888	-2.156464
96	6	0	2.334656	8.546537	-3.318960
97	6	0	-0.021076	8.233256	0.267558
98	6	0	2.721235	7.369581	0.261084
99	6	0	2.005530	7.548833	1.476191
100	6	0	0.638806	7.961419	1.441113
101	6	0	2.615300	7.155771	2.690670
102	6	0	3.812222	6.476857	2.695690
103	6	0	4.449667	6.116431	1.478960
104	6	0	3.918852	6.622074	0.291783
105	6	0	3.153592	8.667981	-4.580947
106	6	0	-2.658260	10.194658	3.226603
107	6	0	-1.871274	9.703341	2.204607
108	6	0	-2.331005	8.680852	1.341229
109	6	0	-3.652781	8.176299	1.537770
110	6	0	-4.427240	8.699836	2.597683
111	6	0	-3.958029	9.690205	3.446721
112	6	0	-1.510726	8.166564	0.253289
113	6	0	-4.175574	7.156500	0.638038
114	6	0	-3.450737	6.893630	-0.557255
115	6	0	-2.121506	7.395850	-0.704846
116	6	0	-3.991234	5.995469	-1.506427
117	6	0	-5.128064	5.270474	-1.226638
118	6	0	-5.766044	5.389734	0.034309
119	6	0	-5.312447	6.366376	0.918909
120	6	0	-4.810069	10.237920	4.565689
121	1	0	6.239203	2.192774	3.142963
122	1	0	4.757225	4.137227	3.272111

123	1	0	6.514823	5.749323	-0.295959
124	1	0	7.654689	0.771514	1.825362
125	1	0	10.307964	1.266542	-2.110984
126	1	0	10.837938	3.117325	-3.638061
127	1	0	8.173912	5.682623	-1.488590
128	1	0	9.586762	5.427519	-4.642397
129	1	0	9.336284	6.588179	-3.330810
130	1	0	10.934027	5.877680	-3.600794
131	1	0	6.416900	-4.158217	-3.651207
132	1	0	7.976896	-4.893048	0.276467
133	1	0	7.389353	-1.900516	-3.628567
134	1	0	8.077710	-0.006666	-2.255412
135	1	0	9.634842	-4.380446	1.455392
136	1	0	10.300847	0.495991	1.942058
137	1	0	11.215946	-1.044664	3.622393
138	1	0	10.640614	-3.564775	4.690205
139	1	0	10.827153	-4.815024	3.452028
140	1	0	12.133101	-3.661783	3.759896
141	1	0	-6.793179	1.832478	2.768512
142	1	0	-5.735000	4.016212	2.341024
143	1	0	-7.891565	4.361296	-1.350365
144	1	0	-7.764234	-0.154414	1.764044
145	1	0	-10.897533	-0.955024	-1.756568
146	1	0	-12.044742	0.448914	-3.412158
147	1	0	-9.794971	3.851364	-2.114180
148	1	0	-11.537329	2.734431	-4.931087
149	1	0	-12.769203	3.120040	-3.732380
150	1	0	-11.336693	4.147233	-3.885088
151	1	0	-5.899835	-4.929682	-4.009602
152	1	0	-5.881979	-5.557358	0.235641
153	1	0	-7.631749	-3.200071	-3.754693
154	1	0	-8.562854	-1.501797	-2.277430
155	1	0	-7.331654	-5.631389	1.798720
156	1	0	-9.812161	-1.387611	2.335844
157	1	0	-9.617311	-2.944641	4.224427
158	1	0	-7.771973	-6.254586	4.040270
159	1	0	-7.794084	-4.883917	5.157909
160	1	0	-9.307468	-5.645799	4.675445
161	1	0	-1.395464	-5.309745	-3.442329
162	1	0	-3.742224	-4.589335	-3.492963
163	1	0	-4.743938	-7.534716	-0.537608
164	1	0	0.385913	-6.412769	-2.265896
165	1	0	0.725584	-10.045185	0.788509
166	1	0	-0.871625	-11.551316	1.902252
167	1	0	-4.140934	-9.369023	0.210371
168	1	0	-3.430501	-12.516558	1.518678
169	1	0	-3.491520	-11.441536	2.912705
170	1	0	-4.637367	-11.224247	1.582314
171	1	0	6.383069	-6.536910	-3.586195
172	1	0	5.691479	-5.366392	0.478434
173	1	0	4.371935	-7.957492	-3.520956
174	1	0	2.180007	-8.394447	-2.487158
175	1	0	4.947535	-6.120467	2.251224
176	1	0	0.228945	-7.520807	1.826891
177	1	0	1.071663	-6.703538	3.966204
178	1	0	4.657844	-5.601276	4.543197
179	1	0	3.034285	-5.041783	4.970359
180	1	0	3.524329	-6.689133	5.356973
181	1	0	2.099362	7.357610	3.625747

182	1	0	4.250416	6.175924	3.641381
183	1	0	4.379727	6.336141	-0.647038
184	1	0	0.080443	7.903702	2.369749
185	1	0	-0.781033	9.259019	-2.135935
186	1	0	0.562038	9.440941	-4.181241
187	1	0	3.912705	7.710554	-2.159170
188	1	0	2.720209	8.073485	-5.393956
189	1	0	3.194966	9.705728	-4.931454
190	1	0	4.180049	8.324379	-4.427495
191	1	0	-5.481167	4.522965	-1.929906
192	1	0	-5.811870	6.469237	1.876850
193	1	0	-3.452603	5.827963	-2.435388
194	1	0	-1.540398	7.016905	-1.539114
195	1	0	-5.442533	8.340757	2.733788
196	1	0	-0.883297	10.119565	2.040858
197	1	0	-2.278229	10.991008	3.861793
198	1	0	-5.803151	9.780897	4.574232
199	1	0	-4.348420	10.053259	5.542957
200	1	0	-4.939701	11.322467	4.474016

Table S15. Cartesian coordinate of *E,R,E,R,E,R,E,S* (13)

SCF Done: E(RB3LYP) = -4621.34200105 A.U. after 5 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.210515	-5.313394	-3.450508
2	6	0	0.344133	-5.999320	-2.261455
3	6	0	-0.776344	-6.552260	-1.591821
4	6	0	-2.065877	-6.317878	-2.152877
5	6	0	-2.162988	-5.632189	-3.385441
6	6	0	-1.054642	-5.134445	-4.049996
7	6	0	-0.655454	-7.326265	-0.362475
8	6	0	-3.247858	-6.741107	-1.419671
9	6	0	-3.094114	-7.608299	-0.304587
10	6	0	-1.775469	-7.905505	0.174547
11	6	0	-4.254651	-8.011833	0.402791
12	6	0	-5.492994	-7.469338	0.120885
13	6	0	-5.636285	-6.493268	-0.897702
14	6	0	-4.522318	-6.203017	-1.682026
15	6	0	-1.181157	-4.417583	-5.371724
16	6	0	-0.211386	-5.312492	3.449901
17	6	0	-0.344974	-5.998698	2.261005
18	6	0	0.775505	-6.551893	1.591588
19	6	0	2.065015	-6.317492	2.152681
20	6	0	2.162091	-5.631529	3.385097
21	6	0	1.053740	-5.133521	4.049447
22	6	0	0.654635	-7.326193	0.362430
23	6	0	3.247018	-6.740980	1.419663
24	6	0	3.093290	-7.608354	0.304715
25	6	0	1.774649	-7.905584	-0.174430
26	6	0	4.253842	-8.012108	-0.402506
27	6	0	5.492222	-7.469701	-0.120574
28	6	0	5.635524	-6.493514	0.897892
29	6	0	4.521511	-6.202996	1.682053
30	6	0	1.180221	-4.416366	5.371019
31	6	0	-1.377486	9.371047	3.419711
32	6	0	-0.743239	8.962971	2.264358

33	6	0	-1.394841	8.142307	1.312739
34	6	0	-2.741820	7.744409	1.571814
35	6	0	-3.358247	8.182644	2.765949
36	6	0	-2.707034	8.981739	3.692514
37	6	0	-0.741580	7.734909	0.079946
38	6	0	-3.441117	6.905162	0.607585
39	6	0	-2.845849	6.717165	-0.671065
40	6	0	-1.500590	7.141405	-0.896983
41	6	0	-3.540708	5.966175	-1.648104
42	6	0	-4.711378	5.309716	-1.339446
43	6	0	-5.245362	5.364623	-0.026635
44	6	0	-4.631336	6.204640	0.901148
45	6	0	-3.393714	9.444039	4.954619
46	6	0	1.378448	9.370831	-3.420040
47	6	0	0.744152	8.962841	-2.264683
48	6	0	1.395675	8.142152	-1.313031
49	6	0	2.742629	7.744143	-1.572072
50	6	0	3.359105	8.182293	-2.766214
51	6	0	2.707968	8.981408	-3.692813
52	6	0	0.742367	7.734844	-0.080232
53	6	0	3.441850	6.904880	-0.607803
54	6	0	2.846549	6.716971	0.670844
55	6	0	1.501320	7.141321	0.896729
56	6	0	3.541337	5.965965	1.647922
57	6	0	4.711965	5.309411	1.339307
58	6	0	5.245979	5.364238	0.026505
59	6	0	4.632029	6.204268	-0.901318
60	6	0	3.394703	9.443619	-4.954921
61	6	0	11.155042	1.419779	2.873087
62	6	0	10.670006	0.603249	1.871740
63	6	0	9.653435	1.038789	0.989116
64	6	0	9.139417	2.362203	1.148869
65	6	0	9.659879	3.168229	2.186555
66	6	0	10.649736	2.725951	3.050656
67	6	0	9.155780	0.189982	-0.081765
68	6	0	8.104388	2.846359	0.243957
69	6	0	7.831494	2.079838	-0.922921
70	6	0	8.367507	0.762541	-1.049151
71	6	0	6.889998	2.564686	-1.860324
72	6	0	6.141603	3.689268	-1.595472
73	6	0	6.291179	4.384662	-0.368370
74	6	0	7.305987	3.982875	0.499823
75	6	0	11.194756	3.612394	4.143971
76	6	0	10.162926	-2.341059	-3.557012
77	6	0	10.005479	-1.573020	-2.420941
78	6	0	9.391945	-2.092878	-1.256757
79	6	0	8.939923	-3.446059	-1.279337
80	6	0	9.114106	-4.201451	-2.460562
81	6	0	9.712123	-3.678526	-3.596755
82	6	0	9.241941	-1.298477	-0.046781
83	6	0	8.315556	-4.010316	-0.091386
84	6	0	8.452569	-3.300728	1.132781
85	6	0	8.916037	-1.948768	1.118648
86	6	0	7.932337	-3.878441	2.316338
87	6	0	7.146915	-5.007963	2.265818
88	6	0	6.821714	-5.607972	1.021089
89	6	0	7.479642	-5.147842	-0.118992
90	6	0	9.899437	-4.510015	-4.842420
91	6	0	-10.162871	-2.340077	3.557351

92	6	0	-10.005402	-1.572098	2.421243
93	6	0	-9.392008	-2.092073	1.257037
94	6	0	-8.940151	-3.445309	1.279636
95	6	0	-9.114351	-4.200637	2.460900
96	6	0	-9.712228	-3.677598	3.597113
97	6	0	-9.241983	-1.297735	0.047024
98	6	0	-8.315934	-4.009686	0.091664
99	6	0	-8.452938	-3.300125	-1.132518
100	6	0	-8.916231	-1.948107	-1.118404
101	6	0	-7.932863	-3.877956	-2.316088
102	6	0	-7.147587	-5.007577	-2.265579
103	6	0	-6.822370	-5.607582	-1.020849
104	6	0	-7.480162	-5.147319	0.119257
105	6	0	-9.899553	-4.509015	4.842824
106	6	0	-11.154955	1.420643	-2.872816
107	6	0	-10.669947	0.604091	-1.871474
108	6	0	-9.653274	1.039545	-0.988925
109	6	0	-9.139122	2.362900	-1.148748
110	6	0	-9.659557	3.168949	-2.186430
111	6	0	-10.649510	2.726751	-3.050462
112	6	0	-9.155646	0.190716	0.081949
113	6	0	-8.103996	2.846975	-0.243905
114	6	0	-7.831107	2.080454	0.922973
115	6	0	-8.367246	0.763216	1.049267
116	6	0	-6.889514	2.565232	1.860315
117	6	0	-6.141038	3.689745	1.595406
118	6	0	-6.290620	4.385131	0.368299
119	6	0	-7.305504	3.983416	-0.499835
120	6	0	-11.194458	3.613199	-4.143808
121	1	0	-4.147645	-8.716875	1.223325
122	1	0	-6.356734	-7.760906	0.711328
123	1	0	-4.609996	-5.423901	-2.428353
124	1	0	-1.683733	-8.510327	1.073031
125	1	0	1.329867	-6.121154	-1.831691
126	1	0	1.095230	-4.910308	-3.937242
127	1	0	-3.139303	-5.505000	-3.841856
128	1	0	-2.225053	-4.337041	-5.686433
129	1	0	-0.768498	-3.403653	-5.314147
130	1	0	-0.631780	-4.941287	-6.162944
131	1	0	6.355983	-7.761438	-0.710902
132	1	0	4.609230	-5.423774	2.428265
133	1	0	4.146830	-8.717263	-1.222942
134	1	0	1.682928	-8.510602	-1.072783
135	1	0	3.138380	-5.504315	3.841559
136	1	0	-1.330687	-6.120549	1.831196
137	1	0	-1.096103	-4.909204	3.936463
138	1	0	2.224100	-4.335848	5.685789
139	1	0	0.767660	-3.402411	5.313179
140	1	0	0.630736	-4.939838	6.162318
141	1	0	-3.095828	5.850790	-2.632970
142	1	0	-5.178540	4.665469	-2.077324
143	1	0	-5.050393	6.264504	1.899791
144	1	0	-1.033998	6.849922	-1.833080
145	1	0	0.271725	9.288422	2.064183
146	1	0	-0.852596	10.012564	4.123264
147	1	0	-4.391946	7.911134	2.955000
148	1	0	-4.425211	9.085321	5.004540
149	1	0	-2.869662	9.082372	5.847225
150	1	0	-3.415117	10.538124	5.018829

151	1	0	5.179070	4.665159	2.077217
152	1	0	5.051113	6.264071	-1.899953
153	1	0	3.096432	5.850647	2.632785
154	1	0	1.034694	6.849909	1.832832
155	1	0	4.392786	7.910697	-2.955243
156	1	0	-0.270787	9.288381	-2.064531
157	1	0	0.853618	10.012369	-4.123619
158	1	0	3.416217	10.537702	-5.019147
159	1	0	4.426164	9.084797	-5.004830
160	1	0	2.870620	9.081992	-5.847525
161	1	0	6.708016	1.989676	-2.764411
162	1	0	5.360432	3.990590	-2.285727
163	1	0	7.436620	4.526594	1.429437
164	1	0	8.000727	0.154449	-1.869766
165	1	0	11.085376	-0.389908	1.738758
166	1	0	11.946753	1.058739	3.524934
167	1	0	9.297000	4.185488	2.295186
168	1	0	11.021425	3.174069	5.133920
169	1	0	12.277257	3.751417	4.041861
170	1	0	10.727203	4.600504	4.129842
171	1	0	6.719106	-5.408578	3.179571
172	1	0	7.226713	-5.587013	-1.077840
173	1	0	8.104887	-3.376432	3.264810
174	1	0	8.826297	-1.383144	2.040774
175	1	0	8.799924	-5.240747	-2.469606
176	1	0	10.373863	-0.552899	-2.405602
177	1	0	10.653307	-1.915900	-4.429265
178	1	0	9.524213	-5.527681	-4.705522
179	1	0	9.370930	-4.070298	-5.696500
180	1	0	10.957276	-4.576823	-5.121982
181	1	0	-8.105415	-3.375963	-3.264569
182	1	0	-6.719911	-5.408287	-3.179353
183	1	0	-7.227223	-5.586468	1.078110
184	1	0	-8.826480	-1.382525	-2.040553
185	1	0	-10.373663	-0.551932	2.405891
186	1	0	-10.653145	-1.914827	4.429619
187	1	0	-8.800298	-5.239972	2.469960
188	1	0	-9.524570	-5.526766	4.705900
189	1	0	-9.370828	-4.069394	5.696819
190	1	0	-10.957367	-4.575583	5.122536
191	1	0	-5.359804	3.991014	2.285613
192	1	0	-7.436142	4.527133	-1.429450
193	1	0	-6.707535	1.990220	2.764402
194	1	0	-8.000481	0.155106	1.869875
195	1	0	-9.296577	4.186166	-2.295113
196	1	0	-11.085424	-0.389014	-1.738431
197	1	0	-11.946750	1.059673	-3.524600
198	1	0	-10.727160	4.601426	-4.129424
199	1	0	-11.020732	3.175051	-5.133768
200	1	0	-12.277022	3.751924	-4.041986

Table S16. Cartesian coordinate of *E,R,Z,R,Z,S,E,S* (14)

SCF Done: E(RB3LYP) = -4621.34167166 A.U. after 14 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.036281	-9.231163	1.327891

2	6	0	-4.900888	-8.862033	0.636559
3	6	0	-4.918905	-7.793779	-0.290735
4	6	0	-6.146033	-7.095167	-0.502738
5	6	0	-7.287573	-7.500352	0.225430
6	6	0	-7.258294	-8.549834	1.131310
7	6	0	-3.731994	-7.414916	-1.034365
8	6	0	-6.187291	-5.994918	-1.457506
9	6	0	-5.087503	-5.846538	-2.347798
10	6	0	-3.875028	-6.562286	-2.097077
11	6	0	-5.146793	-4.856652	-3.354903
12	6	0	-6.169383	-3.934834	-3.378819
13	6	0	-7.172996	-3.945908	-2.376277
14	6	0	-7.205079	-5.014844	-1.482340
15	6	0	-8.495996	-8.974623	1.883807
16	1	0	-4.325644	-4.778325	-4.062510
17	1	0	-6.146373	-3.122263	-4.097798
18	1	0	-7.988315	-5.040722	-0.731753
19	1	0	-3.002395	-6.298910	-2.687775
20	1	0	-3.971273	-9.400497	0.791725
21	1	0	-5.995057	-10.063764	2.025763
22	1	0	-8.232242	-6.995981	0.046175
23	1	0	-8.750805	-10.019944	1.673753
24	1	0	-9.359285	-8.359656	1.615940
25	1	0	-8.349839	-8.893732	2.967419
26	6	0	-2.022458	-6.330740	2.833180
27	6	0	-2.567775	-6.733908	1.632289
28	6	0	-1.775437	-7.322833	0.614977
29	6	0	-0.369900	-7.415109	0.839702
30	6	0	0.149882	-7.016220	2.093101
31	6	0	-0.644947	-6.488238	3.096348
32	6	0	-2.336444	-7.789607	-0.647316
33	6	0	0.500814	-7.854955	-0.239538
34	6	0	-0.084218	-8.408856	-1.410548
35	6	0	-1.508054	-8.382056	-1.565215
36	6	0	0.767171	-8.832235	-2.460789
37	6	0	2.124772	-8.587457	-2.424371
38	6	0	2.705323	-7.911402	-1.321341
39	6	0	1.890174	-7.615067	-0.232101
40	6	0	-0.068246	-6.082162	4.430352
41	1	0	2.748807	-8.878592	-3.264219
42	1	0	2.320491	-7.053534	0.588060
43	1	0	0.324521	-9.303579	-3.334615
44	1	0	-1.927852	-8.749245	-2.498102
45	1	0	1.210470	-7.139154	2.286653
46	1	0	-3.628733	-6.601316	1.468907
47	1	0	-2.665701	-5.890745	3.591281
48	1	0	1.013856	-6.234620	4.462807
49	1	0	-0.513104	-6.659905	5.249209
50	1	0	-0.264728	-5.024748	4.642421
51	6	0	2.536353	10.016450	-3.325494
52	6	0	2.918482	9.427920	-2.136948
53	6	0	1.967012	8.884293	-1.241772
54	6	0	0.586317	8.963717	-1.593793
55	6	0	0.232244	9.571022	-2.819614
56	6	0	1.174824	10.095025	-3.690829
57	6	0	2.359600	8.284091	0.024171
58	6	0	-0.414973	8.419479	-0.687035
59	6	0	-0.010163	8.097807	0.638357
60	6	0	1.382469	8.034888	0.955886

61	6	0	-0.985043	7.655365	1.563414
62	6	0	-2.272309	7.376717	1.157639
63	6	0	-2.642932	7.514312	-0.204089
64	6	0	-1.730834	8.097216	-1.082246
65	6	0	0.769699	10.751177	-4.988308
66	1	0	-0.681626	7.451656	2.586979
67	1	0	-2.977989	6.941532	1.858324
68	1	0	-2.018965	8.223283	-2.120730
69	1	0	1.655382	7.612437	1.917933
70	1	0	3.968437	9.392558	-1.867078
71	1	0	3.292163	10.438107	-3.983524
72	1	0	-0.818598	9.662736	-3.076511
73	1	0	1.211644	10.235279	-5.848865
74	1	0	1.109658	11.792472	-5.031539
75	1	0	-0.315808	10.747755	-5.117925
76	6	0	4.759640	8.784260	3.701755
77	6	0	4.089350	8.727055	2.496911
78	6	0	4.403095	7.751219	1.521208
79	6	0	5.448433	6.819994	1.806411
80	6	0	6.111509	6.909722	3.051370
81	6	0	5.788464	7.865346	4.002242
82	6	0	3.716273	7.702717	0.240594
83	6	0	5.803731	5.811089	0.816134
84	6	0	5.271604	5.950703	-0.495785
85	6	0	4.233976	6.899241	-0.744573
86	6	0	5.658098	5.029058	-1.496584
87	6	0	6.428276	3.930387	-1.188882
88	6	0	6.847949	3.692014	0.144988
89	6	0	6.575518	4.664667	1.106621
90	6	0	6.519809	7.943877	5.320289
91	1	0	6.634542	3.187547	-1.952454
92	1	0	6.914206	4.495949	2.123178
93	1	0	5.271943	5.158320	-2.504212
94	1	0	3.749232	6.863474	-1.715048
95	1	0	6.927349	6.225908	3.263683
96	1	0	3.315137	9.453866	2.276253
97	1	0	4.503367	9.555377	4.424039
98	1	0	7.311668	7.192985	5.385358
99	1	0	5.837078	7.784183	6.163277
100	1	0	6.978487	8.929080	5.463601
101	6	0	10.637560	-2.197000	-2.900838
102	6	0	9.829523	-2.789866	-1.952510
103	6	0	9.071270	-2.018304	-1.039828
104	6	0	9.163673	-0.595063	-1.116173
105	6	0	10.002185	-0.024420	-2.100585
106	6	0	10.736155	-0.791438	-2.991899
107	6	0	8.242068	-2.638630	-0.019980
108	6	0	8.397452	0.225276	-0.186936
109	6	0	7.784391	-0.418995	0.923775
110	6	0	7.725755	-1.845292	0.973530
111	6	0	7.094136	0.365442	1.877416
112	6	0	6.893050	1.712817	1.676452
113	6	0	7.370152	2.347309	0.501017
114	6	0	8.160521	1.604357	-0.375135
115	6	0	11.634878	-0.155229	-4.024226
116	1	0	6.653487	-0.127640	2.739897
117	1	0	6.280487	2.275088	2.373772
118	1	0	8.546087	2.092552	-1.263620
119	1	0	7.121725	-2.294140	1.756162

120	1	0	9.781627	-3.871343	-1.886317
121	1	0	11.217270	-2.819284	-3.578139
122	1	0	10.103098	1.055412	-2.144640
123	1	0	11.339567	-0.443494	-5.039914
124	1	0	12.676775	-0.470248	-3.893556
125	1	0	11.605294	0.935949	-3.964206
126	6	0	8.345709	-5.583075	3.259738
127	6	0	8.419354	-4.721321	2.184673
128	6	0	7.646549	-4.927749	1.016992
129	6	0	6.780717	-6.062298	0.970498
130	6	0	6.732101	-6.922522	2.090899
131	6	0	7.491328	-6.706879	3.230464
132	6	0	7.743848	-4.040959	-0.130537
133	6	0	5.974466	-6.300751	-0.219453
134	6	0	6.273406	-5.549617	-1.390364
135	6	0	7.159408	-4.431794	-1.309026
136	6	0	5.553470	-5.816397	-2.578622
137	6	0	4.480274	-6.679813	-2.579353
138	6	0	4.064777	-7.314952	-1.381255
139	6	0	4.859379	-7.165985	-0.245532
140	6	0	7.429951	-7.648699	4.408319
141	1	0	3.884826	-6.797541	-3.479085
142	1	0	4.559390	-7.674678	0.664277
143	1	0	5.810010	-5.266702	-3.480441
144	1	0	7.241302	-3.793444	-2.183497
145	1	0	6.101249	-7.804804	2.049448
146	1	0	9.095735	-3.874199	2.219486
147	1	0	8.963936	-5.403694	4.135915
148	1	0	6.744216	-8.479787	4.222977
149	1	0	7.091876	-7.130951	5.313763
150	1	0	8.416331	-8.071205	4.632371
151	6	0	-7.655006	1.015786	3.125158
152	6	0	-7.749099	1.802325	1.995689
153	6	0	-8.058890	1.250273	0.727758
154	6	0	-8.188864	-0.168209	0.638629
155	6	0	-8.108739	-0.940353	1.820120
156	6	0	-7.858819	-0.379214	3.061177
157	6	0	-8.203984	2.062415	-0.474929
158	6	0	-8.325030	-0.792875	-0.667681
159	6	0	-8.617818	0.027714	-1.789843
160	6	0	-8.580876	1.451941	-1.644491
161	6	0	-8.740876	-0.580122	-3.064022
162	6	0	-8.407893	-1.905324	-3.255545
163	6	0	-7.952745	-2.696620	-2.170366
164	6	0	-7.997529	-2.146635	-0.891971
165	6	0	-7.797229	-1.220967	4.312064
166	1	0	-9.025301	0.036287	-3.913013
167	1	0	-8.439719	-2.332542	-4.253670
168	1	0	-7.607375	-2.734478	-0.069527
169	1	0	-8.717572	2.057864	-2.536292
170	1	0	-7.591294	2.868364	2.086264
171	1	0	-7.426948	1.480109	4.081472
172	1	0	-8.264919	-2.012680	1.757756
173	1	0	-8.575869	-0.929471	5.026929
174	1	0	-6.834707	-1.102974	4.823181
175	1	0	-7.930010	-2.282761	4.087971
176	6	0	-9.791773	5.545968	1.807866
177	6	0	-9.362825	4.499970	1.017249
178	6	0	-8.129690	4.556406	0.326036

179	6	0	-7.329308	5.733549	0.453195
180	6	0	-7.800625	6.782283	1.275348
181	6	0	-9.008880	6.713080	1.952199
182	6	0	-7.684805	3.465664	-0.520908
183	6	0	-6.068281	5.828421	-0.272537
184	6	0	-5.813895	4.861683	-1.284500
185	6	0	-6.629313	3.691496	-1.365268
186	6	0	-4.656824	4.986912	-2.085470
187	6	0	-3.705419	5.940682	-1.804977
188	6	0	-3.855585	6.803149	-0.688666
189	6	0	-5.055628	6.770713	0.020199
190	6	0	-9.495372	7.854108	2.812396
191	1	0	-2.780751	5.965210	-2.372123
192	1	0	-5.180197	7.443397	0.862638
193	1	0	-4.489502	4.266686	-2.881912
194	1	0	-6.304446	2.898378	-2.031951
195	1	0	-7.213759	7.692156	1.355669
196	1	0	-9.979045	3.613024	0.908247
197	1	0	-10.748923	5.477928	2.318858
198	1	0	-10.467986	8.225442	2.469235
199	1	0	-8.794028	8.692591	2.800945
200	1	0	-9.623923	7.539283	3.854775

Table S17. Cartesian coordinate of *Z,R,E,S,Z,R,Z,S* (15)

SCF Done: E(RB3LYP) = -4621.34096695 A.U. after 5 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.628210	-10.273432	1.906296
2	6	0	-0.692913	-9.626152	1.126030
3	6	0	-1.073683	-8.654732	0.169447
4	6	0	-2.461878	-8.345703	0.028443
5	6	0	-3.389776	-9.033855	0.843162
6	6	0	-3.004624	-9.986004	1.774019
7	6	0	-0.094017	-8.003809	-0.680100
8	6	0	-2.876684	-7.326786	-0.928386
9	6	0	-1.907163	-6.845509	-1.852684
10	6	0	-0.536186	-7.216662	-1.711012
11	6	0	-2.290009	-5.872092	-2.803026
12	6	0	-3.541366	-5.302435	-2.770230
13	6	0	-4.494538	-5.687097	-1.790446
14	6	0	-4.158473	-6.732884	-0.930135
15	6	0	-4.019196	-10.711896	2.623714
16	6	0	3.110378	-9.264303	-3.426215
17	6	0	2.117776	-8.959721	-2.518093
18	6	0	2.398395	-8.244522	-1.329323
19	6	0	3.744047	-7.828501	-1.086677
20	6	0	4.733384	-8.163645	-2.039017
21	6	0	4.446917	-8.869849	-3.196894
22	6	0	1.363050	-7.963623	-0.352394
23	6	0	4.052570	-7.062483	0.115033
24	6	0	3.048436	-6.964932	1.118898
25	6	0	1.727649	-7.439735	0.860170
26	6	0	3.330190	-6.245082	2.301715
27	6	0	4.503432	-5.541472	2.440988
28	6	0	5.478025	-5.530103	1.407946
29	6	0	5.254526	-6.342245	0.295176

30	6	0	5.526765	-9.225084	-4.189926
31	6	0	-1.962135	6.650716	-3.459807
32	6	0	-1.378108	7.177449	-2.326722
33	6	0	-2.106438	7.344824	-1.122213
34	6	0	-3.451141	6.868311	-1.091235
35	6	0	-4.025097	6.359066	-2.279070
36	6	0	-3.316015	6.252478	-3.463475
37	6	0	-1.524115	7.937057	0.076609
38	6	0	-4.175096	6.848999	0.170246
39	6	0	-3.627268	7.539734	1.284813
40	6	0	-2.312837	8.099745	1.186817
41	6	0	-4.325412	7.506207	2.517306
42	6	0	-5.428334	6.695418	2.690952
43	6	0	-5.902432	5.888541	1.625842
44	6	0	-5.308746	6.035291	0.375211
45	6	0	-3.955342	5.722476	-4.723421
46	6	0	0.921426	10.758216	-2.331740
47	6	0	0.159475	9.961184	-1.502570
48	6	0	0.750755	8.959841	-0.697040
49	6	0	2.167491	8.788889	-0.751967
50	6	0	2.914318	9.621283	-1.616377
51	6	0	2.323300	10.598053	-2.403362
52	6	0	-0.044996	8.130939	0.189353
53	6	0	2.800801	7.779288	0.086937
54	6	0	2.023976	7.199988	1.128476
55	6	0	0.605842	7.382227	1.134654
56	6	0	2.641293	6.308847	2.035145
57	6	0	3.932290	5.875749	1.830055
58	6	0	4.658135	6.294527	0.685977
59	6	0	4.106330	7.282331	-0.127726
60	6	0	3.145593	11.486998	-3.304578
61	6	0	10.644892	2.483432	3.568249
62	6	0	10.232615	1.715742	2.497275
63	6	0	9.234313	2.168105	1.603045
64	6	0	8.669137	3.461049	1.821868
65	6	0	9.110547	4.215826	2.931703
66	6	0	10.079533	3.753945	3.809471
67	6	0	8.802134	1.370184	0.463153
68	6	0	7.671111	3.975373	0.893480
69	6	0	7.513750	3.299859	-0.347983
70	6	0	8.074465	1.996800	-0.519092
71	6	0	6.642361	3.843354	-1.320266
72	6	0	5.830466	4.915072	-1.020884
73	6	0	5.833574	5.478095	0.280541
74	6	0	6.795294	5.042399	1.190692
75	6	0	10.541559	4.585096	4.981625
76	6	0	9.719799	-1.063334	-3.115130
77	6	0	9.604589	-0.333589	-1.948845
78	6	0	8.997995	-0.877202	-0.792142
79	6	0	8.521578	-2.221376	-0.850309
80	6	0	8.649807	-2.935715	-2.062483
81	6	0	9.231494	-2.385223	-3.194221
82	6	0	8.880643	-0.118214	0.446164
83	6	0	7.943527	-2.830119	0.340198
84	6	0	8.134437	-2.165245	1.581644
85	6	0	8.582236	-0.808710	1.596415
86	6	0	7.702244	-2.805899	2.766696
87	6	0	6.966717	-3.968460	2.717201
88	6	0	6.580079	-4.534008	1.472990

89	6	0	7.133396	-3.984838	0.314656
90	6	0	9.365261	-3.173271	-4.474522
91	6	0	-9.150200	-3.084027	3.676566
92	6	0	-9.205671	-2.098763	2.711492
93	6	0	-8.575762	-2.257398	1.454377
94	6	0	-7.888900	-3.481241	1.194001
95	6	0	-7.848056	-4.464918	2.207678
96	6	0	-8.457309	-4.291051	3.440732
97	6	0	-8.642546	-1.228873	0.425725
98	6	0	-7.272548	-3.695698	-0.108367
99	6	0	-7.606047	-2.795716	-1.156983
100	6	0	-8.272945	-1.569372	-0.852833
101	6	0	-7.117317	-3.058673	-2.458457
102	6	0	-6.215236	-4.073144	-2.687201
103	6	0	-5.717250	-4.860232	-1.615305
104	6	0	-6.302884	-4.689455	-0.359926
105	6	0	-8.406616	-5.362122	4.502938
106	6	0	-11.124076	1.574447	-1.933577
107	6	0	-10.470196	0.690819	-1.098701
108	6	0	-9.525624	1.135348	-0.143419
109	6	0	-9.271448	2.537666	-0.048282
110	6	0	-9.957072	3.411580	-0.921829
111	6	0	-10.871245	2.961350	-1.861852
112	6	0	-8.845821	0.211546	0.753044
113	6	0	-8.327085	3.031781	0.945082
114	6	0	-7.904567	2.132223	1.962551
115	6	0	-8.169384	0.735258	1.827308
116	6	0	-7.071469	2.610769	3.000573
117	6	0	-6.543884	3.881912	2.954613
118	6	0	-6.807900	4.731495	1.850040
119	6	0	-7.744388	4.317474	0.904135
120	6	0	-11.598001	3.918216	-2.775352
121	1	0	-1.551616	-5.521211	-3.519057
122	1	0	-3.767833	-4.490349	-3.451461
123	1	0	-4.888433	-7.054191	-0.196035
124	1	0	0.186895	-6.736410	-2.364042
125	1	0	0.358913	-9.870591	1.228941
126	1	0	-1.304768	-11.024063	2.623205
127	1	0	-4.449444	-8.832222	0.722521
128	1	0	-3.854552	-10.519209	3.690498
129	1	0	-5.039787	-10.403335	2.381918
130	1	0	-3.954249	-11.796928	2.482115
131	1	0	4.640798	-4.920208	3.318200
132	1	0	6.002661	-6.365122	-0.488934
133	1	0	2.568377	-6.189674	3.074763
134	1	0	0.964677	-7.240069	1.607092
135	1	0	5.764596	-7.882879	-1.849526
136	1	0	1.099145	-9.284362	-2.701768
137	1	0	2.864923	-9.826606	-4.323755
138	1	0	5.319741	-8.790080	-5.174832
139	1	0	6.506146	-8.864630	-3.864107
140	1	0	5.598267	-10.310053	-4.329405
141	1	0	-3.935302	8.078640	3.355040
142	1	0	-5.910466	6.637770	3.662536
143	1	0	-5.639224	5.383310	-0.424465
144	1	0	-1.888100	8.561997	2.074041
145	1	0	-0.339206	7.475288	-2.364791
146	1	0	-1.371151	6.547243	-4.366527
147	1	0	-5.065710	6.051359	-2.270193

148	1	0	-3.978432	6.486374	-5.509804
149	1	0	-3.395642	4.869387	-5.123815
150	1	0	-4.983211	5.395564	-4.545062
151	1	0	4.361270	5.120709	2.481048
152	1	0	4.669369	7.618482	-0.992559
153	1	0	2.054100	5.904177	2.855262
154	1	0	0.025082	6.785057	1.831441
155	1	0	3.994926	9.519199	-1.641156
156	1	0	-0.915672	10.101410	-1.452406
157	1	0	0.439963	11.526868	-2.931174
158	1	0	4.209241	11.240457	-3.249592
159	1	0	2.832478	11.390734	-4.350824
160	1	0	3.031743	12.543163	-3.033636
161	1	0	6.558919	3.349304	-2.284670
162	1	0	5.099339	5.260284	-1.745075
163	1	0	6.811613	5.485141	2.181428
164	1	0	7.758829	1.437236	-1.393136
165	1	0	10.694941	0.750920	2.318832
166	1	0	11.426032	2.111292	4.226584
167	1	0	8.704733	5.211194	3.084778
168	1	0	10.326930	4.083723	5.932859
169	1	0	11.623791	4.755394	4.947784
170	1	0	10.048915	5.560849	5.000343
171	1	0	6.637965	-4.426689	3.643676
172	1	0	6.837392	-4.385881	-0.647849
173	1	0	7.915684	-2.337757	3.724104
174	1	0	8.515186	-0.277383	2.539958
175	1	0	8.314735	-3.967626	-2.101058
176	1	0	10.004142	0.673791	-1.904698
177	1	0	10.205927	-0.619691	-3.980525
178	1	0	8.983255	-4.191278	-4.360674
179	1	0	8.811250	-2.697969	-5.292677
180	1	0	10.411541	-3.240487	-4.794316
181	1	0	-7.428765	-2.413213	-3.275569
182	1	0	-5.848831	-4.240815	-3.694351
183	1	0	-5.918937	-5.262066	0.476479
184	1	0	-8.337165	-0.829917	-1.644508
185	1	0	-9.759385	-1.186812	2.906331
186	1	0	-9.658703	-2.935422	4.625973
187	1	0	-7.352408	-5.408906	2.003770
188	1	0	-7.896094	-5.003051	5.404405
189	1	0	-9.413567	-5.669873	4.807572
190	1	0	-7.876091	-6.250950	4.151161
191	1	0	-5.833269	4.199382	3.711077
192	1	0	-7.966028	4.978019	0.072428
193	1	0	-6.786274	1.930746	3.798930
194	1	0	-7.673644	0.068336	2.525033
195	1	0	-9.790448	4.480627	-0.832682
196	1	0	-10.694989	-0.368668	-1.156687
197	1	0	-11.854841	1.199683	-2.646036
198	1	0	-11.322648	4.956062	-2.569862
199	1	0	-11.369534	3.713361	-3.828022
200	1	0	-12.684706	3.830196	-2.661992

Table S18. Cartesian coordinate of *Z,R,Z,R,Z,S,Z,S* (16)

SCF Done: E(RB3LYP) = -4621.33795807 A.U. after 5 cycles

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.313510	10.419234	-0.876637
2	6	0	0.389355	9.551500	-0.333501
3	6	0	0.790854	8.409859	0.399858
4	6	0	2.189983	8.166759	0.577985
5	6	0	3.104330	9.081688	0.007118
6	6	0	2.698608	10.195082	-0.712471
7	6	0	-0.184338	7.515666	0.990205
8	6	0	2.631754	7.002463	1.339699
9	6	0	1.642146	6.255449	2.037589
10	6	0	0.258202	6.537031	1.838601
11	6	0	2.032642	5.156824	2.833153
12	6	0	3.341452	4.741285	2.867830
13	6	0	4.336511	5.403217	2.101441
14	6	0	3.970071	6.543528	1.386190
15	6	0	3.700054	11.159073	-1.301047
16	1	0	1.269068	4.603624	3.373371
17	1	0	3.601695	3.846721	3.422133
18	1	0	4.733439	7.063799	0.817572
19	1	0	-0.463490	5.874098	2.306312
20	1	0	-0.672383	9.741841	-0.455612
21	1	0	0.974242	11.292080	-1.428856
22	1	0	4.168208	8.926422	0.155651
23	1	0	3.553468	12.173104	-0.911240
24	1	0	4.726746	10.859040	-1.074958
25	1	0	3.600628	11.219200	-2.391294
26	6	0	-1.830296	6.620035	-2.973127
27	6	0	-1.330011	7.004713	-1.746487
28	6	0	-2.156474	7.075719	-0.598333
29	6	0	-3.518574	6.669640	-0.728924
30	6	0	-4.000049	6.298283	-2.005178
31	6	0	-3.190334	6.275053	-3.128923
32	6	0	-1.653955	7.503215	0.699046
33	6	0	-4.357010	6.586138	0.457896
34	6	0	-3.887512	7.172396	1.664597
35	6	0	-2.535879	7.639584	1.739315
36	6	0	-4.702155	7.101018	2.820950
37	6	0	-5.845987	6.331100	2.837839
38	6	0	-6.239656	5.601469	1.687164
39	6	0	-5.532096	5.805000	0.504760
40	6	0	-3.730801	5.889951	-4.484290
41	1	0	-6.421410	6.235993	3.754034
42	1	0	-5.807568	5.217597	-0.363550
43	1	0	-4.371087	7.602850	3.726569
44	1	0	-2.168523	7.980753	2.703537
45	1	0	-5.047889	6.037485	-2.115930
46	1	0	-0.283413	7.268922	-1.662053
47	1	0	-1.168154	6.588154	-3.834912
48	1	0	-4.790426	5.625562	-4.433545
49	1	0	-3.624031	6.710457	-5.203689
50	1	0	-3.189839	5.030816	-4.897766
51	6	0	1.831775	-6.621911	2.973895
52	6	0	1.331071	-7.006222	1.747313
53	6	0	2.157095	-7.076752	0.598827
54	6	0	3.519186	-6.670509	0.729019
55	6	0	4.001105	-6.299504	2.005206
56	6	0	3.191839	-6.276840	3.129286
57	6	0	1.654088	-7.503742	-0.698499

58	6	0	4.357118	-6.586401	-0.458096
59	6	0	3.887227	-7.172269	-1.664832
60	6	0	2.535633	-7.639597	-1.739186
61	6	0	4.701431	-7.100352	-2.821465
62	6	0	5.845158	-6.330287	-2.838493
63	6	0	6.239164	-5.601008	-1.687702
64	6	0	5.532060	-5.805059	-0.505117
65	6	0	3.732874	-5.892491	4.484640
66	1	0	4.370093	-7.601900	-3.727143
67	1	0	6.420237	-6.234800	-3.754864
68	1	0	5.807738	-5.217921	0.363309
69	1	0	2.167881	-7.980407	-2.703389
70	1	0	0.284461	-7.270457	1.663103
71	1	0	1.169965	-6.590362	3.835947
72	1	0	5.048939	-6.038528	2.115605
73	1	0	3.189779	-5.035824	4.900403
74	1	0	3.629607	-6.714651	5.202681
75	1	0	4.791617	-5.624771	4.433003
76	6	0	-1.314011	-10.420160	0.876271
77	6	0	-0.389683	-9.552408	0.333464
78	6	0	-0.790942	-8.410367	-0.399421
79	6	0	-2.190028	-8.166957	-0.577503
80	6	0	-3.104556	-9.081916	-0.006966
81	6	0	-2.699063	-10.195655	0.712213
82	6	0	0.184419	-7.516132	-0.989415
83	6	0	-2.631607	-7.002371	-1.338888
84	6	0	-1.641850	-6.255265	-2.036460
85	6	0	-0.257967	-6.537101	-1.837455
86	6	0	-2.032125	-5.156372	-2.831764
87	6	0	-3.340899	-4.740747	-2.866554
88	6	0	-4.336132	-5.402828	-2.100514
89	6	0	-3.969885	-6.543316	-1.385453
90	6	0	-3.700711	-11.159692	1.300374
91	1	0	-3.601014	-3.846041	-3.420688
92	1	0	-4.733389	-7.063673	-0.817098
93	1	0	-1.268420	-4.603093	-3.371715
94	1	0	0.463861	-5.874073	-2.304833
95	1	0	-4.168398	-8.926380	-0.155447
96	1	0	0.672016	-9.743054	0.455445
97	1	0	-0.974914	-11.293296	1.428140
98	1	0	-3.600983	-11.220664	2.390543
99	1	0	-4.727348	-10.859093	1.074791
100	1	0	-3.554639	-12.173501	0.909785
101	6	0	-9.546259	-3.438786	3.125231
102	6	0	-9.592458	-2.414084	2.201180
103	6	0	-8.882999	-2.486880	0.979429
104	6	0	-8.122292	-3.664586	0.710890
105	6	0	-8.093231	-4.690385	1.681929
106	6	0	-8.782995	-4.600852	2.881359
107	6	0	-8.936828	-1.416231	-0.007260
108	6	0	-7.413245	-3.787288	-0.555459
109	6	0	-7.743184	-2.867683	-1.588154
110	6	0	-8.492681	-1.691482	-1.277775
111	6	0	-7.155127	-3.035639	-2.864000
112	6	0	-6.152512	-3.956772	-3.063534
113	6	0	-5.662147	-4.741678	-1.986663
114	6	0	-6.350615	-4.691671	-0.774637
115	6	0	-8.743968	-5.715736	3.898022
116	1	0	-7.464165	-2.381301	-3.674884

117	1	0	-5.693131	-4.045797	-4.042665
118	1	0	-5.974516	-5.271547	0.061382
119	1	0	-8.545307	-0.924057	-2.042999
120	1	0	-10.199956	-1.537852	2.400435
121	1	0	-10.116805	-3.356895	4.047073
122	1	0	-7.539797	-5.599657	1.468072
123	1	0	-8.301365	-5.376620	4.842133
124	1	0	-9.751595	-6.079244	4.130311
125	1	0	-8.155264	-6.564457	3.539840
126	6	0	-11.261599	1.495112	-2.407367
127	6	0	-10.675007	0.573392	-1.563368
128	6	0	-9.790419	0.970409	-0.533274
129	6	0	-9.525979	2.364990	-0.371211
130	6	0	-10.140030	3.278489	-1.257229
131	6	0	-10.995866	2.874554	-2.270590
132	6	0	-9.181186	0.004883	0.370989
133	6	0	-8.647846	2.810654	0.703222
134	6	0	-8.319055	1.869942	1.717906
135	6	0	-8.585527	0.482053	1.512527
136	6	0	-7.562065	2.297801	2.832627
137	6	0	-7.014484	3.560037	2.871386
138	6	0	-7.177946	4.452191	1.780382
139	6	0	-8.042782	4.086526	0.749728
140	6	0	-11.649479	3.873029	-3.194841
141	1	0	-6.360394	3.838439	3.691252
142	1	0	-8.190845	4.777629	-0.073714
143	1	0	-7.348673	1.586352	3.626000
144	1	0	-8.143082	-0.213575	2.217608
145	1	0	-9.965852	4.341224	-1.119630
146	1	0	-10.908859	-0.480132	-1.673240
147	1	0	-11.948744	1.156184	-3.178744
148	1	0	-11.363253	4.898167	-2.945167
149	1	0	-11.367976	3.691301	-4.238796
150	1	0	-12.742519	3.807799	-3.143365
151	6	0	9.545609	3.439450	-3.125390
152	6	0	9.591961	2.414677	-2.201427
153	6	0	8.882733	2.487395	-0.979538
154	6	0	8.122109	3.665092	-0.710761
155	6	0	8.092855	4.690955	-1.681729
156	6	0	8.782380	4.601498	-2.881299
157	6	0	8.936710	1.416658	0.007046
158	6	0	7.413306	3.787717	0.555730
159	6	0	7.743417	2.868022	1.588294
160	6	0	8.492807	1.691809	1.277667
161	6	0	7.155619	3.035919	2.864262
162	6	0	6.153070	3.957077	3.064053
163	6	0	5.662501	4.742053	1.987330
164	6	0	6.350737	4.692098	0.775164
165	6	0	8.743096	5.716389	-3.897941
166	1	0	7.464786	2.381523	3.675049
167	1	0	5.693901	4.046050	4.043288
168	1	0	5.974486	5.272023	-0.060752
169	1	0	8.545535	0.924310	2.042811
170	1	0	10.199418	1.538454	-2.400855
171	1	0	10.115996	3.357635	-4.047335
172	1	0	7.539455	5.600210	-1.467700
173	1	0	8.154444	6.565100	-3.539642
174	1	0	9.750659	6.079916	-4.130460
175	1	0	8.300270	5.377251	-4.841940

176	6	0	11.261897	-1.495040	2.406283
177	6	0	10.675144	-0.573209	1.562528
178	6	0	9.790308	-0.970083	0.532583
179	6	0	9.525788	-2.364638	0.370419
180	6	0	10.140010	-3.278258	1.256207
181	6	0	10.996078	-2.874462	2.269419
182	6	0	9.180905	-0.004426	-0.371405
183	6	0	8.647393	-2.810156	-0.703855
184	6	0	8.318290	-1.869288	-1.718279
185	6	0	8.584852	-0.481440	-1.512809
186	6	0	7.560960	-2.296978	-2.832855
187	6	0	7.013427	-3.559215	-2.871675
188	6	0	7.177273	-4.451589	-1.780886
189	6	0	8.042378	-4.086064	-0.750422
190	6	0	11.649815	-3.873053	3.193461
191	1	0	6.359115	-3.837514	-3.691398
192	1	0	8.190743	-4.777305	0.072847
193	1	0	7.347329	-1.585389	-3.626036
194	1	0	8.142221	0.214291	-2.217670
195	1	0	9.965759	-4.340969	1.118530
196	1	0	10.909067	0.480295	1.672448
197	1	0	11.949233	-1.156228	3.177543
198	1	0	11.368028	-3.691761	4.237419
199	1	0	11.363955	-4.898192	2.943381
200	1	0	12.742843	-3.807451	3.142249

Table S19. Cartesian coordinate of *Z,R,Z,R,Z,R,Z,S* (17)

SCF Done: E(RB3LYP) = -4621.33608502 A.U. after 14 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	10.894657	-0.991916	2.319348
2	6	0	10.245038	-0.154490	1.434986
3	6	0	9.360443	-0.657423	0.451741
4	6	0	9.167414	-2.070684	0.378625
5	6	0	9.845587	-2.896374	1.303590
6	6	0	10.697700	-2.388842	2.272160
7	6	0	8.681138	0.218732	-0.492761
8	6	0	8.297478	-2.626206	-0.649429
9	6	0	7.889711	-1.766585	-1.706664
10	6	0	8.079958	-0.355699	-1.585585
11	6	0	7.145016	-2.304824	-2.781916
12	6	0	6.688936	-3.603792	-2.746037
13	6	0	6.930767	-4.420084	-1.611857
14	6	0	7.777492	-3.939277	-0.615324
15	6	0	11.418715	-3.294906	3.240368
16	1	0	6.872261	-1.653652	-3.608214
17	1	0	6.048952	-3.975594	-3.540099
18	1	0	7.979553	-4.573403	0.241697
19	1	0	7.586220	0.273828	-2.318586
20	1	0	10.426576	0.913961	1.476043
21	1	0	11.578666	-0.572133	3.052822
22	1	0	9.725081	-3.972924	1.233143
23	1	0	11.146164	-3.065542	4.277315
24	1	0	12.505787	-3.176980	3.162847
25	1	0	11.182015	-4.346461	3.057702
26	6	0	8.916780	3.489769	-3.458693

27	6	0	8.988186	2.520004	-2.479010
28	6	0	8.314740	2.664620	-1.242918
29	6	0	7.566298	3.860128	-1.019241
30	6	0	7.511461	4.828258	-2.047087
31	6	0	8.163699	4.666934	-3.259658
32	6	0	8.398359	1.653030	-0.198452
33	6	0	6.901890	4.064179	0.261097
34	6	0	7.243560	3.191407	1.329967
35	6	0	7.974307	1.993746	1.062816
36	6	0	6.704002	3.441289	2.613710
37	6	0	5.746084	4.410815	2.802624
38	6	0	5.247035	5.163391	1.706692
39	6	0	5.880041	5.016134	0.472186
40	6	0	8.095403	5.721096	-4.337667
41	1	0	5.334192	4.569476	3.793772
42	1	0	5.493898	5.567231	-0.378224
43	1	0	7.021260	2.818686	3.446158
44	1	0	8.047574	1.269429	1.867375
45	1	0	6.967852	5.751085	-1.870271
46	1	0	9.589450	1.632816	-2.644974
47	1	0	9.459674	3.352894	-4.390663
48	1	0	9.096335	6.061604	-4.626737
49	1	0	7.525604	6.594320	-4.008963
50	1	0	7.616542	5.331543	-5.243886
51	6	0	-7.217817	-2.039270	2.813951
52	6	0	-7.648490	-1.565027	1.591938
53	6	0	-7.644655	-2.382414	0.434982
54	6	0	-7.105758	-3.698924	0.553971
55	6	0	-6.690921	-4.157172	1.825106
56	6	0	-6.746830	-3.361933	2.957879
57	6	0	-8.121280	-1.915823	-0.860787
58	6	0	-6.927169	-4.508617	-0.641561
59	6	0	-7.569013	-4.099432	-1.841286
60	6	0	-8.181667	-2.806313	-1.902252
61	6	0	-7.397020	-4.883415	-3.008727
62	6	0	-6.477212	-5.910577	-3.044064
63	6	0	-5.697139	-6.217167	-1.900172
64	6	0	-5.997379	-5.569136	-0.704800
65	6	0	-6.316440	-3.878825	4.308703
66	1	0	-7.939175	-4.607958	-3.909734
67	1	0	-6.301663	-6.449332	-3.970725
68	1	0	-5.375253	-5.773885	0.159014
69	1	0	-8.562272	-2.470143	-2.863135
70	1	0	-8.007369	-0.546628	1.520637
71	1	0	-7.248053	-1.384665	3.681567
72	1	0	-6.331288	-5.176811	1.923057
73	1	0	-7.148212	-3.867404	5.023024
74	1	0	-5.520204	-3.258311	4.736025
75	1	0	-5.944357	-4.904922	4.245606
76	6	0	-11.131126	0.914569	0.830683
77	6	0	-10.255705	0.028759	0.237501
78	6	0	-9.145553	0.480578	-0.514329
79	6	0	-8.945412	1.889913	-0.659263
80	6	0	-9.864747	2.764406	-0.036129
81	6	0	-10.946638	2.309204	0.702064
82	6	0	-8.240596	-0.452049	-1.156500
83	6	0	-7.817240	2.383075	-1.442760
84	6	0	-7.096737	1.438986	-2.225535
85	6	0	-7.329348	0.042318	-2.051912

86	6	0	-6.047590	1.884858	-3.058388
87	6	0	-5.631201	3.194058	-3.026649
88	6	0	-6.239629	4.129490	-2.149094
89	6	0	-7.355494	3.720262	-1.417764
90	6	0	-11.919705	3.267550	1.344984
91	1	0	-4.764184	3.491232	-3.605837
92	1	0	-7.840107	4.439163	-0.765440
93	1	0	-5.522182	1.159539	-3.673854
94	1	0	-6.662213	-0.644527	-2.563657
95	1	0	-9.740899	3.835546	-0.161788
96	1	0	-10.416084	-1.040655	0.333920
97	1	0	-11.980146	0.537032	1.395106
98	1	0	-11.647991	4.308006	1.147910
99	1	0	-11.953603	3.129868	2.432161
100	1	0	-12.938527	3.110689	0.971964
101	6	0	-3.777866	8.388443	3.638836
102	6	0	-2.777624	8.485558	2.692674
103	6	0	-2.955634	7.996085	1.377122
104	6	0	-4.205578	7.396282	1.043718
105	6	0	-5.205069	7.308516	2.038496
106	6	0	-5.017547	7.789538	3.325139
107	6	0	-1.915465	8.114923	0.365588
108	6	0	-4.416899	6.895183	-0.306198
109	6	0	-3.502408	7.299557	-1.317450
110	6	0	-2.259225	7.902983	-0.946804
111	6	0	-3.750960	6.903349	-2.653564
112	6	0	-4.740938	5.992773	-2.948908
113	6	0	-5.523387	5.410756	-1.916758
114	6	0	-5.398169	5.933682	-0.630376
115	6	0	-6.105947	7.699544	4.366976
116	1	0	-3.100556	7.274758	-3.441171
117	1	0	-4.883150	5.669663	-3.975350
118	1	0	-5.972669	5.484029	0.172046
119	1	0	-1.508362	8.015661	-1.723094
120	1	0	-1.837027	8.960581	2.949870
121	1	0	-3.614877	8.789748	4.636042
122	1	0	-6.168503	6.880681	1.778371
123	1	0	-6.386760	8.692600	4.736752
124	1	0	-5.776717	7.117119	5.235513
125	1	0	-7.005582	7.224119	3.967271
126	6	0	1.096828	10.794125	-1.476408
127	6	0	0.152312	10.038935	-0.812229
128	6	0	0.521299	8.954599	0.018694
129	6	0	1.912807	8.656552	0.168961
130	6	0	2.848993	9.454130	-0.527929
131	6	0	2.473201	10.508503	-1.345680
132	6	0	-0.472503	8.177732	0.739267
133	6	0	2.328665	7.552590	1.027663
134	6	0	1.338243	6.949170	1.851775
135	6	0	-0.036608	7.284476	1.684634
136	6	0	1.710834	5.908349	2.731352
137	6	0	2.988852	5.403842	2.727790
138	6	0	3.973407	5.916420	1.842363
139	6	0	3.634578	7.009982	1.044425
140	6	0	3.498001	11.347366	-2.069892
141	1	0	3.222723	4.548446	3.351304
142	1	0	4.389760	7.420572	0.383056
143	1	0	0.950638	5.463776	3.368051
144	1	0	-0.761435	6.702017	2.244013

145	1	0	3.908407	9.255513	-0.400690
146	1	0	-0.899483	10.286441	-0.907446
147	1	0	0.779538	11.628496	-2.097028
148	1	0	3.362034	11.290423	-3.156390
149	1	0	4.516533	11.021146	-1.843117
150	1	0	3.414950	12.404784	-1.793199
151	6	0	1.585054	-6.444200	3.148123
152	6	0	1.197887	-7.080186	1.987073
153	6	0	2.090780	-7.256563	0.900235
154	6	0	3.388714	-6.672480	1.010323
155	6	0	3.759800	-6.052133	2.225781
156	6	0	2.893403	-5.937522	3.299682
157	6	0	1.719109	-7.963584	-0.319978
158	6	0	4.269423	-6.659958	-0.147590
159	6	0	3.924976	-7.450646	-1.277047
160	6	0	2.659167	-8.119031	-1.307171
161	6	0	4.765166	-7.415909	-2.417412
162	6	0	5.811583	-6.520668	-2.505169
163	6	0	6.087980	-5.632469	-1.435868
164	6	0	5.357270	-5.768152	-0.258923
165	6	0	3.318093	-5.285535	4.592549
166	1	0	4.527986	-8.058570	-3.261459
167	1	0	6.402276	-6.462666	-3.414869
168	1	0	5.540303	-5.055905	0.536926
169	1	0	2.393509	-8.665615	-2.208158
170	1	0	0.187543	-7.458158	1.911035
171	1	0	0.871798	-6.337811	3.961801
172	1	0	4.766461	-5.660443	2.330015
173	1	0	3.270540	-5.992471	5.429389
174	1	0	2.662392	-4.444907	4.847510
175	1	0	4.341690	-4.906081	4.533275
176	6	0	-0.863009	-10.783487	1.960560
177	6	0	-0.042336	-9.992569	1.183338
178	6	0	-0.572262	-9.111246	0.211713
179	6	0	-1.989724	-9.061764	0.037875
180	6	0	-2.798089	-9.883165	0.856490
181	6	0	-2.267004	-10.738323	1.809901
182	6	0	0.289449	-8.289437	-0.618442
183	6	0	-2.559587	-8.189359	-0.981368
184	6	0	-1.671862	-7.628081	-1.940778
185	6	0	-0.262147	-7.678484	-1.714084
186	6	0	-2.201010	-6.882016	-3.017608
187	6	0	-3.539215	-6.565174	-3.064278
188	6	0	-4.409239	-6.952977	-2.012514
189	6	0	-3.920934	-7.808363	-1.026778
190	6	0	-3.152309	-11.619359	2.657567
191	1	0	-3.914210	-5.917922	-3.850451
192	1	0	-4.592537	-8.125254	-0.235368
193	1	0	-1.521408	-6.494915	-3.772210
194	1	0	0.372642	-7.089371	-2.369228
195	1	0	-3.874039	-9.873287	0.711357
196	1	0	1.034896	-10.043917	1.305581
197	1	0	-0.425013	-11.458187	2.691913
198	1	0	-4.210438	-11.456360	2.436254
199	1	0	-2.999050	-11.426649	3.725831
200	1	0	-2.934881	-12.680914	2.490716

Table S20. Cartesian coordinate of *E,R,Z,R,E,R,E,S* (18)

SCF Done: E(RB3LYP) = -4621.33534271 A.U. after 14 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.318692	-7.003991	2.668648
2	6	0	2.706042	-7.355913	1.483882
3	6	0	3.330369	-7.140191	0.229805
4	6	0	4.586209	-6.461985	0.224929
5	6	0	5.196118	-6.139442	1.459044
6	6	0	4.597638	-6.407362	2.678626
7	6	0	2.724235	-7.542018	-1.034177
8	6	0	5.172514	-6.051327	-1.041352
9	6	0	4.629312	-6.571984	-2.246677
10	6	0	3.423760	-7.343453	-2.197299
11	6	0	5.188382	-6.158148	-3.481148
12	6	0	6.122160	-5.143760	-3.535704
13	6	0	6.561939	-4.507306	-2.347595
14	6	0	6.136233	-5.024219	-1.127133
15	6	0	5.276774	-6.071121	3.983551
16	1	0	4.811562	-6.599353	-4.400388
17	1	0	6.484888	-4.791624	-4.497104
18	1	0	6.436476	-4.507796	-0.223008
19	1	0	2.986185	-7.665526	-3.138520
20	1	0	1.727432	-7.815178	1.518155
21	1	0	2.810166	-7.196108	3.610247
22	1	0	6.177991	-5.676985	1.454258
23	1	0	5.474524	-6.973912	4.573671
24	1	0	4.649598	-5.417618	4.600859
25	1	0	6.231068	-5.563354	3.819847
26	6	0	0.851529	-11.129944	0.812036
27	6	0	1.438857	-10.073760	0.146733
28	6	0	0.663749	-9.019598	-0.391517
29	6	0	-0.756023	-9.071346	-0.240844
30	6	0	-1.320648	-10.167613	0.450154
31	6	0	-0.550153	-11.192687	0.977465
32	6	0	1.277078	-7.915932	-1.106598
33	6	0	-1.578586	-8.011699	-0.811284
34	6	0	-0.960154	-7.111450	-1.722761
35	6	0	0.464765	-7.080587	-1.827864
36	6	0	-1.751776	-6.146433	-2.385190
37	6	0	-3.075361	-5.970215	-2.050834
38	6	0	-3.664415	-6.736723	-1.012848
39	6	0	-2.926554	-7.778902	-0.454055
40	6	0	-1.179963	-12.360924	1.696548
41	1	0	-3.646285	-5.165852	-2.503159
42	1	0	-3.382987	-8.378232	0.327157
43	1	0	-1.279936	-5.489262	-3.110857
44	1	0	0.909120	-6.270698	-2.398800
45	1	0	-2.400435	-10.231173	0.543466
46	1	0	2.516538	-10.043670	0.020721
47	1	0	1.472644	-11.930491	1.206100
48	1	0	-0.946166	-13.308701	1.197675
49	1	0	-2.268137	-12.265630	1.740591
50	1	0	-0.808367	-12.441669	2.724819
51	6	0	-0.712430	7.570250	-3.879512
52	6	0	-1.194922	7.740130	-2.598732
53	6	0	-0.332254	8.020047	-1.509496
54	6	0	1.071598	8.042958	-1.763911

55	6	0	1.527909	7.889591	-3.093671
56	6	0	0.668298	7.666614	-4.156009
57	6	0	-0.823808	8.241709	-0.155275
58	6	0	1.999815	8.156788	-0.649314
59	6	0	1.489596	8.492114	0.634224
60	6	0	0.072830	8.553263	0.834021
61	6	0	2.393259	8.597360	1.720191
62	6	0	3.716785	8.232314	1.585292
63	6	0	4.207711	7.752981	0.344591
64	6	0	3.359007	7.794544	-0.758206
65	6	0	1.178003	7.521011	-5.568881
66	1	0	2.012202	8.909565	2.689201
67	1	0	4.379418	8.266098	2.445142
68	1	0	3.721412	7.391544	-1.696428
69	1	0	-0.293148	8.741330	1.839964
70	1	0	-2.260173	7.665089	-2.425854
71	1	0	-1.407767	7.366181	-4.690062
72	1	0	2.591357	7.964042	-3.296532
73	1	0	0.763622	8.296646	-6.223684
74	1	0	0.889200	6.554161	-5.997318
75	1	0	2.267973	7.594547	-5.612158
76	6	0	-4.443447	10.356017	-1.604945
77	6	0	-3.323467	9.755012	-1.068964
78	6	0	-3.408967	8.526608	-0.372224
79	6	0	-4.690481	7.913131	-0.225659
80	6	0	-5.814582	8.558400	-0.789914
81	6	0	-5.718046	9.760870	-1.473313
82	6	0	-2.235180	7.901270	0.207495
83	6	0	-4.805623	6.655813	0.502803
84	6	0	-3.683135	6.221763	1.261662
85	6	0	-2.415981	6.857438	1.076280
86	6	0	-3.799115	5.064172	2.064053
87	6	0	-4.927288	4.276545	2.009645
88	6	0	-5.989134	4.599050	1.126622
89	6	0	-5.934129	5.807744	0.434763
90	6	0	-6.936960	10.436490	-2.053149
91	1	0	-4.963939	3.344254	2.563977
92	1	0	-6.754963	6.064603	-0.226843
93	1	0	-2.950515	4.759713	2.670954
94	1	0	-1.549466	6.401404	1.546163
95	1	0	-6.797184	8.115992	-0.657758
96	1	0	-2.352186	10.228658	-1.170165
97	1	0	-4.347833	11.304893	-2.126904
98	1	0	-7.082924	11.433735	-1.621840
99	1	0	-7.844232	9.855622	-1.867164
100	1	0	-6.839850	10.569003	-3.137103
101	6	0	-9.735429	-1.248151	4.334887
102	6	0	-9.490320	-1.671577	3.044038
103	6	0	-8.951552	-0.799704	2.068944
104	6	0	-8.676826	0.549398	2.447641
105	6	0	-8.936249	0.945996	3.778765
106	6	0	-9.453820	0.078044	4.728082
107	6	0	-8.705988	-1.234118	0.701317
108	6	0	-8.147913	1.479143	1.458307
109	6	0	-8.197352	1.090746	0.090900
110	6	0	-8.466982	-0.270934	-0.248171
111	6	0	-7.789529	2.014008	-0.900000
112	6	0	-7.203572	3.211562	-0.553081
113	6	0	-6.978062	3.534942	0.808956

114	6	0	-7.509716	2.695029	1.786438
115	6	0	-9.731535	0.530549	6.141006
116	1	0	-7.867746	1.729056	-1.945877
117	1	0	-6.809738	3.864973	-1.325122
118	1	0	-7.356235	2.950432	2.829834
119	1	0	-8.306437	-0.564337	-1.280431
120	1	0	-9.731673	-2.689431	2.757233
121	1	0	-10.164299	-1.940474	5.055162
122	1	0	-8.757243	1.978219	4.063653
123	1	0	-9.496073	1.589443	6.276800
124	1	0	-9.137042	-0.039944	6.864409
125	1	0	-10.784676	0.383650	6.407209
126	6	0	-10.172598	-3.238152	-2.959950
127	6	0	-9.841868	-2.692678	-1.735590
128	6	0	-8.782906	-3.214043	-0.955853
129	6	0	-8.062705	-4.337957	-1.461117
130	6	0	-8.425413	-4.866884	-2.719965
131	6	0	-9.459439	-4.340219	-3.478989
132	6	0	-8.438768	-2.657167	0.345009
133	6	0	-6.984210	-4.912845	-0.668409
134	6	0	-6.889663	-4.530733	0.698371
135	6	0	-7.620438	-3.394361	1.165658
136	6	0	-5.920878	-5.154797	1.518800
137	6	0	-4.969068	-5.991728	0.977869
138	6	0	-4.930104	-6.228358	-0.419555
139	6	0	-5.975394	-5.742469	-1.203567
140	6	0	-9.835669	-4.931063	-4.815966
141	1	0	-4.172524	-6.381973	1.603587
142	1	0	-5.959440	-5.939612	-2.270609
143	1	0	-5.880647	-4.894727	2.573294
144	1	0	-7.369388	-3.017276	2.151687
145	1	0	-7.900288	-5.740807	-3.093191
146	1	0	-10.414109	-1.857610	-1.346084
147	1	0	-11.002782	-2.823750	-3.526572
148	1	0	-10.886124	-5.243722	-4.832372
149	1	0	-9.222438	-5.803665	-5.055978
150	1	0	-9.707685	-4.200009	-5.623093
151	6	0	11.360214	-0.038644	1.632151
152	6	0	10.423019	0.833919	1.118831
153	6	0	9.454015	0.405474	0.181240
154	6	0	9.464712	-0.960887	-0.234524
155	6	0	10.437154	-1.825943	0.316908
156	6	0	11.380985	-1.394847	1.236682
157	6	0	8.479069	1.324743	-0.375319
158	6	0	8.489743	-1.419821	-1.215815
159	6	0	7.750163	-0.433786	-1.926147
160	6	0	7.756152	0.920047	-1.466831
161	6	0	6.883382	-0.839078	-2.966334
162	6	0	6.627062	-2.172936	-3.191483
163	6	0	7.206651	-3.167112	-2.362114
164	6	0	8.175910	-2.780021	-1.438683
165	6	0	12.420992	-2.334899	1.796473
166	1	0	6.356784	-0.078503	-3.536759
167	1	0	5.889293	-2.464407	-3.932275
168	1	0	8.639009	-3.543694	-0.822182
169	1	0	7.049075	1.608309	-1.920597
170	1	0	10.424612	1.874948	1.426097
171	1	0	12.100014	0.322289	2.342349
172	1	0	10.471990	-2.858741	-0.016134

173	1	0	12.349126	-2.402665	2.888391
174	1	0	13.435496	-1.990160	1.564665
175	1	0	12.309839	-3.343910	1.390619
176	6	0	6.994943	1.735958	3.723798
177	6	0	7.521571	1.628352	2.453599
178	6	0	7.527569	2.724179	1.554300
179	6	0	6.891193	3.929656	1.976338
180	6	0	6.386412	4.012111	3.294735
181	6	0	6.435755	2.948739	4.180071
182	6	0	8.114866	2.647320	0.221851
183	6	0	6.713158	5.016292	1.025740
184	6	0	7.399330	4.957326	-0.217367
185	6	0	8.116817	3.768580	-0.568070
186	6	0	7.215816	6.010955	-1.146748
187	6	0	6.273899	6.996233	-0.932032
188	6	0	5.475414	6.984663	0.239423
189	6	0	5.762932	6.040276	1.221015
190	6	0	5.905066	3.066247	5.587781
191	1	0	6.107380	7.761133	-1.684921
192	1	0	5.126824	6.005409	2.097416
193	1	0	7.783741	5.995862	-2.073544
194	1	0	8.574732	3.721036	-1.552600
195	1	0	5.955963	4.948393	3.635040
196	1	0	7.946287	0.683586	2.142477
197	1	0	7.018156	0.874215	4.386352
198	1	0	5.130360	2.315946	5.784212
199	1	0	5.470739	4.052548	5.771807
200	1	0	6.698759	2.906461	6.327194

Table S21. Cartesian coordinate of *E,R,Z,R,Z,R,Z,S* (19)

SCF Done: E(RB3LYP) = -4621.33468730 A.U. after 14 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	10.307486	-1.465082	3.002743
2	6	0	9.996338	-0.741312	1.869579
3	6	0	9.288662	-1.322821	0.791033
4	6	0	8.907744	-2.695480	0.894055
5	6	0	9.241621	-3.403675	2.070661
6	6	0	9.927573	-2.819268	3.124191
7	6	0	8.978700	-0.571488	-0.415537
8	6	0	8.195904	-3.328466	-0.208689
9	6	0	8.146719	-2.637585	-1.451247
10	6	0	8.537492	-1.265110	-1.515206
11	6	0	7.542977	-3.268226	-2.564233
12	6	0	6.877726	-4.466041	-2.424929
13	6	0	6.768531	-5.086287	-1.154276
14	6	0	7.483260	-4.541442	-0.088385
15	6	0	10.282237	-3.602569	4.364743
16	1	0	7.542627	-2.753257	-3.521313
17	1	0	6.343511	-4.887697	-3.270420
18	1	0	7.422569	-5.030714	0.877915
19	1	0	8.321568	-0.729896	-2.434350
20	1	0	10.315077	0.292134	1.787212
21	1	0	10.865515	-0.991497	3.806724
22	1	0	8.983189	-4.455590	2.142713
23	1	0	11.364552	-3.605490	4.538287

24	1	0	9.951962	-4.642132	4.291155
25	1	0	9.817470	-3.165876	5.256684
26	6	0	10.533559	1.994852	-3.654641
27	6	0	10.175709	1.233535	-2.560356
28	6	0	9.244489	1.704200	-1.604711
29	6	0	8.683382	3.003308	-1.791358
30	6	0	9.070040	3.752580	-2.925443
31	6	0	9.977639	3.276350	-3.859050
32	6	0	8.878960	0.916610	-0.436649
33	6	0	7.738953	3.523127	-0.811912
34	6	0	7.630594	2.844681	0.433760
35	6	0	8.203165	1.543017	0.581408
36	6	0	6.796917	3.387790	1.439546
37	6	0	5.977559	4.464112	1.176224
38	6	0	5.938936	5.038461	-0.119415
39	6	0	6.862797	4.600057	-1.066449
40	6	0	10.384205	4.102214	-5.055252
41	1	0	5.275507	4.807646	1.929564
42	1	0	6.847586	5.051029	-2.053170
43	1	0	6.748091	2.890289	2.404605
44	1	0	7.942155	0.984138	1.474572
45	1	0	8.670608	4.753687	-3.055857
46	1	0	10.628015	0.258942	-2.412098
47	1	0	11.264053	1.609360	-4.361637
48	1	0	9.896472	5.080614	-5.051915
49	1	0	10.119911	3.599531	-5.993140
50	1	0	11.467684	4.267026	-5.075987
51	6	0	-7.424559	-1.227700	2.618850
52	6	0	-7.862364	-0.755580	1.398897
53	6	0	-7.925334	-1.590474	0.255100
54	6	0	-7.433487	-2.923969	0.385142
55	6	0	-7.016940	-3.381527	1.656529
56	6	0	-7.014831	-2.568607	2.777347
57	6	0	-8.423548	-1.129596	-1.036741
58	6	0	-7.297910	-3.755340	-0.800494
59	6	0	-7.915919	-3.330610	-2.007194
60	6	0	-8.502605	-2.025945	-2.072900
61	6	0	-7.766400	-4.130612	-3.167286
62	6	0	-6.902215	-5.206382	-3.184541
63	6	0	-6.161010	-5.551379	-2.026252
64	6	0	-6.430936	-4.867234	-0.844264
65	6	0	-6.582680	-3.083815	4.128132
66	1	0	-8.285076	-3.836601	-4.076249
67	1	0	-6.747585	-5.762474	-4.104733
68	1	0	-5.830561	-5.099733	0.027276
69	1	0	-8.898943	-1.694092	-3.028937
70	1	0	-8.172171	0.277291	1.320803
71	1	0	-7.402181	-0.556202	3.473698
72	1	0	-6.699781	-4.413861	1.764605
73	1	0	-7.399786	-3.024640	4.856899
74	1	0	-5.752165	-2.492781	4.531340
75	1	0	-6.257469	-4.126266	4.074802
76	6	0	-11.312806	1.651687	0.912931
77	6	0	-10.499755	0.778320	0.220202
78	6	0	-9.428177	1.244753	-0.576897
79	6	0	-9.204662	2.653305	-0.661635
80	6	0	-10.053416	3.516179	0.068165
81	6	0	-11.098389	3.046697	0.849528
82	6	0	-8.581110	0.331133	-1.321647

83	6	0	-8.129255	3.160337	-1.504719
84	6	0	-7.535363	2.257813	-2.429665
85	6	0	-7.766974	0.854299	-2.292482
86	6	0	-6.582180	2.743984	-3.352698
87	6	0	-6.104501	4.031491	-3.259034
88	6	0	-6.536279	4.884833	-2.211181
89	6	0	-7.586778	4.461855	-1.398880
90	6	0	-12.004051	3.990888	1.602390
91	1	0	-5.306066	4.361171	-3.916103
92	1	0	-7.936333	5.125002	-0.613950
93	1	0	-6.168498	2.060597	-4.089598
94	1	0	-7.153529	0.185234	-2.888410
95	1	0	-9.907735	4.589061	-0.013422
96	1	0	-10.681271	-0.290619	0.273172
97	1	0	-12.136011	1.264004	1.507918
98	1	0	-13.045401	3.889672	1.274939
99	1	0	-11.707619	5.032972	1.456362
100	1	0	-11.986938	3.784701	2.679011
101	6	0	-2.073361	6.559145	3.475970
102	6	0	-1.390262	7.072606	2.393117
103	6	0	-2.029371	7.298166	1.148389
104	6	0	-3.392484	6.894113	1.022431
105	6	0	-4.067567	6.394714	2.159957
106	6	0	-3.443165	6.231835	3.385165
107	6	0	-1.341095	7.877971	0.001109
108	6	0	-4.031755	6.931931	-0.283733
109	6	0	-3.384798	7.627258	-1.340528
110	6	0	-2.053302	8.117193	-1.146679
111	6	0	-3.997095	7.649131	-2.618202
112	6	0	-5.102512	6.869895	-2.890968
113	6	0	-5.667273	6.047029	-1.884025
114	6	0	-5.170334	6.155656	-0.588191
115	6	0	-4.189425	5.715541	4.590762
116	1	0	-3.532651	8.229507	-3.411358
117	1	0	-5.511360	6.841739	-3.896919
118	1	0	-5.573269	5.493157	0.168922
119	1	0	-1.550202	8.573403	-1.995134
120	1	0	-0.342146	7.315743	2.503655
121	1	0	-1.548647	6.411186	4.416676
122	1	0	-5.119873	6.142174	2.076862
123	1	0	-4.212597	6.461565	5.394045
124	1	0	-3.709658	4.819581	5.001431
125	1	0	-5.222991	5.458978	4.343285
126	6	0	1.205260	10.451534	2.588836
127	6	0	0.421541	9.729700	1.712641
128	6	0	0.972070	8.712682	0.897609
129	6	0	2.373447	8.448575	0.989429
130	6	0	3.142452	9.206071	1.902258
131	6	0	2.590373	10.196511	2.700134
132	6	0	0.152685	7.964142	-0.037018
133	6	0	2.971081	7.428799	0.135673
134	6	0	2.185532	6.917668	-0.934519
135	6	0	0.783472	7.189895	-0.975321
136	6	0	2.769512	6.015118	-1.851505
137	6	0	4.036636	5.519405	-1.643976
138	6	0	4.772684	5.884337	-0.487846
139	6	0	4.251813	6.869201	0.349752
140	6	0	3.438239	11.002357	3.654221
141	1	0	4.438275	4.762506	-2.309861

142	1	0	4.823844	7.162703	1.224025
143	1	0	2.174174	5.658472	-2.687872
144	1	0	0.187800	6.649371	-1.704818
145	1	0	4.212659	9.032860	1.959393
146	1	0	-0.639657	9.943070	1.631699
147	1	0	0.755079	11.233789	3.194927
148	1	0	4.484164	10.685359	3.627487
149	1	0	3.082580	10.899207	4.686103
150	1	0	3.405481	12.070838	3.411016
151	6	0	0.741830	-5.917045	3.180175
152	6	0	0.390900	-6.639852	2.059363
153	6	0	1.349285	-7.013476	1.084047
154	6	0	2.686916	-6.548282	1.256622
155	6	0	3.015370	-5.832053	2.431170
156	6	0	2.077445	-5.517405	3.399766
157	6	0	1.006678	-7.808032	-0.089332
158	6	0	3.662724	-6.763615	0.199247
159	6	0	3.328539	-7.632460	-0.875096
160	6	0	1.998828	-8.156474	-0.968944
161	6	0	4.276914	-7.834433	-1.907913
162	6	0	5.445044	-7.101993	-1.959397
163	6	0	5.731582	-6.133488	-0.964266
164	6	0	4.864867	-6.030189	0.120331
165	6	0	2.455410	-4.764692	4.651836
166	1	0	4.041868	-8.537585	-2.702882
167	1	0	6.132642	-7.238215	-2.789029
168	1	0	5.058313	-5.256278	0.853230
169	1	0	1.749763	-8.765650	-1.833912
170	1	0	-0.642092	-6.932378	1.927649
171	1	0	-0.021747	-5.656674	3.909051
172	1	0	4.044090	-5.526395	2.591405
173	1	0	2.268850	-5.366189	5.549475
174	1	0	1.866698	-3.845887	4.755255
175	1	0	3.512788	-4.486832	4.649583
176	6	0	-1.869848	-10.275552	2.210227
177	6	0	-0.959441	-9.592890	1.430316
178	6	0	-1.380763	-8.742966	0.380715
179	6	0	-2.780671	-8.602679	0.137024
180	6	0	-3.683202	-9.315861	0.958478
181	6	0	-3.258574	-10.146165	1.984558
182	6	0	-0.425800	-8.038511	-0.454248
183	6	0	-3.236349	-7.741398	-0.946566
184	6	0	-2.271298	-7.296408	-1.892532
185	6	0	-0.878642	-7.449053	-1.605070
186	6	0	-2.700670	-6.554507	-3.016408
187	6	0	-4.004651	-6.124488	-3.122525
188	6	0	-4.937852	-6.394888	-2.089314
189	6	0	-4.557523	-7.252471	-1.058803
190	6	0	-4.242339	-10.912382	2.835242
191	1	0	-4.295534	-5.477462	-3.943903
192	1	0	-5.279259	-7.480845	-0.281260
193	1	0	-1.966234	-6.256682	-3.760097
194	1	0	-0.170495	-6.950437	-2.260524
195	1	0	-4.747896	-9.240237	0.759657
196	1	0	0.104586	-9.709646	1.610027
197	1	0	-1.515906	-10.929996	3.002931
198	1	0	-5.274712	-10.698686	2.545909
199	1	0	-4.131736	-10.659656	3.896267
200	1	0	-4.086848	-11.994068	2.747325

Table S22. Cartesian coordinate of *E,R,Z,R,E,R,Z,R* (20)

SCF Done: E(RB3LYP) = -4621.33463794 A.U. after 5 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.070178	2.026077	-3.316032
2	6	0	-10.491733	1.133051	-2.437146
3	6	0	-9.563183	1.556144	-1.456923
4	6	0	-9.231972	2.945532	-1.391113
5	6	0	-9.846696	3.829089	-2.306618
6	6	0	-10.753060	3.400870	-3.264542
7	6	0	-8.978514	0.623053	-0.508641
8	6	0	-8.269381	3.409037	-0.398447
9	6	0	-7.904464	2.507122	0.638376
10	6	0	-8.280781	1.133915	0.557384
11	6	0	-7.006478	2.941484	1.639867
12	6	0	-6.368627	4.155010	1.539061
13	6	0	-6.603784	5.016478	0.434291
14	6	0	-7.605009	4.654173	-0.469556
15	6	0	-11.401727	4.369517	-4.223343
16	6	0	-9.809044	-2.470519	2.519024
17	6	0	-9.700169	-1.538323	1.506978
18	6	0	-8.971317	-1.812597	0.325693
19	6	0	-8.347072	-3.088707	0.197619
20	6	0	-8.476762	-4.017103	1.254876
21	6	0	-9.190479	-3.735088	2.409491
22	6	0	-8.870649	-0.844200	-0.755431
23	6	0	-7.598013	-3.398547	-1.011755
24	6	0	-7.764535	-2.544276	-2.136464
25	6	0	-8.404999	-1.275884	-1.973322
26	6	0	-7.110978	-2.879579	-3.346781
27	6	0	-6.195182	-3.907139	-3.397130
28	6	0	-5.869766	-4.646623	-2.230085
29	6	0	-6.629894	-4.423086	-1.082386
30	6	0	-9.325451	-4.748528	3.519840
31	6	0	10.369636	2.204092	2.346641
32	6	0	10.168801	1.248552	1.370593
33	6	0	9.280688	1.467826	0.291729
34	6	0	8.600186	2.722375	0.221627
35	6	0	8.825949	3.673311	1.241887
36	6	0	9.689623	3.440160	2.301268
37	6	0	9.075364	0.470042	-0.748982
38	6	0	7.705367	2.994935	-0.895732
39	6	0	7.765535	2.119255	-2.013881
40	6	0	8.449243	0.870935	-1.904117
41	6	0	6.977211	2.402362	-3.153928
42	6	0	6.034890	3.403646	-3.124890
43	6	0	5.826359	4.167912	-1.947373
44	6	0	6.711635	4.001450	-0.883738
45	6	0	9.921714	4.478159	3.372253
46	6	0	10.597847	-2.390200	-3.762268
47	6	0	10.301930	-1.508795	-2.741356
48	6	0	9.557432	-1.912266	-1.608330
49	6	0	9.129233	-3.270961	-1.533311
50	6	0	9.442658	-4.143235	-2.599308
51	6	0	10.162188	-3.731853	-3.710954

52	6	0	9.246422	-0.992939	-0.520801
53	6	0	8.402542	-3.727480	-0.357052
54	6	0	8.423286	-2.896104	0.794817
55	6	0	8.831809	-1.531718	0.674190
56	6	0	7.847411	-3.386632	1.991152
57	6	0	7.120009	-4.554995	2.000173
58	6	0	6.884436	-5.276184	0.798674
59	6	0	7.599215	-4.887451	-0.335699
60	6	0	10.496224	-4.686678	-4.831156
61	6	0	0.066805	-6.011587	3.851454
62	6	0	-0.100316	-6.613612	2.622009
63	6	0	1.006153	-6.938072	1.798494
64	6	0	2.306156	-6.566772	2.249374
65	6	0	2.440902	-5.968387	3.523670
66	6	0	1.353612	-5.691541	4.335584
67	6	0	0.850915	-7.593605	0.507458
68	6	0	3.450451	-6.772556	1.374717
69	6	0	3.286495	-7.555727	0.200683
70	6	0	1.968441	-7.952833	-0.199641
71	6	0	4.421839	-7.791483	-0.613707
72	6	0	5.626674	-7.165416	-0.367127
73	6	0	5.758799	-6.242613	0.703683
74	6	0	4.680573	-6.117453	1.578465
75	6	0	1.523848	-5.065099	5.697938
76	6	0	-2.463807	-10.255550	1.737164
77	6	0	-1.412130	-9.484187	1.288264
78	6	0	-1.613210	-8.432802	0.363133
79	6	0	-2.940114	-8.170360	-0.098088
80	6	0	-3.990551	-8.984786	0.383049
81	6	0	-3.780753	-10.017542	1.284278
82	6	0	-0.503325	-7.642056	-0.129630
83	6	0	-3.170799	-7.077773	-1.036480
84	6	0	-2.035146	-6.474289	-1.645816
85	6	0	-0.722898	-6.780881	-1.170141
86	6	0	-2.227349	-5.456887	-2.606405
87	6	0	-3.481992	-4.954471	-2.862152
88	6	0	-4.617082	-5.443340	-2.164202
89	6	0	-4.446485	-6.533471	-1.311000
90	6	0	-4.919346	-10.882301	1.768466
91	6	0	-0.733158	8.034207	3.953358
92	6	0	-0.345678	8.016713	2.629261
93	6	0	-1.288254	7.870716	1.582195
94	6	0	-2.655003	7.655201	1.940067
95	6	0	-3.017082	7.699660	3.305428
96	6	0	-2.090568	7.898795	4.316258
97	6	0	-0.907053	7.892063	0.177659
98	6	0	-3.618920	7.313038	0.902598
99	6	0	-3.250201	7.516866	-0.453935
100	6	0	-1.894861	7.841691	-0.773248
101	6	0	-4.175272	7.175023	-1.469073
102	6	0	-5.326119	6.477199	-1.173438
103	6	0	-5.633051	6.112313	0.164006
104	6	0	-4.821986	6.628552	1.175673
105	6	0	-2.505280	7.967288	5.765727
106	6	0	2.562824	10.653213	0.728824
107	6	0	1.482573	9.825182	0.507155
108	6	0	1.644672	8.524104	-0.025859
109	6	0	2.965883	8.080634	-0.358438
110	6	0	4.045810	8.959989	-0.112540

111	6	0	3.874458	10.226836	0.423384
112	6	0	0.503879	7.665001	-0.273677
113	6	0	3.164151	6.765508	-0.961290
114	6	0	2.003723	6.027876	-1.325116
115	6	0	0.710160	6.495502	-0.954935
116	6	0	2.137795	4.788354	-1.986368
117	6	0	3.378216	4.254539	-2.231648
118	6	0	4.554387	4.924560	-1.803622
119	6	0	4.430366	6.171910	-1.195115
120	6	0	5.048591	11.143970	0.665739
121	1	0	-6.753811	2.260455	2.448165
122	1	0	-5.600869	4.404113	2.262141
123	1	0	-7.818637	5.312833	-1.303752
124	1	0	-7.851450	0.457371	1.289329
125	1	0	-10.763699	0.083631	-2.478113
126	1	0	-11.790697	1.670136	-4.048269
127	1	0	-9.626996	4.890292	-2.242111
128	1	0	-11.085444	5.397996	-4.029980
129	1	0	-11.146493	4.130653	-5.262606
130	1	0	-12.494624	4.334218	-4.147182
131	1	0	-5.676386	-4.118263	-4.326963
132	1	0	-6.372910	-4.961414	-0.176859
133	1	0	-7.292296	-2.268777	-4.227343
134	1	0	-8.347673	-0.577300	-2.802542
135	1	0	-8.030287	-5.001007	1.147732
136	1	0	-10.195081	-0.577888	1.603492
137	1	0	-10.389988	-2.234303	3.407128
138	1	0	-8.821898	-5.686340	3.270524
139	1	0	-8.891247	-4.373796	4.454286
140	1	0	-10.377716	-4.976356	3.725780
141	1	0	7.077905	1.770138	-4.032165
142	1	0	5.400910	3.576776	-3.988921
143	1	0	6.543575	4.571440	0.024252
144	1	0	8.301675	0.159341	-2.709171
145	1	0	10.717194	0.313542	1.412990
146	1	0	11.071385	2.008560	3.153722
147	1	0	8.331870	4.638056	1.178495
148	1	0	9.350529	5.389833	3.177925
149	1	0	9.626953	4.102660	4.359278
150	1	0	10.980859	4.752795	3.438544
151	1	0	6.672382	-4.893174	2.928494
152	1	0	7.434214	-5.415666	-1.267813
153	1	0	7.937687	-2.795196	2.898551
154	1	0	8.622748	-0.878287	1.514730
155	1	0	9.143541	-5.184727	-2.529225
156	1	0	10.661022	-0.486456	-2.793116
157	1	0	11.186697	-2.050776	-4.610845
158	1	0	11.578854	-4.753117	-4.989202
159	1	0	10.125462	-5.693899	-4.623281
160	1	0	10.054924	-4.356640	-5.779060
161	1	0	4.318567	-8.442128	-1.478408
162	1	0	6.467159	-7.349895	-1.028761
163	1	0	4.741972	-5.389578	2.376231
164	1	0	1.853483	-8.461330	-1.153412
165	1	0	-1.100436	-6.851192	2.283144
166	1	0	-0.805445	-5.786385	4.460148
167	1	0	3.433678	-5.733597	3.893694
168	1	0	0.974562	-4.119238	5.771000
169	1	0	1.138489	-5.719844	6.488429

170	1	0	2.575111	-4.859736	5.917011
171	1	0	-3.591091	-4.110009	-3.533708
172	1	0	-5.315295	-6.929096	-0.795863
173	1	0	-1.356804	-5.020302	-3.088653
174	1	0	0.107616	-6.204307	-1.567359
175	1	0	-4.998125	-8.818389	0.014760
176	1	0	-0.403002	-9.685216	1.634305
177	1	0	-2.278059	-11.064040	2.439861
178	1	0	-5.872361	-10.572836	1.331176
179	1	0	-4.757952	-11.935123	1.508913
180	1	0	-5.019047	-10.834611	2.859226
181	1	0	-3.912745	7.371290	-2.505399
182	1	0	-5.944441	6.113107	-1.986844
183	1	0	-5.060177	6.394042	2.206006
184	1	0	-1.619248	7.888056	-1.823217
185	1	0	0.702892	8.129312	2.384359
186	1	0	0.017877	8.161636	4.729136
187	1	0	-4.063242	7.592046	3.575095
188	1	0	-3.576528	7.784765	5.885962
189	1	0	-1.967784	7.226271	6.368652
190	1	0	-2.283406	8.950778	6.196821
191	1	0	3.464431	3.277574	-2.694509
192	1	0	5.334281	6.685201	-0.884203
193	1	0	1.240037	4.243619	-2.265831
194	1	0	-0.135448	5.847672	-1.163406
195	1	0	5.051183	8.646413	-0.374596
196	1	0	0.478978	10.170882	0.734018
197	1	0	2.404265	11.649689	1.133571
198	1	0	5.989096	10.683187	0.352152
199	1	0	4.937506	12.086537	0.117262
200	1	0	5.139428	11.401767	1.727579

Table S23. Cartesian coordinate of *E,R,Z,R,E,R,Z,S* (21)

SCF Done: E(RB3LYP) = -4621.33396968 A.U. after 14 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.758067	1.626166	2.777165
2	6	0	-7.664865	2.398696	1.638041
3	6	0	-7.900852	1.858558	0.348692
4	6	0	-8.147689	0.455762	0.259011
5	6	0	-8.263405	-0.299722	1.448546
6	6	0	-8.089487	0.256521	2.704395
7	6	0	-7.857904	2.660783	-0.870041
8	6	0	-8.195160	-0.179703	-1.048002
9	6	0	-8.282273	0.639558	-2.205127
10	6	0	-8.150802	2.059145	-2.068775
11	6	0	-8.303662	0.017300	-3.478586
12	6	0	-8.069792	-1.336316	-3.615601
13	6	0	-7.827548	-2.142648	-2.474835
14	6	0	-7.971303	-1.561465	-1.217661
15	6	0	-8.237285	-0.564883	3.961472
16	1	0	-8.427641	0.638120	-4.362277
17	1	0	-8.017780	-1.779095	-4.606154
18	1	0	-7.736945	-2.164447	-0.348645
19	1	0	-8.147851	2.659049	-2.975028
20	1	0	-7.412037	3.444871	1.738281

21	1	0	-7.580144	2.083363	3.747462
22	1	0	-8.512968	-1.353660	1.378528
23	1	0	-7.326114	-0.527594	4.569752
24	1	0	-8.445701	-1.613586	3.733283
25	1	0	-9.054827	-0.189715	4.588518
26	6	0	-9.373296	6.229309	1.332085
27	6	0	-8.966704	5.168843	0.548646
28	6	0	-7.678277	5.135333	-0.034522
29	6	0	-6.799307	6.238140	0.192524
30	6	0	-7.248041	7.302761	1.006765
31	6	0	-8.510871	7.320637	1.579244
32	6	0	-7.248730	4.027579	-0.869186
33	6	0	-5.483852	6.249180	-0.434245
34	6	0	-5.238844	5.306578	-1.470930
35	6	0	-6.126789	4.198638	-1.638014
36	6	0	-4.029686	5.379461	-2.198543
37	6	0	-3.027853	6.242409	-1.814151
38	6	0	-3.177202	7.046249	-0.655359
39	6	0	-4.417217	7.081120	-0.021862
40	6	0	-8.972510	8.478282	2.430858
41	1	0	-2.071427	6.230185	-2.327096
42	1	0	-4.537042	7.709246	0.855238
43	1	0	-3.869137	4.687988	-3.021452
44	1	0	-5.809393	3.397945	-2.299278
45	1	0	-6.596183	8.157310	1.160794
46	1	0	-9.643038	4.340323	0.363394
47	1	0	-10.373652	6.231743	1.757747
48	1	0	-8.200687	9.248034	2.513511
49	1	0	-9.227422	8.148869	3.445052
50	1	0	-9.870773	8.947354	2.012732
51	6	0	8.036478	-6.075739	-3.804770
52	6	0	8.138641	-5.267270	-2.691079
53	6	0	7.313022	-5.461691	-1.557947
54	6	0	6.366792	-6.528217	-1.588676
55	6	0	6.286915	-7.333582	-2.747217
56	6	0	7.097077	-7.128962	-3.853089
57	6	0	7.427831	-4.626897	-0.370974
58	6	0	5.518403	-6.762303	-0.429683
59	6	0	5.860735	-6.115578	0.789395
60	6	0	6.812534	-5.047861	0.781977
61	6	0	5.110261	-6.420665	1.950463
62	6	0	3.969365	-7.187871	1.876869
63	6	0	3.493622	-7.665673	0.626738
64	6	0	4.319302	-7.504830	-0.485208
65	6	0	7.001412	-8.009993	-5.074759
66	1	0	5.416283	-5.990932	2.900785
67	1	0	3.398466	-7.383837	2.778634
68	1	0	3.966823	-7.848519	-1.451072
69	1	0	6.907680	-4.456178	1.687610
70	1	0	8.876960	-4.473142	-2.669524
71	1	0	8.697196	-5.909084	-4.651941
72	1	0	5.590395	-8.166151	-2.760687
73	1	0	7.965670	-8.477260	-5.305617
74	1	0	6.707156	-7.432043	-5.958905
75	1	0	6.266441	-8.807767	-4.938076
76	6	0	10.274258	-2.797753	2.488636
77	6	0	9.473862	-3.384887	1.530612
78	6	0	8.779585	-2.612270	0.569387
79	6	0	8.935857	-1.189690	0.599748

80	6	0	9.765058	-0.627435	1.597228
81	6	0	10.430476	-1.395563	2.539739
82	6	0	7.956551	-3.233921	-0.453481
83	6	0	8.251064	-0.362604	-0.388334
84	6	0	7.599910	-1.025723	-1.465732
85	6	0	7.472953	-2.444648	-1.465182
86	6	0	6.966162	-0.260256	-2.469636
87	6	0	6.894107	1.108109	-2.374432
88	6	0	7.454785	1.792620	-1.263858
89	6	0	8.153870	1.047064	-0.314286
90	6	0	11.313739	-0.764437	3.588471
91	1	0	6.334233	1.664136	-3.117812
92	1	0	8.600796	1.570023	0.524326
93	1	0	6.481898	-0.776775	-3.294021
94	1	0	6.864062	-2.889640	-2.245464
95	1	0	9.911769	0.447678	1.615804
96	1	0	9.383074	-4.465032	1.493358
97	1	0	10.802465	-3.422109	3.205023
98	1	0	11.364748	0.321206	3.469916
99	1	0	12.336155	-1.156220	3.536775
100	1	0	10.942780	-0.973860	4.598839
101	6	0	5.353232	6.936060	3.997138
102	6	0	4.764681	7.394685	2.835663
103	6	0	5.022583	6.787163	1.584234
104	6	0	5.935411	5.689143	1.543678
105	6	0	6.512975	5.242820	2.753522
106	6	0	6.238492	5.837022	3.975641
107	6	0	4.413926	7.272411	0.352834
108	6	0	6.267255	5.074328	0.264924
109	6	0	5.879225	5.762282	-0.916926
110	6	0	4.943524	6.837797	-0.837991
111	6	0	6.291465	5.253494	-2.170873
112	6	0	6.918692	4.032835	-2.266362
113	6	0	7.138873	3.236360	-1.111686
114	6	0	6.866847	3.801731	0.134497
115	6	0	6.879282	5.347766	5.251635
116	1	0	6.057528	5.818863	-3.069130
117	1	0	7.205840	3.652816	-3.241281
118	1	0	7.012421	3.195681	1.022178
119	1	0	4.529204	7.198788	-1.773209
120	1	0	4.103481	8.253660	2.872403
121	1	0	5.143654	7.436528	4.939315
122	1	0	7.227596	4.426114	2.723779
123	1	0	6.123533	5.017951	5.974151
124	1	0	7.459336	6.141620	5.736475
125	1	0	7.552574	4.506865	5.065411
126	6	0	3.395220	10.567378	-2.423332
127	6	0	3.738263	9.669206	-1.432240
128	6	0	2.756749	8.931123	-0.730203
129	6	0	1.385442	9.152680	-1.058627
130	6	0	1.071543	10.072609	-2.083904
131	6	0	2.044611	10.779329	-2.774079
132	6	0	3.106821	7.988985	0.325761
133	6	0	0.347688	8.446391	-0.320118
134	6	0	0.721816	7.800537	0.890337
135	6	0	2.105603	7.569623	1.167468
136	6	0	-0.284720	7.223591	1.699162
137	6	0	-1.584933	7.133126	1.251298
138	6	0	-1.930429	7.587572	-0.046388

139	6	0	-0.978320	8.290763	-0.781008
140	6	0	1.682392	11.767452	-3.856026
141	1	0	-2.328475	6.606629	1.841626
142	1	0	-1.245830	8.652680	-1.768729
143	1	0	-0.002665	6.774386	2.647769
144	1	0	2.337025	6.890209	1.980929
145	1	0	0.028195	10.263979	-2.315480
146	1	0	4.781357	9.536124	-1.166285
147	1	0	4.174634	11.130232	-2.931059
148	1	0	0.599112	11.848283	-3.978862
149	1	0	2.107679	11.471934	-4.822469
150	1	0	2.070394	12.767153	-3.628997
151	6	0	-7.000931	-8.593868	1.510730
152	6	0	-5.750311	-8.340325	0.985945
153	6	0	-5.555841	-7.345133	-0.000138
154	6	0	-6.684317	-6.591704	-0.441683
155	6	0	-7.949252	-6.878221	0.119330
156	6	0	-8.130114	-7.861785	1.080272
157	6	0	-4.246596	-7.087456	-0.569098
158	6	0	-6.496427	-5.549156	-1.441886
159	6	0	-5.269596	-5.529338	-2.162437
160	6	0	-4.163463	-6.306865	-1.691278
161	6	0	-5.102951	-4.589036	-3.205040
162	6	0	-6.026638	-3.586530	-3.406356
163	6	0	-7.155605	-3.466963	-2.556193
164	6	0	-7.411575	-4.493212	-1.648441
165	6	0	-9.495082	-8.163432	1.649941
166	1	0	-4.186138	-4.609147	-3.788340
167	1	0	-5.829107	-2.811070	-4.139748
168	1	0	-8.290803	-4.420006	-1.016523
169	1	0	-3.193441	-6.136611	-2.149898
170	1	0	-4.893142	-8.916657	1.319839
171	1	0	-7.123067	-9.373612	2.258424
172	1	0	-8.818303	-6.333169	-0.236801
173	1	0	-9.509204	-8.033715	2.738465
174	1	0	-9.790701	-9.199766	1.448580
175	1	0	-10.260745	-7.509118	1.224693
176	6	0	-3.154725	-5.537084	3.329705
177	6	0	-3.509949	-6.090357	2.117638
178	6	0	-2.599681	-6.868815	1.359326
179	6	0	-1.270931	-7.006606	1.855639
180	6	0	-0.949687	-6.447123	3.114448
181	6	0	-1.862561	-5.725867	3.864905
182	6	0	-2.964677	-7.487751	0.090540
183	6	0	-0.269129	-7.674041	1.039330
184	6	0	-0.682872	-8.369584	-0.128769
185	6	0	-2.044462	-8.263384	-0.565018
186	6	0	0.301033	-9.039862	-0.897467
187	6	0	1.645429	-8.920499	-0.608038
188	6	0	2.083904	-8.106589	0.468358
189	6	0	1.110435	-7.548237	1.293504
190	6	0	-1.499792	-5.150408	5.211848
191	1	0	2.374956	-9.425409	-1.233867
192	1	0	1.428279	-6.886259	2.088110
193	1	0	-0.016361	-9.620502	-1.759958
194	1	0	-2.322295	-8.740600	-1.501294
195	1	0	0.044222	-6.600686	3.521495
196	1	0	-4.511457	-5.928927	1.742306
197	1	0	-3.884146	-4.952310	3.884711

198	1	0	-0.456690	-5.354591	5.467967
199	1	0	-2.128221	-5.569877	6.006406
200	1	0	-1.643746	-4.063874	5.231155

Table S24. Cartesian coordinate of *E,R,Z,R,Z,R,Z,R* (22)

SCF Done: E(RB3LYP) = -4621.33019141 A.U. after 5 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-10.548616	1.642662	-1.974294
2	6	0	-10.130900	0.608956	-1.159144
3	6	0	-9.192176	0.816953	-0.122141
4	6	0	-8.697728	2.140668	0.082407
5	6	0	-9.140004	3.171695	-0.775700
6	6	0	-10.047895	2.950505	-1.800409
7	6	0	-8.747690	-0.266628	0.746838
8	6	0	-7.773944	2.401258	1.178357
9	6	0	-7.645229	1.399174	2.177857
10	6	0	-8.123867	0.077770	1.922304
11	6	0	-6.861053	1.674402	3.322490
12	6	0	-6.086082	2.809098	3.388547
13	6	0	-6.027020	3.713931	2.295497
14	6	0	-6.929507	3.531707	1.246984
15	6	0	-10.513288	4.072069	-2.696931
16	1	0	-6.828529	0.943016	4.125732
17	1	0	-5.466176	2.984372	4.261690
18	1	0	-6.887147	4.207155	0.398968
19	1	0	-7.804779	-0.697945	2.609592
20	1	0	-10.544051	-0.384500	-1.297811
21	1	0	-11.284070	1.450013	-2.751490
22	1	0	-8.785816	4.183695	-0.603933
23	1	0	-10.241661	3.883282	-3.742286
24	1	0	-11.603388	4.182194	-2.665262
25	1	0	-10.070900	5.028266	-2.405128
26	6	0	-9.316035	-3.834871	3.325571
27	6	0	-9.329473	-2.762081	2.455808
28	6	0	-8.652538	-2.806978	1.215144
29	6	0	-7.965278	-4.008708	0.866419
30	6	0	-7.963852	-5.082221	1.784223
31	6	0	-8.618494	-5.019078	3.005257
32	6	0	-8.663898	-1.681689	0.287243
33	6	0	-7.305887	-4.107880	-0.428841
34	6	0	-7.640773	-3.134811	-1.408987
35	6	0	-8.299383	-1.929703	-1.014667
36	6	0	-7.124557	-3.280740	-2.717902
37	6	0	-6.164590	-4.226756	-2.993882
38	6	0	-5.643498	-5.055199	-1.964656
39	6	0	-6.281606	-5.034940	-0.723838
40	6	0	-8.613411	-6.185078	3.963737
41	1	0	-5.754091	-4.297323	-3.995893
42	1	0	-5.888135	-5.653357	0.076138
43	1	0	-7.447070	-2.588225	-3.490929
44	1	0	-8.323527	-1.126680	-1.743033
45	1	0	-7.464573	-6.006267	1.508536
46	1	0	-9.887902	-1.868604	2.714150
47	1	0	-9.861595	-3.772295	4.263916
48	1	0	-9.632379	-6.519109	4.190989

49	1	0	-8.064369	-7.037639	3.555235
50	1	0	-8.146522	-5.912611	4.917612
51	6	0	7.336837	1.263562	3.718686
52	6	0	7.777326	0.994567	2.439645
53	6	0	7.869511	2.009085	1.453721
54	6	0	7.401170	3.311484	1.801365
55	6	0	6.983717	3.557363	3.130001
56	6	0	6.955093	2.568035	4.098119
57	6	0	8.378279	1.761149	0.109423
58	6	0	7.294209	4.333014	0.771142
59	6	0	7.894268	4.095490	-0.494682
60	6	0	8.459860	2.809594	-0.772367
61	6	0	7.769352	5.083907	-1.502786
62	6	0	6.958932	6.187404	-1.327012
63	6	0	6.243534	6.367594	-0.116665
64	6	0	6.482113	5.475087	0.925467
65	6	0	6.524266	2.859480	5.514587
66	1	0	8.272377	4.926801	-2.453591
67	1	0	6.832733	6.901729	-2.135460
68	1	0	5.902129	5.585804	1.833561
69	1	0	8.860961	2.633099	-1.766925
70	1	0	8.065655	-0.017031	2.189274
71	1	0	7.290289	0.458321	4.447780
72	1	0	6.686683	4.562820	3.410137
73	1	0	5.690709	2.215161	5.817229
74	1	0	7.340711	2.679018	6.223975
75	1	0	6.204598	3.898503	5.631030
76	6	0	11.308841	-1.192510	1.681213
77	6	0	10.476259	-0.251416	1.111913
78	6	0	9.444478	-0.624032	0.218376
79	6	0	9.285650	-2.007961	-0.099432
80	6	0	10.154189	-2.943272	0.508474
81	6	0	11.156834	-2.566296	1.388618
82	6	0	8.574703	0.365255	-0.392135
83	6	0	8.259161	-2.414587	-1.050714
84	6	0	7.634419	-1.396006	-1.822694
85	6	0	7.795108	-0.026052	-1.448795
86	6	0	6.734489	-1.760898	-2.848897
87	6	0	6.348020	-3.071243	-3.013110
88	6	0	6.815538	-4.077165	-2.128203
89	6	0	7.801779	-3.744861	-1.202682
90	6	0	12.082182	-3.583827	2.010611
91	1	0	5.596339	-3.326337	-3.753226
92	1	0	8.174530	-4.519620	-0.540382
93	1	0	6.295293	-0.980083	-3.464172
94	1	0	7.165028	0.706676	-1.944267
95	1	0	10.059042	-3.993627	0.250822
96	1	0	10.610942	0.800891	1.340981
97	1	0	12.099472	-0.873863	2.355987
98	1	0	12.016791	-3.564120	3.104864
99	1	0	11.844056	-4.598169	1.679563
100	1	0	13.127892	-3.382804	1.750140
101	6	0	2.081274	-7.235661	2.671853
102	6	0	1.531248	-7.529583	1.441061
103	6	0	2.287393	-7.429439	0.247538
104	6	0	3.624488	-6.937673	0.346068
105	6	0	4.159781	-6.663179	1.625044
106	6	0	3.423031	-6.813335	2.788538
107	6	0	1.739574	-7.763991	-1.059889

108	6	0	4.375931	-6.660516	-0.869156
109	6	0	3.884245	-7.170358	-2.100905
110	6	0	2.573692	-7.745150	-2.148652
111	6	0	4.602849	-6.896995	-3.290696
112	6	0	5.648779	-5.998158	-3.295686
113	6	0	6.044749	-5.349956	-2.098746
114	6	0	5.459864	-5.755446	-0.901919
115	6	0	4.021876	-6.532471	4.144897
116	1	0	4.260105	-7.338276	-4.223114
117	1	0	6.135213	-5.735640	-4.230707
118	1	0	5.736876	-5.231527	0.006020
119	1	0	2.176889	-8.020838	-3.122040
120	1	0	0.500459	-7.855920	1.389450
121	1	0	1.472812	-7.337501	3.567158
122	1	0	5.193082	-6.339293	1.702260
123	1	0	3.452890	-5.762272	4.678551
124	1	0	4.015848	-7.428671	4.776549
125	1	0	5.056418	-6.188390	4.063203
126	6	0	-1.134652	-10.837422	0.447286
127	6	0	-0.241201	-9.928799	-0.080528
128	6	0	-0.681519	-8.749586	-0.727109
129	6	0	-2.089985	-8.515906	-0.839532
130	6	0	-2.971650	-9.471961	-0.285094
131	6	0	-2.527151	-10.619417	0.353533
132	6	0	0.260863	-7.809286	-1.300271
133	6	0	-2.576163	-7.322605	-1.526177
134	6	0	-1.621841	-6.534282	-2.226982
135	6	0	-0.228904	-6.800413	-2.086024
136	6	0	-2.051890	-5.409585	-2.962639
137	6	0	-3.364801	-5.009618	-2.932334
138	6	0	-4.323818	-5.712108	-2.155259
139	6	0	-3.920205	-6.876543	-1.500775
140	6	0	-3.495072	-11.626479	0.925829
141	1	0	-3.654263	-4.096162	-3.438837
142	1	0	-4.655656	-7.426681	-0.923289
143	1	0	-1.314415	-4.825548	-3.506584
144	1	0	0.463713	-6.099920	-2.542111
145	1	0	-4.042006	-9.321231	-0.383620
146	1	0	0.826209	-10.115082	-0.013429
147	1	0	-0.765198	-11.737733	0.931922
148	1	0	-3.347288	-11.750971	2.005055
149	1	0	-4.532743	-11.323124	0.763181
150	1	0	-3.358973	-12.613855	0.469429
151	6	0	-3.696349	10.325538	-0.921031
152	6	0	-2.514203	9.683792	-0.616857
153	6	0	-2.500237	8.458854	0.091671
154	6	0	-3.748542	7.887875	0.498768
155	6	0	-4.937155	8.578352	0.167781
156	6	0	-4.937743	9.777188	-0.528710
157	6	0	-1.253874	7.805111	0.434706
158	6	0	-3.763567	6.631575	1.242696
159	6	0	-2.515404	6.116348	1.690766
160	6	0	-1.295206	6.722428	1.270724
161	6	0	-2.485720	4.932803	2.458770
162	6	0	-3.635647	4.224209	2.705292
163	6	0	-4.886145	4.661275	2.193632
164	6	0	-4.931088	5.874185	1.505518
165	6	0	-6.224044	10.496245	-0.855737
166	1	0	-1.526706	4.556502	2.804505

167	1	0	-3.574490	3.277009	3.228503
168	1	0	-5.888529	6.219800	1.130382
169	1	0	-0.367111	6.235291	1.554069
170	1	0	-1.566109	10.122483	-0.912011
171	1	0	-3.674487	11.269758	-1.459435
172	1	0	-5.890569	8.172450	0.490702
173	1	0	-7.094131	9.956816	-0.472047
174	1	0	-6.237359	11.503939	-0.424386
175	1	0	-6.351377	10.611256	-1.938645
176	6	0	-0.174353	7.442130	-3.802785
177	6	0	-0.525255	7.665332	-2.487375
178	6	0	0.452785	7.885491	-1.486944
179	6	0	1.826854	7.800350	-1.864547
180	6	0	2.148136	7.586296	-3.224370
181	6	0	1.179954	7.417278	-4.200756
182	6	0	0.103000	8.150670	-0.099556
183	6	0	2.856458	7.872291	-0.838158
184	6	0	2.488189	8.312444	0.462068
185	6	0	1.101352	8.460289	0.787173
186	6	0	3.487698	8.399387	1.461729
187	6	0	4.754272	7.899811	1.244708
188	6	0	5.086491	7.292560	0.006830
189	6	0	4.160520	7.366288	-1.031194
190	6	0	1.547542	7.209051	-5.649582
191	1	0	5.488786	7.917232	2.044420
192	1	0	4.398797	6.875731	-1.968051
193	1	0	3.220163	8.799002	2.436608
194	1	0	0.842665	8.682501	1.819059
195	1	0	3.192238	7.572729	-3.521284
196	1	0	-1.573194	7.684581	-2.215276
197	1	0	-0.953164	7.289517	-4.545941
198	1	0	1.153285	8.014462	-6.280527
199	1	0	2.631610	7.176999	-5.787730
200	1	0	1.132072	6.270273	-6.033997

Table S25. Cartesian coordinate of *E,R,Z,R,Z,S,Z,S* (23)

SCF Done: E(RB3LYP) = -4621.32979818 A.U. after 5 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-9.656628	-1.011078	3.199759
2	6	0	-9.558609	-0.170629	2.108837
3	6	0	-9.030742	-0.618194	0.875097
4	6	0	-8.612797	-1.979576	0.774662
5	6	0	-8.722101	-2.808871	1.913161
6	6	0	-9.228932	-2.353886	3.120909
7	6	0	-8.936899	0.257348	-0.285116
8	6	0	-8.103999	-2.482719	-0.494233
9	6	0	-8.315339	-1.686652	-1.652685
10	6	0	-8.717183	-0.323097	-1.511123
11	6	0	-7.933877	-2.202791	-2.913871
12	6	0	-7.213660	-3.371637	-3.010638
13	6	0	-6.809807	-4.073625	-1.844570
14	6	0	-7.324715	-3.653879	-0.617628
15	6	0	-9.345255	-3.263543	4.319727
16	1	0	-8.164554	-1.628741	-3.807443
17	1	0	-6.902284	-3.730494	-3.986388

18	1	0	-7.006918	-4.168317	0.282731
19	1	0	-8.668831	0.299271	-2.398393
20	1	0	-9.911208	0.852347	2.185251
21	1	0	-10.082260	-0.638611	4.128289
22	1	0	-8.432593	-3.852125	1.831819
23	1	0	-10.379213	-3.319300	4.679286
24	1	0	-9.016130	-4.279448	4.085677
25	1	0	-8.735995	-2.898790	5.155156
26	6	0	-10.735384	3.214328	-3.048628
27	6	0	-10.308148	2.332853	-2.075411
28	6	0	-9.239456	2.652485	-1.205599
29	6	0	-8.614307	3.927861	-1.346779
30	6	0	-9.072938	4.801658	-2.357651
31	6	0	-10.114694	4.471481	-3.211234
32	6	0	-8.791372	1.736158	-0.165141
33	6	0	-7.535020	4.300996	-0.442493
34	6	0	-7.354405	3.517468	0.730516
35	6	0	-7.983185	2.236972	0.826608
36	6	0	-6.396196	3.926778	1.687203
37	6	0	-5.528158	4.963347	1.419717
38	6	0	-5.562350	5.622983	0.165309
39	6	0	-6.604205	5.327507	-0.712278
40	6	0	-10.595283	5.428518	-4.274912
41	1	0	-4.735209	5.202090	2.121652
42	1	0	-6.643902	5.844778	-1.665577
43	1	0	-6.293287	3.353657	2.604903
44	1	0	-7.655326	1.587072	1.631042
45	1	0	-8.619547	5.784143	-2.447508
46	1	0	-10.811958	1.379658	-1.955875
47	1	0	-11.570713	2.943135	-3.689532
48	1	0	-10.041483	6.370676	-4.246693
49	1	0	-10.476371	5.000403	-5.277303
50	1	0	-11.659441	5.660379	-4.151257
51	6	0	8.426948	-1.973573	2.713209
52	6	0	8.538602	-1.537851	1.408996
53	6	0	8.318839	-2.405937	0.310088
54	6	0	7.873832	-3.732572	0.598197
55	6	0	7.799020	-4.152699	1.946003
56	6	0	8.082359	-3.309698	3.007495
57	6	0	8.488982	-1.987004	-1.077512
58	6	0	7.422807	-4.587534	-0.490450
59	6	0	7.713211	-4.196772	-1.825081
60	6	0	8.291195	-2.912210	-2.072422
61	6	0	7.250403	-5.011803	-2.885904
62	6	0	6.383487	-6.059037	-2.652658
63	6	0	5.959408	-6.371403	-1.334590
64	6	0	6.569298	-5.689656	-0.282229
65	6	0	8.021708	-3.789682	4.436869
66	1	0	7.506257	-4.738971	-3.906511
67	1	0	5.949532	-6.584226	-3.497024
68	1	0	6.286939	-5.943607	0.731864
69	1	0	8.447865	-2.616956	-3.106384
70	1	0	8.809570	-0.507452	1.225210
71	1	0	8.615491	-1.277332	3.526729
72	1	0	7.524042	-5.180517	2.161385
73	1	0	9.011419	-3.761309	4.908347
74	1	0	7.362464	-3.156581	5.041809
75	1	0	7.652893	-4.817011	4.499982
76	6	0	11.778040	0.789003	0.105115

77	6	0	10.817951	-0.087813	-0.356046
78	6	0	9.623711	0.374728	-0.957717
79	6	0	9.436307	1.784510	-1.100489
80	6	0	10.438398	2.651493	-0.607838
81	6	0	11.598877	2.185650	-0.009287
82	6	0	8.616715	-0.545035	-1.457205
83	6	0	8.247175	2.289710	-1.774938
84	6	0	7.451644	1.355700	-2.493983
85	6	0	7.644787	-0.043985	-2.284371
86	6	0	6.377991	1.824243	-3.284323
87	6	0	6.005637	3.148592	-3.250984
88	6	0	6.664529	4.058703	-2.385069
89	6	0	7.803413	3.631840	-1.707011
90	6	0	12.661441	3.133247	0.492162
91	1	0	5.132833	3.482927	-3.802950
92	1	0	8.317360	4.335809	-1.060291
93	1	0	5.804534	1.109185	-3.868268
94	1	0	6.902539	-0.718093	-2.700784
95	1	0	10.315897	3.722513	-0.736434
96	1	0	10.975052	-1.158031	-0.267487
97	1	0	12.689821	0.401713	0.553038
98	1	0	13.621732	2.954338	-0.005405
99	1	0	12.383523	4.176114	0.317941
100	1	0	12.831325	3.006730	1.567905
101	6	0	2.730503	6.417036	3.427798
102	6	0	2.045114	6.959448	2.360544
103	6	0	2.636936	7.080621	1.078316
104	6	0	3.944663	6.535293	0.901550
105	6	0	4.627138	6.011836	2.023786
106	6	0	4.055802	5.954125	3.283685
107	6	0	1.952380	7.692405	-0.055258
108	6	0	4.511325	6.452896	-0.435674
109	6	0	3.877888	7.164275	-1.489883
110	6	0	2.622713	7.808962	-1.246859
111	6	0	4.403042	7.054734	-2.801290
112	6	0	5.396936	6.143601	-3.095102
113	6	0	5.941706	5.323462	-2.075958
114	6	0	5.546730	5.549933	-0.761134
115	6	0	4.810811	5.407794	4.470364
116	1	0	3.950276	7.640651	-3.597124
117	1	0	5.728325	6.011561	-4.121125
118	1	0	5.934493	4.890106	0.006356
119	1	0	2.126772	8.288438	-2.086618
120	1	0	1.032466	7.306769	2.513300
121	1	0	2.242921	6.352310	4.397475
122	1	0	5.643706	5.652658	1.898940
123	1	0	4.942063	6.172405	5.245274
124	1	0	4.272214	4.573131	4.933870
125	1	0	5.802987	5.048906	4.183840
126	6	0	-0.186360	10.545331	2.618571
127	6	0	0.476317	9.742789	1.713003
128	6	0	-0.213826	8.782804	0.935805
129	6	0	-1.629190	8.667372	1.095214
130	6	0	-2.271871	9.502810	2.037085
131	6	0	-1.583028	10.433832	2.799389
132	6	0	0.477588	7.946473	-0.028364
133	6	0	-2.371628	7.718681	0.274520
134	6	0	-1.697982	7.136566	-0.834742
135	6	0	-0.277358	7.250683	-0.936557

136	6	0	-2.420382	6.316137	-1.729987
137	6	0	-3.721856	5.956853	-1.462369
138	6	0	-4.351808	6.375492	-0.262447
139	6	0	-3.689872	7.289826	0.554705
140	6	0	-2.296248	11.325371	3.786758
141	1	0	-4.237798	5.258462	-2.113376
142	1	0	-4.179123	7.623918	1.464124
143	1	0	-1.909127	5.910339	-2.598927
144	1	0	0.220838	6.647356	-1.689419
145	1	0	-3.350441	9.441337	2.144852
146	1	0	1.548540	9.846309	1.579878
147	1	0	0.370095	11.280901	3.194104
148	1	0	-3.370986	11.125930	3.803798
149	1	0	-1.912102	11.179719	4.803248
150	1	0	-2.155307	12.384456	3.541335
151	6	0	-3.571108	-9.927681	1.933804
152	6	0	-2.524629	-9.371609	1.227999
153	6	0	-2.740784	-8.350869	0.272584
154	6	0	-4.076632	-7.892661	0.049644
155	6	0	-5.121818	-8.489354	0.791152
156	6	0	-4.898465	-9.492559	1.721977
157	6	0	-1.642727	-7.787381	-0.486960
158	6	0	-4.320443	-6.832755	-0.922889
159	6	0	-3.248830	-6.465269	-1.783890
160	6	0	-1.931996	-6.959648	-1.537564
161	6	0	-3.466447	-5.488523	-2.779764
162	6	0	-4.655882	-4.802738	-2.847123
163	6	0	-5.696706	-5.055662	-1.915280
164	6	0	-5.528845	-6.102435	-1.008530
165	6	0	-6.036590	-10.121984	2.488203
166	1	0	-2.650226	-5.231690	-3.449678
167	1	0	-4.762839	-3.993972	-3.561234
168	1	0	-6.331088	-6.317960	-0.310748
169	1	0	-1.119659	-6.552043	-2.132120
170	1	0	-1.510381	-9.722611	1.391214
171	1	0	-3.375796	-10.717810	2.654548
172	1	0	-6.144370	-8.173618	0.608884
173	1	0	-6.095990	-11.200129	2.298804
174	1	0	-5.906381	-9.994942	3.569368
175	1	0	-6.998227	-9.680844	2.212726
176	6	0	-0.008224	-6.152313	3.200130
177	6	0	-0.520423	-6.761553	2.073620
178	6	0	0.324150	-7.259665	1.050855
179	6	0	1.727943	-7.053822	1.185996
180	6	0	2.218556	-6.443204	2.363101
181	6	0	1.383831	-5.997468	3.374479
182	6	0	-0.193859	-7.927420	-0.135579
183	6	0	2.613043	-7.432010	0.094978
184	6	0	2.099105	-8.230215	-0.962173
185	6	0	0.686542	-8.463361	-1.039410
186	6	0	2.983367	-8.628447	-1.994764
187	6	0	4.272670	-8.139315	-2.065950
188	6	0	4.746654	-7.203445	-1.110204
189	6	0	3.918807	-6.919451	-0.024817
190	6	0	1.931675	-5.361049	4.628314
191	1	0	4.911371	-8.441099	-2.890302
192	1	0	4.237234	-6.169468	0.687092
193	1	0	2.613116	-9.289274	-2.774488
194	1	0	0.300393	-8.981093	-1.913649

195	1	0	3.290607	-6.335230	2.492812
196	1	0	-1.592791	-6.869091	1.974960
197	1	0	-0.687310	-5.791982	3.968935
198	1	0	3.022961	-5.300070	4.603356
199	1	0	1.541942	-4.344963	4.760396
200	1	0	1.647617	-5.930525	5.521115

Table S26. Cartesian coordinate of *E,R,E,S,Z,R,E,S* (24)

SCF Done: E(RB3LYP) = -4621.32939801 A.U. after 5 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.736609	-8.461970	2.012456
2	6	0	7.669373	-7.290995	1.286266
3	6	0	6.519616	-6.956490	0.532958
4	6	0	5.411078	-7.859764	0.537795
5	6	0	5.519280	-9.049568	1.293083
6	6	0	6.653018	-9.368381	2.025284
7	6	0	6.460916	-5.739247	-0.251702
8	6	0	4.212647	-7.531764	-0.226589
9	6	0	4.294593	-6.453691	-1.151018
10	6	0	5.426060	-5.583221	-1.134202
11	6	0	3.176836	-6.148617	-1.957608
12	6	0	1.974946	-6.786548	-1.765530
13	6	0	1.824391	-7.770802	-0.752881
14	6	0	2.959865	-8.163403	-0.043510
15	6	0	6.745244	-10.654320	2.810500
16	1	0	3.255715	-5.340369	-2.679701
17	1	0	1.106393	-6.460017	-2.325953
18	1	0	2.859068	-8.929509	0.718014
19	1	0	5.384124	-4.690205	-1.750751
20	1	0	8.513276	-6.608061	1.274819
21	1	0	8.637661	-8.697451	2.573330
22	1	0	4.697658	-9.759117	1.279662
23	1	0	6.900148	-10.458307	3.878044
24	1	0	5.835538	-11.251941	2.708704
25	1	0	7.588956	-11.267596	2.473202
26	6	0	6.656158	-3.469423	3.470373
27	6	0	6.689830	-4.233787	2.322422
28	6	0	7.291520	-3.757806	1.131220
29	6	0	7.803820	-2.427471	1.130917
30	6	0	7.769710	-1.680217	2.330508
31	6	0	7.217731	-2.175050	3.500475
32	6	0	7.362236	-4.555043	-0.086877
33	6	0	8.299658	-1.853877	-0.110555
34	6	0	8.523907	-2.711214	-1.220897
35	6	0	8.049070	-4.062685	-1.166918
36	6	0	9.048714	-2.147713	-2.409960
37	6	0	9.192397	-0.782157	-2.554778
38	6	0	8.800719	0.102289	-1.516105
39	6	0	8.421548	-0.463972	-0.299732
40	6	0	7.208462	-1.365863	4.774189
41	1	0	9.562820	-0.382932	-3.493915
42	1	0	8.070339	0.188492	0.488870
43	1	0	9.283076	-2.806666	-3.242191
44	1	0	8.123222	-4.666163	-2.067874
45	1	0	8.209737	-0.688147	2.344911

46	1	0	6.254384	-5.224193	2.338266
47	1	0	6.195642	-3.873886	4.368404
48	1	0	7.636467	-0.371604	4.620805
49	1	0	6.188819	-1.237397	5.155386
50	1	0	7.784948	-1.860712	5.564827
51	6	0	-8.156011	5.418341	4.336168
52	6	0	-7.787349	5.630770	3.022582
53	6	0	-7.720922	4.567888	2.091544
54	6	0	-8.066787	3.257358	2.539678
55	6	0	-8.432717	3.076070	3.892089
56	6	0	-8.479793	4.124611	4.798212
57	6	0	-7.344612	4.783172	0.700329
58	6	0	-8.049867	2.148289	1.595422
59	6	0	-7.984773	2.461052	0.209707
60	6	0	-7.612096	3.779372	-0.198738
61	6	0	-8.092353	1.414301	-0.735565
62	6	0	-8.088260	0.096007	-0.334072
63	6	0	-7.946881	-0.236256	1.036955
64	6	0	-7.997564	0.790344	1.978309
65	6	0	-8.884318	3.906251	6.235843
66	1	0	-8.091335	1.661194	-1.793997
67	1	0	-8.074667	-0.697559	-1.074722
68	1	0	-7.907480	0.536222	3.029603
69	1	0	-7.369551	3.918904	-1.246839
70	1	0	-7.561592	6.636227	2.684016
71	1	0	-8.212274	6.260810	5.021121
72	1	0	-8.724760	2.085878	4.228355
73	1	0	-8.070430	4.170431	6.921470
74	1	0	-9.744795	4.528628	6.507196
75	1	0	-9.152597	2.863112	6.423021
76	6	0	-7.711754	7.000465	-3.115741
77	6	0	-7.676936	6.451076	-1.849449
78	6	0	-6.498235	6.467229	-1.067650
79	6	0	-5.335845	7.089435	-1.614727
80	6	0	-5.405770	7.634420	-2.916386
81	6	0	-6.563944	7.599189	-3.677935
82	6	0	-6.454374	5.900891	0.274396
83	6	0	-4.119941	7.166853	-0.816410
84	6	0	-4.222754	6.888044	0.574329
85	6	0	-5.392215	6.237340	1.078033
86	6	0	-3.090020	7.082965	1.398794
87	6	0	-1.860294	7.382488	0.852577
88	6	0	-1.702016	7.467858	-0.553123
89	6	0	-2.839453	7.417767	-1.356007
90	6	0	-6.616411	8.201275	-5.061027
91	1	0	-0.982395	7.444515	1.488311
92	1	0	-2.719422	7.497146	-2.431770
93	1	0	-3.184343	6.913720	2.468246
94	1	0	-5.343868	5.854575	2.091958
95	1	0	-4.532071	8.134165	-3.323343
96	1	0	-8.576084	6.013229	-1.429533
97	1	0	-8.639439	6.984844	-3.682497
98	1	0	-5.661187	8.655622	-5.337098
99	1	0	-6.856958	7.442932	-5.815474
100	1	0	-7.389143	8.975712	-5.129544
101	6	0	5.492575	10.157304	0.001526
102	6	0	5.658248	8.855343	-0.423153
103	6	0	4.549494	8.036773	-0.743920
104	6	0	3.238017	8.594718	-0.637501

105	6	0	3.108622	9.930299	-0.191942
106	6	0	4.202576	10.718514	0.130108
107	6	0	4.722114	6.671761	-1.207765
108	6	0	2.080177	7.795904	-1.020132
109	6	0	2.317931	6.575558	-1.711186
110	6	0	3.639662	6.035221	-1.756957
111	6	0	1.222481	5.843695	-2.221917
112	6	0	-0.070908	6.228079	-1.949417
113	6	0	-0.327990	7.344460	-1.113740
114	6	0	0.743441	8.132545	-0.701194
115	6	0	4.035749	12.146918	0.588571
116	1	0	1.415501	4.933618	-2.783705
117	1	0	-0.903822	5.620253	-2.288299
118	1	0	0.541889	8.994353	-0.073107
119	1	0	3.755811	5.026425	-2.141458
120	1	0	6.656514	8.442217	-0.525613
121	1	0	6.365168	10.764057	0.230404
122	1	0	2.118698	10.371912	-0.133003
123	1	0	4.446262	12.292091	1.594851
124	1	0	4.563548	12.842308	-0.074375
125	1	0	2.982891	12.440339	0.611825
126	6	0	6.767303	5.974522	2.630425
127	6	0	6.159919	6.228571	1.418298
128	6	0	6.562810	5.570062	0.229611
129	6	0	7.561079	4.554402	0.342489
130	6	0	8.180890	4.341588	1.595395
131	6	0	7.818550	5.038923	2.735697
132	6	0	5.974460	5.863803	-1.071964
133	6	0	7.855281	3.709505	-0.806558
134	6	0	7.353106	4.095753	-2.078588
135	6	0	6.452362	5.202284	-2.175136
136	6	0	7.617229	3.264625	-3.193255
137	6	0	8.191906	2.021266	-3.033818
138	6	0	8.565751	1.553136	-1.747030
139	6	0	8.475227	2.449313	-0.682570
140	6	0	8.510150	4.809386	4.057095
141	1	0	8.268489	1.360315	-3.890675
142	1	0	8.793494	2.120553	0.298974
143	1	0	7.269714	3.577890	-4.174381
144	1	0	6.039603	5.437573	-3.152396
145	1	0	8.983548	3.614539	1.667957
146	1	0	5.361000	6.956443	1.376146
147	1	0	6.435419	6.509691	3.516759
148	1	0	9.267314	4.024063	3.983330
149	1	0	9.007421	5.720862	4.409395
150	1	0	7.795057	4.516006	4.834471
151	6	0	-4.917400	-7.080423	-3.830730
152	6	0	-5.164452	-6.876729	-2.488703
153	6	0	-4.244095	-7.283777	-1.490540
154	6	0	-2.999277	-7.830672	-1.926837
155	6	0	-2.791380	-8.049255	-3.307956
156	6	0	-3.728024	-7.701679	-4.266966
157	6	0	-4.500503	-7.126973	-0.062296
158	6	0	-1.943851	-8.067892	-0.953613
159	6	0	-2.274266	-8.046901	0.427974
160	6	0	-3.576345	-7.609758	0.830566
161	6	0	-1.244663	-8.266628	1.375346
162	6	0	0.079686	-8.309759	0.990055
163	6	0	0.440103	-8.161755	-0.374206

164	6	0	-0.584507	-8.140723	-1.318536
165	6	0	-3.494397	-7.966430	-5.734054
166	1	0	-1.501712	-8.295088	2.431129
167	1	0	0.855758	-8.349701	1.747993
168	1	0	-0.320090	-8.059241	-2.365973
169	1	0	-3.777509	-7.526277	1.895264
170	1	0	-6.090403	-6.401553	-2.195734
171	1	0	-5.655725	-6.763517	-4.563244
172	1	0	-1.869835	-8.522846	-3.631691
173	1	0	-4.235104	-8.668878	-6.134413
174	1	0	-3.578047	-7.045412	-6.322457
175	1	0	-2.502582	-8.390336	-5.912609
176	6	0	-8.886981	-7.679297	-0.664980
177	6	0	-7.543124	-7.561356	-0.375717
178	6	0	-6.998634	-6.352864	0.118889
179	6	0	-7.877898	-5.246608	0.331398
180	6	0	-9.247032	-5.403530	0.017094
181	6	0	-9.767237	-6.590738	-0.475356
182	6	0	-5.588062	-6.229201	0.439106
183	6	0	-7.352351	-4.005164	0.885698
184	6	0	-6.045776	-4.034797	1.447010
185	6	0	-5.189246	-5.146947	1.180246
186	6	0	-5.554349	-2.891202	2.115810
187	6	0	-6.258799	-1.708697	2.098883
188	6	0	-7.475864	-1.606304	1.377707
189	6	0	-8.028613	-2.764138	0.833793
190	6	0	-11.237146	-6.737275	-0.785816
191	1	0	-5.831469	-0.815243	2.542699
192	1	0	-8.969190	-2.689268	0.297300
193	1	0	-4.573321	-2.936084	2.581290
194	1	0	-4.145339	-5.053542	1.463867
195	1	0	-9.926554	-4.577142	0.201701
196	1	0	-6.881007	-8.409437	-0.519113
197	1	0	-9.277331	-8.624570	-1.033780
198	1	0	-11.783803	-5.812105	-0.584945
199	1	0	-11.396846	-6.999356	-1.838330
200	1	0	-11.693513	-7.533516	-0.186184

Table S27. Cartesian coordinate of *E,R,E,R,E,S,Z,S* (25)

SCF Done: E(RB3LYP) = -4621.32937722 A.U. after 5 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.104769	6.641834	2.680139
2	6	0	3.430803	7.043232	1.545423
3	6	0	3.966101	6.838111	0.249010
4	6	0	5.192536	6.114434	0.149055
5	6	0	5.868662	5.742252	1.333671
6	6	0	5.360090	6.002696	2.594952
7	6	0	3.298819	7.295331	-0.964986
8	6	0	5.676176	5.704733	-1.160157
9	6	0	5.079915	6.274228	-2.317120
10	6	0	3.918534	7.099524	-2.173557
11	6	0	5.527360	5.852236	-3.593815
12	6	0	6.389185	4.782728	-3.727573
13	6	0	6.873289	4.104078	-2.581257
14	6	0	6.574514	4.628927	-1.327224

15	6	0	6.108098	5.612969	3.846132
16	1	0	5.111983	6.328910	-4.478069
17	1	0	6.653705	4.418320	-4.716127
18	1	0	6.909785	4.081128	-0.454180
19	1	0	3.438885	7.464050	-3.078045
20	1	0	2.473575	7.534484	1.653502
21	1	0	3.664144	6.828104	3.656501
22	1	0	6.830503	5.245675	1.254601
23	1	0	6.355480	6.492557	4.452201
24	1	0	5.506540	4.949190	4.477973
25	1	0	7.042224	5.095910	3.610793
26	6	0	1.650420	10.857471	1.137013
27	6	0	2.165538	9.816869	0.392067
28	6	0	1.328167	8.814083	-0.151093
29	6	0	-0.079542	8.905819	0.074876
30	6	0	-0.569296	9.983662	0.847368
31	6	0	0.262464	10.955752	1.381762
32	6	0	1.865086	7.724628	-0.945858
33	6	0	-0.969037	7.910405	-0.510172
34	6	0	-0.429787	7.039364	-1.497089
35	6	0	0.987127	6.957328	-1.666473
36	6	0	-1.290838	6.152297	-2.181753
37	6	0	-2.609611	6.020574	-1.808292
38	6	0	-3.119061	6.747400	-0.702578
39	6	0	-2.310391	7.713567	-0.108053
40	6	0	-0.288348	12.105276	2.190202
41	1	0	-3.240636	5.279471	-2.288542
42	1	0	-2.707570	8.280071	0.728125
43	1	0	-0.878679	5.520528	-2.964118
44	1	0	1.371692	6.160187	-2.295625
45	1	0	-1.639994	10.077451	1.000457
46	1	0	3.233400	9.759063	0.206631
47	1	0	2.318375	11.618286	1.533164
48	1	0	-0.040173	13.069679	1.731863
49	1	0	-1.376320	12.047452	2.280119
50	1	0	0.131602	12.116136	3.202912
51	6	0	-1.230527	-11.336097	-1.327707
52	6	0	-1.891788	-10.212036	-0.878490
53	6	0	-1.197090	-9.148482	-0.255640
54	6	0	0.220293	-9.255026	-0.099121
55	6	0	0.860710	-10.423786	-0.570492
56	6	0	0.168763	-11.460951	-1.177284
57	6	0	-1.897014	-7.979685	0.239183
58	6	0	0.957942	-8.166803	0.533218
59	6	0	0.206206	-7.152896	1.189426
60	6	0	-1.210167	-7.090529	1.020626
61	6	0	0.886095	-6.117179	1.866239
62	6	0	2.253443	-6.004276	1.789405
63	6	0	3.020894	-6.927409	1.030692
64	6	0	2.363494	-8.019358	0.463512
65	6	0	0.877398	-12.703597	-1.659152
66	1	0	0.304691	-5.359473	2.384701
67	1	0	2.739407	-5.142233	2.231732
68	1	0	2.944537	-8.740292	-0.101787
69	1	0	-1.729030	-6.225014	1.422120
70	1	0	-2.968944	-10.133930	-0.989112
71	1	0	-1.792260	-12.141896	-1.793625
72	1	0	1.931633	-10.531575	-0.428992
73	1	0	0.481878	-13.602058	-1.171289

74	1	0	0.745767	-12.842830	-2.738696
75	1	0	1.950709	-12.657850	-1.456439
76	6	0	-2.987718	-7.003602	-3.865459
77	6	0	-2.687793	-7.398151	-2.578299
78	6	0	-3.574510	-7.151757	-1.500863
79	6	0	-4.765333	-6.416466	-1.772492
80	6	0	-5.049014	-6.045025	-3.107079
81	6	0	-4.193647	-6.331066	-4.158116
82	6	0	-3.290555	-7.584299	-0.139267
83	6	0	-5.633068	-6.029528	-0.670656
84	6	0	-5.416801	-6.608444	0.608505
85	6	0	-4.236250	-7.388604	0.833971
86	6	0	-6.299159	-6.262590	1.661782
87	6	0	-7.257063	-5.281990	1.503916
88	6	0	-7.373476	-4.572099	0.280113
89	6	0	-6.594108	-5.006716	-0.791066
90	6	0	-4.527235	-5.940797	-5.577129
91	1	0	-7.898424	-5.024441	2.340954
92	1	0	-6.634998	-4.453808	-1.720153
93	1	0	-6.178012	-6.749186	2.626286
94	1	0	-4.035115	-7.731534	1.845540
95	1	0	-5.981889	-5.535113	-3.324877
96	1	0	-1.756967	-7.917344	-2.390824
97	1	0	-2.287359	-7.220633	-4.668252
98	1	0	-4.605635	-6.822259	-6.224480
99	1	0	-5.476151	-5.400529	-5.632418
100	1	0	-3.749365	-5.298366	-6.005948
101	6	0	-9.457555	1.468582	4.461516
102	6	0	-9.267702	1.994981	3.199630
103	6	0	-9.001665	1.166819	2.083488
104	6	0	-8.955059	-0.245149	2.289373
105	6	0	-9.147288	-0.747788	3.595986
106	6	0	-9.391103	0.076231	4.683732
107	6	0	-8.813583	1.712452	0.745814
108	6	0	-8.741293	-1.130404	1.152779
109	6	0	-8.862485	-0.575469	-0.149445
110	6	0	-8.873749	0.842931	-0.316853
111	6	0	-8.798527	-1.444053	-1.265144
112	6	0	-8.464048	-2.770126	-1.113579
113	6	0	-8.123096	-3.294119	0.162226
114	6	0	-8.337201	-2.477638	1.273831
115	6	0	-9.604540	-0.487387	6.067516
116	1	0	-8.972162	-1.036444	-2.257653
117	1	0	-8.410986	-3.407871	-1.989407
118	1	0	-8.072084	-2.850713	2.256219
119	1	0	-8.765731	1.221603	-1.327872
120	1	0	-9.343668	3.066183	3.048445
121	1	0	-9.676151	2.133500	5.293484
122	1	0	-9.142660	-1.822316	3.750766
123	1	0	-9.566665	-1.579963	6.065683
124	1	0	-8.839187	-0.127322	6.765235
125	1	0	-10.575971	-0.185337	6.475642
126	6	0	-10.171300	4.363208	-2.527502
127	6	0	-9.847367	3.623893	-1.407572
128	6	0	-8.659880	3.866266	-0.677534
129	6	0	-7.803477	4.921546	-1.116005
130	6	0	-8.163897	5.652576	-2.270405
131	6	0	-9.322518	5.393323	-2.986251
132	6	0	-8.316969	3.098784	0.512329

133	6	0	-6.599986	5.234304	-0.357081
134	6	0	-6.466674	4.661460	0.937843
135	6	0	-7.323843	3.585972	1.326491
136	6	0	-5.375244	5.046084	1.751040
137	6	0	-4.369406	5.845539	1.253421
138	6	0	-4.393342	6.270761	-0.098609
139	6	0	-5.529452	6.006219	-0.860393
140	6	0	-9.689567	6.197712	-4.209558
141	1	0	-3.496939	6.064617	1.861123
142	1	0	-5.552836	6.345033	-1.891113
143	1	0	-5.301453	4.639274	2.756139
144	1	0	-7.062139	3.050701	2.233138
145	1	0	-7.530569	6.473861	-2.591185
146	1	0	-10.524959	2.851198	-1.061132
147	1	0	-11.099910	4.159553	-3.055050
148	1	0	-10.667335	6.678961	-4.091620
149	1	0	-8.952963	6.980049	-4.410900
150	1	0	-9.752921	5.560427	-5.099517
151	6	0	11.819401	-0.800694	0.689258
152	6	0	10.705175	-1.561173	0.399085
153	6	0	9.628690	-1.034606	-0.352647
154	6	0	9.723364	0.310340	-0.826023
155	6	0	10.875948	1.061127	-0.501498
156	6	0	11.921064	0.536036	0.243471
157	6	0	8.459730	-1.834374	-0.673601
158	6	0	8.651877	0.861604	-1.645694
159	6	0	7.703143	-0.049860	-2.185314
160	6	0	7.619779	-1.373962	-1.655121
161	6	0	6.736726	0.421376	-3.102322
162	6	0	6.597777	1.768773	-3.346045
163	6	0	7.395863	2.711640	-2.648174
164	6	0	8.450371	2.244253	-1.866574
165	6	0	13.150079	1.352972	0.560759
166	1	0	6.048189	-0.289110	-3.552083
167	1	0	5.793481	2.124840	-3.981993
168	1	0	9.077144	2.965827	-1.351995
169	1	0	6.759938	-1.971580	-1.941887
170	1	0	10.644871	-2.588762	0.743691
171	1	0	12.635516	-1.237499	1.259463
172	1	0	10.965996	2.074424	-0.881192
173	1	0	13.288599	1.458585	1.643257
174	1	0	14.056651	0.877814	0.168282
175	1	0	13.086187	2.356774	0.132452
176	6	0	7.909273	-2.007953	3.700038
177	6	0	8.150636	-1.983165	2.341736
178	6	0	7.726057	-3.032301	1.488266
179	6	0	6.946138	-4.076604	2.071638
180	6	0	6.741123	-4.083967	3.470286
181	6	0	7.219438	-3.082968	4.299025
182	6	0	8.012884	-3.062111	0.056584
183	6	0	6.305146	-5.055564	1.207189
184	6	0	6.724606	-5.146443	-0.146827
185	6	0	7.615159	-4.156509	-0.671674
186	6	0	6.089757	-6.090336	-0.991009
187	6	0	4.963148	-6.771234	-0.576459
188	6	0	4.429233	-6.562373	0.721367
189	6	0	5.168836	-5.784802	1.610290
190	6	0	7.009613	-3.124052	5.792716
191	1	0	4.421541	-7.389459	-1.285608

192	1	0	4.787578	-5.642126	2.614199
193	1	0	6.437556	-6.194272	-2.015603
194	1	0	7.856624	-4.201632	-1.730289
195	1	0	6.202114	-4.913768	3.916834
196	1	0	8.686787	-1.142225	1.925116
197	1	0	8.264432	-1.187805	4.319236
198	1	0	6.498685	-2.221455	6.147483
199	1	0	6.409787	-3.988388	6.090139
200	1	0	7.965337	-3.180318	6.327256

Table S28. Cartesian coordinate of *E,R,E,S,E,S,Z,R* (26)

SCF Done: E(RB3LYP) = -4621.32883562 A.U. after 5 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.243543	-10.817038	-0.455667
2	6	0	-1.159518	-9.977995	-0.610429
3	6	0	-1.300497	-8.689078	-1.176257
4	6	0	-2.601959	-8.259850	-1.586757
5	6	0	-3.686382	-9.149441	-1.413134
6	6	0	-3.535137	-10.412449	-0.860736
7	6	0	-0.155539	-7.821044	-1.366239
8	6	0	-2.773365	-6.930137	-2.163206
9	6	0	-1.599018	-6.213554	-2.524732
10	6	0	-0.316831	-6.686734	-2.115133
11	6	0	-1.722048	-4.949134	-3.138838
12	6	0	-2.949703	-4.346668	-3.268983
13	6	0	-4.129327	-4.979287	-2.793813
14	6	0	-4.023385	-6.283059	-2.306350
15	6	0	-4.709595	-11.347337	-0.702100
16	1	0	-0.820588	-4.419696	-3.435300
17	1	0	-3.000279	-3.333693	-3.649990
18	1	0	-4.921658	-6.785781	-1.964024
19	1	0	0.538005	-6.040514	-2.290414
20	1	0	-0.169795	-10.305065	-0.306557
21	1	0	-2.102832	-11.806326	-0.027363
22	1	0	-4.673647	-8.848330	-1.749991
23	1	0	-4.553526	-12.280444	-1.255875
24	1	0	-4.860506	-11.621602	0.348633
25	1	0	-5.635425	-10.893734	-1.065844
26	6	0	0.326476	-7.619753	2.971247
27	6	0	0.184347	-7.801989	1.611119
28	6	0	1.297594	-7.756326	0.736079
29	6	0	2.571526	-7.444918	1.295759
30	6	0	2.682739	-7.281863	2.695614
31	6	0	1.592208	-7.372807	3.544719
32	6	0	1.177836	-7.969675	-0.700254
33	6	0	3.710957	-7.251441	0.412536
34	6	0	3.602036	-7.658993	-0.943537
35	6	0	2.316718	-8.022104	-1.462820
36	6	0	4.736297	-7.515914	-1.780754
37	6	0	5.864769	-6.848319	-1.351193
38	6	0	5.914546	-6.263289	-0.058149
39	6	0	4.860275	-6.541142	0.811029
40	6	0	1.738092	-7.212763	5.038223
41	1	0	6.701604	-6.727210	-2.031707
42	1	0	4.854607	-6.077623	1.788610

43	1	0	4.684975	-7.889580	-2.800298
44	1	0	2.231547	-8.206513	-2.530584
45	1	0	3.661851	-7.099972	3.127499
46	1	0	-0.800614	-7.995925	1.207149
47	1	0	-0.549916	-7.674826	3.612337
48	1	0	1.424744	-8.119646	5.568751
49	1	0	2.773214	-7.001796	5.319829
50	1	0	1.114351	-6.392606	5.412483
51	6	0	-1.939679	7.482334	-3.880325
52	6	0	-1.404281	7.751894	-2.638075
53	6	0	-2.217055	7.839496	-1.480116
54	6	0	-3.607599	7.552732	-1.624166
55	6	0	-4.125479	7.306137	-2.916631
56	6	0	-3.326315	7.278460	-4.047102
57	6	0	-1.681075	8.167704	-0.164794
58	6	0	-4.443233	7.448789	-0.437876
59	6	0	-3.921882	7.894682	0.806608
60	6	0	-2.544846	8.278024	0.894707
61	6	0	-4.730702	7.780368	1.964310
62	6	0	-5.928268	7.095747	1.932017
63	6	0	-6.385695	6.505058	0.727086
64	6	0	-5.677083	6.764017	-0.443001
65	6	0	-3.904872	7.031407	-5.418742
66	1	0	-4.356981	8.176592	2.905075
67	1	0	-6.499878	6.957491	2.845196
68	1	0	-6.005309	6.280269	-1.355483
69	1	0	-2.152136	8.547160	1.871706
70	1	0	-0.337435	7.907737	-2.550465
71	1	0	-1.283321	7.433629	-4.745740
72	1	0	-5.192690	7.146821	-3.033170
73	1	0	-3.736854	7.888166	-6.082016
74	1	0	-3.438058	6.162102	-5.896357
75	1	0	-4.982165	6.850554	-5.373200
76	6	0	1.271839	10.990299	-1.894216
77	6	0	0.353432	10.170763	-1.271614
78	6	0	0.756616	9.003566	-0.580930
79	6	0	2.148682	8.688077	-0.529272
80	6	0	3.059156	9.550168	-1.182445
81	6	0	2.651605	10.688286	-1.861207
82	6	0	-0.206255	8.148639	0.087921
83	6	0	2.591576	7.508162	0.202972
84	6	0	1.649644	6.856670	1.047171
85	6	0	0.262572	7.189189	0.946370
86	6	0	2.078199	5.783950	1.861621
87	6	0	3.353978	5.276971	1.749833
88	6	0	4.254015	5.802443	0.788879
89	6	0	3.877230	6.935188	0.070802
90	6	0	3.646536	11.599955	-2.537560
91	1	0	3.645310	4.403663	2.324959
92	1	0	4.574150	7.344997	-0.653116
93	1	0	1.362182	5.316496	2.532433
94	1	0	-0.445728	6.563746	1.481790
95	1	0	4.121699	9.335149	-1.124829
96	1	0	-0.702423	10.420618	-1.298122
97	1	0	0.932638	11.885668	-2.409197
98	1	0	3.602573	12.614348	-2.124164
99	1	0	4.670181	11.234686	-2.419687
100	1	0	3.442082	11.684113	-3.611376
101	6	0	9.953642	1.719336	3.901105

102	6	0	9.720679	1.090929	2.694324
103	6	0	8.804870	1.613507	1.750778
104	6	0	8.135323	2.835290	2.066777
105	6	0	8.393645	3.445933	3.314870
106	6	0	9.280648	2.913382	4.237660
107	6	0	8.563311	0.962385	0.470308
108	6	0	7.229748	3.434091	1.094857
109	6	0	7.244168	2.916507	-0.229773
110	6	0	7.896776	1.674015	-0.496815
111	6	0	6.472698	3.555999	-1.227786
112	6	0	5.609239	4.580203	-0.906899
113	6	0	5.451873	4.991257	0.440552
114	6	0	6.296797	4.448265	1.406209
115	6	0	9.546420	3.594367	5.558253
116	1	0	6.518718	3.180204	-2.246519
117	1	0	4.966683	5.009821	-1.669087
118	1	0	6.184561	4.774891	2.434888
119	1	0	7.721446	1.224226	-1.468295
120	1	0	10.264649	0.185759	2.447585
121	1	0	10.675519	1.297087	4.595873
122	1	0	7.908707	4.388392	3.549739
123	1	0	8.968140	4.516829	5.656731
124	1	0	9.284707	2.943296	6.400668
125	1	0	10.606814	3.849081	5.669266
126	6	0	10.152286	-0.786314	-3.264134
127	6	0	9.813844	-0.261947	-2.032875
128	6	0	9.139666	-1.035195	-1.058110
129	6	0	8.832763	-2.393487	-1.371976
130	6	0	9.187421	-2.894172	-2.644834
131	6	0	9.833862	-2.120789	-3.596443
132	6	0	8.788837	-0.494886	0.248821
133	6	0	8.191039	-3.234035	-0.370876
134	6	0	8.151495	-2.756835	0.966597
135	6	0	8.432070	-1.382179	1.236002
136	6	0	7.664585	-3.619191	1.977991
137	6	0	7.082792	-4.825824	1.662607
138	6	0	6.906160	-5.217720	0.308138
139	6	0	7.530482	-4.444478	-0.672106
140	6	0	10.213963	-2.683601	-4.944313
141	1	0	6.705212	-5.456083	2.460557
142	1	0	7.402038	-4.714286	-1.713761
143	1	0	7.710448	-3.291814	3.013430
144	1	0	8.193330	-1.014072	2.228404
145	1	0	8.981700	-3.935074	-2.874737
146	1	0	10.085603	0.760100	-1.792648
147	1	0	10.684275	-0.168176	-3.983136
148	1	0	11.295017	-2.617750	-5.113578
149	1	0	9.923780	-3.733568	-5.036952
150	1	0	9.729505	-2.129486	-5.756928
151	6	0	-9.859321	-3.504316	2.062715
152	6	0	-9.516496	-2.274742	1.538431
153	6	0	-8.600319	-2.161210	0.466886
154	6	0	-8.039694	-3.356053	-0.078189
155	6	0	-8.405121	-4.596261	0.491674
156	6	0	-9.300155	-4.694659	1.546423
157	6	0	-8.242605	-0.871925	-0.098176
158	6	0	-7.133980	-3.267881	-1.215682
159	6	0	-7.091578	-2.038539	-1.927598
160	6	0	-7.629764	-0.859503	-1.325730

161	6	0	-6.344170	-1.970234	-3.125865
162	6	0	-5.513919	-3.002251	-3.496811
163	6	0	-5.348605	-4.138380	-2.659610
164	6	0	-6.223493	-4.284705	-1.581951
165	6	0	-9.692556	-6.032982	2.123774
166	1	0	-6.385710	-1.061758	-3.720962
167	1	0	-4.928018	-2.914843	-4.405577
168	1	0	-6.108675	-5.141132	-0.926176
169	1	0	-7.391437	0.092076	-1.791292
170	1	0	-9.957427	-1.369327	1.943557
171	1	0	-10.576111	-3.560586	2.878174
172	1	0	-8.001968	-5.509077	0.063103
173	1	0	-9.450997	-6.091760	3.191512
174	1	0	-10.771085	-6.206110	2.030698
175	1	0	-9.177104	-6.854179	1.618657
176	6	0	-6.574931	-0.143659	3.909015
177	6	0	-7.158024	-0.383510	2.681862
178	6	0	-7.685611	0.665563	1.887069
179	6	0	-7.500850	1.999856	2.358933
180	6	0	-6.926477	2.206882	3.634069
181	6	0	-6.474909	1.165099	4.426146
182	6	0	-8.356554	0.441605	0.608833
183	6	0	-7.823954	3.117420	1.486877
184	6	0	-8.588476	2.872514	0.315317
185	6	0	-8.875309	1.521401	-0.062772
186	6	0	-8.874789	3.959746	-0.548154
187	6	0	-8.279016	5.191737	-0.365154
188	6	0	-7.385071	5.403840	0.714398
189	6	0	-7.245672	4.391624	1.659954
190	6	0	-5.884443	1.407996	5.793256
191	1	0	-8.450448	5.989388	-1.082290
192	1	0	-6.531583	4.536873	2.461829
193	1	0	-9.509957	3.788097	-1.413562
194	1	0	-9.402263	1.356831	-0.999012
195	1	0	-6.847692	3.220210	4.014904
196	1	0	-7.216135	-1.402408	2.326775
197	1	0	-6.192899	-0.979743	4.489634
198	1	0	-4.878160	0.980844	5.872951
199	1	0	-5.814518	2.476101	6.015992
200	1	0	-6.492029	0.941834	6.578101

Table S29. Cartesian coordinate of *E,R,Z,R,E,S,Z,S* (27)

SCF Done: E(RB3LYP) = -4621.32875230 A.U. after 6 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.061373	6.621548	3.045785
2	6	0	1.373590	6.958881	1.898686
3	6	0	2.008374	6.990819	0.631836
4	6	0	3.372460	6.575384	0.564898
5	6	0	4.052412	6.261378	1.764221
6	6	0	3.432206	6.288693	3.001914
7	6	0	1.315147	7.386789	-0.588194
8	6	0	4.008385	6.411169	-0.733117
9	6	0	3.350903	6.921259	-1.884917
10	6	0	2.020094	7.435742	-1.763897
11	6	0	3.955682	6.740078	-3.153297

12	6	0	5.070180	5.940535	-3.302773
13	6	0	5.653477	5.304801	-2.178115
14	6	0	5.158563	5.613354	-0.914371
15	6	0	4.183748	5.966680	4.270184
16	1	0	3.480012	7.178030	-4.027127
17	1	0	5.474804	5.752432	-4.293120
18	1	0	5.577951	5.090260	-0.062928
19	1	0	1.513615	7.755345	-2.670772
20	1	0	0.324838	7.212757	1.972958
21	1	0	1.539921	6.619034	3.999837
22	1	0	5.105184	6.001576	1.718662
23	1	0	3.708473	5.142819	4.815065
24	1	0	5.217477	5.678461	4.061547
25	1	0	4.206430	6.827353	4.949224
26	6	0	-1.151809	10.375167	1.593180
27	6	0	-0.391129	9.509001	0.835481
28	6	0	-0.971392	8.394543	0.184828
29	6	0	-2.378189	8.183624	0.318306
30	6	0	-3.123238	9.090295	1.106393
31	6	0	-2.542253	10.175713	1.744091
32	6	0	-0.177115	7.493316	-0.629444
33	6	0	-3.007231	7.064638	-0.372413
34	6	0	-2.242224	6.378730	-1.356445
35	6	0	-0.833341	6.603816	-1.439317
36	6	0	-2.857679	5.370463	-2.131889
37	6	0	-4.139017	4.950471	-1.854715
38	6	0	-4.856599	5.501178	-0.762382
39	6	0	-4.301968	6.579633	-0.076052
40	6	0	-3.364485	11.137570	2.566950
41	1	0	-4.569018	4.119328	-2.404321
42	1	0	-4.859325	7.011223	0.749063
43	1	0	-2.277629	4.878570	-2.908222
44	1	0	-0.256293	5.946358	-2.082784
45	1	0	-4.197287	8.956092	1.189331
46	1	0	0.674451	9.680901	0.721266
47	1	0	-0.678958	11.228873	2.072265
48	1	0	-4.422304	10.861616	2.568108
49	1	0	-3.023286	11.161822	3.608647
50	1	0	-3.284778	12.160632	2.181413
51	6	0	0.152981	-6.295746	-3.915457
52	6	0	-0.179687	-6.665792	-2.628983
53	6	0	0.801645	-7.094837	-1.700331
54	6	0	2.165874	-7.061170	-2.117130
55	6	0	2.467700	-6.699517	-3.449960
56	6	0	1.492044	-6.328437	-4.360031
57	6	0	0.469273	-7.547371	-0.354440
58	6	0	3.213842	-7.337066	-1.147531
59	6	0	2.855712	-7.902034	0.106321
60	6	0	1.469342	-8.030563	0.448430
61	6	0	3.877050	-8.148604	1.057503
62	6	0	5.167185	-7.702056	0.851920
63	6	0	5.505029	-7.005086	-0.335034
64	6	0	4.544073	-6.909429	-1.337709
65	6	0	1.835522	-5.964218	-5.783575
66	1	0	3.613394	-8.631522	1.995092
67	1	0	5.918423	-7.837511	1.624663
68	1	0	4.789341	-6.340597	-2.226716
69	1	0	1.223245	-8.403785	1.439073
70	1	0	-1.217069	-6.629668	-2.322725

71	1	0	-0.630397	-5.979890	-4.600104
72	1	0	3.500676	-6.729661	-3.781582
73	1	0	1.377315	-6.661901	-6.494688
74	1	0	1.467643	-4.963298	-6.036955
75	1	0	2.915682	-5.977588	-5.951939
76	6	0	-0.300825	-4.829281	2.945321
77	6	0	-0.070380	-5.718434	1.916461
78	6	0	-1.134944	-6.347543	1.222860
79	6	0	-2.466008	-5.973444	1.575148
80	6	0	-2.664804	-5.078213	2.651301
81	6	0	-1.614118	-4.507791	3.349872
82	6	0	-0.916449	-7.335309	0.172020
83	6	0	-3.579768	-6.472381	0.784655
84	6	0	-3.344952	-7.517416	-0.149623
85	6	0	-2.000753	-7.950691	-0.396691
86	6	0	-4.427608	-7.982753	-0.936901
87	6	0	-5.652098	-7.345288	-0.917098
88	6	0	-5.862423	-6.220070	-0.081235
89	6	0	-4.846222	-5.852126	0.795772
90	6	0	-1.851005	-3.564773	4.503770
91	1	0	-6.447859	-7.678677	-1.577032
92	1	0	-4.991246	-4.961881	1.395932
93	1	0	-4.259797	-8.813955	-1.617102
94	1	0	-1.843482	-8.713972	-1.154197
95	1	0	-3.678277	-4.838011	2.955778
96	1	0	0.949980	-5.942489	1.634163
97	1	0	0.543493	-4.373227	3.456443
98	1	0	-2.918058	-3.398175	4.673593
99	1	0	-1.420434	-3.956394	5.432951
100	1	0	-1.383749	-2.590029	4.321534
101	6	0	-10.271730	-1.276274	3.740477
102	6	0	-10.070481	-0.678690	2.512291
103	6	0	-9.437678	-1.365985	1.449903
104	6	0	-9.017891	-2.712133	1.672768
105	6	0	-9.235425	-3.289383	2.943888
106	6	0	-9.848434	-2.601334	3.979914
107	6	0	-9.239334	-0.750453	0.144994
108	6	0	-8.390453	-3.456694	0.589218
109	6	0	-8.490143	-2.922840	-0.725208
110	6	0	-8.904389	-1.567095	-0.907501
111	6	0	-7.991195	-3.678742	-1.811880
112	6	0	-7.270178	-4.833200	-1.598366
113	6	0	-6.991536	-5.272950	-0.279409
114	6	0	-7.614208	-4.620037	0.782974
115	6	0	-10.082242	-3.246444	5.324340
116	1	0	-8.111445	-3.290401	-2.819812
117	1	0	-6.813757	-5.349187	-2.437365
118	1	0	-7.422568	-4.972134	1.791343
119	1	0	-8.776526	-1.141256	-1.897265
120	1	0	-10.420741	0.333979	2.343698
121	1	0	-10.776481	-0.724753	4.529861
122	1	0	-8.946764	-4.323168	3.107552
123	1	0	-9.556055	-2.707021	6.120823
124	1	0	-11.146333	-3.245039	5.587395
125	1	0	-9.735243	-4.283045	5.337297
126	6	0	-10.877641	1.516766	-3.284661
127	6	0	-10.500843	0.864934	-2.127407
128	6	0	-9.510626	1.396315	-1.268137
129	6	0	-8.912321	2.643993	-1.619038

130	6	0	-9.318781	3.280044	-2.813375
131	6	0	-10.282586	2.742605	-3.652919
132	6	0	-9.119260	0.724713	-0.036410
133	6	0	-7.913839	3.233919	-0.737435
134	6	0	-7.787816	2.697991	0.573994
135	6	0	-8.390256	1.438931	0.882857
136	6	0	-6.908956	3.323447	1.489050
137	6	0	-6.064996	4.334033	1.081969
138	6	0	-6.044013	4.750407	-0.272928
139	6	0	-7.008419	4.239515	-1.139827
140	6	0	-10.706903	3.447722	-4.918191
141	1	0	-5.331645	4.739780	1.771919
142	1	0	-7.004969	4.570992	-2.173178
143	1	0	-6.847482	2.938404	2.503521
144	1	0	-8.107354	0.973390	1.821216
145	1	0	-8.888355	4.243808	-3.067735
146	1	0	-10.984366	-0.066373	-1.852930
147	1	0	-11.653808	1.088520	-3.914109
148	1	0	-10.197641	4.408365	-5.031701
149	1	0	-10.481464	2.842729	-5.804487
150	1	0	-11.786600	3.636228	-4.926861
151	6	0	11.559265	1.674294	1.139353
152	6	0	10.774096	0.661410	0.628412
153	6	0	9.657133	0.938580	-0.194467
154	6	0	9.358114	2.301804	-0.500532
155	6	0	10.181643	3.312106	0.046218
156	6	0	11.270740	3.028021	0.856085
157	6	0	8.838526	-0.124433	-0.748480
158	6	0	8.235510	2.612470	-1.376549
159	6	0	7.658098	1.542267	-2.114236
160	6	0	7.965912	0.193231	-1.756869
161	6	0	6.656914	1.823958	-3.070984
162	6	0	6.127456	3.089490	-3.184536
163	6	0	6.552718	4.127443	-2.316281
164	6	0	7.638267	3.890514	-1.475552
165	6	0	12.144916	4.125349	1.413041
166	1	0	6.253664	1.007795	-3.664615
167	1	0	5.298969	3.271977	-3.861499
168	1	0	7.978224	4.692093	-0.827644
169	1	0	7.371606	-0.593540	-2.211708
170	1	0	11.012802	-0.374320	0.848773
171	1	0	12.417790	1.429176	1.759670
172	1	0	9.978820	4.348676	-0.205414
173	1	0	12.144850	4.115869	2.509438
174	1	0	13.186628	4.005834	1.093350
175	1	0	11.806002	5.112333	1.087269
176	6	0	7.923985	-1.112988	3.437942
177	6	0	8.284290	-0.811773	2.140794
178	6	0	8.354008	-1.808664	1.135545
179	6	0	7.947885	-3.130505	1.489726
180	6	0	7.609917	-3.408334	2.834173
181	6	0	7.603469	-2.433693	3.817680
182	6	0	8.776575	-1.528145	-0.232677
183	6	0	7.812206	-4.139545	0.451051
184	6	0	8.361101	-3.875851	-0.832427
185	6	0	8.871369	-2.569566	-1.121506
186	6	0	8.209831	-4.849592	-1.850902
187	6	0	7.395390	-5.948643	-1.669388
188	6	0	6.709711	-6.139616	-0.443447

189	6	0	6.999317	-5.281204	0.613597
190	6	0	7.259186	-2.757469	5.250693
191	1	0	7.230655	-6.643796	-2.487557
192	1	0	6.446156	-5.403862	1.537429
193	1	0	8.681449	-4.676594	-2.814930
194	1	0	9.213652	-2.370097	-2.133525
195	1	0	7.360041	-4.427374	3.112271
196	1	0	8.527642	0.211827	1.891733
197	1	0	7.894099	-0.319951	4.181184
198	1	0	6.988709	-3.810007	5.370422
199	1	0	8.103232	-2.550684	5.919351
200	1	0	6.416752	-2.151379	5.603718

Table S30. Cartesian coordinate of *E,R,E,S,E,R,E,S* (28)

SCF Done: E(RB3LYP) = -4621.32840465 A.U. after 5 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.410856	1.704645	1.065373
2	6	0	-10.561604	0.762944	0.522163
3	6	0	-9.318944	1.131184	-0.045291
4	6	0	-8.957140	2.513356	-0.055583
5	6	0	-9.851571	3.448064	0.513999
6	6	0	-11.064551	3.074329	1.072081
7	6	0	-8.432321	0.145285	-0.635245
8	6	0	-7.697843	2.923165	-0.664994
9	6	0	-7.002805	1.966820	-1.456168
10	6	0	-7.385177	0.590986	-1.398771
11	6	0	-5.844463	2.363903	-2.161379
12	6	0	-5.303469	3.616926	-1.980951
13	6	0	-5.881914	4.524633	-1.057499
14	6	0	-7.093525	4.184696	-0.458706
15	6	0	-12.008077	4.095200	1.660245
16	1	0	-5.341714	1.638393	-2.795414
17	1	0	-4.367433	3.878951	-2.463700
18	1	0	-7.545209	4.886814	0.234695
19	1	0	-6.731847	-0.132262	-1.877640
20	1	0	-10.845151	-0.284764	0.516493
21	1	0	-12.364006	1.392108	1.484637
22	1	0	-9.598921	4.503510	0.484058
23	1	0	-12.189984	3.901695	2.724014
24	1	0	-11.609883	5.109164	1.568374
25	1	0	-12.983390	4.070901	1.160435
26	6	0	-8.251606	-1.643646	3.372571
27	6	0	-8.378524	-1.089529	2.115661
28	6	0	-8.326873	-1.883580	0.942690
29	6	0	-8.048322	-3.274915	1.098612
30	6	0	-7.948830	-3.812252	2.402621
31	6	0	-8.058841	-3.031504	3.540975
32	6	0	-8.503452	-1.330179	-0.394901
33	6	0	-7.797188	-4.090920	-0.079251
34	6	0	-8.109491	-3.556883	-1.358339
35	6	0	-8.495050	-2.182439	-1.469938
36	6	0	-7.849214	-4.343498	-2.507729
37	6	0	-7.144879	-5.526408	-2.415848
38	6	0	-6.684764	-5.992088	-1.158526
39	6	0	-7.091529	-5.311300	-0.014395

40	6	0	-7.970822	-3.631245	4.922885
41	1	0	-6.888947	-6.078206	-3.315724
42	1	0	-6.707261	-5.645392	0.942351
43	1	0	-8.143812	-3.960888	-3.481642
44	1	0	-8.654388	-1.777916	-2.465963
45	1	0	-7.795967	-4.880446	2.519729
46	1	0	-8.529749	-0.022149	2.028230
47	1	0	-8.308340	-1.000764	4.247569
48	1	0	-7.758234	-4.702918	4.882290
49	1	0	-7.180996	-3.153497	5.514011
50	1	0	-8.908287	-3.496960	5.475633
51	6	0	11.410566	1.707019	-1.065148
52	6	0	10.561509	0.765103	-0.522000
53	6	0	9.318704	1.133025	0.045341
54	6	0	8.956543	2.515106	0.055598
55	6	0	9.850781	3.450037	-0.513920
56	6	0	11.063896	3.076610	-1.071916
57	6	0	8.432299	0.146901	0.635237
58	6	0	7.697105	2.924606	0.664925
59	6	0	7.002232	1.968076	1.456020
60	6	0	7.384959	0.592342	1.398652
61	6	0	5.843735	2.364856	2.161149
62	6	0	5.302468	3.617761	1.980731
63	6	0	5.880784	4.525640	1.057363
64	6	0	7.092509	4.186007	0.458639
65	6	0	12.007104	4.097702	-1.660207
66	1	0	5.341104	1.639201	2.795111
67	1	0	4.366341	3.879567	2.463421
68	1	0	7.544070	4.888252	-0.234713
69	1	0	6.731764	-0.131071	1.877455
70	1	0	10.845340	-0.282527	-0.516268
71	1	0	12.363845	1.394728	-1.484298
72	1	0	9.597868	4.505419	-0.483993
73	1	0	12.983124	4.072303	-1.161853
74	1	0	12.187359	3.905382	-2.724480
75	1	0	11.609547	5.111756	-1.566578
76	6	0	8.252515	-1.642347	-3.372510
77	6	0	8.379177	-1.088117	-2.115623
78	6	0	8.327557	-1.882094	-0.942600
79	6	0	8.049308	-3.273502	-1.098458
80	6	0	7.950066	-3.810945	-2.402442
81	6	0	8.060063	-3.030258	-3.540839
82	6	0	8.503833	-1.328557	0.394968
83	6	0	7.798206	-4.089476	0.079431
84	6	0	8.110264	-3.555282	1.358512
85	6	0	8.495509	-2.180752	1.470062
86	6	0	7.850031	-4.341872	2.507934
87	6	0	7.145926	-5.524916	2.416067
88	6	0	6.686024	-5.990774	1.158727
89	6	0	7.092791	-5.310004	0.014592
90	6	0	7.972525	-3.630150	-4.922713
91	1	0	6.890016	-6.076707	3.315952
92	1	0	6.708701	-5.644246	-0.942173
93	1	0	8.144466	-3.959135	3.481847
94	1	0	8.654646	-1.776126	2.466077
95	1	0	7.797401	-4.879175	-2.519492
96	1	0	8.530147	-0.020695	-2.028249
97	1	0	8.309195	-0.999513	-4.247546
98	1	0	8.910834	-3.497581	-5.474458

99	1	0	7.758116	-4.701461	-4.882120
100	1	0	7.184170	-3.151194	-5.514809
101	6	0	-0.331806	-6.035201	3.523189
102	6	0	-0.423531	-6.668396	2.301140
103	6	0	0.718815	-7.193990	1.646310
104	6	0	1.988691	-6.974964	2.258866
105	6	0	2.042693	-6.345172	3.523326
106	6	0	0.911130	-5.882741	4.173886
107	6	0	0.642821	-7.924439	0.385170
108	6	0	3.198147	-7.341482	1.539991
109	6	0	3.087735	-8.162669	0.385667
110	6	0	1.787387	-8.472369	-0.133159
111	6	0	4.266491	-8.492597	-0.328945
112	6	0	5.476127	-7.900657	-0.023334
113	6	0	5.569919	-6.966619	1.038257
114	6	0	4.451082	-6.770381	1.842847
115	6	0	0.990238	-5.228441	5.531282
116	1	0	4.191594	-9.164616	-1.180154
117	1	0	6.352312	-8.110025	-0.630219
118	1	0	4.511515	-6.025461	2.627375
119	1	0	1.731401	-9.052779	-1.050276
120	1	0	-1.394160	-6.767025	1.833268
121	1	0	-1.233511	-5.652980	3.995396
122	1	0	3.004424	-6.233670	4.013834
123	1	0	0.567607	-4.217235	5.509561
124	1	0	0.423825	-5.794939	6.279907
125	1	0	2.023323	-5.152810	5.881019
126	6	0	0.332969	-6.035838	-3.523615
127	6	0	0.424862	-6.668858	-2.301483
128	6	0	-0.717378	-7.194415	-1.646454
129	6	0	-1.987337	-6.975601	-2.258918
130	6	0	-2.041517	-6.345929	-3.523425
131	6	0	-0.910050	-5.883505	-4.174170
132	6	0	-0.641188	-7.924621	-0.385191
133	6	0	-3.196692	-7.342226	-1.539917
134	6	0	-3.086067	-8.163275	-0.385517
135	6	0	-1.785631	-8.472658	0.133294
136	6	0	-4.264722	-8.493378	0.329179
137	6	0	-5.474489	-7.901697	0.023577
138	6	0	-5.568501	-6.967751	-1.038074
139	6	0	-4.449748	-6.771381	-1.842748
140	6	0	-0.989353	-5.229389	-5.531644
141	1	0	-6.350614	-8.111203	0.630501
142	1	0	-4.510382	-6.026554	-2.627349
143	1	0	-4.189654	-9.165320	1.180434
144	1	0	-1.729514	-9.052852	1.050539
145	1	0	-3.003304	-6.234492	-4.013834
146	1	0	1.395544	-6.767359	-1.833693
147	1	0	1.234605	-5.653667	-3.995994
148	1	0	-0.423711	-5.796430	-6.280447
149	1	0	-2.022553	-5.153097	-5.880898
150	1	0	-0.565986	-4.218488	-5.510307
151	6	0	-0.910440	9.719975	-3.674429
152	6	0	-0.450176	9.419271	-2.408202
153	6	0	-1.193870	8.601443	-1.525222
154	6	0	-2.454443	8.100401	-1.970506
155	6	0	-2.890609	8.423641	-3.275047
156	6	0	-2.146210	9.216612	-4.134966
157	6	0	-0.724090	8.294236	-0.181495

158	6	0	-3.261971	7.287101	-1.071171
159	6	0	-2.900903	7.262167	0.304389
160	6	0	-1.622559	7.758104	0.708161
161	6	0	-3.733238	6.576982	1.220162
162	6	0	-4.789454	5.809642	0.779296
163	6	0	-5.047142	5.671057	-0.607862
164	6	0	-4.321372	6.458098	-1.500217
165	6	0	-2.640644	9.557090	-5.519780
166	1	0	-3.478395	6.597281	2.276507
167	1	0	-5.361775	5.216710	1.485879
168	1	0	-4.530468	6.366024	-2.561126
169	1	0	-1.307941	7.543633	1.724267
170	1	0	0.492855	9.832661	-2.067345
171	1	0	-0.320737	10.364934	-4.321232
172	1	0	-3.861634	8.069428	-3.606771
173	1	0	-2.708115	10.641641	-5.663470
174	1	0	-1.959642	9.175021	-6.289532
175	1	0	-3.629907	9.131831	-5.708797
176	6	0	0.908407	9.720095	3.674364
177	6	0	0.448186	9.419326	2.408136
178	6	0	1.192000	8.601616	1.525150
179	6	0	2.452654	8.100769	1.970424
180	6	0	2.888770	8.424063	3.274968
181	6	0	2.144246	9.216903	4.134900
182	6	0	0.722264	8.294344	0.181422
183	6	0	3.260319	7.287616	1.071079
184	6	0	2.899243	7.262621	-0.304478
185	6	0	1.620811	7.758350	-0.708237
186	6	0	3.731682	6.577584	-1.220263
187	6	0	4.788046	5.810436	-0.779410
188	6	0	5.045780	5.671907	0.607742
189	6	0	4.319875	6.458805	1.500112
190	6	0	2.638572	9.557323	5.519768
191	1	0	5.360475	5.217613	-1.485998
192	1	0	4.528996	6.366752	2.561018
193	1	0	3.476818	6.597832	-2.276604
194	1	0	1.306219	7.543822	-1.724339
195	1	0	3.859854	8.070003	3.606683
196	1	0	-0.494902	9.832587	2.067276
197	1	0	0.318614	10.364972	4.321167
198	1	0	1.958236	9.173986	6.289485
199	1	0	3.628409	9.133206	5.708348
200	1	0	2.704691	10.641880	5.663996

Table S31. Cartesian coordinate of *Z,R,Z,R,Z,R,Z,R* (29)

SCF Done: E(RB3LYP) = -4621.32672366 A.U. after 14 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.257927	6.058561	3.022513
2	6	0	3.984061	6.186119	1.856675
3	6	0	3.465908	6.866990	0.726560
4	6	0	2.122063	7.342612	0.801830
5	6	0	1.417389	7.217773	2.021288
6	6	0	1.960195	6.601164	3.135826
7	6	0	4.229318	7.055718	-0.502076
8	6	0	1.481659	7.871251	-0.392313

9	6	0	2.285835	8.157353	-1.528238
10	6	0	3.664641	7.771681	-1.527445
11	6	0	1.660037	8.645708	-2.701974
12	6	0	0.285026	8.683630	-2.812546
13	6	0	-0.533734	8.262588	-1.734931
14	6	0	0.078490	7.939402	-0.527483
15	6	0	1.196499	6.495513	4.432904
16	6	0	8.046819	7.360272	1.776463
17	6	0	6.909649	7.339878	0.995536
18	6	0	6.667444	6.294556	0.073495
19	6	0	7.637871	5.252580	-0.044980
20	6	0	8.787308	5.304932	0.775975
21	6	0	9.010445	6.331819	1.680430
22	6	0	5.480711	6.277198	-0.762288
23	6	0	7.431565	4.184512	-1.014898
24	6	0	6.416837	4.368346	-1.994184
25	6	0	5.450414	5.406844	-1.821012
26	6	0	6.276622	3.417460	-3.030300
27	6	0	7.000736	2.246883	-3.015015
28	6	0	7.874814	1.956051	-1.936376
29	6	0	8.122558	2.950731	-0.992920
30	6	0	10.254165	6.371562	2.534824
31	6	0	-8.048179	-7.357361	1.778978
32	6	0	-6.911063	-7.338181	0.997942
33	6	0	-6.668513	-6.293877	0.074810
34	6	0	-7.638543	-5.251662	-0.044522
35	6	0	-8.788039	-5.302869	0.776416
36	6	0	-9.011453	-6.328727	1.681982
37	6	0	-5.481772	-6.277727	-0.761145
38	6	0	-7.431854	-4.184334	-1.015103
39	6	0	-6.416903	-4.368820	-1.994044
40	6	0	-5.450911	-5.407744	-1.820225
41	6	0	-6.276120	-3.418261	-3.030429
42	6	0	-6.999772	-2.247282	-3.015641
43	6	0	-7.874255	-1.956090	-1.937443
44	6	0	-8.122677	-2.950496	-0.993922
45	6	0	-10.254918	-6.367080	2.536803
46	6	0	-3.257276	-6.056432	3.022607
47	6	0	-3.983799	-6.184529	1.857052
48	6	0	-3.466563	-6.867007	0.727556
49	6	0	-2.122806	-7.342968	0.802731
50	6	0	-1.417696	-7.217524	2.021865
51	6	0	-1.959951	-6.599845	3.136100
52	6	0	-4.230669	-7.056778	-0.500533
53	6	0	-1.483029	-7.872707	-0.391228
54	6	0	-2.287706	-8.159789	-1.526537
55	6	0	-3.666555	-7.773970	-1.525447
56	6	0	-1.662121	-8.648610	-2.700244
57	6	0	-0.287058	-8.685397	-2.811586
58	6	0	0.531958	-8.263400	-1.734512
59	6	0	-0.079934	-7.940271	-0.526982
60	6	0	-1.196020	-6.494247	4.433078
61	6	0	7.365608	-8.047007	1.775454
62	6	0	7.343931	-6.909776	0.994697
63	6	0	6.295706	-6.666309	0.076220
64	6	0	5.252889	-7.636031	-0.039768
65	6	0	5.306504	-8.785487	0.781095
66	6	0	6.335734	-9.009509	1.682673
67	6	0	6.277283	-5.479623	-0.759730

68	6	0	4.183556	-7.429807	-1.008281
69	6	0	4.366506	-6.415762	-1.988510
70	6	0	5.405337	-5.449327	-1.816970
71	6	0	3.414916	-6.276446	-3.024122
72	6	0	2.244697	-7.001159	-3.007822
73	6	0	1.955047	-7.874817	-1.928582
74	6	0	2.950010	-8.121193	-0.985129
75	6	0	6.376436	-10.253105	2.537174
76	6	0	6.064867	-3.252052	3.022374
77	6	0	6.190972	-3.980010	1.857481
78	6	0	6.870859	-3.463750	0.725924
79	6	0	7.347134	-2.120012	0.798772
80	6	0	7.223851	-1.413510	2.017266
81	6	0	6.608016	-1.954350	3.133205
82	6	0	7.057648	-4.228838	-0.501931
83	6	0	7.874318	-1.481331	-0.396808
84	6	0	8.158329	-2.286902	-1.532230
85	6	0	7.772255	-3.665655	-1.529097
86	6	0	8.644310	-1.662234	-2.707568
87	6	0	8.681278	-0.287311	-2.819914
88	6	0	8.262275	0.532663	-1.742403
89	6	0	7.941964	-0.078429	-0.533644
90	6	0	6.504070	-1.188773	4.429335
91	6	0	-7.364777	8.045339	1.780270
92	6	0	-7.343331	6.908232	0.999233
93	6	0	-6.296808	6.666262	0.078416
94	6	0	-5.254381	7.636347	-0.037973
95	6	0	-5.307411	8.785304	0.783541
96	6	0	-6.335886	9.008786	1.686083
97	6	0	-6.279244	5.480517	-0.758919
98	6	0	-4.185733	7.430791	-1.007383
99	6	0	-4.369713	6.417873	-1.988575
100	6	0	-5.408580	5.451484	-1.817238
101	6	0	-3.418735	6.279137	-3.024784
102	6	0	-2.248089	7.003068	-3.008206
103	6	0	-1.957340	7.875466	-1.928260
104	6	0	-2.951759	8.121576	-0.984063
105	6	0	-6.377072	10.252861	2.539952
106	6	0	-6.058113	3.249802	3.020365
107	6	0	-6.187753	3.978965	1.856583
108	6	0	-6.869355	3.463230	0.725903
109	6	0	-7.344498	2.119067	0.798429
110	6	0	-7.218195	1.411558	2.015996
111	6	0	-6.599791	1.951507	3.131038
112	6	0	-7.058282	4.229048	-0.501105
113	6	0	-7.872778	1.480788	-0.397000
114	6	0	-8.158302	2.286755	-1.531741
115	6	0	-7.773213	3.665791	-1.528055
116	6	0	-8.645033	1.662510	-2.706974
117	6	0	-8.681759	0.287726	-2.820039
118	6	0	-8.261473	-0.532590	-1.743374
119	6	0	-7.940013	0.077961	-0.534657
120	6	0	-6.492855	1.184275	4.425948
121	1	0	2.281001	8.916152	-3.552273
122	1	0	-0.176108	8.987676	-3.747886
123	1	0	-0.548004	7.575014	0.278261
124	1	0	4.240202	7.938815	-2.433939
125	1	0	4.977513	5.761766	1.811771
126	1	0	3.696063	5.537606	3.870284

127	1	0	0.417318	7.632851	2.094771
128	1	0	1.094961	5.451097	4.749888
129	1	0	0.192185	6.918013	4.343431
130	1	0	1.711991	7.025944	5.242415
131	1	0	6.820544	1.487929	-3.769675
132	1	0	8.809294	2.735425	-0.180626
133	1	0	5.530873	3.588152	-3.802216
134	1	0	4.588669	5.404295	-2.481734
135	1	0	9.544063	4.533715	0.670931
136	1	0	6.182427	8.141668	1.075604
137	1	0	8.210549	8.183427	2.467580
138	1	0	10.004484	6.341518	3.602130
139	1	0	10.824140	7.292622	2.366628
140	1	0	10.913230	5.525835	2.321980
141	1	0	-5.530130	-3.589412	-3.802005
142	1	0	-6.819154	-1.488512	-3.770396
143	1	0	-8.809319	-2.734592	-0.181700
144	1	0	-4.588822	-5.405670	-2.480512
145	1	0	-6.183993	-8.139961	1.079104
146	1	0	-8.212180	-8.179742	2.470952
147	1	0	-9.544394	-4.531345	0.670813
148	1	0	-10.825445	-7.287982	2.369591
149	1	0	-10.913619	-5.521186	2.323487
150	1	0	-10.004868	-6.336281	3.604008
151	1	0	0.173903	-8.989332	-3.747046
152	1	0	0.546624	-7.574722	0.278190
153	1	0	-2.283310	-8.919783	-3.550142
154	1	0	-4.242482	-7.941589	-2.431613
155	1	0	-0.417904	-7.633299	2.095414
156	1	0	-4.976814	-5.759278	1.811682
157	1	0	-3.694853	-5.534497	3.870053
158	1	0	-0.191521	-6.916254	4.343280
159	1	0	-1.711038	-7.025347	5.242449
160	1	0	-1.094973	-5.449927	4.750506
161	1	0	3.584983	-5.531163	-3.796628
162	1	0	1.485313	-6.822333	-3.762400
163	1	0	2.735427	-8.807861	-0.172556
164	1	0	5.402300	-4.587754	-2.477908
165	1	0	8.146994	-6.183626	1.071739
166	1	0	8.191120	-8.211972	2.463455
167	1	0	4.534611	-9.541774	0.677777
168	1	0	6.356524	-10.002657	3.604460
169	1	0	5.525879	-10.908276	2.331552
170	1	0	7.293344	-10.827645	2.361592
171	1	0	8.983899	0.172758	-3.756223
172	1	0	7.578224	0.548583	0.272012
173	1	0	8.913444	-2.284056	-3.557657
174	1	0	7.936937	-4.242274	-2.435380
175	1	0	7.639694	-0.413610	2.088709
176	1	0	5.765702	-4.973154	1.814202
177	1	0	5.544549	-3.688741	3.871279
178	1	0	6.926869	-0.184722	4.338138
179	1	0	7.035184	-1.703381	5.238979
180	1	0	5.460062	-1.086400	4.747372
181	1	0	-3.589716	5.534957	-3.798155
182	1	0	-1.489342	6.824802	-3.763562
183	1	0	-2.736450	8.807321	-0.170887
184	1	0	-5.406181	4.590647	-2.479138
185	1	0	-8.145609	6.181351	1.077521

186	1	0	-8.189169	8.209362	2.469823
187	1	0	-4.535888	9.541871	0.679485
188	1	0	-5.531454	10.912266	2.327737
189	1	0	-6.348160	10.003644	3.607345
190	1	0	-7.298126	10.822538	2.370521
191	1	0	-8.985194	-0.171964	-3.756259
192	1	0	-7.575710	-0.549589	0.270281
193	1	0	-8.915244	2.284668	-3.556460
194	1	0	-7.939281	4.242865	-2.433795
195	1	0	-7.632413	0.410992	2.087144
196	1	0	-5.762979	4.972395	1.813329
197	1	0	-5.535718	3.685826	3.868328
198	1	0	-6.915989	0.180379	4.334414
199	1	0	-7.022122	1.697841	5.237475
200	1	0	-5.448067	1.081346	4.741169

Table S32. Cartesian coordinate of *E,R,E,R,Z,R,Z,S* (30)

SCF Done: E(RB3LYP) = -4621.32392142 A.U. after 14 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.488356	9.976287	1.414034
2	6	0	1.608916	9.217570	0.669602
3	6	0	2.069572	8.226591	-0.229012
4	6	0	3.477092	8.025259	-0.357489
5	6	0	4.347122	8.817868	0.425307
6	6	0	3.883905	9.785355	1.303895
7	6	0	1.149184	7.439241	-1.029350
8	6	0	3.975504	7.026978	-1.294192
9	6	0	3.061656	6.493638	-2.245212
10	6	0	1.657670	6.704351	-2.068101
11	6	0	3.544045	5.619597	-3.246254
12	6	0	4.839813	5.153241	-3.212332
13	6	0	5.706101	5.515815	-2.149418
14	6	0	5.284515	6.495228	-1.253126
15	6	0	4.834395	10.631239	2.115959
16	1	0	2.852898	5.254274	-4.001304
17	1	0	5.168185	4.411917	-3.934155
18	1	0	5.956491	6.789381	-0.453358
19	1	0	0.979354	6.141160	-2.702608
20	1	0	0.540006	9.382729	0.759124
21	1	0	2.104763	10.739140	2.087000
22	1	0	5.419397	8.692364	0.309836
23	1	0	4.693029	11.698574	1.910044
24	1	0	5.876915	10.383620	1.899206
25	1	0	4.672795	10.489863	3.191201
26	6	0	-0.311094	5.915653	2.796816
27	6	0	0.134243	6.436049	1.599982
28	6	0	-0.752817	6.700998	0.526308
29	6	0	-2.121361	6.331755	0.691123
30	6	0	-2.546666	5.826901	1.942147
31	6	0	-1.676782	5.623262	2.999685
32	6	0	-0.309162	7.291471	-0.730965
33	6	0	-3.029989	6.419746	-0.441980
34	6	0	-2.589046	7.074555	-1.624382
35	6	0	-1.232869	7.525391	-1.716811
36	6	0	-3.464782	7.138729	-2.736108

37	6	0	-4.671787	6.470133	-2.735326
38	6	0	-5.075621	5.717233	-1.604339
39	6	0	-4.274762	5.755822	-0.466649
40	6	0	-2.158162	5.096853	4.329419
41	1	0	-5.303797	6.490388	-3.618433
42	1	0	-4.563017	5.139438	0.376427
43	1	0	-3.143722	7.678392	-3.623423
44	1	0	-0.909006	7.982603	-2.648105
45	1	0	-3.597196	5.598927	2.088790
46	1	0	1.187713	6.651269	1.483054
47	1	0	0.400520	5.733915	3.598492
48	1	0	-3.229180	4.878147	4.310699
49	1	0	-1.977888	5.820705	5.133081
50	1	0	-1.631936	4.175818	4.605800
51	6	0	-0.757975	-5.530693	-3.321144
52	6	0	-0.763694	-6.123303	-2.075565
53	6	0	0.421743	-6.633367	-1.488586
54	6	0	1.642257	-6.449231	-2.199906
55	6	0	1.608662	-5.859168	-3.484026
56	6	0	0.435537	-5.406018	-4.063753
57	6	0	0.437351	-7.314219	-0.198137
58	6	0	2.894833	-6.824355	-1.566304
59	6	0	2.865473	-7.627321	-0.395616
60	6	0	1.606475	-7.876181	0.246983
61	6	0	4.102378	-7.997552	0.191897
62	6	0	5.299016	-7.468251	-0.252388
63	6	0	5.323750	-6.526166	-1.313925
64	6	0	4.125070	-6.285111	-1.983032
65	6	0	0.419529	-4.792531	-5.442240
66	1	0	4.094511	-8.663128	1.051415
67	1	0	6.221515	-7.738731	0.252560
68	1	0	4.107417	-5.534078	-2.760783
69	1	0	1.612522	-8.417612	1.189555
70	1	0	-1.698646	-6.203514	-1.537162
71	1	0	-1.690281	-5.160427	-3.740398
72	1	0	2.531494	-5.776450	-4.049177
73	1	0	0.030557	-3.767948	-5.415698
74	1	0	-0.224575	-5.360763	-6.123530
75	1	0	1.421299	-4.759415	-5.878907
76	6	0	0.470157	-4.970612	3.451884
77	6	0	0.458958	-5.777798	2.333339
78	6	0	-0.746554	-6.313663	1.815303
79	6	0	-1.965735	-5.935223	2.449891
80	6	0	-1.915508	-5.123987	3.606246
81	6	0	-0.725425	-4.642595	4.126070
82	6	0	-0.781450	-7.211155	0.666236
83	6	0	-3.229592	-6.347288	1.861607
84	6	0	-3.225583	-7.350670	0.855858
85	6	0	-1.973531	-7.783036	0.304470
86	6	0	-4.465980	-7.748666	0.296213
87	6	0	-5.636113	-7.078304	0.594315
88	6	0	-5.627419	-5.969205	1.478622
89	6	0	-4.436290	-5.677378	2.140032
90	6	0	-0.693381	-3.790845	5.371258
91	1	0	-6.563131	-7.374322	0.112188
92	1	0	-4.403113	-4.805566	2.780717
93	1	0	-4.476374	-8.556195	-0.431535
94	1	0	-1.998582	-8.480932	-0.528513
95	1	0	-2.840401	-4.884061	4.121081

96	1	0	1.395211	-6.010815	1.843048
97	1	0	1.416812	-4.586449	3.823880
98	1	0	-1.700038	-3.598166	5.751774
99	1	0	-0.216361	-2.823146	5.177447
100	1	0	-0.119866	-4.275165	6.170430
101	6	0	-10.454977	-2.315199	-3.125196
102	6	0	-10.138592	-1.379516	-2.161077
103	6	0	-9.396457	-1.727419	-1.007531
104	6	0	-8.988976	-3.086575	-0.853051
105	6	0	-9.326273	-4.015912	-1.862573
106	6	0	-10.045138	-3.659746	-2.993120
107	6	0	-9.074755	-0.751588	0.023879
108	6	0	-8.251225	-3.482605	0.338125
109	6	0	-8.214829	-2.572811	1.429544
110	6	0	-8.623110	-1.217300	1.235018
111	6	0	-7.597277	-2.982289	2.636118
112	6	0	-6.889005	-4.160562	2.704760
113	6	0	-6.733279	-4.980177	1.555770
114	6	0	-7.482137	-4.663933	0.422396
115	6	0	-10.404471	-4.674550	-4.050971
116	1	0	-7.638895	-2.320446	3.497283
117	1	0	-6.394065	-4.437189	3.630243
118	1	0	-7.360888	-5.271931	-0.467391
119	1	0	-8.402679	-0.513642	2.031409
120	1	0	-10.478728	-0.355811	-2.273748
121	1	0	-11.040216	-2.016813	-3.991521
122	1	0	-9.044370	-5.056348	-1.732997
123	1	0	-9.973369	-4.405080	-5.022391
124	1	0	-11.489901	-4.738079	-4.190309
125	1	0	-10.041318	-5.672046	-3.789625
126	6	0	-10.507670	2.461577	2.704009
127	6	0	-10.185855	1.480712	1.787971
128	6	0	-9.301085	1.732870	0.712745
129	6	0	-8.753539	3.045879	0.582364
130	6	0	-9.103293	4.023001	1.541743
131	6	0	-9.961231	3.758853	2.598129
132	6	0	-8.972985	0.707794	-0.266743
133	6	0	-7.867764	3.349786	-0.534129
134	6	0	-7.785508	2.402973	-1.592513
135	6	0	-8.335044	1.096005	-1.419093
136	6	0	-7.016556	2.716025	-2.737785
137	6	0	-6.244086	3.855282	-2.782899
138	6	0	-6.183500	4.728236	-1.667232
139	6	0	-7.036529	4.490437	-0.591012
140	6	0	-10.326145	4.824966	3.602323
141	1	0	-5.598377	4.037926	-3.636111
142	1	0	-7.005364	5.173454	0.251414
143	1	0	-6.987850	2.004967	-3.559232
144	1	0	-8.098738	0.355015	-2.175841
145	1	0	-8.714872	5.030576	1.431478
146	1	0	-10.633187	0.496592	1.875292
147	1	0	-11.202692	2.237486	3.509498
148	1	0	-9.857535	5.782263	3.359117
149	1	0	-10.008312	4.543932	4.613408
150	1	0	-11.410303	4.981772	3.641022
151	6	0	7.170810	0.549011	3.081565
152	6	0	7.749966	-0.020313	1.966382
153	6	0	8.069935	0.744134	0.815510
154	6	0	7.668104	2.114031	0.811851

155	6	0	7.106797	2.672434	1.983301
156	6	0	6.865699	1.925552	3.123494
157	6	0	8.739253	0.187556	-0.359069
158	6	0	7.755337	2.881279	-0.419727
159	6	0	8.506557	2.353637	-1.503237
160	6	0	9.030678	1.024385	-1.409141
161	6	0	8.548131	3.080621	-2.719733
162	6	0	7.741613	4.183591	-2.919520
163	6	0	6.879951	4.638377	-1.890209
164	6	0	6.964133	4.027025	-0.642745
165	6	0	6.284703	2.546644	4.369775
166	1	0	9.164689	2.705666	-3.532760
167	1	0	7.727411	4.676916	-3.887275
168	1	0	6.268760	4.343453	0.125487
169	1	0	9.557349	0.624600	-2.271677
170	1	0	7.967257	-1.078128	1.981616
171	1	0	6.953145	-0.074721	3.945112
172	1	0	6.864692	3.730309	1.995361
173	1	0	6.987012	2.485274	5.209696
174	1	0	5.369374	2.030135	4.680818
175	1	0	6.039660	3.600936	4.215856
176	6	0	10.867661	-2.697451	2.315849
177	6	0	10.344446	-1.806091	1.401267
178	6	0	9.414012	-2.220081	0.419818
179	6	0	9.035466	-3.596279	0.380707
180	6	0	9.580290	-4.477319	1.341393
181	6	0	10.485382	-4.057576	2.304782
182	6	0	8.859528	-1.291294	-0.550717
183	6	0	8.128138	-4.058320	-0.660446
184	6	0	7.929128	-3.204740	-1.778413
185	6	0	8.272761	-1.821782	-1.672776
186	6	0	7.203870	-3.699045	-2.887731
187	6	0	6.517623	-4.887624	-2.804397
188	6	0	6.466073	-5.612484	-1.582136
189	6	0	7.351847	-5.236178	-0.570713
190	6	0	11.070655	-5.021121	3.308552
191	1	0	5.944148	-5.232228	-3.658144
192	1	0	7.341722	-5.777139	0.369353
193	1	0	7.141426	-3.094542	-3.788813
194	1	0	7.891384	-1.155196	-2.440242
195	1	0	9.314472	-5.529455	1.297180
196	1	0	10.649732	-0.764606	1.422882
197	1	0	11.590620	-2.351935	3.050609
198	1	0	12.164568	-5.048436	3.243932
199	1	0	10.700530	-6.037768	3.151638
200	1	0	10.818982	-4.727722	4.334596

Table S33. Cartesian coordinate of *E,R,Z,R,Z,R,E,S* (31)

SCF Done: E(RB3LYP) = -4621.31677133 A.U. after 16 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.653657	-9.636067	3.839017
2	6	0	3.232869	-8.940603	2.797393
3	6	0	2.478543	-8.537086	1.670694
4	6	0	1.093926	-8.886063	1.620396
5	6	0	0.532534	-9.587037	2.711501

6	6	0	1.280253	-9.966476	3.815919
7	6	0	3.082172	-7.810107	0.566618
8	6	0	0.310223	-8.547488	0.440003
9	6	0	1.022220	-8.159838	-0.726792
10	6	0	2.390355	-7.765360	-0.617742
11	6	0	0.310438	-7.996076	-1.937399
12	6	0	-1.063741	-8.016486	-1.951998
13	6	0	-1.802102	-8.137627	-0.743176
14	6	0	-1.102767	-8.487761	0.412725
15	6	0	0.661391	-10.730388	4.961269
16	1	0	0.864513	-7.798813	-2.851392
17	1	0	-1.590214	-7.870481	-2.889000
18	1	0	-1.647052	-8.590319	1.345575
19	1	0	2.833726	-7.267098	-1.474391
20	1	0	4.290120	-8.697034	2.830171
21	1	0	3.262792	-9.942427	4.685791
22	1	0	-0.513164	-9.876517	2.666125
23	1	0	1.169509	-11.688177	5.122655
24	1	0	-0.396250	-10.938857	4.779281
25	1	0	0.735070	-10.168097	5.899683
26	6	0	3.831706	-4.780854	3.686688
27	6	0	3.625578	-5.764887	2.742061
28	6	0	4.488309	-5.925625	1.628244
29	6	0	5.524226	-4.957233	1.460048
30	6	0	5.726845	-3.982812	2.464312
31	6	0	4.915400	-3.883680	3.581445
32	6	0	4.333813	-6.993209	0.642930
33	6	0	6.281454	-4.929165	0.219058
34	6	0	6.184426	-6.035589	-0.666168
35	6	0	5.242532	-7.076701	-0.384191
36	6	0	6.871021	-5.980334	-1.905201
37	6	0	7.474425	-4.814198	-2.333808
38	6	0	7.461934	-3.658919	-1.514399
39	6	0	6.941147	-3.764744	-0.228421
40	6	0	5.160889	-2.846975	4.649865
41	1	0	7.913926	-4.762083	-3.325904
42	1	0	6.892969	-2.865188	0.374074
43	1	0	6.837864	-6.846466	-2.561308
44	1	0	5.153025	-7.887271	-1.102513
45	1	0	6.556676	-3.290747	2.362720
46	1	0	2.783639	-6.430630	2.865069
47	1	0	3.150057	-4.701558	4.530023
48	1	0	6.003051	-2.198329	4.394085
49	1	0	5.380604	-3.315717	5.616483
50	1	0	4.279540	-2.211907	4.796211
51	6	0	-2.240789	5.533455	3.916008
52	6	0	-2.589082	6.180400	2.748788
53	6	0	-3.838387	5.955761	2.117476
54	6	0	-4.701091	4.976365	2.688654
55	6	0	-4.323015	4.350959	3.899344
56	6	0	-3.119198	4.615462	4.530110
57	6	0	-4.244537	6.651632	0.901152
58	6	0	-5.920890	4.606572	1.989516
59	6	0	-6.361728	5.405723	0.901837
60	6	0	-5.497811	6.429649	0.390203
61	6	0	-7.579749	5.054186	0.267481
62	6	0	-8.243096	3.883942	0.578589
63	6	0	-7.709951	2.977719	1.533954
64	6	0	-6.597025	3.401610	2.258052

65	6	0	-2.744290	3.948568	5.830709
66	1	0	-7.963585	5.696953	-0.520752
67	1	0	-9.153512	3.634702	0.042675
68	1	0	-6.141410	2.718602	2.961191
69	1	0	-5.810826	6.966872	-0.501422
70	1	0	-1.891007	6.881720	2.312463
71	1	0	-1.276853	5.740770	4.374197
72	1	0	-5.008448	3.651320	4.366712
73	1	0	-2.610139	4.684994	6.631876
74	1	0	-1.798759	3.401714	5.738217
75	1	0	-3.511399	3.239721	6.153751
76	6	0	-2.344293	10.451584	2.146063
77	6	0	-3.016137	9.338884	1.682993
78	6	0	-2.501633	8.560338	0.620268
79	6	0	-1.258237	8.942374	0.033316
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81	6	0	-1.114500	10.846815	1.573425
82	6	0	-3.211837	7.399582	0.117548
83	6	0	-0.708851	8.143526	-1.054224
84	6	0	-1.569068	7.208280	-1.694241
85	6	0	-2.809072	6.853129	-1.072254
86	6	0	-1.093126	6.499602	-2.821317
87	6	0	0.231901	6.571183	-3.193436
88	6	0	1.151049	7.339558	-2.434703
89	6	0	0.652393	8.168310	-1.431374
90	6	0	-0.400045	12.076248	2.079894
91	1	0	0.602128	5.943775	-3.998224
92	1	0	1.350458	8.777472	-0.866140
93	1	0	-1.768009	5.823185	-3.339209
94	1	0	-3.355089	6.007236	-1.480360
95	1	0	0.331811	10.402472	0.070984
96	1	0	-3.964151	9.050962	2.126754
97	1	0	-2.769492	11.039430	2.955740
98	1	0	0.530104	12.253623	1.533534
99	1	0	-0.151666	11.981750	3.143583
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101	6	0	6.117567	4.226455	2.097070
102	6	0	6.552286	3.801193	0.859153
103	6	0	6.123945	4.427715	-0.338507
104	6	0	5.144218	5.459619	-0.226989
105	6	0	4.745103	5.890637	1.059506
106	6	0	5.220767	5.308696	2.222029
107	6	0	6.609177	4.032847	-1.657137
108	6	0	4.521390	5.988953	-1.430043
109	6	0	5.078954	5.656040	-2.693828
110	6	0	6.151170	4.708889	-2.760387
111	6	0	4.447470	6.141901	-3.866043
112	6	0	3.230754	6.791688	-3.806222
113	6	0	2.598189	7.016663	-2.558005
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115	6	0	4.794951	5.798654	3.584127
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117	1	0	2.731704	7.093677	-4.722601
118	1	0	2.779938	6.799757	-0.450658
119	1	0	6.528900	4.435302	-3.742021
120	1	0	7.242911	2.971227	0.807056
121	1	0	6.478366	3.723556	2.990964
122	1	0	4.048838	6.718606	1.143743
123	1	0	5.650239	6.178364	4.155656

124	1	0	4.349661	4.990386	4.175764
125	1	0	4.059481	6.604129	3.509102
126	6	0	10.618228	3.174966	0.071744
127	6	0	9.434356	3.474777	-0.570259
128	6	0	8.636173	2.462976	-1.153726
129	6	0	9.088656	1.110666	-1.076982
130	6	0	10.301736	0.840808	-0.403312
131	6	0	11.072357	1.840722	0.170083
132	6	0	7.395066	2.773236	-1.841801
133	6	0	8.310296	0.056224	-1.712810
134	6	0	7.293586	0.447170	-2.627180
135	6	0	6.843243	1.804688	-2.639588
136	6	0	6.623741	-0.545866	-3.377645
137	6	0	6.826010	-1.882539	-3.115318
138	6	0	7.675789	-2.285235	-2.053249
139	6	0	8.449703	-1.320056	-1.415263
140	6	0	12.374561	1.529172	0.867081
141	1	0	6.244770	-2.634458	-3.640095
142	1	0	9.114100	-1.630776	-0.615151
143	1	0	5.886017	-0.239603	-4.114683
144	1	0	5.937993	2.026875	-3.196866
145	1	0	10.665510	-0.181565	-0.366040
146	1	0	9.102292	4.505609	-0.641543
147	1	0	11.215980	3.975786	0.499927
148	1	0	12.592448	0.458015	0.850060
149	1	0	12.351035	1.849991	1.915211
150	1	0	13.214707	2.049921	0.393011
151	6	0	-5.512378	-2.509376	-3.878622
152	6	0	-6.273723	-2.732145	-2.750937
153	6	0	-6.128101	-3.908043	-1.971012
154	6	0	-5.097242	-4.818171	-2.341509
155	6	0	-4.359339	-4.575859	-3.524141
156	6	0	-4.552605	-3.450802	-4.306542
157	6	0	-6.952918	-4.191110	-0.799296
158	6	0	-4.787445	-5.938437	-1.468435
159	6	0	-5.654937	-6.237729	-0.384165
160	6	0	-6.745725	-5.351901	-0.097341
161	6	0	-5.330523	-7.338846	0.449033
162	6	0	-4.146943	-8.037062	0.299474
163	6	0	-3.210807	-7.665119	-0.699349
164	6	0	-3.581851	-6.652834	-1.581579
165	6	0	-3.763107	-3.220257	-5.571482
166	1	0	-6.014085	-7.604348	1.251610
167	1	0	-3.919447	-8.856167	0.975375
168	1	0	-2.856246	-6.314770	-2.307822
169	1	0	-7.372186	-5.569446	0.764046
170	1	0	-7.000629	-1.986865	-2.461637
171	1	0	-5.660888	-1.597049	-4.450952
172	1	0	-3.621352	-5.303703	-3.843986
173	1	0	-3.037603	-4.019780	-5.744053
174	1	0	-3.214468	-2.272144	-5.529492
175	1	0	-4.420787	-3.169704	-6.447304
176	6	0	-10.474040	-2.553289	-2.920002
177	6	0	-9.481713	-3.153953	-2.172349
178	6	0	-8.891673	-2.492294	-1.070848
179	6	0	-9.340873	-1.178910	-0.744472
180	6	0	-10.352383	-0.591298	-1.536473
181	6	0	-10.927915	-1.250996	-2.612351
182	6	0	-7.849014	-3.115832	-0.275078

183	6	0	-8.746910	-0.489672	0.391797
184	6	0	-8.012282	-1.268111	1.326600
185	6	0	-7.557086	-2.572021	0.949146
186	6	0	-7.567425	-0.644275	2.515717
187	6	0	-7.644549	0.721318	2.667831
188	6	0	-8.116720	1.548041	1.611231
189	6	0	-8.748686	0.914625	0.539773
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191	1	0	-7.266788	1.170845	3.579438
192	1	0	-9.129353	1.512284	-0.280605
193	1	0	-7.097708	-1.251035	3.285490
194	1	0	-6.814137	-3.050005	1.581598
195	1	0	-10.719664	0.395760	-1.270806
196	1	0	-9.145832	-4.156305	-2.418982
197	1	0	-10.920111	-3.090994	-3.752975
198	1	0	-12.265217	0.388455	-3.068109
199	1	0	-12.941732	-1.211528	-3.403382
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