CuH-Catalyzed Enantioselective Alkylation of Indole Derivatives with Ligand-Controlled Regiodivergence

Yuxuan Ye[1], Seoung-Tae Kim[2,3], Jinhoon Jeong[2,3], Mu-Hyun Baik[2,3]*, Stephen L. Buchwald[1]*

[1]Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

[2]Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, 34141, Republic of Korea

[3]Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science (IBS), Daejeon, 34141, Republic of Korea

Table of Contents

I. General Information

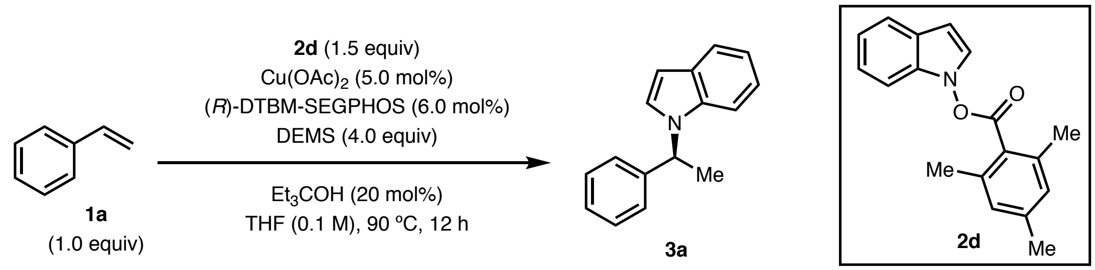
General Reagent Information: All reactions were performed under a nitrogen atmosphere using the indicated method in the general procedures. Tetrahydrofuran (THF) was purchased from J.T. Baker in CYCLE-TAINER® solvent delivery kegs and purified by passage under argon pressure through two packed columns of neutral alumina and copper(II) oxide. Anhydrous 1,4-dioxane was purchased from Aldrich Chemical Company in a Sure-Seal™ bottle and used as received. Copper(II) acetate was purchased from Strem and was used as received. 1,2-Bis((2*S*,5*S*)2,5-diphenylphospholano)ethane, 1,2-Bis((2*R*,5*R*)2,5-diphenylphospholano)ethane (Ph-BPE) ligands were purchased from Namena Corp. and stored in a nitrogen-filled glove box. DTBM-SEGPHOS was purchased from Takasago International Co. and used as received. Diethoxymethylsilane was purchased from TCI America. Dimethoxy(methyl)silane (DMMS) was purchased from Tokyo Chemical Industry Co. (TCI). Both silanes were stored in a nitrogen-filled glove box at −20 °C for long-term storage. (***Caution****: Dimethoxy(methyl)silane (DMMS, CAS#16881-77-9) is listed by several vendors (TCI, Alfa Aesar) SDS or MSDS as a H318, a category 1 Causes Serious Eye Damage Other vendors (Sigma-Aldrich, Gelest) list DMMS as a H319, a category II Eye Irritant. DMMS should be handled in a well-ventilated fumehood using proper precaution as outlined for the handling of hazardous materials in prudent practices in the laboratory*[1]*. At the end of the reaction either ammonium fluoride in methanol, aqueous sodium hydroxide (1 M) or aqueous hydrochloric acid (1 M) should be carefully added to the reaction mixture. This should be allowed to stir for at least 30 min or the time indicated in the detailed reaction procedure*). All other solvents and commercial reagents were used as received from Sigma Aldrich, Alfa Aesar, Acros Organics, TCI and Combi-Blocks, unless otherwise noted. Flash column chromatography was performed using 40-63 µm silica gel (SiliaFlash® F60 from Silicycle), or with the aid of a Biotage Isolera Automated Flash Chromatography System using prepacked SNAP silica cartridges (10-100 g). Organic solutions were concentrated *in vacuo* using a Buchi rotary evaporator.

General Analytical Information: All new compounds were characterized by NMR spectroscopy, IR spectroscopy, elemental analysis or high resolution mass spectrometry, optical rotation and melting point analysis (if solids). ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded in $CDCl_3$ on a Bruker AMX-400 spectrometer. Chemical shifts for ^{1}H NMR are reported as follows: chemical shift in reference to residual $CHCl_3$ at 7.26 ppm (δ ppm), multiplicity (s =

singlet, br s = broad singlet, d = doublet, t = triplet, q = quartet, sex = sextet, sep = septet, ddd = doublet of double of doublets, td = triplet of doublets, m = multiplet), coupling constant (Hz), and integration. Chemical shifts for ^{13}C NMR are reported in terms of chemical shift in reference to the $CDCl_3$ solvent signal (77.16 ppm). Chemical shifts for ^{19}F-NMR are reported in terms of chemical shift in reference to an external standard (α,α,α-trifluorotoluene set to δ -63.7 ppm). IR spectra were recorded on a Thermo Scientific Nicolet iS5 spectrometer (iD5 ATR, diamond) and are reported in terms of frequency of absorption (cm^{-1}). Melting points were measured on a Mel-Temp capillary melting point apparatus. Optical rotations were measured using a Jasco P-1010 digital polarimeter. Elemental analyses were performed by Atlantic Microlabs Inc., Norcross, GA. ESI- and DART-MS spectrometric data were recorded on a Bruker Daltonics APEXIV 4.7 Tesla Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR-MS). Enantiomeric excesses (ee's) were mostly determined by chiral SFC analysis using a Waters Acquity UPC2 instrument; specific columns and analytical methods are provided in the experimental details for individual compounds; the wavelengths of light used for chiral analyses are provided with the associated chromatograms. The enantiomeric excesss of certain compounds were determined by High pressure liquid chromatography (HPLC) performing on Agilent 1200 Series chromatographs using chiral columns (25 cm). Thin-layer chromatography (TLC) was performed on silica gel 60Å F_{254} plates (SiliaPlate from Silicycle) and visualized with UV light or potassium permanganate stain. Preparatory thin-layer chromatography (Prep-TLC) was performed on silica gel GF with UV 254 (20 x 20 cm, 1000 microns, catalog # TLG-R10011B-341 from Silicycle) and visualized with UV light. Isolated yields reported reflect the average values from two independent runs.

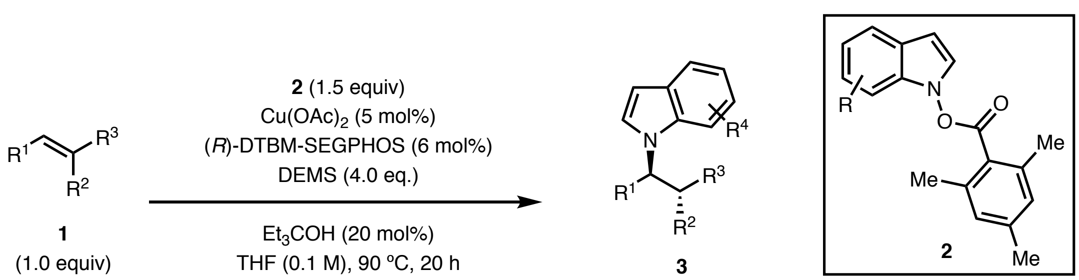
II. CuH-Catalyzed Enantioselective N-Alkylation

Table S1. Optimization of CuH-catalyzed enantioselective N-alkylation.[a]



Entry	Change from the "standard conditions"	Yield (%)	e.e. (%)	r.r.
1	none	91 (85)[b]	91	> 20:1
2	70 °C	75	93	> 20:1
3	DMMS instead of DEMS	69	22	> 20:1
4	1.0 instead of 1.5 equiv of **2d**	86	89	> 20:1
5	0.5 M instead of 0.1 M	71	93	13:1
6	no Et_3COH	68	92	> 20:1

[a]Reactions were conducted on 0.1 mmol scale. Yields were determined by gas chromatography using dodecane as internal standard. The ee was determined by SFC analysis. The regioisomeric ratio (rr) was determined by GC analysis of the crude reaction mixture. [b]Isolated yield on a 0.5 mmol scale.



General Procedure A:

Preparation of CuH solution: In a nitrogen-filled glovebox, an oven-dried screw-top reaction tube (Fisherbrand, 13 x 100 mm, catalog no. 14-959035C) equipped with a magnetic stir bar was charged with $Cu(OAc)_2$ (4.5 mg, 0.025 mmol, 5 mol %) and (*R*)-DTBM-SEGPHOS (35.4 mg, 0.030 mmol, 6 mol %). Anhydrous THF (0.5 mL) was added via syringe and the reaction solution was stirred at room temperature (rt) for 15 min. $HSiMe(OEt)_2$ (0.32 mL, 2.0 mmol, 4.0 equiv) was added sequentially via syringe and the resulting mixture was stirred at rt to afford a pale yellow to orange solution of CuH (about 15 min).

N-Alkylation: In a nitrogen-filled glovebox, a second oven-dried screw-top reaction tube (Fisherbrand, 16 x 125 mm, catalog no. 1495925C) equipped with a stir bar was charged with indole electrophile **2d** (0.21 g, 0.75 mmol, 1.5 equiv). Anhydrous THF (4.2 mL), styrene (0.50 mmol, 1.0 equiv), and 3-ethyl-3-pentanol (14 µl, 0.10 mmol, 0.20 equiv) were added, followed by addition of the CuH solution via syringe from the first reaction tube to the stirred reaction mixture at rt. The reaction tube was sealed with a Teflon-lined screw cap and removed from the glovebox, placed in a 90 °C oil bath and stirred for 20 h. After cooling to rt, the reaction cap was removed and dodecane (50 µl) was added as an internal standard. An aliquot of the solution was transferred into a GC vial and diluted with EtOAc. GC analysis was used for determination of the conversion, yield and regioselectivity. Sat. NH_4F in MeOH (5 mL) was slowly added to the reaction tube to quench the reaction as part of the workup (*Caution*: gas evolution observed). The mixture was stirred uncapped for 30 min, transferred to a 20 mL scintillation vial, the reaction tube was rinsed with EtOAc (2 mL × 3), and concentrated *in vacuo* with the aid of a rotary evaporator. The resulting residue was redissolved in EtOAc, filtered through a short pad of Celite and washed with additional EtOAc (~ 100 mL). The collected EtOAc solution was concentrated *in vacuo* with the aid of a rotary evaporator, and the crude material was purified by silica gel column chromatography.

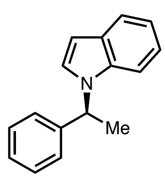
General Procedure B:

Preparation of CuH solution: see General Procedure A.

N-Alkylation: In a nitrogen-filled glovebox, a second oven-dried screw-top reaction tube (Fisherbrand, 16 x 125 mm, catalog no. 1495925C) equipped with a stir bar was charged with indole electrophile **2d** (0.14 g, 0.50 mmol, 1.0 equiv). Anhydrous THF (4.2 mL), styrene (0.75 mmol, 1.5 equiv) and KF (0.0058 g, 0.10 mmol, 0.20 equiv) were added, followed by addition of the CuH solution via syringe from the first reaction tube to the stirred reaction mixture at rt. The reaction tube was sealed with a Teflon-lined screw cap, removed from the glovebox, placed in a oil bath preheated to 70 ºC and stirred for 20 h. After cooling to rt, the reaction cap was removed and dodecane (50 µL) was added as an internal standard. An aliquot of the solution was transferred into a GC vial and diluted with EtOAc. GC analysis was used for determination of the conversion, yield and regioselectivity. Sat. NH_4F in MeOH (5 mL) was slowly added to the reaction tube to quench the reaction as part of the workup (*Caution*: gas evolution observed). The mixture was stirred uncapped for 30 min, transferred to a 20 mL scintillation vial, the reaction tube was rinsed with EtOAc (2 mL × 3), and concentrated *in vacuo* with the aid of a rotary evaporator. The resulting residue was redissolved in EtOAc, filtered through a shot pad of Celite and washed with additional EtOAc (~ 100 mL). The collected EtOAc solution was concentrated *in vacuo* with the aid of a rotary evaporator, and the crude material was purified by silica gel column chromatography.

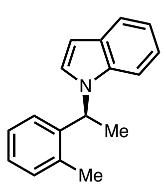
Characterization Data for N-Alkylated Chiral Indoles

(*S*)-1-(1-phenylethyl)-1*H*-indole (3a)



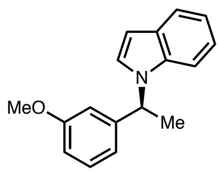
General procedure A was followed using styrene (0.052 g, 0.50 mmol, 1.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 15 : 1) to provide the title compound as a white solid in 85% yield (Run 1: 98 mg, 89%, 91% ee; Run 2: 90 mg, 81%, 91% ee). m.p. 63-67 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70–7.66 (m, 1H), 7.35–7.24 (m, 5H), 7.19–7.10 (m, 4H), 6.61 (dd, *J* = 3.2 Hz, *J* = 0.8, 1H), 5.70 (q, *J* = 7.1 Hz, 1H), 1.95 (d, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.7, 136.1, 128.8, 128.7, 127.5, 125.9, 124.9, 121.5, 120.9, 119.6, 110.1, 101.5, 54.8, 21.8 ppm. IR (thin film) 3028, 1458, 1311, 1300, 1228, 1014, 737, 697 cm^{-1}. EA Calcd. for $C_{16}H_{15}N$: C, 86.84; H, 6.83. Found: C, 86.83; H, 6.98. $[\alpha]_D^{22}$ = -85.0. **SFC** analysis: ODH (5:95 MeOH: $scCO_2$ to 15:85 MeOH: $scCO_2$ linear gradient over 20 min, 2.50 mL/min), 6.66 min (major), 7.15 min (minor), 91% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **3t**.

(*S*)-1-(1-(*o*-tolyl)ethyl)-1*H*-indole (3b)



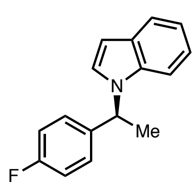
General procedure A was followed using 1-methyl-2-vinylbenzene (0.059 g, 0.50 mmol, 1.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 15 : 1) to provide the title compound as a white solid in 81% yield (Run 1: 99 mg, 84%, 87% ee; Run 2: 92 mg, 78%, 87% ee). m.p. 38-42 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72–7.68 (m, 1H), 7.30–7.12 (m, 8H), 6.57 (dd, *J* = 3.2 Hz, *J* = 0.8 Hz, 1H), 5.85 (q, *J* = 6.9 Hz, 1H), 2.33–2.29 (s, 3H), 1.91 (d, *J* = 7.0 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.1, 140.0, 135.7, 130.8, 128.9, 127.7, 126.6, 125.4, 125.1, 121.5, 121.0, 119.6, 109.7, 101.3, 51.8, 20.5, 19.1 ppm. IR (thin film) 3047, 2976, 1509, 1476, 1458, 1307, 1228, 1012, 758, 737 cm^{-1}. EA Calcd. for $C_{17}H_{17}N$: C, 86.77; H, 7.28. Found: C, 86.81; H, 7.33. $[\alpha]_D^{22}$ = -72.3. **SFC** analysis: ODH (1:99 MeOH: $scCO_2$ over 40 min, 2.50 mL/min), 21.95 min (minor), 22.68 min (major), 87% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **3t**.

(*S*)-1-(1-(3-methoxyphenyl)ethyl)-1*H*-indole (3c)



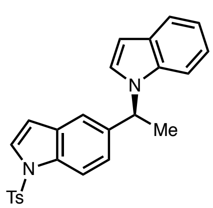
General procedure A was followed using 1-methoxy-3-vinylbenzene (0.067 g, 0.50 mmol, 1.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 10 : 1) to provide the title compound as a colorless oil in 71% yield (Run 1: 83 mg, 66%, 93% ee; Run 2: 96 mg, 76%, 93% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74–7.70 (m, 1H), 7.36 (d, *J* = 3.3 Hz, 1H), 7.34–7.30 (m, 1H), 7.29–7.24 (m, 1H), 7.23–7.14 (m, 2H), 6.68–6.74 (m, 3H), 6.64 (dd, *J* = 3.3 Hz, *J* = 0.8 Hz, 1H), 5.70 (q, *J* = 7.1 Hz, 1H), 3.79–3.76 (s, 3H), 1.96 (d, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 144.5, 136.2, 129.8, 128.9, 124.9, 121.5, 121.0, 119.6, 118.4, 112.4, 112.2, 110.1, 101.6, 55.2, 54.8, 21.8 ppm. IR (thin film) 2978, 2834, 1458, 1309, 1284, 1223, 1042, 738, 717, 696 cm^{-1}. EA Calcd. for $C_{17}H_{17}NO$: C, 81.24; H, 6.82. Found: C, 81.22; H, 6.85. $[\alpha]_D^{23}$ = -52.3. **SFC** analysis: ODH (5:95 MeOH: $scCO_2$ to 15:85 MeOH: $scCO_2$ linear gradient over 20 min, 2.50 mL/min), 9.33 min (major), 10.29 min (minor), 93% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **3t**.

(*S*)-1-(1-(4-fluorophenyl)ethyl)-1*H*-indole (3e)



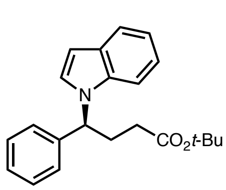
General procedure A was followed using 1-fluoro-4-vinylbenzene (0.061 g, 0.50 mmol, 1.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 15 : 1) to provide the title compound as a white solid in 81% yield (Run 1: 93 mg, 78%, 93% ee; Run 2: 99 mg, 83%, 93% ee). m.p. 78-81 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76–7.69 (m, 1H), 7.33 (d, *J* = 3.3 Hz, 1H), 7.30–7.26 (m, 1H), 7.24–7.12 (m, 4H), 7.06–7.00 (m, 2H), 6.65 (dd, *J* = 3.3 Hz, *J* = 0.8 Hz, 1H), 5.71 (q, *J* = 7.1 Hz, 1H), 1.96 (d, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ (d, *J* = 247.5 Hz), 138.5 (d, *J* = 3.0 Hz), 136.0, 128.9, 127.6 (d, *J* = 8.1 Hz), 124.7, 121.6, 121.0, 119.7, 115.6 (d, *J* = 21.2 Hz), 110.0, 101.8, 54.2, 21.8 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.1 ppm. IR (thin film) 3049, 2979, 1508, 1459, 1310, 1299, 1226, 1158, 1013, 833, 763, 738 cm^{-1}. EA Calcd. for $C_{16}H_{14}FN$: C, 80.31; H, 5.90. Found: C, 80.35; H, 6.04. $[\alpha]_D^{22}$ = -80.6. **SFC** analysis: ODH (5:95 MeOH: $scCO_2$ to 15:85 MeOH: $scCO_2$ linear gradient over 20 min, 2.50 mL/min), 6.66 min (major), 7.15 min (minor), 93% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **3t**.

(*S*)-5-(1-(1*H*-indol-1-yl)ethyl)-1-tosyl-1*H*-indole (3f)



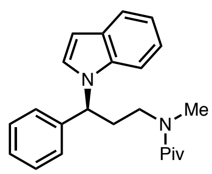
General procedure A was followed using 1-tosyl-5-vinyl-1*H*-indole (0.149 g, 0.50 mmol, 1.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 4 : 1) to provide the title compound as a white solid in 52% yield (Run 1: 101 mg, 49%, 95% ee; Run 2: 114 mg, 55%, 95% ee). m.p. 152-158 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.6 Hz, 1H), 7.79–7.71 (m, 2H), 7.67–7.62 (m, 1H), 7.54 (d, *J* = 3.7 Hz, 1H), 7.33–7.05 (m, 8H), 6.58 (d, *J* = 3.1 Hz, 1H), 6.55 (d, *J* = 3.7 Hz, 1H), 5.74 (q, *J* = 7.1 Hz, 1H), 2.36–2.31 (s, 3H), 1.93 (d, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.0, 138.0, 136.0, 135.3, 134.0, 130.9, 129.9, 128.8, 126.9, 126.8, 124.8, 122.8, 121.4, 120.9, 119.6, 118.5, 113.7, 110.0, 108.9, 101.5, 54.8, 22.1, 21.6 ppm. IR (thin film) 2980, 1461, 1370, 1173, 1129, 742, 676, 576 cm^{-1}. HRMS (DART) m/z calcd. for $C_{25}H_{23}N_2O_2S^+$ $[M+H]^+$: 415.1475; found 415.1456. $[\alpha]_D^{22}$ = -103.1. **SFC** analysis: ADH (5:95 MeOH (0.1% Et_2NH): $scCO_2$ to 30:70 MeOH (0.1% Et_2NH): $scCO_2$ linear gradient over 25 min, 2.50 mL/min), 15.96 (major), 16.49 min (minor), 95% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **3t**.

***tert*-butyl (*S*)-4-(1*H*-indol-1-yl)-4-phenylbutanoate (3g)**



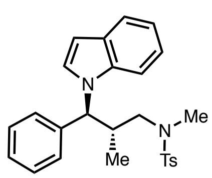
General procedure A was followed using *tert*-butyl (*E*)-4-phenylbut-3-enoate (0.109 g, 0.50 mmol, 1.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 10 : 1) to provide the title compound as a white solid in 78% yield (Run 1: 124 mg, 74%, 96% ee; Run 2: 138 mg, 82%, 96% ee). m.p. 66-69 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.7 Hz, 1H), 7.42–7.34 (m, 9H), 6.66 (d, *J* = 3.2 Hz, 1H), 5.66 (t, *J* = 7.9 Hz, 1H), 2.74–2.60 (m, 2H), 2.34–2.22 (m, 2H), 1.55–1.45 (s, 9H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.2, 141.1, 136.6, 128.8, 128.7, 127.7, 126.5, 124.9, 121.7, 121.0, 119.7, 109.9, 102.3, 80.7, 58.6, 32.2, 30.3, 28.2 ppm. IR (thin film) 2976, 1722, 1458, 1366, 1307, 1244, 1223, 1147, 847, 738, 698 cm^{-1}. EA Calcd. for $C_{22}H_{25}NO_2$: C, 78.77; H, 7.51. Found: C, 78.56; H, 7.35. $[\alpha]_D^{22}$ = -65.8. **SFC** analysis: ODH (5:95 MeOH: $scCO_2$ to 15:85 MeOH: $scCO_2$ linear gradient over 20 min, 2.50 mL/min), 7.17 min (major), 8.40 min (minor), 96% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **3t**.

(*S*)-*N*-(3-(1*H*-indol-1-yl)-3-phenylpropyl)-*N*-methylpivalamide (3h)



General procedure A was followed using *N*-cinnamyl-*N*-methylpivalamide (0.116 g, 0.50 mmol, 1.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 3:1) to provide the title compound as a colorless oil in 69% yield (Run 1: 115 mg, 66%, 96% ee; Run 2: 125 mg, 72%, 96% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.6 Hz, 1H), 7.47 (d, *J* = 3.3 Hz, 1H), 7.38–7.11 (m, 8H), 6.66 (d, *J* = 3.3 Hz, 1H), 5.56 (t, *J* = 7.7 Hz, 1H), 3.49–3.27 (m, 2H), 3.07–3.01 (s, 3H), 2.68–2.56 (m, 2H), 1.33–1.23 (s, 9H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.5, 141.1, 136.3, 128.8, 127.7, 126.3, 124.9, 121.7, 121.0, 119.7, 109.8, 102.3, 57.8, 48.8, 38.7, 37.2, 32.8, 28.2 ppm. IR (thin film) 2956, 1616, 1478, 1458, 1404, 1363, 1304, 1208, 1103, 909, 762, 698 cm^{-1}. EA Calcd. for $C_{22}H_{25}NO_2$: C, 78.77; H, 7.51. Found: C, 78.56; H, 7.35. $[\alpha]_D^{22}$ = -60.2. **SFC** analysis: ODH (5:95 MeOH: $scCO_2$ to 15:85 MeOH: $scCO_2$ linear gradient over 20 min, 2.50 mL/min), 14.86 min (major), 16.75 min (minor), 96% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **3t**.

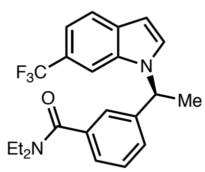
***N*-((2*S*,3*S*)-3-(1*H*-indol-1-yl)-2-methyl-3-phenylpropyl)-*N*,4-dimethylbenzenesulfonamide (3i)**



General procedure B was followed using (*E*)-*N*,4-dimethyl-*N*-(2-methyl-3-phenylallyl)benzenesulfonamide (0.237 g, 0.75 mmol, 1.5 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 5:1) to provide the title compound as a white foam in 41% yield (Run 1: 78 mg, 36%, 99% ee; Run 2: 99 mg, 46%, 99% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.9 Hz, 1H), 7.44–7.37 (m, 3H), 7.33–6.95 (m, 10H), 6.50 (d, *J* = 3.2 Hz, 1H), 4.98 (d, *J* = 10.5 Hz, 1H), 3.00–2.86 (m, 1H), 2.78–2.60 (m, 2H), 2.62–2.57 (s, 3H), 2.28–2.30 (s, 3H), 0.99 (d, *J* = 6.5 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4, 139.3, 136.4, 133.7, 129.7, 128.8, 128.5, 127.9, 127.4, 127.3, 124.2, 121.8, 120.9, 119.6, 109.6, 102.7, 63.5, 54.6, 37.2, 37.0, 21.5, 16.2 ppm. IR (thin film) 2969, 2924, 1458, 1337, 1304, 1159, 1089, 973, 741, 700, 655 cm^{-1}. HRMS (DART) m/z calcd. for $C_{26}H_{29}N_2O_2S^+$ $[M+H]^+$: 433.1944; found 433.1928. $[\alpha]_D^{23}$ = -72.6. **SFC** analysis:

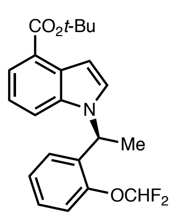
ADH (5:95 MeOH: $scCO_2$ to 20:80 MeOH: $scCO_2$ linear gradient over 15 min, 2.50 mL/min), 11.89 min (major), 12.70 min (minor), 99% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **3t**.

(*S*)-*N*,*N*-diethyl-3-(1-(6-(trifluoromethyl)-1*H*-indol-1-yl)ethyl)benzamide (3j)



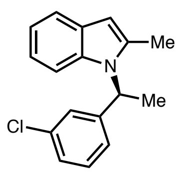
General procedure A was followed using *N*,*N*-diethyl-3-vinylbenzamide (0.102 g, 0.50 mmol, 1.0 equiv), and indole electrophile **2e** (0.26 g, 0.75 mmol, 1.5 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 1:1) to provide the title compound as a colorless oil in 56% yield (Run 1: 99 mg, 51%, 81% ee; Run 2: 117 mg, 60%, 81% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.3 Hz, 1H), 7.46 (d, *J* = 3.3 Hz, 1H), 7.43 (s, 1H), 7.40–7.25 (m, 3H), 7.19 (d, *J* = 7.7 Hz, 1H), 7.03 (s, 1H), 6.65 (d, *J* = 3.3 Hz, 1H), 5.71 (q, *J* = 7.1 Hz, 1H), 3.65–3.35 (m, 2H), 3.15–2.95 (m, 2H), 1.94 (d, *J* = 7.0 Hz, 3H), 1.3–1.1 (m, 3H), 0.9–0.7 (m, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 142.5, 137.8, 134.8, 131.3, 129.2, 127.7, (q, *J* = 31 Hz), 125.2 (q, *J* = 272.9 Hz), 126.6, 125.8, 123.4, 121.4, 116.3 (q, *J* = 3.4 Hz), 107.5 (q, *J* = 4.5 Hz), 102.1, 55.2, 43.2, 39.3, 21.6, 13.7, 12.8 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.5 ppm. IR (thin film) 2978, 2937, 1623, 1338, 1273, 1157, 1111, 1056, 911, 816, 726, 667 cm^{-1}. EA Calcd. for $C_{22}H_{25}NO_2$: C, 78.77; H, 7.51. Found: C, 78.56; H, 7.35. $[\alpha]_D^{22}$ = -63.7. **SFC** analysis: ODH (5:95 MeOH: $scCO_2$ to 15:85 MeOH: $scCO_2$ linear gradient over 20 min, 2.50 mL/min), 8.15 min (major), 8.72 min (minor), 81% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **3t**.

***tert*-butyl (*S*)-1-(1-(2-(difluoromethoxy)phenyl)ethyl)-1*H*-indole-4-carboxylate (3k)**



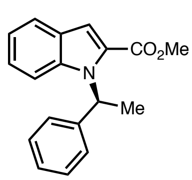
General procedure A was followed using 1-(difluoromethoxy)-2-vinylbenzene (0.085 g, 0.50 mmol, 1.0 equiv), and indole electrophile **2f** (0.28 g, 0.75 mmol, 1.5 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 5:1) to provide the title compound as a colorless oil in 61% yield (Run 1: 112 mg, 58%, 92% ee; Run 2: 124 mg, 64%, 92% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.5 Hz, 1H), 7.53 (d, *J* = 3.3 Hz, 1H), 7.38 (d, *J* = 8.2 Hz, 1H), 7.26–7.10 (m, 4H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.82 (dd, *J* = 7.8 Hz, *J* = 1,7 Hz, 1H), 6.57 (t, *J* = 73.7 Hz, 1H), 6.05 (q, *J* = 7.0 Hz, 1H), 1.92 (d, *J* = 7.0 Hz, 3H), 1,68 (s, 9H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8, 148.0, 136.8, 134.2, 129.0, 128.2, 126.7, 126.5, 126.0, 123.6, 123.3, 120.8, 118.5, 116.2 (t, J = 260.3 Hz), 114.3, 102.9, 80.7, 49.4, 28.5, 20.7 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.7 (dd, J = 169.2 Hz, J = 73.6 Hz), -80.2 (dd, J = 169.2 Hz, J = 73.6 Hz) ppm. IR (thin film) 2979, 1698, 1366, 1291, 1271, 1254, 1166, 1120, 1037, 750.0, 728.2 cm^{-1}. EA Calcd. for $C_{22}H_{25}NO_2$: C, 78.77; H, 7.51. Found: C, 78.56; H, 7.35. $[\alpha]_D^{22}$ = +53.9. **SFC** analysis: ODH (5:95 MeOH: $scCO_2$ to 10:90 MeOH: $scCO_2$ linear gradient over 12 min, 2.50 mL/min), 5.38 min (major), 5.65 min (minor), 92% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **3t**.

(*S*)-1-(1-(3-chlorophenyl)ethyl)-2-methyl-1*H*-indole (3l)



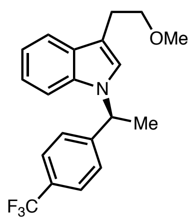
General procedure A was followed using 1-chloro-3-vinylbenzene (0.069 g, 0.50 mmol, 1.0 equiv), and indole electrophile **2g** (0.22 g, 0.75 mmol, 1.5 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a yellow oil in 81% yield (Run 1: 105 mg, 78%, 93% ee; Run 2: 113 mg, 84%, 93% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 7.6 Hz, 1H), 7.35–7.20 (m, 3H), 7.15–7.00 (m, 4H), 6.35 (s, 1H), 5.74 (q, J = 7.2 Hz, 1H), 2.40 (s, 3H), 1.96 (d, J = 7.2 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.8, 136.5, 135.9, 134.7, 129.9, 128.7, 127.4, 126.5, 124.7, 120.5, 119.9, 119.4, 110.8, 101.5, 52.1, 18.6, 14.0 ppm. IR (thin film) 2980, 1596, 1458, 1398, 1308, 782, 748, 720 cm^{-1}. HRMS (DART) m/z calcd. for $C_{17}H_{17}NCl^+$ $[M+H]^+$: 270.1044; found 270.1048. $[\alpha]_D^{22}$ = -42.6. **SFC** analysis: ODH (5:95 MeOH: $scCO_2$ to 15:85 MeOH: $scCO_2$ linear gradient over 20 min, 2.50 mL/min), 7.89 min (minor), 8.81 min (major), 93% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **3t**.

methyl (*S*)-1-(1-phenylethyl)-1*H*-indole-2-carboxylate (3m)



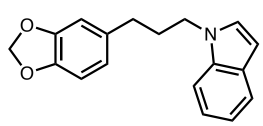
General procedure A was followed using styrene (0.104 g, 1.0 mmol, 2.0 equiv), and indole electrophile **2j** (0.17 g, 1.0 mmol, 1.0 equiv). Dioxane was used as the solvent instead of THF. The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a colorless oil in 43% yield (Run 1: 56 mg, 40%, 0% ee; Run 2: 64 mg, 46%, 0% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60–7.54 (m, 1H), 7.30 (s, 1H), 7.24–7.10 (m, 5H), 7.02–6.92 (m, 3H), 6.92–6.86 (m, 1H), 3.81 (s, 3H), 1.87 (d, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 141.5, 138.0, 128.5, 127.7, 127.0, 126.9, 126.4, 124.5, 122.8, 120.4, 113.6, 111.6, 53.1, 51.8, 18.2 ppm. IR (thin film) 2950, 1703, 1516, 1446, 1436, 1319, 1197, 1162, 1138, 747 cm^{-1}. HRMS (DART) m/z calcd. for $C_{18}H_{18}NO_2^+$ $[M+H]^+$: 280.1332; found 280.1327. **SFC** analysis: ODH (5:95 MeOH: $scCO_2$ to 15:85 MeOH: $scCO_2$ linear gradient over 20 min, 2.50 mL/min), 5.66 min (major), 6.50 min (minor), 0% ee.

(*S*)-3-(2-methoxyethyl)-1-(1-(4-(trifluoromethyl)phenyl)ethyl)-1*H*-indole (3n)



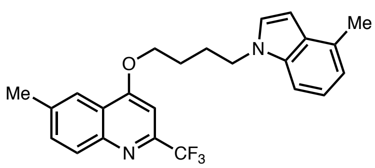
General procedure A was followed using 1-(trifluoromethyl)-4-vinylbenzene (0.086 g, 0.50 mmol, 1.0 equiv), and indole electrophile **2k** (0.506 g, 1.5 mmol, 3.0 equiv). Dioxane was used as the solvent instead of THF. The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a colorless oil in 16% yield (Run 1: 28 mg, 16%, 17% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66–7.61 (m, 1H), 7.53 (d, *J* = 8.1 Hz, 2H), 7.22–7.08 (m, 6H), 5.67 (q, *J* = 7.1 Hz, 1H), 3.71 (t, *J* = 7.2 Hz, 2H), 3.42 (s, 3H), 3.09 (t, *J* = 7.2 Hz, 2H), 1.93 (d, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.0, 136.3, 129.7 (q, *J* = 32.4 Hz), 128.4, 126.2, 125.7 (q, *J* = 3.7 Hz), 124.0 (q, *J* = 272.0 Hz), 122.5, 121.8, 119.3, 119.2, 112.5, 109.9, 73.1, 58.7, 54.4, 25.8, 21.7 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.5 ppm. IR (thin film) 2922, 1619, 1460, 1322, 1163, 1111, 1069, 1014, 840, 737, 617 cm^{-1}. **SFC** analysis: ODH (5:95 MeOH: $scCO_2$ to 10:90 MeOH: $scCO_2$ linear gradient over 12 min, 2.50 mL/min), 4.80 min (major), 5.94 min (minor), 17% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **3t**.

1-(3-(benzo[*d*][1,3]dioxol-5-yl)propyl)-1*H*-indole (3o)



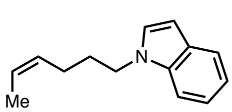
General procedure B was followed using Safrole (0.122 g, 0.75 mmol, 1.5 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as an colorless oil in 61% yield (Run 1: 78 mg, 56%; Run 2: 92 mg, 66%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.9 Hz, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 7.25 (td, *J* = 8.1 Hz, *J* = 1.0 Hz, 1H), 7.19–7.10 (m, 2H), 6.78 (d, *J* = 7.9 Hz, 1H), 6.70 (d, *J* = 1.6 Hz, 1H), 6.64 (dd, *J* = 7.9 Hz, *J* = 1.7 Hz, 1H), 6.55 (dd, *J* = 3.2 Hz, *J* = 0.8 Hz, 1H), 5.96 (s, 2H), 4.15 (d, *J* = 7.0 Hz, 2H), 2.59 (dd, *J* = 8.4 Hz, *J* = 6.8 Hz, 2H), 2.17 (p, *J* = 7.3 Hz, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.8, 145.9, 136.0, 134.8, 128.7, 127.77, 121.4, 121.2, 121.0, 119.3, 109.4, 108.8, 108.3, 101.1, 100.9, 45.6, 32.7, 31.8 ppm. IR (thin film) 2925, 1501, 1487, 1441, 1243, 1036, 926, 808, 738, 719 cm^{-1}. EA Calcd. for $C_{18}H_{17}NO_2$: C, 77.40; H, 6.13. Found: C, 77.10; H, 6.18.

6-methyl-4-(4-(4-methyl-1*H*-indol-1-yl)butoxy)-2-(trifluoromethyl)quinolone (3p)



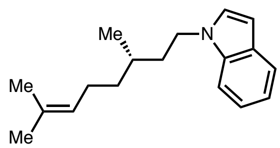
General procedure B was followed using 6-methyl-4-(4-(4-methyl-1*H*-indol-1-yl)butoxy)-2-(trifluoromethyl)quinoline (0.211 g, 0.75 mmol, 1.5 equiv), and indole electrophile **2h** (0.15 g, 1.0 mmol, 1.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 5:1) to provide the title compound as a white solid in 76% yield (Run 1: 151 mg, 73%; Run 2: 163 mg, 79%). m.p. 120-122 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.6 Hz, 1H), 8.08 (s, 1H), 7.75 (dd, *J* = 8.7 Hz, *J* = 2.0 Hz, 1H), 7.45–7.25 (m, 3H), 7.12–7.05 (m, 2H), 6.70 (d, *J* = 3.0 Hz, 1H), 4.42 (t, *J* = 6.8 Hz, 2H), 4.31 (t, *J* = 6.2 Hz, 2H), 2.72 (s, 3H), 2.71 (s, 3H), 2.38 (m, 2H), 2.26 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3, 148.1 (q, *J* = 34.0 Hz), 146.7, 137.8, 135.6, 133.1, 130.6, 129.4 128.6, 127.0, 121.8, 121.7 (q, *J* = 275.2 Hz), 121.6, 120.6, 119.7, 106.9, 100.0, 99.9, 96.6 (q, *J* = 2.3 Hz), 68.3, 46.1, 26.8, 26.4, 21.9, 18.7 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -67.6 ppm. IR (thin film) 2932, 1576, 1368, 1280, 1254, 1180, 1132, 1110, 1093, 745, 715 cm^{-1}. HRMS (DART) m/z calcd. for $C_{24}H_{24}N_2OF_3^+$ $[M+H]^+$: 413.1835; found 413.1834.

(*Z*)-1-(hex-4-en-1-yl)-1*H*-indole (3q)



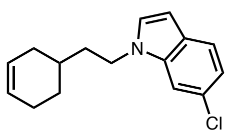
General procedure B was followed using (*Z*)-hexa-1,4-diene (0.062 g, 0.75 mmol, 1.5 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a colorless oil in 73% yield (Run 1: 70 mg, 70%; Run 2: 76 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.8 Hz, 1H), 7.42 (dd, *J* = 8.3 Hz, *J* = 1.0 Hz, 1H), 7.29 (td, *J* = 7.7 Hz, *J* = 1.2 Hz, 1H), 7.19 (td, *J* = 7.5 Hz, *J* = 1.0 Hz, 1H), 7.16 (d, *J* = 3.1 Hz, 1H), 6.57 (dd, *J* = 3.2 Hz, *J* = 0.9 Hz, 1H), 5.67–5.66 (m, 1H), 5.52–5.42 (m, 1H), 4.18 (t, *J* = 7.1 Hz, 2H), 2.14 (q, *J* = 7.2 Hz, 2H), 1.98 (p, *J* = 7.2 Hz, 2H), 1.66 (d, *J* = 6.7 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.0, 129.1, 128.7, 127.9, 125.3, 121.4, 121.0, 119.3, 109.5, 101.0, 45.8, 30.0, 24.2, 13.0 ppm. IR (thin film) 3013, 2927, 1511, 1463, 1334, 1315, 1172, 762, 736, 712 cm^{-1}. HRMS (DART) m/z calcd. for $C_{14}H_{18}N^+$ $[M+H]^+$: 200.1434; found 200.1430.

(*S*)-1-(3,7-dimethyloct-6-en-1-yl)-1*H*-indole (3r)



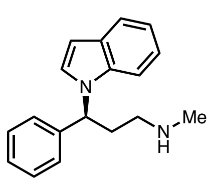
General procedure B was followed using (*S*)-3,7-dimethylocta-1,6-diene (0.104 g, 0.75 mmol, 1.5 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a colorless oil in 71% yield (Run 1: 86 mg, 67%; Run 2: 97 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.9 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.18–7.11 (m, 2H), 6.54 (d, *J* = 2.9 Hz, 1H), 5.13 (t, *J* = 7.1 Hz, 1H), 4.26–4.10 (m, 2H), 2.14–1.86 (m, 3H), 1.73 (s, 3H), 1.71 (m, 1H), 1.64 (m, 3H), 1.60–1.40 (m, 2H), 1.34–1.22 (m, 1H), 1.03 (d, *J* = 6.6 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.9, 131.5, 128.6, 127.6, 124.5, 121.3, 121.0, 119.2, 109.4, 101.0, 44.5, 37.2, 36.9, 30.2, 25.8, 25.4, 19.5, 17.7 ppm. IR (thin film) 2958, 2915, 1512, 1464, 1376, 1334, 1315, 1194, 1085, 1012, 762, 736 cm^{-1}. EA Calcd. for $C_{18}H_{25}N$: C, 84.65; H, 9.87. Found: C, 84.68; H, 9.84.

6-chloro-1-(2-(cyclohex-3-en-1-yl)ethyl)-1*H*-indole (3s)



General procedure B was followed using 4-vinylcyclohex-1-ene (0.081 g, 0.75 mmol, 1.5 equiv), and indole electrophile **2i** (0.16 g, 1.0 mmol, 1.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a colorless oil in 63% yield (Run 1: 79 mg, 61%; Run 2: 84 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.4 Hz, 1H), 7.33 (s, 1H), 7.14–7.00 (m, 2H), 6.46 (d, *J* = 3.0 Hz, 1H), 5.75–5.60 (m, 2H), 4.13 (t, *J* = 7.5 Hz, 2H), 2.25–2.00 (m, 3H), 1.90–1.70 (m, 4H), 1.67–1.55 (m, 1H), 1.40–1.25 (m, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.3, 128.4, 127.4, 127.1, 127.1, 125.9, 121.8, 119.9, 109.3, 101.3, 44.3, 36.6, 31.6, 31.1, 28.6, 24.9 ppm. IR (thin film) 3021, 2914, 2836, 1506, 1464, 1434, 1319, 901, 802, 716, 654 cm^{-1}. EA Calcd. for $C_{16}H_{18}ClN$: C, 73.98; H, 6.98. Found: C, 73.90; H, 6.93.

(*S*)-3-(1*H*-indol-1-yl)-*N*-methyl-3-phenylpropan-1-amine (3t)

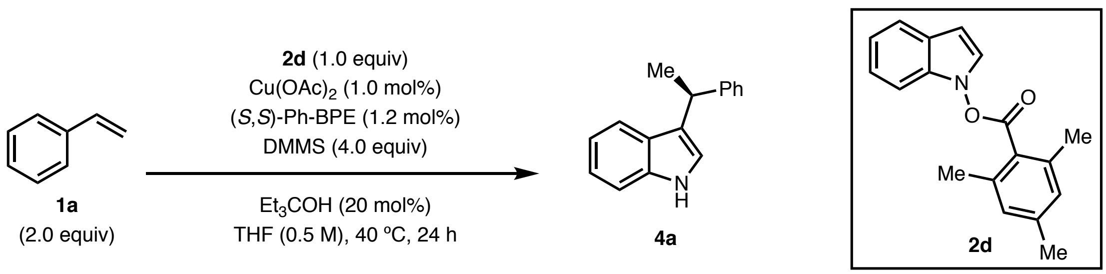


General procedure B was followed using (*E*)-*N*-methyl-3-phenylprop-2-en-1-amine (0.11 g, 0.50 mmol, 1.5 equiv). The crude material was first purified by column (EtOAc ~ EtOAc : MeOH = 5:1), and then by preparative thin layer chromatography (EtOAc : MeOH (2M Ammonium solution) = 10:1) to provide the title compound as an amorphous solid in 15% yield (~95% purity). ^{1}H NMR (400

MHz, $CDCl_3$) δ 7.63 (dt, J = 7.6 Hz, J = 1.0 Hz, 1H), 7.37–7.19 (m, 7H), 7.15 (ddd, J = 8.3 Hz, J = 7.0 Hz, J = 1.3 Hz, 1H), 7.09 (ddd, J = 8.0 Hz, J = 7.0 Hz, J = 1.1 Hz, 1H), 6.58 (d, J = 3.3 Hz, 1H), 5.70 (t, J = 7.8 Hz, 1H), 2.68–2.51 (m, 4H), 2.41 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0, 136.3, 128.8, 128.6, 127.7, 126.4, 124.9, 121.7, 121.0, 119.7, 109.9, 102.2, 57.2, 48.4, 35.6, 34.4 ppm. $[\alpha]_D^{25}$ = -0.128. **SFC** analysis: CEL2 (5:95 MeOH: $scCO_2$ to 20:80 MeOH: $scCO_2$ linear gradient over 8 min, 2.50 mL/min), 5.01 min (major), 5.41 min (minor), 50% ee. ***The absolute stereochemistry was assigned as (S) by comparison to the sign of the specific rotation to the same compound previously reported in the literature.***[6a]

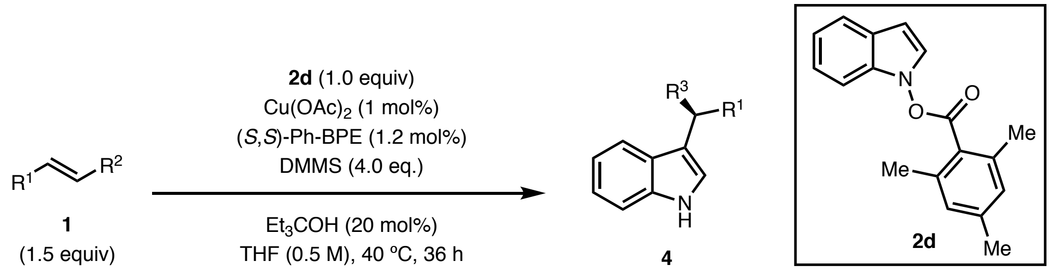
III. CuH-Catalyzed Enantioselective C3-Alkylation

Table S2. Optimization of CuH-catalyzed enantioselective C3-alkylation.[a]



Entry	Change from the "standard conditions"	Yield (%)	e.e. (%)	r.r.
1	none	79 (71)[b]	79	5.3:1
2	90 °C	59	67	2.1:1
3	5 mol% instead of 1 mol% $Cu(OAc)_2$	78	72	6.0:1
4	DEMS instead of DMMS	22	94	2.3:1
5	1.0 instead of 2.0 equiv of **1a**	37	83	4.9:1
6	0.1 M instead of 0.5 M	55	73	3.7:1
7	no Et_3COH	67	73	5.6:1

[a]Reactions were conducted on 0.1 mmol scale. Yields were determined by gas chromatography using dodecane as an internal standard. The ee was determined by SFC analysis. The regioisomeric ratio (rr) was determined by ^1H NMR analysis of the crude reaction mixture. [b]Isolated yield on a 0.5 mmol scale. [d]



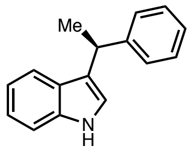
General Procedure C:

Preparation of CuH solution: In a nitrogen-filled glovebox, an oven-dried screw-top reaction tube (Fisherbrand, 13 x 100 mm, catalog no. 14-959035C) equipped with a magnetic stir bar was charged with $Cu(OAc)_2$ (0.9 mg, 0.005 mmol, 1 mol %) and (*S,S*)-Ph-BPE (3.1 mg, 0.006 mmol, 1.2 mol %). Anhydrous THF (0.5 mL) was added via a syringe and the reaction solution was stirred at room temperature (rt) for 15 min. $HSiMe(OMe)_2$ (0.25 mL, 2.0 mmol, 4.0 equiv) [*Note: see warning about* $HSiMe(OMe)_2$ *at the beginning of the experimental section*] was added sequentially via syringe and the resulting mixture was stirred at rt to afford a pale yellow to orange solution of CuH (about 15 min).

C3-Alkylation: In a nitrogen-filled glovebox, a second oven-dried screw-top reaction tube (Fisherbrand, 16 x 125 mm, catalog no. 1495925C) equipped with a stir bar was charged with indole electrophile **2d** (0.14 g, 0.50 mmol, 1.0 equiv). Anhydrous THF (0.25 mL), styrene (1.0 mmol, 2.0 equiv), and 3-ethyl-3-pentanol (14 µl, 0.10 mmol, 0.20 equiv) were added, followed by addition of the CuH solution via syringe from the first reaction tube to the stirred reaction mixture at rt. The reaction tube was sealed with a Teflon-lined screw cap and removed from the glovebox, placed in an oil bath preheated to 40 °C and stirred for 20 h. After cooling to rt, the reaction cap was removed and dodecane (50 µL) was added as an internal standard. An aliquot of the solution was transferred into a GC vial and diluted with EtOAc. GC analysis was used for determination of the conversion, yield and regioselectivity. Sat. NH_4F in MeOH (5 mL) was slowly added to the reaction tube to quench the reaction as part of the workup (*Caution*: gas evolution observed). The mixture was stirred uncapped for 30 min, transferred to a 20 mL scintillation vial, the reaction tube was rinsed with EtOAc (2 mL × 3), and concentrated *in vacuo* with the aid of a rotary evaporator. The resulting residue was redissolved in EtOAc, filtered through a shot pad of Celite and washed with additional EtOAc (about 100 mL). The collected EtOAc solution was concentrated *in vacuo* with the aid of a rotary evaporator, and the crude material was purified by silica gel column chromatography.

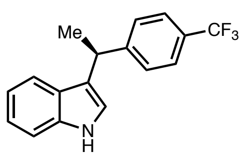
Characterization Data for C3-Alkylated Chiral Indoles

(*S*)-3-(1-phenylethyl)-1*H*-indole (4a)



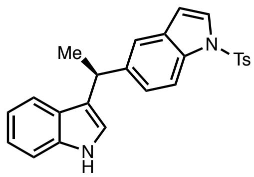
The general procedure C was followed using styrene (0.104 g, 1.0 mmol, 2.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 5:1) to provide the title compound as a white solid in 71% yield (Run 1: 74 mg, 67%, 76% ee; Run 2: 83 mg, 75%, 76% ee) with 6:1 regioselectivity (C3:N). m.p. 98-101 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.35–6.85 (m, 10H), 4.28 (q, *J* = 7.2 Hz, 1H), 1.61 (d, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.8, 136.6, 128.3, 127.5, 126.9, 125.9, 122.0, 121.5, 121.1, 119.7, 119.2, 111.0, 34.0, 22.4 ppm. IR (thin film) 3406, 2966, 2869, 1490, 1456, 1223, 10-95, 1010, 739, 699 cm^{-1}. HRMS (DART) m/z calcd. for $C_{16}H_{16}N^+$ $[M+H]^+$: 222.1277; found 222.1277. $[\alpha]_D^{22}$ = -6.8. **SFC** analysis: ADH (5:95 MeOH: $scCO_2$ to 20:80 MeOH: $scCO_2$ linear gradient over 15 min, 2.50 mL/min), 8.04 min (minor), 8.93 min (major), 76% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **4e**.

(*S*)-3-(1-(4-(trifluoromethyl)phenyl)ethyl)-1*H*-indole (4b)



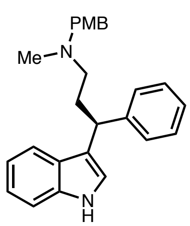
The general procedure C was followed using 1-(trifluoromethyl)-4-vinylbenzene (0.172 g, 1.0 mmol, 2.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 5:1) to provide the title compound as a white solid in 61% yield (Run 1: 84 mg, 58%, 65% ee; Run 2: 93 mg, 64%, 65% ee) with >20:1 regioselectivity (C3:N). m.p. 92-96 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.58 (d, *J* = 8.1 Hz, 2H), 7.45 (d, *J* = 8.1 Hz, 2H), 7.39 (t, *J* = 8.6 Hz, 2H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.14–7.05 (m, 2H), 4.49 (q, *J* = 7.2 Hz, 1H), 1.78 (d, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.0, 136.7, 128.3 (q, *J* = 32.2 Hz), 127.8, 126.7, 125.3 (q, *J* = 3.8 Hz), 124.4 (q, *J* = 271.8 Hz), 122.3, 121.2, 120.4, 119.5, 119.4, 111.2, 36.9, 22.2 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.1 ppm. IR (thin film) 3412, 2968, 1456, 1321, 1161, 1108, 1067, 1015, 841, 767, 740 cm^{-1}. HRMS (DART) m/z calcd. for $C_{17}H_{15}NF_3^+$ $[M+H]^+$: 290.1151; found 290.1145. $[\alpha]_D^{22}$ = -5.4. **SFC** analysis: ADH (5:95 MeOH: $scCO_2$ to 20:80 MeOH: $scCO_2$ linear gradient over 15 min, 2.50 mL/min), 5.53 min (minor), 5.94 min (major), 65% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **4e**.

(*S*)-5-(1-(1*H*-indol-3-yl)ethyl)-1-tosyl-1*H*-indole (4c)



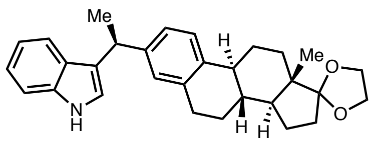
The general procedure C was followed using 1-tosyl-5-vinyl-1*H*-indole (0.297 g, 1.0 mmol, 2.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 3:1) to provide the title compound as a foam solid in 55% yield (Run 1: 106 mg, 51%, 85% ee; Run 2: 122 mg, 59%, 85% ee) with 3:1 regioselectivity (C3:N). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.76 (d, *J* = 8.6 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.38 (d, *J* = 3.7 Hz, 1H), 7.30 (s, 1H), 7.20 (d, *J* = 8.0 Hz, 1H), 7.15 (d, *J* = 8.3 Hz, 2H), 7.05–6.95 (m, 3H), 6.85–6.78 (m, 2H), 6.40 (d, *J* = 3.6 Hz, 1H), 4.30 (q, *J* = 7.2 Hz, 1H), 2.12 (s, 3H), 1.56 (d, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9, 142.3, 136.7, 135.4, 133.4, 131.0, 129.9, 126.9, 126.8, 126.3, 124.7, 122.0, 121.5, 121.3, 119.8, 119.7, 119.2, 113.3, 111.2, 109.2, 36.9, 22.9, 21.6 ppm. IR (thin film) 3422, 2962, 1456, 1367, 1188, 1170, 1142, 1123, 1092, 812, 703, 676 cm^{-1}. HRMS (DART) m/z calcd. for $C_{25}H_{23}N_2O_2S^+$ $[M+H]^+$: 415.1475; found 415.1460. $[\alpha]_D^{22}$ = -12.8. **HPLC** analysis (ADH, 20% IPA in hexanes, 1.0 mL/min, 254 nm) indicated 85% ee: t_R (major) = 18.7 min, t_R (minor) = 25.1 min. The absolute stereochemistry was assigned as (*S*) by analogy to **4e**.

(*S*)-3-(1*H*-indol-3-yl)-*N*-(4-methoxybenzyl)-*N*-methyl-3-phenylpropan-1-amine (4d)



The general procedure C was followed using (*E*)-*N*-(4-methoxybenzyl)-*N*-methyl-3-phenylprop-2-en-1-amine (0.267 g, 1.0 mmol, 2.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 1:1) to provide the title compound as a colorless oil in 61% yield (Run 1: 113 mg, 59%, 67% ee; Run 2: 121 mg, 63%, 67% ee) with 4:1 regioselectivity (C3:N). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.37–7.10 (m, 11H), 6.81 (d, *J* = 8.6 Hz, 2H), 4.30 (t, *J* = 7.0 Hz, 1H), 3.80 (s, 3H), 3.44 (s, 2H), 2.60–2.20 (m, 4H), 2.19 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.6, 145.2, 136.5, 130.3, 128.3, 127.9, 127.0, 126.0, 122.0, 121.0, 119.5, 119.2, 113.6, 111.0, 61.5, 55.5, 55.3, 41.9, 40.5, 33.7 ppm. IR (thin film) 3417, 2934, 2834, 2793, 1510, 1455, 1243, 1032, 740, 700 cm^{-1}. HRMS (DART) m/z calcd. for $C_{26}H_{29}N_2O^+$ $[M+H]^+$: 385.2274; found 385.2287. $[\alpha]_D^{23}$ = +14.2. **SFC** analysis: ADH (5:95 MeOH (0.1% Et_2NH): $scCO_2$ to 30:70 MeOH (0.1% Et_2NH): $scCO_2$ linear gradient over 25 min, 2.50 mL/min), 11.82 min (minor), 12.38 min (major), 67% ee. The absolute stereochemistry was assigned as (*S*) by analogy to **4e**.

3-((*S*)-1-((8*R*,9*S*,13*S*,14*S*)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydrospiro[cyclopenta[*a*]phenanthrene-17,2'-[1,3]dioxolan]-2-yl)ethyl)-1*H*-indole (4e)



The general procedure C was followed using (8*R*,9*S*,13*S*,14*S*)-13-methyl-2-vinyl-6,7,8,9,11,12,13,14,15,16-decahydrospiro[cyclopenta[*a*]phenanthrene-17,2'-[1,3]dioxolane] (0.325 g, 1.0 mmol, 2.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 3:1) to provide the title compound as a white solid in 62% yield (Run 1: 126 mg, 57%, 84% ee; Run 2: 139 mg, 63%, 84% ee) with 5:1 regioselectivity (C3:N). m.p. 169-173 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 7.24–6.98 (m, 6H), 4.34 (q, *J* = 7.1 Hz, 1H), 4.05–3.85 (m, 4H), 2.93–2.75 (m, 2H), 2.40–2.20 (m, 2H), 2.12–2.00 (m, 1H), 1.95–1.75 (m, 4H), 1.71 (d, *J* = 7.2 Hz, 3H), 1.70–1.25 (m, 6H), 0.90 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.9, 137.9, 136.6, 136.5, 127.8, 127.0, 125.2, 124.8, 121.9, 121.8, 121.0, 119.8, 119.5, 119.1, 111.0, 65.3, 64.6, 49.6, 46.2, 44.0, 38.9, 36.4, 34.3, 30.8, 29.7, 27.1, 25.9, 22.5, 22.4, 14.4 ppm. IR (thin film) 3414, 2933, 2870, 1456, 1158, 1102, 1043, 1011, 906, 728, 647 cm^{-1}. HRMS (DART) m/z calcd. for $C_{30}H_{35}NO_2^+$ $[M+H]^+$: 442.2741; found 442.2728. $[\alpha]_D^{22}$ = -4.4. **HPLC** analysis (ADH, 10% IPA in hexanes, 1.0 mL/min, 254 nm) indicated 84% ee: t_R (major) = 11.1 min, t_R (minor) = 9.5 min. The absolute configuration of **4e** was determined by X-ray crystallographic analysis. CCDC 1854713 contains the supplementary crystallographic data for this diastereomer. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Single Crystal X-ray Diffraction Data for 4e (P18006_t4).

Crystal of the complex **4e** was obtained by layering *n*-pentane upon the DCM solution of **4e** at ambient conditions (room temperature, air).

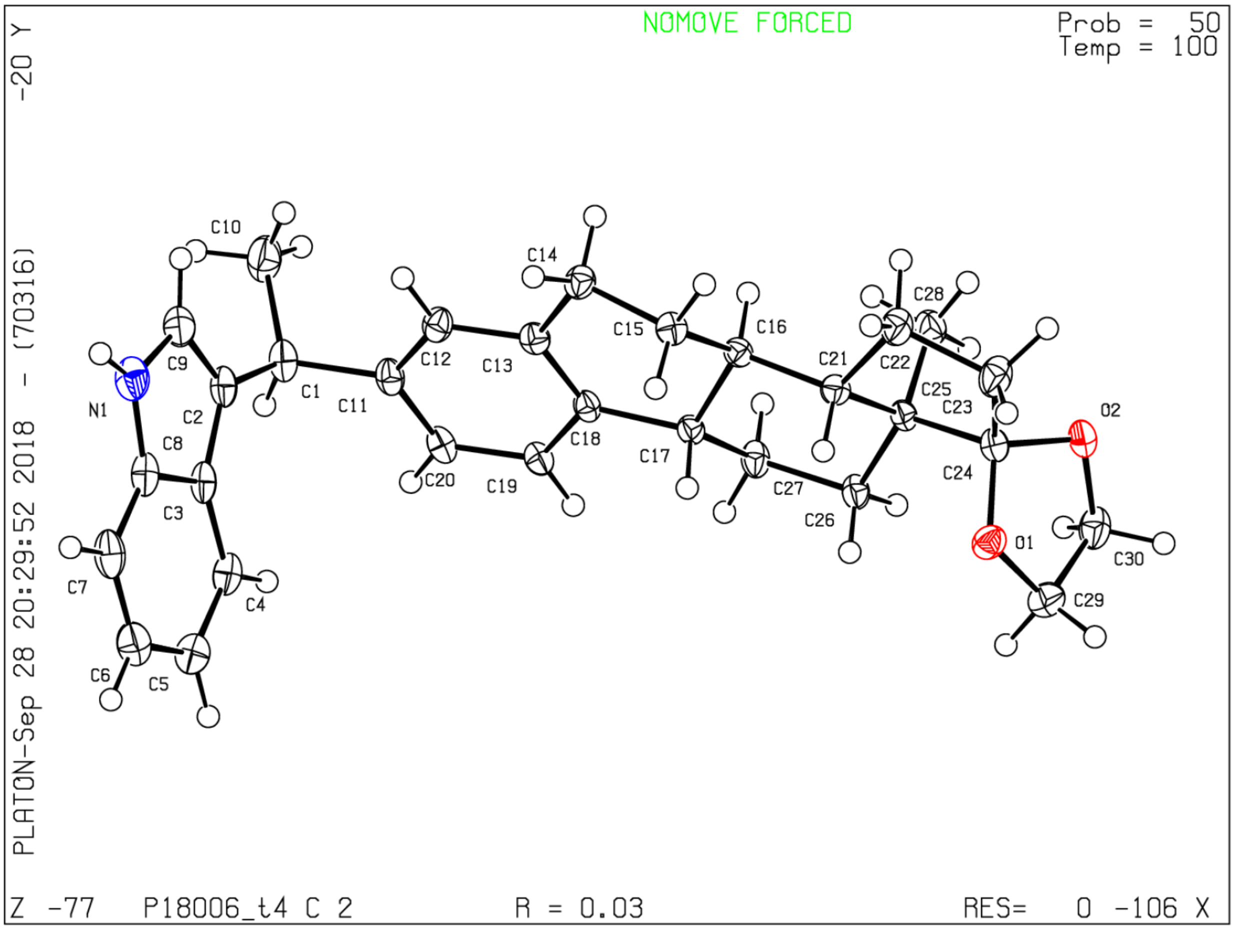


Table S3. Crystal data and structure refinement for 4e (P18006_t4).

Identification code	P18006_t4	
Empirical formula	C30 H35 N O2	
Formula weight	441.59	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2	
Unit cell dimensions	a = 18.0835(5) Å	a= 90°.
b = 7.9265(2) Å	b= 114.1748(13)°.	

c = 18.2000(5) Å	g = 90°.
Volume	2379.98(11) $Å^3$
Z	4
Density (calculated)	1.232 Mg/m^3
Absorption coefficient	0.588 mm^{-1}
F(000)	952
Crystal size	0.160 x 0.075 x 0.030 mm^3
Theta range for data collection	4.913 to 74.460°.
Index ranges	?<=h<=?, ?<=k<=?, ?<=l<=?
Reflections collected	4888
Independent reflections	4888 [R(int) = ?]
Completeness to theta = 67.679°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4888 / 2 / 303
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0277, wR2 = 0.0723
R indices (all data)	R1 = 0.0284, wR2 = 0.0728
Absolute structure parameter	0.06(6)
Extinction coefficient	n/a
Largest diff. peak and hole	0.202 and -0.149 e.$Å^{-3}$

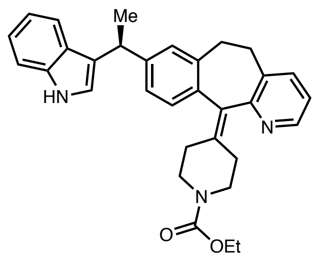
The structure factors and structural output was checked using IUCr's CheckCIF routine. The routine indicated a B-level alert in the structure. The explanation for the alert is attached below.

Alert level B

```
PLAT411_ALERT_2_B Short Inter H...H Contact  H17      ..H17      .       1.89 Ang.
                                                  1-x,y,1-z  =     2_656 Check
```

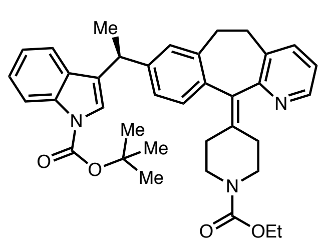
Author Response: Residual density for this hydrogen atom is clearly visible in the difference Fourrier synthesis and this hydrogen atom needs to be in this position for chemical reasons.

Ethyl (*S*)-4-(8-(1-(1*H*-indol-3-yl)ethyl)-5,6-dihydro-11*H*-benzo[5,6]cyclohepta[1,2-*b*]pyridin-11-ylidene)piperidine-1-carboxylate (4f)



The general procedure C was followed using ethyl 4-(8-vinyl-5,6-dihydro-11*H*-benzo[5,6]cyclohepta[1,2-*b*]pyridin-11-ylidene)piperidine-1-carboxylate (0.375 g, 1.0 mmol, 2.0 equiv). The crude material was purified by flash column chromatography (CH_2Cl_2 ~ CH_2Cl_2 : MeOH = 30:1) to provide the title compound as an oil in 41% yield (Run 1: 88 mg, 36%; Run 2: 113 mg, 46%) with 5:1 regioselectivity (C3:N). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (m, 1H), 8.09 (m, 1H), 7.48–7.38 (m, 2H), 7.34 (dd, J = 8.1 Hz, J = 2.7 Hz, 1H), 7.19–6.97 (m, 7H), 4.31 (q, J = 7.2 Hz, 1H), 4.13 (q, J = 7.1 Hz, 2H), 3.90–3.70 (m, 2H), 3.45–3.25 (m, 2H), 3.20–3.05 (m, 2H), 2.90–2.70 (m, 2H), 2.55–2.20 (m, 4H), 1.67 (d, J = 7.1 Hz, 3H), 1.24 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.0, 155.6, 146.3, 146.0, 137.3, 137.2, 136.6, 136.3, 135.3, 134.0, 129.4, 129.3, 128.4, 128.1, 126.9, 125.1, 124.9, 122.1, 121.8, 121.3, 121.2, 121.2, 121.0, 119.6, 119.0, 111.1, 61.3, 45.0, 44.9, 36.6, 32.1, 31.7, 31.7, 30.7, 30.6, 22.5, 22.4, 14.7 ppm. IR (thin film) 2967, 2920, 1695, 1436, 1264, 1226, 1114, 767, 734, 701 cm^{-1}. HRMS (DART) m/z calcd. for $C_{32}H_{34}N_3O_2^+$ [M+H]$^+$: 492.2646; found 492.2620. $[\alpha]_D^{23}$ = -28.4. The absolute stereochemistry was assigned as (*S*) by analogy to **4e**.

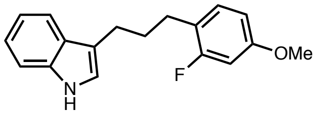
***tert*-butyl (S)-3-(1-(11-(1-(ethoxycarbonyl)piperidin-4-ylidene)-6,11-dihydro-5*H*-benzo[5,6]cyclohepta[1,2-*b*]pyridin-8-yl)ethyl)-1*H*-indole-1-carboxylate (4f')**



The crude material was purified by flash column chromatography (CH_2Cl_2 ~ CH_2Cl_2 : MeOH = 30:1) to provide the title compound as a purple liquid in 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, J = 4.8 Hz, 1H), 8.07 (m, 1H), 7.41 (m, 2H), 7.33–7.20 (m, 2H), 7.13–6.97 (m, 5H), 4.20 (m, 1H), 4.11 (m, 2H), 3.78 (m, 2H), 3.39–3.26 (m, 2H), 3.12 (m, 2H), 2.82–2.69 (m, 2H), 2.55–2.14 (m, 4H), 1.65 (m, 12H), 1.24 (m, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 157.9, 155.5, 146.5, 144.5, 137.6, 137.5, 137.3, 137.2, 136.9, 136.8, 136.5, 135.7, 135.2, 133.8, 130.1, 129.5, 129.4, 128.2, 127.9, 125.5, 125.4, 125.2, 124.9, 124.2, 122.3, 122.3, 122.2, 122.0, 119.9, 119.9, 115.2, 115.2, 83.5, 65.9, 61.3, 60.4, 45.0, 44.8, 36.4, 32.1, 32.0, 31.8, 31.7, 31.7, 30.7, 30.5, 28.3, 22.0, 21.1, 15.3, 14.7, 14.2 ppm. IR (thin film) 3414, 2933, 2870, 1456, 1158, 1102, 1043, 1011, 906, 728, 647 cm^{-1}. HRMS (DART) m/z calcd. for $C_{37}H_{42}N_3O_4^+$ [M+H]$^+$: 592.3170; found 592.3134. $[\alpha]_D^{23}$ = +35.2. **SFC** analysis: OJH (5:95

MeOH (0.1% Et_2NH): $scCO_2$ to 10:90 MeOH (0.1% Et_2NH): $scCO_2$ linear gradient over 20 min, 2.50 mL/min), 12.30 min (major), 13.07 min (minor), 81% ee.

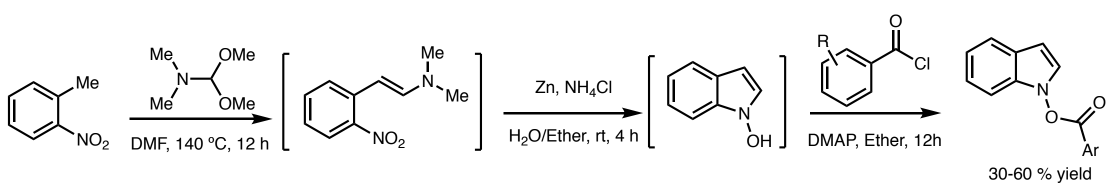
3-(3-(2-fluoro-4-methoxyphenyl)propyl)-1*H*-indole (4g)



The general procedure C was followed using 1-allyl-2-fluoro-4-methoxybenzene (0.166 g, 1.0 mmol, 2.0 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 5:1) to provide the title compound as a white solid in 32% yield (Run 1: 43 mg, 30%; Run 2: 48 mg, 34%) with > 20:1 regioselectivity (C3:N). m.p. 86-89 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.60 (d, *J* = 8.2 Hz, 1H), 7.36 (dt, *J* = 8.1 Hz, *J* = 0.9 Hz, 1H), 7.22–7.16 (m, 1H), 7.14–7.06 (m, 2H), 7.02–6.98 (m, 1H), 6.67–6.57 (m, 2H), 3.78 (s, 3H), 2.80 (t, *J* = 7.6 Hz, 2H), 2.69 (t, *J* = 7.6 Hz, 2H), 2.02 (p, *J* = 7.6 Hz, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.6 (d, *J* = 244.3 Hz), 159.0 (d, *J* = 10.9 Hz), 136.4, 130.8 (d, *J* = 7.3 Hz), 127.6, 121.9, 121.1, 119.1, 119.0, 116.5, 111.0, 109.5 (d, *J* = 3.0 Hz), 101.6, 101.4, 55.5, 30.6, 28.2 (d, *J* = 1.4 Hz), 24.7 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.6 ppm. IR (thin film) 3415, 2930, 2859, 2357, 1625, 1506, 1456, 1283, 1141, 1096, 741, 668 cm^{-1}. HRMS (DART) m/z calcd. for $C_{18}H_{19}NOF^+$ $[M+H]^+$: 284.1445; found 284.1438.

IV. Preparation of Indole Electrophile Reagents

Method A (reduction conditions):[2]



2

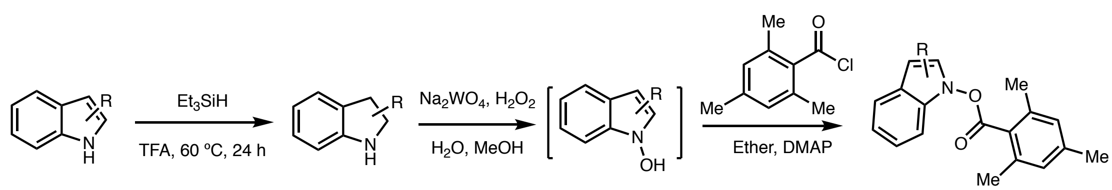
General Procedure:

Hydroxyindole (ether solution) synthesis: A 300 mL round bottom flask equipped with a magnetic stir bar, was charged with 2-nitrotoluene (4.72 mL, 40.0 mmol, 1.0 equiv) and *N*,*N*-dimethylformamide dimethyl acetal (14.3 g, 120 mmol, 3.0 equiv). *N,N*-dimethylformamide (DMF, 90 mL) was added and the solution was heated to 140 ºC for 12 h with stirring. After cooling to rt, the solvent was evaporated under reduced pressure with the aid of a rotary evaporator. The red-colored residue (crude enamine) was then dissolved in Et_2O (240 mL), followed by the addition of zinc powder (52.3 g, 800 mmol, 20.0 equiv), and a solution of NH_4Cl

(7.63 g, 144 mmol, 3.6 equiv) in H_2O (50 mL). The mixture was vigorously stirred for about 4 h at rt until the color of the solution turned yellow from red (*Caution*: hydrogen gas evolution was observed at the beginning of the reaction). The mixture was then filtered through a fritted funnel. The filtrate was collected and the organic phase was separated from the aqueous phase with a separation funnel. The organic layer (crude 1-hydroxyindole in Et_2O) was dried over anhydrous Na_2SO_4 and filtered.

Synthesis of indole electrophiles from hydroxyindoles: To the resulting dried ether solution from above, under argon, was added 4-(dimethylamino)pyridine (5.86 g, 48.0 mmol, 1.2 equiv) followed by the addition of the corresponding benzoyl chloride (44.0 mmol, 1.1 equiv). The reaction mixture was then stirred under argon overnight at rt. Upon completion, the mixture was diluted with Et_2O and quenched with a saturated aqueous $NaHCO_3$ solution. The aqueous phase was extracted with Et_2O and the combined organic phases were dried over Na_2SO_4, filtered and concentrated under reduced pressure with the aid of a rotary evaporator. The crude material was purified by flash column chromatography to provide the corresponding indole electrophile reagents.

Method B (oxidation conditions):[3,4]



General Procedure:

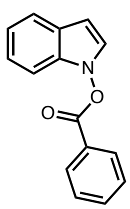
Indoline synthesis: Triethylsilane (4.65 g, 40.0 mmol, 2.0 equiv) was added to a solution of the indole derivative (20.0 mmol, 1.0 equiv) in trifluoroacetic acid (TFA, 60 mL) and the mixture was stirred at 60 ºC for 24 h. After cooling to rt, TFA was removed by distillation under reduced pressure. The crude residue was cooled to 0 ºC with an ice water bath, neutralized with saturated $NaHCO_3$ aqueous solution (100 mL), and extracted with CH_2Cl_2 (50 mL × 3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure with the aid of a rotary evaporator. The crude material was purified by flash column chromatography to provide the corresponding indoline derivative.

Hydroxyindole (ether solution) synthesis: A solution of sodium tungstate dihydrate (0.66 g, 2.0 mmol, 0.2 equiv) in water (10 mL) was added to a solution of the indoline derivative (10 mmol, 1.0 equiv) in MeOH (50 mL) and the mixture was cooled to 0 ºC in an ice/water bath. Hydrogen peroxide aqueous solution (30%, 10 equiv) was added to the resultant solution slowly at 0 ºC while stirring (10 min). Upon the complete addition, the ice bath was removed and the reaction mixture was stirred for another 10 min before quenched with water (200 mL) and extracted with Et_2O (100 mL × 3). The aqueous solution was treated with sat. sodium sulfite solution (Na_2SO_3, 50 equiv) to quench the excess hydrogen peroxide. The combined organic layers were concentrated under reduced pressure with the aid of a rotary evaporator until all the MeOH was removed. The residue was redissolved in Et_2O (100 mL), washed with brine, and dried over Na_2SO_4.

Indole electrophile synthesis from hydroxyindoles: see Method A.

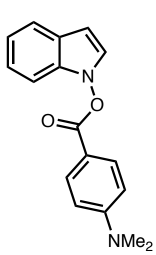
Characterization Data for Indole Electrophiles

1*H*-indol-1-yl benzoate (2a)



Method A was followed using 1-methyl-2-nitrobenzene (5.49 g, 40.0 mmol, 1.0 equiv) and benzoyl chloride (6.19 g, 44 mmol, 1.1 equiv). The crude material was first purified by a silica gel column (Hexanes ~ Hexanes : EtOAc = 10:1), and subsequently an aluminum oxide (activated, basic, Brockmann I) column (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a white solid in 51% yield (4.84 g). (The extra basic alumina column was performed to get rid of benzoic anhydride which was difficult to separate from **2a** on silica gel). m.p. 58-60 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (dd, *J* = 8.3 Hz, *J* = 1.4 Hz, 2H), 7.80–7.72 (m, 1H), 7.68 (d, *J* = 7.9 Hz, 1H), 7.61 (t, *J* = 7.8 Hz, 2H), 7.36–7.17 (m, 4H), 6.60 (d, *J* = 3.2 Hz, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.7, 134.7, 134.3, 130.3, 129.0, 126.4, 125.5, 124.8, 123.1, 121.4, 120.9, 108.5, 100.4 ppm. IR (thin film) 3059, 1766, 1451, 1319, 1232, 1179, 1037, 996, 736, 698 cm^{-1}. EA Calcd. for $C_{15}H_{11}NO_2$: C, 75.94; H, 4.67. Found: C, 76.12; H, 4.86.

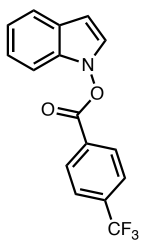
1*H*-indol-1-yl 4-(dimethylamino)benzoate (2b)



Method A was followed using 1-methyl-2-nitrobenzene (5.49 g, 40.0 mmol, 1.0 equiv) and 4-(dimethylamino)benzoyl chloride (8.08 g, 44 mmol, 1.1 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 5:1) to provide the title compound as a white solid in 36% yield (4.04 g). m.p. 138-140 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 9.1 Hz, 2H), 7.63

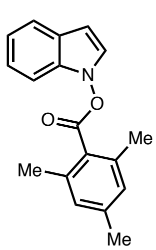
(dt, J = 7.8 Hz, J = 1.0 Hz, 1H), 7.31–7.19 (m, 3H), 7.17–7.10 (m, 1H), 6.73 (d, J = 9.1 Hz, 2H), 6.53 (dd, J = 3.5 Hz, J = 0.9 Hz, 1H), 3.11 (s, 6H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.9, 154.2, 134.2, 132.2, 125.6, 124.6, 122.8, 121.2, 120.4, 112.0, 110.9, 108.5, 99.5, 40.1 ppm. IR (thin film) 2915, 1748, 1599, 1531, 1372, 1258, 1169, 1034, 980, 753 cm^{-1}. EA Calcd. for $C_{17}H_{16}N_2O_2$: C, 72.84; H, 5.75. Found: C, 72.89; H, 5.88.

1*H*-indol-1-yl 4-(trifluoromethyl)benzoate (2c)



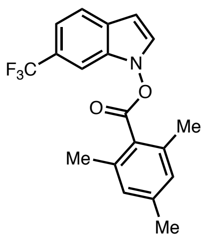
Method A was followed using 1-methyl-2-nitrobenzene (5.49 g, 40.0 mmol, 1.0 equiv) and 4-(trifluoromethyl)benzoyl chloride (9.18 g, 44 mmol, 1.1 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a white solid in 45% yield (5.49 g). m.p. 103-108 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, J = 3.5 Hz, 2H), 7.77 (d, J = 8.3 Hz, 2H), 7.57 (d, J = 7.8 Hz, 1H), 7.25–7.15 (m, 3H), 7.14–7.07 (m, 1H), 6.50 (d, J = 8.1 Hz, 1H), ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.6, 136.0 (q, J = 32.9 Hz), 134.5, 130.7, 126.4 (q, J = 3.6 Hz), 125.6, 124.9, 124.7, 123.3 (q, J = 273.0 Hz), 123.4, 121.5, 121.2, 108.5, 101.0 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.3 ppm. IR (thin film) 1775, 1412, 1321, 1233, 1171, 1128, 1065, 1039, 1000, 858, 736, 695 cm^{-1}. EA Calcd. for $C_{16}H_{10}F_3NO_2$: C, 62.96; H, 3.30. Found: C, 63.12; H, 3.48.

1*H*-indol-1-yl 2,4,6-trimethylbenzoate (2d)



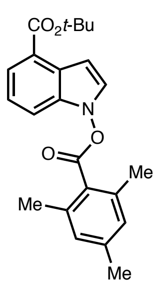
Method A was followed using 1-methyl-2-nitrobenzene (5.49 g, 40.0 mmol, 1.0 equiv) and 2,4,6-trimethylbenzoyl chloride (8.04 g, 44 mmol, 1.1 equiv). The crude material was first purified by a silica gel column (Hexanes ~ Hexanes : EtOAc = 10:1), and subsequently an aluminum oxide (activated, basic, Brockmann I) column (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a white solid in 41% yield (4.58 g). (The extra basic alumina column was performed to get rid of 2,4,6-trimethylbenzoic anhydride which was difficult to separate from **2d** on silica gel). m.p. 80-82 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (dt, J = 7.9 Hz, J = 1.0 Hz, 1H), 7.38 (dd, J = 8.1 Hz, J = 1.1 Hz, 1H), 7.35–7.30 (m, 1H), 7.29 (d, J = 3.5 Hz, 1H), 7.21 (ddd, J = 8.1 Hz, J = 7.0 Hz, J = 1.2 Hz, 1H), 7.01 (s, 2H), 6.60 (dd, J = 3.5 Hz, J = 0.9 Hz, 1H), 2.56 (s, 6H), 2.38 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 141.3, 136.4, 134.3, 128.9, 126.4, 125.3, 124.9, 123.2, 121.4, 120.9, 108.7, 100.4, 21.3, 20.3 ppm. IR (thin film) 1780, 1610, 1445, 1222, 1155, 1028, 982, 946, 734, 699 cm^{-1}. EA Calcd. for $C_{18}H_{17}NO_2$: C, 77.40; H, 6.13. Found: C, 77.49; H, 6.06.

6-(trifluoromethyl)-1*H*-indol-1-yl 2,4,6-trimethylbenzoate (2e)



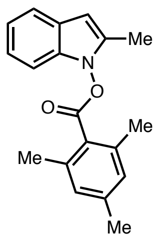
Method A was followed using 1-methyl-2-nitro-4-(trifluoromethyl)benzene (2.05 g, 10.0 mmol, 1.0 equiv) and 2,4,6-trimethylbenzoyl chloride (2.01 g, 11 mmol, 1.1 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a white solid in 38% yield (1.32 g). m.p. 66-68 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.3 Hz, 1H), 7.66 (s, 1H), 7.43–7.37 (m, 2H), 7.00 (s, 2H), 6.63 (dd, *J* = 3.5 Hz, *J* = 0.9 Hz, 1H), 2.53 (s, 6H), 2.36 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 124.8 (d, *J* = 271.6 Hz) 167.7, 141.6, 136.6, 132.8, 129.0, 127.5, 126.9, 125.7, 125.4 (d, *J* = 32.2 Hz), 125.4 (d, *J* = 32.2 Hz), 121.9, 117.4 (q, *J* = 3.6 Hz), 106.1 (q, *J* = 4.4 Hz), 100.2, 21.3, 20.3 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.1 ppm. IR (thin film) 1786, 1611, 1449, 1228, 1280, 1224, 1154, 1114, 1053, 979 cm^{-1}. HRMS (DART) m/z calcd. for $C_{19}H_{17}NO_2F_3^+$ $[M+H]^+$: 348.1206; found 348.1197.

***tert*-butyl 1-((2,4,6-trimethylbenzoyl)oxy)-1*H*-indole-4-carboxylate (2f)**



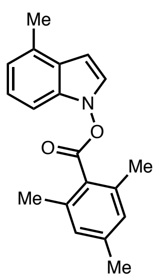
Method A was followed using *tert*-butyl 2-methyl-3-nitrobenzoate (2.37 g, 10.0 mmol, 1.0 equiv) and 2,4,6-trimethylbenzoyl chloride (2.01 g, 11.0 mmol, 1.1 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 6:1) to provide the title compound as a white solid in 32% yield (1.21 g). m.p. 66-68 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 7.4 Hz, *J* = 1.1 Hz, 1H), 7.50 (d, *J* = 8.2 Hz, 1H), 7.36 (d, *J* = 3.5 Hz, 1H), 7.31 (t, *J* = 7.8 Hz, 1H), 7.20 (dd, *J* = 3.6 Hz, *J* = 1.0 Hz, 1H), 6.99 (s, 2H), 2.53 (s, 6H), 2.36 (s, 3H), 1.68 (s, 9H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.8, 166.3, 141.4, 136.5, 134.7, 129.0, 126.5, 126.1, 124.2, 124.1, 124.0, 122.4, 112.8, 101.5, 81.1, 28.4, 21.3, 20.3 ppm. IR (thin film) 2976, 2925, 1786, 1289, 1226, 1162, 1141, 982, 750 cm^{-1}. HRMS (DART) m/z calcd. for $C_{23}H_{26}NO_4^+$ $[M+H]^+$: 380.1856; found 380.1860.

2-methyl-1*H*-indol-1-yl 2,4,6-trimethylbenzoate (2g)



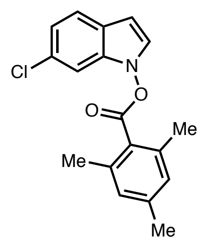
Method B was followed using 2-methylindoline (1.33 g, 10.0 mmol, 1.0 equiv) and 2,4,6-trimethylbenzoyl chloride (2.01 g, 11 mmol, 1.1 equiv). The crude material was first purified by a silica gel column (Hexanes ~ Hexanes : EtOAc = 10:1), and subsequently an aluminum oxide (activated, basic, Brockmann I) column (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a white solid in 28% yield (0.821 g). (The extra basic alumina column was performed to get rid of 2,4,6-trimethylbenzoic anhydride which was difficult to separate from **2g** on silica gel). m.p. 66-68 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, J = 7.8 Hz, 1H), 7.31 (d, J = 8.0 Hz, 1H), 7.22 (t, J = 7.8 Hz, 1H), 7.15 (t, J = 7.5 Hz, 1H), 7.01 (s, 2H), 6.31 (s, 1H), 2.61 (s, 6H), 2.49 (s, 3H), 2.40 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 141.3, 136.7, 135.2, 134.7, 129.1, 126.4, 124.9, 122.0, 120.8, 120.3, 108.3, 98.4, 21.3, 20.8, 12.1 ppm. IR (thin film) 2921, 1777, 1611, 1449, 1220, 1155, 785, 738 cm^{-1}. EA Calcd. for $C_{19}H_{19}NO_2$: C, 77.79; H, 6.53. Found: C, 77.94; H, 6.38.

4-methyl-1*H*-indol-1-yl 2,4,6-trimethylbenzoate (2h)



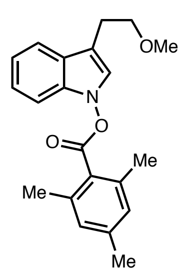
Method A was followed using 1,2-dimethyl-3-nitrobenzene (1.51 g, 10.0 mmol, 1.0 equiv) and 2,4,6-trimethylbenzoyl chloride (2.01 g, 11 mmol, 1.1 equiv). The crude material was first purified by a silica gel column (Hexanes ~ Hexanes : EtOAc = 10:1), and subsequently an aluminum oxide (activated, basic, Brockmann I) column (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a white solid in 43% yield (1.23 g). (The extra basic alumina column was performed to get rid of 2,4,6-trimethylbenzoic anhydride which was difficult to separate from **2h** on silica gel). m.p. 105-108 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, J = 2.1 Hz, 1H), 7.23–7.19 (m, 2H), 7.05–6.95 (m, 3H), 6.61 (d, J = 3.5 Hz, 1H), 2.60 (s, 3H), 2.56 (s, 6H), 2.38 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 141.2, 136.4, 133.84, 130.8, 128.9, 126.4, 124.5, 124.4, 123.3, 121.0, 106.2, 98.7, 21.3, 20.3, 18.3 ppm. IR (thin film) 2920, 1780, 1610, 1453, 1226, 1153, 1001, 982, 742, 697 cm^{-1}. EA Calcd. for $C_{19}H_{19}NO_2$: C, 77.79; H, 6.53. Found: C, 78.01; H, 6.76.

6-chloro-1*H*-indol-1-yl 2,4,6-trimethylbenzoate (2i)



Method A was followed using 4-chloro-1-methyl-2-nitrobenzene (1.72 g, 10.0 mmol, 1.0 equiv) and 2,4,6-trimethylbenzoyl chloride (2.01 g, 11 mmol, 1.1 equiv). The crude material was first purified by a silica gel column (Hexanes ~ Hexanes : EtOAc = 10:1), and subsequently an aluminum oxide (activated, basic, Brockmann I) column (Hexanes ~ Hexanes : EtOAc = 10:1) to provide the title compound as a white solid in 36% yield (1.13 g). (The extra basic alumina column was performed to get rid of 2,4,6-trimethylbenzoic anhydride which was difficult to separate from **2i** on silica gel). m.p. 75-77 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.4 Hz, 1H), 7.33 (s, 1H), 7.26 (d, *J* = 3.5 Hz, 1H), 7.17 (dd, *J* = 8.4 Hz, *J* = 1.8 Hz, 1H), 7.01 (s, 2H), 6.57 (dd, *J* = 3.5 Hz, *J* = 0.9 Hz, 1H), 2.55 (s, 6H), 2.38 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.7, 141.5, 136.6, 134.3, 129.3, 129.0, 125.9, 125.8, 123.3, 122.3, 121.6, 108.7, 100.3, 21.3, 20.4 ppm. IR (thin film) 2922, 1783, 1610, 1225, 1027, 980, 898, 801, 700 cm^{-1}. HRMS (DART) m/z calcd. for $C_{18}H_{17}NO_2Cl^+$ $[M+H]^+$: 314.0942; found 314.0944.

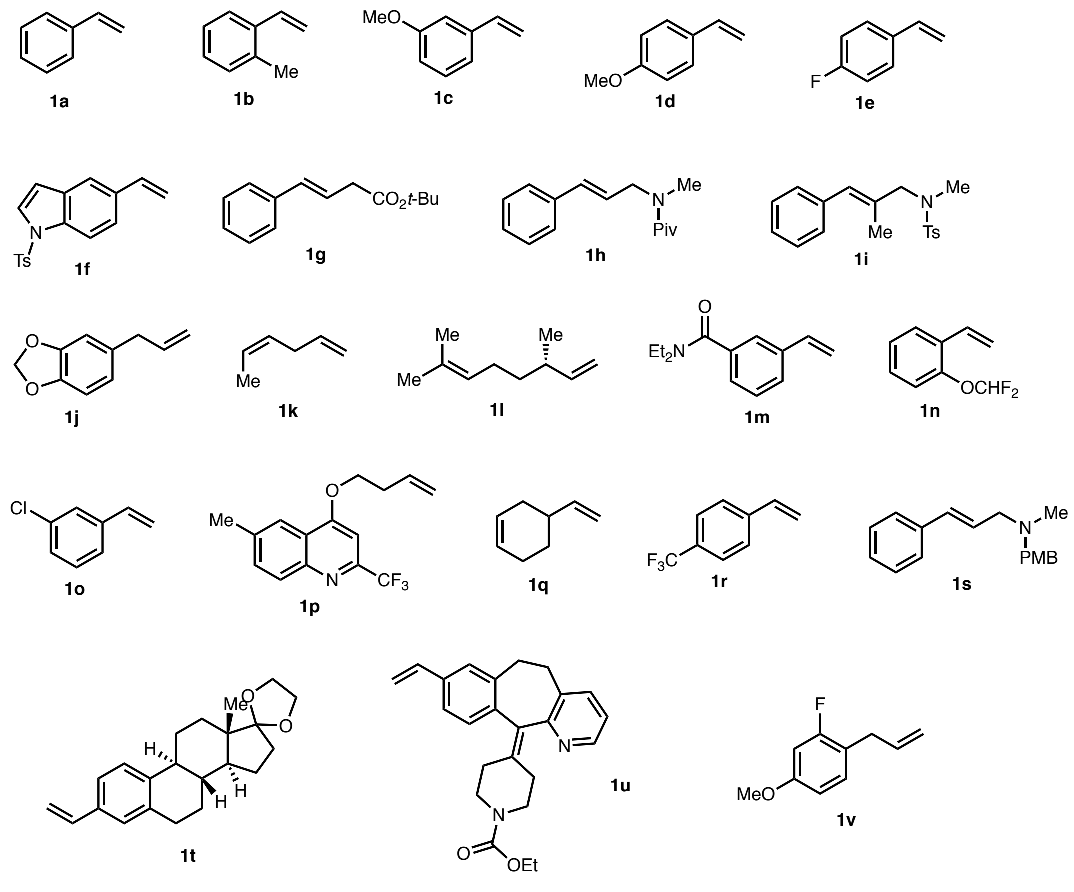
3-(2-methoxyethyl)-1*H*-indol-1-yl 2,4,6-trimethylbenzoate (2k)



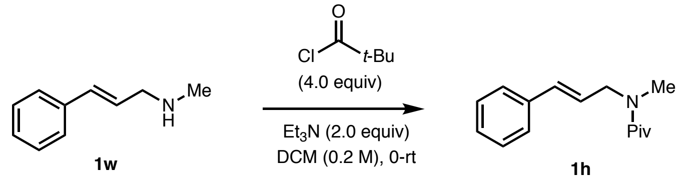
Method B was followed using 3-(2-methoxyethyl)indoline (1.77 g, 10.0 mmol, 1.0 equiv) and 2,4,6-trimethylbenzoyl chloride (2.01 g, 11 mmol, 1.1 equiv). The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 6:1) to provide the title compound as a yellow liquid/solid in 25% yield (0.844 g). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.8 Hz, 1H), 7.36–7.27 (m, 2H), 7.21 (ddd, *J* = 8.0 Hz, *J* = 6.8 Hz, *J* = 1.3 Hz, 1H), 7.15 (s, 1H), 6.99 (s, 2H), 3.74 (t, *J* = 7.1 Hz, 2H), 3.43 (s, 3H), 3.08 (t, *J* = 7.1 Hz, 2H), 2.54 (s, 6H), 2.36 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 141.1, 136.4, 135.6, 128.9, 126.7, 125.2, 123.8, 123.4, 120.7, 119.4, 112.2, 109.2, 72.5, 58.7, 25.6, 21.3, 20.3 ppm. IR (thin film) 2923, 1777, 1611, 1446, 1226, 1155, 1113, 1009, 982, 735 cm^{-1}. HRMS (DART) m/z calcd. for $C_{21}H_{24}NO_3^+$ $[M+H]^+$: 338.1751; found 338.1745.

V. Preparation of Alkene Substrates

All the alkenes used in the paper are listed below. **1a**, **1b**, **1c**, **1d**, **1e**, **1j**, **1k**, **1l**, **1o**, **1q**, and **1r** were purchased from Alfa Aeser, Combi-Blocks or Sigma-Aldrich, and were used as received. **1f**[5], **1g**[6], **1m**[7], **1n**[8], **1p**[9], **1t**[10], **1u**[11] are known compounds and were prepared by previously reported procedures.

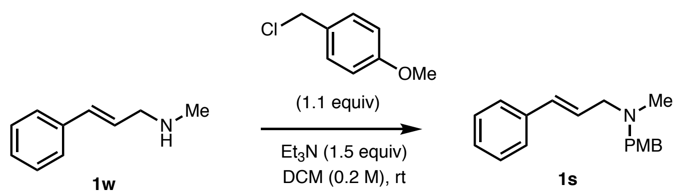


Synthesis of **1h**, **1s**, **1i**, **1v**.



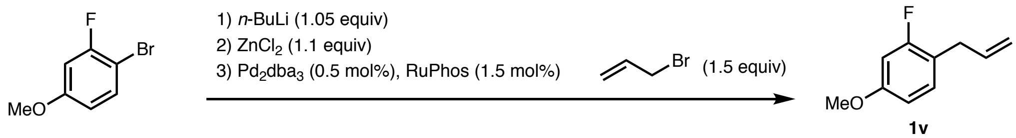
N-cinnamyl-*N*-methylpivalamide (1h)

A 200 mL round bottom flask with a magnetic stir bar was charged with (*E*)-*N*-methyl-3-phenylprop-2-en-1-amine[i] (1.47 g, 10.0 mmol, 1.0 equiv), CH_2Cl_2 (50 mL), and triethylamine (2.02 g, 20.0 mmol, 2.0 equiv). The reaction flask was cooled to 0 ºC in an ice/water bath. Then pivaloyl chloride (4.82 g, 40 mmol, 4.0 equiv) was added slowly via syringe. The ice bath was then removed and the reaction mixture was allowed to warm to rt and stirred overnight. The reaction mixture was diluted with CH_2Cl_2 (50 mL) and quenched with saturated aqueous $NaHCO_3$ solution (100 mL). The aqueous phase was extracted with CH_2Cl_2 (20 mL × 3) and the combined organic phases was dried over Na_2SO_4, filtered and concentrated under reduced pressure with the aid of a rotary evaporator. The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : EtOAc = 1:1) to provide **1h** as liquid in 86% yield (1.99 g). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43–7.32 (m, 4H), 7.29–7.24 (m, 1H), 6.51 (d, *J* = 15.9 Hz, 1H), 6.18 (dt, *J* = 15.9 Hz, *J* = 6.1 Hz, 1H), 4.20 (d, *J* = 5.4 Hz, 2H), 3.07 (s, 3H), 1.35 (s, 9H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.5, 136.6, 132.5, 128.6, 127.7, 126.4, 125.0, 52.1, 38.9, 35.9, 28.4 ppm. IR (thin film) 2973, 1623, 1479, 1449, 1401, 1380, 1363, 1181, 1096, 966 cm^{-1}. HRMS (DART) m/z calcd. for $C_{15}H_{22}NO^+$ $[M+H]^+$: 232.1696; found 232.1684.



(*E*)-*N*-(4-methoxybenzyl)-*N*-methyl-3-phenylprop-2-en-1-amine (1s)

A 200 mL round bottom flask with a magnetic stir bar was charged with (*E*)-*N*-methyl-3-phenylprop-2-en-1-amine (1.47 g, 10.0 mmol, 1.0 equiv), CH_2Cl_2 (50 mL), and triethylamine (1.52 g, 15.0 mmol, 1.5 equiv). 1-(chloromethyl)-4-methoxybenzene (1.72 g, 40 mmol, 4.0 equiv) was added slowly via syringe and the reaction mixture was stirred overnight. The reaction mixture was diluted with CH_2Cl_2 (50 mL) and quenched with saturated aqueous $NaHCO_3$ solution (100 mL). The aqueous phase was extracted with CH_2Cl_2 (20 mL × 3) and the combined organic phases was dried over Na_2SO_4, filtered and concentrated under reduced pressure with the aid of a rotary evaporator. The crude material was purified by flash column chromatography (CH_2Cl_2 ~ CH_2Cl_2 : MeOH = 10:1) to provide **1s** as liquid in 88% yield (2.35 g). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47–7.20 (m, 7H), 6.90 (d, *J* = 8.1 Hz, 2H), 6.56 (d, *J* = 15.8 Hz, 1H), 6.34 (dt, *J* = 15.7 Hz, *J* = 6.6 Hz, 1H), 3.83 (s, 3H), 3.52 (s, 2H), 3.21 (d, *J* = 6.6 Hz, 2H), 2.26 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.7, 137.2, 132.5, 131.0, 130.3, 128.5, 127.7, 127.4, 126.3, 113.6, 61.2, 59.7, 55.3, 42.1 ppm. IR (thin film) 2832, 2783, 1611, 1510, 1495, 1242, 1035, 966, 805, 691 cm^{-1}. EA Calcd. for $C_{18}H_{21}NO$: C, 80.86; H, 7.92. Found: C, 80.64; H, 8.11.



1-allyl-2-fluoro-4-methoxybenzene (1v)

A 300 mL round bottom flask with a magnetic stir bar was charged with 1-bromo-2-fluoro-4-methoxybenzene (10.3 g, 50.0 mmol, 1.0 equiv) and anhydrous tetrahydrofuran (THF, 60 mL) under argon. The reaction mixture was cooled to -78 ºC with a dry ice/acetone bath followed by the slow addition of *n*-BuLi (2.5 M in THF, 1.05 equiv). The reaction mixture was allowed to stir at -78 ºC for 45 min before the addition of solid $ZnCl_2$ (7.50 g, 55.0 mmol, 1.1 equiv) with a counter flow of argon. The reaction mixture was stirred at -78 ºC for 1 h and then was allowed to warm to rt by removing the cooling bath. 3-bromoprop-1-ene (9.07 g, 75.0 mmol, 1.5 equiv), and a 10 mL THF solution of Pd_2dba_3 (0.23 g, 0.25 mmol, 1% mol) and RuPhos (0.35 g, 0.75 mmol, 1.5% mmol) were added via syringe. The round bottom flask was fitted with a reflux condenser and the reaction mixture was heated at 60 ºC for 1 h. After completion, the reaction mixture was cooled to rt and diluted with EtOAc (50 mL). The organic phase was sequentially washed with 1M HCl aqueous solution (50 mL × 2) and brine (50 mL). The combined organic phases was tried over Na_2SO_4, filtered and concentrated under reduced pressure with the aid of a rotary evaporator. The crude material was purified by flash column chromatography (Hexanes ~ Hexanes : CH_2Cl_2 = 10:1) to provide **1v** as liquid in 47% yield (2.35 g). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (t, *J* = 8.5 Hz, 1H), 6.67–6.57 (m, 2H), 5.94 (ddt, *J* = 15.7 Hz, *J* = 11.1 Hz, *J* = 6.5 Hz, 1H), 5.07 (d, *J* = 1.5 Hz, 1H), 5.04 (dd, *J* = 6.9 Hz, *J* = 1.7 Hz, 1H), 3.78 (s, 3H), 3.34 (dd, *J* = 6.5 Hz, *J* = 1.6 Hz, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.3 (d, *J* = 244.9 Hz), 159.3 (d, *J* = 11.0 Hz), 136.32, 130.8 (d, *J* = 6.7 Hz), 118.7 (d, *J* = 16.8 Hz), 115.7, 109.6 (d, *J* = 3.0 Hz), 101.5 (d, *J* = 26.2 Hz), 55.5, 32.4 (d, *J* = 2.8 Hz) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.5 ppm. IR (thin film) 2911, 2837, 1624, 1506, 1278, 1152, 1111, 1032, 952, 914, 832 cm^{-1}. HRMS (DART) m/z calcd. for $C_{10}H_{12}OF^+$ [M+H]$^+$: 167.0867; found 167.0861.

VI. Computational Details

All density functional theory[12] (DFT) calculations were performed using the Jaguar 9.1. Software of ab initio quantum chemistry programs.[13] Geometry optimizations were carried out with the Becke's three-parameter exchange functional[14,15] including Grimme's D3 dispersion correction[16,17] (B3LYP-D3), with the 6-31G** basis set[18]. Cu was described by the LACVP basis set[19–21] which includes relativistic effective core potentials (ECP). The electronic energies were reevaluated by single point calculations using Dunning's correlation-consistent triple-ζ basis set, cc-pVTZ(-f)[22] which includes a double set of polarization functions. For Cu, a modified version of LACVP, designated as LACV3P containing the decontracted exponents to match the effective core potential with triple-ζ quality, was used. The zero-point energy (ZPE) and entropy corrections obtained from the vibrational calculations at the same level of theory as the geometry optimization (B3LYP-D3/6-31G**/LACVP). Solvation energies were evaluated by a self-consistent reaction field (SCRF) approach[23–25] with the dielectric constant ε = 7.6 (THF) using the gas phase optimized structures. All values in the energy profile of SEGPHOS and Ph-BPE are relative free energies (kcal/mol) at 363.15 K and 313.15 K, respectively.

The energy components have been computed with the following protocol. The free energy in solution phase G(sol) has been calculated as follows:

$$G(sol) = G(gas) + G(solv) \quad (1)$$

$$G(gas) = H(gas) - TS(gas) \quad (2)$$

$$H(gas) = E(SCF) + ZPE \quad (3)$$

$$\Delta E(SCF) = \sum E(SCF) \text{ for products} - \sum E(SCF) \text{ for reactants} \quad (4)$$

$$\Delta G(sol) = \sum G(sol) \text{ for products} - \sum G(sol) \text{ for reactants} \quad (5)$$

G(gas) is the free energy in gas phase; G(solv) is the free energy of solvation as computed using the continuum solvation model; H(gas) is the enthalpy in gas phase; T is the temperature; S(gas) is the entropy in gas phase; E(SCF) is the self-consistent field energy, i.e. "raw" electronic energy as computed from the SCF procedure and ZPE is the zero-point energy. Note that by entropy here we refer specifically to the vibrational/rotational/translational entropy of the solute(s); the entropy of the solvent is incorporated implicitly in the continuum solvation model.

Full energy profile of SEGPHOS

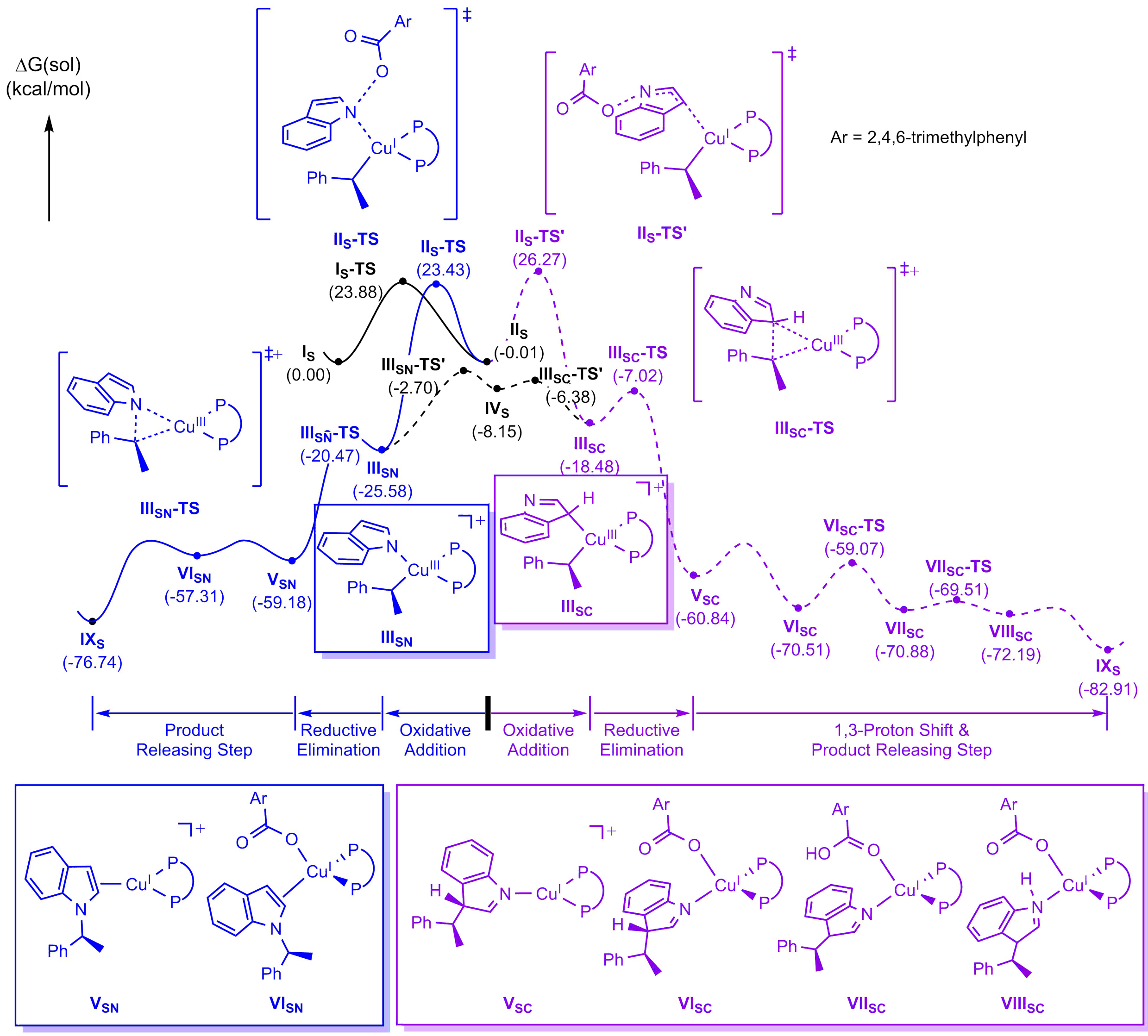


Figure S1. The energy profile of CuH-catalyzed alkylation of indoles with SEGPHOS.

Fig. S1 shows the DFT calculated energy profile for the CuH catalyzed indole alkylation reaction with the SEGPHOS ligand. Instead of DTBM-SEGPHOS, SEGPHOS which gives the same regioselectivity trend with DTBM-SEGPHOS in experiment is used for computational efficiency. The reaction begins with a hydrocupration that furnishes enantioenriched alkylcopper(I) intermediate **II**$_{\mathbf{S}}$ with a barrier of 23.9 kcal/mol. After the olefin insertion step, the intermediate **II**$_{\mathbf{S}}$ would perform either N- or C3-oxidative addition. As described in the main text, SEGPHOS ligand prefers to follow N-oxidative addition pathway which is colored blue in the energy profile across **II**$_{\mathbf{S}}$**-TS** with a barrier of 23.4 kcal/mol and forms cationic Cu(III) complex

III$_{SN}$. This cationic complex **III$_{SN}$** undergoes reductive elimination via **III$_{SN}$-TS** with a negligible barrier of only 5.1 kcal/mol. Then, the association of the benzoate anion to the metal center of **V$_{SN}$** affords **VI$_{SN}$** which would subsequently release the N-alkylated indole as a product and the copper acetate **IX$_S$**. The overall reaction is highly exothermic and thus thermodynamically favored.

Full energy profile of Ph-BPE

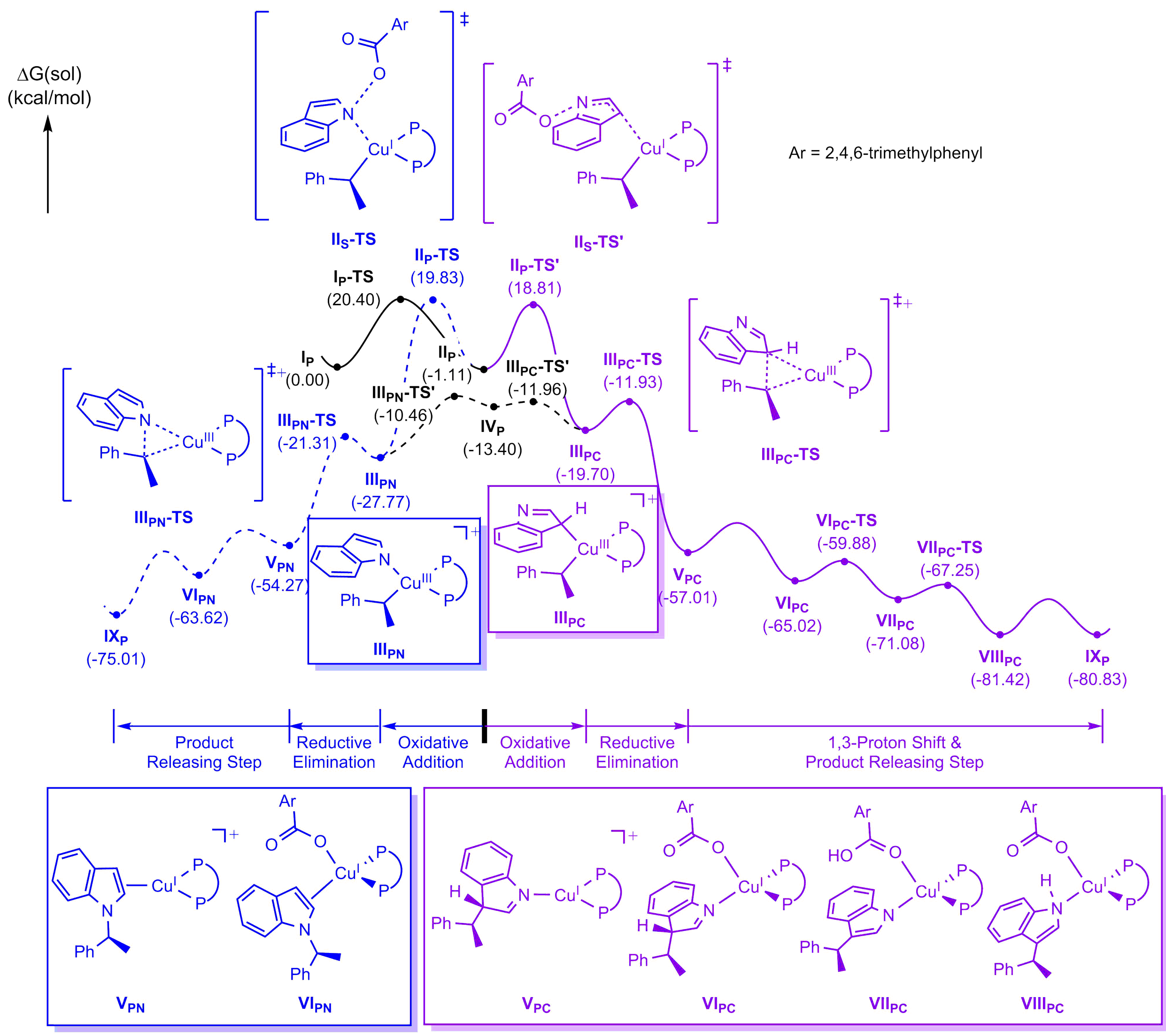


Figure S2. The energy profile of CuH-catalyzed alkylation of indoles with Ph-BPE.

Fig. S2 summarizes the DFT calculated energy profile for the CuH catalyzed indole alkylation reaction with Ph-BPE ligand. Whereas the alkylcopper(I) complex with SEGPHOS ligand prefers oxidative addition toward the N-position of indole substrate, the alkylcopper(I) complex with Ph-BPE ligand, **II$_\mathbf{P}$** shows preference to C3-oxidative addition which is displayed in violet and as explained in the main text. After the C3-oxidative addition, the cationic Cu(III) complex **III$_\mathbf{PC}$** performs either reductive elimination which generates C3-alkylated indole product or 3,1-shift of indole which leads to N bound intermediate **III$_\mathbf{PN}$**. The reductive elimination step **III$_\mathbf{PC}$-TS** requires 7.8 kcal/mol while the 2,1-shift which is one part of 3,1-shift demands 9.2 kcal/mol of free energy. Although the barrier for **III$_\mathbf{PC}$-TS** is slightly lower only by 1.5 kcal/mol than that for **III$_\mathbf{PN}$-TS'**, we assume that the reductive elimination may take place dominantly due to the different pre-exponential factors in two steps. The isomerization, however, may happen occasionally and lower the regio-selectivity. The formation of **V$_\mathbf{PC}$** across **III$_\mathbf{PC}$-TS** is highly exergonic and thus this reaction is irreversible. Next, association of a benzoate anion to the metal center of **V$_\mathbf{PC}$** yields intermediate **VI$_\mathbf{PC}$**. Since the γ-hydrogen in indole moiety of **VI$_\mathbf{PC}$** is very acidic, the benzoate deprotonate it with a small barrier of 5.2 kcal/mol to give intermediate **VII$_\mathbf{PC}$**. A protonation of the nitrogen in the substrate generates intermediate **VIII$_\mathbf{PC}$** and the C–C coupled product with the copper(I) acetate **IX$_\mathbf{P}$** can finally be released.

Hydrocupration which determines enantioselectivity

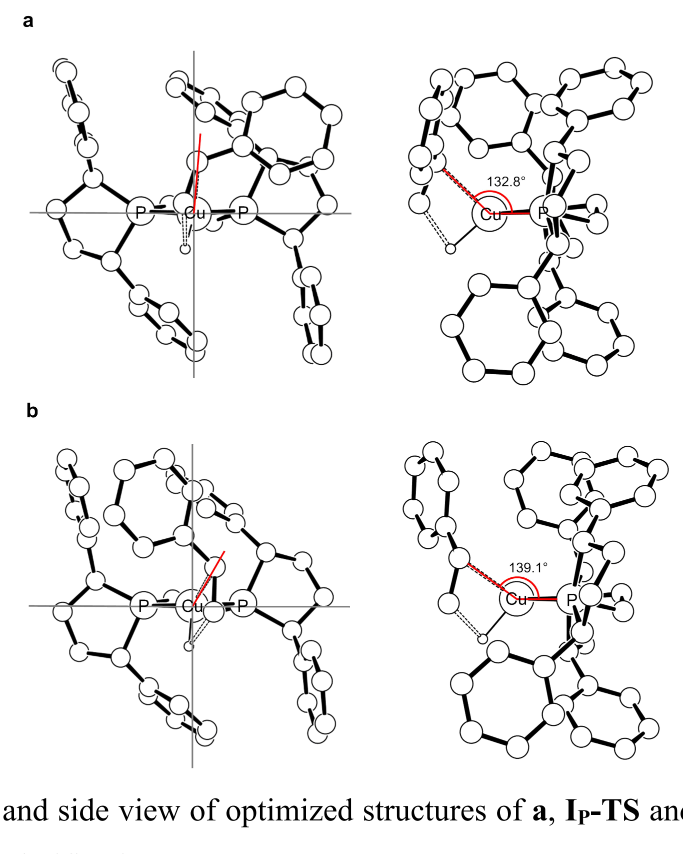


Figure S3. The front and side view of optimized structures of **a**, **I$_\mathbf{P}$-TS** and **b**, **I$_\mathbf{P}$-TS'**. Hydrogen atoms are omitted for clarification.

The enantioselectivity is determined in the hydrocupration step in the early stage of the reaction. The chiral ligand imposes a steric hindrance when an asymmetric alkene substrate approaches to the CuH catalyst. The transition state **I_P-TS** and **I_P-TS'** are related with forming a (S) and (R) form of the subsequent alkylcopper(I) intermediate, respectively. Compared to **I_P-TS**, there is a steric clash between a phenyl of the ligand and that of the substrate in **I_P-TS'**. To release this steric hindrance, the alkene substrate is distorted as shown in Fig. S3 b). In **I_P-TS'**, a benzylic carbon is further away from the virtual central axis which is denoted in gray color and an angle between a P-Cu-P plane and the benzylic carbon is larger than those in **I_P-TS**. These distortions finally weaken the orbital interaction between the substrate and CuH catalyst and increase the hydrocupration barrier. Our DFT calculations show that the barrier for **I_P-TS** is 5.0 kcal/mol higher in energy than that for **I_P-TS'**. Thus, the styrene substrate is selectively inserted into CuH catalyst via **I_P-TS**, which forms the enantioenriched alkylcopper(I) intermediate **II_P**.

Reason for the low yield when C3-substituted indole is used for the substrate.

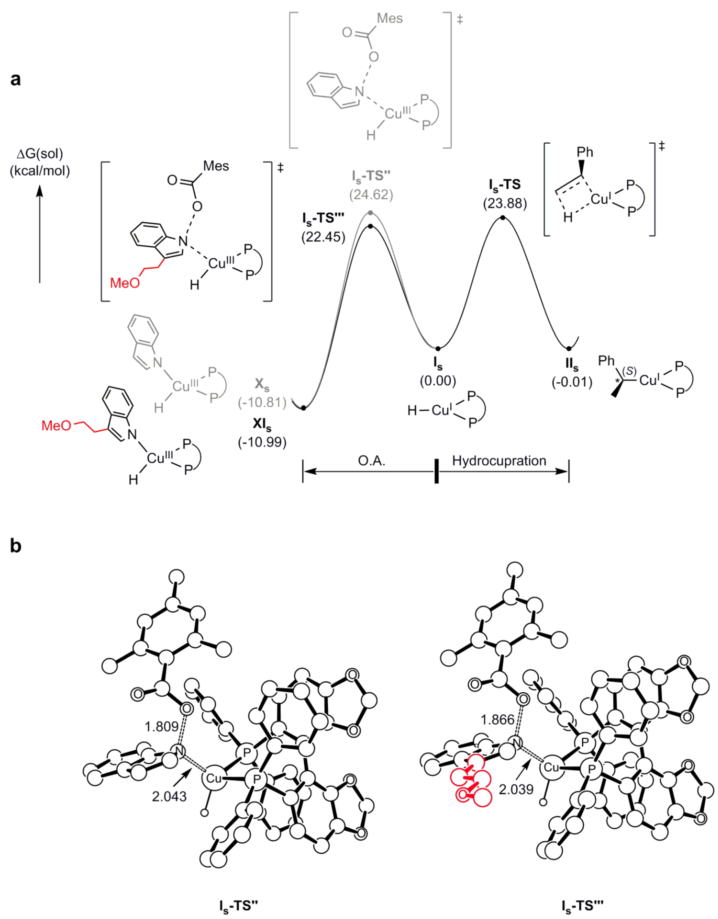


Figure S4. (a) The energy profile of two competitive pathways from $\mathbf{I_S}$; oxidative addition and hydrocupration. (b) The optimized structure fo $\mathbf{I_S}$**-TS''** and $\mathbf{I_S}$**-TS'''**. All hydrogens except the hydride is omitted for clarification

The CuH catalyst $\mathbf{I_S}$ can react with either indole or styrene substrates as shown in Fig. S4a. As a reason for the low yield in C3-substituted indole substrate, we presume that there is a competitive side reaction involving the transition state denoted as $\mathbf{I_S}$**-TS'''**. In the absence of the C3-substitution at the indole substrate, the hydrocupration which leads to the formation of the desired alkylated product through $\mathbf{I_S}$**-TS** is relatively facile than the side reaction which is the direct oxidative addition of indole substrate across $\mathbf{I_S}$**-TS''**. The oxidative addition step is computed to have 0.7 kcal/mol higher in energy than the hydrocupration step. In the case of C3-substituted indole substrate, however, the oxidative addition transition state $\mathbf{I_S}$**-TS'''** associated with a barrier of 22.5 kcal/mol which requires 1.4 kcal/mol lower energy than $\mathbf{I_S}$**-TS**. In other words, the C3-substitution lowers 2.2 kcal/mol of oxidative addition barrier.

We found that the barrier difference between $\mathbf{I_S}$**-TS''** and $\mathbf{I_S}$**-TS'''** is mainly contributed by the variance of interaction energy between the indole moiety and the alkylcopper(I) moiety. With the C3-substitution, the transition state shows ~4 kcal/mol stronger interaction energy in the gas phase. We found that this interaction energy preference mostly originates from 2.7 kcal/mol of van der Waals interaction between C3-substituent and the ligand as shown in Fig. S4 b. Based on this result, we also suppose that the low yield of N-alkylated product using C3-substituted indole with DTBM-SEGPHOS is due to the side-reaction of direct indolyl-benzoate reduction.

Energy decomposition analysis

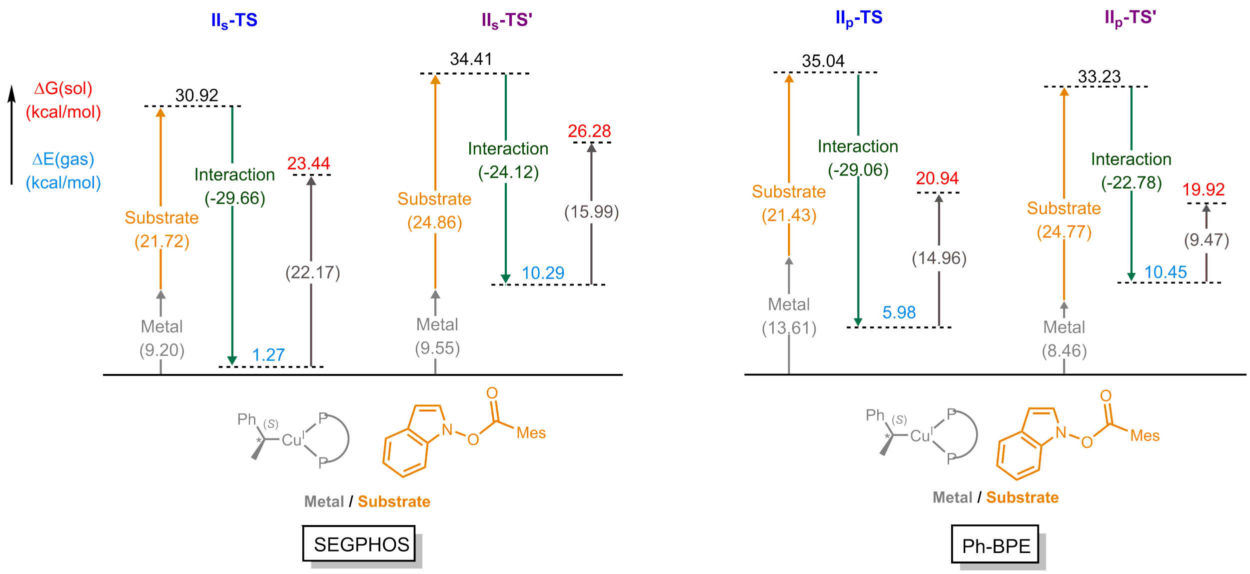


Figure S5. Energy decomposition analysis of transition states **II-TS** and **II-TS'** depending on the ligand

To understand the computed energy differences, we carried out an energy decomposition analysis of the transition states **II-TS** and **II-TS'**. As illustrated in Fig. S5, the transition state was partitioned into substrate and metal fragments. The energies labeled "substrate" in yellow and "metal" in grey represent the distortion energies of each fragments during the structural transformation from the ground to the transition states. The interaction energy between the two fragments is shown in green. This intuitive decomposition scheme divides the electronic energy of the transition state into three chemically meaningful components. In addition, the free energy which involves entropy and solvation corrections are shown in red.

In the case of SEGPHOS system, the distortion energies of the metal fragments are nearly identical in both transition states, but **II_S-TS** requires 3.1 kcal/mol less distortion energy in the substrate fragment than **II_S-TS'**. Furthermore, the interaction energy in **II_S-TS** is greater by 5.5 kcal/mol, which is easy to understand, since the polarity inversion makes the indole-*N* a better electrophile. Taken together, the electronic barrier of **II_S-TS** is ~9 kcal/mol lower than that of **II_S-TS'**. The free energy correction attenuates the preference to **II_S-TS** since the solvation penalty of **II_S-TS** is more substantial due to the reduced exposure of the highly polarized N–O bond**.** Despite the substantial solvation penalty, the electronic energy difference of 9 kcal/mol allows **II_S-TS** to have a free energy barrier that is ~3 kcal/mol lower. In contrast, the Ph-BPE system shows reversed energy ordering in the transition states. Whereas the interaction energy and distortion of substrate fragment show similar trends compared to the SEGPHOS system, the distortion energy of metal fragment is markedly different: The metal fragment in **II_P-TS** is distorted more, affording a 5.2 kcal/mol of distortion energy difference due to the architecture of Ph-BPE ligand. Overall, the electronic energy difference between **II_P-TS** and **II_P-TS'** becomes 4.5 kcal/mol, which is smaller than the difference in the SEGPHOS case. As a result, the small electronic energy gap is overwhelmed by the 5.5 kcal/mol of correction energy variance and gives reversed preference toward C3-oxidative addition.

Catalyst distortion during the N-oxidative addition.

As discussed in the main text, the N-oxidative addition demands higher metal fragment distortion in the Ph-BPE system. Fig. S6 reveals the factors that determine the distortion energy. This distortion of the metal fragment is reflected in the Cu–P bond length and the angle between P–Cu–P plane and the α-carbon of the styrene. Whereas Cu–P bond of the metal fragment in **II_S-TS** is elongated by 0.048 Å and the styrene moiety is bent 26.1°, that in **II_P-TS** is elongated by 0.121 Å and the styrene moiety is bent 31.3°. Consequently, we concluded that the architecture of Ph-BPE is not proper for the N-oxidative addition which results in the preference to the C3-oxidative addition pathway.

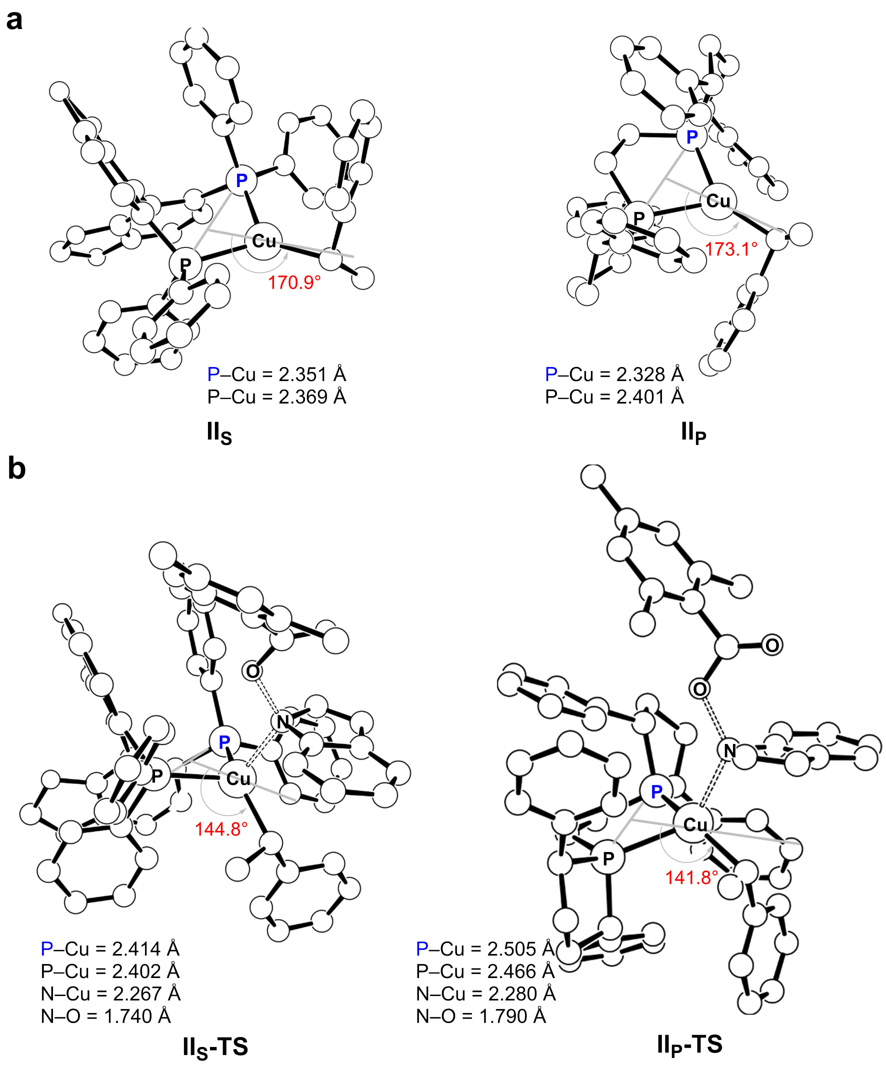


Figure S6. **DFT optimized geometries.** (a) Side view of **II$_S$** and **II$_P$**. **b, II$_S$-TS** and **II$_P$-TS**. Hydrogen atoms are omitted for clarification. (b) Side view of **II$_S$-TS** and **II$_P$-TS**.

Table S4. Computed energy components for DFT-optimized structures

	E(SCF)/(eV)	**ZPE/(kcal/mol)**	**S(gas)/(cal/mol)**	**G(solv)/(kcal/mol)**
	cc-pVTZ(-f)/LACV3P**	6-31G**/LACVP**	6-31G**/LACVP**	6-31G**/LACVP**
styrene	-8428.928	83.82	82.75	-3.08
1*H*-indol-1yl trimethylbenzoate	-24534.758	192.97	142.54	-7.47
C3-substituted benzoate	-29792.582	248.96	176.46	-8.99

trimethylbenzoate	-14650.915	115.96	107.97	-56.79
3a	-18333.031	168.16	117.54	-5.74
4a	-18333.162	168.16	117.28	-7.67
I_S	-72000.119	355.55	241.41	-22.50
IX_S	-86635.578	469.87	294.67	-18.75
I_P	-59793.922	387.34	216.215	-17.48
IX_P	-74429.217	501.56	272.287	-11.97
I_S-TS	-80429.359	440.54	270.69	-15.09
I_S-TS'	-80429.266	441.52	260.87	-15.11
II_S	-80430.508	443.50	271.62	-15.11
II_S-TS	-104965.211	636.53	363.88	-18.73
III_{SN}	-90312.430	520.40	303.45	-36.54
III_{SN}-TS	-90312.172	519.80	303.22	-36.87
V_{SN}	-90313.969	521.68	301.28	-36.72
VI_{SN}	-104968.859	639.58	360.77	-19.52
II_S-TS’	-104964.820	635.04	368.20	-21.85
III_{SC}	-90312.039	520.59	298.43	-40.47
III_{SC}-TS	-90311.469	519.90	302.81	-39.87
V_{SC}	-90314.040	521.24	302.50	-35.85
VI_{SC}	-104969.153	637.69	371.76	-20.05
VI_{SC}-TS	-104968.784	635.49	363.01	-18.10
VII_{SC}	-104969.458	639.08	365.07	-17.22
VII_{SC}-TS	-104969.339	636.87	363.38	-16.99
$VIII_{SC}$	-104969.641	639.60	358.77	-17.11
IV_S	-90311.476	519.51	305.840	-39.36
III_{SN}-TS'	-90311.320	519.14	301.000	-38.89
III_{SC}-TS'	-90311.429	519.67	300.840	-40.65
I_S-TS''	-96534.972	547.98	330.981	-21.84
X_S	-81881.622	431.40	271.806	-38.30
I_S-TS'''	-101793.060	604.35	355.961	-23.08
XI_S	-87139.560	487.52	300.655	-39.35
I_P-TS	-68223.117	472.33	250.139	-10.44
I_P-TS'	-68222.906	472.14	248.925	-10.53
II_P	-68224.351	475.35	240.016	-9.69

II_P-TS	-92758.844	667.76	340.917	-14.81
III_{PN}	-78106.028	552.02	277.736	-35.71
III_{PN}-TS	-78105.818	552.30	276.824	-34.66
V_{PN}	-78107.404	553.78	269.632	-34.78
VI_{PN}	-92762.715	671.17	334.016	-14.56
II_P-TS'	-92758.656	667.88	346.947	-18.39
III_{PC}	-78105.512	552.25	280.069	-39.04
III_{PC}-TS	-78105.234	552.09	279.913	-37.58
V_{PC}	-78107.441	553.93	278.67	-33.99
VI_{PC}	-92762.640	670.54	338.359	-15.70
VI_{PC}-TS	-92762.511	668.65	337.552	-11.90
VII_{PC}	-92763.012	671.28	337.802	-14.10
VII_{PC}-TS	-92762.854	668.42	332.59	-12.68
$VIII_{PC}$	-92763.566	671.76	333.972	-13.34
IV_P	-78105.292	551.76	280.805	-37.10
III_{PN}-TS'	-78105.276	551.18	274.444	-35.93
III_{PC}-TS'	-78105.261	551.68	278.634	-36.97
MF of II_S-TS' [a]	-80430.109	-	-	-
SF of II_S-TS' [b]	-24533.816	-	-	-
MF of II_S-TS [a]	-80430.094	-	-	-
SF of II_S-TS [b]	-24533.680	-	-	-
MF of II_P-TS' [a]	-68223.761	-	-	-
SF of II_P-TS' [b]	-24533.829	-	-	-
MF of II_P-TS [a]	-68223.984	-	-	-
SF of II_P-TS [b]	-24533.684	-	-	-

[a] MF represents metal fragment at energy decomposition analysis
[b] SF represents substrate fragment at energy decomposition analysis

Table S5. Cartesian Coordinates of the Optimized Geometries.

==============================

Styrene

==============================

C	0.199031353	0.049974460	-3.052597284
C	-0.929726839	-0.436844438	-2.371161938
C	1.337207556	0.465258241	-2.362348795
H	2.196619749	0.838231444	-2.912503958
C	-0.879624009	-0.490713060	-0.965755343
C	1.369908571	0.404559940	-0.969662964
H	-1.736751318	-0.853960693	-0.407453090
H	2.253000975	0.730012298	-0.427438527
C	0.254625887	-0.075089119	-0.275637835
H	0.270930201	-0.123049319	0.809633076
H	0.181362525	0.100314222	-4.138609409
C	-2.103086710	-0.862714350	-3.152635336
H	-1.997781873	-0.732833683	-4.229802608
C	-3.248414993	-1.381706834	-2.692831516
H	-3.437100887	-1.552695155	-1.637118101
H	-4.045801640	-1.660042763	-3.374152422

==============================

1*H*-indol-1yl trimethylbenzoate

==============================

C	-0.801888168	-8.081636429	-3.842875719
C	-0.555720270	-7.985819340	-5.214999199
C	-0.618603468	-6.944793701	-3.052886963
H	-0.687634587	-8.865172386	-5.840485573
H	-0.784220994	-7.011914253	-1.980700374
C	-0.138139188	-6.794278145	-5.808949471
C	-0.225963175	-5.718533039	-3.596892834
C	0.007074779	-5.647951603	-4.989100456
C	0.432841301	-4.389021873	-5.653863430
O	1.254618168	-4.256315231	-6.521327019
O	-0.322722912	-3.302493811	-5.172417164
C	-0.231754556	-0.152692273	-8.798052788
C	0.134592131	-0.696394384	-7.555431843
C	-0.589307666	-1.819355011	-7.074403286
C	-1.624319553	-2.427338839	-7.784778118
C	-1.948254228	-1.874886394	-9.019197464
C	-1.262770891	-0.746276438	-9.516497612
C	1.149342299	-0.392449021	-6.580141068
C	1.030927062	-1.303261399	-5.566598892
N	-0.057331849	-2.115961313	-5.836276531
H	0.294812292	0.711231828	-9.194070816
H	-2.141812325	-3.293732882	-7.385998726
H	-2.743145704	-2.319236040	-9.610752106
H	-1.545222163	-0.338893294	-10.482913017
H	1.872094035	0.409705698	-6.626288414
H	1.593953371	-1.443638563	-4.656606674
C	-0.036502078	-4.539743423	-2.665739059
H	-0.861458540	-3.826799870	-2.754817009
H	0.011652730	-4.880306721	-1.627948046
H	0.884164095	-3.991527319	-2.883363962
C	0.126200274	-6.764344215	-7.297892094
H	1.193256617	-6.648975849	-7.503815651
H	-0.224228933	-7.687802315	-7.766490936
H	-0.372789443	-5.920814991	-7.785421371
C	-1.278827190	-9.380313873	-3.238348722
H	-2.362327099	-9.492677689	-3.368303776
H	-0.803370893	-10.242155075	-3.717076302
H	-1.069544196	-9.425775528	-2.165844679

==============================

C3-substituted 1*H*-indol-1yl trimethylbenzoate

==============================

C	1.054493785	-6.467426777	-0.379361302
C	0.782510936	-6.860335350	-1.690058112
C	1.546123624	-5.175523758	-0.163577095
H	0.400846839	-7.861212730	-1.875717163
H	1.776860595	-4.860735416	0.851609707
C	0.990037203	-6.008859158	-2.779013634
C	1.751646757	-4.274344444	-1.208831072
C	1.467543364	-4.700563431	-2.528818130
C	1.656921625	-3.820068836	-3.711609364
O	2.068941832	-4.137459278	-4.796539783
O	1.214009523	-2.511090517	-3.445270538
C	-0.241556674	-1.108659625	-7.787586212
C	0.621373713	-1.186855435	-6.683901310
C	0.159210145	-1.826818585	-5.506949425
C	-1.097991228	-2.419242382	-5.404116154
C	-1.921455622	-2.346163988	-6.523568630
C	-1.501096487	-1.691791415	-7.699287415
C	1.980744123	-0.755436718	-6.448281288
C	2.297384024	-1.137576342	-5.171078682
N	1.173088312	-1.702266932	-4.575857162
H	0.077674158	-0.612112164	-8.699584961
H	-1.410000801	-2.911427975	-4.488669872
H	-2.908123016	-2.798954725	-6.489233017
H	-2.173567533	-1.648611307	-8.551027298
H	3.201401949	-1.022052765	-4.593216419
C	0.835235655	-7.405745506	0.782560647
H	0.138675570	-6.974474430	1.510530114
H	0.428745031	-8.366289139	0.454533398
H	1.774511814	-7.600489616	1.312956810
C	0.683770478	-6.516185284	-4.170289993
H	1.602462411	-6.654312134	-4.746863842
H	0.154175431	-7.471023083	-4.118870735
H	0.071408674	-5.810341835	-4.739583492
C	2.295829296	-2.899662733	-0.884480655
H	1.514274359	-2.138289690	-0.954905152
H	2.703687191	-2.881988049	0.129624590
H	3.089216709	-2.600524187	-1.575164437
C	2.831391335	-0.017435167	-7.439487934
H	2.422895432	0.984552741	-7.627112865
H	2.804188490	-0.538814545	-8.404849052
C	4.287414074	0.128658995	-7.018703938
H	4.357808590	0.685939908	-6.067669392
H	4.734581470	-0.865981460	-6.846637726
O	4.971688271	0.817522526	-8.047914505
C	6.338100910	1.017173648	-7.758121490
H	6.482374191	1.619969964	-6.845997334
H	6.875235558	0.063584879	-7.624482155
H	6.777287483	1.551652431	-8.604720116

==============================

Trimethylbenzoate

==============================

C	-0.813101113	-8.104188919	-3.837814808
C	-0.602982283	-7.986446857	-5.214809895
C	-0.614932299	-6.968132019	-3.048749924
H	-0.745719135	-8.861642838	-5.850365639
H	-0.768498957	-7.037028313	-1.971006989
C	-0.203813463	-6.779388428	-5.799291611
C	-0.233491555	-5.740730286	-3.604359865
C	-0.018978070	-5.634036541	-4.995024681
C	0.420908988	-4.287554264	-5.625574589
O	1.467193365	-4.334072590	-6.319912910
O	-0.319135040	-3.305649996	-5.369139671
C	-0.055480529	-4.533597469	-2.711824417
H	-0.655403674	-3.705527782	-3.096832991
H	-0.321168274	-4.760569572	-1.672307134
H	0.983188629	-4.180176258	-2.732013226
C	0.043363705	-6.707864285	-7.289153099
H	1.044029474	-6.308560848	-7.472239017
H	-0.081466220	-7.688117504	-7.764156818
H	-0.649679303	-6.003588200	-7.766441822
C	-1.272820830	-9.410702705	-3.229873896
H	-2.364574432	-9.529813766	-3.288637161
H	-0.831148028	-10.272727966	-3.744703054
H	-0.999515176	-9.478807449	-2.170406103

==============================

3a

==============================

H	1.024832368	-2.010401726	-2.898260832
C	-0.046641670	-2.069233656	-3.111347198

C	-0.404076606	-1.227559924	-4.341845512
C	-0.163027063	0.270976543	-4.204216480
C	-0.649517119	1.112359405	-5.216578960
C	0.557726860	0.835936606	-3.149964809
C	-0.425835937	2.484818697	-5.173542976
C	0.783806562	2.215632915	-3.103631258
C	0.295421958	3.041979551	-4.112863064
H	-1.194525123	0.674701810	-6.049143791
H	0.948675394	0.209343657	-2.355343819
H	-0.807509720	3.120527029	-5.967395782
H	1.350078583	2.639200449	-2.279044151
H	0.477959692	4.112202644	-4.079456329
H	-1.473123908	-1.360765219	-4.548866272
H	-0.293165416	-3.116378546	-3.303354740
H	-0.601481915	-1.734217644	-2.229552031
C	0.740123391	-4.127322197	-8.163410187
C	0.914671719	-3.075723648	-7.248808861
C	-0.107338227	-2.816638470	-6.290883064
C	-1.270010948	-3.592518330	-6.217678547
C	-1.411682367	-4.627589703	-7.135631561
C	-0.417852193	-4.891509533	-8.100512505
C	1.954266667	-2.115286827	-7.015055656
C	1.547639489	-1.331024408	-5.968965054
N	0.295577496	-1.733248353	-5.529985905
H	1.505095243	-4.338715076	-8.905725479
H	-2.036471128	-3.399518967	-5.473010540
H	-2.303443909	-5.246919155	-7.105829239
H	-0.561496675	-5.709493160	-8.800699234
H	2.877242088	-2.008103132	-7.567090511
H	2.036059618	-0.490813285	-5.498693943

==============================

4a

==============================

H	0.845597982	-0.517036378	-3.429801464
C	0.027124684	-1.194643974	-3.167725325
C	-1.175778031	-1.005279541	-4.108928680
C	-1.831622839	0.376684964	-4.024751663
C	-2.951646566	0.635415614	-4.829482079
C	-1.363535881	1.401865602	-3.196164846
C	-3.584886074	1.874277592	-4.807639599
C	-1.995060325	2.650051117	-3.173093319
C	-3.106186152	2.891539574	-3.977318048
H	-3.310942411	-0.145957813	-5.494232178
H	-0.499709398	1.239974618	-2.560293198
H	-4.449170589	2.050717115	-5.442318439
H	-1.610557556	3.433152676	-2.525187969
H	-3.595740318	3.861154318	-3.960359812
H	-1.940955043	-1.734530926	-3.806021929
H	0.404420704	-2.216934919	-3.255802393
H	-0.247854099	-1.018934488	-2.122603893
C	0.721058607	0.666500509	-6.286903381
C	0.051705152	-0.563454270	-6.410642147
C	0.156161100	-1.282575488	-7.633199692
C	0.912739992	-0.816475272	-8.712934494
C	1.570481420	0.398023069	-8.556719780
C	1.472746849	1.133713484	-7.357332706
C	-0.796046317	-1.334748864	-5.532831669
C	-1.167718649	-2.451689482	-6.236266136
N	-0.599125385	-2.429382324	-7.498758316
H	0.629341364	1.247373462	-5.374820709
H	0.982287228	-1.381199121	-9.638576508
H	2.167320967	0.789474249	-9.375564575
H	1.992341161	2.084024906	-7.274999142
H	-1.796760678	-3.275917053	-5.929625511
H	-0.712612391	-3.139406681	-8.202519417

==============================

I_S

==============================

Cu	-7.554090023	-1.529623032	4.081732750
H	-9.075405121	-1.726476669	3.799596310
P	-5.685937405	-1.150449872	2.622682095
C	-4.313284874	-0.201517522	3.404674292
C	-4.850702763	-2.659301519	1.990760326
C	-6.117038727	-0.171549439	1.127537608
C	-3.549935102	-0.817351043	4.443989277
C	-4.104572773	1.146458745	3.087012053
C	-2.585426331	-0.024108810	5.037312508
C	-3.685735941	-2.232013226	4.904942989
C	-3.150777340	1.939500213	3.749263287
H	-4.695890903	1.602463841	2.301112413
C	-2.400402069	1.318684340	4.723394871
O	-1.731960058	-0.381909370	6.053758621
C	-2.668081284	-3.118503571	4.603336334
C	-4.756146431	-2.756678820	5.694694519
H	-3.009577990	2.986568689	3.506263971
O	-1.432571530	1.856218338	5.535064220
C	-0.880987942	0.750883758	6.260372162
C	-2.691044807	-4.462886333	4.961228848
O	-1.533082008	-2.853996038	3.875422716
C	-4.759627819	-4.108971119	6.059418678
P	-6.221773624	-1.701328158	6.067253590
H	-0.853111923	0.995092511	7.326639175
H	0.126355961	0.525343418	5.878700733
C	-3.730559111	-4.994499207	5.692252636
O	-1.580522537	-5.096033096	4.461728096
C	-0.764502883	-4.061736107	3.898574352
H	-5.581730366	-4.493258476	6.652739525
C	-7.070796967	-2.572441578	7.446231842
C	-5.495353222	-0.207864091	6.848650932
H	-3.750152349	-6.041649342	5.972227573
H	0.127797589	-3.914314270	4.525233269
H	-0.487664372	-4.335089207	2.875464439
C	-6.521914005	-2.719329596	8.730375290
C	-8.332697868	-3.118348837	7.171939373
C	-7.225520611	-3.399442911	9.721406937
H	-5.552870274	-2.291030169	8.962646484
C	-9.031975746	-3.805263758	8.167251587
H	-8.764391899	-2.983983278	6.181489944
C	-8.480820656	-3.946720839	9.440253258
C	-6.097353458	1.025835514	6.566817760
C	-4.363513947	-0.242553890	7.676836014
C	-5.585602283	2.203265905	7.113302708
H	-6.959479809	1.057595968	5.904894829
C	-3.858260393	0.933546782	8.227814674
H	-3.845473051	-1.180861712	7.848574638
C	-4.467006683	2.158877373	7.946734428
C	-5.560020447	-3.867164373	2.062411308
C	-3.536968470	-2.665971279	1.498764157
C	-4.967933178	-5.058927536	1.642283797
H	-6.571414948	-3.866003513	2.462942362
C	-2.950700760	-3.857279778	1.073262095
H	-2.955317974	-1.749384403	1.492745161
C	-3.662464142	-5.057137012	1.146443009
C	-7.366694450	0.464481443	1.118997574
C	-5.262012005	-0.018474847	0.024291791
C	-7.746221542	1.256981969	0.033200037
H	-8.045598030	0.311668307	1.955608249
C	-5.648389816	0.765149653	-1.061432481
H	-4.299579620	-0.519930601	0.008783017
C	-6.888857841	1.410145998	-1.056647062
H	-2.978286505	0.895566046	8.865266800
H	-4.065135002	3.075815439	8.368418694
H	-6.050263882	3.156052589	6.875215054
H	-10.009867668	-4.223988056	7.946043015
H	-9.028866768	-4.473214149	10.216866493
H	-6.794860840	-3.505200624	10.713806152
H	-5.520831585	-5.991234779	1.718232274
H	-3.200112581	-5.986208916	0.825407445
H	-1.930358410	-3.850029469	0.697786033
H	-4.984408855	0.870213807	-1.915501714
H	-7.186800480	2.021918535	-1.903499246
H	-8.719607353	1.739609361	0.033886287

==============================

IX_S

==============================

Cu	-0.629524112	-0.178741902	-3.383583069
P	-1.935043693	-1.256434917	-1.808645248

C	-0.924609840	-2.460940838	-0.853605330
C	0.122593731	-1.968607545	-0.012535505
C	-1.081790328	-3.838016272	-1.047245741
C	0.901247382	-2.932314873	0.603989244
C	0.398222804	-0.534070492	0.313575834
C	-0.251508713	-4.788713455	-0.426054478
H	-1.874632359	-4.194297314	-1.695525289
C	0.735870183	-4.299290180	0.400054961
O	1.941706538	-2.718387604	1.473589301
C	0.090903804	-0.094945066	1.589076757
C	1.032881737	0.425163537	-0.537423730
H	-0.383811474	-5.853384018	-0.582808554
O	1.665091038	-4.996575832	1.128039002
C	2.462004423	-4.011667728	1.801795840
C	0.324524373	1.203356028	2.031696081
O	-0.480222553	-0.830831468	2.598810911
C	1.267433643	1.725424290	-0.077737458
P	1.414687395	-0.026588587	-2.287396908
H	3.499359369	-4.085210323	1.452889204
H	2.396126747	-4.167041779	2.886001825
C	0.914501488	2.144598246	1.217527747
O	-0.091347381	1.335795045	3.331529379
C	-0.688492835	0.080285572	3.684692621
H	1.739994287	2.443519592	-0.738074303
H	1.102410793	3.155178785	1.562008381
H	-0.205970183	-0.312959701	4.587309837
H	-1.765960455	0.221914798	3.838427544
C	2.515772104	1.311250567	-2.887441397
C	3.916591883	1.256660700	-2.869320869
C	1.875934720	2.443327665	-3.424611807
C	4.666304588	2.323107719	-3.368909597
H	4.426777363	0.382006913	-2.478765965
C	2.632914305	3.511455297	-3.908500671
H	0.788717151	2.482379198	-3.466117144
C	4.028857708	3.454334974	-3.883599520
C	2.459822655	-1.518298626	-2.096710682
C	2.189303398	-2.619950056	-2.919395447
C	3.465004206	-1.618739247	-1.122301340
C	2.910854816	-3.805082083	-2.771437168
H	1.390804291	-2.549946785	-3.654316664
C	4.198853016	-2.796809435	-0.989812672
H	3.650442123	-0.786665797	-0.449317813
C	3.918170214	-3.893857718	-1.808566809
C	-2.636144876	-0.151081666	-0.523596048
C	-2.735129356	1.215075612	-0.827475131
C	-3.062447309	-0.617854655	0.728852570
C	-3.256269217	2.100498676	0.118279926
H	-2.387833595	1.580877781	-1.792256117
C	-3.598296642	0.269258797	1.660484314
H	-2.938418388	-1.663686395	0.993503273
C	-3.690511227	1.631328940	1.359116316
C	-3.370593548	-2.200193644	-2.449285746
C	-3.612100840	-2.127515078	-3.829271793
C	-4.242993832	-2.943219662	-1.636538029
C	-4.706396580	-2.794713736	-4.387012005
H	-2.952667952	-1.529280186	-4.456002235
C	-5.332120419	-3.607294321	-2.196710587
H	-4.073288918	-3.000181675	-0.565868378
C	-5.564926147	-3.536132097	-3.574398041
H	-4.887980938	-2.727476597	-5.456028938
H	-6.417156696	-4.052348614	-4.008104324
H	-6.002023697	-4.178526402	-1.559076786
H	-3.938711882	-0.101122111	2.624724627
H	-4.094415665	2.323568106	2.093317986
H	-3.315960169	3.159812927	-0.115688905
H	2.126487255	4.380759716	-4.318783760
H	4.617004871	4.281516075	-4.271370411
H	5.751816750	2.267256498	-3.355366707
H	4.982965946	-2.862559795	-0.239484176
H	4.478356838	-4.817691803	-1.690794349
H	2.680414200	-4.660632133	-3.399892569
C	-2.420994997	4.300973415	-8.226397514
C	-1.236497164	3.556047678	-8.236549377
C	-3.277459860	4.169883251	-7.128461838
H	-0.555277348	3.651977539	-9.081545830
H	-4.204417706	4.741911411	-7.104830265
C	-0.903348863	2.685337067	-7.193987846
C	-2.972655773	3.328475475	-6.052601814
C	-1.785583615	2.572357178	-6.099934101
C	-1.438648582	1.664900541	-4.952762604
O	-1.142853022	0.447501749	-5.223608494
O	-1.425794363	2.138307095	-3.782664776
C	-3.911302567	3.241923332	-4.867746353
H	-3.436076403	3.652735949	-3.972043991
H	-4.840929985	3.787159920	-5.062215328
H	-4.166298389	2.202630758	-4.628898621
C	0.393188715	1.904670000	-7.242331028
H	0.198782131	0.829263568	-7.253486633
H	0.980206966	2.174686670	-8.126228333
H	1.008212924	2.095993996	-6.354135990
C	-2.744984388	5.248876095	-9.359300613
H	-2.251311779	6.219225407	-9.216220856
H	-2.404572964	4.853530884	-10.322715759
H	-3.821869373	5.437789440	-9.430492401

==============================

I_P

==============================

P	1.084397674	-0.422823101	-1.020244002
C	0.903518617	1.382680178	-1.475933433
C	0.152009547	2.224195004	-0.424514323
P	-1.195083141	1.285123467	0.474748373
C	-2.755076408	1.505355954	-0.579134166
C	-1.751107693	2.556334734	1.758041382
C	-3.376634359	2.830240250	-0.106572509
C	-3.240360022	2.835073709	1.423008204
C	1.848064899	-1.133085966	-2.593450308
C	2.699117899	-0.542994857	-0.044044580
C	3.246865273	-1.650850654	-2.159662962
C	3.799926996	-0.674036205	-1.109874010
Cu	-0.705164671	-1.082077622	0.394903064
H	-1.373489022	-2.360477209	0.978196859
C	-1.497626901	2.152762890	3.194077730
C	-1.070666790	3.112833738	4.120888233
C	-1.690803766	0.834653735	3.633754492
C	-0.834607542	2.769820213	5.453027248
C	-1.454421401	0.489106804	4.964210033
C	-1.024124622	1.453758001	5.878820419
C	-2.469916582	1.280116081	-2.043582439
C	-2.283004045	-0.039895862	-2.490544558
C	-2.282952309	2.323727608	-2.957579613
C	-1.897958994	-0.310134530	-3.801658869
C	-1.903675199	2.055110216	-4.276925087
C	-1.700666904	0.741434872	-4.702146053
C	2.775864601	0.533503890	1.011905193
C	3.559968233	1.684562445	0.877910256
C	1.952428460	0.414156437	2.146059752
C	3.509949923	2.695725918	1.844106436
C	1.896124721	1.420847535	3.106758356
C	2.674514771	2.573081255	2.955029726
C	0.998570681	-2.158539772	-3.314426661
C	0.986598611	-2.181521177	-4.715418339
C	0.225076631	-3.101901293	-2.621472836
C	0.217094675	-3.114361048	-5.412060738
C	-0.547602057	-4.032608509	-3.316006422
C	-0.555792212	-4.043197155	-4.712687969
H	0.341613263	1.370701551	-2.415792465
H	1.885675192	1.823973775	-1.681700230
H	0.842308164	2.536811590	0.366341233
H	-0.255437255	3.129838467	-0.889315903
H	-3.400392056	0.689481139	-0.229798853
H	-1.182705283	3.470547199	1.546911955
H	-4.418803692	2.923293352	-0.432955801
H	-2.829534769	3.686801672	-0.520569324
H	-3.863105774	2.042587519	1.857432127
H	-3.563516140	3.779789448	1.873565555
H	2.002519369	-0.277580351	-3.263344526
H	2.610310793	-1.511699200	0.464493841
H	3.903984070	-1.752706528	-3.030433416
H	3.140863895	-2.650599957	-1.719556689

H	3.999497175	0.295560956	-1.584556222
H	4.743557453	-1.022281885	-0.673708320
H	-0.907638371	4.136609554	3.791220188
H	-1.983583331	0.063037850	2.925825357
H	-0.493536413	3.526638508	6.154603958
H	-1.594901443	-0.540541768	5.281322002
H	-0.832068861	1.180432439	6.912817478
H	-2.412615299	-0.862039685	-1.788289666
H	-2.427873135	3.353947639	-2.646333456
H	-1.737135887	-1.336944580	-4.113173008
H	-1.763279557	2.879930973	-4.970882416
H	-1.395193338	0.534777939	-5.723835945
H	4.214897633	1.800921559	0.019505715
H	1.327114820	-0.470171213	2.258576393
H	4.127002716	3.582267046	1.721781850
H	1.236565471	1.312028289	3.962051868
H	2.628798962	3.363544941	3.698646069
H	1.573962212	-1.449615240	-5.265929222
H	0.180454031	-3.080256462	-1.535173178
H	0.213683933	-3.109211683	-6.498891354
H	-1.155547380	-4.740979195	-2.760014057
H	-1.165224314	-4.763821602	-5.251213551

==============================

IX$_P$

==============================

P	1.196146250	-0.368236005	-1.207234144
C	1.020888805	1.471947670	-1.512159467
C	0.213297531	2.224701405	-0.428126067
P	-1.233716011	1.251548767	0.253543347
C	-2.702396393	1.698065162	-0.833367109
C	-1.836942315	2.307509661	1.695648789
C	-3.153920174	3.073553324	-0.321292758
C	-3.174209118	2.953754187	1.212559819
C	2.024306297	-0.967081130	-2.792003632
C	2.757128477	-0.574694932	-0.169197619
C	3.446985960	-1.429431796	-2.355395555
C	3.908985376	-0.543627858	-1.185800076
Cu	-0.624318063	-0.959927499	0.027875841
C	-1.978027701	1.501568556	2.971957922
C	-1.584347010	2.040659904	4.202714443
C	-2.507400513	0.201022223	2.947790384
C	-1.714298368	1.300992489	5.380888462
C	-2.631255388	-0.542949975	4.119266033
C	-2.234873772	0.006152481	5.341188908
C	-2.359284878	1.473410726	-2.284390211
C	-2.209968567	0.145177841	-2.725960970
C	-2.065879107	2.512826681	-3.173110247
C	-1.746402621	-0.135620192	-4.008823872
C	-1.614104867	2.232309341	-4.467189312
C	-1.442034006	0.911853552	-4.884376526
C	2.742158413	0.355291307	1.019274831
C	3.475633860	1.546384573	1.064862370
C	1.867958307	0.057443280	2.081475735
C	3.326515675	2.430497885	2.138413191
C	1.710764289	0.944077194	3.144452810
C	2.438635349	2.137982130	3.174361944
C	1.231602192	-2.020965576	-3.540089846
C	1.243927956	-2.035486460	-4.941462040
C	0.484733075	-3.003079653	-2.868630648
C	0.524063408	-2.994647264	-5.656465530
C	-0.240530521	-3.959146738	-3.580025673
C	-0.227363110	-3.958462000	-4.978137016
H	0.505745828	1.544000626	-2.476515770
H	2.008077145	1.934929252	-1.628499866
H	0.851131439	2.414278269	0.441703379
H	-0.114976995	3.196154594	-0.816283464
H	-3.463825703	0.961456597	-0.541989803
H	-1.090756774	3.095636606	1.850137949
H	-4.134296894	3.356730700	-0.722432613
H	-2.443630695	3.852784157	-0.625964761
H	-4.003015518	2.300569057	1.512023091
H	-3.335468292	3.917926073	1.706684232
H	2.131418467	-0.085979737	-3.436917543
H	2.667481661	-1.603367925	0.204883844
H	4.137647629	-1.398599267	-3.205198765
H	3.395070553	-2.474162102	-2.023328066
H	4.085738659	0.479293883	-1.543662786
H	4.848008156	-0.899485171	-0.745309591
H	-1.162407756	3.043520212	4.236906528
H	-2.780951262	-0.256519467	1.999495149
H	-1.399477243	1.733773947	6.327484608
H	-3.014307737	-1.559119225	4.071066380
H	-2.323148966	-0.575551927	6.254847527
H	-2.428072214	-0.671971500	-2.040413141
H	-2.180189371	3.546251535	-2.858883619
H	-1.605659842	-1.167406440	-4.316714764
H	-1.390303850	3.051527262	-5.145864010
H	-1.074525714	0.695929706	-5.883710384
H	4.165060520	1.793406725	0.262512386
H	1.285181403	-0.861042082	2.059306860
H	3.905108452	3.350648642	2.160336971
H	1.008394599	0.707971931	3.938572884
H	2.317010880	2.831570625	4.002256870
H	1.813312650	-1.278419971	-5.478445530
H	0.429004163	-2.998680353	-1.782464981
H	0.543216050	-2.982470751	-6.743820190
H	-0.828601778	-4.694982529	-3.036487103
H	-0.798381567	-4.698606491	-5.531788349
C	-3.218340397	-6.284166336	3.360255957
C	-4.052666664	-5.289047718	2.846106291
C	-1.842480421	-6.165167332	3.145632505
H	-5.126681328	-5.360542297	3.009540319
H	-1.176858068	-6.932431698	3.539117813
C	-3.551828861	-4.205193520	2.115769863
C	-1.291136622	-5.085602283	2.449493647
C	-2.156482697	-4.097205162	1.920885324
C	-1.583508849	-2.926590681	1.169822216
O	-2.173861265	-2.478882790	0.134032518
O	-0.503696203	-2.399050474	1.594703317
C	0.213095844	-5.019905567	2.290120125
H	0.668223858	-5.983183384	2.546472311
H	0.505898178	-4.754221439	1.270241022
H	0.637134135	-4.245619774	2.936301947
C	-4.523211479	-3.174531698	1.579545856
H	-4.523581505	-3.168037653	0.486826360
H	-5.536874771	-3.375614405	1.940757871
H	-4.245470524	-2.161859989	1.889861822
C	-3.781553507	-7.474459648	4.103483677
H	-4.781398296	-7.266850948	4.498479366
H	-3.863363743	-8.348459244	3.443840265
H	-3.138886929	-7.763797760	4.942288876

==============================

I$_S$-TS

==============================

P	1.397578835	1.172733665	0.301739514
C	0.471935689	2.272930622	1.458502293
C	-0.132385567	1.700329661	2.619274378
C	0.162277177	3.584667206	1.083670020
C	-1.015593171	2.512350082	3.307199955
C	0.180579305	0.357213169	3.194897175
C	-0.746117592	4.382851601	1.802306771
H	0.621381700	4.005164146	0.196484610
C	-1.333251715	3.808793783	2.908487320
O	-1.695894837	2.207426548	4.461248875
C	1.030253291	0.298373193	4.283126831
C	-0.376352251	-0.884389102	2.768978834
H	-0.977011383	5.398218155	1.499321461
O	-2.231170893	4.359065533	3.788307428
C	-2.623623848	3.282558441	4.652600288
C	1.372313619	-0.888692975	4.923451900
O	1.685209036	1.349231243	4.876098633
C	-0.047001641	-2.068274736	3.437499762
P	-1.430733562	-0.881954432	1.256938577
H	-3.631844997	2.941945076	4.378405571
H	-2.580545902	3.618489742	5.693127155
C	0.841334343	-2.096678495	4.527766228
O	2.257623672	-0.634065211	5.937979698
C	2.455198288	0.786980629	5.944549561

H	-0.481193721	-3.004870653	3.109005451
H	1.097418308	-3.021705389	5.032211304
H	2.109248638	1.200204372	6.901264191
H	3.516889811	1.004733920	5.780614376
C	-1.958635449	-2.629471779	1.088066697
C	-3.252006292	-3.093405724	1.357031703
C	-0.993555427	-3.531844378	0.605631351
C	-3.572882652	-4.437550068	1.150927067
H	-4.011206150	-2.410180330	1.723869681
C	-1.312369227	-4.874567986	0.418209940
H	0.005267488	-3.171218634	0.375311345
C	-2.606506824	-5.330103874	0.686725259
C	-2.929607868	0.036190946	1.776370406
C	-3.487414598	0.938157201	0.861091137
C	-3.517221212	-0.122746810	3.039988518
C	-4.633650780	1.659425020	1.197295904
H	-2.996294260	1.078028440	-0.100952454
C	-4.667877674	0.592673779	3.370382071
H	-3.069009781	-0.798733711	3.762635469
C	-5.228088856	1.483361959	2.448702097
C	2.756995678	0.445303947	1.283992171
C	3.109806299	-0.882050037	1.005444050
C	3.441568375	1.147188425	2.287381887
C	4.133183002	-1.501276612	1.724102020
H	2.583943605	-1.427119493	0.228239611
C	4.463909626	0.523781300	3.002911329
H	3.154206276	2.166685581	2.526958704
C	4.809801102	-0.802814126	2.726351261
C	2.218089819	2.308275223	-0.882770360
C	1.455476999	2.730802774	-1.984941244
C	3.555616617	2.711355925	-0.781949520
C	2.015481949	3.560053110	-2.955079079
H	0.427193135	2.385026932	-2.073937416
C	4.117835999	3.528654337	-1.764219046
H	4.164948463	2.375763416	0.050792173
C	3.350781441	3.957393408	-2.848588467
H	5.368479729	-2.307240248	-2.222491980
C	4.291296482	-2.168997288	-2.235341549
C	3.730770111	-0.950734913	-2.635599375
C	3.433406353	-3.205094814	-1.853865504
C	2.352840900	-0.765190363	-2.645365000
C	2.053138018	-3.021828651	-1.855168104
C	1.465959191	-1.791327477	-2.237061501
H	4.375520229	-0.126161516	-2.931026697
H	3.843357086	-4.166029930	-1.549236894
H	1.954564810	0.202045530	-2.932504892
H	1.402139783	-3.840001583	-1.554401040
C	0.021415366	-1.630783200	-2.179762363
C	-0.710384011	-0.531739295	-2.708038568
H	-0.550386190	-2.497886658	-1.864538074
H	-1.755419493	-0.702746332	-2.943563223
H	-1.153142095	0.741759956	-1.737571239
Cu	-0.306969315	-0.104977310	-0.590081751
H	-0.214710072	0.145911694	-3.397783041
H	-0.555281639	-5.562367916	0.051074296
H	-2.860298872	-6.375017643	0.529519796
H	-4.581623077	-4.785977364	1.356825948
H	-5.125908852	0.460078478	4.347286224
H	-6.123030663	2.042833805	2.709293127
H	-5.058740616	2.361634731	0.485232800
H	1.415592313	3.881075621	-3.802577257
H	3.793824911	4.590497017	-3.612702370
H	5.159496784	3.827804089	-1.682254076
H	4.397952557	-2.529634237	1.494683504
H	5.602566242	-1.286966681	3.290271997
H	4.995157719	1.074866533	3.775147200

==============================

I$_S$-TS'

==============================

P	1.138113737	1.242212296	0.278895140
C	0.292609453	2.284821272	1.539123416
C	-0.213182434	1.641373396	2.709702730
C	0.017411601	3.635630846	1.301634550
C	-0.943959892	2.442769289	3.568244696
C	0.093008690	0.239153579	3.132021189
C	-0.751956820	4.413921833	2.184218407
H	0.407607615	4.108617783	0.407885969
C	-1.224791646	3.781591892	3.312672138
O	-1.497645378	2.076671839	4.770632267
C	1.004395604	0.084835790	4.162480831
C	-0.481890827	-0.967986465	2.623283386
H	-0.957870543	5.460894585	1.992172837
O	-1.972612023	4.305897713	4.335838795
C	-2.225869179	3.218494415	5.236203194
C	1.386132121	-1.149556994	4.675813675
O	1.678899407	1.086077213	4.818295956
C	-0.098960176	-2.202499866	3.161272287
P	-1.596892118	-0.911095142	1.146124721
H	-3.299319744	2.990127325	5.234981060
H	-1.878420830	3.487156391	6.240660667
C	0.844690263	-2.321347952	4.196334362
O	2.313392162	-0.976350367	5.671182632
C	2.575063467	0.433547884	5.724462509
H	-0.540756226	-3.110930443	2.769399881
H	1.131556511	-3.286259651	4.598603249
H	2.395666599	0.800348997	6.741929531
H	3.609463215	0.622074187	5.410006523
C	-2.438670635	-2.544492006	1.154649854
C	-3.704519272	-2.775197029	1.715038061
C	-1.753675461	-3.614490509	0.555745184
C	-4.257863998	-4.055763721	1.700574160
H	-4.265127659	-1.959072113	2.157349348
C	-2.303171873	-4.897080898	0.560900927
H	-0.793510437	-3.447381496	0.077721119
C	-3.555267334	-5.121876717	1.134568810
C	-2.874576569	0.302921385	1.662837386
C	-3.273072004	1.281302333	0.742904246
C	-3.426862955	0.303549707	2.953069687
C	-4.211838245	2.247000217	1.107350230
H	-2.813363791	1.289580584	-0.243893698
C	-4.380055904	1.257244587	3.306835651
H	-3.091673374	-0.424624979	3.685900450
C	-4.768821716	2.234981060	2.387162209
C	2.560002089	0.528515518	1.194136500
C	2.812798262	-0.841443479	1.039498448
C	3.366334200	1.282557964	2.060639381
C	3.860531092	-1.447755218	1.734516144
H	2.161693573	-1.427712917	0.395202994
C	4.424449444	0.677937925	2.739209175
H	3.152994871	2.336616278	2.214915037
C	4.671611786	-0.689337492	2.581099510
C	1.876973271	2.432680845	-0.907111526
C	1.013851643	2.967224360	-1.881017923
C	3.233770132	2.784617662	-0.937029541
C	1.493179798	3.857407093	-2.840673208
H	-0.031267077	2.665363550	-1.881223083
C	3.712408543	3.664505005	-1.909366846
H	3.922594070	2.368847370	-0.209531456
C	2.845359802	4.207323551	-2.857975245
H	-0.536048830	-6.586758614	-2.318401098
C	-0.298251987	-5.526963234	-2.302277565
C	0.945245087	-5.079110146	-1.840551257
C	-1.226744652	-4.578687668	-2.743474245
C	1.252273083	-3.722105503	-1.831561923
C	-0.927514374	-3.219702959	-2.727684736
C	0.330256760	-2.747421741	-2.282097578
H	1.684255481	-5.795670509	-1.488626480
H	-2.205358982	-4.901206493	-3.091195583
H	2.227161646	-3.392354965	-1.476440310
H	-1.682460308	-2.509155750	-3.051349163
C	0.702538431	-1.340733767	-2.283123016
C	-0.074635267	-0.303356290	-2.864736557
H	-0.894508958	-0.569085181	-3.523655415
H	-1.173524022	0.572749376	-1.938725710
Cu	-0.433096886	-0.224803716	-0.700899899
H	0.445848912	0.602856338	-3.157740593
H	-1.754598737	-5.704940796	0.088292502
H	-3.987926483	-6.118538857	1.129108429
H	-5.240475178	-4.219036102	2.135524988

H	-4.812985897	1.242664099	4.303877354
H	-5.499770641	2.987742901	2.670301199
H	-4.503034115	3.012447834	0.393299580
H	0.813326836	4.266752720	-3.582915783
H	3.222541094	4.892299652	-3.612397194
H	4.767362118	3.925397396	-1.923398256
H	4.037234306	-2.513620377	1.620806694
H	5.487617016	-1.160889626	3.121582031
H	5.054313660	1.273122549	3.395807743
H	1.731892228	-1.111280680	-2.021430492

==============================

II$_S$

==============================

Cu	0.341290265	-1.576453090	-1.690577745
H	-0.851242959	-3.127178907	-4.222526073
H	-4.161387920	2.042347193	-2.941020012
C	-3.311563492	1.388395190	-3.116652727
C	-2.020885229	1.910147429	-3.244381428
C	-3.484795332	0.004619900	-3.232421637
C	-0.934053004	1.068008184	-3.471993208
C	-2.398630857	-0.838699162	-3.448162556
C	-1.074173689	-0.340536177	-3.558792830
H	-1.859738588	2.984879494	-3.181581974
H	-4.480059147	-0.425516009	-3.139925957
H	0.055792965	1.499124646	-3.607125759
H	-2.566436291	-1.909970045	-3.502942085
C	0.108268052	-1.224130869	-3.678342104
C	-0.050666053	-2.463261604	-4.563923836
H	0.973084748	-0.640743375	-4.018959522
H	-0.280049294	-2.207785845	-5.612397194
P	-1.248250604	-2.393435717	-0.136222407
C	-0.370348394	-3.396269560	1.138289690
C	0.493603021	-2.752352953	2.078005791
C	-0.396664798	-4.794705868	1.058810711
C	1.243023634	-3.591129541	2.883327246
C	0.597502470	-1.280173779	2.312419653
C	0.405269295	-5.616123199	1.870941997
H	-1.057088017	-5.271693707	0.343573183
C	1.224391699	-4.978199959	2.776110172
O	2.141781569	-3.215941668	3.852810383
C	0.020968452	-0.759396970	3.455846786
C	1.285437822	-0.346099794	1.480720162
H	0.380230546	-6.697053432	1.790802121
O	2.116898775	-5.526925087	3.662687540
C	2.608265638	-4.432497978	4.446873188
C	0.036000561	0.595452547	3.772161722
O	-0.705319226	-1.445261240	4.400667191
C	1.311872840	1.012055516	1.820626020
P	1.971383691	-0.926768661	-0.125307932
H	3.703245163	-4.441779137	4.436886787
H	2.220729113	-4.511353970	5.473179340
C	0.677830398	1.513898253	2.970678091
O	-0.680732727	0.812182307	4.922199249
C	-1.017212272	-0.488749415	5.419592381
H	1.836696029	1.709127426	1.177356124
H	0.690997720	2.569783688	3.215987206
H	-0.421711564	-0.703880310	6.319548130
H	-2.089019775	-0.527488410	5.638158798
C	2.976117373	0.488841653	-0.710542917
C	4.307188988	0.728162527	-0.343078524
C	2.331738710	1.380106449	-1.582321048
C	4.979322910	1.845466495	-0.839769602
H	4.822543621	0.039381590	0.319250017
C	2.999956131	2.504473209	-2.064280033
H	1.307157755	1.181271911	-1.882288337
C	4.327270985	2.736133337	-1.696218848
C	3.165018797	-2.233079672	0.341315001
C	3.284636974	-3.332332611	-0.521504223
C	3.921392679	-2.199466228	1.521818876
C	4.148399353	-4.381878853	-0.210282281
H	2.683121681	-3.362153053	-1.427755833
C	4.788797855	-3.247628927	1.828157306
H	3.802074671	-1.373489857	2.216527462
C	4.901175022	-4.340719700	0.965425789
C	-2.208320856	-1.137095571	0.785117209
C	-2.372989178	0.115867980	0.177290514
C	-2.777323484	-1.372591734	2.046279907
C	-3.098043680	1.118588090	0.823332012
H	-1.938549638	0.306800157	-0.799238503
C	-3.494470119	-0.364793450	2.690889597
H	-2.625567198	-2.328089476	2.539618015
C	-3.655213833	0.883799195	2.081882477
C	-2.508113861	-3.530197620	-0.831298649
C	-2.115674019	-4.294476032	-1.941301107
C	-3.821501970	-3.639081478	-0.355906546
C	-3.013363361	-5.166924000	-2.554904938
H	-1.106948614	-4.181266308	-2.329670429
C	-4.722849369	-4.502810955	-0.979363978
H	-4.145774364	-3.039999008	0.489027560
C	-4.321457386	-5.268815041	-2.075664520
H	0.871738553	-3.055642366	-4.563122749
H	4.225741386	-5.235016346	-0.878461659
H	5.568988323	-5.161542892	1.212117195
H	5.371993065	-3.214273214	2.744972229
H	6.014357090	2.020412207	-0.558127165
H	4.854806900	3.605168104	-2.079814434
H	2.488819599	3.189128876	-2.735756397
H	-2.698105097	-5.748990536	-3.416339636
H	-5.028630257	-5.936654568	-2.559900999
H	-5.742560387	-4.573910713	-0.610057175
H	-3.220806360	2.081737518	0.336529911
H	-4.209819794	1.668652534	2.588906288
H	-3.925602913	-0.552745700	3.671186209

==============================

II$_S$-TS

==============================

Cu	-0.225367934	-0.640409172	-3.275611639
H	-3.287765980	0.239022851	-2.958347082
C	-2.991525173	0.164878532	-4.008861542
C	-1.566022754	0.644347548	-4.274747372
C	-1.284786224	2.067005157	-4.025138855
C	-0.376012027	2.758244276	-4.864307880
C	-1.890365720	2.827951908	-2.996723175
C	-0.073450968	4.101628304	-4.674347878
C	-1.565601230	4.169029713	-2.790973425
C	-0.649511337	4.822366238	-3.620262384
H	0.091145538	2.208366871	-5.678743839
H	-2.639273643	2.365931273	-2.361276388
H	0.622136235	4.593084812	-5.351623058
H	-2.049079657	4.715878010	-1.983794212
H	-0.411429375	5.871422768	-3.468255520
H	-1.304944158	0.421686471	-5.309515953
H	-3.097308159	-0.886818111	-4.292779922
P	-1.387740850	-2.107519150	-1.769847393
C	-0.324418843	-3.191905975	-0.719692111
C	0.580032349	-2.563976526	0.194005519
C	-0.301685214	-4.581977367	-0.879331887
C	1.438460112	-3.410557032	0.871523261
C	0.607995868	-1.112561584	0.559981525
C	0.599410117	-5.410557747	-0.186826944
H	-1.002571106	-5.052361012	-1.557851076
C	1.469974279	-4.788738251	0.679166913
O	2.375960588	-3.055171251	1.809542775
C	0.077728279	-0.757325768	1.787873507
C	1.195356846	-0.051650207	-0.197503909
H	0.607145607	-6.485544682	-0.327287942
O	2.432326555	-5.350288391	1.477882385
C	3.097407818	-4.252434254	2.120175123
C	0.062537178	0.547463179	2.272257566
O	-0.522172749	-1.593513489	2.696728945
C	1.197824478	1.251419783	0.311500728
P	1.759526610	-0.415499955	-1.919710398
H	4.120007992	-4.170460224	1.729564786
H	3.094270706	-4.408373356	3.204602242
C	0.630388796	1.579331636	1.556981325
O	-0.554216802	0.585649431	3.495597601
C	-1.017053962	-0.751229763	3.743483782
H	1.649809361	2.047635555	-0.268510073

H 0.635978639 2.596044302 1.933432102
H -0.626060784 -1.098821282 4.706513882
H -2.114418745 -0.762799442 3.727979183
C 2.814553499 1.008071423 -2.413791180
C 4.208359718 0.943529129 -2.570273161
C 2.153195858 2.203532457 -2.743374109
C 4.922836781 2.058154821 -3.013914824
H 4.743046284 0.025304545 -2.353624105
C 2.874154329 3.321431875 -3.161710739
H 1.070171833 2.258233547 -2.691142559
C 4.262199879 3.254368305 -3.298058748
C 2.961827040 -1.783753276 -1.647360206
C 2.871776581 -2.952230930 -2.416358709
C 3.959451437 -1.689067960 -0.662928641
C 3.779591322 -3.995286226 -2.218351126
H 2.077932835 -3.064517736 -3.147220373
C 4.871574879 -2.727305889 -0.477759123
H 4.015078068 -0.802184701 -0.038171511
C 4.784219265 -3.885722160 -1.256139278
C -2.317340612 -1.143084526 -0.517174363
C -2.226512194 0.254041255 -0.570867658
C -3.052203417 -1.743366718 0.515004396
C -2.879249096 1.043245554 0.373863935
H -1.616690040 0.715933800 -1.340397835
C -3.717907906 -0.952884614 1.452443123
H -3.097338676 -2.826500654 0.587016284
C -3.633201838 0.440878302 1.382804513
C -2.611881733 -3.231709003 -2.550123215
C -2.137506485 -4.123642921 -3.529605627
C -3.991035461 -3.174152613 -2.303066969
C -3.012150764 -4.968504906 -4.211620808
H -1.084672093 -4.137961864 -3.786798954
C -4.867172718 -4.006601334 -3.002380848
H -4.388828278 -2.473869324 -1.576865435
C -4.382868290 -4.910552979 -3.948804617
H -3.732673168 0.738831997 -4.589735031
C -1.135896087 -7.945042610 -6.234514236
C -1.124826550 -7.031476498 -7.289062500
C -0.355087608 -7.661466599 -5.107564449
H -1.708698273 -7.244875431 -8.181900978
H -0.326923937 -8.376249313 -4.287419796
C -0.379315436 -5.846222401 -7.243443489
C 0.387566537 -6.484118938 -5.003474236
C 0.354616374 -5.561863422 -6.071314335
C 1.055969954 -4.225040913 -5.993088722
O 1.752868652 -3.772104502 -6.878770351
O 0.728636146 -3.563192368 -4.862174511
C -0.285077751 -0.323914558 -8.200492859
C 0.391224623 -0.771864057 -7.068568707
C -0.263982475 -1.621677160 -6.154591560
C -1.559716105 -2.069571972 -6.350989819
C -2.222385168 -1.630377054 -7.503755569
C -1.595827818 -0.768055677 -8.412425041
C 1.721158862 -0.532830954 -6.527576447
C 1.822528839 -1.225153089 -5.369771004
N 0.581287384 -1.837248206 -5.023423672
H 0.190344617 0.358336210 -8.899393082
H -2.037365913 -2.728915453 -5.637247086
H -3.240086794 -1.960879326 -7.689260006
H -2.137941599 -0.434051543 -9.292605400
H 2.485481501 0.099269010 -6.960596561
H 2.654304743 -1.320465088 -4.690282822
H -2.615680456 -5.653172493 -4.956475735
H -5.070513248 -5.557521820 -4.486964703
H -5.934049129 -3.945173025 -2.803978682
H -4.298470497 -1.424812913 2.241110325
H -4.145527363 1.054092765 2.119274616
H -2.787466764 2.124392033 0.323847115
H 2.335648298 4.232270718 -3.400804996
H 4.822177887 4.121437073 -3.637614727
H 6.000894070 1.987490892 -3.134592295
H 5.648088455 -2.633316517 0.277384788
H 5.490767002 -4.698061466 -1.109071374
H 3.695280075 -4.897756100 -2.815048456
C -1.953007698 -9.214097023 -6.302588463
H -2.663625717 -9.271857262 -5.469507217
H -2.522584200 -9.277316093 -7.234438896
H -1.312909365 -10.102234840 -6.240034580
C -0.385784537 -4.923728466 -8.441552162
H 0.618897438 -4.832370758 -8.862243652
H -1.061725616 -5.302425861 -9.213601112
H -0.700963795 -3.911104441 -8.175846100
C 1.245124459 -6.243788719 -3.782419920
H 0.911992550 -5.379168987 -3.204405069
H 1.242656589 -7.115897655 -3.122560740
H 2.282502890 -6.050940990 -4.077297688

===============================

III$_{SN}$

===============================

Cu -0.941248715 -3.405044556 -2.113626957
H -4.241759777 -3.797001839 -3.461281776
C -3.413094997 -3.711453915 -4.161592484
C -2.385308266 -2.703941107 -3.779937744
C -2.698173285 -1.465458274 -3.103135347
C -3.924449205 -1.241199255 -2.430175066
C -1.759628654 -0.402786791 -3.164711952
C -4.203781605 -0.002279116 -1.871256709
C -2.042342424 0.830161512 -2.592112541
C -3.267928600 1.037500739 -1.948919535
H -4.649509907 -2.043085575 -2.349260807
H -0.814217865 -0.567136526 -3.673044682
H -5.150686741 0.159922823 -1.365559459
H -1.315773010 1.634555340 -2.658095121
H -3.495316505 2.005377054 -1.511623621
H -1.562960148 -2.628087521 -4.484436512
H -2.958239079 -4.693258286 -4.312847137
P -2.357319832 -4.148876190 -0.428008765
C -1.357126474 -5.448640347 0.411266565
C -0.271869749 -5.078576565 1.271783233
C -1.535414577 -6.791591167 0.050274882
C 0.547210634 -6.117006779 1.682573795
C 0.046410624 -3.719604969 1.815153956
C -0.674689293 -7.816876888 0.477766871
H -2.375964642 -7.072553158 -0.570264459
C 0.378189802 -7.444683075 1.285735846
O 1.634925246 -6.020606041 2.503897667
C -0.244241908 -3.435865879 3.135759354
C 0.748745620 -2.704892397 1.098846555
H -0.831849635 -8.848822594 0.186349690
O 1.353713036 -8.222141266 1.828376055
C 2.217744350 -7.332671642 2.558348656
C 0.093717843 -2.227320433 3.747338295
O -0.927548945 -4.225970745 4.019544125
C 1.103874564 -1.506197810 1.724655628
P 1.027644753 -3.034695148 -0.676308870
H 3.201788902 -7.309210300 2.077359438
H 2.280576706 -7.661645889 3.600401878
C 0.781039476 -1.243019342 3.068981171
O -0.370754331 -2.215049982 5.031768799
C -0.905795634 -3.525660038 5.273937702
H 1.647634387 -0.752387047 1.166215777
H 1.056139350 -0.311308384 3.549781322
H -0.259940624 -4.061779499 5.981645107
H -1.926527143 -3.435861111 5.657167912
C 1.887263775 -1.574769497 -1.367244124
C 3.157941341 -1.656146765 -1.953903079
C 1.184210062 -0.358268321 -1.430356979
C 3.713982344 -0.540391445 -2.585374117
H 3.710579634 -2.589508057 -1.927950859
C 1.749468207 0.755578697 -2.047268152
H 0.189727455 -0.283708721 -0.999269724
C 3.016306400 0.667032301 -2.633368492
C 2.248261690 -4.402463913 -0.675732791
C 2.076785088 -5.506516933 -1.522449493
C 3.337500334 -4.377920628 0.210382745
C 2.979013443 -6.569663048 -1.483686686
H 1.245828509 -5.526475430 -2.212634325
C 4.247875214 -5.434909821 0.232705578
H 3.467231035 -3.538866043 0.888128400

C	4.068242550	-6.536403656	-0.610064864
C	-2.730984449	-2.898166895	0.841080844
C	-2.419900656	-1.556851506	0.588431776
C	-3.304619074	-3.259502649	2.070870399
C	-2.680495024	-0.583386421	1.551841259
H	-1.965435386	-1.279974580	-0.356843114
C	-3.570942879	-2.282325745	3.027135134
H	-3.518681049	-4.302292347	2.285681486
C	-3.257119179	-0.944535792	2.770034313
C	-3.969679594	-4.884983063	-0.895062864
C	-4.011149883	-5.874557972	-1.894391894
C	-5.180161953	-4.419827938	-0.356558532
C	-5.225339890	-6.416132450	-2.309224367
H	-3.100000143	-6.194805622	-2.386664391
C	-6.395527363	-4.953039169	-0.788945079
H	-5.182838917	-3.640408754	0.396739572
C	-6.422730923	-5.957376957	-1.756713748
H	-3.820540428	-3.410029888	-5.139501095
C	-0.544993937	-5.648005486	-6.661582470
C	-0.088488705	-4.694295883	-5.741239071
C	-0.261079699	-4.935260296	-4.351596832
C	-0.855981946	-6.107459545	-3.873082161
C	-1.322212696	-7.036766529	-4.806313038
C	-1.169618368	-6.802717686	-6.185461044
C	0.568854094	-3.412297726	-5.830834866
C	0.740218997	-2.965425968	-4.535883427
N	0.244271189	-3.868708611	-3.614537239
H	-0.416618228	-5.496808052	-7.729448318
H	-0.939991474	-6.282469749	-2.802478790
H	-1.791231036	-7.955520630	-4.465747833
H	-1.532159209	-7.542798519	-6.892841339
H	0.914612532	-2.922778368	-6.732078075
H	1.213245988	-2.054876804	-4.190268993
H	4.696887970	-0.619356453	-3.040881872
H	3.452830315	1.531513572	-3.124489546
H	1.200847983	1.693155885	-2.076118946
H	-2.428585529	0.453555852	1.350377440
H	-3.455135822	-0.187217921	3.522905111
H	-4.016476631	-2.564303160	3.976795912
H	-7.322858334	-4.581732750	-0.362208307
H	-7.370905876	-6.369750977	-2.088715076
H	-5.234985828	-7.180368900	-3.080843687
H	2.830621719	-7.421040535	-2.141647100
H	4.775593758	-7.360579014	-0.588620722
H	5.094665051	-5.400120735	0.912603140

==============================

III$_{SN}$-TS

==============================

Cu	-1.216004848	-3.395395517	-2.088064671
H	-3.883001566	-4.118024826	-3.352836609
C	-3.372238159	-3.779512405	-4.254199982
C	-2.350223780	-2.714123487	-4.006773949
C	-2.655247927	-1.551225066	-3.157772303
C	-3.837274790	-1.488326311	-2.378054857
C	-1.846572876	-0.392656505	-3.256195068
C	-4.203565121	-0.302539855	-1.751417756
C	-2.205621958	0.782656550	-2.601492405
C	-3.390239239	0.834531844	-1.856127024
H	-4.470039845	-2.364923239	-2.272737265
H	-0.942931056	-0.423471183	-3.859510422
H	-5.119151115	-0.265459418	-1.166178107
H	-1.573665619	1.664147735	-2.691998959
H	-3.678883076	1.757240772	-1.358463883
H	-1.810294509	-2.429884672	-4.902696609
H	-2.932358980	-4.639178753	-4.765150547
P	-2.509649754	-4.114159584	-0.296270162
C	-1.503993988	-5.421860695	0.532951713
C	-0.334988326	-5.053030014	1.275123596
C	-1.762436628	-6.770828724	0.258631617
C	0.490972877	-6.100656509	1.648210168
C	0.046552610	-3.694848299	1.777808070
C	-0.901879251	-7.807677269	0.657290280
H	-2.668465614	-7.047736645	-0.264539152
C	0.237717241	-7.436093330	1.335866928
O	1.646903753	-6.012612820	2.375249624
C	-0.168745354	-3.402845860	3.111278772
C	0.728142262	-2.693024397	1.025403976
H	-1.123615384	-8.847290039	0.444659948
O	1.226627111	-8.228251457	1.839260340
C	2.213201523	-7.332781792	2.379769087
C	0.227417633	-2.204178095	3.704233408
O	-0.821861029	-4.179685116	4.030883789
C	1.151685953	-1.509109855	1.636817098
P	0.883295596	-2.980558872	-0.775971234
H	3.104888678	-7.344560623	1.740764976
H	2.445978642	-7.625618458	3.407800436
C	0.909791648	-1.239333510	2.995986223
O	-0.171467006	-2.181327105	5.011555195
C	-0.732741296	-3.475364447	5.279465199
H	1.684740424	-0.767430842	1.053084970
H	1.237717986	-0.317895710	3.463530302
H	-0.076465413	-4.027066708	5.965557098
H	-1.735546112	-3.355500698	5.701056480
C	1.831669331	-1.547875166	-1.417889953
C	3.137099028	-1.655830503	-1.918633819
C	1.178089499	-0.304073870	-1.490867972
C	3.774721384	-0.544045568	-2.474881172
H	3.658558607	-2.606598377	-1.880865335
C	1.822448492	0.806868255	-2.033679247
H	0.163046181	-0.204335168	-1.115477920
C	3.124272346	0.689528704	-2.532551527
C	2.042170048	-4.397178173	-0.871100247
C	1.798198104	-5.434995651	-1.780578017
C	3.165377617	-4.467213154	-0.030591505
C	2.670847416	-6.520698071	-1.861166596
H	0.926600158	-5.398311615	-2.421476126
C	4.042520523	-5.547227859	-0.122102186
H	3.346876860	-3.682124376	0.697888494
C	3.798009396	-6.575019836	-1.038594484
C	-2.777131796	-2.844657898	0.987351716
C	-2.416964054	-1.518146157	0.721720934
C	-3.290170670	-3.183785200	2.250475168
C	-2.576331615	-0.537294328	1.699529529
H	-1.989570618	-1.262508869	-0.242401421
C	-3.458990335	-2.199116230	3.222113848
H	-3.533528090	-4.217801094	2.477658272
C	-3.101990938	-0.875721693	2.947289944
C	-4.163981438	-4.824517250	-0.650314033
C	-4.273640633	-5.811395168	-1.648207068
C	-5.339384556	-4.329413891	-0.064857736
C	-5.517489910	-6.311597824	-2.026084185
H	-3.382541656	-6.182443142	-2.145806313
C	-6.585606098	-4.821045399	-0.457328945
H	-5.288561821	-3.557981253	0.695345938
C	-6.679814816	-5.813141346	-1.433123589
H	-4.123981476	-3.349682331	-4.933583736
C	0.778198540	-5.818166733	-6.487513065
C	0.548945963	-4.725937366	-5.643411636
C	-0.338563949	-4.870450974	-4.542869091
C	-0.966935337	-6.086143970	-4.257175922
C	-0.736913979	-7.158850193	-5.119616032
C	0.119476467	-7.021422386	-6.227291584
C	1.097597718	-3.391562939	-5.543346405
C	0.546949565	-2.818603516	-4.430922508
N	-0.339940816	-3.696741819	-3.797154427
H	1.473028541	-5.738049984	-7.319270134
H	-1.585015535	-6.186782360	-3.368628263
H	-1.212710023	-8.116053581	-4.925059319
H	0.288507760	-7.875885963	-6.876696587
H	1.850802541	-2.952569723	-6.184644222
H	0.740016937	-1.849344134	-3.994585037
H	4.785603046	-0.645265579	-2.860505342
H	3.626179934	1.551684499	-2.961754560
H	1.310263157	1.765101194	-2.069432974
H	-2.280012131	0.486517698	1.490221620
H	-3.221368790	-0.112753741	3.711277008
H	-3.860227585	-2.464164019	4.196326256
H	-7.485166073	-4.424875259	0.005129644
H	-7.651754379	-6.191425800	-1.735105157

H	-5.578285694	-7.078677177	-2.792640924
H	2.468725681	-7.319112778	-2.569488287
H	4.482836246	-7.415957451	-1.107432127
H	4.916465759	-5.588511944	0.523052573

================================

V_{SN}

================================

Cu	-0.065299295	-3.325263739	-1.537607193
H	-2.735490561	-0.993741155	0.620119035
C	-3.158489943	-1.983013034	0.421131670
C	-3.848958015	-2.032958746	-0.945600569
C	-4.970593452	-1.020645976	-1.147762537
C	-5.470602512	-0.242823407	-0.098009773
C	-5.522490025	-0.864074588	-2.426516294
C	-6.498505592	0.676463664	-0.322545558
C	-6.545572758	0.053292040	-2.652228832
C	-7.036379337	0.829468012	-1.598976135
H	-5.065133572	-0.338934749	0.903270185
H	-5.132612228	-1.453043699	-3.252659559
H	-6.872524738	1.274976969	0.503478169
H	-6.957443714	0.167642102	-3.650830746
H	-7.830639839	1.549130440	-1.774192810
H	-4.265810013	-3.039696217	-1.072156787
H	-2.348992586	-2.712091923	0.434923708
P	-0.636594653	-4.900348186	0.111830652
C	0.652252495	-6.172454357	-0.205465317
C	2.013421297	-5.820338726	0.068092607
C	0.350661427	-7.359437466	-0.880056024
C	2.966767311	-6.705734253	-0.399906605
C	2.469733715	-4.702731609	0.952256083
C	1.347878575	-8.239445686	-1.338610530
H	-0.683677495	-7.629453182	-1.054311872
C	2.654287815	-7.870972633	-1.102771401
O	4.322094440	-6.618470669	-0.235616237
C	2.781432390	-5.017788410	2.262669325
C	2.671357393	-3.342472315	0.572438240
H	1.102054000	-9.164276123	-1.847712517
O	3.800059319	-8.539353371	-1.423359871
C	4.882768154	-7.687202454	-1.015189171
C	3.242974520	-4.082386017	3.188820362
O	2.647137403	-6.238020897	2.868087292
C	3.161973476	-2.417478561	1.501621127
P	2.167635202	-2.809676886	-1.112873077
H	5.372058868	-7.265775681	-1.903423309
H	5.583746433	-8.258335114	-0.399550200
C	3.461205721	-2.769445658	2.830315590
O	3.410013914	-4.675673008	4.405518055
C	3.100244522	-6.067116261	4.220195770
H	3.315947771	-1.388538361	1.198637247
H	3.833789825	-2.042108059	3.542398930
H	4.002999306	-6.668495178	4.383727074
H	2.299206972	-6.353354931	4.909303188
C	2.525507927	-1.018860340	-1.135922432
C	3.746680737	-0.475309014	-1.559800506
C	1.519116402	-0.164488301	-0.658383548
C	3.959218979	0.903198361	-1.489565611
H	4.530459404	-1.124952078	-1.938566208
C	1.742842793	1.208350897	-0.570515990
H	0.550716996	-0.572576106	-0.374681711
C	2.964368820	1.745583177	-0.985923469
C	3.348653793	-3.639946461	-2.228026628
C	2.884108543	-4.085906506	-3.474042177
C	4.681155205	-3.878715515	-1.860611081
C	3.740886211	-4.754951000	-4.347151279
H	1.844311237	-3.918038845	-3.747218847
C	5.538440228	-4.540965080	-2.739398479
H	5.037796974	-3.568594456	-0.882973135
C	5.070068359	-4.980320454	-3.980643988
C	-0.473787010	-4.445782661	1.875890374
C	-0.300020903	-3.098707676	2.222056866
C	-0.470008433	-5.421207905	2.885983467
C	-0.131731406	-2.728763580	3.556577921
H	-0.259953231	-2.344893694	1.440786004
C	-0.311625093	-5.047003746	4.220219612
H	-0.576404393	-6.470510483	2.626420975
C	-0.137880579	-3.701640844	4.558539391
C	-2.282974720	-5.691019058	-0.047863439
C	-2.687093973	-6.145449162	-1.317692637
C	-3.208525419	-5.729474068	1.005638242
C	-3.970545769	-6.649789810	-1.520656109
H	-1.991614699	-6.104777336	-2.152695656
C	-4.499310493	-6.220728874	0.795037329
H	-2.931834459	-5.370175362	1.990427375
C	-4.883120537	-6.684842587	-0.462746233
H	-3.853584528	-2.237447739	1.224888802
C	-0.146508098	-0.208323747	-3.701390743
C	-1.030627728	-1.172664881	-3.194480419
C	-2.072250843	-0.778693259	-2.312918663
C	-2.221919775	0.550050139	-1.893609405
C	-1.329229116	1.483443975	-2.409295321
C	-0.308809400	1.112474680	-3.309000015
C	-1.152215719	-2.606313944	-3.380848408
C	-2.284661531	-2.992270470	-2.656717062
N	-2.834180117	-1.913048625	-2.014901876
H	0.651059449	-0.496566951	-4.380198479
H	-3.023169041	0.845086217	-1.225918531
H	-1.427880883	2.525407791	-2.117685556
H	0.368659347	1.872079730	-3.686836243
H	-0.677158833	-3.196141243	-4.156123638
H	-2.769544601	-3.954881907	-2.599778891
H	4.906715870	1.317952991	-1.822742820
H	3.137288094	2.816459179	-0.927633405
H	0.954539478	1.858738899	-0.203736693
H	0.020958340	-1.684247971	3.811514616
H	-0.000328141	-3.415004730	5.596860886
H	-0.318666399	-5.806743622	4.996953964
H	-5.204781532	-6.240139484	1.620950341
H	-5.887010098	-7.067620277	-0.620851815
H	-4.261126041	-7.007430553	-2.504340649
H	3.373176575	-5.104007721	-5.307774544
H	5.738957882	-5.500545979	-4.660473824
H	6.571400166	-4.718646526	-2.452956676

================================

VI_{SN}

================================

Cu	0.514613450	-3.694612265	-1.204445362
H	-3.468926430	-2.748766899	-2.346891642
C	-3.110935926	-3.770434141	-2.211446762
C	-2.631195307	-4.356493950	-3.543224335
C	-3.672697783	-4.364928246	-4.659927368
C	-5.030729771	-4.135473728	-4.413408756
C	-3.264476061	-4.607232571	-5.979648590
C	-5.956084251	-4.133370876	-5.461108208
C	-4.184276104	-4.604547977	-7.025489807
C	-5.537259102	-4.365693569	-6.770034790
H	-5.375771999	-3.928609133	-3.405994654
H	-2.208793402	-4.760947227	-6.186236382
H	-7.004377842	-3.936214685	-5.250644684
H	-3.843095541	-4.774388790	-8.043507576
H	-6.254590988	-4.348729134	-7.586486816
H	-2.333055735	-5.396001816	-3.361178875
H	-2.278944969	-3.731281281	-1.506418943
P	0.123572357	-5.570338726	0.005012481
C	1.746282339	-6.309712410	0.454502463
C	2.690382957	-5.450645924	1.103989482
C	2.136686087	-7.575755596	0.007185197
C	3.978646040	-5.943446159	1.202782989
C	2.403360844	-4.150219917	1.793307781
C	3.459541321	-8.045776367	0.124174997
H	1.403960824	-8.223125458	-0.460151881
C	4.365604401	-7.190555096	0.711324692
O	5.051221371	-5.331169128	1.798244119
C	2.102918625	-4.180763721	3.141870022
C	2.584743023	-2.851228476	1.220557451
H	3.751554966	-9.027882576	-0.229485825
O	5.695961952	-7.395310402	0.960279822
C	6.182458401	-6.168006897	1.527756929
C	1.997827530	-3.032089472	3.929629803

O	1.899466872	-5.290945053	3.923651218
C	2.518230438	-1.714674950	2.028291941
P	2.604459524	-2.745873213	-0.617219388
H	6.836753845	-5.665799618	0.803328872
H	6.707122803	-6.382774353	2.464508057
C	2.235680103	-1.781499028	3.406233549
O	1.705729723	-3.382237196	5.221843719
C	1.419364929	-4.788402081	5.177845478
H	2.644832134	-0.737164795	1.579177260
H	2.175946712	-0.888514221	4.018009186
H	1.944193959	-5.290634155	5.994825363
H	0.333192587	-4.942656994	5.235569477
C	2.765735626	-0.968096375	-1.044066072
C	3.836446285	-0.144687176	-0.650903285
C	1.739656687	-0.424349338	-1.828027010
C	3.857000351	1.199379921	-1.016493559
H	4.651986599	-0.545017779	-0.057710674
C	1.761352539	0.924474895	-2.189855099
H	0.901692748	-1.031407833	-2.148268223
C	2.816739082	1.738036871	-1.782388926
C	4.236305237	-3.440124512	-1.088390231
C	4.308930874	-4.230022907	-2.244938612
C	5.414469719	-3.145233393	-0.385018528
C	5.542235374	-4.683820248	-2.717113972
H	3.389181614	-4.495714188	-2.762832403
C	6.647723198	-3.587136507	-0.863602519
H	5.362246513	-2.586071253	0.545119524
C	6.714488983	-4.351509571	-2.034025669
C	-0.791342914	-5.319225788	1.566907525
C	-1.424172282	-4.082139492	1.768480182
C	-0.874902666	-6.319260597	2.547311306
C	-2.138488531	-3.854518890	2.946543694
H	-1.343998790	-3.298379183	1.014627099
C	-1.603459835	-6.088441849	3.713676453
H	-0.367031634	-7.268721104	2.399851084
C	-2.234188080	-4.854944706	3.915187836
C	-0.848820746	-6.801128864	-0.947764218
C	-0.331599951	-7.316051960	-2.152581930
C	-2.202204466	-7.024525642	-0.652590156
C	-1.144774437	-8.026926994	-3.034381151
H	0.709772229	-7.142694473	-2.411810637
C	-3.017371178	-7.724408627	-1.545428395
H	-2.628345490	-6.626877785	0.263172895
C	-2.498162031	-8.221662521	-2.742119789
H	-3.911119699	-4.380266190	-1.781017780
C	0.502990127	-0.838571727	-5.087854385
C	0.096311331	-2.082742453	-4.577650070
C	-1.286769271	-2.410666466	-4.537327290
C	-2.263186455	-1.520439506	-5.005099297
C	-1.831407905	-0.301650137	-5.507714272
C	-0.463190079	0.041697562	-5.548930645
C	0.808510482	-3.189991951	-4.013472080
C	-0.134730026	-4.135626793	-3.658902884
N	-1.403087139	-3.679980993	-3.987834215
H	1.556172490	-0.570479035	-5.101967335
H	-3.317386866	-1.765491843	-4.966824532
H	-2.567842007	0.410287619	-5.871481419
H	-0.168362290	1.010430694	-5.944407940
H	1.880405545	-3.280181646	-3.916835070
H	-0.010690260	-5.161050320	-3.340519190
H	4.684622288	1.830236793	-0.701790273
H	2.836131334	2.789846659	-2.057102203
H	0.939372599	1.314852715	-2.782064199
H	-2.615286827	-2.889701843	3.099340200
H	-2.797214270	-4.677214146	4.828200817
H	-1.677428603	-6.867672443	4.468081951
H	-4.067879200	-7.868132114	-1.307357311
H	-3.139568090	-8.748963356	-3.441958666
H	-0.725798249	-8.406262398	-3.962567329
H	5.588205338	-5.292819977	-3.616894722
H	7.677234173	-4.692078590	-2.407092571
H	7.558144093	-3.334137201	-0.324198216
C	-3.519299746	1.707165599	1.535956264
C	-2.294865608	1.166016459	1.930392742
C	-4.047222137	1.282021761	0.314728260
H	-1.842601418	1.500662208	2.863147020
H	-4.991219997	1.704340696	-0.026657762
C	-1.611200452	0.226908803	1.148696899
C	-3.390445948	0.357775718	-0.507307351
C	-2.159780264	-0.198399842	-0.081332192
C	-1.351632476	-1.108778477	-1.009191036
O	-1.234295368	-0.757492721	-2.192317009
O	-0.815437198	-2.165899038	-0.489177406
C	-4.027158737	0.007221133	-1.835516453
H	-4.381435871	-1.030492544	-1.844558239
H	-4.893355846	0.648365974	-2.029376507
H	-3.307179451	0.106344774	-2.649550915
C	-0.257019311	-0.249644548	1.611553431
H	0.503807247	-0.054150712	0.849163592
H	0.044548661	0.261074424	2.531944036
H	-0.239989907	-1.325301170	1.788004041
C	-4.243972301	2.715313911	2.398243427
H	-4.888620377	2.221435308	3.137119293
H	-3.540928602	3.345530272	2.954180717
H	-4.882447243	3.372196198	1.797875285

==============================

II_S-TS’

==============================

Cu	-2.243358135	0.947758377	-4.128157616
H	-5.454327583	0.836856008	-4.336148739
C	-5.045289993	1.490248680	-5.111362934
C	-3.784198284	2.209934950	-4.666051865
C	-3.859062433	3.000041962	-3.427607059
C	-2.977535725	4.099092007	-3.235530615
C	-4.794065475	2.746393681	-2.392783880
C	-3.016028166	4.877756119	-2.084095001
C	-4.840610504	3.541522264	-1.248423696
C	-3.951872110	4.607666016	-1.076124787
H	-2.300059319	4.356111526	-4.043592930
H	-5.487143517	1.914962530	-2.487394571
H	-2.343202829	5.728693485	-1.994670630
H	-5.573534966	3.319497585	-0.475164562
H	-3.998761892	5.227835178	-0.184075251
H	-3.336556196	2.792867184	-5.469541073
H	-4.851037979	0.875150383	-5.992285728
P	-2.782873154	-0.570287228	-2.227044106
C	-1.654040694	-2.031051159	-2.148486614
C	-0.318026364	-1.859830737	-1.667411447
C	-2.051546097	-3.265728235	-2.677314281
C	0.502237380	-2.971558809	-1.751019120
C	0.252250046	-0.635700226	-1.029461980
C	-1.185464621	-4.370670795	-2.760110855
H	-3.069360018	-3.388992786	-3.029481173
C	0.097130552	-4.187343597	-2.292132854
O	1.812674761	-3.058447361	-1.351022720
C	0.552049637	-0.690110624	0.319696695
C	0.603762388	0.576713920	-1.696685076
H	-1.510082960	-5.320704937	-3.169774771
O	1.135089040	-5.082629204	-2.258366346
C	2.268985748	-4.349366665	-1.770588279
C	1.127203584	0.364861220	1.021330953
O	0.327263147	-1.742487907	1.171103001
C	1.194663167	1.625169158	-0.981516540
P	0.190870956	0.760078013	-3.486068249
H	2.999655962	-4.228572369	-2.581605673
H	2.705003262	-4.878037930	-0.915750206
C	1.469063044	1.542191505	0.394462973
O	1.283226609	0.019846981	2.337973595
C	0.704004526	-1.286120415	2.475387573
H	1.462130427	2.538751125	-1.497899294
H	1.926723599	2.362432718	0.935936034
H	1.445773363	-1.971517682	2.901853323
H	-0.189147562	-1.221427321	3.110421658
C	1.106587648	2.270674467	-3.977610111
C	2.310628653	2.298912525	-4.694329262
C	0.470832020	3.483188868	-3.656116486
C	2.873863935	3.522890806	-5.065998077
H	2.801388264	1.375570536	-4.984907627
C	1.036899805	4.702370644	-4.020861149

H -0.482767165 3.469367504 -3.135311127
C 2.243356466 4.722556591 -4.728609085
C 1.078019381 -0.677102864 -4.214342594
C 0.343868971 -1.580483794 -4.996605873
C 2.424783468 -0.954936743 -3.935705185
C 0.947505951 -2.725151062 -5.515532017
H -0.718988955 -1.413850784 -5.147446632
C 3.033581495 -2.090976000 -4.469074249
H 2.985631704 -0.298453659 -3.276361227
C 2.297602654 -2.975224257 -5.262917519
C -2.680911779 0.095495664 -0.522487581
C -2.450248003 1.466993213 -0.357248843
C -2.752274990 -0.733175695 0.610301495
C -2.307203054 2.006384373 0.921858072
H -2.377654791 2.111729145 -1.226287484
C -2.625942945 -0.188346997 1.887146831
H -2.879586458 -1.805582762 0.490736097
C -2.399159908 1.182839036 2.044569731
C -4.454613686 -1.304661274 -2.391539097
C -4.858294487 -1.634589076 -3.697752953
C -5.348620892 -1.514126182 -1.330871701
C -6.111127853 -2.199553490 -3.933740139
H -4.193823814 -1.417939782 -4.532884598
C -6.609202385 -2.064150333 -1.571462512
H -5.071114063 -1.236624241 -0.318920225
C -6.989025116 -2.417244673 -2.868315935
H -5.839618206 2.206186533 -5.383438587
C -2.217523336 8.621003151 -3.697443724
C -1.126302242 8.314389229 -4.526375771
C -3.436906338 7.976104736 -3.934424639
H -0.177193716 8.829212189 -4.371520519
H -4.295362473 8.209068298 -3.304334641
C -1.226342559 7.366901398 -5.549651623
C -3.583261013 7.024502754 -4.953903675
C -2.464925051 6.722043991 -5.751651764
C -2.565639019 5.646946907 -6.821142197
O -3.133205891 5.792104244 -7.893986225
O -1.948027968 4.583721638 -6.355744362
C -3.155797720 0.111675754 -7.833762169
C -2.294358969 1.150107741 -7.496131420
C -2.550225973 2.465711594 -7.954411983
C -3.696002722 2.785571098 -8.669532776
C -4.577460289 1.736664176 -8.975018501
C -4.302162170 0.420083970 -8.583624840
C -1.047228336 1.236366391 -6.738349438
C -0.592783630 2.530791044 -6.880033493
N -1.445275307 3.296747446 -7.642566681
H -2.944446564 -0.913148701 -7.533792019
H -3.885377407 3.818273544 -8.944736481
H -5.485466003 1.949829340 -9.533448219
H -4.994555950 -0.374232322 -8.854042053
H -0.467120409 0.390915543 -6.400495529
H 0.316787124 2.969095230 -6.498388767
H -6.409533024 -2.447680473 -4.949334621
H -7.971660614 -2.845297813 -3.050464869
H -7.295876980 -2.215430260 -0.741546154
H -2.696537971 -0.834286273 2.759374857
H -2.286353588 1.604002714 3.040416002
H -2.128936052 3.072028160 1.030732870
H 0.517313361 5.628833294 -3.789197445
H 2.678361893 5.670346260 -5.034311771
H 3.804248571 3.535905600 -5.629527569
H 4.080362797 -2.292109966 -4.256031036
H 2.770999193 -3.864790916 -5.669872761
H 0.361432582 -3.424837112 -6.104445457
C -2.062387466 9.602464676 -2.555048704
H -1.605086684 9.122124672 -1.678984404
H -1.415305495 10.443428040 -2.832482100
H -3.029469967 10.007470131 -2.236737251
C -0.045673881 7.053543091 -6.442589760
H 0.833448231 7.647607803 -6.164748192
H 0.211166039 5.991415501 -6.387116909
H -0.283987403 7.267558575 -7.492959023
C -4.902655125 6.325357914 -5.194417000
H -4.793979645 5.240412235 -5.076537132
H -5.668220997 6.667191029 -4.490073681
H -5.253054619 6.504903316 -6.216828823

==============================

III$_{SC}$

==============================

Cu -1.274702072 1.303786039 -3.165694475
H -4.717835426 1.962405920 -2.943298101
C -4.110347271 2.541728020 -3.635876656
C -2.761164665 2.908166885 -3.108015537
C -2.536068439 3.245383501 -1.712148309
C -1.337360859 3.922984600 -1.367830753
C -3.471281290 2.982682705 -0.683302224
C -1.083953738 4.310992718 -0.057230014
C -3.221122265 3.393517971 0.620065629
C -2.026638985 4.049067497 0.944411516
H -0.626187623 4.148631573 -2.157160044
H -4.394977093 2.463634491 -0.914791763
H -0.163863599 4.836311817 0.183370635
H -3.954162598 3.194217682 1.395828724
H -1.838460445 4.363402367 1.966652036
H -2.193191051 3.534777164 -3.786427498
H -4.026097298 1.996239066 -4.577320576
P -2.368277550 -0.475143075 -1.952397108
C -1.623944879 -2.093449831 -2.432034969
C -0.318760991 -2.432021379 -1.952099562
C -2.266954184 -2.933199406 -3.350732803
C 0.236584440 -3.587653875 -2.472049236
C 0.477515042 -1.691891074 -0.926805198
C -1.670532465 -4.099504948 -3.861841440
H -3.269062281 -2.696257353 -3.684209824
C -0.398329169 -4.391520977 -3.419188738
O 1.473510385 -4.097086906 -2.191869736
C 0.609211028 -2.232690334 0.337930799
C 1.207941175 -0.489998341 -1.169811010
H -2.184336901 -4.734197140 -4.574569225
O 0.413708180 -5.425265789 -3.772952795
C 1.630149364 -5.257544994 -3.023804903
C 1.377404451 -1.644652247 1.345790029
O 0.025798295 -3.374852419 0.809566915
C 1.999250531 0.076536663 -0.163704172
P 0.924089253 0.332096308 -2.776839256
H 2.461674690 -5.092942715 -3.718266964
H 1.796470761 -6.139411449 -2.395899534
C 2.100852489 -0.491976708 1.119921207
O 1.291486144 -2.386549234 2.485433817
C 0.399406523 -3.475920200 2.192594528
H 2.564600229 0.977449059 -0.369590342
H 2.718073130 -0.048875209 1.892697334
H 0.915185273 -4.426632881 2.363501310
H -0.497117758 -3.385707617 2.816802740
C 2.110381842 1.712580323 -2.910117865
C 3.074666262 1.792942762 -3.923408270
C 1.945977569 2.800550699 -2.033264399
C 3.864300728 2.938489437 -4.050526619
H 3.203084469 0.975862443 -4.625106335
C 2.747164249 3.933202982 -2.153369665
H 1.181112528 2.763977528 -1.262705564
C 3.706465006 4.006566525 -3.168035507
C 1.386465669 -0.905399442 -4.043811798
C 0.453403831 -1.266735554 -5.027285099
C 2.632194042 -1.550254941 -4.011215687
C 0.763789713 -2.240180254 -5.974787235
H -0.532360673 -0.813597500 -5.024097919
C 2.943708658 -2.519623518 -4.965782642
H 3.351531267 -1.302432179 -3.235963821
C 2.011872530 -2.866973400 -5.948879242
C -2.222966671 -0.445788115 -0.132292166
C -1.538802266 0.607185423 0.486115456
C -2.707811117 -1.507592201 0.649058998
C -1.345451117 0.606505752 1.866918802
H -1.141439557 1.417305708 -0.114085920
C -2.529265642 -1.495324373 2.032063246
H -3.209625483 -2.346395969 0.175397873
C -1.841754794 -0.441715509 2.643974781

C	-4.143495083	-0.594615161	-2.361052513
C	-4.496603012	-0.604592860	-3.722569942
C	-5.158011436	-0.567223310	-1.393772125
C	-5.834013939	-0.630841136	-4.107617855
H	-3.724613428	-0.547985911	-4.485325813
C	-6.498738289	-0.572041571	-1.785225749
H	-4.909750938	-0.535810411	-0.338433087
C	-6.839644909	-0.613469720	-3.137676239
H	-4.646324635	3.474388838	-3.870486259
C	-2.524482250	1.093943357	-6.567823410
C	-1.708738804	2.058247805	-5.969294071
C	-1.974293590	3.440023184	-6.160249233
C	-3.062950373	3.866786242	-6.916890144
C	-3.880893469	2.893083811	-7.500349522
C	-3.611963034	1.525221229	-7.335918903
C	-0.547813416	2.007033825	-5.085061550
C	-0.174085572	3.414242029	-4.940608978
N	-1.013317347	4.244711399	-5.511558533
H	-2.320076942	0.031908695	-6.449400425
H	-3.253031015	4.926546574	-7.056062698
H	-4.732511520	3.199640989	-8.100795746
H	-4.254608631	0.793439925	-7.817474842
H	0.226869822	1.262291193	-5.222444057
H	0.690900683	3.772232056	-4.391574860
H	-6.090692520	-0.635913908	-5.162880898
H	-7.884006977	-0.618866622	-3.435529947
H	-7.277397633	-0.545563459	-1.028338313
H	-2.919697046	-2.313324213	2.631178379
H	-1.691380382	-0.441115707	3.719638824
H	-0.804532588	1.425171852	2.331353903
H	2.614438295	4.765086174	-1.467284083
H	4.320896626	4.895729542	-3.273343563
H	4.601381779	2.994184494	-4.846199036
H	3.914930820	-3.005874395	-4.940640926
H	2.254964113	-3.625267506	-6.687223434
H	0.027554164	-2.517877579	-6.723091602

===============================

III$_{SC}$-TS

===============================

Cu	-1.353717804	1.168999672	-3.019933462
H	-4.426602840	1.715111136	-3.255159378
C	-4.040067673	2.531322002	-3.860211372
C	-2.680062771	3.004946947	-3.436697483
C	-2.443067312	3.305996180	-2.009422779
C	-1.342450023	4.117346287	-1.645765901
C	-3.356004477	2.924369812	-0.996609747
C	-1.164832592	4.534142017	-0.329690605
C	-3.187173843	3.367197752	0.311655849
C	-2.091708422	4.168612480	0.653120577
H	-0.639125943	4.427056313	-2.413259029
H	-4.210509300	2.300318241	-1.238213539
H	-0.316606194	5.164722443	-0.074448220
H	-3.907154083	3.077370644	1.072560430
H	-1.963766217	4.508024693	1.677685261
H	-2.291263342	3.784674644	-4.078156471
H	-4.050849438	2.230613947	-4.909228802
P	-2.492333651	-0.512660623	-1.772308111
C	-1.766078472	-2.124092579	-2.305805683
C	-0.426490873	-2.451987267	-1.916502237
C	-2.448494196	-2.936911345	-3.219722986
C	0.109720401	-3.581054211	-2.512143850
C	0.432377577	-1.764528632	-0.897891402
C	-1.869603753	-4.075720310	-3.808181524
H	-3.471786022	-2.701878786	-3.484398365
C	-0.572241724	-4.363182068	-3.444198847
O	1.362671256	-4.092762470	-2.312935352
C	0.604989886	-2.365598202	0.334736854
C	1.207970023	-0.586661577	-1.120965958
H	-2.415158749	-4.694906712	-4.510794640
O	0.227431849	-5.383826733	-3.867305994
C	1.516853452	-5.147218704	-3.275755882
C	1.453902721	-1.860153794	1.321237445
O	-0.020842489	-3.490471601	0.796121240
C	2.081502914	-0.106112495	-0.140143752
P	0.892005503	0.324905634	-2.669502735
H	2.220114946	-4.824383259	-4.054346085
H	1.858291864	-6.055529594	-2.771540642
C	2.223567486	-0.736542106	1.109342456
O	1.379893422	-2.639752865	2.438764095
C	0.496984482	-3.726429939	2.115141153
H	2.675279856	0.778349042	-0.339366972
H	2.900187254	-0.360308021	1.867605090
H	1.056538820	-4.669810772	2.125866175
H	-0.331285238	-3.745036364	2.831108570
C	2.033252001	1.749770641	-2.724343777
C	2.960350513	1.957151771	-3.754826546
C	1.833440900	2.765558720	-1.770232081
C	3.685011864	3.150265217	-3.817896128
H	3.111602306	1.201404929	-4.518027306
C	2.567739248	3.946706295	-1.830142379
H	1.090626836	2.636575699	-0.987893820
C	3.494505644	4.143958569	-2.858727694
C	1.387558699	-0.817813396	-4.012141228
C	0.429996669	-1.230641246	-4.952263355
C	2.688759327	-1.339117765	-4.085720539
C	0.773788214	-2.118612289	-5.970145226
H	-0.598560333	-0.891925216	-4.864502430
C	3.033128738	-2.224465847	-5.107174873
H	3.428876162	-1.053600192	-3.343142986
C	2.078801632	-2.608071566	-6.054417610
C	-2.196331978	-0.463543147	0.029485106
C	-1.506915927	0.623761356	0.581234157
C	-2.579554319	-1.530482888	0.859115362
C	-1.211276174	0.652381837	1.943430543
H	-1.187101364	1.436711073	-0.061573692
C	-2.296213865	-1.492070436	2.223012686
H	-3.075519562	-2.397747993	0.432767302
C	-1.609038115	-0.403005004	2.767035007
C	-4.304669857	-0.665592790	-1.997935057
C	-4.800653458	-0.647446632	-3.315468073
C	-5.217230320	-0.706514299	-0.932588458
C	-6.170532703	-0.709417462	-3.562201738
H	-4.109858036	-0.562712789	-4.152013302
C	-6.590415955	-0.751650572	-1.183170080
H	-4.864553928	-0.695947051	0.092935823
C	-7.069329739	-0.760559380	-2.493542433
H	-4.728689194	3.384251356	-3.763282061
C	-2.702512503	1.283363938	-6.707688332
C	-1.792854905	2.156584501	-6.116035461
C	-1.547713518	3.433011055	-6.672794819
C	-2.229423046	3.867145061	-7.803911209
C	-3.160140753	2.992999077	-8.382074356
C	-3.385399103	1.715448260	-7.852317333
C	-0.948240638	2.078207254	-4.918974876
C	-0.172343016	3.346059084	-4.987074375
N	-0.544066131	4.132616520	-5.951731682
H	-2.882834435	0.293686420	-6.292083740
H	-2.031670570	4.848092079	-8.224044800
H	-3.709851980	3.306800842	-9.264913559
H	-4.104013920	1.056448460	-8.332082748
H	-0.328866571	1.177700758	-4.893414497
H	0.591751873	3.637718916	-4.272226334
H	-6.536298752	-0.701012909	-4.585197449
H	-8.138195038	-0.797568381	-2.682911873
H	-7.285645485	-0.780936778	-0.348794341
H	-2.602968693	-2.316903114	2.860301256
H	-1.376908302	-0.381827474	3.827983856
H	-0.666151285	1.495066285	2.358400822
H	2.410558701	4.718760967	-1.082113504
H	4.058350563	5.070201397	-2.914119244
H	4.395361900	3.302119970	-4.625160694
H	4.045579910	-2.614044189	-5.165100098
H	2.349742651	-3.295586586	-6.850570202
H	0.022028506	-2.435021639	-6.686970711

===============================

V$_{SC}$

===============================

Cu	-1.352560997	1.080864549	-2.843912125

H -2.438981771 5.987091541 -7.580699444
C -2.971875429 5.030909061 -7.607537270
C -2.309637070 3.991930246 -6.694238186
C -0.897910237 3.611794233 -7.121682644
C -0.557686687 2.262228489 -7.289445877
C 0.116308041 4.573162556 -7.235452652
C 0.759099662 1.877317190 -7.550236702
C 1.434246182 4.192661762 -7.494608402
C 1.762287378 2.843371630 -7.646686077
H -1.332021713 1.502511382 -7.200105667
H -0.118500195 5.626601219 -7.104682446
H 0.999709785 0.823901296 -7.660997391
H 2.207809925 4.951883316 -7.569866180
H 2.789368153 2.549243689 -7.840569496
H -2.919165373 3.079883575 -6.712249756
H -4.009208679 5.210566521 -7.310920715
P -2.390276670 -0.693137109 -1.782233357
C -1.528805256 -2.211515427 -2.350175381
C -0.141301483 -2.360942125 -2.037723303
C -2.175380468 -3.130513668 -3.183692455
C 0.478896260 -3.466121674 -2.590386152
C 0.654544413 -1.478750229 -1.125011563
C -1.506103992 -4.232647419 -3.748672485
H -3.228158712 -2.996556759 -3.406833887
C -0.171392888 -4.368803501 -3.433641911
O 1.786348820 -3.839122057 -2.435372353
C 0.883140683 -1.901988745 0.171689332
C 1.299976826 -0.256582320 -1.499832153
H -2.012661219 -4.941754818 -4.392999172
O 0.702653706 -5.335796356 -3.839539051
C 1.965165257 -5.022463799 -3.230024576
C 1.654207110 -1.184412122 1.088643909
O 0.411191821 -3.043309927 0.760637045
C 2.086288691 0.443635166 -0.578852057
P 0.859972060 0.489615321 -3.120827436
H 2.705157757 -4.822768688 -4.013408184
H 2.277181864 -5.852086067 -2.585096598
C 2.280021667 -0.006763267 0.741249084
O 1.682645679 -1.841344714 2.285173178
C 0.849639893 -3.001353025 2.128804684
H 2.565448284 1.368044853 -0.881542623
H 2.893410683 0.539643943 1.448218465
H 1.431033134 -3.902697563 2.352639675
H -0.024851806 -2.911181688 2.784749031
C 1.966755867 1.923480988 -3.366281271
C 3.071475744 1.929607153 -4.228446007
C 1.612407804 3.109451294 -2.696074486
C 3.813322544 3.099335194 -4.406438351
H 3.345892906 1.031631827 -4.773056507
C 2.365343332 4.270195007 -2.862968206
H 0.736696422 3.118113995 -2.048697233
C 3.467354298 4.266568184 -3.723504066
C 1.276795864 -0.741075814 -4.398634911
C 0.323207498 -1.002475142 -5.392598152
C 2.491647720 -1.443404913 -4.405568123
C 0.578832984 -1.949235439 -6.384652138
H -0.625888586 -0.471895635 -5.372347832
C 2.753375292 -2.374247313 -5.411867142
H 3.220280647 -1.274222732 -3.617906809
C 1.797642231 -2.632677078 -6.399114609
C -2.366733789 -0.769229770 0.042249877
C -2.182530880 0.420710474 0.761035740
C -2.532155752 -1.977058768 0.738150418
C -2.173793077 0.406744093 2.156909943
H -2.036019802 1.354342341 0.221616939
C -2.538913250 -1.984809995 2.133660078
H -2.638327360 -2.908482790 0.189709470
C -2.356306076 -0.795583963 2.845599174
C -4.136545658 -0.898819268 -2.290196180
C -4.478334904 -0.433682173 -3.572249174
C -5.134020805 -1.453126073 -1.473886609
C -5.787090302 -0.537804425 -4.039432526
H -3.714094162 0.029413568 -4.195307255
C -6.447587013 -1.545219183 -1.939645290
H -4.892802238 -1.801503778 -0.474059522
C -6.774819374 -1.093022108 -3.220445156
H -2.973109961 4.676265717 -8.642770767
C -4.873236179 4.899250984 -4.605994225
C -3.625472784 4.300242424 -4.474092960
C -3.447567701 3.281056404 -3.521055222
C -4.472338200 2.822428703 -2.704500675
C -5.726664543 3.424670696 -2.853812695
C -5.921268940 4.450102329 -3.786928415
C -2.301229715 4.474202633 -5.188455105
C -1.437430382 3.531479597 -4.389202118
N -2.094008207 2.829020500 -3.520584345
H -5.041855335 5.705968857 -5.313407421
H -4.297074318 2.024416685 -1.989911675
H -6.556689739 3.094897985 -2.235088825
H -6.901491642 4.910801888 -3.876574516
H -1.910658598 5.499782562 -5.157636642
H -0.378242910 3.369293928 -4.551500797
H -6.040420532 -0.170667857 -5.030603409
H -7.799169540 -1.165411115 -3.576340675
H -7.216198921 -1.970586419 -1.299121737
H -2.682096243 -2.921636343 2.665686131
H -2.354569912 -0.806023896 3.932003021
H -2.022644758 1.331236839 2.706376553
H 2.087135077 5.176998615 -2.332116604
H 4.049525738 5.172896862 -3.864773273
H 4.664285183 3.096931458 -5.082635880
H 3.703282595 -2.902166605 -5.423026085
H 1.999907494 -3.367929697 -7.172377110
H -0.172222644 -2.157326937 -7.141160965

================================

VI_{SC}

================================

Cu -1.225280046 0.909941137 -3.188374996
H -1.382622004 4.692094803 -9.075039864
C -2.028090954 3.814960003 -9.194811821
C -1.709871054 2.739605665 -8.147155762
C -0.298772424 2.178671122 -8.258227348
C -0.101237170 0.791609108 -8.293207169
C 0.826136172 3.008967638 -8.160720825
C 1.180186510 0.243947700 -8.205489159
C 2.107939482 2.467108965 -8.066496849
C 2.289008856 1.082366943 -8.080473900
H -0.965322375 0.132675156 -8.356287956
H 0.699435234 4.087377071 -8.111547470
H 1.308288813 -0.835393310 -8.202478409
H 2.964479208 3.124661922 -7.949531555
H 3.284866571 0.661467493 -7.977591515
H -2.406692743 1.904851079 -8.288467407
H -3.066649675 4.148796558 -9.110011101
P -2.229854822 -0.861506522 -2.039065123
C -1.264738202 -2.435802698 -2.046604156
C 0.070134453 -2.384844303 -1.543687701
C -1.773543239 -3.627659559 -2.576680422
C 0.780526519 -3.571043015 -1.594977736
C 0.702317655 -1.184432864 -0.908508301
C -1.012130141 -4.809967041 -2.643254280
H -2.789072752 -3.650535822 -2.954743624
C 0.270422906 -4.746335983 -2.142292023
O 2.073583603 -3.779283762 -1.179480433
C 0.737145066 -1.131363869 0.473289818
C 1.324928045 -0.089154020 -1.589245081
H -1.412437201 -5.725269318 -3.064613819
O 1.219682097 -5.734157085 -2.095083237
C 2.355846643 -5.159866333 -1.433117270
C 1.313833714 -0.083407134 1.188746929
O 0.235309005 -2.064399958 1.348042727
C 1.916750073 0.946836352 -0.857402742
P 0.989104509 0.179678306 -3.380527020
H 3.233034134 -5.238843441 -2.086030722
H 2.526547194 -5.680634975 -0.480815202
C 1.930090189 0.970425129 0.549498260
O 1.184594393 -0.317355484 2.535269022
C 0.307416141 -1.448893905 2.640892029
H 2.355559349 1.783826709 -1.389882326

H	2.384319782	1.784508109	1.102718949
H	0.721340835	-2.163038254	3.359388590
H	-0.695714295	-1.111478567	2.935849428
C	2.261328220	1.369888425	-3.975021124
C	3.516879082	1.002226472	-4.484938622
C	1.903822660	2.728617668	-3.954537153
C	4.398488522	1.974983335	-4.957071304
H	3.805373430	-0.042266525	-4.532272339
C	2.794962406	3.697374582	-4.421461105
H	0.925626218	3.042024612	-3.592980385
C	4.042527199	3.326482058	-4.925551414
C	1.392896891	-1.398525238	-4.219532490
C	0.518523157	-1.815788388	-5.232957363
C	2.498387098	-2.201560259	-3.897576809
C	0.744424045	-3.011056900	-5.917911530
H	-0.346634209	-1.199727416	-5.468507290
C	2.727805614	-3.391851187	-4.588203907
H	3.152014494	-1.916751146	-3.077697992
C	1.851034641	-3.799685001	-5.597342491
C	-2.616189241	-0.600974619	-0.264763951
C	-2.490188837	0.700673938	0.245765030
C	-3.012765646	-1.645646453	0.586441517
C	-2.791067839	0.956914485	1.586209297
H	-2.117016792	1.496861219	-0.396085173
C	-3.314626455	-1.382610559	1.923195124
H	-3.078362942	-2.661185503	0.203634933
C	-3.209313869	-0.078865796	2.425199986
C	-3.823655128	-1.305430412	-2.839433432
C	-3.803506374	-1.459631205	-4.238956928
C	-5.053186893	-1.378303885	-2.169232368
C	-4.978353500	-1.705290198	-4.945002556
H	-2.858704567	-1.364729047	-4.771349430
C	-6.234209061	-1.605568171	-2.883431673
H	-5.092614651	-1.250988960	-1.091118336
C	-6.202551842	-1.774087310	-4.268756866
H	-1.878301144	3.423138380	-10.205945969
C	-4.568438053	3.784231901	-6.587111950
C	-3.382563829	3.178367138	-6.193309307
C	-3.391060591	2.268116951	-5.120627403
C	-4.546674728	1.937911868	-4.427141666
C	-5.737547398	2.548586369	-4.836662769
C	-5.748802185	3.458746672	-5.898988724
C	-1.951451063	3.265325546	-6.683623791
C	-1.275771260	2.367087841	-5.676513672
N	-2.080266476	1.788712978	-4.852537632
H	-4.590448380	4.508663654	-7.396461964
H	-4.511596203	1.238738179	-3.598446608
H	-6.662692547	2.317963362	-4.314938068
H	-6.684083462	3.929236174	-6.191443443
H	-1.536645532	4.279073715	-6.593161583
H	-0.209113389	2.190800190	-5.633701801
H	-4.943933010	-1.820539713	-6.025761127
H	-7.122760296	-1.947724104	-4.819725037
H	-7.181471825	-1.651523471	-2.350170135
H	-3.628815413	-2.194518805	2.575159550
H	-3.449021339	0.122466177	3.466513634
H	-2.692001104	1.970976353	1.965100765
H	2.497101545	4.742229939	-4.395497799
H	4.733402252	4.080493927	-5.293968201
H	5.366090775	1.675269246	-5.352540970
H	3.586668968	-4.008517742	-4.333570480
H	2.024230242	-4.735166073	-6.123257637
H	0.051234957	-3.331325531	-6.692051888
C	-0.925609648	5.972761154	0.933617115
C	-2.265986204	6.055634975	1.328152776
C	-3.222121954	5.377796650	0.562330365
C	-2.661013842	6.830101967	2.565645695
H	-0.166579545	6.497187138	1.513693810
C	-0.533189416	5.230731010	-0.184852064
H	-4.272182941	5.440545082	0.846108794
C	-2.866476774	4.619803905	-0.560068607
C	-1.511445761	4.549206734	-0.928675592
C	0.920212328	5.133606434	-0.591593027
C	-3.918183565	3.891966820	-1.371192455
C	-1.086372256	3.691000223	-2.104377747
O	-0.725837886	4.223445415	-3.171600103
O	-1.113611221	2.432755232	-1.843387365
H	-3.773012877	2.806645632	-1.323811769
H	-4.927529335	4.120268345	-1.013001323
H	-3.861093044	4.164917469	-2.432579041
H	1.050608277	5.448937893	-1.631871700
H	1.561064005	5.746113300	0.049969465
H	1.269066572	4.094367981	-0.532187402
H	-2.578261852	6.209873199	3.468557119
H	-2.016173840	7.703336239	2.715372086
H	-3.696728468	7.181435108	2.507549524

==============================

VI$_{SC}$-TS

==============================

Cu	-1.334688425	0.411165118	-3.616971970
H	-0.620450556	5.615609646	-6.174464226
C	-1.316222310	5.476768017	-7.005830288
C	-1.404090524	3.993868828	-7.417032719
C	-0.097928092	3.490478039	-8.009995461
C	-0.079144768	2.842061758	-9.250885963
C	1.104341269	3.589485884	-7.297274590
C	1.101316333	2.299559355	-9.762077332
C	2.285732508	3.042695999	-7.798959732
C	2.289261103	2.392677307	-9.035105705
H	-1.004335284	2.751058578	-9.816151619
H	1.106315136	4.076463223	-6.327677250
H	1.088659763	1.795870304	-10.725389481
H	3.196590185	3.108561993	-7.211246967
H	3.206579208	1.960729122	-9.425515175
H	-2.169532537	3.910052299	-8.200412750
H	-2.288069963	5.848374844	-6.668920517
P	-2.360745668	-1.075970292	-2.110917807
C	-1.358732939	-2.603391886	-1.857976794
C	-0.052615575	-2.470518351	-1.301162958
C	-1.824357510	-3.857960224	-2.267894268
C	0.672175109	-3.641359806	-1.178879023
C	0.552169621	-1.209109664	-0.773212492
C	-1.046626091	-5.024058342	-2.161063671
H	-2.819956064	-3.946060658	-2.685026884
C	0.208090052	-4.879212379	-1.612700582
O	1.953470111	-3.772715330	-0.697956204
C	0.625708580	-1.063898683	0.600975096
C	1.145525455	-0.160931274	-1.543196321
H	-1.413886070	-5.988540173	-2.493358612
O	1.175999403	-5.832621098	-1.423371792
C	2.234618187	-5.176622868	-0.714039624
C	1.191931486	0.042243943	1.228432775
O	0.170902729	-1.947464347	1.548249602
C	1.724483609	0.938699663	-0.897680879
P	0.908041298	-0.101044007	-3.373294353
H	3.182304382	-5.351592064	-1.234188199
H	2.275436401	-5.554828644	0.317988157
C	1.758158326	1.066192746	0.501698375
O	1.108184695	-0.099999450	2.589572668
C	0.322805494	-1.281508565	2.807935953
H	2.166024208	1.730456471	-1.491531253
H	2.205255508	1.927424073	0.985256553
H	0.846655667	-1.942338705	3.506748438
H	-0.667745531	-0.995894790	3.186382055
C	2.219699621	1.056844711	-3.931972504
C	3.552487850	0.683995724	-4.161126137
C	1.854618192	2.405741692	-4.045781136
C	4.507395267	1.650609016	-4.470906258
H	3.846854448	-0.358420938	-4.102574825
C	2.820935249	3.374795437	-4.320898056
H	0.819985986	2.702321768	-3.912633181
C	4.147691250	2.999870777	-4.533802509
C	1.399034858	-1.745482326	-4.002068520
C	0.609689653	-2.285395622	-5.027171612
C	2.486931086	-2.482409000	-3.510560274
C	0.908104956	-3.538990021	-5.561481476
H	-0.250118941	-1.722608566	-5.384690762
C	2.784307241	-3.733922958	-4.048330784
H	3.066056967	-2.102193356	-2.674320936

C	1.996925235	-4.263262272	-5.074228287
C	-2.629215479	-0.457588047	-0.408588558
C	-2.492910862	0.921027303	-0.187211767
C	-2.913615704	-1.310413361	0.669361949
C	-2.662258625	1.443988919	1.096523762
H	-2.235836506	1.576274037	-1.015306473
C	-3.092154980	-0.782235742	1.947824001
H	-2.979836702	-2.383187294	0.510112882
C	-2.967488527	0.595124781	2.162286282
C	-3.976688623	-1.729905963	-2.682865858
C	-4.070587635	-2.060388803	-4.046248913
C	-5.104824543	-1.886460423	-1.867298365
C	-5.258408070	-2.564553261	-4.573481560
H	-3.217779636	-1.882934570	-4.696821213
C	-6.299574375	-2.373740911	-2.403224468
H	-5.059174538	-1.618889451	-0.816573560
C	-6.379488945	-2.720511198	-3.753043890
H	-0.986577034	6.092670441	-7.848874569
C	-4.316128731	3.938710928	-5.762754440
C	-3.261204958	3.022463799	-5.799892426
C	-3.431679726	1.729396105	-5.251455307
C	-4.632793427	1.346302867	-4.652667522
C	-5.680926323	2.263747692	-4.637351513
C	-5.526967049	3.545506239	-5.190685749
C	-1.854710698	3.097471952	-6.249733925
C	-1.396767378	1.737485170	-6.053894997
N	-2.255825520	0.965100586	-5.399801731
H	-4.204105854	4.938675880	-6.171068192
H	-4.743226528	0.361752242	-4.217489243
H	-6.628149986	1.985898614	-4.182607767
H	-6.358976841	4.244557858	-5.163588524
H	-1.302264690	3.566768646	-5.123258114
H	-0.398704201	1.379305363	-6.277918339
H	-5.316835403	-2.810317039	-5.630118370
H	-7.311217308	-3.097356796	-4.165754318
H	-7.170292377	-2.480376720	-1.761241198
H	-3.322151899	-1.444918156	2.778838634
H	-3.101518631	1.001353741	3.162036419
H	-2.552326918	2.514335632	1.252406120
H	2.528620481	4.419316769	-4.377893925
H	4.898401260	3.753307343	-4.757564545
H	5.536356926	1.352025628	-4.653302670
H	3.624758005	-4.303409576	-3.659527302
H	2.224496126	-5.244083881	-5.482822418
H	0.284814239	-3.953275204	-6.349080086
C	-0.656501412	5.838197231	0.093298554
C	-1.916034937	5.927922249	0.698660672
C	-2.993462801	5.297307491	0.074824698
C	-2.085381508	6.678675652	1.999488950
H	0.194455191	6.330452919	0.561473310
C	-0.461083323	5.135773659	-1.096172929
H	-3.985080719	5.375606537	0.517366290
C	-2.841034651	4.566421986	-1.111854553
C	-1.560870409	4.483091831	-1.688623190
C	0.914266288	5.054631233	-1.716480970
C	-4.047891617	3.886956930	-1.723127127
C	-1.376844764	3.634932280	-2.921493769
O	-0.947031617	4.209366798	-3.984790325
O	-1.669628859	2.419701815	-2.824243784
H	-4.187970161	2.885327578	-1.301673412
H	-4.956138134	4.460077286	-1.508447766
H	-3.970060110	3.769348621	-2.804517746
H	0.899112284	5.433941841	-2.742083073
H	1.644960761	5.626801968	-1.137579560
H	1.263768792	4.017257690	-1.769106150
H	-1.601665139	6.146466732	2.828458786
H	-1.627509356	7.673318863	1.948967457
H	-3.140710592	6.806455135	2.258279324

==============================

VII$_{SC}$

==============================

Cu	-1.200962186	1.074407220	-3.072218657
H	-1.655954361	4.209404469	-8.560672760
C	-2.564104557	3.675522566	-8.860870361
C	-2.592101574	2.258863926	-8.255377769
C	-1.490264654	1.330994725	-8.763828278
C	-1.567948580	-0.036573388	-8.444839478
C	-0.392207742	1.770774126	-9.510969162
C	-0.588969767	-0.934905469	-8.863169670
C	0.597973168	0.873619139	-9.930402756
C	0.504215419	-0.480980307	-9.612658501
H	-2.407187223	-0.391066164	-7.850419998
H	-0.297689855	2.820535421	-9.773065567
H	-0.676862359	-1.988840222	-8.606679916
H	1.443548322	1.239496112	-10.509200096
H	1.269530296	-1.178802848	-9.945659637
H	-3.545644522	1.800676346	-8.563188553
H	-3.418074131	4.251327038	-8.490045547
P	-2.316359758	-0.874405384	-2.641897202
C	-1.161733747	-2.268156767	-2.995078802
C	0.040199369	-2.375858545	-2.231582642
C	-1.357721090	-3.087704659	-4.114048004
C	0.943702281	-3.332396984	-2.661299944
C	0.369531214	-1.621534109	-0.979130089
C	-0.407438785	-4.037411213	-4.535673141
H	-2.270411491	-2.985336542	-4.689743519
C	0.743979394	-4.133292675	-3.784630775
O	2.151840925	-3.641792774	-2.085468531
C	0.174304008	-2.267143726	0.228460968
C	0.996321559	-0.336059332	-0.906314194
H	-0.572735369	-4.662987232	-5.405740738
O	1.812996626	-4.973350525	-3.957470655
C	2.758932829	-4.621816158	-2.936374664
C	0.545282781	-1.729488373	1.459595203
O	-0.378502458	-3.510725498	0.419464678
C	1.393766046	0.173990294	0.335411251
P	1.016921282	0.723016322	-2.425296783
H	3.652860165	-4.191071033	-3.404903412
H	3.007252932	-5.512576580	-2.347289801
C	1.178974390	-0.510338664	1.546686292
O	0.230760053	-2.606154442	2.465862989
C	-0.504366100	-3.667152882	1.838159561
H	1.885855556	1.137286544	0.382489234
H	1.495995164	-0.098684832	2.498321295
H	-0.079451598	-4.631143570	2.136939287
H	-1.563502312	-3.589030266	2.118557453
C	2.121417999	2.137835979	-2.009291649
C	3.356652021	2.359348536	-2.638173819
C	1.671635985	3.077887774	-1.061988354
C	4.126418591	3.479184628	-2.313713312
H	3.723085880	1.663351655	-3.385763645
C	2.450412035	4.186531544	-0.730472028
H	0.704621673	2.946502686	-0.589448035
C	3.682286978	4.393298626	-1.356450319
C	1.937737226	-0.235736161	-3.686418295
C	1.395080566	-0.303907990	-4.978492737
C	3.151410103	-0.887227416	-3.417392254
C	2.054822683	-1.003397703	-5.990538597
H	0.443395108	0.178957865	-5.187796116
C	3.815690517	-1.576300144	-4.432366848
H	3.568313360	-0.858063221	-2.414576530
C	3.268453598	-1.638362408	-5.718767166
C	-2.893388271	-1.084892154	-0.919932663
C	-2.966029406	0.076722242	-0.134045914
C	-3.257044315	-2.319100380	-0.361745805
C	-3.409363747	0.004570324	1.187388539
H	-2.653707266	1.030315399	-0.553208530
C	-3.713337183	-2.383423090	0.956189871
H	-3.167894840	-3.227139950	-0.951440275
C	-3.788351059	-1.223377943	1.734449506
C	-3.752558231	-1.184819341	-3.734254837
C	-3.659698248	-0.669670284	-5.037927628
C	-4.920034409	-1.854789853	-3.345260382
C	-4.707492828	-0.839630604	-5.940204620
H	-2.777828217	-0.111434020	-5.338475227
C	-5.969806671	-2.016030788	-4.251378536
H	-5.021525860	-2.234951496	-2.333556414
C	-5.866003513	-1.514137268	-5.550601482
H	-2.610514402	3.651323557	-9.955759048

C -5.136267662 2.659328461 -6.159495831
C -3.761656046 2.501713991 -5.911305904
C -3.293604851 2.469490290 -4.567452431
C -4.173467159 2.584627628 -3.483088255
C -5.530107021 2.732333183 -3.751295805
C -6.006155491 2.770658016 -5.080121994
C -2.603290319 2.310252905 -6.743920326
C -1.531797171 2.205212831 -5.879626274
N -1.910298109 2.300069809 -4.544140339
H -5.515231133 2.688381910 -7.179293156
H -3.788885355 2.544328928 -2.468201160
H -6.234954357 2.820269108 -2.928404331
H -7.071866512 2.890458822 -5.259671688
H -1.422945976 3.551186800 -3.718811274
H -0.488906890 2.062810183 -6.135835648
H -4.630188942 -0.408373415 -6.933666706
H -6.690951824 -1.630616188 -6.247975826
H -6.875365734 -2.528280973 -3.936563253
H -4.011482716 -3.340727568 1.376893163
H -4.137162685 -1.278996229 2.762175798
H -3.453978300 0.909397304 1.787889361
H 2.072358847 4.903807163 -0.007063450
H 4.283750534 5.263751507 -1.108648419
H 5.078775883 3.634168625 -2.814842224
H 4.765903473 -2.061400890 -4.221149921
H 3.787525415 -2.181379080 -6.503935814
H 1.617242455 -1.042388320 -6.984254837
C -0.006965951 7.363766670 -0.403097153
C -0.642645121 7.404943943 0.839758515
C -1.504701257 6.357465744 1.171148896
C -0.377900392 8.537307739 1.803647041
H 0.667920053 8.172132492 -0.678019464
C -0.211405367 6.323949337 -1.314898968
H -2.019227743 6.378337383 2.129654408
C -1.728220224 5.278117657 0.310714036
C -1.079582453 5.262063980 -0.948706269
C 0.535318911 6.386620045 -2.630608559
C -2.674392700 4.186520576 0.765521646
C -1.306135774 4.103317261 -1.868310571
O -1.242976069 4.396737099 -3.144906044
O -1.521895289 2.953323841 -1.449043751
H -2.129987717 3.266896486 0.999141634
H -3.223277092 4.507530689 1.656251431
H -3.395605803 3.922130823 -0.012023987
H -0.145885810 6.589968204 -3.460381031
H 1.292237401 7.176334858 -2.595773697
H 1.033797860 5.442029476 -2.858114481
H 0.505866468 8.328272820 2.420470953
H -0.187878832 9.476801872 1.274335265
H -1.221199870 8.693260193 2.483534336

==============================

VII$_{SC}$-TS

==============================

Cu -1.428796291 1.257205129 -3.037506104
H -0.195497438 3.401874781 -8.477038383
C -1.187323332 3.312035561 -8.937683105
C -1.979426146 2.143658161 -8.319055557
C -1.344409704 0.765042663 -8.535676956
C -2.014011383 -0.363705486 -8.026816368
C -0.131376639 0.562845469 -9.204564095
C -1.489568353 -1.645858169 -8.169813156
C 0.398769826 -0.726666927 -9.357171059
C -0.273341238 -1.834638476 -8.838885307
H -2.956094742 -0.223065376 -7.502687931
H 0.417048812 1.408245444 -9.611836433
H -2.029975414 -2.498921394 -7.761981964
H 1.343579292 -0.858884931 -9.882036209
H 0.142895281 -2.833786964 -8.952796936
H -2.959002256 2.114589930 -8.821982384
H -1.719987512 4.252925396 -8.763332367
P -2.373110533 -0.749310315 -2.636500835
C -1.167389989 -2.025563955 -3.198621988
C 0.058502551 -2.192058802 -2.485814095
C -1.360860348 -2.681589127 -4.420141697
C 0.979901075 -3.052299976 -3.057998419
C 0.408233851 -1.585736275 -1.164061904
C -0.387231141 -3.521345377 -4.990093708
H -2.286871195 -2.531033039 -4.963030338
C 0.781850100 -3.688969374 -4.280094147
O 2.207838535 -3.399680614 -2.551479816
C 0.356982440 -2.405714035 -0.051875263
C 0.905888796 -0.262353331 -0.947058439
H -0.546151698 -4.008274555 -5.945451736
O 1.874604225 -4.454010010 -4.592556477
C 2.829698086 -4.222673416 -3.545075417
C 0.740073025 -1.999547720 1.222112060
O -0.064490728 -3.712599993 -0.011226571
C 1.315034032 0.119984604 0.335515529
P 0.846310079 0.949408412 -2.351246595
H 3.698991299 -3.696749687 -3.958587646
H 3.117243528 -5.180754185 -3.096368074
C 1.239739537 -0.737422705 1.447704911
O 0.569178939 -3.027646780 2.112606764
C -0.032999530 -4.095978737 1.368227005
H 1.715499043 1.112522364 0.494867504
H 1.563013315 -0.421010286 2.433126688
H 0.569605172 -5.004611015 1.480460763
H -1.058969855 -4.253133774 1.725547552
C 1.862345219 2.366304636 -1.764275670
C 3.094503641 2.725762129 -2.333420515
C 1.358987331 3.144786119 -0.705863416
C 3.813187599 3.815252066 -1.837012172
H 3.499338388 2.160707951 -3.165891409
C 2.092650414 4.215754032 -0.197359860
H 0.380604088 2.924814939 -0.292664677
C 3.323430538 4.556889534 -0.760935545
C 1.857562542 0.133594319 -3.643970013
C 1.301639557 -0.022086920 -4.921260357
C 3.139016628 -0.377678871 -3.386377335
C 2.014081717 -0.668411732 -5.931926250
H 0.293813109 0.331751078 -5.116308212
C 3.860502720 -1.002735496 -4.402111530
H 3.564663172 -0.290975422 -2.390655279
C 3.297688007 -1.152542949 -5.673918724
C -2.703959703 -1.088830590 -0.873522043
C -2.677484274 0.008284226 0.002003334
C -2.954840660 -2.373608351 -0.369256020
C -2.900878906 -0.181945816 1.366029024
H -2.459763527 1.002614975 -0.382704288
C -3.195338249 -2.554055929 0.992515445
H -2.935976267 -3.231244564 -1.035709262
C -3.161432028 -1.460290909 1.862111092
C -3.916416645 -1.093951464 -3.550534725
C -4.006762505 -0.519946396 -4.828940392
C -5.003216267 -1.817200184 -3.042593479
C -5.156728745 -0.684238255 -5.596652508
H -3.182490110 0.076360241 -5.206986904
C -6.158249378 -1.969900727 -3.810721159
H -4.961492062 -2.242135525 -2.044984579
C -6.235774040 -1.408467770 -5.086241722
H -1.054904342 3.188319206 -10.018969536
C -4.857299805 2.637359858 -6.690222263
C -3.533715963 2.570678949 -6.221508980
C -3.283465624 2.713318348 -4.830532074
C -4.311540127 2.925591469 -3.908273935
C -5.613080502 2.990686417 -4.395233631
C -5.882063866 2.847866535 -5.772960186
C -2.247749805 2.376367092 -6.846336842
C -1.322042346 2.430197716 -5.830644608
N -1.912512183 2.618498564 -4.577778816
H -5.078304768 2.534043074 -7.750751495
H -4.078235626 3.019546509 -2.851079702
H -6.437354565 3.151555538 -3.705141068
H -6.910462379 2.904746771 -6.121234894
H -1.542048454 3.634338379 -3.810874939
H -0.244909212 2.347598314 -5.904801846
H -5.224107265 -0.206060395 -6.568460941
H -7.142292023 -1.520213485 -5.674901009
H -7.002386570 -2.522877455 -3.407084465

H	-3.407443762	-3.548515797	1.377248406
H	-3.334773540	-1.606958747	2.924904823
H	-2.865412235	0.669522941	2.040265799
H	1.677779794	4.807250977	0.612035096
H	3.887677193	5.401014328	-0.374475420
H	4.762897968	4.080407143	-2.294628382
H	4.859386444	-1.381882787	-4.199329853
H	3.857058287	-1.654152036	-6.459394932
H	1.559058547	-0.797603428	-6.909086704
C	0.150025278	7.319141388	-0.279103607
C	-0.473880500	7.368403435	0.969274104
C	-1.429453015	6.394410133	1.262962341
C	-0.091874108	8.423743248	1.980178475
H	0.905515909	8.064255714	-0.521113873
C	-0.152100280	6.339242935	-1.228468060
H	-1.932642341	6.420442104	2.227662802
C	-1.758183837	5.378898621	0.357928067
C	-1.119348407	5.353145599	-0.904485643
C	0.624437809	6.356579781	-2.527637720
C	-2.787930727	4.353929043	0.785337210
C	-1.431775689	4.248680115	-1.875417590
O	-1.337232113	4.559459209	-3.126912594
O	-1.744856238	3.105368137	-1.466090560
H	-2.310620070	3.399847507	1.031780601
H	-3.331542015	4.708270550	1.666951895
H	-3.507384539	4.135573864	-0.007164459
H	-0.015002115	6.626708984	-3.371083021
H	1.450092912	7.071804523	-2.461739779
H	1.041392803	5.372021675	-2.754473448
H	0.791549504	8.114778519	2.553695202
H	0.155986443	9.373099327	1.493902445
H	-0.898075104	8.607914925	2.696793795

================================

VIII$_{SC}$

================================

Cu	-1.346984744	1.588208675	-2.978189230
H	0.759692609	1.876413107	-8.085754395
C	-0.056048457	2.242515087	-8.720762253
C	-1.415316701	1.700499535	-8.247342110
C	-1.501455069	0.164032042	-8.258664131
C	-2.638854980	-0.470892280	-7.729524136
C	-0.500110626	-0.649147749	-8.809896469
C	-2.776357412	-1.857522488	-7.754338264
C	-0.630090296	-2.042687416	-8.831796646
C	-1.770115972	-2.654220581	-8.310659409
H	-3.427898884	0.125170112	-7.284601212
H	0.395581394	-0.204719782	-9.233441353
H	-3.671167612	-2.310740948	-7.331971645
H	0.164834946	-2.648112059	-9.263329506
H	-1.874785066	-3.736709356	-8.337208748
H	-2.173620701	2.055154800	-8.962267876
H	-0.055348594	3.335146427	-8.673297882
P	-2.331989050	-0.495642483	-2.712441683
C	-1.153581381	-1.788110256	-3.301382542
C	0.071759701	-2.037320852	-2.609699011
C	-1.400420189	-2.413552523	-4.529913902
C	0.931250632	-2.941924572	-3.211226940
C	0.500677168	-1.465797424	-1.296723843
C	-0.489739954	-3.302511454	-5.126495838
H	-2.318957090	-2.197313070	-5.062217712
C	0.677152932	-3.547976971	-4.436821461
O	2.153015375	-3.352687836	-2.737185240
C	0.534237027	-2.314266920	-0.204864189
C	0.996909201	-0.144091681	-1.076545477
H	-0.688769400	-3.748726130	-6.092950821
O	1.728336453	-4.356579304	-4.786557198
C	2.703578949	-4.209328651	-3.743577719
C	0.970582306	-1.926934004	1.056691885
O	0.122721471	-3.625819206	-0.168182284
C	1.458565116	0.222862288	0.192941397
P	0.927281737	1.067443848	-2.477535725
H	3.608678579	-3.746273041	-4.156379700
H	2.922261000	-5.191578388	-3.306759596
C	1.448741078	-0.657010972	1.289072037
O	0.843759358	-2.970814705	1.937286973
C	0.386987865	-4.086535931	1.161748528
H	1.853446245	1.218134046	0.350828797
H	1.806131482	-0.353421360	2.266631842
H	1.168395042	-4.859214783	1.133452296
H	-0.536932766	-4.479147434	1.601729155
C	1.966072202	2.465301514	-1.905882001
C	3.205046177	2.806576252	-2.467515945
C	1.457087278	3.249511719	-0.854442954
C	3.933450460	3.884863615	-1.961779237
H	3.607819796	2.235133171	-3.296854258
C	2.197837353	4.311277390	-0.339129329
H	0.472163647	3.035774231	-0.453137368
C	3.441064835	4.629138947	-0.889424980
C	1.903849959	0.212483779	-3.772364616
C	1.309625268	0.005093109	-5.024751663
C	3.187169313	-0.301299661	-3.528580666
C	1.992364645	-0.685229063	-6.026555538
H	0.293018013	0.343185991	-5.199513435
C	3.876391649	-0.976111174	-4.535344124
H	3.637966156	-0.181556389	-2.547286272
C	3.279444695	-1.168904305	-5.785151005
C	-2.573652983	-0.871257901	-0.933671951
C	-2.697320461	0.218605742	-0.059308447
C	-2.621859312	-2.176731825	-0.419919848
C	-2.880088568	0.003493676	1.307996511
H	-2.617142439	1.230141640	-0.449001193
C	-2.808693647	-2.386135340	0.945391834
H	-2.456673861	-3.027610779	-1.075164795
C	-2.938570738	-1.296919107	1.811904550
C	-3.925454855	-0.956306994	-3.505513191
C	-4.343390465	-0.169002309	-4.593927383
C	-4.714136600	-2.056705475	-3.098355770
C	-5.515605450	-0.485701382	-5.284365177
H	-3.755768061	0.696126640	-4.898192406
C	-5.888540268	-2.366156340	-3.781813383
H	-4.422775269	-2.664951086	-2.241647482
C	-6.288062096	-1.586213231	-4.881170750
H	0.162004337	1.946068406	-9.751550674
C	-4.411466122	2.524430513	-7.031868935
C	-3.133885860	2.587290525	-6.445528507
C	-3.015832186	3.047893763	-5.110759735
C	-4.116493702	3.448112249	-4.350450993
C	-5.368225574	3.379610300	-4.953484535
C	-5.513921738	2.924253941	-6.281319141
C	-1.795193672	2.272936106	-6.898905754
C	-0.956310689	2.592267036	-5.861918926
N	-1.672409415	3.006770849	-4.735260487
H	-4.535642147	2.173136473	-8.053621292
H	-3.981003284	3.784685135	-3.327693224
H	-6.249391079	3.678764820	-4.391825676
H	-6.505942822	2.885153770	-6.723359108
H	-1.366718769	3.785960913	-4.053528786
H	0.121568732	2.545619965	-5.813201427
H	-5.821208000	0.145807996	-6.119067192
H	-7.205380917	-1.830550551	-5.410558701
H	-6.494320393	-3.216920853	-3.455280781
H	-2.842433453	-3.400808096	1.335537553
H	-3.071931601	-1.462797761	2.877756357
H	-2.964823008	0.854339123	1.979383588
H	1.782339573	4.908223629	0.466940552
H	4.014645100	5.463742256	-0.495301843
H	4.892220020	4.138334751	-2.406745434
H	4.874865532	-1.360431910	-4.341487408
H	3.811953306	-1.709138870	-6.563522339
H	1.502196193	-0.864836276	-6.978436947
C	-0.267353714	7.242946148	0.407243758
C	-0.914578259	6.994018078	1.617745519
C	-1.775346041	5.897390366	1.681297660
C	-0.668958426	7.859387398	2.831536770
H	0.404279143	8.096403122	0.334070921
C	-0.445390999	6.431950092	-0.720211267
H	-2.303119421	5.692524433	2.611225843
C	-1.974911690	5.043329239	0.592212558
C	-1.298384190	5.301354885	-0.626156211

C	0.330410540	6.794681072	-1.968491912
C	-2.907968283	3.868900061	0.794745386
C	-1.437469244	4.368698597	-1.810899019
O	-1.289626598	4.856164455	-2.965971231
O	-1.663107038	3.130592346	-1.575224280
H	-2.332933903	2.951885700	0.951585174
H	-3.542913675	4.034592628	1.671456456
H	-3.543743610	3.686090946	-0.073722459
H	-0.337426960	7.123685360	-2.767607212
H	1.046077847	7.593607426	-1.747242451
H	0.878741920	5.935586929	-2.362000465
H	0.056374602	7.389806747	3.508929253
H	-0.269811690	8.839733124	2.553606987
H	-1.588692427	8.016578674	3.405334234

===============================

IV_S

===============================

Cu	-0.840274096	-3.669593811	-2.142092228
H	-4.276721478	-4.321354866	-3.373173237
C	-3.453622818	-4.146824360	-4.065643311
C	-2.465946436	-3.128362656	-3.604769707
C	-2.863988638	-1.897208571	-2.968402863
C	-4.140262604	-1.690865278	-2.390352249
C	-1.934896588	-0.820779383	-2.978121996
C	-4.476478100	-0.452413321	-1.862451553
C	-2.279620409	0.410936505	-2.435684443
C	-3.551525116	0.600425601	-1.881907344
H	-4.857879162	-2.503837585	-2.359515429
H	-0.957846642	-0.983363569	-3.430109024
H	-5.458730698	-0.298886865	-1.425607085
H	-1.566885591	1.230569601	-2.458518267
H	-3.825613499	1.567386985	-1.469310164
H	-1.608770132	-3.016451120	-4.257297993
H	-2.959692955	-5.090436935	-4.298278809
P	-2.270853758	-4.451168060	-0.403517008
C	-1.275918484	-5.611198902	0.620367885
C	-0.249365106	-5.086131573	1.468516469
C	-1.427749634	-6.997303486	0.477929860
C	0.560303450	-6.026244164	2.079746485
C	-0.013345994	-3.653606653	1.828348398
C	-0.585950494	-7.924958229	1.115294576
H	-2.232043266	-7.389628887	-0.129630834
C	0.420006037	-7.403275013	1.898902059
O	1.603399515	-5.779119492	2.927949667
C	-0.374893576	-3.228190899	3.092221260
C	0.659427524	-2.690119743	1.018696189
H	-0.722654402	-8.993535995	0.998080552
O	1.371681690	-8.064336777	2.614201546
C	2.219514132	-7.051127911	3.182795286
C	-0.129603758	-1.937584639	3.563516855
O	-1.036846519	-3.950004101	4.046105385
C	0.931061208	-1.409486175	1.512727022
P	1.018813968	-3.152521372	-0.710355520
H	3.199823856	-7.081724644	2.691028118
H	2.301541805	-7.208619595	4.262113571
C	0.542789519	-1.006570578	2.802253485
O	-0.640279293	-1.799343228	4.820537090
C	-1.170205355	-3.084555864	5.184718609
H	1.462485552	-0.698002160	0.892552078
H	0.755896151	-0.012793477	3.178927660
H	-0.596227169	-3.493017197	6.025374413
H	-2.230377674	-2.980089664	5.437670231
C	1.959174156	-1.771879673	-1.447531939
C	3.259816408	-1.917160988	-1.946067810
C	1.288128853	-0.549688339	-1.631487489
C	3.882463217	-0.851463318	-2.600337505
H	3.789471865	-2.857633829	-1.834830523
C	1.919627666	0.513960719	-2.268984556
H	0.268487602	-0.430796713	-1.275274038
C	3.220221758	0.365197062	-2.759934902
C	2.134964705	-4.594108582	-0.581658781
C	1.769352198	-5.797285080	-1.203008771
C	3.305422306	-4.545267582	0.190171674
C	2.566787243	-6.931804657	-1.069999933
H	0.843409061	-5.852189064	-1.768684149
C	4.108074665	-5.679536819	0.314324021
H	3.581166506	-3.626187563	0.699425995
C	3.739742756	-6.872442722	-0.314461797
C	-2.856282234	-3.182994843	0.771040142
C	-2.566362381	-1.833622694	0.538867652
C	-3.523249626	-3.556537628	1.949565649
C	-2.944221973	-0.865156114	1.467219114
H	-2.033006191	-1.544101119	-0.358739316
C	-3.915374994	-2.583327055	2.866398335
H	-3.722153187	-4.604516506	2.153685331
C	-3.623576880	-1.237051010	2.628189564
C	-3.751921654	-5.370337486	-0.950084507
C	-3.588129282	-6.430075169	-1.860716701
C	-5.050617695	-4.987694740	-0.580998659
C	-4.693462849	-7.123899937	-2.347208738
H	-2.594458103	-6.694250107	-2.212922335
C	-6.156688213	-5.670971394	-1.090039611
H	-5.205559254	-4.157648087	0.099181116
C	-5.982197285	-6.744620323	-1.963418365
H	-3.881792307	-3.776112556	-5.010514736
C	-1.302127481	-4.906627655	-6.715166569
C	-0.503892899	-4.398967743	-5.651763916
C	-0.120171331	-2.986927748	-5.638625622
C	-0.551618040	-2.127354860	-6.685063362
C	-1.322600722	-2.660197020	-7.692183495
C	-1.697683692	-4.045207024	-7.709908009
C	0.043901335	-4.938209534	-4.485495090
C	0.712176681	-3.832835197	-3.839374065
N	0.622609258	-2.662288666	-4.551376820
H	-1.587723851	-5.955606937	-6.739036560
H	-0.263854176	-1.079513669	-6.675304890
H	-1.659080625	-2.021826506	-8.505473137
H	-2.303069115	-4.410723209	-8.535249710
H	0.022881955	-5.965409279	-4.143796921
H	1.533567190	-3.956384420	-3.145369053
H	4.889099598	-0.978826523	-2.987767935
H	3.708646297	1.190057397	-3.269722700
H	1.393445253	1.456369042	-2.395945549
H	-2.704640865	0.177369580	1.281991720
H	-3.917396069	-0.481953919	3.351549864
H	-4.440667152	-2.876263142	3.771130085
H	-7.156410217	-5.363114357	-0.797155797
H	-6.845462799	-7.276350021	-2.352259874
H	-4.550970554	-7.945528984	-3.042847633
H	2.269645691	-7.860912800	-1.546995997
H	4.364414215	-7.755288124	-0.212976292
H	5.019682407	-5.632746696	0.903300881

===============================

III$_{SN}$-TS'

===============================

Cu	-0.823786378	-3.853306770	-2.048249006
H	-4.426306725	-4.436753750	-3.305467367
C	-3.596511602	-4.307339191	-4.002959728
C	-2.615408897	-3.264432669	-3.609330893
C	-2.980191469	-1.986794710	-3.068788767
C	-4.269419670	-1.702665210	-2.553420544
C	-2.001581192	-0.955416441	-3.073886633
C	-4.570114613	-0.430658847	-2.087873697
C	-2.312468529	0.311766982	-2.603745699
C	-3.598879814	0.579269052	-2.115821123
H	-5.021553993	-2.483833075	-2.518993855
H	-1.008785844	-1.182289720	-3.451612473
H	-5.560406208	-0.216323748	-1.697289109
H	-1.561019182	1.095856547	-2.623322248
H	-3.845660925	1.573921442	-1.754664302
H	-1.697597623	-3.281807899	-4.186821938
H	-3.090834856	-5.260385513	-4.168183327
P	-2.317965269	-4.511965275	-0.358317226
C	-1.333247185	-5.642676353	0.706289470
C	-0.274795473	-5.096077919	1.499223590
C	-1.491189957	-7.032046795	0.610949755
C	0.564993501	-6.017165184	2.097861767
C	-0.024621254	-3.655994177	1.816062450

C -0.620472908 -7.939944744 1.238087773
H -2.319040060 -7.442218304 0.048220538
C 0.421726197 -7.398451328 1.958338618
O 1.652828336 -5.745370865 2.877964735
C -0.403104305 -3.186728001 3.058866024
C 0.698443234 -2.739422321 0.996702075
H -0.758914769 -9.011838913 1.154658675
O 1.418761134 -8.038237572 2.628878117
C 2.295809746 -7.007091999 3.119002104
C -0.121284537 -1.895340323 3.505382776
O -1.100286126 -3.866794825 4.019162655
C 1.007773519 -1.458911061 1.468143344
P 1.072598100 -3.265681267 -0.714179575
H 3.241639614 -7.040897369 2.564330816
H 2.448361635 -7.141365051 4.193751335
C 0.603387892 -1.009400845 2.737808466
O -0.641284525 -1.713243365 4.753627777
C -1.285502076 -2.947913647 5.107758999
H 1.577126861 -0.781440079 0.843323290
H 0.847715259 -0.015927533 3.096347570
H -0.823427856 -3.356034756 6.013744831
H -2.357242823 -2.768786192 5.251305580
C 1.888376713 -1.855145216 -1.533646345
C 3.124285460 -1.956003666 -2.181999445
C 1.144717693 -0.668041289 -1.655894160
C 3.613395452 -0.882155418 -2.928189754
H 3.697517633 -2.875456810 -2.134649515
C 1.639873147 0.403575122 -2.392878056
H 0.171848491 -0.583273411 -1.178480744
C 2.877401114 0.297058165 -3.035656691
C 2.283116579 -4.627130032 -0.531327128
C 1.888964891 -5.935727119 -0.854346871
C 3.562410831 -4.408160210 0.002650746
C 2.772085667 -7.001126289 -0.685206294
H 0.873221040 -6.129882336 -1.190733552
C 4.447877407 -5.474241257 0.162954047
H 3.865899324 -3.406033516 0.292840570
C 4.057585716 -6.769564629 -0.189780891
C -2.881613493 -3.180206537 0.749969125
C -2.587976694 -1.849843025 0.428726345
C -3.562027693 -3.474699259 1.942399740
C -2.971410275 -0.820664585 1.286862850
H -2.045145273 -1.623465061 -0.482246101
C -3.960128784 -2.441375971 2.788328409
H -3.764624834 -4.506758213 2.213253736
C -3.661745310 -1.114295721 2.464249134
C -3.811186314 -5.430593014 -0.871027708
C -3.658056498 -6.531276226 -1.734400392
C -5.106082439 -5.017014503 -0.522788227
C -4.770615101 -7.232809067 -2.193614244
H -2.666695833 -6.822683334 -2.071771383
C -6.219168663 -5.709663868 -1.004311323
H -5.252922058 -4.156877041 0.120990932
C -6.056077957 -6.822077274 -1.830755353
H -4.016720772 -3.997750044 -4.977369308
C -1.294628263 -4.253833771 -7.011888981
C -0.586566567 -4.293839931 -5.783214092
C 0.044195805 -3.080116034 -5.274398327
C -0.063726313 -1.859137774 -6.000641823
C -0.761397004 -1.860541940 -7.186690331
C -1.374382973 -3.053702831 -7.690212250
C -0.313945293 -5.294317245 -4.818521023
C 0.431038350 -4.648650646 -3.816234589
N 0.655403554 -3.287383795 -4.088416576
H -1.763675570 -5.150735855 -7.411151886
H 0.420011967 -0.962556362 -5.618558407
H -0.850251317 -0.943602145 -7.765643120
H -1.911532044 -3.003507137 -8.635261536
H -0.574143052 -6.344705582 -4.860126972
H 1.057761908 -5.128382683 -3.073051929
H 4.570520878 -0.974719286 -3.433936357
H 3.261914730 1.128629684 -3.619374275
H 1.061333776 1.320860982 -2.471299410
H -2.729167223 0.207382679 1.034874558
H -3.961412907 -0.312546641 3.133099318
H -4.498336792 -2.671311140 3.703860044
H -7.216093540 -5.378845215 -0.726600409
H -6.924802780 -7.361348152 -2.196945429
H -4.635540962 -8.085968971 -2.852125406
H 2.452910423 -8.009446144 -0.932108998
H 4.750942707 -7.597513676 -0.070116542
H 5.441742897 -5.294312954 0.563553214

================================
III_{SC}-TS'
================================
Cu -0.700339794 -3.834658384 -2.084500790
H -4.269134521 -4.050202847 -3.242482662
C -3.431284666 -3.967231035 -3.933312893
C -2.353105783 -3.047969818 -3.473814964
C -2.679010630 -1.765162945 -2.897544146
C -3.952841043 -1.457354665 -2.358418941
C -1.705276608 -0.735887468 -2.972363949
C -4.241164684 -0.170994535 -1.926951647
C -2.002185822 0.547610760 -2.529738903
C -3.269401789 0.835085988 -2.010074615
H -4.708786488 -2.230955124 -2.278195381
H -0.735447824 -0.966645896 -3.408456087
H -5.221607208 0.056770366 -1.519386053
H -1.254365802 1.330904841 -2.607267857
H -3.504667521 1.841957450 -1.676308632
H -1.486080170 -3.008081436 -4.124628544
H -3.041583061 -4.958607197 -4.158849716
P -2.303879023 -4.444435120 -0.419791669
C -1.336258531 -5.649159431 0.569080353
C -0.277949750 -5.155136108 1.394577622
C -1.504656196 -7.027574062 0.389151484
C 0.550541878 -6.113528728 1.945325136
C -0.057937503 -3.737003803 1.808761597
C -0.644121110 -7.975348949 0.967545450
H -2.334479094 -7.396037102 -0.198744997
C 0.396479607 -7.483571529 1.725283027
O 1.619110942 -5.897177219 2.768226624
C -0.497840345 -3.344281197 3.059306383
C 0.648751199 -2.752057314 1.056385994
H -0.794024527 -9.039527893 0.827638149
O 1.368399620 -8.169964790 2.386709690
C 2.244160414 -7.177355289 2.950514078
C -0.293227047 -2.062015057 3.569899082
O -1.216816545 -4.089008808 3.952391863
C 0.887112439 -1.484106779 1.597883701
P 1.100088954 -3.182656527 -0.666272402
H 3.200639486 -7.189541340 2.413259983
H 2.373698711 -7.371955872 4.018678665
C 0.419160366 -1.112464428 2.870380402
O -0.887007117 -1.950403929 4.792347908
C -1.448392510 -3.239771605 5.088622570
H 1.449143291 -0.753921926 1.029227734
H 0.598728061 -0.124437422 3.278392315
H -0.951476872 -3.662456512 5.969730854
H -2.526769161 -3.135738611 5.248260021
C 1.937703252 -1.710808277 -1.362245321
C 3.217803001 -1.771536827 -1.927847743
C 1.215014338 -0.507111847 -1.444666266
C 3.760581970 -0.650586247 -2.561409473
H 3.792121649 -2.691498280 -1.886218667
C 1.767168045 0.611564517 -2.062511206
H 0.217082262 -0.441512913 -1.023486972
C 3.041622877 0.541892886 -2.631076097
C 2.348716021 -4.502590656 -0.521999896
C 2.142186403 -5.701802731 -1.217137098
C 3.468431234 -4.368364334 0.311190724
C 3.047350883 -6.753748894 -1.093400598
H 1.259388208 -5.815071106 -1.839029312
C 4.379578114 -5.417309761 0.425710261
H 3.622616291 -3.447434425 0.866326511
C 4.169865131 -6.609213352 -0.275319964
C -2.855255365 -3.153457880 0.750186741
C -2.519003868 -1.813901067 0.520795465
C -3.602840662 -3.493717909 1.890380621

C	-2.938480854	-0.822502136	1.406916857
H	-1.924237967	-1.547998071	-0.344420850
C	-4.032758236	-2.497876644	2.765527725
H	-3.843796253	-4.532892227	2.093192816
C	-3.700211525	-1.161201835	2.525702000
C	-3.831108093	-5.285544395	-0.974474728
C	-3.726078987	-6.357606888	-1.879867792
C	-5.109581470	-4.816057682	-0.630161643
C	-4.867991924	-6.980597973	-2.378262758
H	-2.748804331	-6.681489468	-2.226543188
C	-6.250855923	-5.430047989	-1.149206638
H	-5.224046230	-3.968448877	0.035393190
C	-6.134874821	-6.518996716	-2.013005495
H	-3.811532021	-3.560782909	-4.884706020
C	-1.529834270	-5.187751770	-6.303341389
C	-0.570039928	-4.549709797	-5.480601311
C	-0.227355570	-3.161249638	-5.713493347
C	-0.841099739	-2.444922924	-6.759773254
C	-1.777311325	-3.099556208	-7.543107986
C	-2.118224859	-4.463088036	-7.320358276
C	0.137086198	-4.908436298	-4.311702728
C	0.951935470	-3.742928743	-4.004777908
N	0.706661224	-2.697007179	-4.806296825
H	-1.801555991	-6.226747036	-6.133643627
H	-0.574579358	-1.407551289	-6.937497616
H	-2.264383316	-2.563649416	-8.353399277
H	-2.853516817	-4.933346272	-7.966840267
H	0.257852048	-5.902669430	-3.901155949
H	1.811065555	-3.727141380	-3.346371412
H	4.749538898	-0.715331197	-3.004859447
H	3.466987848	1.409641266	-3.125774622
H	1.201181293	1.538226604	-2.105837584
H	-2.668311596	0.212413967	1.220849395
H	-4.029724121	-0.388389945	3.214201212
H	-4.626546383	-2.764250040	3.635638952
H	-7.231706142	-5.053881645	-0.872059762
H	-7.026187897	-6.995178699	-2.410557508
H	-4.769649029	-7.811967373	-3.069813251
H	2.876109362	-7.681509972	-1.631078720
H	4.881347179	-7.424759865	-0.184080690
H	5.251739502	-5.306567192	1.063352585

==============================

I_S-TS''

==============================

Cu	-0.125766084	-0.422624946	-3.334456921
P	-0.706540167	-2.444012403	-2.237899542
C	0.687170625	-3.226526976	-1.309167385
C	1.273892879	-2.500641108	-0.224822134
C	1.228140950	-4.456608295	-1.701008081
C	2.366600990	-3.096897364	0.377713144
C	0.756543994	-1.224834204	0.362882078
C	2.355367184	-5.022055626	-1.078620791
H	0.771315098	-5.006462097	-2.514316082
C	2.909596443	-4.309043884	-0.039955042
O	3.079655170	-2.619488955	1.449348092
C	0.076377325	-1.283654690	1.565642953
C	0.968084335	0.084114864	-0.167649075
H	2.764442444	-5.973941326	-1.397998214
O	3.986354351	-4.633993149	0.743108332
C	4.180763245	-3.518214703	1.624435186
C	-0.421744913	-0.158621609	2.217704296
O	-0.215169311	-2.407800913	2.297737122
C	0.471355021	1.207518935	0.500180244
P	1.734002948	0.230069220	-1.831123114
H	5.113512993	-3.004428625	1.357796669
H	4.200351715	-3.871631384	2.661401033
C	-0.239900470	1.108781338	1.709504604
O	-1.049120307	-0.533102512	3.379062414
C	-1.045311332	-1.967892289	3.379110336
H	0.633613467	2.191110134	0.073392496
H	-0.621919990	1.984979272	2.221352577
H	-0.630803347	-2.331142664	4.325849056
H	-2.068114281	-2.334014654	3.220817804
C	2.092207670	2.024859667	-2.045606852
C	3.327887774	2.622515917	-1.754002690
C	1.071576715	2.812203407	-2.608675003
C	3.534760237	3.978486061	-2.010776043
H	4.137626171	2.031667709	-1.339650154
C	1.279264569	4.169700623	-2.850703716
H	0.125162244	2.342715979	-2.870734453
C	2.511666775	4.756148338	-2.555300236
C	3.401022434	-0.510933042	-1.602958918
C	3.937923670	-1.256520391	-2.661942482
C	4.152091980	-0.340485781	-0.430096328
C	5.216569424	-1.806665182	-2.554439783
H	3.343766451	-1.422691226	-3.556875944
C	5.433270454	-0.882237256	-0.330962837
H	3.726868391	0.205623955	0.406776160
C	5.967062950	-1.616999984	-1.393309474
C	-1.995951653	-2.235183001	-0.953111410
C	-2.694513798	-1.021807432	-0.899347007
C	-2.292150974	-3.249687195	-0.029548272
C	-3.684363604	-0.829217613	0.065802082
H	-2.437977076	-0.236025840	-1.607361555
C	-3.292988062	-3.058675051	0.921471596
H	-1.735302091	-4.182130814	-0.054719601
C	-3.988748789	-1.846369624	0.971799016
C	-1.349472642	-3.777382851	-3.325449467
C	-0.548311710	-4.171342850	-4.412336349
C	-2.614604712	-4.361567497	-3.169033766
C	-0.983520091	-5.155945778	-5.297997475
H	0.407939106	-3.688315630	-4.579298496
C	-3.057224274	-5.330641747	-4.072003365
H	-3.257920980	-4.063004017	-2.348266602
C	-2.242722750	-5.736644745	-5.129748821
C	2.162830353	-6.670386791	-7.166060448
C	1.544147253	-5.808603764	-8.074189186
C	2.819919348	-6.109322071	-6.066433430
H	1.032441616	-6.227353096	-8.938423157
H	3.319367647	-6.764531612	-5.355103016
C	1.552979350	-4.418380737	-7.907299995
C	2.847993135	-4.729914665	-5.848940849
C	2.201874733	-3.882484674	-6.773278236
C	2.132395029	-2.382483244	-6.571043015
O	2.360925913	-1.576842427	-7.454407692
O	1.712038636	-2.076764822	-5.337461472
C	-0.785479903	0.922061503	-8.082598686
C	0.072306275	0.633791924	-7.026745796
C	-0.161848798	-0.504391015	-6.232541561
C	-1.197749257	-1.388966799	-6.474816799
C	-2.037224531	-1.107256651	-7.560846806
C	-1.836950302	0.033193991	-8.347308159
C	1.245670319	1.291112423	-6.466130733
C	1.667248249	0.555277467	-5.413542747
N	0.784772694	-0.533074319	-5.160248280
H	-0.645621836	1.812594771	-8.688887596
H	-1.346260309	-2.260143042	-5.848422527
H	-2.858921289	-1.780312419	-7.787171364
H	-2.510150671	0.234925956	-9.175916672
H	1.685882807	2.216773272	-6.812184811
H	2.500928879	0.704704762	-4.746299744
H	-0.341953844	-5.451670647	-6.122444153
H	-2.590887785	-6.495695114	-5.825431824
H	-4.042707920	-5.770887375	-3.942396402
H	-3.527244329	-3.852393627	1.626483321
H	-4.763503075	-1.695361614	1.719184995
H	-4.215631008	0.117624566	0.109944597
H	0.480473250	4.764880180	-3.285493135
H	2.677554131	5.811379910	-2.756411076
H	4.499836445	4.425895691	-1.787127137
H	6.014966488	-0.731611609	0.575273335
H	6.963268280	-2.044119835	-1.313709140
H	5.625748634	-2.389219999	-3.374382496
C	2.136951685	-8.167615891	-7.364631176
H	1.841638923	-8.684151649	-6.444332123
H	1.435864568	-8.456808090	-8.153194427
H	3.127208948	-8.547685623	-7.644252300
C	0.850449443	-3.546186924	-8.922994614
H	1.557258964	-2.872216225	-9.412816048

H	0.356406212	-4.160670757	-9.681188583
H	0.095581457	-2.907884359	-8.452256203
C	3.571818352	-4.181360245	-4.641495705
H	2.875517368	-3.862142086	-3.861133575
H	4.239116669	-4.933308125	-4.209417820
H	4.172491550	-3.307225466	-4.908555984
H	-1.256164551	0.668214083	-3.276262760

==============================

X_S

==============================

Cu	0.148355648	-0.664085090	-3.323302507
P	-0.581784487	-2.481903553	-2.138465643
C	0.789106965	-3.200754166	-1.186528802
C	1.308001161	-2.482956409	-0.062926963
C	1.385424614	-4.399079323	-1.609532237
C	2.393206358	-3.060714483	0.563311458
C	0.740022302	-1.218196034	0.488506645
C	2.494619846	-4.952561855	-0.953434289
H	0.979844272	-4.927578926	-2.463307142
C	2.983056545	-4.253023624	0.130628511
O	3.064525604	-2.586586475	1.653491139
C	0.013664606	-1.257737517	1.663081169
C	0.930797160	0.075787634	-0.084465548
H	2.945275784	-5.883076668	-1.278043389
O	4.032530785	-4.566089630	0.933425665
C	4.176914215	-3.472911119	1.857774019
C	-0.544055223	-0.120527461	2.253395557
O	-0.291902184	-2.361313820	2.408008337
C	0.378067225	1.210343361	0.518436015
P	1.691539526	0.185402364	-1.739829183
H	5.110552788	-2.941333771	1.640825868
H	4.156536102	-3.857079506	2.881788015
C	-0.372778624	1.133573771	1.705933213
O	-1.214519262	-0.471000284	3.386862516
C	-1.158368945	-1.904543281	3.461646318
H	0.528272271	2.182529688	0.061368629
H	-0.796510935	2.016672850	2.169850349
H	-0.745534658	-2.205405712	4.429411888
H	-2.163376093	-2.315232277	3.304885864
C	1.978108525	1.950514555	-2.094275951
C	3.188970089	2.598780394	-1.810847878
C	0.951117396	2.653679609	-2.747421980
C	3.362964153	3.935038805	-2.172596455
H	4.000655651	2.060225964	-1.332183838
C	1.126203299	3.990740538	-3.096503258
H	0.024751609	2.145344019	-3.006308794
C	2.334769011	4.631037235	-2.812192917
C	3.307686567	-0.646330118	-1.673228979
C	3.681729794	-1.434438109	-2.772266626
C	4.174491882	-0.519457817	-0.576709628
C	4.914429665	-2.088586807	-2.774610519
H	3.002741575	-1.534030914	-3.615956068
C	5.410354614	-1.166078091	-0.591956854
H	3.874157429	0.060599815	0.291179776
C	5.780933857	-1.953599930	-1.687181830
C	-1.939416885	-2.152901173	-0.990809321
C	-2.613013983	-0.925214767	-1.050571799
C	-2.312220812	-3.117537498	-0.040193141
C	-3.656430721	-0.661475420	-0.164427936
H	-2.309251308	-0.183031052	-1.783851862
C	-3.369514227	-2.853804588	0.829061389
H	-1.774899483	-4.059224606	0.023489865
C	-4.034647465	-1.624566555	0.773864448
C	-1.098631144	-3.722857952	-3.360592127
C	-0.269000411	-3.921482563	-4.479003429
C	-2.311080933	-4.419947147	-3.255850792
C	-0.633378506	-4.838642597	-5.462752342
H	0.644301057	-3.340303898	-4.591326714
C	-2.674030542	-5.327146053	-4.252803326
H	-2.969485044	-4.258610249	-2.408182859
C	-1.837148190	-5.541090965	-5.350413799
C	0.726176560	-0.171233073	-8.638603210
C	1.075947642	0.052593190	-7.301325321
C	0.321672440	-0.552121758	-6.259462357
C	-0.796638310	-1.332280040	-6.541815281
C	-1.130066752	-1.553057790	-7.881488323
C	-0.379674971	-0.976893842	-8.918110847
C	2.122414112	0.796022713	-6.652641296
C	1.972872376	0.595397413	-5.296556473
N	0.928138137	-0.261416614	-5.023153305
H	1.313510537	0.261354506	-9.444017410
H	-1.406420827	-1.733312607	-5.737752438
H	-1.992906690	-2.168260098	-8.120172501
H	-0.665655911	-1.159021020	-9.950031281
H	2.910197258	1.361298323	-7.132893085
H	2.591516256	0.977569640	-4.498775959
H	0.008913457	-4.984104156	-6.326616764
H	-2.126952410	-6.247820377	-6.122983456
H	-3.613971472	-5.866497040	-4.170415878
H	-3.671646357	-3.605844498	1.552690148
H	-4.850298882	-1.418944836	1.461423993
H	-4.170637131	0.294081599	-0.203996599
H	0.330469966	4.524507046	-3.607608318
H	2.479489803	5.668420792	-3.099610090
H	4.306051254	4.430418968	-1.960770488
H	6.088887215	-1.050867677	0.249101296
H	6.741731644	-2.460078239	-1.691918969
H	5.197619438	-2.702466965	-3.624809265
H	-1.268193841	-0.853129447	-3.807264090

==============================

I_S-TS'''

==============================

Cu	-0.136550590	-0.431478769	-3.357699871
P	-0.719528258	-2.445119143	-2.248220444
C	0.686188579	-3.230678320	-1.343284965
C	1.297017455	-2.506132603	-0.271713465
C	1.215965867	-4.461112499	-1.748225689
C	2.401763678	-3.104026794	0.306930125
C	0.788837612	-1.233392358	0.330092758
C	2.353114128	-5.030638218	-1.147916555
H	0.744199216	-5.004934788	-2.557328224
C	2.930812836	-4.319108486	-0.120974213
O	3.138513327	-2.629088163	1.364023685
C	0.126865730	-1.302798510	1.542134404
C	0.984999239	0.079856142	-0.196173772
H	2.753703594	-5.982974529	-1.476561904
O	4.021613121	-4.648269176	0.640697300
C	4.240822792	-3.531110048	1.514080644
C	-0.365345776	-0.184479669	2.210052490
O	-0.145973936	-2.432888031	2.272108555
C	0.494113386	1.196542859	0.487244517
P	1.730158806	0.235641718	-1.868333220
H	5.168230057	-3.020386219	1.223442316
H	4.284951687	-3.882065296	2.551036119
C	-0.196574256	1.086935759	1.707744837
O	-0.969559550	-0.569704056	3.379467249
C	-0.967193246	-2.004350185	3.364785194
H	0.645412564	2.184046984	0.065718040
H	-0.573291481	1.958077550	2.231980085
H	-0.545259297	-2.378149271	4.303900242
H	-1.991628051	-2.367799759	3.211062431
C	2.071763039	2.035415888	-2.082502604
C	3.312783718	2.639329195	-1.829603672
C	1.023966908	2.822984695	-2.594532013
C	3.495770454	4.003558159	-2.064491510
H	4.142826557	2.048459530	-1.457265973
C	1.208053231	4.187567234	-2.814825296
H	0.075165756	2.346861839	-2.835630655
C	2.444167614	4.782326698	-2.550283194
C	3.404082537	-0.494896293	-1.660681486
C	3.934786797	-1.238792300	-2.724710703
C	4.165365696	-0.318210304	-0.494989157
C	5.217535496	-1.781550527	-2.627557278
H	3.332942724	-1.414326787	-3.613069534
C	5.449664116	-0.853895903	-0.406861544
H	3.745872974	0.229052052	0.344157338
C	5.976755142	-1.588398695	-1.472666144
C	-1.992355943	-2.237277985	-0.947427690

C	-2.725461960	-1.044161797	-0.912726104
C	-2.254122734	-3.242056608	-0.002989435
C	-3.716689348	-0.862640858	0.053506915
H	-2.494816065	-0.264626920	-1.636390090
C	-3.256957054	-3.063371658	0.948290646
H	-1.671253681	-4.158576965	-0.014245789
C	-3.988194704	-1.871579528	0.979225874
C	-1.382519245	-3.780777216	-3.321014166
C	-0.620349526	-4.140778065	-4.446147442
C	-2.606537104	-4.426116467	-3.094018459
C	-1.052679777	-5.153661251	-5.301304340
H	0.306937695	-3.619140625	-4.658478737
C	-3.047441959	-5.422521591	-3.967018366
H	-3.220271349	-4.154177189	-2.242185831
C	-2.269305468	-5.796710014	-5.063194752
C	2.101536036	-6.758780003	-7.099951267
C	1.504150271	-5.896461487	-8.022441864
C	2.767055273	-6.193107128	-6.007029533
H	0.984886289	-6.316540241	-8.881795883
H	3.248723507	-6.847122192	-5.282163620
C	1.544389009	-4.503838062	-7.876345158
C	2.826280594	-4.810857773	-5.812731266
C	2.203498125	-3.962925196	-6.751795292
C	2.160207510	-2.455970764	-6.562172413
O	2.451124907	-1.662587166	-7.442256927
O	1.691593409	-2.140103102	-5.358399391
C	-0.574750781	0.929017305	-8.207568169
C	0.210031658	0.633191109	-7.100578308
C	-0.108909063	-0.474537939	-6.295467377
C	-1.161102891	-1.326349258	-6.574627876
C	-1.930295706	-1.040084243	-7.712556362
C	-1.644240856	0.071386315	-8.511822701
C	1.376616716	1.275169134	-6.486796856
C	1.698429346	0.531591296	-5.395359039
N	0.782143891	-0.520974219	-5.175951958
H	-0.367500216	1.798419476	-8.825408936
H	-1.374334335	-2.177141905	-5.937895298
H	-2.763315916	-1.688043356	-7.969317913
H	-2.262453318	0.276973754	-9.381436348
H	2.494410992	0.672099710	-4.682795525
H	-0.437928855	-5.428412914	-6.152261257
H	-2.612908602	-6.580333710	-5.733618259
H	-4.000961781	-5.911153793	-3.782894611
H	-3.466681957	-3.851802588	1.666975260
H	-4.765086174	-1.730285406	1.726318479
H	-4.275749207	0.068708912	0.082540318
H	0.389166057	4.782313347	-3.210497379
H	2.590800047	5.843252182	-2.734284878
H	4.464217663	4.456589699	-1.868008137
H	6.038191319	-0.700501859	0.494428366
H	6.975263119	-2.011558294	-1.401319623
H	5.621990204	-2.363695145	-3.449985266
C	2.049721241	-8.257410049	-7.279732227
H	1.805651069	-8.762331963	-6.338404655
H	1.301049590	-8.547648430	-8.023017883
H	3.018135071	-8.649726868	-7.614533424
C	0.865811765	-3.627064228	-8.903939247
H	1.586148858	-2.957256317	-9.379483223
H	0.380435795	-4.236537933	-9.671834946
H	0.106754273	-2.984297752	-8.445414543
C	3.557438135	-4.254104614	-4.613725185
H	2.865010738	-3.866958380	-3.862059355
H	4.177245617	-5.020888805	-4.138847828
H	4.208196640	-3.424429893	-4.906002522
H	-1.269517303	0.657747865	-3.312683821
C	2.030089140	2.533618450	-6.952515125
H	1.284359813	3.337501049	-7.023769855
H	2.416259289	2.387603521	-7.971215248
C	3.165434122	2.991743088	-6.043222427
H	2.793555021	3.138176203	-5.016450882
H	3.951073885	2.216985941	-6.003457546
O	3.683776855	4.201214314	-6.565896988
C	4.768377781	4.694651127	-5.806925297
H	4.482341766	4.887855530	-4.760991096
H	5.619146347	3.992562532	-5.802538872
H	5.089920521	5.632548332	-6.268558025

==============================

XI$_S$

==============================

Cu	0.241930068	-0.489052534	-3.220114231
P	-0.476752073	-2.412495375	-2.180478096
C	0.868113875	-3.157541752	-1.206080914
C	1.299063444	-2.503947973	-0.008759812
C	1.530725718	-4.303534985	-1.672151327
C	2.366341829	-3.090058565	0.641397476
C	0.657724202	-1.298001647	0.592094183
C	2.621029139	-4.865494251	-0.989899397
H	1.191848397	-4.784822464	-2.581700325
C	3.023474932	-4.229684353	0.167069197
O	2.954586506	-2.671232700	1.800738573
C	-0.127610177	-1.442071915	1.719385266
C	0.825749636	0.038434029	0.117267102
H	3.120950460	-5.756825924	-1.350343943
O	4.034483910	-4.564761162	1.010042429
C	4.079188824	-3.538503885	2.017658710
C	-0.757538378	-0.367213070	2.350918055
O	-0.429631650	-2.603521585	2.372134924
C	0.199433818	1.109513283	0.763071299
P	1.661500096	0.294221193	-1.484304190
H	5.007088184	-2.966121197	1.905851126
H	4.002654552	-3.997422218	3.007823229
C	-0.608304858	0.926407397	1.899404764
O	-1.473244190	-0.817093849	3.420728683
C	-1.371510386	-2.249629259	3.400087595
H	0.334524304	2.115188837	0.380591601
H	-1.090340376	1.759362221	2.397665977
H	-1.005566001	-2.605451584	4.367835045
H	-2.350324631	-2.679503202	3.154707432
C	1.905967355	2.091177225	-1.679080486
C	3.074071169	2.753261328	-1.275314331
C	0.888129830	2.812931538	-2.325809717
C	3.215008020	4.121337414	-1.511114478
H	3.878524065	2.203069687	-0.797802389
C	1.028450012	4.181003094	-2.548264503
H	-0.003684388	2.296764612	-2.675542593
C	2.194795847	4.835556030	-2.143438101
C	3.302049875	-0.486642927	-1.389519215
C	3.756709576	-1.184911489	-2.518167257
C	4.105410576	-0.417601764	-0.240856782
C	5.006182671	-1.805715203	-2.498718739
H	3.124264956	-1.245351791	-3.400734663
C	5.358211040	-1.031058788	-0.232953474
H	3.741095781	0.087440357	0.649142087
C	5.809453964	-1.727672815	-1.358690500
C	-1.901133180	-2.219993114	-1.080065489
C	-2.631001949	-1.023592949	-1.097299337
C	-2.275573730	-3.262327433	-0.215515614
C	-3.732573271	-0.869536102	-0.256354839
H	-2.326662779	-0.221580967	-1.764654756
C	-3.390616655	-3.108179808	0.606849730
H	-1.696724176	-4.180905819	-0.183503956
C	-4.113454342	-1.910900712	0.592926145
C	-0.904088318	-3.587487698	-3.501709223
C	-0.034937240	-3.675020456	-4.603575230
C	-2.090857029	-4.333933830	-3.489116907
C	-0.335215956	-4.527884483	-5.664113522
H	0.860023081	-3.057608366	-4.640823364
C	-2.389849663	-5.176108360	-4.561357975
H	-2.780204296	-4.260435104	-2.654351473
C	-1.514629245	-5.277218342	-5.644334793
C	1.101406693	0.587931812	-8.418428421
C	1.368103504	0.657594740	-7.047630787
C	0.598046005	-0.106060825	-6.132429600
C	-0.455509454	-0.902717113	-6.566689014
C	-0.710222781	-0.967492819	-7.941269398
C	0.054791573	-0.228956223	-8.855780602
C	2.349344969	1.370286822	-6.261435986
C	2.126462936	0.991479218	-4.946297646
N	1.122127533	0.061271451	-4.833450794

H	1.702510834	1.146517158	-9.130858421
H	-1.075521231	-1.435078382	-5.851736546
H	-1.524315238	-1.589967489	-8.301570892
H	-0.170519188	-0.293045133	-9.916314125
H	2.680838108	1.300192595	-4.074069977
H	0.337961346	-4.586975574	-6.514110088
H	-1.755416393	-5.932656765	-6.476478100
H	-3.310790300	-5.752280712	-4.549310684
H	-3.694014549	-3.921345949	1.260680199
H	-4.975420952	-1.791167498	1.243355989
H	-4.291883469	0.061265320	-0.263202846
H	0.238903299	4.730220795	-3.052407742
H	2.311926842	5.899178505	-2.329087257
H	4.124722481	4.628638268	-1.203175187
H	5.985499859	-0.962420404	0.651756585
H	6.782200336	-2.210259199	-1.345180035
H	5.350540638	-2.351600170	-3.372278214
H	-1.147376299	-0.615957856	-3.812054873
C	3.414327145	2.281538963	-6.777609348
H	2.957586050	3.076268435	-7.384099483
H	4.081455231	1.737555623	-7.462336063
C	4.254206657	2.922981262	-5.676959038
H	3.605121613	3.484097481	-4.979503155
H	4.763567448	2.140395164	-5.084841728
O	5.195371628	3.777457237	-6.289127827
C	6.046614647	4.415712357	-5.357120037
H	5.479823112	5.038146496	-4.643285275
H	6.641844749	3.687504530	-4.781066895
H	6.727282524	5.057299614	-5.922958374

==============================

I_P-TS

==============================

P	1.222771645	-0.540600896	-0.740547717
C	1.053233504	1.239948273	-1.293736339
C	0.158122003	2.091896534	-0.371675193
P	-1.390880585	1.229849815	0.234487742
C	-2.706310987	1.535727620	-1.097148180
C	-2.104445457	2.561508179	1.385308027
C	-3.395539522	2.853525877	-0.705524743
C	-3.519918680	2.838644981	0.822232425
C	2.050769567	-1.339672685	-2.253246784
C	2.827715635	-0.552580297	0.264376253
C	3.491487980	-1.702295899	-1.793405652
C	3.951662302	-0.648905158	-0.778245151
C	-2.048391581	2.241674423	2.856509686
C	-1.273250222	3.020740509	3.723533392
C	-2.774873972	1.167217970	3.390576124
C	-1.225255013	2.738972664	5.090749264
C	-2.728251457	0.882250547	4.753292561
C	-1.952786207	1.667835951	5.610350609
C	-2.138238907	1.397909999	-2.487046480
C	-1.825104594	0.110305831	-2.956182241
C	-1.841030002	2.493644714	-3.306895971
C	-1.240095615	-0.076388270	-4.206242085
C	-1.247057557	2.309566259	-4.558936133
C	-0.943865716	1.026000500	-5.013525486
C	2.850881100	0.562855363	1.280086637
C	3.631531715	1.714957237	1.128773689
C	1.989874125	0.474826127	2.388569117
C	3.549584866	2.756594181	2.058044434
C	1.900379062	1.515978694	3.308845997
C	2.681491613	2.664098024	3.145823002
C	1.302433014	-2.516947031	-2.838020802
C	1.167080522	-2.653011799	-4.225819111
C	0.766300321	-3.520039082	-2.016066313
C	0.503304541	-3.750848770	-4.779802322
C	0.101385526	-4.617320061	-2.563820124
C	-0.036230616	-4.736518383	-3.950143814
H	0.619566858	1.196874738	-2.296534777
H	2.043397903	1.702334166	-1.378546119
H	0.705247819	2.355190754	0.540478289
H	-0.114182882	3.024872780	-0.879546523
H	-3.418652058	0.719805837	-0.934289992
H	-1.494736552	3.455134869	1.199695110
H	-4.367056370	2.950243950	-1.202313542
H	-2.789383411	3.717961073	-1.004818916
H	-4.210183620	2.042560577	1.125580430
H	-3.909358740	3.781338930	1.222721219
H	2.116788864	-0.550904691	-3.012453794
H	2.780830622	-1.507920742	0.803351521
H	4.161172390	-1.778967977	-2.657310963
H	3.474130630	-2.689482212	-1.314801931
H	4.091515541	0.313130558	-1.287853837
H	4.910354614	-0.910732627	-0.314478904
H	-0.695704579	3.851306915	3.323674440
H	-3.369513512	0.547681153	2.728063583
H	-0.619569898	3.357555389	5.748306751
H	-3.296819210	0.043788522	5.147286415
H	-1.916530132	1.445666194	6.673331738
H	-2.017372847	-0.741086185	-2.312910557
H	-2.073303699	3.501485586	-2.977208853
H	-1.004689932	-1.081768155	-4.541137695
H	-1.024076700	3.174213648	-5.179068089
H	-0.484606147	0.884721339	-5.988521576
H	4.312779903	1.806782007	0.288252026
H	1.351173997	-0.399306476	2.494560242
H	4.167142391	3.641409397	1.926993847
H	1.207080960	1.437710762	4.140769005
H	2.614250898	3.477548361	3.863421679
H	1.577521801	-1.885185838	-4.879070759
H	0.846007109	-3.425701380	-0.935522020
H	0.405485809	-3.832110643	-5.859902859
H	-0.320572913	-5.373323441	-1.906223536
H	-0.560092688	-5.586814880	-4.378134251
C	-3.480885744	-1.969285965	-0.145344600
C	-4.066153526	-1.434530020	1.029622078
H	-3.521782160	-1.502457857	1.966475725
C	-5.302985668	-0.796439826	1.000693679
H	-5.714844227	-0.392380565	1.923415184
C	-6.014393806	-0.665360451	-0.197571173
H	-6.976656437	-0.162097335	-0.218858838
H	-6.004151344	-1.125352502	-2.306037188
C	-5.465462208	-1.206374288	-1.364644051
C	-4.230127335	-1.847913980	-1.339953065
H	-3.823094606	-2.262901068	-2.259164095
C	-2.170281649	-2.594309568	-0.149969518
H	-1.771643043	-2.919483662	-1.105870008
C	-1.471471071	-2.968683720	1.028963447
H	-0.667089939	-3.690280199	0.924510121
H	-2.027236462	-3.079677343	1.954628706
H	-0.478367388	-1.880258679	1.845705032
Cu	-0.729433119	-0.968923450	0.518255353

==============================

I_P-TS'

==============================

P	1.185198307	-0.424962431	-1.073373079
C	0.797197998	1.354812980	-1.501539111
C	-0.011506124	2.127758026	-0.443621457
P	-1.348679066	1.113659859	0.378967226
C	-2.874931812	1.382080555	-0.708233416
C	-1.971038938	2.317908287	1.713612795
C	-3.439408302	2.742224216	-0.270489722
C	-3.395370483	2.746739626	1.262891293
C	2.057437897	-0.953243673	-2.669571400
C	2.813677549	-0.411183745	-0.085570447
C	3.390743256	-1.569081545	-2.186358929
C	3.941950798	-0.625474155	-1.110392451
C	-1.906977534	1.740195155	3.108465672
C	-1.117212296	2.335568428	4.097929478
C	-2.628216267	0.582587302	3.440536976
C	-1.040422678	1.788556695	5.381986618
C	-2.555493116	0.033388302	4.719076633
C	-1.756801128	0.633587122	5.696874142
C	-2.569633722	1.140166640	-2.166305780
C	-2.436283350	2.178920269	-3.095220327
C	-2.328611851	-0.178238794	-2.593232870
C	-2.060921431	1.908249855	-4.415023327
C	-1.948219419	-0.448264748	-3.905252934
C	-1.808779836	0.598017216	-4.821413517

C	2.896914959	0.766041815	0.855652273
C	3.528342009	1.970542908	0.516128302
C	2.233256340	0.686680198	2.092017651
C	3.494009256	3.065114260	1.383844614
C	2.195909739	1.778553724	2.957197428
C	2.825294018	2.975674868	2.605432034
C	1.278558969	-1.811206937	-3.632595539
C	1.274266601	-1.479118943	-4.994022846
C	0.587581575	-2.957089186	-3.217345953
C	0.604687572	-2.273246050	-5.924841881
C	-0.081343882	-3.754667997	-4.145567894
C	-0.074094154	-3.416410923	-5.500983715
H	0.228911564	1.289191842	-2.435580015
H	1.729727149	1.888906360	-1.717090130
H	0.648554742	2.439697742	0.372550100
H	-0.437949091	3.033641815	-0.890920222
H	-3.568656921	0.601047456	-0.367943794
H	-1.311116099	3.191509008	1.659184694
H	-4.453370094	2.901357412	-0.655556917
H	-2.817382336	3.559513330	-0.656152189
H	-4.131196022	2.030953169	1.648762941
H	-3.652612686	3.723258734	1.687626004
H	2.305040121	-0.010585520	-3.175612926
H	2.719893217	-1.321566224	0.516355693
H	4.079201698	-1.694019556	-3.029578447
H	3.207729340	-2.567709684	-1.768316984
H	4.224077702	0.321851969	-1.586194754
H	4.841596127	-1.019976020	-0.624512136
H	-0.547969699	3.230316401	3.857574940
H	-3.240766764	0.095811605	2.684997320
H	-0.419836581	2.266689301	6.135437965
H	-3.117152691	-0.867499530	4.951292992
H	-1.695456743	0.204589099	6.692958355
H	-2.626056194	3.205849648	-2.797912121
H	-2.402847052	-0.994014084	-1.879930377
H	-1.964105844	2.727521420	-5.123010159
H	-1.743741512	-1.470937610	-4.205173969
H	-1.501784921	0.387001842	-5.841746330
H	4.051259041	2.066295862	-0.430757344
H	1.704455853	-0.228597045	2.345504999
H	3.991312027	3.989436150	1.101249814
H	1.663235307	1.692667365	3.899496794
H	2.799335957	3.828587770	3.278611422
H	1.798385978	-0.585417628	-5.325845718
H	0.539635718	-3.217499495	-2.163173914
H	0.610260904	-1.996281147	-6.976006508
H	-0.626890123	-4.624724865	-3.798914194
H	-0.603116751	-4.036370754	-6.219809532
C	-2.200840473	-3.588407993	-0.438658327
C	-3.215201855	-3.682168484	-1.420359135
H	-3.981102705	-2.909818172	-1.456179500
C	-3.274751186	-4.749666214	-2.310224056
H	-4.079711437	-4.790281296	-3.040550232
C	-2.320292473	-5.771991253	-2.265838861
H	-2.374868393	-6.613821507	-2.950197697
H	-0.521183372	-6.451894283	-1.286501646
C	-1.286783576	-5.679893970	-1.326351404
C	-1.217442274	-4.608014584	-0.440194398
H	-0.396222115	-4.559708118	0.270025551
C	-2.229661703	-2.516191483	0.544026315
C	-1.450174332	-2.508802652	1.730852962
H	-0.948181391	-3.423552513	2.026642561
H	-1.796957970	-1.914601207	2.569258451
H	0.075009070	-1.756407976	1.780537009
Cu	-0.475045919	-1.092005014	0.391974896
H	-3.059563160	-1.815868735	0.477184892

==============================

II$_P$

==============================

P	0.957749784	-0.444071054	-1.065972209
C	0.807801366	1.381166220	-1.444361448
C	0.053313896	2.181992531	-0.361726642
P	-1.330806494	1.243005514	0.485353798
C	-2.888874769	1.439738512	-0.582453132
C	-1.911854506	2.520431995	1.755862117
C	-3.606600761	2.691668987	-0.047993042
C	-3.429316282	2.669395924	1.475649595
C	1.654500484	-1.131092310	-2.680214882
C	2.588938713	-0.662787914	-0.141406313
C	3.072501898	-1.660614967	-2.320504904
C	3.662221909	-0.743506908	-1.237468243
C	-1.567596674	2.181079388	3.184930086
C	-0.938568890	3.115675449	4.014574528
C	-1.887233138	0.921800673	3.712377310
C	-0.635753453	2.803249598	5.342014313
C	-1.584511280	0.605036080	5.034735680
C	-0.956008494	1.545990348	5.856313229
C	-2.572420835	1.337898612	-2.053580046
C	-2.413803101	0.058880728	-2.612802267
C	-2.332311630	2.453187466	-2.866076469
C	-2.013480425	-0.105276451	-3.936786175
C	-1.932057261	2.292665720	-4.195753098
C	-1.764451265	1.015829325	-4.733891964
C	2.706968069	0.333054811	0.984419703
C	3.512263060	1.474304318	0.914833426
C	1.889072537	0.155931935	2.114932537
C	3.488056660	2.422492743	1.943243146
C	1.850139499	1.105361223	3.131311178
C	2.652062893	2.247284174	3.045816183
C	0.772841930	-2.148350239	-3.375211239
C	0.749440849	-2.194760084	-4.775227547
C	-0.017353158	-3.063182354	-2.662206650
C	-0.049318045	-3.118698835	-5.450636864
C	-0.821727276	-3.983140707	-3.335339308
C	-0.843719542	-4.013187408	-4.731555939
H	0.252480447	1.420314431	-2.388086796
H	1.796507955	1.821602345	-1.621208429
H	0.737406492	2.438714266	0.456225783
H	-0.323254675	3.118840218	-0.788530529
H	-3.488070726	0.565451801	-0.299930096
H	-1.424553633	3.466641903	1.487233162
H	-4.661882401	2.691176176	-0.343291163
H	-3.155660629	3.607796192	-0.449389398
H	-3.966052771	1.810517788	1.897929788
H	-3.819672346	3.571055889	1.960698366
H	1.774621010	-0.267690927	-3.346472502
H	2.486370564	-1.663622379	0.298479795
H	3.699627161	-1.713416457	-3.217187643
H	2.984271765	-2.682841301	-1.930945635
H	3.859466314	0.248999327	-1.663172245
H	4.612651348	-1.123850703	-0.844847023
H	-0.676268697	4.093328953	3.616654634
H	-2.362488747	0.184397414	3.074281216
H	-0.144841939	3.540429592	5.971778870
H	-1.833017588	-0.380107999	5.420623302
H	-0.716620922	1.299245834	6.886925697
H	-2.600014448	-0.811341882	-1.991603613
H	-2.451467991	3.455757618	-2.466279268
H	-1.885958672	-1.105477095	-4.339748859
H	-1.748574853	3.170561075	-4.810101509
H	-1.447573185	0.893711984	-5.766164780
H	4.161439419	1.631759882	0.058474962
H	1.251762748	-0.724992812	2.177683592
H	4.123006344	3.302130938	1.875413299
H	1.186270952	0.963388383	3.978158236
H	2.620508432	2.992174625	3.835713863
H	1.351897478	-1.487812161	-5.341830254
H	-0.043089125	-3.027611971	-1.575704336
H	-0.059207018	-3.131318092	-6.537333965
H	-1.441016912	-4.669454098	-2.764029741
H	-1.477103710	-4.724420071	-5.254190445
C	-2.997658253	-2.332071304	1.038985729
C	-3.814597845	-1.752279401	2.039236784
H	-3.444647551	-1.691103458	3.057723045
C	-5.085985184	-1.253976583	1.750494719
H	-5.672762871	-0.801823616	2.548129797
C	-5.617931366	-1.343297124	0.462490171
H	-6.606936932	-0.952976048	0.240243703
H	-5.259641647	-2.082923651	-1.536088705

C -4.858283997 -1.976772308 -0.530347705
C -3.587952614 -2.464715242 -0.246026590
H -3.001152515 -2.935017824 -1.034262538
C -1.585732460 -2.709761858 1.254838347
H -1.335234165 -3.587879896 0.645935357
C -1.142637134 -2.919151783 2.703301668
H -0.112352684 -3.292201281 2.733087301
H -1.771589756 -3.643414736 3.250778437
H -1.152652502 -1.986602664 3.281607151
Cu -0.732225180 -1.081050515 0.402343661

==============================

II$_{P}$-TS

==============================

P 1.103844881 -0.551119626 -0.920286000
C 0.809843063 1.219982028 -1.427813292
C -0.042985912 2.021294832 -0.426197857
P -1.436579943 1.070538402 0.389230192
C -2.923747778 1.265219092 -0.793227673
C -2.081053019 2.421049595 1.564320087
C -3.701992750 2.500977278 -0.298148483
C -3.585206509 2.552879572 1.229121566
C 1.966903925 -1.246724010 -2.453480721
C 2.712773323 -0.519997120 0.096307859
C 3.272084475 -1.871762395 -1.901189208
C 3.844395638 -0.867777467 -0.892219961
C -1.775415421 2.245911360 3.031635046
C -1.077181458 3.240730047 3.729698658
C -2.218675852 1.119990349 3.740315676
C -0.842819810 3.125680685 5.101836205
C -1.995634794 1.005900860 5.110944271
C -1.307014346 2.009107828 5.799085617
C -2.556046724 1.222086906 -2.263668060
C -2.029842854 0.030895060 -2.798766136
C -2.713938475 2.317924738 -3.123740196
C -1.682219148 -0.064092368 -4.143897057
C -2.364959240 2.226351976 -4.476495266
C -1.848438859 1.038505197 -4.991942406
C 2.846816063 0.737754703 0.926152349
C 3.606067181 1.844861031 0.523541689
C 2.117446899 0.831998229 2.123823881
C 3.632039785 3.011754990 1.293375611
C 2.143864393 1.992070079 2.894173861
C 2.899929047 3.091848373 2.478908062
C 1.143712878 -2.176046848 -3.316731691
C 1.283728838 -2.132966757 -4.711312771
C 0.257721514 -3.112054110 -2.763527393
C 0.554240882 -2.992397785 -5.534509659
C -0.473578513 -3.972278595 -3.583366394
C -0.331860989 -3.913563013 -4.972582340
H 0.296441317 1.157246351 -2.391498804
H 1.767968655 1.727137327 -1.587427855
H 0.583525419 2.365190506 0.404229045
H -0.459484547 2.907772541 -0.919663966
H -3.522154808 0.370229214 -0.601464093
H -1.596987247 3.345136404 1.222277403
H -4.743401051 2.468720198 -0.640839040
H -3.258834839 3.419027090 -0.703030765
H -4.148931980 1.736649632 1.695132971
H -3.984894514 3.485689640 1.644395471
H 2.252301931 -0.375850588 -3.058762789
H 2.589146614 -1.359082580 0.786860049
H 3.968760014 -2.089758158 -2.719130754
H 3.044353485 -2.826025724 -1.409055829
H 4.172829628 0.025173588 -1.437962174
H 4.719375610 -1.258625150 -0.359771401
H -0.714239776 4.114939213 3.192972660
H -2.733885527 0.321265042 3.217936754
H -0.300977319 3.910542488 5.624849319
H -2.350431919 0.123590738 5.638038158
H -1.130487323 1.919523716 6.867793083
H -1.894319773 -0.826234579 -2.148354530
H -3.133660316 3.249888182 -2.756586790
H -1.275476933 -0.996277988 -4.526420593
H -2.504780531 3.089745760 -5.125729084
H -1.580652714 0.968355417 -6.043954849
H 4.187530041 1.808219790 -0.393355250
H 1.515194654 -0.006572132 2.450727940
H 4.228230000 3.858749390 0.962007165
H 1.564138889 2.032103777 3.811467409
H 2.921802759 4.000557423 3.075691223
H 1.964617372 -1.410146713 -5.156672478
H 0.129812583 -3.147850752 -1.686486006
H 0.672047615 -2.936327219 -6.614191055
H -1.160575151 -4.690412521 -3.141945839
H -0.909337580 -4.578061581 -5.609445572
C 0.753543079 -2.408727169 2.840760708
C 2.146303177 -2.594014168 3.002772093
H 2.700435400 -3.179189444 2.274913549
C 2.832738638 -2.046602249 4.088023663
H 3.906316996 -2.200195313 4.173219681
C 2.156422853 -1.309037566 5.059016705
H 2.693520546 -0.875876725 5.898421288
H 0.229018360 -0.549322963 5.671254635
C 0.772233307 -1.130192876 4.931353092
C 0.088761158 -1.666986346 3.848188400
H -0.979594946 -1.497192264 3.737814665
C -0.007685808 -2.943797112 1.700469732
H -0.971015513 -3.329029560 2.044076920
C 0.723395288 -3.975155830 0.851468265
H 0.041798435 -4.449967861 0.143111631
H 1.171106935 -4.778558254 1.460203767
H 1.542493582 -3.534133196 0.268390685
Cu -0.725167632 -1.326729536 0.540212214
C -5.952045918 -1.241797447 -4.915658951
C -6.991589546 -0.334590286 -4.672555923
H -5.634367466 -1.425751328 -5.941768169
C -5.299565315 -1.910453081 -3.873319387
C -7.384693146 -0.105420895 -3.346808434
C -5.725405693 -1.664438367 -2.555075884
H -8.188065529 0.603309453 -3.143388271
C -6.766928673 -0.758019388 -2.275930405
C -5.021512985 -2.328967810 -1.394168854
O -5.493176460 -3.195450544 -0.684071779
O -3.826641083 -1.753080964 -1.280867815
N -2.717458725 -2.301947832 0.012011468
C -4.117750168 -3.845529318 2.989281416
C -3.494663954 -3.614560366 1.764106512
C -4.747206688 -2.772894144 3.632272482
H -4.127864361 -4.838599205 3.429824829
C -3.462435484 -2.308507442 1.233429909
C -2.836949348 -4.464625359 0.784260690
C -4.763268948 -1.494652152 3.058280468
H -5.245748043 -2.937548876 4.583748817
C -4.115066051 -1.250036955 1.842341542
C -2.445827484 -3.670674324 -0.243339583
H -2.677375555 -5.531202316 0.869289160
H -5.278491497 -0.681523502 3.562234640
H -4.138068676 -0.274289340 1.376296520
H -1.952995777 -3.920182943 -1.168293118
C -4.160928249 -2.868594885 -4.151439190
H -4.058751106 -3.061385870 -5.225138664
H -3.210872173 -2.465501070 -3.783887148
H -4.322182178 -3.829214811 -3.645645142
C -7.178904533 -0.484284014 -0.845524848
H -7.406509876 -1.415145993 -0.317220092
H -6.362290859 -0.004453958 -0.288797110
H -8.051867485 0.174826816 -0.799524844
C -7.697853088 0.366419196 -5.812599182
H -7.980410576 1.389838934 -5.539261818
H -7.068243027 0.414823234 -6.708278179
H -8.621408463 -0.160439417 -6.088278770

==============================

III$_{PN}$

==============================

P 0.983174503 0.066894881 -1.010012031
C 0.796702564 1.870543957 -1.427083135
C 0.057451498 2.712017298 -0.376180440
P -1.407168865 1.848778248 0.381542176

C	-2.942531347	2.131369591	-0.685792148
C	-1.966758013	3.101046562	1.695140839
C	-3.558436394	3.452449560	-0.179618344
C	-3.444499493	3.407343864	1.346781850
C	1.831754923	-0.615839958	-2.575275421
C	2.528407335	-0.128276095	0.047822814
C	3.229708195	-1.080096126	-2.097345114
C	3.683355093	-0.146798790	-0.967311919
C	-1.730788589	2.747601748	3.144205332
C	-1.014335513	3.626102924	3.966959953
C	-2.262780666	1.578885198	3.705388784
C	-0.829896033	3.346224546	5.321990490
C	-2.070731401	1.291613579	5.056194305
C	-1.354361057	2.173901796	5.869708538
C	-2.752843618	1.952340961	-2.168465614
C	-3.145376205	0.745662093	-2.768989086
C	-2.201108932	2.953434706	-2.982048273
C	-3.000976801	0.545509398	-4.141016960
C	-2.047277212	2.751448393	-4.354629993
C	-2.449035168	1.547451973	-4.940495968
C	2.545610428	0.828242183	1.213089824
C	3.328146458	1.985978842	1.236718178
C	1.669756532	0.582424998	2.282671213
C	3.234302282	2.875015497	2.313141823
C	1.557029963	1.473163366	3.344624996
C	2.347136259	2.626647234	3.360104084
C	1.028935671	-1.589053512	-3.412684441
C	0.121591695	-1.085995436	-4.357687950
C	1.158368945	-2.980101347	-3.289020777
C	-0.626310289	-1.946740508	-5.161497116
C	0.404468507	-3.842751026	-4.087179661
C	-0.486453086	-3.330452681	-5.030911446
H	0.239048988	1.881260514	-2.371137381
H	1.792903066	2.282433987	-1.626901984
H	0.719175160	2.918834925	0.472661763
H	-0.229854420	3.676869154	-0.808552444
H	-3.597450018	1.329136610	-0.333772331
H	-1.386160374	4.000965595	1.452283740
H	-4.596349239	3.540634871	-0.517721474
H	-3.012667418	4.318464279	-0.574052572
H	-4.090929031	2.618939638	1.751088619
H	-3.745272875	4.346571445	1.822157860
H	1.978106380	0.291774362	-3.174139261
H	2.430729866	-1.148236275	0.445195764
H	3.925558090	-1.087639451	-2.942005873
H	3.184843063	-2.104842424	-1.711221457
H	3.874753952	0.858987451	-1.361110926
H	4.609283924	-0.490481406	-0.494608104
H	-0.600805998	4.539612293	3.545598030
H	-2.820428848	0.883353353	3.087123156
H	-0.279095203	4.042835236	5.948194981
H	-2.477504492	0.372042686	5.465214252
H	-1.210878849	1.952316165	6.923528194
H	-3.579354525	-0.043428641	-2.160033941
H	-1.906979322	3.904922247	-2.547215462
H	-3.327337265	-0.391555697	-4.583248138
H	-1.626769543	3.541440248	-4.970646381
H	-2.345854044	1.400788665	-6.011744976
H	4.020982265	2.198601723	0.428044438
H	1.063660502	-0.319899887	2.270899296
H	3.857800484	3.764499426	2.328013659
H	0.848644733	1.282132030	4.144810677
H	2.264349461	3.325039387	4.186709881
H	-0.005855107	-0.011652543	-4.467798710
H	1.860600710	-3.406928778	-2.579006195
H	-1.313143969	-1.533849478	-5.894520760
H	0.520287037	-4.916980743	-3.974545240
H	-1.067597747	-4.002424240	-5.655584335
C	-1.929189324	-3.131617785	-0.611185551
C	-2.804902554	-3.861186028	0.228495002
H	-2.514121771	-4.090060234	1.247697353
C	-4.036954880	-4.289593220	-0.248682231
H	-4.695981026	-4.855799675	0.402039170
C	-4.439720631	-3.970047951	-1.550429463
H	-5.408039093	-4.301878452	-1.913738489
H	-3.917896986	-2.958341360	-3.388593674
C	-3.604119778	-3.208842278	-2.379120111
C	-2.361727238	-2.795335531	-1.919440866
H	-1.701517820	-2.225298643	-2.566555023
C	-0.586726725	-2.780105591	-0.217686504
H	0.043876518	-2.560605526	-1.071730375
C	0.143957868	-3.453031301	0.907142997
H	1.048852563	-2.900303841	1.177736402
H	0.462549865	-4.448133945	0.563187718
H	-0.461083740	-3.577256441	1.804071426
Cu	-0.828988433	-0.617154062	0.313834548
C	-4.973044395	-2.051231384	3.361621380
C	-3.605219841	-1.871226788	3.110443592
C	-5.895650387	-1.712918162	2.372203588
H	-5.310966015	-2.440732241	4.318548679
C	-3.194648981	-1.305702925	1.864266157
C	-2.397339344	-2.090475798	3.860192060
C	-5.476555824	-1.196351290	1.130074143
H	-6.956729412	-1.849614859	2.560549974
C	-4.126187801	-0.987141073	0.867366493
N	-1.830148339	-1.143007159	1.863090158
C	-1.364318252	-1.650536895	3.061923265
H	-2.313004255	-2.471157789	4.869081497
H	-3.788527012	-0.641086519	-0.103392601
H	-6.215812683	-0.963352859	0.369031787
H	-0.309218973	-1.623524904	3.296107769

===============================

III$_{PN}$-TS

===============================

P	3.197735071	-0.068751089	-3.134894371
C	3.017554045	1.778029561	-3.363404036
C	2.520188570	2.541461706	-2.127539158
P	0.949032307	1.897422552	-1.338191271
C	-0.472845376	2.838901758	-2.171835184
C	0.915458977	3.076995134	0.174447462
C	-0.374555230	4.276543140	-1.618167877
C	-0.188990951	4.137374401	-0.105527721
C	3.753736496	-0.528429508	-4.875885010
C	4.928739548	-0.339640945	-2.396540880
C	5.231670380	-0.042376943	-4.910815716
C	5.925018787	-0.440993488	-3.593369961
C	0.791501582	2.407772064	1.523298502
C	1.881600261	2.392015219	2.403725863
C	-0.409240603	1.806075335	1.935132027
C	1.781094432	1.787572026	3.659316778
C	-0.515484035	1.205541492	3.190844774
C	0.581581771	1.194351673	4.058586597
C	-0.627148271	2.713750124	-3.667953968
C	0.230479449	3.378229141	-4.561635494
C	-1.678862929	1.952609777	-4.202763081
C	0.064537838	3.252747059	-5.942287922
C	-1.853877783	1.830017209	-5.584083080
C	-0.975081086	2.472503901	-6.460197926
C	5.238903999	0.665966809	-1.310856938
C	5.882635593	1.884174347	-1.571018696
C	4.809682846	0.400957882	-0.001237109
C	6.085462093	2.814845085	-0.550248742
C	5.012584686	1.328628659	1.018879414
C	5.648784637	2.542539835	0.747958839
C	3.610143900	-1.986737132	-5.261575699
C	3.070668697	-2.303317070	-6.516522408
C	4.063865185	-3.040624380	-4.453058243
C	2.984829187	-3.625777245	-6.953559875
C	3.974921942	-4.364533424	-4.884073734
C	3.435253620	-4.664292336	-6.136290073
H	2.310526133	1.892867923	-4.191904545
H	3.970800638	2.209598541	-3.684058189
H	3.269348145	2.482522249	-1.332383633
H	2.409428596	3.604881525	-2.367702723
H	-1.359012246	2.380341768	-1.705964446
H	1.889748096	3.577941656	0.132186309
H	-1.275590420	4.846120834	-1.872033238
H	0.473682225	4.807621479	-2.068301916
H	-1.137203455	3.813546896	0.341567874

H	0.076267794	5.086528301	0.375084460
H	3.152173519	0.069841281	-5.568537235
H	4.843106270	-1.317154288	-1.910831571
H	5.247726917	1.046402454	-5.032804489
H	5.747873306	-0.464504600	-5.779380322
H	6.811876774	0.173649475	-3.419874430
H	6.280039787	-1.472676039	-3.667353630
H	2.818558216	2.851485729	2.098466635
H	-1.270935535	1.805702567	1.270320654
H	2.638803482	1.785922527	4.327514172
H	-1.454241395	0.748169363	3.494076014
H	0.499544472	0.728010714	5.036915779
H	1.027485013	4.011856079	-4.179701328
H	-2.380982637	1.461296558	-3.529736996
H	0.739901781	3.777044773	-6.614924908
H	-2.683856249	1.242942929	-5.973361969
H	-1.109830141	2.382169962	-7.535153866
H	6.227625847	2.115917921	-2.575146914
H	4.309054375	-0.536474228	0.218165591
H	6.590634823	3.751305103	-0.769749820
H	4.674236298	1.096157312	2.024231195
H	5.816242695	3.264086723	1.542579770
H	2.727311850	-1.501525402	-7.166528702
H	4.496489525	-2.841612577	-3.479261398
H	2.573871613	-3.843531132	-7.935592651
H	4.337574959	-5.162523746	-4.241412640
H	3.377527237	-5.694143772	-6.476298332
C	-0.117906235	-2.278073788	-2.063459873
C	-0.581720710	-1.255855918	-2.939964056
H	-1.040073514	-0.356552243	-2.544115305
C	-0.491208166	-1.424091101	-4.321103573
H	-0.843129992	-0.633203268	-4.974819660
C	0.058263026	-2.591902256	-4.852729321
H	0.143709987	-2.711723804	-5.927968979
H	0.944024444	-4.511980534	-4.430850029
C	0.507194221	-3.613497257	-4.007388115
C	0.420147121	-3.463522673	-2.631480694
H	0.765106618	-4.252065659	-1.971525431
C	-0.138974607	-2.148935080	-0.608791649
H	0.120183542	-3.057257175	-0.077558286
C	-1.113076210	-1.258456469	0.095276855
H	-0.831881166	-1.104002953	1.137684822
H	-2.089194298	-1.769181371	0.079910651
H	-1.230144382	-0.284760296	-0.386313647
Cu	1.477749228	-0.601887882	-1.585961342
C	3.841084957	-4.087189198	1.747828484
C	2.988051176	-3.008628368	1.485729575
C	4.321246147	-4.842971325	0.674764454
H	4.138567448	-4.324272156	2.766476870
C	2.651325703	-2.693127632	0.142193332
C	2.349766731	-2.000058174	2.302323580
C	3.143073797	-3.437213421	-0.931871712
N	1.857664824	-1.537335396	0.120356061
C	3.976083994	-4.523735523	-0.649760902
H	2.895674467	-3.164934874	-1.951511025
H	4.370973110	-5.122414589	-1.467489958
H	4.984252453	-5.682587147	0.865587771
C	1.693325520	-1.152326107	1.450749755
H	2.428666592	-1.887862325	3.376046419
H	1.143962145	-0.255300969	1.684127212

==============================

V$_{PN}$

==============================

P	1.049706697	0.186113015	-0.917251050
C	0.954391241	2.016636133	-1.283021331
C	0.260570347	2.855979443	-0.191208318
P	-1.341428161	2.150942802	0.476350993
C	-2.729095459	2.805993795	-0.627530873
C	-1.714028716	3.387452364	1.869042039
C	-2.972170830	4.243772507	-0.125043660
C	-2.976514339	4.168332577	1.403275013
C	1.712730408	-0.550248325	-2.528702736
C	2.659485340	-0.065011308	0.012715833
C	3.157903671	-1.000078201	-2.191699266
C	3.722846746	-0.075934954	-1.097292423
C	-1.850572824	2.803468227	3.255721569
C	-1.025793910	3.247446299	4.297104359
C	-2.841872692	1.853175998	3.542096615
C	-1.185577154	2.755650997	5.595186234
C	-3.008177280	1.365383029	4.837487698
C	-2.178968668	1.813132048	5.869916439
C	-2.539690256	2.614307642	-2.113496780
C	-3.151541948	1.523896575	-2.750464916
C	-1.777349353	3.496329069	-2.894356966
C	-3.004419088	1.317985773	-4.123268604
C	-1.613469124	3.280679941	-4.264539719
C	-2.222193241	2.187784195	-4.886310101
C	2.747959852	0.883385718	1.182442904
C	3.563183546	2.018889189	1.188764095
C	1.891942859	0.662071764	2.276382685
C	3.514932394	2.917663813	2.259941101
C	1.832925320	1.560282350	3.338382244
C	2.646998882	2.697514772	3.329697847
C	0.755848229	-1.581438780	-3.106794596
C	-0.534186244	-1.158839822	-3.474421263
C	1.079713702	-2.932517767	-3.272018671
C	-1.470969915	-2.057805777	-3.979175568
C	0.139206052	-3.838275433	-3.776278019
C	-1.139241099	-3.408643007	-4.130026340
H	0.395018756	2.092912674	-2.221432686
H	1.958870649	2.413753510	-1.469081402
H	0.911545157	2.934634686	0.685628474
H	0.092911728	3.874194860	-0.559088707
H	-3.586742640	2.194884777	-0.315285921
H	-0.859559178	4.075040340	1.858819604
H	-3.914453030	4.635934830	-0.523311734
H	-2.175189972	4.914889812	-0.467389047
H	-3.874819279	3.637277126	1.739603043
H	-2.996962309	5.156723022	1.874323368
H	1.765707374	0.295079172	-3.226794004
H	2.584011078	-1.087560415	0.407198399
H	3.780994415	-1.009051204	-3.091254234
H	3.146390676	-2.023283005	-1.798835516
H	3.881879568	0.933164716	-1.496840715
H	4.688830376	-0.432088941	-0.723641336
H	-0.254567325	3.987107038	4.091211796
H	-3.489389896	1.491080523	2.747841835
H	-0.541326702	3.117179394	6.392757416
H	-3.792359591	0.640380383	5.045233727
H	-2.311781168	1.436866760	6.880601883
H	-3.757946968	0.841525555	-2.161133528
H	-1.313419223	4.366524220	-2.439043045
H	-3.508316517	0.481347203	-4.600025177
H	-1.019589186	3.977784872	-4.849387646
H	-2.104375362	2.028197527	-5.953893661
H	4.242033005	2.208369255	0.362916231
H	1.255197287	-0.221803710	2.283570290
H	4.159809113	3.791831732	2.254686594
H	1.149758816	1.382576466	4.162990570
H	2.610577822	3.400178432	4.157214165
H	-0.810237586	-0.112090491	-3.373618126
H	2.070610285	-3.295722485	-3.020270348
H	-2.456800222	-1.700538754	-4.263504505
H	0.414438874	-4.882032394	-3.897168636
H	-1.862793922	-4.111664295	-4.532039165
C	-2.198016882	-4.321193695	-0.026530253
C	-2.444849014	-5.002139568	1.173114657
H	-1.938866854	-4.700400352	2.085428238
C	-3.357039928	-6.056283474	1.215469360
H	-3.543682337	-6.568872452	2.154839039
C	-4.030399323	-6.452294827	0.057074677
H	-4.741406918	-7.272386551	0.091630638
H	-4.301168919	-6.084605217	-2.049878597
C	-3.782699585	-5.785630226	-1.143155575
C	-2.875644922	-4.725121021	-1.181476593
H	-2.690132856	-4.205237865	-2.115826130
C	-1.246194839	-3.137590408	-0.079453513
H	-1.244749665	-2.721012592	-1.090152860
C	0.194584027	-3.503483534	0.275637358

H	0.817704082	-2.605906010	0.340698093
H	0.594694316	-4.144724846	-0.512590766
H	0.257269710	-4.050594807	1.219704151
Cu	-0.864674568	-0.130741805	0.345434397
C	-4.933322906	-0.730106413	1.960112453
C	-3.632887125	-1.252535343	1.886196256
C	-5.658002853	-0.574593961	0.782973826
H	-5.368360043	-0.466731191	2.919870615
C	-3.088603258	-1.571734190	0.621514618
C	-2.620134354	-1.551925182	2.867907047
C	-5.109117031	-0.935359895	-0.463477790
H	-6.670456886	-0.184017226	0.823511302
C	-3.814931393	-1.440797210	-0.564226151
N	-1.747299314	-2.016631842	0.799230993
C	-1.530121922	-2.028630257	2.209225893
H	-2.688179016	-1.382835507	3.932157040
H	-3.386244535	-1.717191339	-1.521520615
H	-5.709110260	-0.823990643	-1.362005591
H	-0.579838276	-2.364482403	2.594414234

================================

VI$_{PN}$

================================

P	0.975587368	1.009310365	-0.772716641
C	-0.067777336	2.571760416	-0.759829462
C	-1.040576100	2.696483135	0.433103353
P	-2.078584909	1.150253057	0.657747507
C	-3.655894041	1.333695650	-0.397812307
C	-3.036032677	1.498440623	2.270557880
C	-4.798842430	1.706375718	0.574826419
C	-4.472481728	1.062675714	1.922228336
C	1.674346805	1.019961238	-2.539255619
C	2.647775412	1.440887213	0.014740908
C	3.201688051	0.973264098	-2.342070580
C	3.531272888	1.899616599	-1.161902189
C	-2.441203833	0.914129674	3.530251265
C	-3.004876614	-0.192430273	4.178992748
C	-1.296870470	1.499389172	4.097185135
C	-2.439417601	-0.707752824	5.346111774
C	-0.731570661	0.987561941	5.264258862
C	-1.298914909	-0.122681499	5.894062519
C	-3.531072617	2.197080135	-1.625079393
C	-3.232413530	1.593585253	-2.856518745
C	-3.703070164	3.590730906	-1.595797062
C	-3.133298159	2.351675749	-4.024064064
C	-3.596993208	4.352361202	-2.760551453
C	-3.317823172	3.735540867	-3.981967449
C	2.540268898	2.323751926	1.232163429
C	2.385585308	1.735013366	2.497638226
C	2.530735731	3.725065947	1.153480768
C	2.221990347	2.511909008	3.642585516
C	2.361011982	4.506530285	2.297657490
C	2.202961922	3.904850245	3.547869205
C	1.012098312	-0.037778489	-3.396868944
C	-0.251130700	0.237121925	-3.938565016
C	1.550023556	-1.314617276	-3.590437412
C	-0.983918488	-0.747563660	-4.596314907
C	0.826303542	-2.295464277	-4.273369312
C	-0.454800338	-2.029077768	-4.756086826
H	-0.643912375	2.526814938	-1.691593647
H	0.578624189	3.453897953	-0.821345806
H	-0.473058790	2.819077253	1.363570333
H	-1.663204432	3.589085579	0.304247022
H	-3.803987503	0.292934507	-0.705277145
H	-3.036456585	2.593437672	2.374428034
H	-5.760357857	1.365926743	0.172726050
H	-4.872092724	2.792638302	0.707057893
H	-4.527901649	-0.028352372	1.819436193
H	-5.172904968	1.359029770	2.712552547
H	1.419862032	2.008695602	-2.943704605
H	3.023831844	0.461093068	0.335491866
H	3.723036289	1.267302632	-3.259516954
H	3.526420832	-0.045294978	-2.096601009
H	3.300762415	2.935332298	-1.439449072
H	4.592372894	1.866482496	-0.889411151
H	-3.892846346	-0.666130543	3.773896933
H	-0.848909199	2.371806383	3.627413511
H	-2.894207716	-1.570939183	5.824570179
H	0.144605622	1.466420174	5.692821980
H	-0.861377180	-0.521025121	6.805570126
H	-3.058296680	0.521887481	-2.887322426
H	-3.933621168	4.089630604	-0.658305883
H	-2.909626245	1.859402061	-4.967542171
H	-3.739934683	5.429416180	-2.713569880
H	-3.245676994	4.327486515	-4.890766144
H	2.396854401	0.653200090	2.588454485
H	2.661418915	4.216773510	0.193806216
H	2.115532160	2.024400949	4.607571602
H	2.355629683	5.590082169	2.210514307
H	2.072370291	4.513933659	4.437942505
H	-0.679795384	1.226789236	-3.810793877
H	2.527442455	-1.562921405	-3.189360619
H	-1.979339004	-0.520829320	-4.971162319
H	1.258996725	-3.283813953	-4.409832478
H	-1.036051154	-2.810210705	-5.236023903
C	2.870777130	-2.912275553	1.009357452
C	4.078169823	-3.579956293	1.232300997
H	4.547669411	-3.551885366	2.210748672
C	4.688727379	-4.307092190	0.205764994
H	5.624442101	-4.825741768	0.398217887
C	4.091926575	-4.380122185	-1.051216364
H	4.556470871	-4.959788799	-1.844629407
H	2.394987345	-3.784805059	-2.247484684
C	2.884762526	-3.713900089	-1.282188296
C	2.282021284	-2.978924274	-0.264536053
H	1.323199511	-2.498736858	-0.450106591
C	2.141297579	-2.148577213	2.105287075
H	2.078701735	-1.110796690	1.757501960
C	2.807457924	-2.151004553	3.483876944
H	2.212072849	-1.544060826	4.172985077
H	3.818907022	-1.733651280	3.440709114
H	2.860974312	-3.166073084	3.889595747
Cu	-0.475192487	-0.580312669	-0.132065922
C	-2.063858509	-4.725974083	1.538606048
C	-1.231848240	-3.624559879	1.802775025
C	-1.496228099	-5.989228725	1.458848953
H	-3.127184391	-4.572999477	1.382334113
C	0.170990363	-3.813314915	1.960966706
C	-1.493214846	-2.225862503	1.956718683
C	-0.105894811	-6.163710594	1.629570603
H	-2.122114182	-6.851914883	1.248618364
C	0.743844330	-5.090445995	1.875196934
N	0.735328257	-2.566359520	2.205817699
C	-0.286546111	-1.614968181	2.194777727
H	-2.450675249	-1.743144870	1.867713690
H	1.811400175	-5.239517212	1.986032486
H	0.316347063	-7.162618160	1.558052182
H	-0.076380484	-0.598904192	2.500316143
O	-1.216947556	-1.883687496	-1.408635139
C	-2.439799309	-2.268329144	-1.304416895
O	-3.278914690	-1.831188321	-0.486748099
C	-2.856299639	-3.330842495	-2.302872181
C	-2.018433571	-4.437745094	-2.560368776
C	-4.089554310	-3.210658073	-2.984359503
C	-2.433678389	-5.401936531	-3.489007473
C	-4.448167324	-4.183638096	-3.920536041
C	-3.636552334	-5.291026115	-4.187249184
H	-1.790814877	-6.261153221	-3.674077034
H	-5.392799854	-4.078775883	-4.452711105
C	-4.062681675	-6.327089310	-5.202188015
H	-3.347839594	-7.154021263	-5.259845257
H	-5.044222832	-6.749113083	-4.953002930
H	-4.149426937	-5.889883041	-6.205249310
C	-0.679970324	-4.615363121	-1.881724954
H	-0.748202562	-4.509249687	-0.797898293
H	-0.262258083	-5.603807449	-2.101123571
H	0.014831884	-3.846575260	-2.224324226
C	-5.036062717	-2.054630995	-2.739373922
H	-5.911852360	-2.124901056	-3.392482519
H	-5.360750198	-2.034920692	-1.697242379

H -4.555844307 -1.088134050 -2.926415920

==============================

II$_P$-TS'

==============================

P 1.552207589 -0.433497280 -0.347039580
C 0.803309798 1.114454269 -1.103900790
C -0.413246989 1.689554095 -0.359916091
P -1.732558250 0.462177217 0.127420425
C -2.993044853 0.584953010 -1.283405542
C -2.783313751 1.533219576 1.280158162
C -3.850874662 1.816473365 -0.948501706
C -4.141287804 1.727272391 0.553770185
C 3.046311140 -0.634564102 -1.534865975
C 2.665996313 0.248764455 1.041304946
C 4.300409794 -0.413844317 -0.662221134
C 3.966033459 0.687271118 0.348897904
C -2.917335510 1.117779493 2.731684446
C -3.287245274 2.108104706 3.655644417
C -2.699557781 -0.182210907 3.198663473
C -3.430841684 1.810173750 5.008289814
C -2.830334663 -0.482427537 4.554875851
C -3.197477579 0.509025753 5.463389874
C -2.338809729 0.496341139 -2.640368223
C -1.802113295 -0.736021698 -3.051223278
C -2.198143482 1.598429441 -3.492756844
C -1.157067060 -0.870641172 -4.277210712
C -1.545827508 1.469038725 -4.722750187
C -1.023548961 0.237538517 -5.120234013
C 1.961767077 1.237346292 1.938021541
C 2.184928894 2.618555546 1.865039229
C 1.001632214 0.758530200 2.846678495
C 1.455304980 3.501287222 2.666934490
C 0.281744242 1.636963964 3.653418779
C 0.499995917 3.015324593 3.559444666
C 2.976147175 -1.908006310 -2.346964598
C 2.240452766 -1.902967572 -3.544569969
C 3.560265064 -3.114610195 -1.932448149
C 2.082707644 -3.064073801 -4.298612595
C 3.409330845 -4.279600620 -2.689300299
C 2.666675806 -4.261471748 -3.872558594
H 0.518914819 0.822543502 -2.122245073
H 1.565896988 1.898106694 -1.194422722
H -0.090658374 2.148244619 0.577509940
H -0.876209199 2.479232073 -0.964858532
H -3.634119272 -0.294195771 -1.152063131
H -2.273350239 2.504566431 1.266123414
H -4.764430523 1.837254763 -1.552950382
H -3.303220272 2.744328976 -1.157833695
H -4.799998283 0.875475585 0.761832654
H -4.648881912 2.619228363 0.936626852
H 2.972990274 0.211550355 -2.229857206
H 2.882881880 -0.647310972 1.636635900
H 5.165882587 -0.165924370 -1.287624240
H 4.555555820 -1.326739669 -0.111502595
H 3.826379061 1.637923956 -0.181665435
H 4.771040916 0.842143238 1.077731371
H -3.451120615 3.126257181 3.306881428
H -2.405833960 -0.973902941 2.519104958
H -3.714695215 2.593870163 5.706271648
H -2.649181128 -1.495078444 4.892431736
H -3.297613144 0.264030516 6.516914368
H -1.887423754 -1.593284249 -2.389307976
H -2.608724594 2.563753605 -3.210309982
H -0.754136384 -1.837346554 -4.567271233
H -1.451126695 2.335479021 -5.372612000
H -0.521916449 0.137965560 -6.078860760
H 2.925835848 3.017037630 1.178926826
H 0.816562414 -0.309126616 2.918729544
H 1.637355566 4.570724487 2.591433287
H -0.458177596 1.246367216 4.344375134
H -0.071687490 3.700727463 4.179358006
H 1.777111650 -0.976964891 -3.880061626
H 4.131982803 -3.160454035 -1.008180737
H 1.508028984 -3.035802603 -5.223772049
H 3.868977070 -5.204275608 -2.345876932
H 2.545999050 -5.169302940 -4.457935810
C 0.408840895 -3.187856674 2.267024279
C 1.816830277 -3.045451641 2.305877924
H 2.398613691 -3.254272223 1.412668705
C 2.469108105 -2.645597219 3.472164631
H 3.553382397 -2.551784039 3.472402573
C 1.748127699 -2.368752718 4.637181759
H 2.261749983 -2.054358721 5.541287899
H -0.227583826 -2.309749603 5.521079540
C 0.353571177 -2.507287264 4.624217987
C -0.300663531 -2.912974358 3.467065334
H -1.381442189 -3.032453537 3.465940952
C -0.330547065 -3.582618952 1.057212710
H -1.254238486 -4.103661537 1.310894370
C 0.447841853 -4.275262356 -0.050849479
H -0.221410096 -4.568386555 -0.864404082
H 0.950850308 -5.189989090 0.305995077
H 1.219347835 -3.633003712 -0.486955106
Cu -0.844205499 -1.710446954 0.479010552
N -4.768986225 -3.335892439 1.680386543
C -2.980148315 -5.301344395 -0.791842520
C -3.483404160 -4.263678551 -0.016624460
C -3.243602037 -6.618695259 -0.385598898
H -2.402424097 -5.103729248 -1.689900756
C -4.284210205 -4.544749737 1.112038374
C -3.415002108 -2.808472395 -0.086557373
C -4.017158031 -6.882583141 0.748252153
H -2.846132517 -7.445823669 -0.967177629
C -4.564873695 -5.840340137 1.513513327
C -4.190054417 -2.325780153 0.952174544
H -3.041283369 -2.249433041 -0.929583430
H -4.207151890 -7.911986828 1.038844347
H -5.175204277 -6.015313148 2.392491579
H -4.398271561 -1.299417496 1.216659784
O -3.829151392 -3.307559013 3.331943512
C -4.474554539 -3.949291945 4.283363819
O -5.581092834 -4.459529400 4.232806206
C -3.596441507 -3.962373257 5.522679329
C -3.947838783 -3.135340214 6.612766743
C -2.430060387 -4.744177341 5.550232887
C -3.087440968 -3.079918623 7.709363937
C -1.604409695 -4.668272495 6.681559563
C -1.901383996 -3.830389500 7.756261826
H -3.342137575 -2.433793068 8.548764229
H -0.691705167 -5.260409355 6.703454494
C -2.077928066 -5.689436913 4.423100471
H -0.997352600 -5.855182648 4.377315998
H -2.565927744 -6.660230637 4.577355862
H -2.401928425 -5.309556961 3.450954437
C -5.220114231 -2.321148872 6.573089123
H -6.086107731 -2.967698336 6.402627945
H -5.365599155 -1.768750072 7.506530762
H -5.195684910 -1.596133351 5.750495434
C -0.976708174 -3.715149641 8.946225166
H -0.681789517 -2.671850681 9.117812157
H -1.465137124 -4.064379215 9.864324570
H -0.063762590 -4.303373337 8.806899071

==============================

III$_{PC}$

==============================

P 1.378480196 -0.534830689 -0.641304493
C 0.974058568 1.063487411 -1.510998368
C 0.131551474 2.043240786 -0.682939589
P -1.331681132 1.257131457 0.168787867
C -2.807703972 1.467210889 -0.988816202
C -1.898325443 2.658337116 1.309994817
C -3.142476082 2.968319416 -0.882003725
C -3.145605803 3.297987700 0.617839813
C 2.307425976 -1.478907943 -2.003890276
C 2.945218325 -0.195214435 0.354979873
C 3.690328836 -1.766030788 -1.382665634
C 4.104898930 -0.510350108 -0.607340813
C -2.151252508 2.207904339 2.731164932

C	-1.441494346	2.771068096	3.796190023
C	-3.117314339	1.230142117	3.012476206
C	-1.677439332	2.359206200	5.110219479
C	-3.354692459	0.811949432	4.320603371
C	-2.632024050	1.376617193	5.376761436
C	-2.669999361	0.858631432	-2.365967751
C	-3.290556908	-0.368400186	-2.652490377
C	-1.935452700	1.481635332	-3.387204885
C	-3.159130335	-0.971435070	-3.903205156
C	-1.802687407	0.882063627	-4.641153336
C	-2.409882545	-0.349137276	-4.902960777
C	2.913785458	1.141250253	1.055495620
C	3.582925558	2.271630287	0.571580291
C	2.133314610	1.270016074	2.215142250
C	3.469733000	3.499693871	1.230167031
C	2.029384613	2.489221573	2.878811121
C	2.692281723	3.615032673	2.383244753
C	1.568894267	-2.624472141	-2.662314892
C	0.508759677	-2.331458807	-3.535015583
C	1.923110008	-3.966081381	-2.474598885
C	-0.169240087	-3.346532822	-4.206724167
C	1.243432522	-4.985086918	-3.144736767
C	0.199230149	-4.680363178	-4.017103672
H	0.436519384	0.773308277	-2.420046329
H	1.911450863	1.541541696	-1.818725109
H	0.740749836	2.463160276	0.123091646
H	-0.193618894	2.883542299	-1.304746747
H	-3.609948874	0.929133773	-0.463942736
H	-1.069971919	3.374424219	1.310541749
H	-4.111160278	3.179109573	-1.347579479
H	-2.397952080	3.572073936	-1.413328886
H	-4.052658081	2.884266376	1.072060943
H	-3.164338350	4.375869751	0.803784847
H	2.456807852	-0.708072901	-2.771658421
H	2.926843405	-0.976369202	1.122731328
H	4.408153057	-2.037152529	-2.163474321
H	3.636239052	-2.614474535	-0.689271510
H	4.267183304	0.313884586	-1.312241197
H	5.038830280	-0.650555611	-0.052998427
H	-0.704507351	3.544150114	3.596066713
H	-3.694870234	0.794230819	2.199789286
H	-1.123238206	2.816170216	5.925462723
H	-4.110512733	0.056608807	4.519658089
H	-2.823824883	1.060778379	6.398101330
H	-3.898442268	-0.858344615	-1.897378922
H	-1.472074747	2.448339224	-3.212522984
H	-3.652058840	-1.921048522	-4.094240189
H	-1.235877275	1.385044575	-5.419812202
H	-2.313347101	-0.809098959	-5.882221699
H	4.206001759	2.204179287	-0.314803958
H	1.601875186	0.408285379	2.599379063
H	3.998340845	4.365630150	0.842045367
H	1.431358695	2.552028418	3.782600403
H	2.615321398	4.568761826	2.897246599
H	0.214807272	-1.297898293	-3.706725597
H	2.745046377	-4.231122494	-1.818089008
H	-0.982122004	-3.091691494	-4.880610943
H	1.538919687	-6.018852234	-2.989268541
H	-0.318553269	-5.473604679	-4.548792362
C	0.669492960	-2.211736917	2.751006126
C	2.056869507	-2.367851973	2.986166716
H	2.648184299	-2.991464138	2.324052334
C	2.654906750	-1.792310476	4.101846695
H	3.714908123	-1.943038702	4.283232212
C	1.895779252	-1.029098153	4.997004509
H	2.371843815	-0.577543139	5.862252712
H	-0.071621239	-0.255872339	5.461081028
C	0.525758028	-0.851500690	4.777950287
C	-0.080937438	-1.441570520	3.677505732
H	-1.145767808	-1.314913750	3.514996529
C	-0.030031372	-2.884042025	1.665137768
H	-1.019555569	-3.211697817	1.951790571
C	0.655174196	-3.809512615	0.710050285
H	0.060404651	-3.936738729	-0.197906077
H	0.737747014	-4.805972576	1.170658708
H	1.655006886	-3.478198290	0.424827427
Cu	-0.613465846	-1.074788690	0.606337607
N	-3.259624481	-3.434337616	2.179095745
C	-2.250739336	-3.753793955	-1.318449497
C	-2.583395720	-3.254635096	-0.055399217
C	-2.294794559	-5.138732433	-1.513520479
H	-1.952692151	-3.091452122	-2.124892235
C	-2.943582058	-4.140507221	0.995179832
C	-2.610047817	-1.921114445	0.534074128
C	-2.647998333	-6.007595539	-0.469567835
H	-2.038477898	-5.546411514	-2.486586094
C	-2.977227926	-5.518791676	0.801433623
C	-3.113274097	-2.165592909	1.892647982
H	-2.952338457	-1.063947797	-0.031222807
H	-2.670449972	-7.078878403	-0.651077688
H	-3.261348724	-6.181918144	1.613552570
H	-3.315114975	-1.398018837	2.631384850

===============================

$\mathbf{III_{PC}}$-TS

===============================

P	1.640460730	-0.452586621	-0.677778482
C	1.097558498	1.150641918	-1.463872194
C	0.232928306	2.053350210	-0.566339791
P	-1.142480969	1.182919979	0.359073848
C	-2.687559605	1.335670948	-0.719632387
C	-1.725133896	2.574877024	1.513354301
C	-3.035860062	2.835458517	-0.656266451
C	-2.965209723	3.236769676	0.822685540
C	2.527131796	-1.311676145	-2.113029718
C	3.244271278	-0.071198642	0.247146964
C	3.941536188	-1.586983681	-1.561053753
C	4.364688873	-0.337698549	-0.774815142
C	-2.012203455	2.134008408	2.932798386
C	-1.300904036	2.683350563	4.005117416
C	-3.030696630	1.209270716	3.213409424
C	-1.595439434	2.321517706	5.322065353
C	-3.320960999	0.834423125	4.523933887
C	-2.604288816	1.394154549	5.586014271
C	-2.658443451	0.697219193	-2.087258816
C	-3.365832090	-0.494576007	-2.306790829
C	-1.968347907	1.267987013	-3.167529106
C	-3.360533953	-1.117889881	-3.554970026
C	-1.963621140	0.649145663	-4.418826103
C	-2.655816317	-0.548445523	-4.616150379
C	3.175088644	1.261588335	0.953391254
C	3.766192436	2.426316977	0.450214565
C	2.406260490	1.353219509	2.125368118
C	3.590735435	3.650648594	1.102015615
C	2.239070892	2.569544315	2.781685829
C	2.827264071	3.728732824	2.267425776
C	1.771998048	-2.461958885	-2.744721651
C	0.549157858	-2.205813169	-3.389261484
C	2.266907930	-3.770983219	-2.754278183
C	-0.145693153	-3.222570419	-4.039071560
C	1.567501426	-4.794545650	-3.400690079
C	0.364864439	-4.524154663	-4.051586151
H	0.534791768	0.854015648	-2.355098486
H	1.979657292	1.706394911	-1.802008390
H	0.856450558	2.498429298	0.213729963
H	-0.174352869	2.882768393	-1.153568625
H	-3.440930128	0.802657902	-0.123514146
H	-0.891784489	3.284506798	1.532507539
H	-4.032270432	3.012313366	-1.075449228
H	-2.333328485	3.421206474	-1.259697914
H	-3.873065472	2.890565872	1.326794505
H	-2.929801464	4.322253227	0.954194129
H	2.623465776	-0.524735928	-2.873589039
H	3.290906191	-0.857248664	1.010393381
H	4.634356499	-1.825028419	-2.374121189
H	3.927294016	-2.453099012	-0.886156917
H	4.469679356	0.504386127	-1.469237447
H	5.329715252	-0.466886461	-0.273844212
H	-0.527133346	3.420764923	3.808603525
H	-3.627117634	0.796397388	2.403317928

H	-1.043189168	2.773304462	6.141343117
H	-4.115067959	0.118634947	4.716835022
H	-2.840515137	1.117541194	6.609410286
H	-3.932700396	-0.937673390	-1.492058635
H	-1.445040345	2.211089611	-3.040952206
H	-3.915464640	-2.040983200	-3.696220875
H	-1.429293513	1.109569669	-5.244942188
H	-2.657467604	-1.023541212	-5.592918396
H	4.372826099	2.389590263	-0.449086994
H	1.928449035	0.464345902	2.520407677
H	4.058509827	4.543866634	0.697957575
H	1.650071859	2.606019735	3.693075657
H	2.700291634	4.680844307	2.774404526
H	0.139048427	-1.198370218	-3.406746387
H	3.212525368	-4.004078865	-2.275533915
H	-1.086028337	-2.994797945	-4.531515121
H	1.973722100	-5.802097321	-3.403139114
H	-0.171679169	-5.318335056	-4.562746525
C	0.402660459	-2.324827671	2.561068535
C	1.794417858	-2.317487955	2.830884695
H	2.470094204	-2.872196913	2.190231800
C	2.294969320	-1.663691759	3.950970888
H	3.360034704	-1.695442438	4.160415173
C	1.434136868	-0.961490631	4.801920414
H	-0.611108243	-0.378912002	5.184256077
C	0.062863827	-0.929135203	4.537247181
C	-0.452126503	-1.616761088	3.442699671
H	-1.522226572	-1.627928972	3.265984774
C	-0.172135442	-3.153610706	1.479848623
H	-1.086263537	-3.645993471	1.784474134
C	0.741908610	-3.995888710	0.638605297
H	0.209004685	-4.454254627	-0.192519680
H	1.135235429	-4.815436840	1.257882833
H	1.586107969	-3.432555676	0.237307698
Cu	-0.213345066	-1.042989969	0.672287464
N	-3.670047760	-2.920063496	1.450511217
C	-1.953624368	-4.708494663	-1.225919843
C	-2.339332104	-3.755103350	-0.284720153
C	-2.572080612	-5.964585304	-1.188002944
H	-1.200935125	-4.484993935	-1.973349810
C	-3.361279488	-4.047781944	0.653488755
C	-1.923815131	-2.382597685	-0.005937772
C	-3.557848454	-6.256408691	-0.237234399
H	-2.283329248	-6.723632336	-1.909234524
C	-3.973175287	-5.294907570	0.693379343
C	-2.899930000	-1.960085273	1.025857210
H	-1.636016726	-1.745969892	-0.843256772
H	-4.018390179	-7.240077019	-0.229669645
H	-4.756744862	-5.501201153	1.415471315
H	-2.945366621	-0.972110271	1.467274666
H	1.833142877	-0.442819178	5.668517113

==============================

V_{PC}

==============================

P	1.756395578	0.108887658	-0.987736046
C	0.655908763	1.432345867	-1.717575788
C	-0.089703679	2.298851728	-0.684695780
P	-0.871453881	1.363025188	0.734643281
C	-2.558640957	0.838333786	0.084852099
C	-1.589174867	2.795767069	1.752833009
C	-3.379582405	2.136257887	0.085289262
C	-3.119203568	2.803346395	1.441651940
C	2.423470497	-0.729591250	-2.552715540
C	3.387015343	0.980025589	-0.638809979
C	3.864423513	-0.161393210	-2.760461092
C	4.010482788	1.181319356	-2.028708935
C	-1.278261065	2.781957626	3.233436823
C	-0.525745809	3.816044092	3.803413153
C	-1.777369380	1.778391242	4.078115940
C	-0.281081975	3.855725288	5.177793503
C	-1.551263809	1.825558662	5.453835487
C	-0.797677159	2.862691641	6.010094166
C	-2.450252771	0.019717965	-1.178712368
C	-1.962841868	-1.295068502	-1.085313559
C	-2.747416019	0.532437146	-2.445883274
C	-1.753195643	-2.067601442	-2.225027084
C	-2.544870138	-0.243716508	-3.591583967
C	-2.040416241	-1.539864898	-3.487154484
C	3.203216076	2.162671089	0.280505627
C	3.305080652	3.486752272	-0.157111004
C	2.844514847	1.924797773	1.619245172
C	3.037878752	4.545748711	0.716755569
C	2.564085484	2.975876331	2.488303900
C	2.658501387	4.295272827	2.035002708
C	2.360905170	-2.240873098	-2.524980545
C	1.513529062	-2.930943251	-3.400258780
C	3.153441668	-2.984206915	-1.636592150
C	1.471301794	-4.327492237	-3.403324604
C	3.114720583	-4.376535892	-1.637575746
C	2.276489258	-5.054203033	-2.525986195
H	-0.063057952	0.888534904	-2.339492321
H	1.235705972	2.078757763	-2.385560989
H	0.607801199	2.995404243	-0.208813563
H	-0.850700498	2.901477337	-1.192780614
H	-2.950566769	0.191500485	0.881888270
H	-1.134363055	3.690875530	1.314995050
H	-4.444589615	1.932500958	-0.068858206
H	-3.061280966	2.797476530	-0.729125917
H	-3.646121979	2.243388414	2.221580267
H	-3.501107216	3.828134298	1.480453372
H	1.775273204	-0.371123075	-3.359065533
H	3.977541924	0.218353137	-0.110569634
H	4.080706120	-0.074781083	-3.829557180
H	4.590658188	-0.871184289	-2.351078749
H	3.485387087	1.972201824	-2.576911926
H	5.059161186	1.488656998	-1.954469919
H	-0.132452831	4.602072716	3.164299011
H	-2.368731499	0.964855254	3.662599325
H	0.298205703	4.672805786	5.598504066
H	-1.979243159	1.062120438	6.096712589
H	-0.631076455	2.905154943	7.082441807
H	-1.745404959	-1.713805079	-0.104352616
H	-3.139975786	1.538990974	-2.549666882
H	-1.370671511	-3.079282284	-2.130771160
H	-2.786611319	0.168581113	-4.567080498
H	-1.887506366	-2.141343355	-4.378638744
H	3.595654249	3.702301502	-1.180369258
H	2.784880638	0.897631884	1.978080630
H	3.129428864	5.568428993	0.362091392
H	2.267143965	2.771503687	3.512440681
H	2.451179266	5.120022297	2.710473299
H	0.886787653	-2.370882750	-4.089591026
H	3.811323643	-2.471421957	-0.938410938
H	0.817762852	-4.845622540	-4.099946976
H	3.737540245	-4.934291363	-0.944237173
H	2.251486063	-6.140040874	-2.531426907
C	0.141548589	-2.687099695	6.306277752
C	1.067236066	-3.220173359	7.213993073
H	1.389432907	-4.253825188	7.120202065
C	1.580318332	-2.440660000	8.251318932
H	2.290003538	-2.875410080	8.949566841
C	1.185373545	-1.108833075	8.394767761
H	1.586007237	-0.503241539	9.202149391
H	-0.035849411	0.472491145	7.583114624
C	0.271568120	-0.564684093	7.491292000
C	-0.245806351	-1.350953341	6.460503578
H	-0.953049600	-0.919561327	5.756804466
C	-0.396229297	-3.510946751	5.143540382
H	-1.273789167	-2.993610144	4.734967232
C	-0.839374602	-4.919922829	5.565132141
H	-1.389381528	-5.413551331	4.761266232
H	-1.496292233	-4.856411457	6.437188625
H	0.011742459	-5.554461479	5.833719730
Cu	0.574434340	-0.451023132	0.992238224
N	0.720594823	-2.072214365	2.168162107
C	0.095838077	-5.636830807	2.452424765
C	0.355331331	-4.299704075	2.730185509
C	-0.129421920	-6.013369560	1.121134281
H	0.076994427	-6.382172108	3.240325212

C	0.409996420	-3.376176834	1.675137877
C	0.684420586	-3.549509764	4.001363277
C	-0.063818306	-5.078439236	0.082682513
H	-0.341339290	-7.053466320	0.891805708
C	0.223994941	-3.736439705	0.346701980
C	0.911031365	-2.164268255	3.446702719
H	1.611560106	-3.930438519	4.453722477
H	-0.203908637	-5.399353027	-0.944095254
H	0.336239934	-3.009556293	-0.450175375
H	1.139870882	-1.292493105	4.049593925

VI_{PC}

P	1.537976027	-0.465126663	-0.563125730
C	0.734153569	0.996896863	-1.407114387
C	0.015562691	1.923581958	-0.406455457
P	-1.217566490	1.029374599	0.696961701
C	-2.867149115	1.364972949	-0.173073351
C	-1.596595049	2.351119757	2.004695415
C	-3.090844393	2.878012180	-0.006598552
C	-2.772557259	3.231719732	1.458133459
C	2.056487799	-1.544160247	-2.038516760
C	3.332584858	0.057180744	-0.188234419
C	3.527638674	-1.878277183	-1.726177454
C	4.192399025	-0.563507140	-1.306718707
C	-1.886688590	1.712495923	3.349787474
C	-0.963474214	1.815790534	4.395949364
C	-3.052471876	0.959388137	3.563128948
C	-1.186979890	1.183581114	5.618309975
C	-3.284378052	0.327454746	4.785372257
C	-2.348758459	0.436163098	5.817248344
C	-2.972552299	0.785380661	-1.560223103
C	-3.415187359	-0.537968934	-1.715006590
C	-2.621832132	1.504032373	-2.712158680
C	-3.512528419	-1.121726274	-2.976252794
C	-2.709432840	0.917734325	-3.976861000
C	-3.158132315	-0.396052629	-4.115831852
C	3.486547470	1.537790298	0.078799918
C	3.906944990	2.460199356	-0.895087540
C	3.157392263	2.019221783	1.362087846
C	3.992810249	3.823554754	-0.599893749
C	3.236138105	3.379287720	1.654645562
C	3.655977249	4.289740086	0.673468411
C	1.144059777	-2.703978300	-2.374807358
C	-0.045856826	-2.461394310	-3.081157684
C	1.458095789	-4.033054352	-2.055974960
C	-0.878901362	-3.507318974	-3.476979971
C	0.631373644	-5.082779884	-2.461891413
C	-0.540264666	-4.829410553	-3.177387714
H	0.015913133	0.587771297	-2.127242804
H	1.481314778	1.568592668	-1.970161796
H	0.752590299	2.360106707	0.275943369
H	-0.456368208	2.754809141	-0.940875411
H	-3.592884302	0.845235348	0.465717286
H	-0.682443500	2.946745634	2.095303297
H	-4.118237495	3.152795076	-0.275516570
H	-2.434376955	3.437280655	-0.680997550
H	-3.660161972	3.052347898	2.073454142
H	-2.534292936	4.295693398	1.564283252
H	2.051455975	-0.862802327	-2.900921345
H	3.527402878	-0.464791775	0.755373895
H	4.016213417	-2.337768078	-2.593403578
H	3.586461544	-2.596736908	-0.900212586
H	4.234330654	0.097778186	-2.180535555
H	5.223772049	-0.708759427	-0.965542555
H	-0.038726024	2.362952471	4.237162590
H	-3.789877176	0.859422803	2.768434525
H	-0.437217772	1.246343136	6.401140213
H	-4.195025444	-0.250425756	4.929792881
H	-2.518578529	-0.063419305	6.767663479
H	-3.682326317	-1.113569736	-0.832694530
H	-2.279561043	2.531007528	-2.629252672
H	-3.868117094	-2.143734694	-3.073024511
H	-2.433128595	1.494808435	-4.855556965
H	-3.234439850	-0.848334670	-5.100858688
H	4.182626724	2.124288797	-1.892990351
H	2.817954779	1.312598348	2.115402937
H	4.326745033	4.520110130	-1.370208144
H	2.974935770	3.727001667	2.654032946
H	3.723459721	5.350380421	0.901636660
H	-0.320948958	-1.441708684	-3.340750694
H	2.353247881	-4.263415337	-1.489317894
H	-1.787681460	-3.284703732	-4.029190540
H	0.905281901	-6.102517128	-2.205229521
H	-1.185289145	-5.647519112	-3.486028433
C	-3.265050650	-5.064625263	0.149479568
C	-4.164412022	-5.650682449	1.049935102
H	-3.818678617	-6.423170090	1.733011127
C	-5.502912998	-5.255625725	1.083639264
H	-6.184506893	-5.722312450	1.789939642
C	-5.967337608	-4.265016079	0.215140745
H	-7.009315014	-3.958882093	0.240073457
H	-5.428860664	-2.899793863	-1.364470124
C	-5.079252720	-3.672677040	-0.684948444
C	-3.740176916	-4.068975925	-0.713845968
H	-3.047656059	-3.603919029	-1.411109924
C	-1.799195647	-5.466597080	0.100911878
H	-1.328296065	-4.910998344	-0.713959277
C	-1.624540806	-6.962471485	-0.192211941
H	-0.574825406	-7.203862190	-0.372632980
H	-2.193343878	-7.238136768	-1.085792184
H	-1.982823491	-7.581589222	0.637472630
Cu	0.160036936	-0.845133603	1.337583542
N	-0.117526285	-2.878200054	1.588590384
C	1.350229740	-6.180925369	1.246561050
C	0.454783261	-5.123162270	1.357400894
C	2.723368883	-5.898135185	1.212772369
H	1.006643176	-7.209227562	1.199667454
C	0.949731648	-3.813120365	1.455884814
C	-1.055557609	-5.032619953	1.408946753
C	3.194841623	-4.584193707	1.315214634
H	3.431917667	-6.717454910	1.124941945
C	2.306794643	-3.511230469	1.451781273
C	-1.222773314	-3.543271065	1.613221765
H	-1.480402112	-5.591145039	2.254935741
H	4.264258862	-4.393530369	1.318520069
H	2.638551950	-2.491763115	1.625303984
H	-2.179462433	-3.040405273	1.694253206
O	0.938314259	0.071113415	2.980244637
C	1.919996619	-0.485787719	3.590566635
O	2.937498808	-0.980328619	3.063686371
C	1.786979437	-0.491324902	5.102057457
C	0.968348265	-1.454966903	5.713571072
C	2.455235958	0.469700038	5.877709389
C	0.825928569	-1.440495133	7.104879856
C	2.285711288	0.458058059	7.265540600
C	1.473962426	-0.491372585	7.900005341
H	0.184498385	-2.183372021	7.576984882
H	2.798453331	1.207301021	7.867835045
C	3.313974619	1.513171196	5.201474190
H	3.847450256	2.133137941	5.928182125
H	4.043219566	1.043889046	4.533155441
H	2.696846008	2.175997019	4.580834866
C	0.201200172	-2.441465855	4.867273808
H	-0.522622585	-1.910566211	4.239434242
H	0.869168460	-2.983358622	4.189794540
H	-0.334988654	-3.171745539	5.482013702
C	1.311888337	-0.482127160	9.403419495
H	0.573705912	-1.221377254	9.732164383
H	2.258640289	-0.710891247	9.910251617
H	0.985016167	0.501068234	9.764890671

VI_{PC}-TS

P	2.528069019	-0.860606551	-0.888522446
C	1.701743007	0.574146569	-1.778817534
C	1.113212824	1.683996677	-0.886647582
P	0.200134858	1.034728646	0.608251512

C	-1.586780071	0.881422400	0.009828702
C	-0.183106646	2.630671024	1.568126082
C	-2.108666182	2.326100349	-0.037488479
C	-1.679300427	2.973167181	1.283753991
C	3.063987970	-1.870709658	-2.418050528
C	4.293107510	-0.264983147	-0.555395663
C	4.612164021	-1.879096866	-2.373308182
C	5.066123486	-0.508810043	-1.860149145
C	0.106963187	2.497216225	3.045626879
C	0.895561278	3.433191538	3.720479250
C	-0.430007994	1.424888611	3.774564266
C	1.160345316	3.290456057	5.085855484
C	-0.163982168	1.272423625	5.131716251
C	0.638862312	2.206572533	5.791306973
C	-1.753171563	0.015043186	-1.213510990
C	-1.684206605	-1.380189896	-1.061198950
C	-1.951230407	0.540058315	-2.496079683
C	-1.811320186	-2.225725174	-2.160397053
C	-2.079490900	-0.308578968	-3.599939108
C	-2.009784937	-1.691811681	-3.436929226
C	4.312895775	1.114239216	0.055871788
C	4.695656300	2.259252310	-0.652360857
C	3.852580547	1.261605263	1.375573754
C	4.608237267	3.523625612	-0.060889676
C	3.769051790	2.519824743	1.966101408
C	4.141728401	3.659717321	1.247025609
C	2.408296824	-3.219268322	-2.575166941
C	1.328593850	-3.374052048	-3.454626083
C	2.852467060	-4.338972569	-1.860194325
C	0.721749663	-4.618198872	-3.631123066
C	2.250913620	-5.582520485	-2.035274744
C	1.188624024	-5.730431557	-2.929672003
H	0.901196182	0.107808135	-2.365722179
H	2.413812160	1.013441920	-2.488242626
H	1.917440772	2.309651852	-0.487439543
H	0.463535577	2.330826521	-1.488119602
H	-2.081834316	0.373281181	0.848489165
H	0.461479217	3.406386852	1.140327811
H	-3.196820974	2.350733757	-0.172793731
H	-1.669889450	2.870297670	-0.882758677
H	-2.291397095	2.565676689	2.096712589
H	-1.830785394	4.057960510	1.287708521
H	2.761667490	-1.247981668	-3.268718958
H	4.661472797	-0.976075590	0.191354185
H	5.015537262	-2.114683151	-3.364626884
H	4.971157074	-2.649948835	-1.683037281
H	4.827239990	0.258098096	-2.607816219
H	6.147787094	-0.469341725	-1.686442494
H	1.314387202	4.273316860	3.171011209
H	-1.050315976	0.688970268	3.267133474
H	1.779864788	4.025372982	5.593639851
H	-0.567840636	0.425260037	5.675811768
H	0.852999210	2.078998327	6.848195553
H	-1.514710784	-1.792987466	-0.070546411
H	-2.019695282	1.613779664	-2.642271519
H	-1.750693202	-3.300698280	-2.020071745
H	-2.241549969	0.116318390	-4.587292671
H	-2.115313292	-2.350501299	-4.294948578
H	5.061634064	2.176126242	-1.671201825
H	3.535103083	0.383487284	1.930300117
H	4.907405853	4.402122498	-0.627119184
H	3.397417784	2.606843472	2.982310295
H	4.073827267	4.643638611	1.704115033
H	0.952771425	-2.511503935	-3.999794722
H	3.669784069	-4.235421658	-1.156397700
H	-0.113137834	-4.718043804	-4.320250511
H	2.602556467	-6.434424877	-1.460210681
H	0.721625447	-6.701784134	-3.069075108
C	-0.215117723	-2.612702608	6.310953140
C	1.066366911	-2.062882662	6.477831841
H	1.893869758	-2.441226959	5.886253834
C	1.287260175	-1.040903449	7.400200367
H	2.286248684	-0.628233671	7.513506413
C	0.234624714	-0.547266781	8.174780846
H	0.410525829	0.242600918	8.900503159
H	-1.876956344	-0.689450920	8.592644691
C	-1.047238111	-1.071354508	8.003191948
C	-1.266511440	-2.093639135	7.076251507
H	-2.266058207	-2.506114960	6.956379414
C	-0.441803336	-3.814257145	5.403529644
H	-1.515969992	-4.044616699	5.423039436
C	0.307607681	-5.025933743	6.004351616
H	0.041662440	-5.956591129	5.500117779
H	0.059321869	-5.136201859	7.064735889
H	1.390001178	-4.891390800	5.916944504
Cu	1.245843172	-1.079000950	1.070092082
N	-0.101567343	-2.372995615	1.959077597
C	-0.287891090	-5.908215523	2.743278980
C	-0.190143496	-4.515336990	2.843802691
C	-0.353247762	-6.492641926	1.479079485
H	-0.322982401	-6.536864281	3.626150370
C	-0.153470814	-3.739695549	1.655900955
C	-0.036754381	-3.553084373	3.951377630
C	-0.280841112	-5.713015079	0.312694103
H	-0.450698048	-7.572242260	1.395360947
C	-0.161653325	-4.327971935	0.387948066
C	-0.137056768	-2.278745413	3.285109520
H	1.310015678	-3.393388510	3.933741570
H	-0.303066641	-6.193421364	-0.659675419
H	-0.055996429	-3.718700409	-0.503372252
H	-0.038611617	-1.316014647	3.767791510
C	6.798555374	-2.872772217	0.967993259
C	6.653177261	-1.849784017	1.904791236
C	5.766294003	-3.814019203	0.847257495
C	8.043426514	-2.992579460	0.120525889
H	7.457062721	-1.127644420	2.035866499
C	5.488899708	-1.710186601	2.672950983
H	5.881711483	-4.639396667	0.146287605
C	4.595916748	-3.729008198	1.604459524
C	4.444513321	-2.633077145	2.487324476
C	5.434099197	-0.612090647	3.714887857
C	3.524391413	-4.788357735	1.466608405
C	3.099320412	-2.408123016	3.128859043
O	2.513240814	-1.316005349	2.909417391
O	2.628885746	-3.379004955	3.821553946
H	5.807564735	0.332410842	3.307268858
H	4.423647881	-0.439100116	4.085242748
H	6.071483135	-0.878488243	4.567559242
H	2.568474293	-4.368783474	1.136542320
H	3.824373245	-5.554376602	0.745867968
H	3.332148314	-5.269581795	2.427868366
H	8.705409050	-3.782981396	0.495929331
H	7.794705391	-3.246853113	-0.916005433
H	8.614804268	-2.059487820	0.112247616

================================

VII_{PC}

================================

P	2.512200594	-0.994356811	-0.939637840
C	1.744001627	0.397029132	-1.937637568
C	1.140780091	1.550744176	-1.113604188
P	0.228846535	0.972386539	0.413627595
C	-1.573466659	0.938536763	-0.123977743
C	-0.001817187	2.581708670	1.389327049
C	-1.993865967	2.416507959	-0.160493150
C	-1.481687784	3.027489901	1.151193976
C	3.140489817	-2.101869822	-2.354331493
C	4.267348289	-0.399214953	-0.512742877
C	4.654056549	-2.254412651	-2.086670160
C	5.167733669	-0.872866631	-1.667296052
C	0.327366084	2.419234991	2.856848240
C	1.070496202	3.385889053	3.542752981
C	-0.139582559	1.305541992	3.568607092
C	1.358847857	3.233619690	4.901961327
C	0.145519078	1.146782398	4.920968533
C	0.900264978	2.111176014	5.592739105
C	-1.796272397	0.068432644	-1.334056377
C	-1.800032139	-1.326828003	-1.163451195
C	-1.945750356	0.589280307	-2.624683619
C	-1.957795143	-2.177697659	-2.254628658
C	-2.103834629	-0.264726967	-3.720347643

C	-2.111875057	-1.647751927	-3.538893461
C	4.336155891	1.054568291	-0.113137126
C	4.782377720	2.064668179	-0.974862397
C	3.877745390	1.417977810	1.163427591
C	4.772169590	3.403342962	-0.571589768
C	3.874281645	2.749706268	1.567635059
C	4.319356441	3.752250433	0.701103091
C	2.360072613	-3.370493650	-2.584455490
C	1.289698482	-3.359221697	-3.489602804
C	2.659946918	-4.568083763	-1.920502424
C	0.552098870	-4.515097141	-3.742075682
C	1.926357865	-5.725964546	-2.174006462
C	0.875820756	-5.706736088	-3.092442989
H	0.960109055	-0.092906736	-2.528807163
H	2.487608433	0.792761624	-2.640306711
H	1.940034389	2.202767849	-0.750960410
H	0.487649709	2.155549765	-1.752957940
H	-2.076173544	0.466686577	0.731260180
H	0.680244803	3.315096378	0.945165932
H	-3.080690861	2.520187378	-0.264959127
H	-1.540399313	2.930005789	-1.017337441
H	-2.092383623	2.656970263	1.982787848
H	-1.558452725	4.120191097	1.162382603
H	3.040660143	-1.475706220	-3.250360966
H	4.524466515	-0.994037986	0.368698150
H	5.161691666	-2.640103579	-2.977995396
H	4.835215569	-2.968837976	-1.276580215
H	5.096314907	-0.193511173	-2.525232077
H	6.218271732	-0.893244267	-1.355069995
H	1.432048440	4.261301041	3.007148981
H	-0.706616282	0.533872604	3.053388596
H	1.942478657	3.992751598	5.417201996
H	-0.212103143	0.270667493	5.449798107
H	1.127356529	1.981150389	6.647316933
H	-1.654859781	-1.743897080	-0.169482127
H	-1.949951410	1.663874984	-2.782632589
H	-1.951201916	-3.251228571	-2.094034195
H	-2.228297472	0.156122610	-4.714943409
H	-2.241975784	-2.309471846	-4.391215801
H	5.148963928	1.818154812	-1.966609836
H	3.498657227	0.651942313	1.831490159
H	5.122448921	4.172076225	-1.255959153
H	3.507939577	3.004601717	2.557078362
H	4.313663483	4.793223858	1.013981104
H	1.026954174	-2.433872223	-3.997407436
H	3.465389729	-4.601883888	-1.193626165
H	-0.274862468	-4.482675552	-4.446646690
H	2.166714430	-6.641277790	-1.640981078
H	0.306076914	-6.610514641	-3.289318323
C	-0.594361484	-2.819532633	6.101399899
C	0.764538467	-2.513287783	6.294934750
H	1.522724748	-3.053198576	5.735819817
C	1.159996510	-1.518834114	7.189646244
H	2.218098879	-1.300804257	7.320015430
C	0.202872634	-0.806970298	7.919254780
H	0.509456873	-0.037319895	8.624079704
H	-1.905837297	-0.536668301	8.281709671
C	-1.150565267	-1.089212656	7.727473259
C	-1.541184545	-2.083676815	6.824142933
H	-2.598730326	-2.299647331	6.685955524
C	-1.015724540	-3.955007315	5.172399044
H	-2.098980665	-4.100231171	5.308291435
C	-0.328542739	-5.268550396	5.621519566
H	-0.683273673	-6.119942665	5.037318230
H	-0.529827535	-5.466410160	6.679896832
H	0.756178737	-5.208629608	5.484091759
Cu	1.053758860	-1.244966984	0.849052429
N	-0.083568782	-2.538262129	1.801392913
C	-1.416943192	-5.844412327	2.408815145
C	-0.919115663	-4.537850857	2.585220337
C	-1.423939943	-6.403654099	1.138467908
H	-1.812747955	-6.406654835	3.250612736
C	-0.458391368	-3.809357882	1.438176036
C	-0.752721786	-3.654068708	3.709474564
C	-0.921703517	-5.692513466	0.024854312
H	-1.814859390	-7.408567905	0.997294724
C	-0.432491779	-4.399932861	0.163484961
C	-0.278019279	-2.463015318	3.166903019
H	1.616140723	-3.041946650	3.369725227
H	-0.912127197	-6.163769245	-0.953077972
H	-0.035941217	-3.849876642	-0.684611022
H	-0.036511257	-1.549543619	3.690795183
C	7.280759811	-1.213055491	2.717187643
C	6.529211044	-0.393173367	3.563308239
C	6.639364243	-2.288295031	2.087753773
C	8.754891396	-0.963579178	2.492303610
H	7.016855240	0.439927906	4.067133427
C	5.159840107	-0.597970128	3.765583992
H	7.214155197	-2.934343100	1.425327897
C	5.279760361	-2.554998159	2.278858423
C	4.539087772	-1.680269957	3.109036922
C	4.389178753	0.341587126	4.670382023
C	4.638685703	-3.723443985	1.557322621
C	3.053000927	-1.798697233	3.181313515
O	2.314175844	-0.838072360	2.973683596
O	2.606102943	-3.025276899	3.447277069
H	3.895297050	1.132403731	4.095351696
H	3.598486185	-0.168484256	5.228554726
H	5.068213463	0.819661498	5.385046005
H	3.704858780	-3.437664032	1.059932351
H	5.323072910	-4.133800030	0.807203114
H	4.375654221	-4.522779465	2.256733418
H	9.366669655	-1.669799685	3.067733526
H	9.022424698	-1.091888666	1.436806679
H	9.043401718	0.047927812	2.795113325

===============================

VII$_{PC}$-TS

===============================

P	2.393763542	-0.825541496	-1.255217075
C	1.753639340	0.573553324	-2.322870731
C	1.283938766	1.797515512	-1.497436643
P	0.237642795	1.343095183	-0.006745802
C	-1.527658224	1.573847651	-0.614130676
C	0.190928236	2.932152987	1.013079405
C	-1.717205405	3.097778559	-0.654107153
C	-1.178920150	3.618401766	0.687008619
C	2.849218130	-2.194374084	-2.477888107
C	4.200325012	-0.391902655	-0.929927289
C	4.405010223	-2.148024559	-2.629940748
C	4.916978836	-0.756292641	-2.239330292
C	0.356415719	2.683827877	2.499008417
C	1.140704751	3.536798716	3.282683611
C	-0.330888480	1.637144089	3.133029222
C	1.236780643	3.351559639	4.664882660
C	-0.239496872	1.448524237	4.509538174
C	0.543989658	2.309740305	5.281317711
C	-1.805810332	0.745491743	-1.841499329
C	-1.935611248	-0.645461500	-1.688077092
C	-1.867966175	1.287931442	-3.129803896
C	-2.116392612	-1.472877502	-2.793009996
C	-2.052487373	0.458478510	-4.240085602
C	-2.173299551	-0.921579957	-4.076571465
C	4.383933067	0.991467297	-0.355910212
C	4.903649807	2.057321548	-1.099132061
C	3.962610483	1.227349401	0.964344621
C	4.987803936	3.336712599	-0.541219652
C	4.046302319	2.502198935	1.518101931
C	4.554592133	3.565390825	0.764961600
C	2.366806746	-3.555195332	-2.017444849
C	1.761846423	-4.447734833	-2.908862591
C	2.558067322	-3.963394165	-0.687425196
C	1.365828753	-5.719707012	-2.485185146
C	2.151978493	-5.223646641	-0.258269757
C	1.560866594	-6.110784531	-1.160829067
H	0.905206025	0.153233513	-2.876253128
H	2.502607822	0.891446650	-3.057392597
H	2.151442289	2.335028648	-1.102723718
H	0.738695085	2.487776041	-2.150607347
H	-2.136298418	1.180388451	0.211806640

H	1.017090797	3.557611704	0.657591999
H	-2.769553900	3.367687464	-0.803444743
H	-1.153370142	3.538181782	-1.485532761
H	-1.889054775	3.357658148	1.480076194
H	-1.073689818	4.708334923	0.700079679
H	2.376030207	-1.942754149	-3.433417559
H	4.495694160	-1.121281862	-0.162991583
H	4.700924873	-2.433323860	-3.644988775
H	4.838196754	-2.891923904	-1.951306224
H	4.672766209	-0.030838534	-3.025485039
H	6.006687641	-0.740928590	-2.116607428
H	1.681519508	4.351951122	2.806722879
H	-0.927445114	0.941754878	2.546805620
H	1.855142236	4.022050381	5.256348133
H	-0.768858314	0.626788020	4.978426456
H	0.618918777	2.153273821	6.353733540
H	-1.878048182	-1.085865140	-0.695342302
H	-1.779656172	2.360629320	-3.274551868
H	-2.212719202	-2.543116808	-2.638871193
H	-2.104436398	0.895867109	-5.233835220
H	-2.318756580	-1.563661814	-4.941172123
H	5.246458530	1.899138570	-2.117229700
H	3.552603960	0.408886582	1.550091863
H	5.394965649	4.153535366	-1.131645203
H	3.701724291	2.662607670	2.535510302
H	4.621043205	4.561072826	1.195819616
H	1.598345280	-4.146086693	-3.941327095
H	2.983388901	-3.279348135	0.041217607
H	0.894548953	-6.399641514	-3.190107107
H	2.271822691	-5.488509655	0.787083864
H	1.232671738	-7.091019630	-0.826911390
C	-1.856342316	-1.933923006	5.422451496
C	-0.524420083	-2.241718292	5.751782894
H	0.014390160	-2.979682684	5.165965080
C	0.126109198	-1.594545007	6.800770760
H	1.165425658	-1.831581473	7.013616562
C	-0.552709222	-0.641629934	7.565868855
H	-0.048720635	-0.137717262	8.386489868
H	-2.421104193	0.394561678	7.856506348
C	-1.882642388	-0.343834788	7.267997265
C	-2.523848057	-0.982570231	6.202072144
H	-3.557706118	-0.735415578	5.970792770
C	-2.583054543	-2.676038265	4.305245876
H	-3.566032171	-2.200286865	4.175464153
C	-2.834116697	-4.130833149	4.781369686
H	-3.406991243	-4.706391335	4.052281857
H	-3.380875587	-4.129309654	5.730389118
H	-1.881485343	-4.646753788	4.938823700
Cu	0.884847164	-0.810922742	0.516377985
N	-0.130116776	-2.357102394	1.451699495
C	-3.247710228	-4.207330227	1.378070951
C	-2.164914131	-3.406742096	1.781093836
C	-3.217342377	-4.811612129	0.124334939
H	-4.107829571	-4.346964359	2.025911570
C	-1.083202839	-3.210874081	0.877749562
C	-1.842622042	-2.651985168	2.981468439
C	-2.122198820	-4.632805347	-0.742959499
H	-4.052996159	-5.431932449	-0.189685121
C	-1.046790361	-3.826585054	-0.375067919
C	-0.662488639	-2.016001701	2.706272364
H	0.996030688	-2.909838676	1.785127759
H	-2.110069275	-5.130854130	-1.709065795
H	-0.204021603	-3.671731949	-1.038469791
H	-0.073885575	-1.374084711	3.343320847
C	5.310244560	-2.889548540	6.168749809
C	4.614604473	-1.690469146	6.010701180
C	5.123703003	-3.886287451	5.208863735
C	6.216277599	-3.118776560	7.355483055
H	4.747932434	-0.900365293	6.747128963
C	3.751877546	-1.462517619	4.932425499
H	5.665797710	-4.824622631	5.309386730
C	4.257933617	-3.723206997	4.124266624
C	3.564928770	-2.495340347	3.978704691
C	3.045529127	-0.125672609	4.866386414
C	4.119485855	-4.876351357	3.152556181
C	2.614314795	-2.275041580	2.835044146
O	2.435312033	-1.125179052	2.374387026
O	1.976473451	-3.313625336	2.390257597
H	3.442916632	0.499926597	4.062110901
H	1.978461623	-0.229342967	4.665304184
H	3.162223101	0.412285030	5.812395096
H	4.189389706	-4.548116207	2.112514734
H	4.899485588	-5.622369766	3.334127188
H	3.142811060	-5.357628345	3.255846739
H	5.693627357	-3.670455217	8.147636414
H	7.096634865	-3.708829403	7.079237461
H	6.561560631	-2.174201012	7.787003040

==============================

$VIII_{PC}$

==============================

P	2.313867807	-0.946683228	-0.991821289
C	1.503466725	0.490467161	-1.882762551
C	0.936070323	1.565167546	-0.923494637
P	-0.010672640	0.884244621	0.540667117
C	-1.810732603	0.643137574	-0.020786870
C	-0.401170284	2.434550762	1.543830633
C	-2.552995682	1.920878410	0.420083970
C	-1.934213638	2.365258694	1.749807715
C	2.691808701	-2.199945211	-2.358739138
C	4.119524002	-0.434296936	-0.836379588
C	4.207232952	-2.012939453	-2.713030815
C	4.688590527	-0.632186890	-2.248674870
C	0.386198014	2.599044561	2.820830345
C	1.139415145	3.759680033	3.036055565
C	0.343486845	1.627939820	3.832016945
C	1.828992248	3.956056595	4.233549595
C	1.024032116	1.826624751	5.031412125
C	1.770565391	2.988786697	5.237369537
C	-1.897969723	0.222521260	-1.469412446
C	-1.713206410	-1.132206798	-1.781551838
C	-2.055621862	1.128885865	-2.526918888
C	-1.665778637	-1.570884466	-3.102648258
C	-2.015844345	0.691516399	-3.853801489
C	-1.811300516	-0.657811224	-4.150785446
C	4.287356377	0.898308694	-0.147587836
C	4.604146004	2.073334455	-0.837727249
C	4.048365116	0.970078468	1.236612201
C	4.671028614	3.296364307	-0.162288815
C	4.101055145	2.190109491	1.905328155
C	4.413326263	3.360258102	1.206863046
C	2.406706572	-3.635467768	-1.956310153
C	1.889916778	-4.552333355	-2.879247904
C	2.735489130	-4.097242832	-0.673190236
C	1.719060302	-5.896350861	-2.532809496
C	2.556473017	-5.432838917	-0.318595976
C	2.053649426	-6.343663216	-1.252455831
H	0.692215204	0.055990286	-2.476026773
H	2.204529047	0.962753415	-2.580071211
H	1.756884336	2.138268232	-0.476470113
H	0.307153434	2.263892651	-1.486783624
H	-2.154987812	-0.190207019	0.603377104
H	-0.187195659	3.283906937	0.881935716
H	-3.630168915	1.734943271	0.501748741
H	-2.419730663	2.721644878	-0.316437483
H	-2.162032843	1.637535572	2.536371946
H	-2.315107346	3.335001707	2.089715004
H	2.068504095	-1.930322409	-3.218878984
H	4.544379234	-1.211858153	-0.186708704
H	4.373829365	-2.175285339	-3.783134699
H	4.776906490	-2.783984900	-2.181847811
H	4.316321850	0.145656094	-2.926690340
H	5.783056736	-0.561694324	-2.253399134
H	1.189536452	4.515843391	2.255770922
H	-0.221796334	0.711726010	3.687243700
H	2.409647703	4.863260269	4.380775452
H	0.969459772	1.066711664	5.802104473
H	2.305011988	3.135484219	6.172263622
H	-1.591107130	-1.847769737	-0.980233133
H	-2.208765030	2.185011148	-2.325802088

H	-1.517330527	-2.629373550	-3.297970533
H	-2.141262531	1.412688732	-4.657283306
H	-1.777507901	-0.992729545	-5.183697701
H	4.803855896	2.043959379	-1.904902816
H	3.784808874	0.069816492	1.786394238
H	4.924821854	4.199244976	-0.712136805
H	3.882094145	2.229479313	2.968542814
H	4.455012798	4.312600613	1.728685737
H	1.619774938	-4.214060307	-3.877477884
H	3.092664719	-3.409668207	0.086196192
H	1.312436581	-6.591094017	-3.263266563
H	2.787572384	-5.737187862	0.697019875
H	1.905622482	-7.384661198	-0.979509294
C	-2.557867527	-1.027819514	4.582277775
C	-1.677066207	-1.585668445	5.523453712
H	-1.333905101	-2.607884645	5.393330574
C	-1.244063497	-0.850103557	6.626391411
H	-0.559438586	-1.302381635	7.339416504
C	-1.694700122	0.457971185	6.820530415
H	-1.357103109	1.032223225	7.678962708
H	-2.934906244	2.038010359	6.040964127
C	-2.578953266	1.020858645	5.901459217
C	-3.006493092	0.280903459	4.796683311
H	-3.711317539	0.722913027	4.095727921
C	-3.091655731	-1.850278854	3.420214415
H	-3.730453014	-1.187724710	2.817682743
C	-4.001665592	-2.979435682	3.968920469
H	-4.436078548	-3.567734480	3.157294512
H	-4.812919617	-2.559931517	4.573379517
H	-3.422420979	-3.660845995	4.599898815
Cu	1.225372076	-0.957962811	1.074803472
N	-0.044616014	-3.085220098	1.595722318
C	-3.464125395	-3.407210112	0.543268979
C	-2.293555975	-3.123018265	1.270916700
C	-3.370515108	-4.132519722	-0.639531136
H	-4.430378437	-3.058820009	0.896479964
C	-1.040313721	-3.556262493	0.753512859
C	-2.026760817	-2.417299986	2.505686522
C	-2.121236086	-4.587359905	-1.112640977
H	-4.270735741	-4.353152752	-1.206194162
C	-0.944066346	-4.301868916	-0.426145613
C	-0.659981251	-2.433585882	2.660986662
H	0.919719994	-3.469529390	1.715384483
H	-2.071287632	-5.166286469	-2.030793667
H	0.015513092	-4.634160995	-0.795999527
H	-0.039618559	-2.020860672	3.440987110
C	6.285379887	-2.840051889	5.610587120
C	5.308159828	-1.854822874	5.754780769
C	6.147243023	-3.746114492	4.557765007
C	7.437275887	-2.953561544	6.581666946
H	5.392316818	-1.142465353	6.573536873
C	4.218455315	-1.751945853	4.882825375
H	6.899983406	-4.521468163	4.426392555
C	5.067392349	-3.700745583	3.671282291
C	4.092626095	-2.682969809	3.823957443
C	3.205586672	-0.658930004	5.140960693
C	5.006388664	-4.754886150	2.585855246
C	2.916143179	-2.615680456	2.875329494
O	2.442209482	-1.451244473	2.616538048
O	2.465732813	-3.689025640	2.398908854
H	3.228993654	0.107714295	4.364540100
H	2.181891441	-1.044836044	5.136518955
H	3.392890930	-0.183308616	6.109468937
H	4.799547195	-4.326036930	1.602279186
H	5.952812672	-5.303030491	2.533700943
H	4.198213100	-5.464774609	2.782366991
H	7.219666004	-3.690839052	7.365609169
H	8.354361534	-3.279668093	6.079247952
H	7.642440319	-1.999816895	7.077887535

==============================

IV$_P$

==============================

P	1.103152633	-0.371492326	-0.721076727
C	0.180707037	1.233615637	-0.953634441
C	-0.562657893	1.725230217	0.298801869
P	-1.565457225	0.380767882	1.110597968
C	-3.305303335	0.600753069	0.408964157
C	-2.027809143	1.120465875	2.793838263
C	-3.884340048	1.773543596	1.222414374
C	-3.545084715	1.464604259	2.684326649
C	1.809930325	-0.693453789	-2.447331190
C	2.766115189	0.101952210	0.020817626
C	3.343126774	-0.646059155	-2.251205206
C	3.643477917	0.431081921	-1.200734615
C	-1.724795222	0.262864560	4.003101826
C	-1.153043270	0.836195409	5.146079063
C	-2.105041981	-1.085987329	4.046999931
C	-0.967134655	0.081603713	6.306906223
C	-1.922964573	-1.841210842	5.204417706
C	-1.356610775	-1.259197235	6.341755867
C	-3.367317915	0.643135905	-1.097336173
C	-3.517784834	-0.561124921	-1.805750370
C	-3.252832174	1.834925413	-1.825797915
C	-3.530188322	-0.577607810	-3.199830532
C	-3.262257576	1.818954468	-3.222893238
C	-3.390011549	0.613965452	-3.915025949
C	2.639976978	1.113391161	1.134886861
C	2.980719805	2.461632013	0.981131017
C	2.087886810	0.694366038	2.355477810
C	2.773234367	3.368511677	2.025278330
C	1.884496331	1.593985558	3.397857666
C	2.223181963	2.940643311	3.234102726
C	1.232836604	-1.909579515	-3.144655943
C	-0.158883393	-2.089931726	-3.185075521
C	2.046993494	-2.859059095	-3.772006035
C	-0.718366325	-3.196562290	-3.821393728
C	1.488221645	-3.973626137	-4.401901722
C	0.104969129	-4.148855686	-4.428791523
H	-0.530841231	1.053037643	-1.767902255
H	0.887320697	1.997871637	-1.297559977
H	0.145005718	2.084760666	1.049080968
H	-1.214078665	2.564766169	0.035766501
H	-3.838122368	-0.300225288	0.740353823
H	-1.455236197	2.053205729	2.856859207
H	-4.964067459	1.857980609	1.058649063
H	-3.435914278	2.727125645	0.918673813
H	-4.126200199	0.596083879	3.016342402
H	-3.788991928	2.290514469	3.359529972
H	1.522626758	0.199535578	-3.019937754
H	3.133585215	-0.834380209	0.456045300
H	3.849272251	-0.447512895	-3.201083422
H	3.706292391	-1.616443038	-1.889656305
H	3.390942335	1.417959094	-1.607136607
H	4.702594280	0.457575828	-0.924054265
H	-0.866775632	1.885554314	5.133571625
H	-2.539638042	-1.577251792	3.182432175
H	-0.529946387	0.546101809	7.186366558
H	-2.225614786	-2.884421110	5.204678535
H	-1.224514723	-1.842954397	7.248297215
H	-3.650370598	-1.490924239	-1.259465337
H	-3.174981356	2.786339521	-1.308045149
H	-3.662152767	-1.518602371	-3.727503777
H	-3.179095030	2.753381252	-3.770435810
H	-3.400414467	0.604299963	-5.000761032
H	3.416593313	2.816459894	0.052688178
H	1.802257657	-0.342506707	2.485104322
H	3.046822786	4.411202908	1.891174912
H	1.455440879	1.240454793	4.330214500
H	2.067974806	3.647748947	4.043976784
H	-0.819148481	-1.363832712	-2.715367317
H	3.125801802	-2.743484020	-3.771943808
H	-1.798532844	-3.315047741	-3.846502066
H	2.138754845	-4.702814102	-4.876192570
H	-0.328255445	-5.014157772	-4.921860695
C	1.575983644	-3.069205523	1.889956474
C	2.982594967	-2.880791903	1.901697516
H	3.561916351	-3.086680889	1.007539272
C	3.627584696	-2.487184525	3.064832687
H	4.706547260	-2.364209890	3.072134018

C	2.890003920	-2.248600245	4.234447956
H	3.403104305	-1.932723522	5.138473034
H	0.926551938	-2.223431826	5.142278671
C	1.501614332	-2.417742014	4.242640972
C	0.847908020	-2.837375641	3.090209484
H	-0.227574825	-3.002074957	3.090600252
C	0.853513241	-3.528819799	0.734132469
H	-0.074143618	-4.038494110	0.969208419
C	1.522403240	-4.009255409	-0.512289166
H	0.794902861	-4.144932747	-1.312796474
H	1.977165461	-4.990513325	-0.305722475
H	2.315593719	-3.348199606	-0.866647184
Cu	-0.433805317	-1.726162672	0.530105710
N	-2.262975693	-3.675447702	1.959309578
C	-1.373937964	-6.199645996	-0.544653475
C	-1.786598325	-4.985063553	0.075226456
C	-1.107753634	-7.288803101	0.253526360
H	-1.280336738	-6.261107922	-1.626535177
C	-1.893873215	-4.914165020	1.528906822
C	-2.093616962	-3.697711229	-0.382594258
C	-1.219922066	-7.213238239	1.679499865
H	-0.804503322	-8.229660988	-0.198212370
C	-1.586905718	-6.046935558	2.318046331
C	-2.371576786	-2.938569069	0.815422058
H	-2.134099007	-3.338396788	-1.400392890
H	-0.994698346	-8.099209785	2.267714977
H	-1.667279124	-5.989578247	3.400309801
H	-2.939306259	-2.018379688	0.841043651

==============================

III$_{PN}$-TS'

==============================

P	1.274037480	-0.215126395	-0.760349751
C	0.299770385	1.376450896	-0.817650318
C	-0.452404350	1.722460866	0.473893821
P	-1.351061583	0.269228935	1.231771827
C	-3.136612654	0.317547798	0.644778609
C	-1.794828773	1.009742141	2.924474955
C	-3.736896276	1.536398888	1.377233505
C	-3.302149057	1.431933522	2.841967583
C	1.813049555	-0.418744236	-2.551295519
C	2.984057665	0.199810356	-0.112076677
C	3.356728792	-0.460995585	-2.457357645
C	3.781235218	0.557028115	-1.380360365
C	-1.523231983	0.150676236	4.136977673
C	-0.847065210	0.686416030	5.240019321
C	-2.055873632	-1.144706368	4.231287479
C	-0.730944812	-0.039004538	6.429952145
C	-1.944445491	-1.866379857	5.418488979
C	-1.288853049	-1.316061258	6.526050568
C	-3.439040899	0.240694895	-0.833816707
C	-4.139212132	-0.867603064	-1.337383509
C	-3.109628439	1.280192256	-1.720210552
C	-4.474489212	-0.952493370	-2.691159964
C	-3.437361479	1.195736766	-3.076043606
C	-4.117009163	0.075843833	-3.567471981
C	2.892585754	1.166894913	1.046547651
C	3.139834881	2.538775682	0.919823229
C	2.414645672	0.683380961	2.275345564
C	2.904543400	3.404223204	1.992915034
C	2.180823088	1.542235851	3.345803022
C	2.418867826	2.912526369	3.205410957
C	1.082403660	-1.549674273	-3.249507427
C	-0.315073460	-1.461926818	-3.379585981
C	1.728248954	-2.685800314	-3.744810820
C	-1.048185587	-2.488771439	-3.966613531
C	0.994599819	-3.717710972	-4.339429379
C	-0.392874926	-3.626539469	-4.446972847
H	-0.401520044	1.247042894	-1.648925066
H	0.981549740	2.190917730	-1.088876247
H	0.262250155	2.045878887	1.236349344
H	-1.132988334	2.563326359	0.302307010
H	-3.520920515	-0.599881947	1.112297893
H	-1.170275450	1.909420133	2.990801573
H	-4.828477383	1.534678698	1.278798103
H	-3.380288363	2.469733953	0.921324551
H	-3.905688047	0.662620962	3.343338251
H	-3.459314823	2.367581129	3.395502329
H	1.535072088	0.525858223	-3.037488937
H	3.355087757	-0.759750962	0.272570431
H	3.811700583	-0.253706634	-3.430792809
H	3.690190554	-1.461139441	-2.152842522
H	3.534568310	1.569694877	-1.721815825
H	4.859124184	0.530917525	-1.190142870
H	-0.431979656	1.690311551	5.176683426
H	-2.543678284	-1.591769934	3.367234945
H	-0.220262975	0.399404705	7.283743382
H	-2.374083042	-2.861411333	5.482949257
H	-1.222909570	-1.875162244	7.456151009
H	-4.413490772	-1.674374223	-0.661301732
H	-2.611021280	2.173189163	-1.350284576
H	-5.019750595	-1.820490956	-3.055998564
H	-3.174420357	2.010898829	-3.746621132
H	-4.378352642	0.013345694	-4.621012688
H	3.521728277	2.943603754	-0.012367068
H	2.208657980	-0.373999178	2.388366699
H	3.102018356	4.466191292	1.877815366
H	1.803320527	1.138465405	4.280290604
H	2.234293938	3.589936972	4.034372807
H	-0.845196605	-0.581714034	-3.021326542
H	2.807990074	-2.776028156	-3.679306507
H	-2.127759933	-2.395965099	-4.042939186
H	1.513619065	-4.593461037	-4.718774796
H	-0.959347427	-4.431309223	-4.906582355
C	1.697481513	-3.114777088	1.907544255
C	3.105463743	-2.941867113	2.010595560
H	3.737296581	-3.161788464	1.156501651
C	3.678125381	-2.551344872	3.211252928
H	4.756324291	-2.449882984	3.290549517
C	2.867649555	-2.273007393	4.324485779
H	3.324462414	-1.956215501	5.257790089
H	0.849775970	-2.188316345	5.094800472
C	1.478691578	-2.405575275	4.238006115
C	0.896348298	-2.839707136	3.053516388
H	-0.176434025	-2.987694979	2.994903803
C	1.047366023	-3.551628828	0.698886991
H	0.085552387	-4.037137032	0.843494415
C	1.781475544	-3.968321323	-0.531203389
H	1.092852116	-4.026870251	-1.374153733
H	2.211906195	-4.969384193	-0.373561203
H	2.601270676	-3.293195963	-0.790589988
Cu	0.030488983	-1.634286642	0.572142601
N	-2.057005644	-2.876200914	0.949736595
C	-1.876387358	-6.483676434	0.512706399
C	-1.870774865	-5.091560364	0.280011207
C	-2.062810659	-6.937508583	1.804904699
H	-1.741215348	-7.181910992	-0.308644116
C	-2.070744276	-4.163074493	1.382995725
C	-1.730446577	-4.283526421	-0.883888721
C	-2.248566389	-6.034163952	2.891485929
H	-2.067223787	-8.005331039	2.006124258
C	-2.254986286	-4.668733597	2.703259468
C	-1.805475712	-2.973608255	-0.446098447
H	-1.583120823	-4.609924793	-1.903279305
H	-2.384161949	-6.440899372	3.889761448
H	-2.424443245	-4.023852825	3.560099125
H	-1.919048905	-2.101386786	-1.077985406

==============================

III$_{PC}$-TS'

==============================

P	1.199340940	-0.362062544	-0.756513000
C	0.257787794	1.237622142	-0.940292835
C	-0.473619699	1.687088847	0.331659794
P	-1.453250766	0.315724075	1.131493688
C	-3.210313559	0.583624482	0.457878590
C	-1.899294972	1.087225318	2.812616587
C	-3.717984915	1.824676871	1.216757059
C	-3.378727198	1.577484250	2.687887907
C	1.825874090	-0.656472802	-2.508107901

C	2.875250101	0.148089215	-0.071944922
C	3.364466667	-0.598060727	-2.373622417
C	3.694316387	0.486924738	-1.332839727
C	-1.723432183	0.220415086	4.039050579
C	-1.160108566	0.753724575	5.204901218
C	-2.227717161	-1.086734056	4.076270103
C	-1.100349784	-0.002271297	6.378655434
C	-2.168852568	-1.845485091	5.243085384
C	-1.604951262	-1.304948211	6.402315617
C	-3.333349466	0.570453584	-1.045177341
C	-3.685629606	-0.625571668	-1.690664530
C	-3.101940155	1.707172155	-1.833373189
C	-3.770943403	-0.695121646	-3.080915928
C	-3.183924675	1.639064789	-3.225930214
C	-3.504750490	0.435414612	-3.855547905
C	2.734764814	1.162771225	1.040371418
C	3.038894653	2.518348932	0.872020125
C	2.178084373	0.747370660	2.261765480
C	2.792638779	3.434744358	1.899677753
C	1.936016917	1.656662583	3.287829638
C	2.239976883	3.009559631	3.107930899
C	1.185657263	-1.861093760	-3.168434858
C	-0.216934115	-1.960097194	-3.183842897
C	1.931303620	-2.874350309	-3.776732683
C	-0.852982461	-3.047838688	-3.776290417
C	1.294397593	-3.972290039	-4.362781048
C	-0.097195849	-4.065981865	-4.364700794
H	-0.465080291	1.067095995	-1.746325850
H	0.948120773	2.019137383	-1.278460264
H	0.236882657	2.047205687	1.077621102
H	-1.140346050	2.523183107	0.100419424
H	-3.775072813	-0.267604262	0.853223026
H	-1.246131063	1.963086724	2.894243240
H	-4.794963360	1.951586127	1.060539842
H	-3.235368729	2.739871979	0.855269372
H	-4.038495541	0.796510994	3.082633972
H	-3.529676676	2.464727163	3.310425282
H	1.508494496	0.239542723	-3.058830261
H	3.282574654	-0.775567114	0.356575131
H	3.832540751	-0.395103872	-3.341902256
H	3.749459505	-1.565149188	-2.025741816
H	3.406914711	1.468473911	-1.729554892
H	4.764550209	0.531763256	-1.106729984
H	-0.794301629	1.778146863	5.203684330
H	-2.686319590	-1.528858423	3.199415684
H	-0.671565235	0.433081448	7.277114868
H	-2.563158751	-2.857218027	5.234173775
H	-1.568802238	-1.888156414	7.317937374
H	-3.916437149	-1.505335212	-1.095813870
H	-2.882057905	2.661624670	-1.364859939
H	-4.061053276	-1.627685308	-3.557182789
H	-3.007403374	2.532216549	-3.818314791
H	-3.572130680	0.385098040	-4.938126564
H	3.467668772	2.873484850	-0.059845544
H	1.902576923	-0.291179508	2.397406816
H	3.034091711	4.483525276	1.751440763
H	1.500786066	1.306193829	4.218954563
H	2.051845789	3.724800348	3.903477907
H	-0.828397512	-1.179706097	-2.735290289
H	3.015120029	-2.819089174	-3.796933651
H	-1.938591719	-3.096057892	-3.781943798
H	1.891425848	-4.753486156	-4.824098110
H	-0.589734495	-4.917045116	-4.825702667
C	1.575082779	-3.068119049	1.983808517
C	2.965245485	-2.795885563	2.075266123
H	3.608570576	-2.994895697	1.224564672
C	3.509279966	-2.325529099	3.260407925
H	4.576519489	-2.137455940	3.331765890
C	2.684488297	-2.088889599	4.371327877
H	3.120174408	-1.709730029	5.291833401
H	0.668131411	-2.144345045	5.158021927
C	1.309326291	-2.335460901	4.303667068
C	0.758364618	-2.841943264	3.130978107
H	-0.302325875	-3.082350254	3.078807116
C	0.954033613	-3.587516308	0.794054210
H	0.044619650	-4.148113251	0.983620405
C	1.707958102	-4.011359692	-0.425381631
H	1.022061467	-4.204870701	-1.252102613
H	2.240813494	-4.949718475	-0.209332988
H	2.449880838	-3.277364969	-0.750343621
Cu	-0.235049158	-1.776044846	0.538713694
N	-2.431359768	-3.851222754	2.020401955
C	-1.186082482	-6.026428699	-0.652900636
C	-1.722903848	-4.925793171	0.055003718
C	-0.950185299	-7.210140705	0.033123866
H	-0.975424290	-5.946276188	-1.716366053
C	-1.955867171	-5.038578987	1.474010587
C	-1.994166970	-3.567148209	-0.255510330
C	-1.212586522	-7.317227840	1.420991898
H	-0.556737661	-8.070899010	-0.499364197
C	-1.684973717	-6.228642941	2.149038315
C	-2.501636267	-3.014504671	0.989381671
H	-2.058245897	-3.121104717	-1.238803387
H	-1.021653175	-8.259796143	1.925656796
H	-1.873260379	-6.299187183	3.216822386
H	-3.002706766	-2.065145731	1.079973221

==============================

MF of $\mathbf{II_S}$**-TS'**

==============================

Cu	-0.225367934	-0.640409172	-3.275611639
H	-3.287765980	0.239022851	-2.958347082
C	-2.991525173	0.164878532	-4.008861542
C	-1.566022754	0.644347548	-4.274747372
C	-1.284786224	2.067005157	-4.025138855
C	-0.376012027	2.758244276	-4.864307880
C	-1.890365720	2.827951908	-2.996723175
C	-0.073450968	4.101628304	-4.674347878
C	-1.565601230	4.169029713	-2.790973425
C	-0.649511337	4.822366238	-3.620262384
H	0.091145538	2.208366871	-5.678743839
H	-2.639273643	2.365931273	-2.361276388
H	0.622136235	4.593084812	-5.351623058
H	-2.049079657	4.715878010	-1.983794212
H	-0.411429375	5.871422768	-3.468255520
H	-1.304944158	0.421686471	-5.309515953
H	-3.097308159	-0.886818111	-4.292779922
P	-1.387740850	-2.107519150	-1.769847393
C	-0.324418843	-3.191905975	-0.719692111
C	0.580032349	-2.563976526	0.194005519
C	-0.301685214	-4.581977367	-0.879331887
C	1.438460112	-3.410557032	0.871523261
C	0.607995868	-1.112561584	0.559981525
C	0.599410117	-5.410557747	-0.186826944
H	-1.002571106	-5.052361012	-1.557851076
C	1.469974279	-4.788738251	0.679166913
O	2.375960588	-3.055171251	1.809542775
C	0.077728279	-0.757325768	1.787873507
C	1.195356846	-0.051650207	-0.197503909
H	0.607145607	-6.485544682	-0.327287942
O	2.432326555	-5.350288391	1.477882385
C	3.097407818	-4.252434254	2.120175123
C	0.062537178	0.547463179	2.272257566
O	-0.522172749	-1.593513489	2.696728945
C	1.197824478	1.251419783	0.311500728
P	1.759526610	-0.415499955	-1.919710398
H	4.120007992	-4.170460224	1.729564786
H	3.094270706	-4.408373356	3.204602242
C	0.630388796	1.579331636	1.556981325
O	-0.554216802	0.585649431	3.495597601
C	-1.017053962	-0.751229763	3.743483782
H	1.649809361	2.047635555	-0.268510073
H	0.635978639	2.596044302	1.933432102
H	-0.626060784	-1.098821282	4.706513882
H	-2.114418745	-0.762799442	3.727979183
C	2.814553499	1.008071423	-2.413791180
C	4.208359718	0.943529129	-2.570273161
C	2.153195858	2.203532457	-2.743374109
C	4.922836781	2.058154821	-3.013914824
H	4.743046284	0.025304545	-2.353624105

C	2.874154329	3.321431875	-3.161710739
H	1.070171833	2.258233547	-2.691142559
C	4.262199879	3.254368305	-3.298058748
C	2.961827040	-1.783753276	-1.647360206
C	2.871776581	-2.952230930	-2.416358709
C	3.959451437	-1.689067960	-0.662928641
C	3.779591322	-3.995286226	-2.218351126
H	2.077932835	-3.064517736	-3.147220373
C	4.871574879	-2.727305889	-0.477759123
H	4.015078068	-0.802184701	-0.038171511
C	4.784219265	-3.885722160	-1.256139278
C	-2.317340612	-1.143084526	-0.517174363
C	-2.226512194	0.254041255	-0.570867658
C	-3.052203417	-1.743366718	0.515004396
C	-2.879249096	1.043245554	0.373863935
H	-1.616690040	0.715933800	-1.340397835
C	-3.717907906	-0.952884614	1.452443123
H	-3.097338676	-2.826500654	0.587016284
C	-3.633201838	0.440878302	1.382804513
C	-2.611881733	-3.231709003	-2.550123215
C	-2.137506485	-4.123642921	-3.529605627
C	-3.991035461	-3.174152613	-2.303066969
C	-3.012150764	-4.968504906	-4.211620808
H	-1.084672093	-4.137961864	-3.786798954
C	-4.867172718	-4.006601334	-3.002380848
H	-4.388828278	-2.473869324	-1.576865435
C	-4.382868290	-4.910552979	-3.948804617
H	-3.732673168	0.738831997	-4.589735031
H	-2.615680456	-5.653172493	-4.956475735
H	-5.070513248	-5.557521820	-4.486964703
H	-5.934049129	-3.945173025	-2.803978682
H	-4.298470497	-1.424812913	2.241110325
H	-4.145527363	1.054092765	2.119274616
H	-2.787466764	2.124392033	0.323847115
H	2.335648298	4.232270718	-3.400804996
H	4.822177887	4.121437073	-3.637614727
H	6.000894070	1.987490892	-3.134592295
H	5.648088455	-2.633316517	0.277384788
H	5.490767002	-4.698061466	-1.109071374
H	3.695280075	-4.897756100	-2.815048456

================================

SF of II_S-TS'

================================

C	-1.135896087	-7.945042610	-6.234514236
C	-1.124826550	-7.031476498	-7.289062500
C	-0.355087608	-7.661466599	-5.107564449
H	-1.708698273	-7.244875431	-8.181900978
H	-0.326923937	-8.376249313	-4.287419796
C	-0.379315436	-5.846222401	-7.243443489
C	0.387566537	-6.484118938	-5.003474236
C	0.354616374	-5.561863422	-6.071314335
C	1.055969954	-4.225040913	-5.993088722
O	1.752868652	-3.772104502	-6.878770351
O	0.728636146	-3.563192368	-4.862174511
C	-0.285077751	-0.323914558	-8.200492859
C	0.391224623	-0.771864057	-7.068568707
C	-0.263982475	-1.621677160	-6.154591560
C	-1.559716105	-2.069571972	-6.350989819
C	-2.222385168	-1.630377054	-7.503755569
C	-1.595827818	-0.768055677	-8.412425041
C	1.721158862	-0.532830954	-6.527576447
C	1.822528839	-1.225153089	-5.369771004
N	0.581287384	-1.837248206	-5.023423672
H	0.190344617	0.358336210	-8.899393082
H	-2.037365913	-2.728915453	-5.637247086
H	-3.240086794	-1.960879326	-7.689260006
H	-2.137941599	-0.434051543	-9.292605400
H	2.485481501	0.099269010	-6.960596561
H	2.654304743	-1.320465088	-4.690282822
C	-1.953007698	-9.214097023	-6.302588463
H	-2.663625717	-9.271857262	-5.469507217
H	-2.522584200	-9.277316093	-7.234438896
H	-1.312909365	-10.102234840	-6.240034580
C	-0.385784537	-4.923728466	-8.441552162
H	0.618897438	-4.832370758	-8.862243652
H	-1.061725616	-5.302425861	-9.213601112
H	-0.700963795	-3.911104441	-8.175846100
C	1.245124459	-6.243788719	-3.782419920
H	0.911992550	-5.379168987	-3.204405069
H	1.242656589	-7.115897655	-3.122560740
H	2.282502890	-6.050940990	-4.077297688

================================

MF of II_S-TS

================================

Cu	-2.243358135	0.947758377	-4.128157616
H	-5.454327583	0.836856008	-4.336148739
C	-5.045289993	1.490248680	-5.111362934
C	-3.784198284	2.209934950	-4.666051865
C	-3.859062433	3.000041962	-3.427607059
C	-2.977535725	4.099092007	-3.235530615
C	-4.794065475	2.746393681	-2.392783880
C	-3.016028166	4.877756119	-2.084095001
C	-4.840610504	3.541522264	-1.248423696
C	-3.951872110	4.607666016	-1.076124787
H	-2.300059319	4.356111526	-4.043592930
H	-5.487143517	1.914962530	-2.487394571
H	-2.343202829	5.728693485	-1.994670630
H	-5.573534966	3.319497585	-0.475164562
H	-3.998761892	5.227835178	-0.184075251
H	-3.336556196	2.792867184	-5.469541073
H	-4.851037979	0.875150383	-5.992285728
P	-2.782873154	-0.570287228	-2.227044106
C	-1.654040694	-2.031051159	-2.148486614
C	-0.318026364	-1.859830737	-1.667411447
C	-2.051546097	-3.265728235	-2.677314281
C	0.502237380	-2.971558809	-1.751019120
C	0.252250046	-0.635700226	-1.029461980
C	-1.185464621	-4.370670795	-2.760110855
H	-3.069360018	-3.388992786	-3.029481173
C	0.097130552	-4.187343597	-2.292132854
O	1.812674761	-3.058447361	-1.351022720
C	0.552049637	-0.690110624	0.319696695
C	0.603762388	0.576713920	-1.696685076
H	-1.510082960	-5.320704937	-3.169774771
O	1.135089040	-5.082629204	-2.258366346
C	2.268985748	-4.349366665	-1.770588279
C	1.127203584	0.364861220	1.021330953
O	0.327263147	-1.742487907	1.171103001
C	1.194663167	1.625169158	-0.981516540
P	0.190870956	0.760078013	-3.486068249
H	2.999655962	-4.228572369	-2.581605673
H	2.705003262	-4.878037930	-0.915750206
C	1.469063044	1.542191505	0.394462973
O	1.283226609	0.019846981	2.337973595
C	0.704004526	-1.286120415	2.475387573
H	1.462130427	2.538751125	-1.497899294
H	1.926723599	2.362432718	0.935936034
H	1.445773363	-1.971517682	2.901853323
H	-0.189147562	-1.221427321	3.110421658
C	1.106587648	2.270674467	-3.977610111
C	2.310628653	2.298912525	-4.694329262
C	0.470832020	3.483188868	-3.656116486
C	2.873863935	3.522890806	-5.065998077
H	2.801388264	1.375570536	-4.984907627
C	1.036899805	4.702370644	-4.020861149
H	-0.482767165	3.469367504	-3.135311127
C	2.243356466	4.722556591	-4.728609085
C	1.078019381	-0.677102864	-4.214342594
C	0.343868971	-1.580483794	-4.996605873
C	2.424783468	-0.954936743	-3.935705185
C	0.947505951	-2.725151062	-5.515532017
H	-0.718988955	-1.413850784	-5.147446632
C	3.033581495	-2.090976000	-4.469074249
H	2.985631704	-0.298453659	-3.276361227
C	2.297602654	-2.975224257	-5.262917519
C	-2.680911779	0.095495664	-0.522487581
C	-2.450248003	1.466993213	-0.357248843
C	-2.752274990	-0.733175695	0.610301495

C	-2.307203054	2.006384373	0.921858072
H	-2.377654791	2.111729145	-1.226287484
C	-2.625942945	-0.188346997	1.887146831
H	-2.879586458	-1.805582762	0.490736097
C	-2.399159908	1.182839036	2.044569731
C	-4.454613686	-1.304661274	-2.391539097
C	-4.858294487	-1.634589076	-3.697752953
C	-5.348620892	-1.514126182	-1.330871701
C	-6.111127853	-2.199553490	-3.933740139
H	-4.193823814	-1.417939782	-4.532884598
C	-6.609202385	-2.064150333	-1.571462512
H	-5.071114063	-1.236624241	-0.318920225
C	-6.989025116	-2.417244673	-2.868315935
H	-5.839618206	2.206186533	-5.383438587
H	-6.409533024	-2.447680473	-4.949334621
H	-7.971660614	-2.845297813	-3.050464869
H	-7.295876980	-2.215430260	-0.741546154
H	-2.696537971	-0.834286273	2.759374857
H	-2.286353588	1.604002714	3.040416002
H	-2.128936052	3.072028160	1.030732870
H	0.517313361	5.628833294	-3.789197445
H	2.678361893	5.670346260	-5.034311771
H	3.804248571	3.535905600	-5.629527569
H	4.080362797	-2.292109966	-4.256031036
H	2.770999193	-3.864790916	-5.669872761
H	0.361432582	-3.424837112	-6.104445457

==============================

SF of **II$_S$-TS**

==============================

C	-2.217523336	8.621003151	-3.697443724
C	-1.126302242	8.314389229	-4.526375771
C	-3.436906338	7.976104736	-3.934424639
H	-0.177193716	8.829212189	-4.371520519
H	-4.295362473	8.209068298	-3.304334641
C	-1.226342559	7.366901398	-5.549651623
C	-3.583261013	7.024502754	-4.953903675
C	-2.464925051	6.722043991	-5.751651764
C	-2.565639019	5.646946907	-6.821142197
O	-3.133205891	5.792104244	-7.893986225
O	-1.948027968	4.583721638	-6.355744362
C	-3.155797720	0.111675754	-7.833762169
C	-2.294358969	1.150107741	-7.496131420
C	-2.550225973	2.465711594	-7.954411983
C	-3.696002722	2.785571098	-8.669532776
C	-4.577460289	1.736664176	-8.975018501
C	-4.302162170	0.420083970	-8.583624840
C	-1.047228336	1.236366391	-6.738349438
C	-0.592783630	2.530791044	-6.880033493
N	-1.445275307	3.296747446	-7.642566681
H	-2.944446564	-0.913148701	-7.533792019
H	-3.885377407	3.818273544	-8.944736481
H	-5.485466003	1.949829340	-9.533448219
H	-4.994555950	-0.374232322	-8.854042053
H	-0.467120409	0.390915543	-6.400495529
H	0.316787124	2.969095230	-6.498388767
C	-2.062387466	9.602464676	-2.555048704
H	-1.605086684	9.122124672	-1.678984404
H	-1.415305495	10.443428040	-2.832482100
H	-3.029469967	10.007470131	-2.236737251
C	-0.045673881	7.053543091	-6.442589760
H	0.833448231	7.647607803	-6.164748192
H	0.211166039	5.991415501	-6.387116909
H	-0.283987403	7.267558575	-7.492959023
C	-4.902655125	6.325357914	-5.194417000
H	-4.793979645	5.240412235	-5.076537132
H	-5.668220997	6.667191029	-4.490073681
H	-5.253054619	6.504903316	-6.216828823

==============================

MF of **II$_P$-TS'**

==============================

P	1.097514868	-0.559144616	-0.919190943
C	0.795758069	1.208102107	-1.434713244
C	-0.065575913	2.009594917	-0.440777838
P	-1.457924962	1.056273341	0.373810202
C	-2.944852829	1.238459110	-0.812577665
C	-2.112553120	2.411374569	1.538310170
C	-3.737152576	2.466042280	-0.319718480
C	-3.618761301	2.524439573	1.207071662
C	1.967608929	-1.255334020	-2.448110819
C	2.703383207	-0.517477095	0.101212859
C	3.273719549	-1.873427391	-1.890554190
C	3.839130640	-0.864042461	-0.883024931
C	-1.798710346	2.254671335	3.005655050
C	-1.104496479	3.262405157	3.688748598
C	-2.229370832	1.133415341	3.729140759
C	-0.861629784	3.164500713	5.060571194
C	-1.997839808	1.036440849	5.099529266
C	-1.313089252	2.052263021	5.772625446
C	-2.578006744	1.198596835	-2.283378124
C	-2.032783031	0.015850060	-2.817620993
C	-2.759223461	2.288539886	-3.146090269
C	-1.689569116	-0.076887369	-4.164026737
C	-2.414699316	2.199337006	-4.500075340
C	-1.879338861	1.019680262	-5.014547348
C	2.829806089	0.743574679	0.927217364
C	3.586597204	1.852061033	0.523811698
C	2.096191883	0.838748217	2.122188807
C	3.606419802	3.021070004	1.290615678
C	2.116519213	2.000890017	2.889478683
C	2.870454073	3.101913452	2.473673105
C	1.150147796	-2.189276695	-3.311541796
C	1.285633922	-2.141711712	-4.706408024
C	0.273951530	-3.134194136	-2.757962227
C	0.561035872	-3.005327702	-5.529559612
C	-0.452563524	-3.998468637	-3.577771425
C	-0.315631002	-3.935118198	-4.967272282
H	0.286706328	1.138196349	-2.400213718
H	1.751963615	1.719367385	-1.592737913
H	0.555640459	2.359970570	0.390984058
H	-0.483664542	2.891992569	-0.940123975
H	-3.534454823	0.337754220	-0.620934129
H	-1.639947295	3.337156296	1.185182452
H	-4.778336048	2.419535398	-0.661224008
H	-3.305874825	3.388186932	-0.727810800
H	-4.172572136	1.703649640	1.677012920
H	-4.028139591	3.454099655	1.619825482
H	2.251221895	-0.384565592	-3.054337740
H	2.581256628	-1.354672551	0.794300079
H	3.973484993	-2.090748072	-2.706020832
H	3.048718452	-2.827210665	-1.396305919
H	4.165779591	0.028443586	-1.430597186
H	4.714005947	-1.249865174	-0.346811414
H	-0.751214743	4.133224487	3.140427589
H	-2.741220474	0.325060040	3.218671560
H	-0.322892338	3.959082365	5.571749210
H	-2.343366861	0.157760739	5.638503075
H	-1.129842281	1.975728750	6.841107845
H	-1.880174756	-0.837289631	-2.165889502
H	-3.194320440	3.213648081	-2.779986858
H	-1.268471837	-1.002952933	-4.545620918
H	-2.572535515	3.058185816	-5.150944233
H	-1.615077615	0.951165378	-6.067549706
H	4.171074867	1.814789772	-0.391135246
H	1.495769739	-0.000962132	2.449572802
H	4.200929642	3.869084358	0.958827198
H	1.533958912	2.041538715	3.804897308
H	2.887572765	4.012227535	3.068146229
H	1.959202409	-1.412276626	-5.151992321
H	0.150212586	-3.174145699	-1.680546045
H	0.675347626	-2.945852041	-6.609421253
H	-1.131700158	-4.723832607	-3.136111021
H	-0.889267623	-4.602976322	-5.604075432
C	0.753153086	-2.406432152	2.848875761
C	2.146453142	-2.579854012	3.018432140
H	2.708700418	-3.163349628	2.295493364
C	2.823168516	-2.022977114	4.104898930
H	3.897451878	-2.167780161	4.195854664
C	2.136247873	-1.287407517	5.069801331

H	2.665635586	-0.847136736	5.910346508
H	0.200413346	-0.540817976	5.669814587
C	0.751443326	-1.119947791	4.934458256
C	0.077511162	-1.665846348	3.849928379
H	-0.991639972	-1.504722238	3.733704567
C	0.002034192	-2.952872038	1.707489729
H	-0.958955526	-3.345334530	2.049116850
C	0.744785309	-3.982131004	0.866093278
H	0.069293432	-4.465417862	0.157541633
H	1.196636915	-4.779232979	1.480033755
H	1.562473536	-3.537448168	0.283825696
Cu	-0.723907650	-1.349559426	0.530492187

===============================

SF of **II**$_P$**-TS'**

===============================

C	-5.930175781	-1.159552455	-4.882779121
C	-6.941804409	-0.228960276	-4.615285873
H	-5.623552322	-1.332061291	-5.914062977
C	-5.290955067	-1.865723014	-3.858184338
C	-7.319998264	-0.014535896	-3.283088207
C	-5.701135635	-1.633148313	-2.532740831
H	-8.102010727	0.711429477	-3.060783386
C	-6.714113712	-0.703659415	-2.229115248
C	-5.002838135	-2.332342863	-1.389473796
O	-5.485211372	-3.198105574	-0.686156809
O	-3.795216084	-1.782765985	-1.281542778
N	-2.696113586	-2.335818052	0.012296468
C	-4.103980064	-3.884889364	2.983101368
C	-3.479003906	-3.651715279	1.759246469
C	-4.730436802	-2.812494278	3.629152536
H	-4.117094517	-4.879279137	3.420539618
C	-3.443085670	-2.344312429	1.232649803
C	-2.820689440	-4.500400066	0.778455675
C	-4.741293907	-1.532017231	3.059840441
H	-5.230163097	-2.978693962	4.579729080
C	-4.091590881	-1.285511971	1.845251560
C	-2.425652504	-3.704859257	-0.246009588
H	-2.663710356	-5.567576885	0.860859156
H	-5.253876686	-0.718783498	3.566344738
H	-4.109388828	-0.307979345	1.383061528
H	-1.931620717	-3.952447891	-1.170753121
C	-4.180278301	-2.847609997	-4.161909103
H	-4.094736099	-3.028115749	-5.238998890
H	-3.216947079	-2.472640991	-3.800327063
H	-4.359652042	-3.810314655	-3.666885376
C	-7.106694221	-0.441699028	-0.791239858
H	-7.336849689	-1.375305891	-0.269145072
H	-6.279460907	0.025681041	-0.239732102
H	-7.972607136	0.224986821	-0.728274822
C	-7.634313107	0.512474179	-5.737074375
H	-7.898195744	1.533419013	-5.438867092
H	-7.003353119	0.571018219	-6.631148338
H	-8.566912651	0.009645576	-6.025473595

===============================

MF of **II**$_P$**-TS**

===============================

P	1.552207589	-0.433497280	-0.347039580
C	0.803309798	1.114454269	-1.103900790
C	-0.413246989	1.689554095	-0.359916091
P	-1.732558250	0.462177217	0.127420425
C	-2.993044853	0.584953010	-1.283405542
C	-2.783313751	1.533219576	1.280158162
C	-3.850874662	1.816473365	-0.948501706
C	-4.141287804	1.727272391	0.553770185
C	3.046311140	-0.634564102	-1.534865975
C	2.665996313	0.248764455	1.041304946
C	4.300409794	-0.413844317	-0.662221134
C	3.966033459	0.687271118	0.348897904
C	-2.917335510	1.117779493	2.731684446
C	-3.287245274	2.108104706	3.655644417
C	-2.699557781	-0.182210907	3.198663473
C	-3.430841684	1.810173750	5.008289814
C	-2.830334663	-0.482427537	4.554875851
C	-3.197477579	0.509025753	5.463389874
C	-2.338809729	0.496341139	-2.640368223
C	-1.802113295	-0.736021698	-3.051223278
C	-2.198143482	1.598429441	-3.492756844
C	-1.157067060	-0.870641172	-4.277210712
C	-1.545827508	1.469038725	-4.722750187
C	-1.023548961	0.237538517	-5.120234013
C	1.961767077	1.237346292	1.938021541
C	2.184928894	2.618555546	1.865039229
C	1.001632214	0.758530200	2.846678495
C	1.455304980	3.501287222	2.666934490
C	0.281744242	1.636963964	3.653418779
C	0.499995917	3.015324593	3.559444666
C	2.976147175	-1.908006310	-2.346964598
C	2.240452766	-1.902967572	-3.544569969
C	3.560265064	-3.114610195	-1.932448149
C	2.082707644	-3.064073801	-4.298612595
C	3.409330845	-4.279600620	-2.689300299
C	2.666675806	-4.261471748	-3.872558594
H	0.518914819	0.822543502	-2.122245073
H	1.565896988	1.898106694	-1.194422722
H	-0.090658374	2.148244619	0.577509940
H	-0.876209199	2.479232073	-0.964858532
H	-3.634119272	-0.294195771	-1.152063131
H	-2.273350239	2.504566431	1.266123414
H	-4.764430523	1.837254763	-1.552950382
H	-3.303220272	2.744328976	-1.157833695
H	-4.799998283	0.875475585	0.761832654
H	-4.648881912	2.619228363	0.936626852
H	2.972990274	0.211550355	-2.229857206
H	2.882881880	-0.647310972	1.636635900
H	5.165882587	-0.165924370	-1.287624240
H	4.555555820	-1.326739669	-0.111502595
H	3.826379061	1.637923956	-0.181665435
H	4.771040916	0.842143238	1.077731371
H	-3.451120615	3.126257181	3.306881428
H	-2.405833960	-0.973902941	2.519104958
H	-3.714695215	2.593870163	5.706271648
H	-2.649181128	-1.495078444	4.892431736
H	-3.297613144	0.264030516	6.516914368
H	-1.887423754	-1.593284249	-2.389307976
H	-2.608724594	2.563753605	-3.210309982
H	-0.754136384	-1.837346554	-4.567271233
H	-1.451126695	2.335479021	-5.372612000
H	-0.521916449	0.137965560	-6.078860760
H	2.925835848	3.017037630	1.178926826
H	0.816562414	-0.309126616	2.918729544
H	1.637355566	4.570724487	2.591433287
H	-0.458177596	1.246367216	4.344375134
H	-0.071687490	3.700727463	4.179358006
H	1.777111650	-0.976964891	-3.880061626
H	4.131982803	-3.160454035	-1.008180737
H	1.508028984	-3.035802603	-5.223772049
H	3.868977070	-5.204275608	-2.345876932
H	2.545999050	-5.169302940	-4.457935810
C	0.408840895	-3.187856674	2.267024279
C	1.816830277	-3.045451641	2.305877924
H	2.398613691	-3.254272223	1.412668705
C	2.469108105	-2.645597219	3.472164631
H	3.553382397	-2.551784039	3.472402573
C	1.748127699	-2.368752718	4.637181759
H	2.261749983	-2.054358721	5.541287899
H	-0.227583826	-2.309749603	5.521079540
C	0.353571177	-2.507287264	4.624217987
C	-0.300663531	-2.912974358	3.467065334
H	-1.381442189	-3.032453537	3.465940952
C	-0.330547065	-3.582618952	1.057212710
H	-1.254238486	-4.103661537	1.310894370
C	0.447841853	-4.275262356	-0.050849479
H	-0.221410096	-4.568386555	-0.864404082
H	0.950850308	-5.189989090	0.305995077
H	1.219347835	-3.633003712	-0.486955106
Cu	-0.844205499	-1.710446954	0.479010552

===============================

SF of **II$_P$-TS**

==============================

N	-4.768986225	-3.335892439	1.680386543
C	-2.980148315	-5.301344395	-0.791842520
C	-3.483404160	-4.263678551	-0.016624460
C	-3.243602037	-6.618695259	-0.385598898
H	-2.402424097	-5.103729248	-1.689900756
C	-4.284210205	-4.544749737	1.112038374
C	-3.415002108	-2.808472395	-0.086557373
C	-4.017158031	-6.882583141	0.748252153
H	-2.846132517	-7.445823669	-0.967177629
C	-4.564873695	-5.840340137	1.513513327
C	-4.190054417	-2.325780153	0.952174544
H	-3.041283369	-2.249433041	-0.929583430
H	-4.207151890	-7.911986828	1.038844347
H	-5.175204277	-6.015313148	2.392491579
H	-4.398271561	-1.299417496	1.216659784
O	-3.829151392	-3.307559013	3.331943512
C	-4.474554539	-3.949291945	4.283363819
O	-5.581092834	-4.459529400	4.232806206
C	-3.596441507	-3.962373257	5.522679329
C	-3.947838783	-3.135340214	6.612766743
C	-2.430060387	-4.744177341	5.550232887
C	-3.087440968	-3.079918623	7.709363937
C	-1.604409695	-4.668272495	6.681559563
C	-1.901383996	-3.830389500	7.756261826
H	-3.342137575	-2.433793068	8.548764229
H	-0.691705167	-5.260409355	6.703454494
C	-2.077928066	-5.689436913	4.423100471
H	-0.997352600	-5.855182648	4.377315998
H	-2.565927744	-6.660230637	4.577355862
H	-2.401928425	-5.309556961	3.450954437
C	-5.220114231	-2.321148872	6.573089123
H	-6.086107731	-2.967698336	6.402627945
H	-5.365599155	-1.768750072	7.506530762
H	-5.195684910	-1.596133351	5.750495434
C	-0.976708174	-3.715149641	8.946225166
H	-0.681789517	-2.671850681	9.117812157
H	-1.465137124	-4.064379215	9.864324570
H	-0.063762590	-4.303373337	8.806899071

Table S6. Vibrational Frequencies (in cm^{-1}) of the Optimized Geometries

==============================
Styrene
==============================
37.09 206.57 243.54 412.15 447.67 453.34
563.83 633.33 654.65 712.69 789.82 798.70
852.50 924.57 926.34 970.57 996.29 1013.70
1035.49 1047.03 1066.76 1122.27 1196.77 1219.74
1235.81 1329.32 1365.31 1372.50 1463.86 1494.10
1541.30 1633.65 1661.33 1710.02 3142.47 3163.49
3171.16 3178.79 3189.01 3198.90 3207.27 3246.49
==============================
1*H*-indol-1yl trimethylbenzoate
==============================
23.79 32.02 43.63 60.11 69.57 76.88
143.55 172.15 192.33 194.16 202.31 222.90
229.56 234.07 274.54 298.84 314.76 350.77
363.55 412.04 434.14 494.62 514.80 532.38
534.95 543.81 560.73 576.12 579.84 593.35
606.39 627.25 707.27 716.01 743.09 756.45
771.85 781.03 789.63 836.50 853.12 863.83
873.49 889.03 901.94 935.97 960.23 975.41
976.09 1004.24 1037.97 1043.54 1047.65 1059.59
1062.62 1065.03 1067.17 1073.01 1100.43 1152.77
1184.59 1188.87 1213.28 1252.37 1257.70 1293.69
1319.53 1329.24 1340.12 1366.11 1392.55 1425.95
1428.92 1430.61 1434.00 1455.44 1472.60 1488.01
1498.04 1501.67 1504.47 1505.90 1512.78 1523.35
1525.17 1564.60 1620.21 1631.81 1662.40 1673.90
1853.59 3039.50 3055.90 3056.23 3100.87 3122.39
3124.51 3128.11 3131.57 3137.94 3175.57 3177.67
3178.29 3189.17 3200.54 3210.94 3259.76 3289.92
==============================
C3-substituted 1*H*-indol-1yl trimethylbenzoate
==============================
11.61 15.91 19.70 24.67 33.59 52.83
71.48 83.36 87.19 108.51 143.03 163.09
171.85 189.63 199.84 205.25 207.91 229.47
238.07 244.48 259.72 280.68 288.01 314.44
331.00 351.88 378.40 411.14 435.08 448.87
516.04 531.80 535.23 543.68 562.01 576.18
582.31 583.27 601.83 604.59 621.34 683.05
717.86 755.74 763.14 771.15 781.05 787.85
809.69 827.82 844.08 865.87 874.87 902.45
936.87 960.29 974.54 975.60 997.32 1001.04
1023.90 1038.90 1040.39 1049.46 1062.17 1064.10
1066.13 1072.13 1076.74 1098.43 1122.17 1145.70
1168.70 1184.47 1185.56 1190.06 1199.81 1228.86
1248.48 1253.79 1255.94 1293.33 1314.39 1316.38
1319.82 1339.22 1344.65 1376.52 1392.78 1411.88
1425.89 1430.26 1433.45 1451.03 1454.72 1472.19
1489.16 1494.63 1496.43 1497.84 1498.88 1503.32
1504.28 1506.25 1514.45 1516.93 1524.40 1525.93
1550.93 1610.28 1618.86 1633.37 1662.70 1674.85
1847.41 2952.52 2972.35 2985.16 3014.71 3031.61
3039.65 3055.37 3056.74 3066.44 3097.55 3120.66
3121.80 3124.60 3127.03 3132.53 3134.83 3170.25
3176.21 3178.14 3188.39 3200.51 3209.81 3281.54
==============================
Trimethylbenzoate
==============================
58.06 69.95 78.97 132.45 151.18 169.49
232.86 234.67 241.72 297.15 314.36 351.72
428.87 504.69 520.24 535.61 577.64 597.67
605.13 730.21 798.88 806.06 862.76 874.24
957.46 974.87 1035.38 1043.76 1057.67 1061.09
1065.17 1066.20 1112.72 1210.19 1275.24 1311.39
1340.97 1376.61 1412.71 1416.35 1420.66 1450.26
1467.85 1474.58 1478.96 1500.31 1508.20 1517.88
1526.49 1614.95 1655.81 1733.62 3004.27 3021.60
3022.77 3058.77 3079.35 3080.69 3090.70 3122.10
3125.50 3131.99 3133.17
==============================
3a
==============================
24.76 38.22 58.29 102.39 166.82 208.58
224.24 247.80 263.21 310.76 349.67 415.60
434.10 454.36 471.41 496.82 556.47 587.77
595.59 613.31 630.80 644.39 707.02 717.72
731.23 753.96 775.33 781.28 793.13 810.62
857.25 861.90 864.64 894.90 928.34 934.28
971.17 979.15 997.78 1003.39 1016.38 1033.47
1043.51 1058.62 1081.43 1101.55 1118.60 1137.53
1157.00 1191.10 1197.82 1222.27 1228.69 1233.54
1246.84 1323.35 1337.67 1349.46 1369.84 1382.28
1392.04 1395.76 1422.85 1447.71 1494.03 1501.45
1508.08 1517.41 1524.41 1543.06 1569.21 1627.49
1644.53 1666.14 1668.93 3042.01 3052.82 3130.12
3138.49 3173.83 3175.63 3182.46 3182.48 3192.80
3192.88 3203.75 3204.11 3211.78 3254.04 3280.04
==============================
4a
==============================
32.03 44.61 56.98 119.31 161.87 199.14
225.36 251.49 293.00 313.05 331.12 388.14
416.66 432.32 436.33 472.54 496.30 543.18
586.96 588.95 632.49 635.81 661.18 703.36
717.42 755.93 773.53 780.58 787.17 794.42
815.33 861.07 861.60 888.75 927.89 936.21
975.90 976.20 981.24 997.55 1016.76 1042.58
1049.82 1069.33 1079.21 1110.44 1115.70 1133.02
1163.36 1189.95 1196.15 1215.85 1223.05 1234.68
1278.25 1305.21 1325.95 1343.03 1362.05 1368.78
1388.84 1391.07 1422.76 1458.08 1490.39 1496.75
1515.14 1518.18 1536.50 1541.37 1605.20 1632.33
1641.56 1664.10 1678.51 3010.30 3046.83 3120.27
3128.92 3170.63 3175.12 3178.10 3185.28 3188.44
3198.62 3199.96 3209.48 3209.69 3256.74 3692.94
==============================
I_S
==============================
17.75 23.72 30.32 31.59 38.72 39.89
42.30 45.90 51.24 51.90 61.25 63.79
69.27 73.35 92.77 98.28 107.97 112.63
118.29 125.52 132.60 142.04 155.58 174.29
185.35 190.30 203.89 218.27 220.43 230.07
235.83 250.20 257.39 259.33 306.69 315.18
320.76 331.58 343.88 350.95 365.43 407.91
410.18 412.47 419.34 420.53 420.88 437.65
438.37 461.58 468.39 474.87 476.59 503.42
516.52 519.68 524.35 550.78 578.32 597.11
624.70 626.60 629.27 629.97 632.55 633.40
643.98 697.12 701.74 709.34 710.08 710.34
711.36 714.36 715.40 718.45 719.86 736.64
755.14 758.37 763.38 763.77 767.86 770.95
772.94 825.32 825.98 865.31 867.84 869.98
870.50 871.99 894.53 908.18 938.12 939.34
940.06 941.43 943.19 945.75 973.44 976.69
986.29 987.44 988.21 990.52 1004.85 1006.33
1009.39 1012.36 1014.80 1015.06 1017.44 1019.24
1031.83 1049.52 1052.04 1053.27 1054.77 1074.56
1090.15 1108.12 1108.87 1114.44 1114.94 1121.09
1121.45 1123.44 1124.73 1133.22 1137.01 1143.58
1144.81 1156.27 1197.32 1197.58 1199.03 1199.78
1200.09 1208.78 1210.98 1212.02 1217.47 1219.82
1227.74 1229.84 1272.17 1285.56 1297.91 1326.89
1327.35 1331.20 1332.96 1361.01 1361.79 1366.67
1368.29 1371.26 1377.14 1442.75 1445.58 1465.83
1476.08 1476.82 1477.86 1478.54 1482.68 1497.40
1503.63 1523.71 1524.28 1528.29 1529.65 1552.67
1553.12 1611.52 1626.59 1628.46 1628.95 1630.82
1644.97 1646.05 1646.33 1646.76 1647.67 1650.17
1670.78 1673.86 3005.16 3008.08 3093.98 3098.09
3160.75 3167.62 3169.67 3171.29 3173.67 3175.50
3178.08 3178.75 3188.58 3189.21 3189.96 3190.32
3198.17 3199.31 3203.19 3203.35 3205.77 3205.97
3209.52 3209.86 3210.49 3214.74 3224.80 3225.33

==============================
IX_S
==============================
3.15 17.67 22.24 29.09 29.81 32.52
34.54 37.27 40.12 41.24 47.07 49.72
52.99 57.77 66.74 68.20 73.05 74.04
75.71 82.27 84.84 91.49 101.41 113.22
115.82 116.46 124.74 133.39 139.18 148.48
159.40 164.58 174.44 176.58 181.94 187.74
190.07 202.33 210.70 216.75 228.17 228.73
236.83 238.89 249.97 252.36 254.08 259.56
272.15 295.90 305.34 312.05 330.75 335.63
339.01 351.27 403.43 407.76 410.97 414.38
418.72 420.55 422.07 437.40 442.35 459.41
464.03 465.36 482.09 482.73 506.88 514.46
515.53 523.26 524.91 528.59 535.53 550.56
572.60 576.43 596.69 605.26 623.98 624.71
626.69 627.73 628.75 631.00 631.83 637.89
697.25 700.22 707.63 709.55 712.19 712.87
716.98 717.39 720.12 721.60 733.42 735.75
755.00 759.44 762.80 764.53 767.11 768.72
773.58 809.29 826.37 826.65 837.10 860.41
867.49 868.53 874.45 877.36 882.37 892.03
896.27 905.97 938.51 940.50 940.85 943.39
950.76 955.27 958.25 973.14 976.01 976.41
986.71 989.00 996.03 998.13 1006.34 1010.86
1010.94 1012.79 1014.15 1017.83 1028.04 1029.41
1036.23 1040.08 1044.29 1047.86 1051.28 1051.64
1051.89 1062.27 1064.61 1068.08 1069.15 1072.01
1089.81 1107.14 1108.26 1113.92 1115.09 1121.95
1123.23 1123.32 1125.96 1131.45 1134.07 1137.86
1142.55 1144.26 1157.19 1196.77 1196.94 1197.99
1198.11 1200.98 1204.52 1207.63 1211.31 1215.84
1218.91 1223.47 1228.98 1232.10 1273.44 1286.77
1286.93 1296.74 1317.50 1325.32 1325.94 1329.50
1330.92 1334.40 1360.06 1365.26 1367.87 1372.52
1374.29 1377.60 1424.63 1426.08 1426.77 1431.97
1445.43 1447.98 1450.65 1465.51 1473.67 1475.73
1477.69 1478.05 1483.22 1487.82 1493.35 1496.04
1496.17 1501.02 1502.92 1505.95 1514.27 1522.32
1526.06 1529.71 1530.06 1531.05 1554.13 1554.24
1595.22 1624.60 1625.40 1627.89 1628.10 1628.88
1643.22 1643.53 1643.90 1645.42 1645.65 1646.85
1660.14 1669.52 1672.72 3025.20 3029.39 3030.47
3036.43 3037.13 3080.84 3083.73 3083.90 3098.21
3099.36 3109.15 3121.33 3131.65 3148.15 3150.61
3162.60 3164.71 3165.23 3168.32 3170.05 3174.39
3175.48 3175.51 3183.57 3186.76 3188.10 3188.19
3193.96 3195.78 3200.15 3201.18 3201.33 3203.33
3206.51 3207.78 3207.99 3211.58 3223.17 3225.48
==============================
I_P
==============================
19.31 23.69 26.54 44.79 45.87 47.01
49.47 53.36 58.24 66.02 85.97 91.86
103.65 105.11 107.09 114.18 116.76 144.77
158.55 174.83 181.09 199.57 223.64 227.82
230.71 239.07 251.45 271.36 272.21 280.43
304.25 315.09 340.55 347.44 353.10 371.30
382.02 415.25 416.43 423.78 424.73 438.72
474.75 481.89 491.26 492.22 508.22 512.86
535.09 536.21 606.28 607.74 614.31 625.69
631.66 633.18 633.69 633.99 644.20 648.23
682.01 682.69 700.81 701.92 716.44 717.84
721.91 722.59 770.78 771.57 783.75 785.79
810.92 838.79 847.73 857.24 859.04 863.77
864.43 872.19 872.86 893.61 911.07 911.46
928.23 929.27 931.73 932.63 941.53 942.39
976.21 976.77 978.50 979.01 999.77 1000.87
1002.19 1009.07 1010.40 1012.09 1013.81 1015.51
1016.09 1016.22 1016.56 1017.09 1020.01 1057.56
1057.75 1059.47 1060.11 1067.13 1068.02 1111.95
1112.38 1117.56 1117.97 1130.45 1146.34 1150.75
1173.71 1186.56 1189.26 1195.88 1195.90 1196.45
1196.96 1215.68 1216.12 1222.97 1223.26 1225.56
1225.61 1232.15 1232.72 1248.14 1248.89 1263.98
1269.64 1291.21 1301.92 1302.75 1315.28 1316.60
1319.88 1343.86 1344.08 1354.82 1355.40 1365.51
1365.79 1368.44 1368.54 1375.79 1376.72 1400.25
1401.43 1464.98 1478.49 1492.01 1492.62 1493.70
1494.32 1506.28 1506.33 1515.64 1515.99 1539.72
1539.85 1540.62 1540.85 1624.70 1636.12 1636.53
1637.07 1637.29 1659.83 1660.10 1660.50 1660.97
3032.75 3034.18 3036.01 3037.47 3040.43 3040.92
3041.93 3044.25 3045.07 3046.65 3082.47 3083.17
3094.23 3095.23 3096.08 3107.89 3156.05 3157.62
3163.32 3163.58 3168.62 3171.67 3173.60 3173.92
3179.99 3180.01 3189.79 3190.16 3190.78 3190.83
3199.10 3199.29 3202.64 3202.83 3213.74 3214.14
==============================
IX_P
==============================
8.46 10.58 17.78 21.34 29.34 33.93
39.89 41.33 45.15 48.96 50.86 54.99
59.38 64.03 76.37 77.03 78.45 84.97
91.01 100.82 110.92 114.46 125.25 128.60
133.62 141.95 155.75 160.90 165.02 180.87
182.47 199.77 204.12 214.48 229.53 232.79
233.48 242.40 244.75 250.32 260.14 269.52
276.95 278.58 293.69 308.98 310.09 334.88
350.92 357.11 368.00 380.27 404.13 416.52
417.83 425.30 425.65 436.40 438.12 483.45
489.00 494.14 499.91 512.26 517.15 523.87
532.09 536.31 539.29 543.44 572.06 600.58
603.17 605.21 614.61 620.57 625.61 632.39
632.66 633.19 633.64 641.41 648.22 682.68
686.12 706.08 707.63 717.23 717.35 722.11
725.10 725.64 768.66 769.88 783.34 785.07
811.20 813.86 836.99 845.07 845.17 852.40
856.45 861.66 862.07 874.14 874.87 876.01
893.79 897.36 902.04 906.02 925.61 929.23
930.30 932.72 937.90 941.42 958.86 974.11
974.78 978.00 980.20 983.18 994.44 999.84
1001.16 1004.65 1005.99 1011.76 1013.80 1014.34
1014.81 1015.57 1017.01 1017.62 1026.24 1040.02
1044.96 1055.86 1056.71 1058.00 1059.71 1062.78
1063.22 1065.95 1067.00 1067.27 1067.96 1112.05
1112.69 1116.74 1118.04 1128.44 1131.14 1146.17
1150.72 1173.67 1182.18 1187.67 1195.22 1195.67
1197.30 1197.77 1210.37 1212.16 1220.60 1222.51
1225.22 1226.02 1229.10 1230.31 1232.97 1246.58
1247.62 1254.33 1261.98 1285.59 1291.73 1296.12
1298.86 1312.31 1313.61 1314.30 1321.48 1332.43
1342.76 1344.19 1353.15 1354.43 1360.89 1363.21
1367.97 1370.15 1373.19 1375.31 1398.62 1401.55
1424.74 1427.42 1428.86 1431.49 1448.10 1464.12
1475.94 1481.83 1489.71 1490.72 1491.78 1492.98
1494.81 1496.48 1498.84 1502.67 1506.71 1507.08
1511.25 1515.51 1516.08 1522.84 1537.32 1540.18
1540.40 1542.80 1579.18 1624.82 1631.72 1634.46
1635.13 1636.70 1657.53 1658.66 1658.78 1659.65
1660.40 3026.94 3027.56 3029.87 3036.90 3037.71
3040.07 3041.68 3043.59 3045.77 3046.00 3047.34
3050.30 3054.84 3081.55 3082.11 3086.55 3095.94
3098.40 3098.93 3110.92 3112.46 3113.63 3114.59
3117.34 3132.53 3151.40 3155.55 3157.61 3158.31
3164.62 3167.05 3169.17 3170.05 3172.47 3176.82
3177.43 3181.22 3185.08 3185.34 3186.88 3187.87
3195.21 3196.62 3200.03 3200.12 3206.11 3207.39
==============================
I_S-TS
==============================
-827.22 15.54 24.27 32.93 34.42 36.09
37.02 42.70 44.29 50.34 54.28 56.18
59.38 63.88 65.88 69.76 72.82 82.72
89.86 97.14 100.70 109.78 115.69 117.15
125.84 133.88 155.52 164.40 170.65 180.40
184.66 194.52 197.04 210.78 220.89 225.70
230.44 232.58 246.03 250.54 260.81 262.15
288.71 306.42 313.15 327.67 334.33 349.57

386.45 410.88 412.35 414.88 417.39 417.93
422.61 426.06 438.08 438.65 455.51 467.80
471.36 481.09 485.91 496.43 508.62 515.60
516.26 528.18 549.30 555.42 569.09 572.99
596.67 620.94 627.17 631.21 631.33 632.47
633.00 634.18 641.30 697.43 698.66 709.34
710.79 712.26 713.07 713.47 715.39 716.16
721.81 723.77 735.77 753.63 758.75 761.11
763.37 765.12 767.02 768.57 770.36 788.83
801.43 826.70 827.84 849.32 858.79 870.46
872.37 874.83 876.26 883.97 894.05 906.99
939.84 940.41 941.66 944.15 947.14 949.14
959.04 967.41 974.70 976.31 978.41 988.33
988.92 991.06 993.81 1003.66 1007.70 1008.42
1010.18 1012.44 1014.41 1015.14 1016.07 1016.33
1029.44 1050.57 1051.83 1053.25 1054.02 1054.28
1071.40 1088.16 1108.03 1109.15 1109.80 1113.53
1114.22 1120.52 1120.90 1123.43 1125.56 1132.10
1133.82 1137.16 1141.80 1153.41 1154.33 1155.86
1189.56 1193.78 1196.55 1197.86 1198.07 1202.02
1203.51 1209.66 1212.96 1216.86 1217.88 1220.28
1223.02 1224.15 1226.51 1275.52 1280.90 1288.39
1297.61 1328.54 1328.77 1330.69 1333.03 1341.31
1360.65 1364.47 1365.53 1368.28 1368.55 1370.04
1380.07 1415.28 1443.26 1446.79 1447.80 1466.10
1475.40 1475.49 1477.97 1479.26 1484.71 1485.97
1494.65 1503.69 1521.42 1524.04 1524.46 1526.79
1527.68 1542.87 1554.99 1556.03 1612.37 1626.33
1626.71 1627.97 1628.38 1644.31 1645.21 1645.99
1646.45 1647.05 1648.20 1651.34 1669.64 1675.77
3026.65 3027.19 3082.97 3103.83 3147.23 3152.08
3152.63 3156.72 3167.50 3169.25 3171.40 3172.80
3173.98 3175.54 3181.77 3183.46 3184.57 3186.20
3189.57 3192.81 3193.63 3195.30 3195.55 3199.31
3200.43 3200.72 3201.52 3208.10 3208.27 3209.33
3210.40 3214.00 3214.83 3223.40 3227.00 3232.64

==============================

I_S-TS'

==============================

-791.87 29.95 36.39 39.64 49.18 50.38
50.89 54.61 56.24 63.68 67.01 68.92
70.80 71.71 77.58 81.81 85.92 92.77
93.52 99.12 114.10 116.77 118.00 125.37
135.76 148.43 151.52 160.48 162.80 176.63
183.64 192.67 201.41 217.05 224.64 232.16
235.45 236.76 253.92 258.66 262.71 265.25
289.48 304.79 312.46 328.75 337.06 350.39
404.37 406.26 417.81 419.23 422.54 423.77
426.48 429.73 439.22 444.69 454.87 467.71
469.78 480.62 484.41 511.30 514.54 516.62
519.51 528.29 546.52 551.83 568.38 575.68
596.07 621.08 626.28 631.53 632.06 633.51
633.89 634.91 639.37 697.52 699.31 710.07
710.55 711.34 715.34 715.98 719.57 720.14
722.28 722.73 735.36 754.54 759.60 764.96
765.83 769.28 770.88 772.64 775.22 792.42
798.60 825.47 832.86 844.69 856.72 874.70
876.46 881.35 882.42 884.96 891.20 906.62
939.00 944.89 945.60 948.49 953.39 954.11
958.55 974.42 975.45 977.40 978.74 991.91
992.38 997.99 999.54 1004.34 1010.42 1010.94
1013.76 1015.14 1016.05 1017.01 1017.37 1019.00
1027.32 1051.75 1054.30 1054.51 1054.71 1055.23
1071.95 1089.74 1108.19 1109.03 1113.64 1115.95
1116.94 1118.24 1118.95 1122.67 1124.73 1132.23
1138.34 1138.83 1143.97 1145.60 1155.46 1156.10
1190.88 1198.11 1199.47 1199.64 1199.79 1200.81
1206.83 1207.69 1212.86 1214.48 1217.97 1224.41
1226.39 1227.95 1228.56 1273.83 1276.48 1288.91
1297.34 1326.71 1329.35 1331.39 1334.96 1343.14
1361.13 1366.11 1367.29 1369.92 1370.13 1370.21
1377.90 1438.74 1445.14 1448.29 1451.21 1466.11
1475.95 1476.17 1479.76 1481.79 1484.28 1487.40
1492.69 1502.04 1524.05 1524.85 1527.83 1527.90
1529.08 1545.92 1554.26 1554.58 1614.33 1626.38
1628.27 1628.50 1630.69 1643.85 1644.69 1645.06
1647.89 1648.54 1649.36 1653.92 1671.01 1674.71
3031.58 3033.49 3084.49 3086.33 3152.19 3158.14
3160.13 3167.20 3168.38 3172.30 3173.97 3175.80
3176.08 3179.63 3179.75 3181.60 3188.75 3190.43
3191.38 3193.32 3196.47 3196.50 3197.34 3199.85
3204.47 3205.07 3207.69 3208.57 3211.08 3215.22
3215.33 3217.10 3221.89 3224.77 3229.36 3242.19

==============================

II_S

==============================

9.82 18.94 24.04 28.61 32.01 34.05
36.57 40.38 44.66 50.61 51.10 52.60
55.91 59.26 65.37 66.91 75.59 86.49
90.49 94.87 98.78 105.23 109.72 116.40
121.65 125.64 151.84 156.73 172.58 181.58
184.77 192.44 204.60 212.30 221.73 224.20
226.97 231.23 235.23 247.52 254.34 258.82
261.13 308.78 314.82 328.14 332.71 350.44
394.53 409.54 412.60 415.14 416.23 418.24
421.56 424.27 436.33 438.96 454.78 467.58
473.21 478.26 479.02 509.45 513.21 517.46
522.71 537.04 553.04 566.99 575.33 597.91
624.25 625.29 630.55 631.00 632.32 632.97
634.19 644.12 696.32 701.25 709.29 710.32
711.68 712.72 714.39 714.93 715.48 722.43
722.99 737.18 754.63 757.99 763.44 764.27
765.01 765.96 767.57 771.33 778.10 824.30
826.54 848.41 865.50 868.86 869.43 871.60
872.50 888.60 894.57 907.69 929.78 938.09
939.31 940.04 941.28 944.15 945.90 963.15
973.28 975.97 977.77 984.60 985.04 988.13
989.04 992.72 1005.23 1006.18 1007.37 1009.25
1012.53 1015.00 1015.23 1016.35 1016.77 1031.51
1050.35 1052.33 1053.18 1053.37 1056.64 1058.86
1073.66 1088.74 1090.44 1109.12 1109.91 1113.13
1114.60 1120.83 1123.72 1124.60 1126.21 1129.78
1133.82 1137.64 1143.34 1144.51 1155.77 1188.91
1193.72 1196.74 1197.37 1197.67 1200.14 1207.46
1209.64 1212.04 1212.33 1218.19 1218.42 1222.99
1226.04 1235.84 1272.85 1287.27 1299.02 1316.57
1327.13 1329.05 1330.61 1331.96 1361.03 1362.01
1363.22 1364.61 1367.20 1367.59 1377.83 1393.79
1413.45 1442.87 1445.62 1466.48 1474.48 1476.52
1477.49 1478.56 1483.92 1490.24 1496.80 1502.43
1503.91 1516.49 1523.29 1524.04 1525.92 1526.77
1528.11 1553.01 1553.77 1607.84 1625.70 1627.45
1628.75 1629.13 1642.99 1645.11 1645.81 1646.08
1646.43 1647.58 1648.97 1670.09 1673.87 2967.21
3007.01 3011.78 3038.28 3060.16 3089.71 3094.70
3099.92 3149.41 3160.52 3165.64 3169.44 3170.68
3173.63 3175.10 3175.52 3180.95 3184.89 3186.58
3187.64 3188.80 3191.06 3195.81 3196.07 3197.88
3198.47 3201.91 3202.13 3202.51 3204.53 3206.65
3208.40 3209.76 3211.03 3211.36 3224.06 3225.84

==============================

II_S-TS

==============================

-434.67 12.56 14.80 21.40 24.70 29.20
31.60 33.79 38.73 40.26 42.31 45.04
49.37 52.21 55.23 55.69 60.44 63.45
64.90 69.34 71.42 71.74 75.27 78.14
82.79 90.73 93.70 95.56 99.09 105.12
105.57 115.04 116.56 119.90 128.03 129.67
133.60 139.11 142.65 146.30 152.44 156.95
162.60 170.48 173.72 181.72 187.23 191.74
194.46 203.43 209.39 219.98 221.83 227.98
229.67 232.25 233.99 235.74 238.86 245.05
255.10 264.02 266.48 276.84 283.29 285.62
308.38 310.44 316.61 325.84 329.17 333.83
351.40 361.52 365.73 411.09 414.62 417.59
420.03 421.81 422.66 427.68 429.68 432.65
436.80 441.77 443.52 449.13 459.42 462.25
479.42 482.53 509.83 513.50 514.45 517.09
527.68 528.79 535.56 536.98 552.82 553.69

570.19 572.10 573.91 574.46 584.89 597.63
599.85 606.10 625.62 626.62 628.78 631.24
631.99 633.02 633.52 640.51 646.25 695.86
696.19 708.40 710.11 711.42 712.46 715.51
715.80 720.05 721.64 723.01 725.53 733.76
737.10 754.30 759.18 763.29 765.84 766.93
768.06 768.24 770.17 770.50 771.78 784.19
784.71 794.52 827.92 828.29 828.99 851.64
863.60 866.04 873.09 873.58 873.66 878.62
882.20 884.50 893.79 894.18 895.38 897.15
905.47 912.21 929.31 939.44 942.54 946.31
947.06 950.32 951.47 955.56 959.47 966.48
971.69 974.09 978.15 982.13 982.83 990.45
992.34 993.79 998.15 998.54 1011.08 1011.34
1013.54 1014.46 1015.30 1016.01 1019.90 1020.22
1023.45 1026.33 1029.07 1038.40 1045.36 1045.88
1048.73 1050.84 1051.76 1053.35 1053.93 1057.18
1063.27 1064.81 1066.54 1071.95 1072.56 1072.73
1084.78 1090.67 1107.46 1110.74 1111.29 1114.34
1115.71 1116.56 1119.22 1120.15 1126.97 1133.52
1135.76 1137.67 1145.00 1145.25 1145.99 1157.16
1182.21 1187.65 1189.40 1194.28 1195.56 1196.25
1197.01 1199.79 1200.37 1207.80 1210.29 1212.12
1214.70 1222.28 1222.59 1227.67 1234.10 1239.08
1246.57 1249.01 1274.89 1288.27 1288.83 1297.18
1303.41 1318.37 1323.34 1326.08 1327.11 1330.00
1334.80 1335.65 1359.48 1363.47 1365.87 1366.39
1366.67 1368.48 1374.06 1378.62 1396.97 1407.92
1420.63 1426.16 1430.84 1433.98 1445.04 1447.44
1451.62 1465.77 1470.46 1472.36 1473.79 1476.95
1479.41 1483.40 1484.01 1491.59 1494.80 1495.52
1496.21 1497.31 1501.01 1503.70 1506.81 1507.96
1515.55 1515.70 1525.20 1525.71 1525.92 1527.26
1529.47 1531.49 1552.61 1552.77 1581.91 1609.80
1617.52 1624.39 1625.17 1626.96 1628.68 1642.39
1643.07 1643.79 1644.56 1644.80 1646.89 1647.23
1648.64 1655.05 1660.17 1668.83 1671.82 1767.58
2973.76 3031.78 3032.50 3034.68 3049.06 3058.60
3077.86 3087.81 3090.69 3090.91 3112.34 3113.28
3120.55 3133.34 3134.06 3135.58 3144.34 3153.91
3160.01 3162.88 3167.46 3171.22 3171.28 3173.35
3174.67 3174.95 3180.61 3184.57 3188.26 3188.54
3191.38 3192.39 3192.79 3193.05 3196.38 3199.15
3199.91 3201.43 3202.50 3204.41 3208.54 3209.54
3211.09 3212.25 3213.86 3214.04 3219.17 3219.31
3220.40 3224.29 3227.21 3239.59 3244.06 3293.11

==============================

III$_{SN}$

==============================

18.83 24.23 28.75 32.82 36.51 39.25
39.49 41.14 47.91 49.99 54.63 55.80
57.88 63.16 65.61 72.43 75.08 77.58
79.54 86.09 91.21 94.46 98.56 101.72
109.06 116.94 123.89 127.63 134.43 140.19
142.37 147.48 156.16 171.95 175.46 185.25
194.37 205.59 210.73 217.41 222.42 228.39
233.98 240.35 251.02 253.23 258.08 262.21
264.81 288.14 307.99 314.46 321.09 329.24
334.51 350.97 352.73 408.01 409.99 414.18
415.51 422.36 424.18 426.69 427.94 434.07
443.97 445.72 450.09 452.79 462.86 476.76
491.27 507.14 510.18 514.16 517.55 528.04
554.66 555.21 565.14 573.78 586.19 598.40
619.50 620.86 623.20 627.09 627.66 629.09
630.81 632.24 640.20 647.26 692.94 693.48
695.16 705.03 708.42 709.88 712.34 713.20
718.12 721.37 723.88 736.12 752.74 757.50
760.46 762.45 764.79 766.15 769.28 769.75
772.38 780.57 783.63 793.85 804.84 824.51
832.38 854.58 862.98 864.58 867.91 868.95
879.73 881.27 889.26 895.14 895.31 910.43
935.50 940.16 940.34 942.87 943.40 945.22
947.34 947.94 951.05 961.55 965.32 966.46
981.35 985.04 988.01 989.24 989.79 999.19
1001.67 1009.49 1010.20 1010.64 1012.90 1013.63
1014.81 1015.11 1016.87 1021.18 1022.72 1031.28
1037.36 1042.96 1045.65 1046.19 1052.26 1052.40
1058.51 1065.60 1086.29 1093.97 1103.32 1108.81
1112.73 1113.57 1113.79 1115.30 1119.37 1119.47
1126.48 1132.91 1137.79 1139.90 1141.63 1143.28
1153.60 1163.48 1164.71 1186.69 1198.76 1200.02
1200.59 1201.45 1202.74 1204.20 1205.78 1210.07
1214.01 1217.69 1219.38 1219.65 1221.69 1225.93
1231.48 1264.08 1273.47 1282.45 1293.54 1302.92
1305.46 1326.85 1327.71 1332.52 1333.83 1347.94
1361.62 1363.45 1366.63 1370.62 1372.69 1376.08
1377.48 1383.95 1405.33 1410.42 1428.90 1442.69
1445.56 1466.86 1470.03 1473.91 1474.34 1476.32
1477.05 1480.11 1484.11 1496.07 1496.22 1501.26
1504.43 1513.37 1518.72 1522.39 1524.47 1526.18
1526.97 1540.20 1552.82 1554.70 1612.67 1621.27
1624.08 1625.36 1625.60 1630.02 1639.59 1642.10
1642.81 1643.39 1644.24 1644.72 1644.87 1646.70
1661.90 1667.66 3010.35 3036.29 3054.17 3107.86
3109.24 3116.23 3163.67 3177.72 3179.18 3180.96
3184.49 3184.79 3188.93 3189.94 3190.38 3190.75
3191.91 3194.15 3195.37 3196.03 3196.83 3198.44
3199.60 3200.84 3206.54 3207.65 3207.77 3208.52
3209.09 3210.25 3210.81 3213.87 3214.47 3216.06
3219.69 3222.05 3223.66 3225.48 3228.64 3233.64
3241.47 3253.25 3275.87

==============================

III$_{SN}$-TS

==============================

-198.78 10.17 17.78 26.25 28.68 34.19
36.18 38.99 42.01 45.75 50.12 54.56
56.21 57.83 61.08 64.92 69.71 75.74
77.15 79.86 87.12 93.65 97.01 103.19
105.02 107.91 118.11 127.50 127.83 136.29
140.79 148.95 156.89 165.75 173.22 185.00
195.68 207.44 212.16 224.75 229.07 231.57
234.24 247.11 249.82 253.12 259.38 262.99
270.39 276.44 282.42 308.61 320.25 325.50
332.93 351.44 372.46 408.96 413.71 414.41
416.77 421.22 425.77 428.24 429.26 431.74
438.17 444.19 449.79 451.83 462.39 475.64
489.15 506.06 510.99 517.22 519.22 528.57
546.05 555.10 557.57 572.71 584.86 598.03
616.09 621.37 622.06 626.40 627.64 629.75
632.11 632.26 633.99 639.05 691.85 694.70
702.73 707.57 708.49 710.12 711.14 712.20
717.64 718.49 723.70 736.02 746.82 752.14
754.08 757.04 762.29 764.62 766.30 766.50
769.75 770.56 773.27 789.81 797.23 824.08
830.23 862.81 865.86 867.44 869.04 870.05
871.26 879.38 880.22 894.42 898.19 908.41
933.50 937.00 939.16 942.14 943.81 946.47
946.90 955.69 957.05 964.24 967.66 968.02
984.43 985.84 989.51 991.00 995.98 996.56
1006.71 1008.04 1009.34 1012.66 1014.26 1014.81
1016.52 1017.55 1018.64 1019.62 1030.41 1033.51
1035.31 1046.92 1049.03 1050.36 1051.69 1057.42
1059.16 1066.79 1085.90 1088.03 1110.73 1111.74
1112.86 1113.76 1114.34 1116.84 1117.16 1119.31
1124.81 1131.76 1137.70 1139.86 1140.96 1146.12
1147.08 1161.09 1161.37 1183.80 1198.65 1199.06
1199.91 1201.49 1202.21 1202.73 1205.78 1212.75
1213.67 1216.09 1219.18 1220.36 1221.27 1226.14
1228.14 1249.30 1273.11 1284.89 1292.57 1301.25
1302.59 1324.18 1324.35 1330.43 1331.07 1332.13
1362.45 1362.78 1365.48 1367.39 1368.65 1372.13
1372.30 1383.63 1401.76 1408.20 1420.92 1442.74
1445.15 1467.36 1471.34 1473.53 1474.28 1478.08
1479.74 1481.57 1484.64 1494.30 1495.17 1503.19
1507.06 1518.17 1523.58 1524.39 1524.98 1525.74
1536.02 1549.85 1553.92 1554.94 1611.51 1622.44
1622.70 1624.43 1626.62 1629.02 1638.89 1641.82
1642.07 1643.46 1644.65 1645.53 1646.56 1648.34
1665.53 1669.78 3018.62 3033.45 3045.58 3103.60
3112.96 3115.74 3170.17 3172.11 3173.97 3175.25

3176.77 3181.15 3182.77 3183.21 3184.91 3186.11
3187.84 3188.44 3190.81 3190.89 3193.56 3194.41
3196.52 3196.67 3197.17 3199.84 3200.20 3202.91
3204.61 3205.05 3205.29 3206.37 3210.07 3211.61
3212.19 3213.11 3218.66 3221.40 3227.06 3236.75
3244.63 3247.54 3271.55

===============================

V$_{SN}$

===============================

3.89 12.65 23.12 25.94 28.84 33.44
34.45 36.41 39.45 41.92 45.81 50.59
53.27 56.00 57.94 59.55 66.95 69.88
71.69 83.07 89.92 93.46 96.04 102.23
109.42 115.22 119.38 123.57 126.32 136.42
147.97 169.42 174.94 179.30 185.98 190.41
193.56 209.58 217.14 220.09 227.95 230.12
234.85 246.41 249.16 255.09 262.62 279.91
291.63 304.80 306.05 316.99 322.26 336.99
353.79 369.48 408.28 412.77 413.31 414.43
417.71 421.15 424.49 426.47 437.52 440.80
441.35 453.81 468.89 480.49 482.00 483.94
486.93 506.72 514.00 517.22 528.11 545.52
556.12 571.03 588.35 590.30 598.62 623.19
625.44 627.30 629.27 629.93 630.44 631.59
631.72 641.41 642.72 694.12 696.43 699.92
707.65 708.30 710.99 711.27 715.62 717.28
718.02 725.17 725.54 736.19 751.46 756.86
761.10 763.44 765.05 767.88 768.14 768.60
770.75 771.14 780.72 802.48 813.62 828.89
831.68 862.26 863.07 864.42 865.67 866.22
869.16 876.02 879.48 890.05 895.93 908.27
935.39 937.95 940.43 941.94 943.12 943.53
952.81 957.52 964.86 967.66 975.99 977.68
982.39 983.75 985.46 991.56 998.82 1010.26
1010.67 1012.71 1013.18 1013.95 1014.30 1014.32
1015.25 1016.36 1018.92 1031.83 1044.59 1046.36
1050.43 1050.94 1051.61 1053.02 1064.67 1067.14
1073.96 1086.87 1101.61 1108.79 1111.14 1113.64
1114.45 1116.98 1117.71 1120.81 1122.67 1126.25
1137.57 1137.85 1138.41 1140.16 1147.33 1162.00
1162.45 1195.71 1199.37 1199.77 1200.33 1201.37
1202.10 1202.43 1205.08 1212.50 1213.61 1216.47
1216.89 1218.68 1222.09 1225.88 1227.15 1228.14
1260.00 1275.23 1292.76 1302.01 1308.00 1315.89
1323.08 1327.16 1329.80 1330.28 1330.68 1358.97
1360.28 1361.06 1361.96 1366.51 1368.92 1374.02
1378.50 1385.20 1393.86 1420.14 1434.28 1443.18
1445.60 1466.43 1473.49 1475.80 1478.09 1478.47
1485.67 1491.77 1496.51 1497.36 1503.15 1504.79
1508.70 1513.99 1523.23 1523.75 1524.36 1525.93
1535.13 1543.21 1553.58 1555.02 1624.19 1624.41
1624.88 1626.60 1627.50 1641.63 1642.20 1642.31
1643.40 1643.89 1644.53 1644.89 1663.86 1664.53
1665.28 1669.20 3034.90 3042.21 3047.59 3066.20
3104.60 3114.22 3140.29 3159.39 3165.18 3168.05
3169.81 3179.07 3180.43 3182.64 3183.60 3183.83
3184.48 3186.09 3188.54 3191.46 3192.91 3194.11
3195.50 3196.47 3197.02 3200.59 3201.09 3202.20
3207.68 3208.50 3208.88 3210.26 3210.55 3211.97
3214.85 3216.38 3219.08 3219.37 3225.90 3229.49
3231.91 3232.98 3280.96

===============================

VI$_{SN}$

===============================

5.47 12.38 13.66 18.36 22.43 28.98
31.01 34.99 41.17 42.30 44.92 46.62
48.81 52.39 53.93 56.59 58.05 59.93
60.69 64.86 66.67 72.73 75.94 79.90
86.21 87.29 90.74 94.26 96.04 99.39
108.91 114.69 118.78 120.68 122.61 124.98
132.16 147.68 153.54 156.98 160.12 164.94
173.86 175.43 186.22 187.39 189.81 194.59
199.80 208.05 212.03 213.32 226.69 230.01
233.98 236.86 248.40 253.85 260.36 265.44
266.94 269.59 280.71 308.29 309.47 310.39
314.97 316.65 330.30 338.02 344.67 354.45
374.20 381.10 412.78 416.42 416.65 418.00
421.81 424.97 429.23 431.77 433.10 437.51
441.37 450.34 458.70 465.24 478.44 483.55
486.80 488.52 506.85 514.26 523.39 524.93
532.22 534.07 542.81 548.23 562.81 570.00
584.25 584.69 593.72 597.62 602.71 613.62
624.04 627.16 628.04 629.29 629.87 631.73
632.12 634.20 641.60 646.55 694.16 699.17
706.44 709.52 710.51 714.24 714.36 717.75
719.05 719.25 720.06 725.96 730.58 735.18
739.74 750.88 758.61 759.32 763.05 764.23
764.47 772.27 773.38 777.71 782.55 789.41
812.17 816.96 820.86 829.06 838.32 845.42
860.23 864.19 864.70 871.36 872.42 874.13
875.60 882.26 891.80 900.03 900.46 907.52
929.08 931.29 935.05 942.27 948.64 949.75
953.59 957.52 964.66 965.68 968.06 970.36
974.25 977.57 982.10 990.91 993.54 995.48
997.60 999.31 1006.48 1007.37 1010.88 1012.91
1013.75 1016.09 1017.07 1030.92 1040.92 1041.32
1046.37 1047.01 1048.67 1050.36 1051.01 1051.72
1052.64 1062.34 1063.23 1067.17 1069.63 1070.38
1074.62 1079.36 1083.36 1086.88 1101.90 1105.50
1111.46 1111.65 1112.33 1117.61 1118.02 1120.65
1124.68 1127.65 1130.08 1134.30 1135.85 1136.96
1149.32 1153.46 1156.31 1165.36 1195.01 1195.58
1196.01 1196.99 1197.52 1198.17 1200.45 1207.84
1212.56 1214.94 1217.95 1219.54 1220.64 1223.50
1225.98 1226.50 1227.66 1235.47 1258.44 1276.29
1285.29 1287.66 1292.80 1311.69 1318.82 1322.02
1322.54 1327.09 1328.29 1332.16 1332.67 1339.23
1357.11 1358.05 1361.25 1365.06 1367.14 1368.59
1372.04 1380.37 1385.56 1385.85 1403.17 1418.83
1425.73 1432.12 1436.14 1438.17 1442.38 1446.28
1450.87 1463.27 1472.15 1472.54 1473.35 1475.92
1477.60 1484.45 1488.33 1489.99 1490.96 1495.33
1499.18 1500.43 1503.62 1506.21 1509.66 1514.56
1517.05 1520.73 1523.61 1525.26 1525.52 1530.06
1535.95 1542.20 1549.91 1555.26 1556.24 1615.40
1620.82 1623.29 1626.44 1626.56 1627.59 1640.63
1641.17 1642.56 1642.58 1644.58 1645.44 1649.75
1660.16 1663.57 1665.87 1669.82 1670.59 1683.23
3026.09 3033.17 3035.15 3038.88 3047.40 3058.01
3063.41 3084.02 3095.29 3099.59 3109.66 3110.30
3115.24 3120.68 3147.57 3148.22 3150.56 3152.82
3155.37 3163.00 3167.24 3167.67 3169.13 3169.70
3170.91 3171.57 3172.11 3178.73 3180.06 3180.40
3181.21 3181.97 3186.70 3189.77 3189.84 3190.27
3190.51 3193.53 3196.37 3198.11 3198.98 3202.86
3207.30 3209.31 3210.89 3211.29 3212.73 3216.53
3227.25 3229.10 3229.34 3229.43 3254.81 3272.30

===============================

II$_{S}$-TS'

===============================

-202.33 10.00 11.23 20.01 21.98 28.00
32.54 33.31 34.13 41.74 43.57 48.13
48.67 51.07 52.91 55.07 57.05 60.90
63.90 64.61 71.49 73.43 74.35 79.23
82.19 89.11 95.38 95.93 101.84 103.53
106.66 108.65 112.66 115.45 116.49 122.26
124.55 128.30 133.56 135.28 141.99 152.67
161.68 167.89 174.71 181.95 185.77 190.64
197.82 203.83 207.93 218.19 219.30 224.51
226.85 231.26 233.79 236.59 244.14 245.89
250.78 258.51 259.39 259.48 273.98 284.78
295.54 301.84 306.62 313.82 324.69 331.71
336.44 351.02 395.12 404.45 408.80 411.62
414.13 416.55 422.23 429.55 430.72 432.91
440.11 441.95 445.87 450.68 454.49 463.02
478.33 480.24 494.78 509.26 513.44 513.73
517.28 525.37 530.23 535.23 541.90 549.66
550.76 558.83 573.74 576.36 590.50 596.78
599.39 604.83 622.75 624.89 627.43 628.86
630.66 631.10 631.84 635.13 640.49 693.19

694.98 706.52 707.23 709.62 712.24 715.53
717.86 718.39 721.28 722.71 733.58 737.39
750.67 752.34 756.59 757.03 761.18 765.45
766.60 767.95 771.57 772.37 774.70 776.53
781.39 784.68 812.05 825.06 825.66 855.24
859.29 861.45 868.42 870.05 875.88 876.19
878.34 882.18 886.98 890.71 893.54 898.38
904.96 905.94 920.74 939.87 940.00 941.66
943.36 947.71 949.81 951.10 953.19 962.48
971.83 974.62 976.02 986.52 986.92 990.23
994.10 997.01 997.35 1003.92 1005.99 1008.55
1010.41 1012.88 1014.57 1016.21 1016.76 1018.29
1025.68 1029.10 1035.24 1037.70 1042.27 1045.18
1050.10 1050.18 1051.07 1054.71 1063.32 1063.69
1068.51 1071.12 1072.28 1073.28 1075.56 1088.08
1090.16 1093.43 1108.05 1109.08 1109.40 1114.58
1115.58 1118.82 1119.05 1119.86 1120.49 1132.98
1137.44 1138.56 1143.15 1145.83 1146.16 1157.80
1185.36 1192.71 1195.44 1196.08 1197.74 1198.44
1200.83 1201.69 1203.08 1205.73 1208.96 1213.58
1216.05 1217.48 1218.40 1225.37 1230.78 1235.37
1238.68 1245.54 1271.83 1287.05 1288.53 1300.22
1301.18 1302.17 1322.18 1323.83 1327.37 1328.26
1329.83 1331.05 1360.31 1360.66 1364.92 1365.32
1366.99 1367.46 1370.18 1380.37 1399.95 1407.91
1419.18 1425.15 1427.45 1430.80 1444.63 1444.80
1447.39 1459.56 1466.54 1468.01 1472.96 1474.23
1477.48 1479.21 1482.78 1490.08 1491.71 1494.35
1496.00 1497.95 1500.48 1502.16 1502.31 1508.47
1513.68 1515.65 1516.85 1522.54 1523.59 1525.44
1526.58 1527.39 1530.42 1553.82 1554.41 1604.59
1610.16 1622.89 1623.27 1626.46 1627.15 1637.24
1638.71 1642.14 1642.73 1643.10 1643.59 1644.39
1645.18 1647.22 1648.57 1668.81 1672.11 1743.44
2971.10 3019.52 3026.17 3027.04 3028.91 3035.89
3076.43 3084.01 3087.80 3089.15 3092.44 3100.83
3105.97 3117.08 3121.96 3138.10 3141.08 3147.77
3155.66 3155.80 3156.31 3163.84 3165.09 3166.12
3170.81 3171.37 3172.89 3173.06 3179.60 3179.84
3181.73 3182.34 3183.12 3187.95 3189.13 3189.17
3190.81 3191.56 3195.69 3196.06 3199.27 3201.72
3204.45 3206.79 3206.85 3208.21 3209.02 3215.56
3219.01 3221.34 3222.47 3228.87 3270.81 3288.28

==============================

III$_{SC}$

==============================

17.48 24.42 29.82 35.85 38.89 39.49
42.45 45.50 54.01 58.05 59.53 62.73
64.02 68.61 72.30 77.96 80.65 85.20
92.59 98.63 100.87 103.55 106.60 108.77
119.81 124.27 126.52 131.72 132.73 137.64
147.10 158.05 174.25 176.37 184.57 192.72
195.32 208.15 208.73 220.43 222.09 231.00
232.11 235.90 247.09 259.89 262.18 266.40
266.56 308.44 313.75 317.84 319.08 329.17
336.99 348.72 368.18 400.35 409.02 411.70
416.96 418.60 422.36 427.93 429.55 438.43
441.11 445.56 446.95 452.27 462.31 481.90
487.39 508.45 513.22 516.20 519.18 528.85
548.73 553.47 570.15 573.09 584.20 598.75
612.43 622.89 623.70 625.47 628.94 629.14
630.00 632.18 638.24 645.95 694.02 697.99
698.53 709.00 709.98 712.80 713.59 716.76
718.62 725.17 726.86 735.75 744.24 754.19
757.94 762.25 764.86 765.47 767.26 767.95
768.61 779.29 781.53 791.70 830.14 830.99
840.38 857.61 866.52 868.23 870.92 873.23
877.43 878.07 881.57 895.60 907.89 910.27
935.45 940.55 942.03 943.79 944.58 948.09
949.64 949.82 957.41 958.18 966.67 967.87
985.13 988.01 988.69 992.91 996.35 997.13
1002.03 1010.02 1011.21 1011.96 1012.96 1014.90
1015.34 1016.41 1018.87 1019.75 1020.93 1025.51
1032.82 1037.79 1037.88 1049.81 1050.45 1051.03
1053.84 1059.19 1068.45 1088.91 1100.31 1110.68
1112.55 1116.23 1117.46 1120.11 1121.05 1121.50
1121.94 1122.47 1137.06 1138.89 1139.27 1141.42
1161.34 1166.87 1184.04 1189.38 1198.26 1199.39
1200.09 1202.57 1203.18 1203.85 1204.10 1211.09
1215.75 1217.68 1219.08 1222.32 1227.52 1228.55
1229.29 1254.37 1255.32 1276.51 1295.04 1303.58
1325.96 1326.52 1328.18 1333.28 1333.80 1343.54
1345.68 1361.01 1363.71 1368.00 1370.21 1373.50
1373.80 1385.51 1386.59 1407.63 1419.07 1444.77
1446.77 1467.48 1472.92 1474.23 1474.47 1477.39
1478.74 1479.34 1485.70 1494.48 1499.33 1505.87
1506.43 1512.61 1519.25 1523.82 1524.59 1526.87
1527.20 1536.27 1552.03 1552.62 1610.73 1621.49
1624.17 1624.83 1626.90 1627.42 1640.70 1641.05
1642.66 1643.15 1643.88 1644.53 1644.94 1650.97
1662.03 1666.40 3012.72 3047.60 3048.54 3107.81
3108.12 3121.31 3162.55 3179.53 3180.58 3180.99
3182.10 3183.55 3184.97 3186.05 3189.88 3191.65
3191.92 3192.98 3194.92 3197.91 3198.79 3199.06
3199.44 3200.00 3202.21 3205.53 3206.85 3209.25
3209.71 3210.08 3210.47 3210.92 3212.16 3214.11
3216.21 3217.12 3218.49 3218.91 3221.99 3222.25
3225.29 3231.82 3234.91

==============================

III$_{SC}$-TS

==============================

-131.79 10.41 13.23 17.08 33.07 36.93
38.96 40.47 44.35 46.96 53.05 56.31
59.62 61.31 63.92 67.72 69.72 79.92
81.22 83.60 91.05 94.63 99.44 101.48
105.97 117.63 120.11 125.69 129.89 134.35
143.07 144.54 153.17 167.76 173.30 184.36
192.34 199.10 207.28 215.35 226.64 228.45
234.41 235.65 248.16 256.50 262.76 266.22
269.12 287.24 298.70 311.99 319.87 327.24
334.87 348.75 355.37 406.29 408.63 413.16
415.11 417.64 420.49 426.47 431.48 438.05
440.97 446.15 447.87 453.41 462.70 480.08
488.08 507.61 512.76 518.59 522.40 529.73
538.66 555.02 556.78 573.14 581.83 599.36
612.61 620.91 623.96 626.00 627.16 628.64
630.16 630.85 632.17 644.12 696.79 698.10
702.37 709.13 710.25 712.26 713.36 716.74
719.34 724.91 726.10 736.93 753.23 755.05
757.83 762.22 764.89 766.96 768.13 769.08
773.11 775.34 779.96 790.20 828.01 829.64
830.85 862.99 866.58 867.66 871.04 871.67
873.21 879.87 884.03 896.33 909.95 911.13
940.11 940.68 945.01 948.75 949.61 951.38
951.98 958.68 964.07 964.71 968.15 978.16
983.78 990.40 991.37 991.88 995.27 996.59
1004.09 1009.44 1011.69 1013.23 1013.87 1014.21
1014.79 1016.74 1017.13 1018.37 1019.51 1030.75
1035.34 1038.90 1050.74 1051.04 1053.33 1053.76
1061.06 1067.41 1068.21 1087.05 1111.95 1113.64
1116.70 1117.00 1117.56 1118.02 1119.81 1122.14
1123.70 1123.98 1136.59 1138.64 1141.20 1146.73
1163.59 1164.93 1183.05 1187.41 1199.39 1201.23
1201.50 1202.31 1202.39 1202.88 1205.80 1209.32
1212.78 1215.35 1219.28 1221.16 1223.22 1227.83
1228.77 1241.79 1250.25 1273.49 1293.10 1300.65
1321.60 1323.12 1324.70 1329.45 1331.75 1333.28
1338.33 1362.37 1364.49 1366.77 1369.10 1369.94
1372.44 1384.46 1388.44 1395.16 1417.34 1443.46
1445.70 1468.00 1474.01 1474.36 1479.25 1479.48
1481.40 1483.93 1484.66 1492.60 1496.03 1503.49
1506.39 1518.49 1524.33 1524.99 1526.02 1527.42
1535.48 1553.83 1554.12 1564.28 1615.27 1624.14
1624.58 1626.95 1627.31 1633.64 1641.51 1641.72
1643.29 1643.61 1644.16 1645.11 1645.84 1657.31
1664.79 1668.22 3019.05 3039.13 3042.18 3103.13
3105.93 3118.04 3124.82 3159.95 3163.34 3177.82
3179.47 3180.45 3180.93 3183.83 3186.50 3186.59
3187.15 3189.45 3191.62 3193.01 3193.79 3195.52
3197.47 3197.55 3199.44 3200.64 3201.79 3204.25

3205.12 3207.26 3208.44 3209.98 3211.03 3211.38
3212.28 3215.08 3215.60 3216.23 3217.30 3220.55
3227.63 3231.31 3232.95

==============================

V_{SC}

==============================

0.69 16.79 18.97 22.79 27.59 29.80
34.02 36.67 37.24 40.37 46.94 51.12
51.87 55.88 58.93 60.99 65.67 66.85
71.11 75.52 77.64 85.61 93.17 102.31
107.00 110.82 114.00 128.81 137.18 140.05
144.84 156.79 171.48 183.52 187.81 194.12
208.32 215.10 217.02 222.47 225.66 228.94
232.24 247.57 252.21 259.48 259.75 267.21
272.18 300.01 307.62 314.53 326.57 329.27
334.26 348.15 409.48 410.10 415.86 416.43
417.05 418.05 425.39 427.79 438.88 440.35
442.72 459.18 470.07 478.77 485.04 487.99
509.44 514.78 515.69 525.73 528.51 552.15
554.24 570.47 573.42 597.69 599.33 616.20
623.11 626.41 629.66 630.54 630.75 632.30
634.38 643.15 652.09 697.68 699.81 706.53
709.44 710.71 711.93 714.86 715.84 717.71
723.10 725.88 736.88 751.07 754.01 757.97
763.38 764.07 766.56 767.12 768.55 770.15
780.83 789.44 797.76 829.17 830.21 842.63
860.82 864.36 865.56 867.75 870.81 871.11
885.47 895.99 897.30 909.59 924.03 928.88
935.77 940.41 941.05 941.80 944.41 945.03
953.53 961.59 967.22 969.73 976.14 982.73
984.63 987.58 988.59 1001.05 1001.92 1003.78
1012.01 1013.13 1013.39 1014.30 1014.51 1014.68
1014.79 1016.09 1017.44 1029.32 1032.13 1043.78
1049.94 1050.16 1050.70 1051.82 1059.51 1068.52
1086.92 1087.44 1097.68 1107.66 1107.96 1115.45
1116.22 1119.71 1120.82 1121.14 1123.63 1123.70
1127.20 1136.16 1137.54 1140.88 1143.87 1163.21
1174.13 1195.15 1198.84 1199.15 1199.17 1201.32
1201.59 1204.25 1204.84 1205.62 1209.16 1211.68
1216.21 1216.82 1221.09 1223.51 1225.58 1225.75
1240.87 1251.91 1274.07 1290.69 1297.44 1310.02
1325.36 1325.91 1327.98 1328.25 1330.14 1343.50
1358.64 1359.03 1360.10 1361.57 1364.40 1366.21
1373.01 1382.10 1382.34 1389.79 1431.70 1445.72
1447.80 1465.45 1474.91 1475.24 1477.48 1478.22
1483.26 1490.27 1494.75 1495.81 1504.62 1506.19
1508.10 1515.53 1522.69 1523.25 1525.34 1525.63
1539.34 1554.19 1554.37 1615.92 1623.77 1624.39
1625.44 1626.37 1637.29 1641.08 1642.51 1642.53
1643.12 1643.71 1643.79 1644.11 1657.82 1663.82
1664.48 1669.25 3041.19 3041.20 3043.73 3050.85
3058.50 3100.33 3100.81 3124.31 3132.54 3149.18
3154.94 3160.74 3164.83 3169.28 3174.82 3179.38
3180.12 3180.53 3181.26 3183.62 3188.29 3188.52
3189.23 3192.63 3193.22 3195.18 3197.00 3198.50
3199.34 3200.32 3202.73 3204.45 3206.18 3208.77
3208.80 3209.30 3209.77 3210.19 3210.62 3213.60
3229.44 3229.84 3238.96

==============================

VI_{SC}

==============================

1.95 11.35 11.82 13.70 19.18 23.58
28.53 29.65 31.89 33.08 37.23 40.93
44.57 46.39 50.45 53.54 54.86 57.26
59.44 61.96 64.36 66.03 69.08 70.66
76.01 78.05 78.15 85.06 85.72 91.97
94.38 100.94 105.49 112.03 114.23 119.02
122.82 127.62 146.37 150.93 152.72 157.52
160.28 161.36 170.57 182.48 187.71 194.67
197.77 200.61 211.71 215.39 219.40 220.92
228.93 231.22 238.74 242.22 248.98 255.36
257.27 261.25 261.86 265.82 285.00 303.91
307.03 309.64 314.55 326.21 331.92 333.32
349.27 386.67 406.57 411.67 414.61 415.16
418.37 418.86 423.79 425.53 434.24 435.73
437.84 454.87 468.62 473.68 478.37 480.17
481.32 501.10 508.66 512.24 516.76 521.40
524.51 526.93 534.41 554.04 555.55 572.32
573.54 577.71 595.54 597.87 609.60 612.72
615.55 619.68 627.38 630.30 630.82 632.54
633.14 634.52 637.61 644.66 694.57 697.28
707.43 709.67 710.51 712.66 714.17 715.50
717.50 721.40 721.89 734.47 741.41 750.54
755.12 755.42 756.63 761.36 764.46 765.52
768.99 772.98 774.21 783.03 798.04 801.75
821.30 822.25 825.01 835.43 856.70 858.63
866.68 869.01 871.65 880.30 882.77 883.50
892.86 893.01 893.95 904.81 920.71 926.59
933.58 935.95 937.79 940.60 950.92 953.78
954.68 955.11 958.66 964.49 968.87 974.09
974.29 981.29 983.51 988.27 991.78 994.09
994.66 1001.81 1004.96 1005.44 1011.83 1013.08
1013.59 1016.22 1016.35 1028.45 1038.57 1040.26
1042.21 1042.55 1048.61 1049.91 1051.04 1051.94
1054.47 1059.33 1061.17 1062.94 1066.15 1067.79
1070.04 1072.31 1085.46 1086.85 1105.01 1105.36
1109.02 1110.48 1110.76 1117.53 1119.61 1120.43
1124.49 1124.57 1125.10 1131.15 1131.53 1134.55
1141.89 1153.59 1156.09 1174.36 1192.05 1195.08
1195.29 1195.84 1196.33 1198.74 1199.07 1202.78
1206.85 1208.89 1214.28 1217.27 1218.62 1220.93
1222.76 1224.67 1230.46 1231.51 1240.17 1253.55
1270.99 1283.64 1285.94 1292.43 1309.26 1319.84
1322.23 1323.60 1326.85 1327.57 1328.60 1333.89
1345.21 1357.71 1362.60 1362.73 1364.99 1368.90
1371.33 1374.46 1377.14 1383.87 1390.73 1404.22
1420.75 1425.18 1428.40 1428.60 1442.42 1445.94
1453.36 1463.40 1471.87 1472.93 1476.33 1476.71
1481.59 1484.55 1490.25 1491.30 1491.54 1493.97
1497.03 1500.87 1503.41 1505.47 1507.82 1509.57
1513.51 1516.17 1523.08 1524.29 1528.55 1530.60
1531.67 1539.96 1556.78 1557.55 1620.15 1620.94
1622.03 1624.46 1626.91 1633.21 1638.75 1639.39
1641.85 1642.95 1643.45 1644.02 1644.40 1653.69
1659.82 1660.39 1665.50 1669.25 1669.90 1672.96
3020.43 3022.19 3030.76 3031.67 3031.84 3038.86
3044.51 3052.95 3076.98 3080.56 3092.00 3092.93
3104.75 3109.27 3110.11 3116.10 3121.70 3124.71
3145.62 3146.21 3148.24 3150.49 3160.14 3160.79
3163.84 3165.15 3168.88 3169.42 3169.68 3174.11
3176.05 3177.51 3180.26 3181.01 3183.08 3184.26
3186.62 3187.32 3190.69 3194.80 3195.11 3195.89
3196.98 3197.62 3198.25 3200.81 3204.87 3207.63
3210.06 3210.67 3223.02 3223.80 3224.32 3252.87

==============================

VI_{SC}-TS

==============================

-938.92 5.45 12.82 17.15 22.67 25.37
27.05 29.83 32.46 36.53 37.92 42.42
44.17 45.70 46.55 51.19 53.29 55.03
57.34 58.43 62.26 65.49 68.43 75.04
78.06 78.63 84.77 86.32 92.44 95.82
99.20 109.25 111.42 115.59 118.18 119.05
123.64 126.21 138.78 147.58 151.70 159.24
166.94 169.22 172.40 181.50 184.40 190.17
200.09 207.84 215.40 218.75 222.25 229.34
231.40 233.52 234.04 234.98 239.15 253.19
254.60 257.21 259.85 279.09 285.36 290.62
296.73 305.99 315.18 326.82 329.37 332.33
350.01 368.73 407.37 409.79 410.82 415.61
418.78 419.78 421.57 422.37 430.29 436.85
438.65 444.25 456.83 469.02 478.46 481.63
485.27 487.57 502.88 509.91 511.11 519.10
524.37 524.76 529.60 533.46 552.83 562.06
571.66 574.20 590.35 596.90 603.58 606.34
618.79 623.24 625.25 628.80 629.50 630.58
632.46 633.02 639.36 640.49 657.14 694.56
699.24 708.20 709.65 710.87 713.55 717.05
718.60 718.82 722.62 722.80 734.71 739.20
747.97 750.07 755.41 762.23 764.96 765.45

767.26 771.26 773.81 777.07 782.30 798.85
802.11 805.77 812.66 823.67 827.62 859.56
865.74 866.60 868.24 869.76 872.93 882.14
886.46 890.94 892.32 895.26 905.58 926.91
930.21 933.05 938.05 940.04 942.06 943.82
954.02 955.18 958.87 969.64 969.83 972.84
973.49 974.65 984.14 986.12 990.14 996.32
997.32 998.95 1004.96 1005.99 1014.17 1014.97
1015.74 1016.00 1017.70 1025.90 1028.48 1030.24
1038.67 1045.83 1047.48 1050.46 1052.22 1052.32
1052.57 1052.95 1061.65 1062.19 1064.13 1066.47
1071.86 1073.09 1079.08 1088.70 1106.76 1108.85
1110.77 1113.17 1114.15 1118.43 1119.98 1126.94
1127.41 1127.77 1132.22 1134.71 1135.90 1138.34
1143.94 1150.32 1155.77 1175.58 1193.57 1195.29
1197.01 1197.22 1197.43 1197.49 1200.56 1207.81
1208.82 1212.22 1214.44 1217.72 1218.49 1222.12
1223.49 1224.59 1227.46 1232.14 1267.54 1271.99
1282.51 1286.73 1288.08 1298.89 1302.97 1314.15
1326.19 1327.36 1330.06 1331.00 1332.39 1338.74
1342.34 1350.31 1361.22 1363.88 1364.52 1364.70
1367.49 1376.20 1379.03 1387.94 1392.40 1419.40
1424.10 1427.30 1433.36 1434.58 1443.43 1446.50
1450.82 1452.06 1467.16 1474.21 1475.44 1478.41
1478.82 1484.10 1485.45 1494.26 1495.53 1496.24
1497.75 1498.80 1503.09 1504.12 1509.35 1511.08
1512.37 1514.16 1515.27 1524.59 1525.66 1526.76
1530.50 1531.40 1534.32 1540.78 1554.17 1555.43
1621.38 1624.82 1626.49 1626.81 1627.44 1629.48
1639.52 1643.43 1643.91 1644.98 1645.99 1646.85
1649.32 1661.64 1663.11 1663.36 1669.26 1674.18
1675.59 3011.53 3019.71 3030.45 3030.93 3046.18
3048.00 3052.77 3086.18 3088.31 3095.01 3102.03
3109.84 3118.14 3125.03 3129.81 3138.05 3155.57
3157.89 3161.38 3163.65 3165.56 3166.50 3169.59
3172.97 3173.98 3175.10 3176.18 3177.90 3179.03
3181.20 3185.21 3186.41 3189.02 3190.08 3190.56
3190.63 3195.97 3196.68 3198.30 3201.00 3201.69
3202.47 3203.27 3208.59 3212.29 3212.60 3213.85
3214.85 3223.99 3225.48 3225.93 3228.63 3248.38
==============================
VII$_{SC}$
==============================
10.87 13.38 21.63 26.03 27.74 31.05
33.28 35.31 35.57 39.58 42.16 44.14
47.18 48.42 49.51 54.04 57.21 58.41
60.87 63.40 66.07 68.11 72.76 79.14
82.36 85.47 89.61 95.90 100.15 108.32
112.65 115.98 118.34 126.72 127.97 138.76
142.11 143.42 152.07 157.44 165.09 170.78
182.68 185.04 185.09 196.75 204.40 213.84
216.90 222.05 222.81 229.77 234.24 235.61
239.53 251.36 257.29 258.47 259.50 262.03
263.79 270.45 288.65 294.27 305.92 313.85
322.04 323.83 327.59 330.59 348.36 358.42
369.18 386.05 413.27 416.26 419.13 419.55
422.14 424.69 426.58 434.70 439.79 441.57
450.18 454.36 461.70 469.77 483.92 486.08
491.45 502.71 509.56 514.92 517.25 528.22
530.22 538.37 545.72 556.04 558.04 569.30
571.88 594.64 598.32 605.24 606.61 617.16
623.17 626.50 630.72 631.29 632.20 632.49
633.13 639.75 640.82 670.55 695.09 699.07
708.84 711.89 712.14 713.59 714.15 714.86
716.44 719.23 724.58 724.81 725.06 737.62
752.95 757.58 759.20 762.44 763.41 767.47
770.50 772.20 778.61 786.84 796.01 801.30
807.41 809.84 825.75 828.08 852.00 861.86
863.29 864.42 870.07 875.11 876.35 876.53
883.49 893.66 900.95 904.90 905.54 924.86
927.92 939.26 940.69 942.58 944.04 949.24
955.69 959.95 963.40 969.40 973.13 973.79
982.48 989.46 991.31 993.86 994.96 998.42
999.44 1012.96 1013.24 1013.87 1014.28 1015.23
1016.67 1017.91 1019.34 1025.61 1029.87 1040.82
1042.35 1043.19 1049.01 1050.08 1050.79 1052.77
1055.05 1058.95 1062.27 1064.97 1068.35 1070.44
1071.40 1083.41 1088.17 1097.72 1108.94 1109.92
1113.73 1114.43 1115.42 1121.68 1124.88 1126.75
1128.05 1129.29 1131.50 1132.29 1134.75 1143.86
1148.77 1148.83 1155.55 1168.55 1190.08 1193.94
1195.54 1197.13 1198.14 1199.09 1199.74 1206.51
1210.07 1214.28 1219.73 1220.66 1222.41 1222.84
1223.13 1227.40 1231.41 1244.26 1271.88 1285.79
1287.86 1292.99 1294.58 1308.02 1314.56 1321.41
1321.71 1326.91 1328.28 1329.71 1330.17 1332.15
1360.75 1363.27 1364.82 1366.01 1366.46 1367.24
1370.31 1371.51 1376.35 1389.81 1402.03 1419.51
1426.23 1429.05 1431.75 1444.28 1446.87 1451.07
1463.80 1466.48 1473.16 1474.03 1477.26 1477.61
1482.39 1483.62 1488.26 1490.90 1494.22 1499.62
1499.98 1501.18 1504.05 1510.32 1511.31 1515.49
1520.34 1520.53 1525.15 1525.26 1527.11 1527.53
1528.62 1538.26 1552.74 1553.51 1570.12 1613.23
1613.52 1621.89 1624.93 1625.09 1627.70 1633.86
1642.65 1642.85 1643.24 1643.67 1645.48 1646.46
1656.37 1657.28 1660.42 1664.93 1670.15 1682.40
2459.95 2982.60 3029.38 3031.87 3032.13 3034.06
3050.18 3056.08 3085.65 3092.70 3096.47 3107.79
3116.38 3118.61 3121.01 3127.74 3129.11 3141.62
3154.96 3157.75 3161.88 3165.79 3167.62 3168.17
3169.35 3169.50 3173.69 3174.82 3179.08 3179.70
3179.75 3184.69 3186.35 3187.69 3188.05 3188.06
3189.88 3194.21 3194.61 3195.09 3198.66 3199.14
3200.42 3201.46 3203.45 3204.71 3207.96 3208.44
3210.90 3215.42 3218.77 3223.91 3224.68 3229.90
==============================
VII$_{SC}$-TS
==============================
-637.04 10.30 15.95 17.96 24.68 26.04
28.22 30.16 34.47 36.79 38.28 43.70
46.21 47.54 48.45 49.99 55.56 56.68
58.56 61.67 64.50 70.22 71.44 78.65
79.16 82.88 88.42 95.26 98.26 102.88
109.47 111.17 115.89 120.14 126.20 133.64
146.10 148.58 152.03 155.98 160.75 171.14
171.61 182.59 184.12 186.37 198.92 209.89
215.81 218.39 220.72 224.37 229.47 231.50
235.48 244.83 250.21 253.06 256.82 262.29
264.28 268.88 272.06 288.56 305.07 306.61
312.82 326.85 327.67 331.96 338.74 349.71
364.95 379.69 408.20 413.95 414.83 417.65
419.81 422.66 424.15 430.00 441.22 444.37
445.89 453.67 462.44 466.90 468.70 483.10
489.53 502.94 509.00 515.55 516.11 523.20
526.79 537.92 541.83 547.65 553.41 559.81
572.67 573.00 593.49 599.10 605.29 608.81
623.14 625.99 630.56 631.12 632.56 632.78
633.49 636.30 643.80 656.43 696.17 699.98
703.81 708.46 710.50 712.76 713.71 715.42
716.84 720.69 723.55 724.92 727.24 735.30
736.14 754.24 758.51 762.14 763.28 765.01
765.49 770.37 771.45 780.42 789.46 791.59
806.31 814.97 819.35 820.23 826.96 850.14
866.25 866.41 867.37 869.47 874.34 876.21
876.50 881.56 893.19 899.16 905.68 909.97
929.26 929.76 933.27 940.59 942.65 943.86
948.56 954.35 960.88 969.54 971.95 975.18
977.59 983.02 989.06 989.85 994.23 995.52
996.56 998.00 1006.93 1011.10 1012.90 1013.44
1014.70 1016.63 1017.61 1018.62 1021.14 1031.07
1039.46 1041.73 1045.28 1048.45 1051.49 1052.90
1054.22 1056.84 1058.31 1061.33 1064.09 1068.29
1069.33 1073.86 1089.51 1091.15 1093.00 1111.63
1111.93 1115.34 1117.05 1117.40 1126.46 1126.92
1130.34 1130.77 1132.56 1134.66 1137.84 1144.06
1144.38 1149.70 1158.07 1160.99 1187.96 1194.02
1197.27 1199.00 1199.12 1200.86 1201.33 1206.53
1208.02 1210.61 1212.84 1220.98 1223.59 1224.32
1224.48 1229.31 1232.00 1243.76 1274.87 1286.93

1288.35 1288.90 1298.98 1312.80 1315.11 1323.46
1324.73 1325.83 1328.82 1332.08 1334.37 1334.46
1356.22 1362.77 1366.14 1368.14 1368.58 1370.42
1370.70 1379.16 1387.04 1394.82 1407.82 1424.57
1425.58 1427.86 1428.58 1430.82 1445.19 1447.82
1450.44 1466.68 1473.38 1475.41 1476.32 1479.95
1480.21 1485.68 1486.55 1487.72 1492.70 1495.90
1497.98 1500.66 1502.99 1503.81 1510.54 1514.26
1517.17 1520.00 1521.08 1526.85 1528.69 1529.05
1529.30 1535.73 1552.53 1554.53 1559.88 1591.15
1614.27 1619.89 1623.65 1627.48 1628.01 1630.31
1630.61 1643.93 1644.89 1645.74 1646.02 1647.76
1649.83 1653.31 1661.22 1662.58 1668.60 1674.54
1692.67 2996.20 3027.49 3031.12 3031.97 3035.02
3046.33 3053.98 3085.91 3088.38 3091.82 3097.24
3108.33 3111.57 3120.68 3127.76 3132.72 3135.83
3152.10 3156.88 3159.74 3160.84 3162.14 3168.25
3169.79 3171.37 3175.92 3176.02 3176.53 3177.71
3184.92 3185.76 3186.11 3190.37 3191.52 3192.85
3193.82 3194.73 3195.02 3196.69 3197.03 3201.24
3201.40 3205.51 3208.19 3210.93 3212.37 3214.21
3214.29 3215.89 3218.32 3224.93 3231.72 3233.80

==============================

VIII$_{SC}$

==============================

11.70 16.86 19.22 24.61 34.19 35.32
36.92 40.86 43.21 45.66 48.10 53.61
53.95 55.85 59.63 61.19 62.82 64.36
68.30 70.16 71.41 73.05 77.64 85.22
87.13 93.12 96.14 102.97 108.28 110.89
113.54 116.21 119.06 122.31 127.10 131.40
140.29 144.25 148.23 158.99 162.68 173.39
179.96 184.46 185.26 187.68 202.39 216.86
219.53 220.49 223.31 226.01 229.58 234.72
245.38 253.79 254.38 260.12 261.82 268.11
268.98 277.36 296.92 300.08 307.86 315.08
329.09 333.99 337.64 345.73 352.69 364.69
383.54 400.07 405.79 417.38 418.14 419.98
422.00 424.70 428.87 433.73 442.48 442.88
443.44 454.31 456.93 470.03 473.07 481.88
484.97 506.43 510.27 512.42 516.84 523.64
527.27 539.11 540.46 552.14 553.57 568.04
575.65 588.25 599.26 600.87 608.78 615.54
620.87 624.05 626.64 630.31 631.25 632.88
633.24 634.55 644.05 664.15 696.80 702.31
703.23 709.26 712.47 713.53 715.42 715.74
717.84 721.46 721.94 725.00 728.17 736.06
754.92 759.10 764.50 764.58 766.63 769.49
770.81 774.49 777.08 784.25 793.97 803.85
812.03 818.01 826.42 826.98 843.40 864.97
866.06 874.19 875.25 875.47 878.16 879.25
883.91 891.90 893.87 898.40 905.72 933.92
940.60 942.01 942.15 945.67 950.57 954.97
955.46 955.47 973.72 973.97 974.00 976.75
986.04 990.50 993.60 995.43 997.18 1004.27
1009.95 1010.88 1011.91 1012.77 1014.19 1015.25
1018.66 1019.74 1023.86 1029.67 1030.84 1039.62
1040.00 1040.22 1047.33 1047.87 1051.18 1054.29
1054.85 1062.41 1062.45 1064.55 1067.49 1070.70
1074.95 1088.15 1092.23 1097.44 1109.79 1111.54
1113.01 1116.32 1116.45 1121.15 1121.74 1123.47
1126.10 1129.11 1135.22 1138.86 1139.88 1142.28
1144.03 1154.67 1157.81 1179.43 1196.43 1196.73
1197.76 1197.92 1200.47 1201.24 1204.23 1204.90
1206.01 1208.48 1214.40 1219.03 1222.02 1227.90
1231.10 1232.09 1233.01 1248.60 1274.53 1278.99
1285.53 1289.06 1301.40 1305.85 1306.02 1309.02
1321.77 1324.42 1329.54 1330.43 1332.06 1337.83
1349.85 1361.17 1363.42 1368.01 1370.80 1371.20
1373.63 1378.73 1386.22 1396.17 1406.84 1425.13
1427.55 1427.86 1430.42 1444.58 1446.55 1447.61
1466.34 1467.02 1473.97 1474.58 1474.85 1478.69
1479.87 1485.96 1486.87 1491.37 1496.68 1497.14
1498.46 1500.16 1502.44 1502.63 1510.59 1515.34
1517.91 1520.33 1524.81 1527.27 1528.10 1530.10
1531.63 1540.81 1553.41 1555.92 1597.06 1602.27
1602.67 1622.87 1625.56 1627.92 1628.24 1630.64
1636.41 1637.62 1642.42 1644.97 1646.30 1647.09
1648.77 1656.43 1660.20 1668.32 1670.20 1674.87
2484.03 2999.22 3016.02 3028.68 3029.42 3038.68
3048.90 3049.47 3078.76 3080.10 3088.50 3107.42
3115.37 3117.12 3118.27 3126.07 3126.62 3137.83
3138.29 3155.89 3158.09 3158.93 3159.27 3160.94
3166.37 3166.69 3168.89 3169.92 3175.16 3178.39
3178.72 3179.11 3183.41 3185.88 3189.31 3190.37
3190.52 3193.25 3194.38 3194.72 3197.87 3197.95
3199.65 3202.56 3210.57 3212.82 3213.33 3214.73
3216.57 3223.49 3224.96 3232.12 3239.94 3267.19

==============================

IV$_{S}$

==============================

10.17 13.10 26.21 30.94 35.15 37.45
40.03 47.30 52.49 54.07 55.73 59.69
61.11 61.41 67.83 71.00 76.50 80.88
84.21 89.35 91.49 98.31 100.38 103.55
106.29 113.98 116.72 121.41 130.69 132.03
138.39 155.94 168.92 174.12 179.33 184.86
187.55 198.77 205.05 216.94 226.35 230.14
231.22 234.44 243.36 256.59 261.19 262.36
266.17 280.33 308.62 309.06 318.12 326.90
335.39 348.43 360.75 408.65 412.81 414.59
416.54 418.57 421.32 425.15 427.76 440.92
444.25 448.20 451.47 454.98 462.31 480.64
487.01 507.13 512.34 516.25 520.74 529.20
549.78 552.62 556.63 566.50 571.65 591.12
598.89 619.68 620.91 624.98 626.21 627.58
628.49 629.48 631.83 637.84 693.56 695.44
701.25 706.78 707.87 711.91 712.35 714.20
716.91 722.78 723.78 733.58 735.43 752.45
757.18 760.16 760.58 762.11 765.17 767.97
768.22 769.25 786.35 788.72 791.30 826.63
833.66 861.62 863.61 864.39 865.32 868.91
869.72 874.36 877.39 885.40 893.74 895.57
907.90 911.24 940.80 941.53 945.20 947.95
953.81 957.16 960.77 962.45 964.62 968.12
980.94 986.44 988.27 991.91 993.71 998.32
1007.01 1007.33 1008.32 1009.72 1010.64 1012.33
1012.80 1013.11 1013.74 1016.61 1019.74 1027.78
1030.47 1031.18 1036.29 1046.43 1047.96 1050.92
1052.08 1057.76 1065.86 1086.71 1099.57 1112.44
1113.66 1116.23 1116.52 1117.36 1119.54 1121.14
1123.46 1136.90 1138.26 1141.86 1142.92 1144.11
1153.82 1163.47 1164.98 1182.49 1200.12 1201.37
1201.44 1202.16 1202.47 1203.61 1205.23 1211.36
1215.23 1218.09 1219.61 1224.51 1227.69 1228.59
1229.51 1242.80 1270.58 1274.31 1295.34 1303.87
1314.20 1325.65 1327.66 1333.50 1334.55 1354.72
1362.79 1365.92 1368.43 1368.74 1369.35 1372.91
1380.40 1386.13 1390.85 1399.78 1404.86 1414.99
1443.76 1445.78 1467.98 1474.17 1474.78 1475.06
1479.32 1480.01 1485.18 1488.12 1489.71 1497.83
1505.39 1505.73 1523.28 1524.60 1525.40 1528.44
1535.66 1541.79 1552.21 1553.65 1570.19 1609.47
1624.83 1625.93 1628.21 1629.08 1640.64 1642.28
1643.47 1644.53 1644.83 1645.47 1646.11 1655.40
1662.57 1668.08 3007.36 3042.80 3043.24 3104.01
3116.54 3123.86 3165.66 3171.09 3175.42 3176.36
3178.14 3179.38 3181.62 3182.96 3185.28 3186.69
3189.42 3190.16 3193.16 3193.17 3193.87 3194.50
3196.58 3199.58 3200.77 3201.55 3202.14 3205.87
3206.88 3208.49 3209.58 3211.34 3211.59 3214.48
3216.52 3218.69 3219.03 3225.43 3226.47 3228.63
3231.20 3242.00 3243.38

==============================

III$_{SN}$-TS'

==============================

-59.90 11.18 17.13 28.46 34.51 37.42
38.42 41.80 48.07 48.24 54.48 55.91
57.49 61.04 65.78 69.26 75.11 76.40
80.20 88.83 91.24 95.62 100.05 103.85

106.38 111.90 113.93 118.55 128.07 132.80
141.00 147.11 166.63 168.33 175.28 184.20
188.45 202.51 205.13 217.03 224.42 226.88
230.01 237.42 242.43 254.67 261.67 262.54
266.89 280.58 312.02 316.60 319.21 327.59
335.62 348.29 353.81 407.22 409.87 411.83
414.66 418.76 422.79 424.14 425.76 442.81
444.64 446.25 453.24 457.35 463.67 481.14
488.61 506.80 510.43 514.23 518.85 530.51
543.95 556.45 567.95 568.81 571.77 592.26
599.68 621.03 622.24 624.31 626.15 628.26
630.16 631.92 632.36 641.57 692.04 696.54
697.50 708.19 709.12 711.83 712.64 717.58
718.25 724.85 727.80 737.49 739.85 751.27
753.24 758.21 760.91 763.29 767.04 769.48
770.04 779.78 784.79 787.50 792.35 826.04
828.87 835.32 840.68 865.97 866.49 868.94
869.58 870.22 876.05 878.54 886.65 897.41
898.40 910.21 939.80 941.12 946.40 952.88
956.40 958.18 958.69 962.91 963.33 968.82
984.98 986.69 990.90 992.64 994.29 998.59
1001.49 1008.82 1010.44 1011.67 1012.19 1013.23
1013.66 1014.27 1016.91 1017.51 1019.06 1020.17
1032.31 1035.41 1048.71 1049.90 1051.10 1052.30
1053.18 1057.29 1067.20 1087.96 1097.79 1102.35
1112.20 1112.53 1116.67 1117.38 1118.10 1121.95
1123.41 1124.58 1138.64 1139.04 1142.44 1142.96
1145.53 1163.74 1164.05 1180.93 1199.92 1200.98
1201.08 1202.63 1202.84 1203.41 1205.55 1212.85
1215.34 1216.93 1218.91 1221.97 1226.99 1228.76
1230.22 1247.33 1275.57 1276.59 1296.16 1304.82
1323.22 1325.31 1333.18 1333.82 1350.87 1357.83
1362.60 1362.84 1364.90 1368.27 1368.55 1370.23
1374.21 1382.04 1386.51 1397.83 1413.07 1424.17
1443.89 1446.47 1467.93 1473.44 1474.26 1474.60
1480.11 1480.47 1486.81 1487.76 1490.22 1498.62
1506.10 1506.66 1523.88 1524.15 1525.58 1526.14
1529.37 1537.64 1553.85 1554.39 1565.15 1609.14
1623.98 1624.22 1628.54 1628.83 1641.88 1642.54
1643.15 1643.18 1644.76 1645.21 1646.04 1646.96
1663.24 1669.21 2975.58 3044.04 3045.95 3101.09
3106.19 3118.76 3162.48 3163.55 3169.73 3169.76
3172.25 3175.09 3180.80 3181.71 3182.03 3183.80
3187.10 3188.39 3190.01 3190.20 3190.87 3191.87
3196.37 3197.87 3198.45 3199.63 3199.97 3204.56
3204.88 3207.72 3208.64 3209.97 3211.57 3215.87
3216.91 3217.31 3217.55 3218.13 3221.09 3223.03
3229.58 3238.14 3240.21

==============================

III_{SC}-TS'

==============================

-16.51 12.09 18.61 24.64 33.94 35.13
37.97 42.98 47.44 51.57 54.73 55.92
56.75 60.28 65.29 68.64 70.39 77.98
78.61 83.79 90.80 94.92 96.16 102.24
105.19 111.63 117.16 118.51 131.67 139.12
144.45 154.02 167.05 168.14 173.28 184.27
185.76 192.68 204.99 214.15 229.04 232.13
235.10 240.16 245.54 257.37 260.92 266.77
268.40 287.05 306.71 319.02 322.55 335.58
342.83 348.00 366.75 408.09 412.51 414.32
416.21 421.63 423.32 425.62 431.47 436.90
441.95 448.29 450.16 456.31 463.85 481.55
486.99 505.83 510.99 518.17 523.24 529.83
548.51 555.09 564.56 566.30 570.50 598.71
607.27 620.03 621.19 625.02 625.79 626.38
628.57 629.92 631.70 637.87 693.33 694.89
699.87 705.27 710.41 711.84 712.84 715.56
715.82 722.73 723.62 730.59 736.10 751.89
757.19 760.80 762.37 765.61 767.58 768.80
770.26 772.28 781.69 787.29 793.70 827.31
834.70 861.36 862.32 863.57 869.62 870.24
872.38 877.89 881.85 888.41 895.31 896.39
905.04 908.69 940.20 941.44 943.22 948.57
954.44 956.74 958.35 963.00 963.87 967.05
979.48 984.56 988.63 990.96 992.99 999.12
1006.62 1008.35 1009.77 1011.23 1012.59 1013.22
1013.49 1013.88 1016.72 1020.31 1021.40 1024.65
1025.29 1032.39 1032.55 1046.79 1048.36 1050.73
1053.49 1058.76 1065.50 1087.24 1101.16 1110.44
1113.59 1113.76 1115.68 1117.95 1119.13 1119.35
1125.77 1138.10 1139.36 1140.02 1142.85 1146.22
1162.05 1163.71 1173.64 1200.10 1200.47 1200.90
1201.57 1202.64 1203.17 1203.84 1205.84 1212.88
1214.03 1216.29 1217.96 1221.86 1229.43 1229.59
1233.91 1239.96 1276.87 1287.69 1296.65 1298.48
1304.86 1323.30 1327.89 1331.75 1335.42 1351.60
1361.39 1361.97 1364.40 1368.56 1369.09 1375.01
1379.44 1387.34 1390.28 1394.30 1407.31 1414.72
1443.82 1446.07 1468.08 1468.64 1473.85 1475.10
1479.25 1479.37 1480.72 1487.46 1489.75 1498.52
1504.61 1508.29 1522.77 1524.11 1525.08 1528.41
1530.07 1534.60 1553.72 1554.00 1583.62 1611.51
1623.88 1626.72 1628.31 1629.14 1642.56 1642.62
1643.83 1644.29 1644.56 1645.19 1646.00 1651.04
1663.81 1669.01 2999.36 3045.70 3046.06 3105.21
3121.15 3132.20 3172.38 3174.37 3179.62 3181.09
3181.88 3182.34 3184.23 3184.83 3188.36 3189.65
3189.90 3193.37 3193.58 3194.30 3197.08 3199.74
3200.20 3200.25 3201.07 3201.62 3204.56 3206.16
3208.72 3209.40 3209.97 3212.41 3212.91 3215.71
3217.68 3220.42 3221.94 3225.68 3229.20 3229.23
3232.61 3242.33 3244.54

==============================

I_S-TS''

==============================

-273.61 13.26 18.99 27.28 28.53 31.54
33.65 35.19 37.88 39.84 41.60 45.89
48.48 53.06 53.79 57.04 59.36 63.14
67.93 72.82 79.49 80.71 83.43 86.99
93.59 94.77 100.79 106.14 110.24 117.24
128.10 137.00 140.06 145.31 148.50 156.91
168.31 171.13 177.09 184.75 188.02 193.12
196.38 206.41 213.29 218.32 223.45 224.77
232.78 234.95 238.39 246.97 251.04 262.13
265.39 272.81 284.90 304.47 312.40 312.74
326.05 326.88 332.02 350.15 369.75 386.34
410.18 412.47 415.80 417.22 419.15 421.29
422.53 430.40 433.33 435.97 443.12 451.73
463.73 475.88 481.03 494.14 509.32 513.11
515.12 515.46 528.08 531.08 540.18 552.08
552.58 570.47 573.39 576.54 591.33 596.29
599.01 606.05 623.07 626.65 628.17 629.73
632.63 633.39 641.48 647.59 696.19 697.87
709.92 710.56 711.23 712.42 715.37 716.67
719.51 722.21 723.88 733.24 734.86 752.92
758.68 761.99 765.47 767.44 768.34 768.44
769.44 770.57 789.12 794.29 827.00 827.67
828.25 859.84 871.28 872.78 873.16 874.74
879.16 880.40 883.76 893.05 897.00 898.78
907.49 918.72 939.67 940.75 943.57 946.19
946.57 951.81 952.64 963.04 971.79 974.72
978.42 979.29 991.29 993.26 993.90 996.91
1012.03 1012.78 1013.22 1014.65 1018.16 1018.70
1019.19 1020.93 1028.47 1028.53 1040.07 1044.04
1048.67 1052.17 1054.00 1054.56 1055.58 1061.78
1063.64 1067.48 1071.34 1076.04 1083.70 1088.57
1106.54 1110.19 1110.97 1113.24 1115.93 1120.21
1120.86 1124.22 1125.51 1132.02 1137.52 1140.03
1146.34 1147.92 1155.78 1184.46 1188.53 1190.89
1196.12 1198.23 1198.49 1200.65 1200.87 1209.57
1212.05 1212.81 1223.46 1224.78 1234.07 1234.11
1239.55 1244.88 1273.38 1286.82 1289.36 1294.65
1302.63 1321.50 1327.51 1328.33 1330.67 1333.48
1335.09 1357.35 1367.50 1368.37 1368.77 1373.80
1375.96 1377.17 1407.85 1426.15 1432.05 1435.66
1444.44 1447.58 1452.34 1465.48 1470.23 1474.70
1475.47 1478.43 1479.35 1483.01 1486.04 1492.99
1495.18 1498.65 1500.69 1501.62 1506.52 1506.84
1514.43 1524.88 1526.03 1528.80 1530.52 1531.21

1536.94 1552.65 1553.04 1583.69 1618.90 1625.85
1625.97 1627.83 1628.87 1644.64 1645.38 1645.92
1646.38 1646.93 1648.97 1649.14 1657.66 1659.47
1668.73 1673.24 1756.63 3031.82 3032.54 3034.72
3051.81 3053.18 3089.94 3091.88 3092.45 3119.72
3120.71 3122.52 3128.72 3138.05 3153.73 3159.38
3160.52 3164.33 3169.60 3169.98 3172.61 3173.69
3179.58 3182.65 3184.13 3184.34 3189.75 3190.51
3192.39 3192.90 3196.88 3197.55 3199.69 3203.58
3205.87 3207.49 3208.97 3211.23 3211.93 3214.98
3221.68 3222.40 3228.64 3235.28 3248.59 3293.80
==============================

X_S

==============================

10.81 25.08 28.08 30.45 34.87 36.53
40.18 43.35 45.13 50.20 55.43 56.63
58.63 65.14 73.89 80.89 81.55 92.62
98.91 105.06 110.16 116.30 130.12 138.12
144.69 151.48 161.27 171.18 180.91 196.67
197.62 210.00 216.31 224.67 226.52 230.08
234.00 251.99 259.76 261.70 280.84 293.01
307.31 317.07 332.20 336.83 345.94 400.52
406.74 410.28 412.68 418.29 419.64 428.84
429.92 437.62 441.13 450.07 461.18 468.44
486.09 493.55 509.08 509.39 515.01 521.20
526.95 549.56 561.76 572.07 580.77 595.47
619.52 621.25 624.23 627.39 628.68 630.18
630.52 633.59 641.57 698.45 699.86 704.59
707.32 708.47 711.32 716.49 719.80 727.10
732.26 734.93 749.97 752.21 755.26 758.63
760.09 763.79 765.32 765.56 769.68 771.32
790.01 831.26 835.01 859.01 864.62 865.49
868.54 871.10 874.79 881.55 889.93 896.60
912.79 941.01 943.44 943.81 946.11 948.10
948.54 949.13 953.08 963.56 964.68 979.27
986.95 987.23 988.67 993.68 1012.46 1013.07
1013.82 1014.24 1018.45 1019.15 1019.82 1020.27
1032.56 1042.68 1050.42 1050.98 1051.77 1052.82
1063.89 1084.78 1096.48 1110.90 1115.69 1117.75
1118.24 1119.98 1121.37 1123.70 1126.23 1128.59
1135.54 1139.71 1141.32 1143.91 1154.71 1164.08
1187.76 1200.22 1202.59 1203.96 1204.25 1204.32
1205.62 1206.22 1211.35 1213.00 1221.23 1221.26
1227.51 1228.74 1263.32 1275.08 1294.09 1301.69
1306.69 1327.80 1329.15 1331.58 1331.77 1363.78
1364.45 1367.46 1368.25 1374.60 1379.76 1386.12
1419.22 1443.80 1446.13 1457.94 1466.61 1476.11
1476.19 1478.42 1479.16 1483.51 1495.23 1497.53
1509.04 1516.22 1522.02 1524.32 1525.06 1526.81
1551.75 1552.15 1623.65 1624.39 1625.15 1625.73
1627.36 1638.65 1640.61 1641.29 1641.56 1641.76
1642.54 1643.45 1658.25 1665.89 1696.44 3045.19
3054.24 3113.35 3121.56 3165.93 3166.86 3176.68
3179.13 3181.19 3181.37 3184.99 3185.64 3186.03
3189.31 3194.02 3195.14 3195.43 3196.87 3198.66
3199.37 3203.07 3206.71 3206.90 3207.87 3208.97
3210.44 3211.77 3212.07 3214.33 3223.95 3230.30
3235.89 3247.32 3278.09
==============================

I_S-TS'''

==============================

-177.16 13.20 17.38 25.58 28.54 30.96
32.78 36.82 38.66 39.62 43.30 46.07
48.05 50.78 51.84 54.27 56.88 59.58
60.78 67.11 68.52 71.83 77.58 79.69
82.92 84.17 88.52 94.17 100.57 103.24
111.95 113.16 117.28 126.10 128.15 129.49
137.73 142.64 145.80 157.54 161.75 163.47
169.37 174.54 184.57 185.41 188.63 196.46
205.47 212.09 215.31 219.19 223.79 229.80
232.87 238.40 241.63 249.81 251.45 261.93
264.16 265.18 279.81 295.39 300.84 304.66
312.94 313.48 326.31 332.31 350.89 356.34
373.85 402.01 410.38 413.00 416.81 419.30
421.40 423.95 426.12 431.86 436.80 437.64
448.46 452.53 464.34 475.78 480.72 486.36
510.17 513.27 513.34 515.31 520.63 526.69
529.89 539.05 552.83 572.27 573.64 577.74
586.40 596.69 599.30 603.50 605.42 624.42
626.19 628.07 629.82 632.10 632.66 634.88
642.55 696.32 698.50 710.64 711.13 711.91
713.30 715.50 716.91 719.95 721.83 726.05
735.27 742.97 753.86 759.11 760.33 762.65
768.27 769.26 769.67 771.15 771.20 791.01
794.09 808.29 825.40 826.97 828.35 847.47
863.71 872.91 873.80 876.02 880.03 881.31
885.57 893.57 894.06 896.07 908.13 939.39
941.87 945.31 946.41 947.63 953.34 954.10
962.80 971.74 974.61 978.88 979.35 992.11
994.69 996.01 998.86 999.04 1012.50 1013.00
1013.70 1014.76 1017.68 1019.13 1020.24 1025.08
1030.34 1040.28 1042.89 1047.53 1048.51 1052.23
1053.51 1053.84 1055.78 1061.84 1063.56 1066.73
1069.66 1073.25 1075.52 1089.30 1091.93 1094.14
1100.03 1110.33 1110.88 1112.78 1116.29 1118.96
1121.30 1123.79 1125.90 1127.25 1134.62 1138.05
1146.84 1148.37 1156.60 1165.01 1180.67 1186.66
1193.71 1194.90 1196.44 1198.48 1198.86 1201.05
1201.62 1210.65 1212.73 1214.11 1222.74 1224.70
1228.72 1233.16 1235.23 1242.31 1246.01 1266.64
1274.10 1288.08 1289.02 1296.10 1304.88 1315.90
1321.43 1323.49 1327.34 1329.44 1330.25 1333.52
1334.25 1367.52 1367.72 1369.30 1372.49 1375.14
1375.76 1378.81 1414.67 1426.24 1431.00 1433.82
1445.04 1447.83 1451.75 1455.02 1466.46 1470.71
1474.20 1475.90 1478.31 1479.59 1481.24 1483.68
1489.11 1494.39 1495.10 1495.91 1498.58 1498.66
1499.88 1502.60 1506.79 1508.09 1514.51 1519.51
1525.22 1525.84 1526.73 1528.43 1529.91 1532.46
1553.07 1553.44 1553.84 1610.58 1617.88 1624.46
1626.41 1628.08 1628.50 1644.03 1645.14 1645.30
1645.52 1646.46 1647.29 1648.81 1658.35 1660.71
1669.30 1673.78 1741.89 2963.03 2976.31 3017.12
3024.89 3025.25 3031.11 3033.34 3033.44 3050.92
3051.71 3058.77 3090.21 3091.42 3093.87 3117.09
3117.97 3118.67 3118.84 3134.67 3138.49 3152.60
3157.96 3160.84 3161.57 3169.62 3169.92 3172.96
3173.41 3178.66 3182.67 3183.11 3185.38 3188.03
3190.05 3191.09 3193.51 3196.77 3198.93 3199.66
3202.36 3203.72 3206.48 3208.02 3210.12 3212.58
3214.78 3218.69 3222.82 3227.67 3227.88 3292.11
==============================

XI_S

==============================

10.82 12.18 23.07 25.91 28.13 35.50
37.58 39.46 40.95 45.70 47.50 52.63
55.34 56.35 58.67 67.85 70.17 76.04
84.27 90.06 96.61 101.01 109.46 111.33
115.93 119.79 130.04 136.30 141.86 148.45
153.64 170.04 173.34 180.41 190.85 196.55
209.62 212.53 217.73 224.86 229.10 233.12
237.97 251.97 256.39 259.67 260.34 262.50
306.99 315.12 316.92 331.56 337.15 345.62
364.88 401.75 406.52 410.91 413.78 418.31
419.71 430.16 435.37 439.01 440.81 446.90
459.64 467.00 484.63 490.83 507.04 509.72
514.83 516.99 525.82 548.73 552.20 572.58
582.75 595.28 595.70 604.15 620.91 623.20
625.40 626.96 627.85 630.01 639.18 642.26
698.60 699.18 705.10 707.59 708.18 711.31
716.15 718.99 726.36 731.21 734.29 753.01
756.60 758.72 760.68 762.45 764.57 765.59
770.13 770.83 771.39 790.02 805.89 831.45
834.08 843.50 860.27 865.42 866.83 868.73
874.43 881.39 896.12 912.48 916.85 943.72
944.28 946.33 946.65 947.84 948.77 952.10
963.92 965.39 981.51 986.40 987.64 989.80
993.38 998.57 1012.34 1012.82 1013.19 1014.22
1017.53 1018.15 1019.24 1019.72 1032.15 1043.34
1049.26 1050.18 1050.38 1051.94 1052.58 1064.16

1085.32 1087.17 1096.87 1110.97 1114.62 1117.17
1117.89 1119.05 1120.85 1123.38 1126.36 1126.63
1135.70 1139.27 1141.59 1143.20 1163.51 1165.14
1170.59 1185.75 1194.95 1200.20 1202.56 1203.42
1203.87 1204.19 1206.08 1206.62 1211.33 1212.87
1220.73 1221.67 1227.31 1228.45 1230.04 1246.35
1274.83 1281.54 1294.21 1305.40 1306.66 1318.16
1328.51 1329.47 1331.38 1331.73 1341.57 1363.66
1364.83 1367.94 1368.27 1374.03 1379.83 1385.78
1406.44 1443.63 1445.96 1450.04 1466.69 1473.53
1475.88 1476.12 1478.36 1478.67 1483.60 1484.78
1494.81 1495.53 1500.23 1506.28 1508.18 1515.93
1521.80 1524.89 1525.60 1526.82 1540.91 1552.00
1552.32 1555.30 1624.54 1624.95 1626.08 1627.17
1628.61 1640.20 1640.81 1640.99 1641.88 1642.28
1643.62 1644.31 1658.31 1666.77 1679.02 2940.34
2966.24 2969.16 3011.22 3019.70 3046.47 3051.14
3053.54 3114.87 3119.70 3126.17 3164.14 3170.36
3177.40 3180.06 3181.36 3181.81 3183.58 3187.94
3188.48 3188.94 3194.26 3194.54 3197.49 3198.79
3199.34 3199.63 3201.59 3207.90 3208.15 3209.27
3210.85 3211.45 3211.55 3214.35 3214.42 3220.71
3231.25 3234.08 3279.91

==============================

I_P-TS

==============================

-783.19 12.21 16.77 26.84 30.37 33.59
38.59 44.64 47.13 51.43 55.90 59.68
67.93 77.55 83.62 95.51 96.70 100.51
107.22 110.55 119.56 128.26 140.08 149.79
155.01 174.26 186.14 195.73 208.80 226.84
228.98 232.21 239.45 248.98 259.88 278.72
282.17 286.55 287.82 310.18 339.40 356.45
373.76 382.29 391.25 415.07 416.45 421.57
421.93 426.85 430.23 437.34 481.96 484.72
492.00 493.09 497.92 505.32 510.73 529.56
536.63 542.39 569.21 604.11 605.42 614.46
624.13 627.09 630.90 631.40 632.24 632.88
641.04 648.10 676.32 678.96 682.97 695.46
707.55 714.37 715.92 717.87 718.58 763.56
770.38 776.34 781.75 782.33 784.47 787.44
817.51 836.50 844.71 845.80 852.65 856.30
858.02 859.33 862.29 866.00 888.90 895.12
907.65 916.29 923.07 925.92 927.24 931.22
939.09 943.98 962.16 963.16 970.29 971.05
975.36 977.94 979.87 996.40 997.65 1001.77
1002.39 1004.04 1005.19 1009.11 1012.03 1014.48
1015.77 1016.25 1017.53 1019.30 1023.84 1053.58
1056.48 1057.59 1058.60 1060.79 1067.83 1069.74
1105.77 1108.77 1109.54 1116.61 1117.56 1120.46
1135.26 1148.34 1155.68 1157.66 1180.81 1188.12
1190.93 1193.73 1195.34 1195.67 1197.70 1197.89
1213.79 1215.24 1219.96 1220.97 1224.63 1226.09
1227.32 1229.13 1231.56 1231.94 1246.98 1253.13
1260.30 1265.66 1277.21 1295.89 1300.85 1310.21
1314.09 1321.51 1324.90 1340.11 1345.17 1347.08
1356.54 1361.46 1362.32 1367.09 1369.29 1370.61
1370.87 1376.76 1392.99 1397.85 1405.52 1443.33
1464.71 1477.18 1479.45 1491.79 1492.34 1492.38
1493.75 1497.23 1506.07 1506.73 1515.69 1516.26
1524.74 1538.37 1541.96 1542.41 1542.71 1543.67
1611.32 1633.97 1635.11 1635.61 1639.52 1650.08
1657.33 1660.19 1660.74 1662.75 3032.21 3035.04
3037.41 3038.28 3041.61 3043.20 3048.80 3050.00
3055.62 3079.71 3080.70 3091.55 3094.72 3099.75
3101.99 3126.02 3152.11 3158.56 3159.96 3162.99
3164.35 3168.92 3169.18 3170.67 3172.78 3175.44
3178.35 3178.50 3184.17 3186.02 3186.18 3186.54
3191.63 3196.27 3198.56 3198.83 3199.41 3199.73
3200.53 3206.78 3207.97 3220.18 3228.36 3231.93

==============================

I_P-TS'

==============================

-759.86 15.07 16.22 19.97 31.59 39.37
44.30 49.08 53.09 55.36 60.47 62.08
77.03 79.52 88.89 92.95 97.87 100.76
101.96 110.05 112.04 123.24 139.07 151.66
158.07 165.70 188.34 198.81 204.27 225.25
229.74 231.69 238.32 256.15 259.47 278.47
280.44 287.92 295.58 309.92 332.69 351.85
374.25 384.30 396.21 414.13 416.49 420.16
422.76 423.68 428.36 437.62 473.26 486.88
494.41 499.53 502.76 504.48 509.19 531.86
534.27 539.74 562.85 601.25 604.12 616.98
625.66 629.38 631.98 632.88 634.35 634.74
642.54 649.41 678.57 679.81 688.27 690.14
707.91 714.24 716.11 716.75 719.30 759.69
763.18 772.81 775.28 775.84 782.91 785.32
816.95 837.15 839.58 845.22 851.54 858.14
859.00 863.44 864.33 868.00 884.22 896.12
910.84 918.65 924.16 924.98 925.49 929.89
939.65 946.04 955.43 959.78 972.82 973.55
974.22 975.78 976.67 993.15 996.08 1001.01
1003.48 1007.66 1011.48 1011.89 1014.74 1016.08
1016.42 1017.24 1017.72 1019.30 1025.15 1048.60
1058.01 1058.44 1059.98 1061.19 1067.78 1069.35
1105.81 1108.25 1109.70 1117.98 1118.86 1120.04
1136.06 1149.31 1153.62 1154.23 1181.90 1187.68
1189.78 1191.52 1195.27 1195.80 1197.50 1197.92
1212.03 1217.44 1220.03 1220.60 1222.65 1225.12
1225.48 1228.11 1228.88 1229.22 1246.55 1249.44
1255.35 1268.89 1273.91 1299.00 1303.60 1308.94
1314.12 1316.23 1323.79 1338.54 1344.05 1345.49
1356.96 1358.50 1363.48 1364.87 1366.74 1368.38
1368.53 1383.47 1385.97 1394.21 1402.31 1438.00
1462.28 1465.17 1477.90 1486.24 1490.56 1494.08
1494.43 1496.22 1505.17 1507.75 1514.69 1516.78
1522.00 1538.79 1540.30 1540.63 1541.36 1542.05
1611.40 1635.08 1635.20 1638.40 1639.25 1649.59
1658.92 1659.04 1660.04 1660.37 3025.39 3026.33
3039.90 3040.32 3041.75 3044.77 3047.66 3051.20
3054.23 3061.45 3084.20 3086.81 3095.65 3098.26
3100.57 3113.91 3154.04 3158.83 3160.66 3162.49
3165.68 3166.60 3169.50 3170.58 3172.49 3175.18
3176.59 3177.99 3182.58 3182.76 3185.09 3186.19
3189.63 3191.12 3193.99 3196.41 3196.78 3199.09
3201.54 3203.73 3206.39 3220.44 3226.39 3248.53

==============================

II_P

==============================

2.96 9.73 21.36 23.91 28.18 41.97
45.28 48.37 53.67 54.25 57.18 58.69
69.25 74.24 81.30 91.74 96.92 101.59
105.33 110.99 121.41 137.85 142.38 157.25
173.39 178.69 190.46 199.17 215.27 220.72
227.58 229.26 238.35 239.72 249.67 273.78
278.86 281.47 288.12 306.72 326.83 350.68
368.67 382.33 414.59 416.56 419.56 420.40
423.47 427.28 436.24 453.44 474.49 480.79
490.93 497.19 505.63 512.11 532.27 534.54
537.20 569.14 602.72 606.82 615.38 625.19
631.26 633.09 633.79 633.97 634.48 643.03
648.04 680.25 684.26 692.84 704.20 713.79
716.76 717.80 718.29 721.60 759.32 769.20
773.46 777.53 782.74 785.06 809.73 837.87
846.47 850.53 855.16 858.20 861.48 865.09
867.04 870.54 880.36 892.29 908.84 911.23
915.27 924.50 927.79 929.57 933.07 940.94
944.95 966.30 974.72 975.67 976.46 978.84
978.89 992.89 997.63 1000.85 1002.81 1007.34
1008.42 1011.83 1012.08 1012.69 1014.85 1016.03
1017.42 1017.54 1018.06 1022.30 1055.61 1057.52
1058.09 1059.93 1060.66 1062.50 1067.17 1068.35
1085.09 1109.82 1112.33 1117.36 1117.46 1129.30
1131.61 1146.83 1153.64 1175.52 1186.71 1189.26
1193.23 1194.85 1196.26 1196.36 1196.60 1212.50
1214.20 1221.74 1222.72 1223.63 1224.86 1225.16
1230.97 1232.33 1236.70 1247.15 1255.30 1263.04
1268.73 1292.05 1300.31 1306.48 1314.61 1318.65
1321.97 1324.09 1343.56 1345.47 1353.58 1360.61

1363.85 1364.31 1367.76 1367.85 1368.75 1374.11
1381.72 1386.08 1399.58 1409.45 1414.05 1463.29
1476.52 1488.85 1491.69 1492.81 1494.87 1496.33
1499.91 1503.98 1506.21 1515.27 1515.73 1518.35
1526.15 1539.63 1540.32 1540.96 1541.48 1607.60
1635.67 1636.49 1636.61 1638.97 1646.49 1659.33
1659.74 1660.36 1661.72 2954.46 3030.31 3033.89
3034.21 3037.27 3038.42 3038.96 3040.19 3044.74
3045.67 3046.06 3047.30 3057.68 3082.81 3083.10
3088.13 3091.87 3096.07 3098.72 3107.01 3143.16
3153.80 3155.89 3163.62 3166.52 3168.77 3171.25
3171.34 3174.07 3177.73 3181.18 3186.38 3187.27
3189.87 3190.40 3191.36 3196.51 3197.90 3199.31
3200.79 3201.75 3203.09 3210.87 3213.26 3215.13

==============================

II$_P$-TS

==============================

-317.82 13.48 18.10 22.22 29.12 29.99
33.18 35.82 38.39 41.80 44.58 48.18
50.42 53.16 57.12 59.15 63.90 64.39
71.09 76.14 79.62 81.86 90.05 97.24
98.57 105.23 106.43 108.66 110.44 111.95
115.15 120.04 123.76 129.98 132.72 137.91
141.28 150.07 157.56 170.53 181.86 187.42
190.18 192.31 196.65 202.45 208.58 220.54
222.03 227.45 229.61 233.00 238.79 247.80
268.59 269.33 276.23 278.81 287.83 288.29
291.07 295.19 302.70 306.32 324.12 334.49
355.50 364.80 370.85 383.87 396.42 412.31
418.30 419.75 422.20 425.01 431.08 434.65
439.53 444.13 448.64 463.13 475.90 482.73
499.03 500.05 503.32 506.05 523.99 532.59
532.82 534.01 543.14 551.28 560.85 568.59
575.06 591.21 599.41 602.35 606.77 607.97
617.79 625.16 630.15 632.36 633.47 633.57
634.61 643.03 644.38 648.41 673.39 681.72
683.46 696.00 713.20 716.34 717.89 719.15
723.14 739.88 742.77 761.90 768.06 770.17
770.60 777.49 778.43 782.80 783.29 785.10
794.35 816.00 829.94 836.39 846.21 852.75
854.43 856.31 861.27 863.73 864.80 867.95
875.19 875.73 876.71 892.57 897.23 899.25
901.71 905.35 911.09 915.28 919.55 927.68
928.79 930.84 932.00 936.43 943.54 945.01
955.34 966.63 970.33 973.83 975.69 978.77
979.32 984.16 987.54 995.62 998.22 1002.82
1007.99 1008.63 1011.32 1013.70 1014.53 1014.86
1015.32 1015.76 1017.68 1019.98 1021.81 1025.01
1039.91 1042.01 1043.34 1044.25 1056.32 1056.65
1057.35 1060.49 1060.97 1062.63 1064.14 1064.89
1065.82 1067.12 1069.25 1069.36 1078.73 1093.23
1105.85 1110.24 1110.62 1115.53 1120.82 1134.69
1138.37 1140.27 1150.79 1155.48 1184.55 1186.28
1187.02 1191.54 1194.03 1194.72 1195.31 1196.95
1198.02 1198.66 1201.47 1216.45 1217.42 1221.09
1222.54 1223.18 1223.76 1225.69 1226.53 1232.93
1240.23 1240.92 1247.34 1253.46 1259.83 1264.80
1270.50 1289.55 1298.97 1301.16 1305.92 1310.11
1313.18 1315.67 1317.75 1323.81 1329.49 1330.25
1341.75 1343.01 1355.68 1355.81 1356.94 1364.65
1364.85 1365.69 1366.20 1367.76 1376.43 1381.25
1388.79 1396.81 1401.39 1406.62 1413.86 1424.28
1425.28 1428.58 1453.03 1464.86 1472.82 1478.82
1480.57 1489.65 1490.28 1493.34 1494.74 1495.17
1495.91 1498.11 1503.03 1503.91 1504.28 1505.76
1507.39 1508.34 1511.14 1515.22 1515.98 1517.68
1526.96 1529.51 1539.58 1539.93 1540.56 1542.11
1572.70 1613.09 1616.16 1630.43 1634.71 1635.47
1636.44 1644.01 1645.70 1650.93 1656.53 1656.92
1657.77 1658.42 1660.10 1773.21 2972.75 3022.85
3024.52 3027.27 3030.40 3031.90 3036.43 3040.05
3041.24 3042.36 3045.29 3051.43 3056.20 3076.33
3080.00 3081.38 3088.79 3090.05 3093.61 3095.23
3099.15 3099.95 3101.57 3101.70 3106.28 3116.35
3123.60 3126.42 3131.69 3143.26 3150.08 3154.65
3161.06 3161.32 3162.88 3166.28 3172.21 3172.92
3175.67 3176.48 3176.84 3180.71 3181.03 3181.25
3183.60 3188.62 3192.11 3192.72 3193.10 3195.57
3197.94 3199.88 3200.47 3202.37 3205.77 3211.86
3218.65 3220.90 3241.68 3247.37 3247.52 3307.82

==============================

III$_{PN}$

==============================

5.47 16.55 17.80 26.17 27.39 33.33
37.36 43.73 47.85 53.53 57.76 63.84
66.10 68.97 70.88 80.12 88.62 91.00
93.48 96.36 101.35 106.01 115.34 118.81
122.87 142.15 148.48 159.21 163.21 172.89
181.80 189.28 192.94 196.92 221.22 223.68
225.68 229.06 243.74 246.24 253.78 259.61
265.84 280.72 283.13 290.46 304.04 313.75
330.71 337.97 356.70 373.06 391.22 408.75
417.83 419.35 420.86 422.01 432.57 434.64
440.59 444.74 474.65 486.05 488.93 499.96
506.90 513.81 514.72 519.29 533.28 560.42
561.87 584.32 603.95 607.14 613.40 617.54
621.73 624.94 630.40 631.34 632.67 634.03
635.98 642.85 647.64 661.23 676.92 689.49
691.72 693.06 717.72 718.55 719.43 721.22
734.97 756.20 777.35 778.59 779.84 781.99
783.35 784.86 785.46 794.05 814.19 840.03
845.89 851.02 851.34 856.09 860.19 862.87
865.29 866.93 867.65 869.13 893.61 893.89
918.00 919.23 925.56 928.81 931.34 932.67
934.59 935.11 946.12 946.93 951.40 956.05
973.78 975.31 983.30 983.99 985.50 985.56
1000.80 1003.33 1006.05 1009.90 1010.73 1011.67
1013.97 1015.59 1015.77 1016.43 1016.88 1017.88
1019.32 1020.21 1020.90 1024.63 1040.06 1041.93
1056.97 1057.69 1057.99 1059.23 1060.97 1066.94
1068.51 1095.68 1100.32 1109.10 1110.84 1119.77
1125.13 1136.51 1140.16 1151.33 1155.26 1157.56
1171.12 1181.21 1182.43 1192.34 1197.75 1198.33
1199.52 1199.80 1200.50 1202.41 1218.59 1221.73
1222.42 1222.42 1223.03 1223.69 1227.18 1230.53
1231.81 1233.69 1252.75 1257.52 1260.28 1264.03
1270.22 1299.45 1300.23 1305.13 1309.54 1316.55
1318.48 1322.55 1328.50 1343.64 1348.14 1355.80
1358.66 1360.81 1365.09 1365.29 1366.18 1367.55
1379.30 1382.03 1385.00 1391.95 1395.26 1401.47
1403.99 1411.14 1430.02 1463.19 1476.42 1477.25
1480.24 1492.41 1493.29 1495.44 1496.62 1500.05
1504.55 1505.75 1506.97 1511.03 1514.54 1515.30
1524.94 1536.60 1539.11 1539.40 1540.22 1540.68
1611.57 1613.84 1635.33 1636.94 1638.31 1639.12
1642.75 1649.85 1657.05 1658.95 1659.64 1659.76
3018.18 3023.63 3032.61 3043.20 3046.23 3046.75
3050.28 3053.99 3055.55 3059.38 3086.81 3096.02
3097.49 3101.32 3102.79 3109.63 3110.52 3113.01
3165.49 3168.03 3175.23 3176.15 3177.80 3178.48
3179.79 3183.26 3184.74 3185.58 3186.12 3186.49
3188.91 3192.66 3196.90 3197.18 3198.84 3199.45
3200.42 3200.65 3206.55 3206.98 3207.10 3207.93
3210.92 3211.24 3211.31 3213.75 3217.54 3218.80
3223.57 3238.94 3258.36

==============================

III$_{PN}$-TS

==============================

-200.00 19.03 23.13 24.88 28.66 32.05
35.70 42.79 44.73 51.36 58.99 61.45
66.70 71.11 72.58 81.17 88.12 91.74
93.42 101.31 104.99 110.28 116.90 122.85
127.11 133.39 137.71 151.91 153.93 155.12
169.22 197.05 208.38 216.94 221.05 228.87
236.60 240.14 244.60 247.36 248.28 262.07
267.15 274.91 282.84 284.63 296.02 313.86
324.39 341.39 343.50 367.75 374.31 419.90
420.29 426.42 426.71 428.07 429.55 431.38
453.41 464.70 483.75 494.16 499.61 512.29
518.37 523.02 530.45 543.37 550.77 556.72

558.23 587.53 590.65 599.09 616.12 616.55
625.84 628.15 629.14 630.91 631.76 632.62
636.70 641.71 653.23 669.95 678.34 695.44
709.24 721.03 721.98 722.72 726.26 742.38
758.60 767.57 772.25 775.08 776.87 780.36
781.44 783.11 786.97 789.60 809.61 812.49
827.73 844.80 851.49 862.92 865.63 866.16
871.65 875.29 883.16 887.91 894.54 898.05
905.30 913.53 917.64 921.19 932.92 934.97
937.05 937.98 947.87 949.14 952.27 965.36
981.81 983.08 986.29 986.66 987.85 992.52
998.17 1003.49 1004.14 1005.86 1007.17 1009.16
1010.60 1014.52 1014.71 1016.20 1016.33 1021.09
1022.04 1031.66 1033.29 1044.24 1045.50 1047.70
1054.43 1057.53 1058.27 1060.28 1061.87 1064.85
1066.20 1090.85 1104.24 1109.03 1117.96 1118.99
1121.72 1135.52 1142.64 1152.40 1153.83 1160.08
1162.01 1180.65 1189.64 1192.87 1197.46 1199.14
1199.59 1199.88 1205.62 1208.14 1210.19 1215.71
1218.80 1221.26 1221.90 1222.14 1223.17 1225.66
1227.42 1227.56 1232.80 1247.38 1262.12 1265.87
1271.55 1276.05 1294.10 1301.63 1307.89 1309.72
1311.67 1321.48 1334.91 1341.60 1344.08 1346.10
1360.18 1360.89 1361.43 1365.17 1366.51 1367.89
1368.54 1373.84 1381.38 1389.08 1389.61 1395.28
1405.29 1408.60 1426.97 1471.95 1475.33 1478.94
1479.58 1490.78 1492.97 1494.73 1494.82 1495.34
1504.77 1508.14 1509.13 1509.41 1517.88 1524.29
1529.84 1537.70 1538.35 1539.11 1541.30 1545.15
1612.36 1625.61 1629.57 1633.78 1635.71 1636.43
1640.06 1648.10 1653.68 1655.61 1658.46 1659.99
2998.21 3010.90 3045.57 3046.29 3052.47 3053.94
3058.72 3061.87 3065.42 3073.55 3080.46 3088.48
3099.11 3100.02 3112.18 3112.38 3121.13 3124.26
3149.54 3160.21 3163.76 3169.01 3169.63 3172.32
3174.09 3174.85 3176.42 3180.94 3182.09 3182.20
3186.03 3186.19 3189.72 3191.73 3196.94 3198.14
3199.18 3201.34 3202.50 3205.95 3206.38 3208.76
3211.67 3215.59 3216.94 3218.07 3221.28 3223.15
3226.67 3245.32 3314.92
==============================
V_{PN}
==============================
5.86 9.63 19.92 24.30 26.94 29.70
35.38 38.40 45.01 46.67 52.56 55.64
58.16 67.93 71.78 73.30 81.24 82.08
95.63 96.83 111.25 112.70 114.37 121.41
131.76 140.50 142.90 160.18 162.97 178.83
192.31 204.03 211.36 213.26 219.21 227.77
235.97 243.57 249.42 259.33 263.25 268.24
270.08 281.63 297.08 304.61 321.04 345.12
347.04 368.25 374.90 390.76 405.05 412.40
418.75 420.77 421.51 424.05 431.16 436.50
475.86 478.24 489.19 494.41 497.80 513.93
515.10 519.89 534.93 537.47 569.82 577.75
587.79 602.35 604.80 613.53 615.72 623.24
630.35 631.66 633.71 634.38 634.71 639.65
647.09 675.87 678.10 679.40 684.96 688.08
707.87 717.06 719.21 720.26 720.65 721.95
740.05 770.02 778.09 779.72 781.29 783.89
784.24 787.14 788.61 795.16 817.68 837.86
841.81 850.24 852.64 859.56 862.74 865.60
867.38 871.06 875.23 891.51 892.52 895.75
912.25 924.48 926.26 927.60 932.90 935.14
935.46 939.77 945.88 952.50 975.36 978.61
980.50 981.06 983.56 984.46 992.62 1002.92
1006.75 1008.20 1008.86 1009.26 1010.01 1011.42
1012.66 1013.79 1014.12 1015.08 1016.40 1017.89
1019.45 1021.62 1022.60 1046.43 1053.63 1055.89
1057.72 1059.54 1061.90 1066.37 1066.94 1068.07
1105.94 1108.43 1109.97 1116.31 1119.62 1123.75
1137.73 1139.21 1153.29 1156.67 1158.49 1169.78
1180.02 1186.81 1195.30 1197.45 1198.39 1198.59
1199.69 1200.40 1204.10 1211.52 1220.06 1221.74
1222.62 1223.03 1223.93 1224.23 1225.77 1228.27
1229.65 1234.71 1245.99 1252.78 1262.47 1266.73
1293.65 1300.01 1302.96 1308.07 1310.92 1312.32
1318.45 1324.65 1332.09 1345.68 1346.00 1351.89
1361.97 1363.37 1363.84 1366.45 1366.73 1366.94
1373.39 1385.86 1387.19 1387.57 1394.10 1397.81
1400.00 1419.28 1431.89 1466.22 1477.65 1487.00
1487.49 1492.29 1494.01 1495.82 1497.60 1504.35
1505.93 1509.88 1510.53 1515.69 1516.36 1517.00
1539.15 1539.56 1540.31 1540.61 1542.05 1580.64
1634.51 1634.58 1635.01 1636.14 1636.33 1642.14
1656.46 1657.19 1658.47 1658.85 1660.65 1661.83
3027.22 3033.48 3041.24 3048.14 3049.13 3049.92
3053.35 3055.98 3056.33 3057.97 3061.02 3096.07
3096.40 3099.10 3105.27 3107.82 3111.31 3117.43
3133.22 3149.17 3150.66 3165.22 3168.47 3177.58
3179.62 3182.13 3183.49 3184.50 3184.92 3185.69
3186.69 3187.63 3188.24 3193.65 3193.96 3195.31
3195.85 3198.15 3199.32 3202.06 3204.20 3205.50
3206.03 3207.25 3210.39 3212.27 3212.65 3213.26
3214.51 3270.12 3289.45
==============================
VI_{PN}
==============================
2.35 7.51 16.87 18.14 20.97 26.37
28.05 34.09 36.74 38.43 40.58 42.55
49.04 50.36 54.20 55.66 58.75 60.05
62.09 63.12 69.84 76.27 81.68 87.18
92.31 95.83 102.60 109.58 111.81 115.26
118.66 121.12 127.19 128.78 138.28 143.67
150.57 160.11 167.33 176.38 183.56 187.37
204.16 212.39 214.22 218.63 221.07 226.15
238.41 239.17 247.04 253.64 254.58 259.92
266.64 270.37 270.76 289.97 298.64 309.58
314.04 319.03 320.19 336.20 343.10 343.40
351.11 387.69 393.37 397.28 413.81 415.25
416.65 421.86 421.94 426.68 433.90 444.10
460.12 468.75 479.02 484.95 491.69 493.74
500.31 505.88 510.03 515.03 518.15 525.14
530.09 541.10 549.84 577.86 582.12 598.41
599.45 604.55 609.77 610.85 617.50 620.96
624.61 633.06 633.31 634.20 635.23 635.99
637.49 646.13 648.03 660.22 671.70 674.25
679.02 703.91 710.19 714.02 714.94 720.58
722.08 726.54 735.33 760.07 776.80 778.64
779.20 782.25 782.99 783.46 789.49 813.13
817.06 818.20 823.32 839.59 843.11 848.06
854.47 855.39 856.89 859.43 864.50 867.02
870.66 872.15 872.86 883.39 890.84 902.81
919.12 923.50 924.02 930.96 933.86 935.11
935.75 938.35 942.29 950.02 959.76 966.04
972.12 975.10 976.66 979.05 980.42 983.49
983.85 995.31 996.15 998.17 1003.39 1004.76
1008.32 1013.51 1015.22 1015.64 1016.71 1018.07
1018.50 1020.30 1023.43 1030.07 1038.93 1043.48
1044.50 1052.85 1058.33 1060.15 1060.98 1062.67
1063.20 1064.58 1065.13 1068.96 1069.70 1072.02
1074.57 1084.39 1107.98 1109.05 1112.41 1117.81
1121.27 1123.81 1127.18 1129.35 1141.00 1149.98
1155.49 1162.57 1175.26 1183.00 1193.91 1195.52
1195.79 1197.21 1198.34 1199.43 1202.00 1217.34
1219.47 1219.71 1221.08 1221.96 1224.93 1227.79
1228.56 1229.48 1234.72 1235.11 1236.67 1247.38
1253.53 1254.87 1256.15 1268.34 1283.80 1289.98
1309.66 1314.03 1314.19 1314.84 1317.17 1323.30
1328.76 1331.13 1336.74 1339.71 1345.16 1345.89
1358.35 1360.44 1365.20 1367.23 1367.82 1369.18
1370.34 1373.97 1380.33 1395.14 1397.02 1398.89
1401.34 1404.87 1423.69 1424.07 1424.87 1426.05
1428.98 1432.19 1450.88 1464.32 1472.12 1475.83
1488.14 1490.70 1491.81 1491.97 1494.27 1495.33
1495.80 1498.13 1498.42 1505.85 1505.88 1507.04
1509.04 1513.77 1514.78 1515.38 1517.57 1523.19
1526.12 1539.23 1540.39 1541.42 1542.81 1545.52
1559.40 1613.86 1623.00 1635.04 1635.10 1637.29
1640.73 1641.22 1651.11 1658.10 1660.09 1661.23

1661.73 1661.90 1662.62 1665.00 3009.50 3025.57
3030.16 3038.20 3038.53 3041.16 3044.04 3044.89
3045.17 3047.41 3047.89 3048.26 3051.83 3054.99
3067.77 3079.07 3082.65 3088.58 3094.57 3096.53
3099.82 3105.46 3107.79 3111.64 3120.31 3126.08
3139.25 3140.88 3149.36 3153.43 3162.68 3166.44
3169.09 3170.35 3171.96 3173.19 3174.13 3174.50
3174.94 3175.30 3178.19 3184.13 3185.33 3188.66
3189.32 3190.59 3193.27 3194.47 3195.22 3199.61
3199.91 3201.02 3201.99 3202.74 3206.72 3209.18
3209.90 3210.41 3218.90 3221.86 3249.20 3321.25

==============================

II$_{P}$-TS'

==============================

-184.18 10.00 15.79 19.17 21.32 24.45
27.34 33.24 34.34 38.29 41.89 45.96
47.17 51.19 53.24 54.83 59.09 63.22
67.06 75.10 77.39 79.89 82.58 84.14
89.47 91.19 101.92 105.32 105.98 109.69
112.46 119.30 121.71 128.47 133.39 139.07
146.70 152.46 163.36 164.38 173.46 184.89
191.10 192.40 197.13 208.38 218.70 220.43
222.45 223.62 227.34 233.50 236.69 238.46
249.36 255.62 264.48 276.69 277.82 280.34
284.67 289.46 300.72 306.70 321.40 328.33
360.32 362.63 369.51 392.49 413.81 414.64
417.48 419.97 422.45 425.10 432.42 436.93
440.63 448.18 457.00 467.25 477.47 490.03
490.60 500.58 501.00 510.39 515.93 520.49
531.51 539.18 545.89 554.29 562.61 571.32
577.52 595.57 602.93 603.07 608.89 610.17
611.70 623.05 629.66 630.27 630.96 631.47
631.89 636.83 638.64 648.06 657.21 668.82
678.39 698.29 712.41 715.44 717.32 718.23
720.27 740.37 744.04 765.24 769.95 773.60
775.90 780.94 781.44 782.60 782.69 783.70
786.98 818.95 827.02 837.95 841.15 851.15
853.18 854.65 861.28 863.38 863.88 867.91
871.61 873.34 875.80 893.48 894.63 897.74
900.64 906.34 914.96 921.15 922.78 923.46
926.80 931.93 938.60 943.69 944.80 959.39
961.15 972.62 972.80 975.93 977.48 978.85
981.95 993.26 995.18 1000.02 1001.72 1008.01
1011.20 1012.22 1013.03 1014.73 1016.39 1017.70
1018.42 1019.35 1021.38 1023.16 1023.78 1029.98
1039.92 1040.80 1048.40 1055.26 1055.59 1057.64
1058.85 1061.80 1062.14 1064.47 1065.40 1068.45
1069.50 1069.88 1073.31 1077.30 1087.07 1107.50
1110.57 1112.10 1116.34 1120.49 1123.56 1135.85
1140.33 1142.82 1149.59 1157.10 1186.03 1189.50
1193.56 1194.62 1195.70 1196.31 1196.52 1197.52
1198.36 1199.42 1207.89 1217.55 1220.16 1221.74
1224.15 1225.13 1226.03 1227.56 1230.73 1231.46
1239.62 1241.47 1248.54 1251.52 1255.92 1256.94
1281.39 1287.46 1303.14 1303.93 1307.81 1309.90
1312.10 1318.80 1322.37 1330.23 1332.90 1344.80
1345.25 1346.36 1355.06 1358.42 1362.36 1365.05
1365.93 1367.19 1367.93 1369.17 1371.12 1392.36
1398.28 1400.14 1404.66 1417.16 1418.51 1426.55
1427.90 1432.23 1451.96 1453.72 1468.16 1468.38
1477.80 1490.19 1491.23 1491.98 1492.70 1493.28
1494.62 1495.85 1498.17 1498.84 1503.78 1507.79
1508.09 1512.00 1513.23 1514.66 1517.10 1517.27
1518.66 1526.34 1529.69 1538.17 1538.96 1539.29
1540.63 1608.07 1619.32 1631.70 1634.21 1634.48
1636.43 1641.41 1647.43 1651.91 1655.44 1656.79
1657.81 1660.79 1662.44 1759.21 2970.80 3026.07
3031.25 3034.13 3035.57 3036.86 3037.64 3038.53
3039.57 3046.80 3048.12 3052.04 3052.61 3064.02
3078.58 3080.83 3081.37 3086.57 3090.07 3094.78
3101.03 3104.10 3104.27 3111.35 3118.23 3126.72
3133.16 3138.81 3140.87 3150.90 3151.56 3156.73
3157.40 3164.43 3165.45 3170.15 3171.07 3173.27
3177.99 3178.62 3180.04 3180.23 3180.89 3186.50
3188.73 3189.41 3190.31 3191.04 3194.40 3195.88
3197.94 3199.36 3200.14 3202.81 3204.48 3206.12
3213.42 3218.80 3229.89 3244.30 3261.96 3291.34

==============================

III$_{PC}$

==============================

17.45 21.79 24.40 27.20 33.16 36.16
40.94 45.93 51.74 60.36 64.27 69.22
71.29 76.17 83.59 87.21 91.44 93.71
96.54 108.29 108.67 116.75 120.62 123.44
124.69 131.86 142.05 150.71 161.13 174.15
182.44 188.09 196.04 203.91 211.26 217.47
222.24 231.16 235.14 243.93 262.04 266.15
269.71 279.61 291.80 303.04 313.61 314.90
334.87 342.39 368.15 378.74 393.72 406.83
412.87 415.80 418.99 421.70 428.85 432.33
437.63 445.15 472.43 493.26 496.88 502.79
506.08 513.37 518.36 519.02 536.53 552.94
571.86 582.43 596.78 608.89 614.67 616.40
622.84 626.26 630.30 632.82 634.19 634.98
639.30 641.59 648.10 663.33 681.16 686.92
694.26 701.34 717.36 717.88 719.09 723.92
766.31 774.24 776.18 777.85 780.51 781.75
783.59 787.35 793.21 797.38 818.86 837.42
845.08 848.69 854.33 860.46 861.62 862.12
865.55 871.79 873.70 885.18 893.20 904.35
912.15 919.77 924.09 927.38 932.95 934.32
938.50 942.77 943.16 946.67 949.85 957.23
976.52 980.88 982.07 989.23 992.95 993.52
999.73 1000.67 1002.51 1006.92 1008.71 1009.88
1012.33 1012.84 1014.41 1015.04 1016.57 1017.76
1018.91 1019.06 1019.50 1021.68 1027.36 1034.65
1040.03 1056.10 1056.96 1057.74 1059.82 1060.54
1065.21 1068.79 1104.71 1109.92 1111.56 1119.41
1120.51 1126.55 1138.75 1152.90 1156.36 1158.41
1183.25 1184.97 1187.75 1193.83 1197.28 1198.45
1198.55 1199.79 1200.14 1202.60 1217.03 1219.37
1222.57 1222.81 1224.27 1224.78 1225.78 1226.39
1228.56 1230.49 1249.24 1252.73 1255.25 1256.08
1258.75 1261.74 1294.78 1302.14 1310.89 1311.14
1321.53 1331.88 1335.09 1342.80 1343.42 1345.27
1346.64 1357.80 1361.48 1363.71 1365.85 1366.75
1367.81 1374.27 1381.77 1388.85 1390.23 1395.36
1396.36 1400.94 1415.48 1466.88 1474.54 1477.06
1478.60 1487.08 1491.97 1493.77 1493.93 1495.74
1502.95 1507.11 1507.47 1508.71 1515.94 1517.00
1523.64 1531.14 1539.08 1540.67 1540.94 1541.40
1611.84 1623.87 1634.22 1637.85 1638.07 1638.76
1641.78 1648.94 1657.43 1659.88 1660.11 1660.50
3011.43 3020.10 3030.57 3046.51 3049.81 3051.47
3056.96 3063.37 3066.54 3068.83 3072.04 3100.71
3101.25 3101.92 3106.12 3107.57 3117.39 3124.29
3148.58 3163.24 3167.19 3178.89 3179.15 3183.45
3184.13 3184.44 3185.11 3187.45 3191.38 3193.35
3193.80 3194.40 3195.93 3198.84 3200.31 3201.11
3203.81 3204.81 3205.88 3207.98 3208.36 3209.51
3211.59 3212.33 3213.46 3215.50 3224.06 3228.96
3243.56 3246.84 3247.37

==============================

III$_{PC}$-TS

==============================

-143.21 13.96 17.38 21.40 24.42 32.36
37.81 43.98 45.39 48.98 52.46 67.50
68.91 72.11 74.63 78.71 81.24 85.82
94.53 99.01 101.92 110.88 114.10 120.96
121.46 126.90 133.52 137.09 159.82 162.58
165.38 185.53 194.12 197.01 212.28 215.22
227.25 233.83 241.75 251.30 262.54 266.43
269.19 276.85 282.79 294.29 298.02 315.40
338.68 343.39 368.36 374.96 393.18 412.22
414.47 414.95 417.89 424.66 425.81 429.47
438.08 450.13 464.31 491.75 496.19 503.79
509.63 512.74 515.33 522.10 541.11 544.60
559.83 585.03 591.36 607.36 615.00 616.15
622.52 625.53 629.84 631.35 632.16 633.87
635.50 640.30 647.52 671.99 677.43 683.82

691.27 702.61 716.07 716.71 724.75 725.35
763.59 772.12 775.75 776.68 780.81 783.46
784.37 786.56 787.96 818.28 828.91 837.12
844.32 848.25 855.01 859.08 860.79 862.13
868.55 871.47 873.31 887.84 892.82 903.48
909.02 917.10 925.22 929.51 936.89 937.47
941.77 946.30 946.89 949.98 961.10 971.83
976.44 979.46 985.47 987.42 992.67 997.96
1000.25 1000.34 1005.51 1005.96 1008.46 1010.22
1010.95 1012.01 1013.62 1015.50 1016.57 1017.14
1019.43 1020.31 1021.49 1025.40 1033.11 1042.50
1055.45 1055.66 1057.16 1058.38 1060.10 1062.48
1066.70 1068.17 1109.71 1111.02 1112.21 1119.83
1120.52 1126.42 1141.19 1152.73 1154.46 1159.47
1184.91 1189.45 1192.67 1194.91 1198.18 1198.96
1199.55 1199.87 1202.84 1203.99 1218.02 1220.35
1221.24 1222.69 1223.80 1224.28 1227.05 1229.76
1230.57 1232.00 1241.02 1249.86 1251.07 1254.71
1257.88 1267.38 1292.58 1304.83 1310.55 1311.10
1321.60 1328.61 1333.04 1335.52 1345.07 1345.62
1350.22 1355.83 1362.24 1363.46 1365.68 1366.16
1367.83 1371.47 1379.78 1384.11 1385.70 1394.13
1396.90 1397.07 1420.89 1465.78 1478.54 1481.66
1485.20 1487.63 1490.52 1493.43 1494.57 1495.77
1499.53 1507.43 1508.55 1509.40 1517.18 1518.34
1526.63 1538.54 1540.15 1540.42 1540.88 1548.30
1614.45 1633.94 1636.34 1636.73 1636.92 1637.17
1642.67 1657.14 1658.27 1659.00 1659.64 1660.11
3022.02 3025.23 3030.64 3038.71 3049.02 3052.82
3057.05 3057.37 3068.74 3070.54 3073.40 3099.11
3101.81 3106.87 3107.66 3119.29 3121.31 3130.02
3136.46 3171.08 3172.23 3178.55 3178.73 3179.17
3183.56 3184.27 3185.18 3187.78 3189.85 3192.14
3192.42 3195.13 3196.11 3198.31 3200.86 3201.86
3204.05 3206.12 3206.28 3209.47 3209.88 3211.37
3212.45 3215.49 3215.92 3221.84 3223.71 3225.20
3230.37 3231.14 3232.12

==============================

V_{PC}

==============================

6.38 12.52 17.46 19.40 23.69 29.78
32.20 39.52 45.94 48.51 53.15 55.46
61.34 64.27 64.86 76.09 80.50 84.76
86.84 94.87 103.28 114.95 119.05 124.05
132.39 133.74 150.70 153.76 158.39 166.72
189.24 204.98 217.34 228.29 229.49 231.32
236.67 242.68 243.90 246.30 248.55 269.27
284.39 289.50 294.31 313.54 317.15 334.47
335.36 354.50 380.40 384.45 414.55 415.32
420.36 420.49 423.49 431.10 435.54 441.64
480.27 483.91 489.14 499.89 508.10 514.08
517.35 519.77 531.78 534.78 553.84 567.96
595.02 595.97 600.70 608.42 615.92 625.48
631.20 632.60 633.59 634.25 635.14 641.07
648.67 654.77 678.73 680.34 688.42 689.71
717.22 717.36 719.26 722.79 724.05 750.23
770.38 774.00 776.38 779.42 782.38 784.75
788.66 795.80 818.89 831.45 835.14 843.70
850.57 854.14 859.06 860.29 863.18 867.16
868.40 892.35 894.96 896.44 906.45 906.91
919.95 922.49 927.07 930.27 931.52 933.74
939.74 941.67 963.68 971.11 973.30 975.42
981.46 981.67 983.16 1001.99 1002.94 1004.04
1004.64 1005.13 1005.48 1007.00 1007.92 1010.32
1013.51 1014.16 1015.70 1016.26 1017.33 1017.96
1018.96 1021.83 1041.68 1053.82 1057.99 1059.50
1060.52 1060.67 1066.19 1067.98 1070.09 1085.30
1095.85 1109.93 1110.56 1121.47 1122.85 1126.03
1129.15 1136.43 1152.50 1158.18 1183.43 1184.67
1190.86 1196.18 1196.87 1198.42 1199.42 1199.91
1200.59 1202.26 1211.14 1219.54 1220.09 1221.88
1222.18 1222.65 1223.21 1225.30 1226.05 1226.77
1228.00 1242.13 1248.86 1250.17 1252.05 1255.20
1260.53 1297.71 1298.53 1304.58 1314.99 1315.31
1315.85 1329.47 1333.18 1341.04 1346.97 1347.91
1353.08 1360.46 1362.15 1363.37 1364.56 1365.73
1366.10 1367.07 1382.20 1384.10 1385.79 1388.85
1392.28 1395.01 1429.90 1469.66 1478.89 1491.53
1492.18 1495.30 1496.14 1496.59 1497.79 1508.15
1508.21 1508.35 1509.53 1518.01 1518.48 1523.59
1539.86 1540.07 1540.32 1540.44 1541.87 1616.86
1636.57 1637.22 1637.92 1639.23 1640.57 1648.50
1658.63 1659.10 1659.17 1660.29 1661.48 1667.03
3024.17 3026.66 3028.60 3043.45 3050.93 3052.13
3054.60 3057.29 3061.28 3063.64 3066.28 3066.92
3069.51 3097.43 3098.05 3107.25 3115.04 3117.03
3119.70 3125.97 3144.16 3144.90 3161.22 3162.61
3167.05 3175.62 3178.78 3179.10 3180.52 3184.10
3184.96 3187.73 3189.46 3192.19 3194.11 3195.34
3196.04 3196.31 3198.84 3202.33 3205.10 3205.54
3208.10 3209.70 3209.93 3211.72 3212.07 3214.13
3216.47 3224.41 3229.90

==============================

VI_{PC}

==============================

5.16 15.40 21.50 26.60 27.81 28.77
32.15 38.02 39.33 44.39 46.20 49.58
52.18 53.48 58.28 58.54 65.87 66.77
67.71 76.15 78.27 79.66 83.79 86.24
90.94 94.23 98.23 100.22 109.68 116.90
120.63 125.82 128.69 131.33 137.65 147.15
148.92 153.15 157.97 167.33 170.03 185.85
191.41 195.90 205.98 212.36 218.27 225.50
228.19 233.06 238.04 242.42 242.55 245.69
251.50 259.83 266.76 269.08 278.39 282.77
296.35 305.88 309.49 320.44 328.48 335.39
346.41 375.10 384.31 393.81 414.84 416.93
417.65 419.02 420.25 423.06 428.12 439.71
467.28 470.62 477.74 495.82 496.33 500.80
502.39 505.62 513.19 517.38 522.40 529.44
529.77 552.20 553.07 569.73 574.25 583.56
599.65 601.59 604.52 610.49 612.42 617.27
624.71 629.53 633.74 634.10 634.49 635.01
639.76 650.60 651.99 665.34 669.77 681.00
697.97 713.63 713.81 714.63 715.03 720.57
750.74 756.71 771.43 773.41 779.15 783.41
784.90 786.56 788.59 799.66 802.35 816.43
821.11 830.05 836.50 840.78 844.74 851.44
856.04 861.85 865.74 867.80 869.87 870.55
886.48 887.64 890.71 892.99 897.18 907.12
920.25 921.68 923.32 926.69 931.89 933.65
934.33 946.07 959.79 960.05 964.67 968.73
971.71 974.01 975.31 977.99 983.36 994.11
997.06 998.06 998.35 1000.26 1001.37 1002.23
1008.49 1012.25 1012.82 1014.61 1015.84 1016.48
1016.64 1019.50 1020.84 1027.57 1038.46 1040.95
1044.17 1055.11 1055.56 1059.03 1059.84 1061.49
1063.71 1065.10 1066.82 1068.03 1069.79 1070.04
1071.07 1087.94 1107.60 1108.95 1111.88 1119.65
1122.44 1123.82 1125.44 1128.69 1128.92 1155.72
1159.16 1177.94 1184.64 1185.36 1193.02 1195.01
1195.57 1195.65 1195.99 1198.19 1201.39 1215.37
1215.51 1216.10 1219.56 1221.54 1222.91 1225.08
1225.38 1226.10 1228.86 1231.10 1235.69 1239.34
1248.89 1251.38 1254.73 1257.12 1268.41 1286.14
1293.74 1298.60 1311.98 1315.88 1319.20 1319.50
1320.50 1327.82 1335.00 1340.22 1341.09 1345.33
1345.43 1357.20 1361.63 1361.87 1365.23 1365.98
1366.21 1368.35 1372.60 1375.47 1385.26 1398.28
1399.63 1401.16 1406.47 1412.70 1420.41 1423.24
1425.67 1428.30 1454.32 1469.21 1477.84 1486.36
1489.84 1492.38 1493.20 1493.50 1495.20 1495.48
1498.75 1498.96 1499.73 1506.37 1507.70 1507.99
1510.01 1510.35 1518.62 1519.21 1520.43 1521.27
1531.36 1538.26 1539.02 1539.29 1542.35 1542.93
1622.37 1623.78 1628.09 1633.41 1636.26 1637.37
1639.75 1648.21 1654.04 1657.66 1658.21 1659.51
1659.84 1661.89 1664.35 1665.34 3017.28 3022.22
3029.75 3035.47 3038.55 3038.86 3041.49 3043.56
3045.91 3047.49 3048.39 3057.92 3059.63 3065.09

3071.84 3076.02 3085.15 3085.99 3091.90 3096.19
3099.39 3100.56 3105.79 3106.99 3108.02 3113.20
3114.04 3118.56 3123.58 3140.45 3141.94 3148.04
3151.57 3151.97 3153.63 3168.63 3168.75 3169.62
3171.71 3173.25 3175.73 3177.95 3178.27 3181.10
3184.64 3184.70 3188.35 3188.37 3188.61 3189.45
3190.45 3191.24 3197.76 3198.00 3201.58 3203.82
3204.77 3206.34 3208.44 3212.86 3218.56 3230.31

==============================

VI$_{PC}$-TS

==============================

-1051.09 13.17 18.16 19.77 26.96 32.60
35.17 38.46 40.29 43.56 44.16 47.16
49.60 53.98 56.86 59.07 62.44 63.50
69.62 72.49 75.21 82.13 86.04 92.82
96.82 98.33 101.58 109.98 112.30 117.55
122.81 127.59 132.22 140.11 142.44 150.91
157.92 160.50 176.48 186.33 187.36 190.27
200.74 203.50 207.11 220.93 225.67 228.39
231.15 234.38 238.14 239.22 245.42 248.45
252.45 270.54 273.98 277.28 281.50 285.99
290.52 307.05 309.82 314.52 334.45 339.24
353.50 361.30 377.29 391.14 403.08 417.97
418.33 420.14 420.64 429.67 435.62 442.10
444.97 480.51 485.63 490.09 491.22 494.22
498.88 503.79 509.15 511.65 518.77 522.88
535.06 540.48 544.15 547.55 568.89 592.45
599.34 604.97 605.76 609.41 613.57 619.63
626.31 629.73 630.18 632.82 634.19 634.62
639.53 641.07 648.57 664.20 665.49 678.67
680.27 696.43 716.66 718.58 720.44 721.50
728.89 736.14 752.98 774.11 774.66 777.38
779.36 781.88 783.45 785.25 798.99 802.53
809.85 817.79 821.46 838.57 845.76 848.13
854.59 859.32 862.10 867.30 869.96 874.11
878.19 881.24 896.60 899.85 903.26 904.60
920.18 923.17 927.86 931.99 934.53 935.76
937.41 940.20 942.37 948.24 953.28 961.22
975.02 978.23 978.89 979.08 979.23 984.21
986.29 999.11 1002.49 1007.11 1007.61 1009.46
1010.07 1012.32 1014.36 1015.32 1016.28 1016.80
1019.37 1022.47 1023.83 1037.03 1038.65 1046.38
1049.28 1051.24 1057.80 1059.31 1060.32 1060.64
1061.91 1062.57 1063.15 1063.44 1070.00 1071.11
1071.94 1080.06 1109.78 1109.87 1110.93 1119.78
1123.78 1125.64 1126.63 1137.18 1144.21 1152.94
1158.79 1182.05 1184.78 1191.40 1194.85 1194.98
1195.64 1196.77 1197.71 1198.03 1209.87 1215.32
1215.92 1216.51 1222.93 1225.28 1225.69 1227.30
1227.50 1228.79 1232.39 1234.27 1240.29 1251.02
1253.34 1254.83 1262.24 1273.95 1285.06 1295.69
1301.46 1302.15 1303.32 1307.57 1311.87 1313.99
1320.54 1322.23 1328.37 1340.53 1343.69 1347.42
1349.66 1361.20 1364.35 1364.56 1365.95 1368.88
1369.17 1370.97 1375.30 1377.94 1384.27 1392.87
1397.51 1398.91 1404.50 1415.47 1424.67 1426.31
1428.97 1431.29 1449.02 1451.52 1467.27 1478.79
1480.58 1493.19 1493.57 1494.01 1494.27 1494.87
1497.90 1498.60 1499.79 1505.84 1506.61 1507.73
1509.14 1511.46 1513.16 1516.15 1516.88 1517.49
1517.95 1523.13 1535.17 1541.29 1541.57 1542.93
1543.87 1547.65 1618.82 1623.58 1636.17 1636.93
1637.61 1639.90 1640.10 1657.20 1659.25 1661.01
1661.37 1662.35 1662.75 1663.56 1664.27 3016.29
3029.26 3032.00 3034.25 3037.21 3037.98 3040.08
3044.76 3050.26 3051.43 3054.18 3054.53 3054.57
3062.37 3079.35 3081.12 3089.30 3089.84 3092.24
3101.33 3101.83 3106.53 3117.26 3117.32 3121.63
3124.86 3140.43 3147.81 3153.64 3160.56 3163.90
3164.17 3165.19 3165.33 3167.64 3169.78 3171.32
3172.97 3173.27 3178.47 3183.07 3184.71 3184.94
3185.60 3188.31 3191.70 3193.25 3195.94 3198.74
3198.84 3199.21 3200.85 3204.70 3207.97 3209.87
3210.76 3211.70 3221.08 3222.21 3227.70 3261.94

==============================

VII$_{PC}$

==============================

8.83 14.81 16.97 21.17 23.95 26.86
29.67 32.69 35.86 39.87 45.27 47.27
49.90 51.59 53.33 60.17 63.13 67.88
70.55 76.26 83.12 85.83 88.42 89.02
97.88 101.53 106.17 109.39 111.04 117.03
122.11 122.98 128.85 135.27 145.06 148.08
152.06 159.82 167.02 182.50 191.56 193.41
200.65 214.16 219.27 226.78 229.43 232.11
233.16 236.51 239.78 245.77 248.78 250.51
252.98 263.13 271.23 273.50 275.81 290.24
296.97 299.40 316.97 325.93 333.90 349.46
355.40 373.36 374.26 393.24 413.24 415.97
420.96 423.05 426.17 432.01 434.09 450.85
454.53 479.25 491.27 494.18 498.61 500.37
505.15 512.85 514.55 518.50 532.72 538.99
540.87 541.09 564.84 573.15 593.88 597.17
599.98 607.74 608.34 610.88 614.51 627.39
630.34 631.01 633.35 634.39 634.81 635.02
641.75 650.15 662.73 663.84 676.13 683.96
702.16 711.94 714.10 719.30 720.65 722.06
722.91 736.32 759.50 760.02 771.54 775.21
776.74 778.98 783.40 785.00 786.18 800.86
802.14 811.84 813.97 839.38 847.33 849.52
853.86 855.63 859.25 860.76 870.63 875.38
876.22 877.13 887.24 895.25 901.67 903.79
920.98 924.25 926.15 930.83 931.76 932.73
935.24 935.52 939.17 947.46 960.60 964.70
970.83 975.41 975.79 979.84 981.20 983.31
986.33 997.96 1001.08 1002.67 1005.43 1010.17
1013.05 1013.42 1014.40 1015.58 1016.10 1017.57
1021.79 1022.60 1023.27 1027.68 1037.27 1041.48
1044.11 1050.41 1057.37 1058.10 1058.12 1059.70
1060.90 1062.96 1064.13 1065.09 1067.97 1070.06
1071.99 1072.20 1106.05 1109.32 1111.55 1118.22
1118.38 1124.30 1125.74 1134.29 1147.66 1150.90
1157.16 1179.82 1181.53 1189.47 1193.80 1194.34
1194.83 1196.55 1197.46 1197.89 1200.02 1210.90
1214.58 1219.71 1220.44 1223.35 1227.15 1227.62
1229.23 1233.53 1234.54 1239.80 1248.32 1252.77
1253.58 1256.50 1261.13 1264.21 1290.06 1294.39
1297.33 1300.48 1302.50 1313.16 1313.43 1313.69
1322.72 1325.00 1329.66 1334.81 1345.75 1348.16
1355.02 1356.99 1358.49 1360.94 1364.80 1365.90
1368.01 1370.30 1373.51 1374.66 1386.63 1394.28
1397.94 1399.29 1405.04 1410.86 1426.84 1426.92
1430.50 1432.91 1451.83 1464.39 1476.75 1477.24
1484.13 1491.64 1492.88 1493.88 1495.20 1496.06
1497.91 1501.04 1502.95 1506.72 1507.30 1507.64
1508.44 1510.96 1515.35 1516.78 1517.36 1518.02
1524.47 1538.84 1541.51 1541.80 1541.93 1548.11
1548.67 1601.65 1616.92 1634.05 1637.19 1637.39
1639.03 1640.07 1656.12 1656.22 1656.77 1660.46
1662.13 1662.99 1663.32 1730.02 2986.81 3029.77
3031.38 3032.05 3035.42 3037.27 3040.20 3041.88
3044.93 3046.62 3049.57 3056.94 3058.35 3062.09
3081.28 3081.35 3087.01 3089.26 3094.09 3100.93
3103.98 3109.08 3112.39 3114.58 3116.60 3117.83
3121.98 3124.58 3144.32 3153.71 3158.85 3160.06
3160.63 3162.68 3165.62 3167.18 3169.86 3170.52
3173.63 3176.21 3178.13 3179.76 3181.72 3181.98
3184.88 3185.85 3188.63 3189.34 3190.07 3194.41
3196.36 3197.80 3198.33 3203.92 3205.09 3206.40
3208.68 3211.01 3217.43 3231.99 3268.22 3324.49

==============================

VII$_{PC}$-TS

==============================

-1159.28 8.82 17.38 21.06 24.50 27.47
31.74 35.04 38.60 42.02 42.91 46.41
50.28 53.04 54.93 59.31 62.25 63.31
66.46 70.90 72.65 76.77 77.45 83.17
87.40 89.25 95.73 101.76 103.68 117.27
119.79 129.61 131.23 140.17 144.06 152.14
154.70 161.26 176.45 179.12 180.50 190.10

200.75 208.40 211.89 216.82 228.00 231.07
233.38 236.60 239.56 243.13 247.02 248.32
255.85 260.16 269.63 274.29 286.30 290.92
293.37 309.77 319.49 334.28 335.47 353.41
357.91 364.91 370.29 379.97 398.28 415.11
415.98 416.69 421.96 424.06 428.08 432.22
453.16 484.68 490.26 497.41 499.57 499.94
506.84 514.57 516.35 527.20 534.85 539.72
543.53 544.85 545.22 563.41 566.21 595.44
598.18 599.10 603.26 608.81 618.81 621.77
625.91 631.55 632.02 632.45 633.80 634.41
640.03 649.18 656.77 679.24 683.92 697.55
704.05 706.79 717.14 718.85 719.62 720.93
722.55 723.06 743.73 768.00 770.34 772.31
773.24 784.23 786.52 787.24 793.38 802.97
810.10 818.41 829.72 837.42 843.79 850.31
855.03 857.60 858.92 869.00 872.44 874.11
874.54 876.99 893.07 897.50 898.07 901.52
903.24 914.64 922.47 922.75 926.94 928.94
934.34 935.47 939.69 941.03 958.18 972.96
973.05 974.00 975.85 978.45 981.91 982.41
984.22 989.68 1000.71 1001.39 1003.34 1004.48
1009.96 1013.59 1014.54 1015.46 1016.08 1016.34
1016.79 1017.61 1020.32 1030.75 1040.44 1041.24
1044.97 1045.72 1056.67 1057.91 1058.12 1059.51
1059.97 1060.68 1062.69 1066.16 1067.08 1067.67
1069.31 1075.41 1106.54 1111.50 1112.62 1118.11
1119.92 1122.17 1125.63 1125.82 1145.19 1149.51
1152.74 1163.59 1170.24 1183.72 1187.93 1188.66
1194.33 1195.42 1196.84 1197.05 1198.34 1210.51
1212.03 1217.60 1219.93 1221.36 1222.70 1223.57
1224.64 1229.63 1231.35 1237.77 1239.55 1248.01
1252.28 1253.44 1253.87 1282.39 1286.72 1289.49
1291.99 1295.94 1301.84 1313.24 1313.92 1314.16
1316.75 1320.89 1330.47 1332.61 1345.64 1346.99
1355.13 1357.33 1359.14 1363.76 1364.19 1364.81
1368.12 1370.88 1371.62 1372.67 1374.63 1384.67
1396.91 1397.20 1399.06 1413.11 1424.97 1425.24
1426.30 1430.59 1449.21 1465.84 1475.13 1475.65
1487.44 1492.05 1492.65 1493.05 1493.75 1494.07
1494.65 1497.34 1500.61 1502.99 1506.57 1507.33
1507.45 1509.80 1510.41 1512.90 1516.95 1517.37
1520.96 1537.12 1538.54 1540.11 1540.42 1547.85
1598.27 1605.19 1613.20 1621.78 1636.30 1636.51
1637.45 1638.21 1638.30 1658.12 1659.25 1659.87
1660.72 1660.82 1661.09 1662.23 1685.41 3004.73
3027.01 3028.11 3031.60 3037.91 3041.38 3043.65
3049.51 3051.07 3051.14 3052.03 3055.81 3059.00
3061.51 3064.75 3081.17 3083.06 3091.36 3095.28
3102.84 3104.02 3118.43 3119.09 3120.89 3121.00
3121.98 3127.78 3149.42 3153.42 3160.77 3162.67
3163.83 3163.89 3164.66 3167.48 3170.27 3170.81
3172.37 3173.94 3180.97 3181.41 3182.30 3182.67
3183.34 3184.77 3186.57 3187.43 3191.99 3195.47
3196.61 3197.19 3197.26 3198.11 3198.21 3204.66
3204.96 3212.56 3219.16 3232.43 3237.87 3277.51
==============================

VIII$_{PC}$

==============================

7.51 15.88 21.62 23.33 26.78 31.52
34.14 36.69 37.42 41.64 45.09 50.61
52.49 56.16 58.01 63.23 67.92 69.74
71.82 74.50 75.31 85.22 88.12 91.25
97.55 98.46 109.43 111.46 115.31 119.63
120.84 127.43 133.75 139.47 141.22 144.65
155.07 160.01 169.66 180.48 182.86 202.61
206.64 208.03 213.66 225.82 231.00 232.61
236.43 241.53 242.83 250.73 251.89 253.35
264.27 271.12 273.24 283.10 289.20 291.26
294.40 313.39 330.07 334.24 345.65 355.54
365.46 370.88 383.10 396.95 417.28 418.05
421.45 421.81 422.20 423.83 430.73 445.28
466.71 472.79 481.04 488.77 498.19 504.56
508.11 513.98 529.45 531.26 536.53 536.69
545.02 548.29 557.05 574.06 591.20 595.19
596.67 601.97 610.20 617.64 620.69 625.44
629.58 631.42 632.60 633.98 634.22 634.89
641.07 649.52 650.32 679.33 683.82 692.09
706.27 714.84 715.91 717.18 718.51 720.58
725.69 731.91 747.05 764.47 773.76 778.19
780.33 783.06 785.08 789.19 807.18 814.22
818.69 823.28 836.25 843.86 850.89 854.89
859.35 863.39 864.51 865.44 867.28 869.59
873.31 877.28 877.59 893.42 895.75 896.45
914.65 921.83 926.21 926.97 930.64 935.84
938.76 941.60 944.27 959.11 973.71 974.28
975.76 977.15 978.18 983.27 983.44 985.19
991.99 999.94 1000.87 1002.19 1002.56 1006.32
1009.03 1013.05 1014.98 1015.59 1016.04 1017.46
1019.07 1019.75 1022.91 1028.29 1038.74 1039.09
1041.41 1046.77 1056.91 1057.94 1058.24 1059.56
1060.42 1061.58 1062.96 1065.80 1067.98 1068.75
1069.55 1076.39 1102.66 1109.84 1111.34 1119.03
1119.51 1122.71 1127.83 1130.40 1145.17 1152.52
1155.14 1164.29 1175.48 1185.75 1186.21 1190.99
1192.99 1193.62 1196.40 1196.79 1197.74 1208.74
1219.17 1219.21 1219.85 1222.90 1223.32 1223.94
1224.83 1226.60 1228.16 1237.88 1243.71 1249.64
1252.54 1253.74 1266.74 1284.40 1286.46 1288.51
1296.49 1304.72 1306.52 1313.60 1315.60 1318.59
1320.51 1322.32 1329.66 1332.99 1346.56 1347.11
1357.42 1359.29 1361.93 1362.63 1365.73 1367.19
1367.57 1369.57 1374.10 1390.13 1390.38 1398.67
1399.17 1402.25 1406.79 1424.91 1425.90 1426.44
1429.22 1450.18 1465.85 1469.92 1475.60 1478.12
1488.62 1491.03 1491.56 1492.71 1493.24 1495.41
1495.97 1496.46 1500.58 1502.73 1504.62 1506.23
1508.69 1510.84 1514.96 1516.48 1516.94 1521.60
1528.74 1535.07 1539.01 1540.21 1541.52 1546.96
1594.35 1606.30 1620.08 1633.86 1635.18 1636.96
1638.41 1639.19 1640.42 1657.76 1659.07 1661.57
1661.61 1662.11 1662.20 1670.12 2999.20 3028.22
3029.29 3034.29 3035.07 3040.02 3045.23 3047.42
3047.68 3048.09 3049.27 3051.72 3054.58 3056.42
3057.92 3060.24 3081.43 3088.66 3089.17 3100.96
3103.52 3109.63 3113.65 3116.94 3117.73 3120.43
3120.72 3127.89 3139.88 3141.94 3156.91 3159.02
3163.10 3164.18 3164.61 3169.91 3172.90 3173.93
3174.63 3177.98 3178.20 3181.10 3185.20 3185.25
3185.58 3185.59 3192.10 3193.45 3194.06 3195.07
3195.55 3196.57 3199.74 3202.80 3203.39 3203.58
3207.20 3220.67 3226.69 3261.44 3278.26 3287.42
==============================

IV$_{P}$

==============================

11.47 22.87 29.54 30.88 33.38 39.70
43.71 49.80 52.52 55.61 59.28 67.45
71.16 77.57 82.81 86.77 89.41 91.00
95.38 104.88 106.98 115.35 118.12 119.49
127.10 134.90 141.32 147.95 156.71 163.36
181.94 183.71 195.37 201.95 210.46 215.49
225.13 231.00 231.86 236.24 263.99 264.73
270.82 280.44 287.01 293.30 297.17 329.12
343.85 350.48 367.59 373.49 397.85 415.64
417.66 418.32 420.96 421.27 425.64 430.97
442.69 455.85 458.80 490.15 492.74 500.90
507.30 508.95 515.66 519.62 540.26 550.91
559.56 569.07 602.40 603.12 608.58 617.63
624.66 625.10 629.91 631.12 633.30 634.80
635.29 642.94 649.18 673.30 682.38 688.69
693.95 706.92 715.29 719.39 721.25 722.40
744.22 767.53 773.85 776.24 777.00 784.57
786.90 789.45 792.53 796.37 818.12 829.85
841.08 848.07 852.27 855.94 860.33 864.10
868.83 869.52 870.04 874.49 888.90 890.99
894.41 897.68 906.10 925.58 928.24 929.09
935.03 936.30 943.04 946.62 961.18 970.36
978.00 982.40 984.25 987.23 987.69 994.64
1003.97 1006.21 1007.57 1010.07 1010.32 1011.34
1012.47 1013.52 1013.83 1015.04 1015.42 1017.07

1017.49 1019.30 1021.50 1022.75 1032.78 1038.05
1039.45 1053.39 1057.31 1058.68 1059.55 1062.55
1066.27 1068.73 1098.61 1111.86 1112.02 1119.09
1126.72 1133.18 1141.29 1149.82 1153.73 1154.93
1166.53 1179.48 1183.34 1192.45 1193.91 1197.99
1199.60 1200.42 1200.99 1205.21 1213.22 1216.61
1220.46 1221.98 1225.50 1226.47 1228.76 1229.46
1230.39 1232.78 1246.45 1250.86 1256.52 1258.52
1262.15 1273.75 1292.58 1298.83 1308.07 1310.01
1314.72 1318.02 1327.65 1344.26 1344.78 1353.30
1355.69 1359.96 1361.37 1365.27 1366.09 1367.18
1368.07 1375.15 1379.31 1384.00 1391.68 1394.88
1400.69 1402.71 1406.99 1423.64 1467.22 1476.61
1479.07 1482.33 1486.40 1489.03 1491.69 1493.89
1494.23 1500.92 1507.08 1510.85 1515.83 1518.61
1534.32 1534.80 1539.90 1541.44 1542.07 1542.47
1570.87 1607.11 1636.35 1636.64 1637.02 1638.03
1641.29 1654.71 1656.77 1658.76 1660.01 1660.43
3011.90 3023.41 3034.02 3044.15 3047.51 3049.44
3050.64 3054.20 3059.94 3060.66 3077.15 3099.89
3100.93 3101.96 3107.20 3113.28 3115.04 3142.15
3166.05 3169.43 3169.47 3172.43 3172.62 3180.21
3181.37 3183.51 3185.11 3185.74 3186.22 3190.55
3191.02 3192.92 3194.59 3196.46 3196.85 3197.10
3200.90 3201.08 3202.44 3203.85 3206.23 3206.51
3211.86 3212.11 3212.35 3212.69 3215.95 3218.38
3241.04 3250.33 3276.15

==============================

$\mathbf{III}_{PN}$-TS'

==============================

-65.29 20.74 23.10 36.00 38.50 39.25
41.71 47.46 53.71 56.26 57.34 62.67
68.03 74.93 79.62 81.18 88.94 92.97
94.58 99.32 106.98 110.12 116.27 124.40
129.53 132.76 138.00 144.58 158.60 166.89
174.70 179.68 194.37 201.84 207.30 216.68
221.67 229.93 235.78 243.85 254.86 268.60
272.51 275.23 276.86 283.81 296.61 317.30
340.64 346.88 363.04 369.38 391.02 412.60
413.89 416.05 418.01 425.14 428.04 434.03
438.73 446.39 468.91 492.22 494.57 507.46
508.92 511.97 519.81 531.05 539.56 543.27
566.44 568.79 595.47 605.87 607.95 614.98
621.30 622.18 624.87 629.41 632.72 634.50
635.49 640.57 648.44 681.26 685.07 691.93
695.16 697.14 717.16 717.95 724.21 727.24
741.80 763.30 773.36 777.22 780.66 784.77
786.73 786.79 787.83 792.67 815.49 840.15
846.33 850.40 852.87 857.54 861.06 862.66
864.63 871.45 871.64 879.65 880.95 889.16
891.15 895.98 902.94 918.64 923.46 929.97
933.55 939.76 940.67 947.19 948.64 955.48
979.03 981.63 985.36 987.59 988.05 993.06
995.94 999.95 1005.22 1008.68 1010.90 1011.94
1012.79 1013.46 1014.20 1014.56 1015.79 1016.55
1019.07 1020.24 1022.32 1025.89 1026.34 1034.46
1042.79 1055.29 1055.80 1057.23 1059.67 1060.40
1065.52 1067.08 1100.44 1108.80 1109.93 1112.75
1117.80 1125.83 1141.17 1149.32 1153.32 1157.75
1158.59 1177.66 1180.91 1185.78 1199.03 1199.23
1199.78 1200.08 1205.35 1211.89 1217.02 1218.26
1221.98 1222.58 1224.54 1225.40 1226.47 1226.58
1229.23 1230.08 1246.16 1247.43 1253.22 1263.75
1273.46 1287.82 1295.98 1299.30 1306.48 1307.50
1309.10 1317.94 1337.43 1344.92 1347.01 1351.32
1353.88 1356.04 1360.88 1362.44 1363.50 1365.84
1372.48 1379.11 1382.18 1383.68 1387.10 1392.08
1401.82 1402.01 1426.10 1431.10 1464.14 1477.23
1479.85 1486.14 1490.39 1493.94 1494.94 1495.91
1498.05 1505.22 1507.99 1508.48 1515.09 1518.88
1526.41 1531.87 1537.83 1539.65 1540.62 1541.49
1576.16 1602.93 1630.39 1634.36 1636.72 1637.56
1638.34 1646.66 1653.06 1657.11 1658.95 1660.07
3010.07 3030.09 3032.56 3033.08 3033.92 3042.31
3045.85 3046.03 3051.37 3053.44 3066.46 3076.23
3092.19 3101.00 3103.53 3105.30 3109.68 3124.79
3164.74 3165.95 3166.22 3167.26 3169.60 3171.89
3174.73 3179.01 3180.72 3182.33 3183.49 3184.11
3186.88 3188.08 3192.23 3193.29 3193.67 3194.09
3197.80 3200.97 3202.36 3203.37 3203.76 3204.45
3210.09 3210.58 3211.84 3215.02 3220.72 3231.56
3231.89 3243.33 3264.50

==============================

$\mathbf{III}_{PC}$-TS'

==============================

-28.41 10.21 23.73 26.05 29.07 35.41
40.94 45.00 45.53 51.87 57.31 59.89
66.25 74.91 76.78 80.54 85.34 88.13
91.44 93.88 108.14 109.18 114.97 120.55
126.90 134.30 137.46 143.61 160.69 162.37
170.60 177.65 190.79 195.54 209.13 218.52
221.36 231.43 234.18 241.67 252.03 261.87
270.16 276.13 286.14 289.96 295.73 327.96
343.17 350.64 364.67 371.25 393.96 413.08
415.89 417.55 420.57 422.48 423.67 431.78
437.80 445.31 461.56 491.21 492.98 500.70
507.36 510.78 512.98 519.56 541.56 550.72
560.46 574.10 599.48 608.48 614.20 617.99
623.94 624.46 626.92 630.85 633.78 634.54
636.08 642.53 648.29 677.20 680.13 688.67
691.37 704.72 714.87 719.89 720.23 721.62
760.92 775.99 776.33 777.51 778.39 785.04
786.78 788.41 791.83 795.27 819.42 838.98
842.47 846.08 852.51 856.99 858.24 860.73
863.27 868.24 868.93 878.96 885.82 887.01
894.42 901.84 906.26 924.30 924.94 927.97
932.51 936.01 940.40 942.14 959.66 967.33
977.18 980.87 982.89 986.39 987.06 991.50
1001.45 1005.60 1006.59 1007.85 1009.86 1011.19
1011.91 1012.20 1015.11 1015.57 1017.12 1017.30
1019.83 1021.66 1025.86 1027.46 1031.67 1034.67
1037.62 1052.95 1056.51 1058.35 1059.06 1061.11
1065.73 1067.01 1095.57 1110.49 1111.17 1118.90
1125.68 1133.60 1135.36 1149.08 1152.97 1155.01
1173.90 1182.16 1189.11 1194.24 1198.04 1199.30
1200.01 1200.72 1203.46 1205.64 1215.07 1217.19
1220.05 1223.04 1224.54 1225.44 1226.09 1227.80
1229.58 1242.48 1247.81 1254.32 1257.35 1258.37
1264.12 1280.43 1291.63 1301.11 1310.23 1311.53
1316.98 1320.03 1332.10 1344.16 1345.32 1352.91
1353.76 1360.66 1360.78 1361.92 1364.07 1365.45
1365.66 1375.95 1378.70 1379.55 1384.38 1389.52
1396.06 1405.74 1430.72 1441.28 1470.14 1479.56
1482.06 1482.19 1484.75 1488.61 1492.58 1493.00
1494.25 1501.28 1506.74 1510.95 1516.41 1517.66
1522.57 1532.58 1534.71 1540.71 1541.01 1541.09
1595.89 1605.18 1635.79 1636.30 1636.74 1637.56
1637.89 1654.40 1657.92 1658.64 1659.09 1660.47
3013.65 3026.81 3043.55 3046.79 3049.28 3053.29
3056.79 3058.11 3062.02 3064.22 3084.45 3098.63
3101.38 3101.89 3102.53 3107.49 3114.17 3152.36
3154.58 3165.41 3165.93 3169.35 3179.45 3179.50
3184.36 3184.96 3186.29 3187.24 3188.60 3189.19
3190.87 3192.05 3194.56 3194.67 3198.71 3198.93
3200.64 3201.00 3202.34 3203.35 3209.14 3210.32
3210.50 3211.71 3212.12 3213.17 3220.13 3230.94
3242.67 3258.60 3291.89

VII. References and Notes

(1) "Prudent Practices in the Laboratory [electronic resource]: Handling and Management of Chemical Hazards / Committee on Prudent Practices in the Laboratory: An Update."; Board on Chemical Sciences and Technology, Division of Earth and Life Studies, National Research Council of the National Academies. Washington, D.C.: National Academies Press, 2011.

(2) Vo, Q. V.; Trenerry, C.; Rochfort, S.; Wadeson, J.; Leyton, C.; Hughes, A., Synthesis and Anti-Inflammatory Activity of Indole Glucosinolates. *Bioorg. Med. Chem.* **2014**, *22*, 856–864.

(3) Tomakinian, T.; Kouklovsky, C.; Vincent, G., Investigation of the Synthesis of Benzofuroindolines from N-Hydroxyindoles: An O-Arylation/[3,3]-Sigmatropic Rearrangement Sequence. *Synlett* **2015**, *26*, 1269–1275.

(4) For using Na_2WO_4/H_2O_2 for oxidation, see: Somei, M.; Kawasaki, T.; Shimizu, K.; Fukui, Y.; Ohta, T., The Chemistry of 1-Hydroxyindoles: Synthesis of Methyl 1-Hydroxyindole-3-Acetate, N_b-Acetyl-1-Hydroxytryptamine, (+)-and (S)-1-Hydroxytryptophan Derivatives. *Chem. Pharm. Bull.* **1991**, *39*, 1905–1907; Yamada, K.; Tanaka, Y.; Somei, M., Synthesis of N_b-Acyltryptamines and Their 1-Hydroxy-Tryptamine Derivatives as New α_2-Blockers. *Heterocycles* **2009**, *79*, 635–645.

(5) Molander, G. A.; Brown, A. R., Suzuki−Miyaura Cross-Coupling Reactions of Potassium Vinyltrifluoroborate with Aryl and Heteroaryl Electrophiles. *J. Org. Chem.* **2006**, *71*, 9681–9686.

(6) Bartoli, G.; Bosco, M.; Carlone, A.; Dalpozzo, R.; Marcantoni, E.; Melchiorre, P.; Sambri, L., Reaction of Dicarbonates with Carboxylic Acids Catalyzed by Weak Lewis Acids: General Method for the Synthesis of Anhydrides and Esters. *Synthesis* **2007**, *22*, 3489–3496.

(7) Wang, Y.-M.; Buchwald, S. L., Enantioselective CuH-Catalyzed Hydroallylation of Vinylarenes. *J. Am. Chem. Soc.* **2016**, *138*, 5024–5027.

(8) Zhou, Y.; Engl, O. D.; Bandar, J. S.; Chant, E. D.; Buchwald, S. L., CuH-Catalyzed Asymmetric Hydroamidation of Vinylarenes. *Angew. Chem. Int. Ed.* **2018**, *57*, 6672–6675.

(9) Friis, S. D.; Pirnot, M. T.; Dupuis, L. N.; Buchwald, S. L., A Dual Palladium and Copper Hydride Catalyzed Approach for Alkyl–Aryl Cross-Coupling of Aryl Halides and Olefins. *Angew. Chem., Int. Ed*. **2017**, *56*, 7242–7246.

(10) Maltais, R.; Ayan, D.; Poirier, D., Crucial Role of 3-Bromoethyl in Removing the Estrogenic Activity of 17β-HSD1 Inhibitor 16β-(*m*-Carbamoylbenzyl)estradiol. *ACS Med. Chem. Lett.* **2011**, *2*, 678–681.

(11) Niu, D.; Buchwald, S. L., Design of Modified Amine Transfer Reagents Allows the Synthesis of α-Chiral Secondary Amines via CuH-Catalyzed Hydroamination. *J. Am. Chem. Soc.* **2015**, *137*, 9716–9721.
(12) Parr, R. G.; Yang, W., Density Functional Theory of Atoms and Molecules (Oxford University Press, New York, 1989).
(13) Bochevarov, A. D.; Harder, E.; Hughes, T. F.; Greenwood, J. R.; Braden, D. A.; Philipp, D. M.; Rinaldo, D.; Halls, M. D.; Zhang, J.; Friesner, R. A., Jaguar: A High-Performance Quantum Chemistry Software Program with Strengths in Life and Materials Sciences. *Int. J. Quantum Chem.* **2013**, *113*, 2110–2142.
(14) Becke, A. D., A New Mixing of Hartree–Fock and Local Density‐Functional Theories *J. Chem. Phys.* **1993**, *98*, 1372–1377.
(15) Becke, A. D., Density-Functional Exchange-Energy Approximation with Correct Asymptotic Behavior *Phys. Rev. A* **1988**, *38*, 3098–3100.
(16) Grimme, S., Semiempirical GGA-Type Density Functional Constructed with a Long-Range Dispersion Correction *J. Comput. Chem.* **2006**, *27*, 1787–1799.
(17) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H., A Consistent and Accurate ab initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.* **2010**, *132*, 154104–154119.
(18) Ditchfield, R.; Hehre, W. J.; Pople, J. A., Self‐Consistent Molecular‐Orbital Methods. IX. An Extended Gaussian‐Type Basis for Molecular‐Orbital Studies of Organic Molecules. *J. Chem. Phys.* **1971**, *54*, 724–728.
(19) Hay, P. J.; Wadt, W. R., *Ab initio* Effective Core Potentials for Molecular Calculations. Potentials for the Transition Metal Atoms Sc to Hg. *J. Chem. Phys*. **1985**, *82*, 270-283.
(20) Hay, P. J.; Wadt, W. R., *Ab initio* Effective Core Potentials for Molecular Calculations. Potentials for Main Group Elements Na to Bi. *J. Chem. Phys*. **1985**, *82*, 284-298.
(21) Hay, P. J.; Wadt, W. R., *Ab initio* Effective Core Potentials for Molecular Calculations. Potentials for K to Au Including the Outermost Core Orbitals. *J. Chem. Phys*. **1985**, *82*, 299-310.
(22) Dunning, T. H. Jr., Gaussian Basis Sets for Use in Correlated Molecular Calculations. I. The Atoms Boron through Neon and Hydrogen. *J. Chem. Phys.* **1989**, *90*, 1007–1023.
(23) Marten, B.; Kim, K.; Cortis, C.; Friesner, R. A.; Murphy, R. B.; Ringnalda, M. N.; Sitkoff, D.; Honig, B., New Model for Calculation of Solvation Free Energies: Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-range Hydrogen-Bonding Effects. *J. Phys. Chem.* **1996**, *100*, 11775-11788.

(24) Edinger, S. R.; Cortis, C.; Shenkin, P. S.; Friesner, R. A., Solvation Free Energies of Peptides: Comparison of Approximate Continuum Solvation Models with Accurate Solution of the Poisson-Boltzmann Equation. *J. Phys. Chem. B* **1997**, *101*, 1190-1197.
(25) Friedrichs, M.; Zhou, R. H.; Edinger, S. R.; Friesner, R. A., Poisson-Boltzmann Analytical Gradients for Molecular Modeling Calculations. *J. Phys. Chem. B* **1999**, *103*, 3057-3061.