Supporting Information

Tripodal S-Ligand Complexes of Copper(I) as Catalysts for Alkene Aziridination, Sulfide Sulfimidation, and C–H Amination

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Experimental Section

Reagents. All reactions were carried out under inert atmosphere using Schlenk techniques unless otherwise stated. 1-Phenylimidazole-2-thione,[1] K[Tm^{Ph}],[2] [Cu(Tm^{tBu})(PPh$_3$)] (**Cu3**),[3] and [Au(PPh$_3$)Cl],[4] and the vinyl azides[5] employed in the intramolecular aryl C–H amination reactions, were prepared according to the literature methods. Other reagents were purchased commercially and used without purification.

Physical Measurements. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AV-400 spectrometer; chemical shifts were reported in ppm and were determined with tetramethylsilane (TMS) as internal reference. Positive-ion-mode FAB mass spectra were recorded on a Thermo Scientific DFS high-resolution magnetic sector mass spectrometer. HRMS-ESI spectrum was obtained on an Agilent 6540 Accurate-Mass Q-TOF mass spectrometer. Infra-red (IR) spectra were measured on a Bio-Rad PTS-165 spectrometer. Elemental analyses were performed at the Institute of Chemistry, the Chinese Academy of Sciences, Beijing.

Synthesis of (MeIm)Tm^{Ph}. To a solution of 1-phenylimidazole-2-thione (528.7 mg, 3 mmol) and *N*-methylimidazole (79.7 μL, 1 mmol) in toluene (10 mL) was added B(NMe$_2$)$_3$ (175 μL, 1 mmol). The reaction mixture was refluxed for 48 h and then cooled to room temperature. The precipitate was collected, washed with Et$_2$O and dried *in vacuo* to give the product as an off-white solid. Yield: 65%. ^{1}H NMR (400 MHz, CDCl$_3$): δ 9.21 (br, s, 1H), 7.63 (br, s, 6H), 7.47 (t, J = 7.7 Hz, 6H), 7.38 (t, J = 7.4 Hz, 3H), 7.07 (br, s, 3H), 6.88 (s, 3H), 6.79 (br, s, 1 H), 6.59 (br, s, 1H), 3.80 (s, 3H). EI-MS: m/z 618.2 (M$^+$).

Synthesis of [Cu(Tm^{Ph})(PPh$_3$)] (Cu1). To a solution of K[Tm^{Ph}] (576.6 mg, 1 mmol) and PPh$_3$ (262.3 mg, 1 mmol) in MeOH (20 mL) was added CuCl (99 mg, 1 mmol). White precipitate appeared in a few minutes. The suspension was allowed to stir for 12 h at room temperature. The

precipitate was filtered off, washed with MeOH and then Et_2O. The product was obtained after re-precipitation from CH_2Cl_2 solution by adding excess Et_2O. Off-white solid. Yield: 72%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38–7.17 (m, 30H), 7.06 (s, 3H), 6.87 (s, 3H). ^{31}P NMR (162 MHz, $CDCl_3$): δ –6.5 (br). IR (KBr): 2376 cm^{-1} (ν(B–H)). FAB-MS: *m*/*z* 863 ([M + H]$^+$). Anal. calcd (%) for $C_{45}H_{37}CuBN_6PS_3 \cdot 0.5H_2O$: C 61.99, H 4.40, N 9.64; found C 61.95, H 4.25, N 9.66.

[Cu(Tm^{Ph})(PCy$_3$)] (Cu2). This complex was prepared according to the same procedure as that for **Cu1** except that PCy_3 (280.4 mg, 1 mmol) was used in place of PPh_3. Off-white solid. Yield: 48%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 7.7 Hz, 6H), 7.39 (t, *J* = 7.4, 6H), 7.38–7.34 (m, 3H), 7.05 (s, 3H), 6.87 (s, 3H), 1.84–1.12 (m, 33H). ^{31}P NMR (162 MHz, $CDCl_3$): δ 12.9 (br). IR (KBr): 2376 cm^{-1} (ν(B–H)). FAB-MS: *m*/*z* 880 (M$^+$). Anal. calcd (%) for $C_{45}H_{55}CuBN_6PS_3 \cdot 0.5H_2O$: C 60.72, H 6.35, N 9.45; found C 60.78, H 6.37, N 9.35.

[Ag(Tm^{Ph})(PPh$_3$)] (Ag1). This complex was prepared according to the same procedure as that for **Cu1** except that $AgNO_3$ (169.9 mg, 1 mmol) was used in place of CuCl. Off-white solid. Yield: 78%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41–7.26 (m, 30H), 7.07 (s, 3H), 6.89 (d, *J* = 1.7 Hz, 3H). ^{31}P NMR (162 MHz, $CDCl_3$): δ 2.9 (br). IR (KBr): 2376 cm^{-1} (ν(B–H)). FAB-MS: *m*/*z* 906 (M$^+$). Anal. calcd (%) for $C_{45}H_{37}AgBN_6PS_3$: C 59.55, H 4.11, N 9.26; found C 59.40, H 4.06, N 9.36.

[Au(Tm^{Ph})(PPh$_3$)] (Au1). This complex was prepared according to the same procedure as that for **Cu1** except that [Au(PPh_3)Cl] (494.7 mg, 1 mmol) was used in place of CuCl. Brown solid. Yield: 80%. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.51–7.42 (m, 21H), 7.33–7.31 (m, 9H), 7.08 (d, *J* = 2.2 Hz, 3H), 6.92 (d, *J* = 2.2 Hz, 3H). ^{31}P NMR (162 MHz, CD_2Cl_2): δ 35.6. IR (KBr): 2372 cm^{-1} (ν(B–H)). FAB-MS: *m*/*z* 996 (M$^+$). Anal. calcd (%) for $C_{45}H_{37}AuBN_6PS_3 \cdot 0.5H_2O$: C 53.72, H 3.81, N 8.36; found C 53.50, H 3.61, N 8.15.

Synthesis of [Cu{(MeIm)Tm^{Ph}}(PPh$_3$)]PF$_6$ (Cu4). To a solution of [Cu(MeCN)$_4$]PF$_6$ (149.0 mg, 0.4 mmol) and triphenylphosphine (104.9 mg, 0.4 mmol) in CH_2Cl_2 (10 mL) was added (MeIm)Tm^{Ph} (127.4 mg, 0.4 mmol). The reaction mixture was stirred at room temperature for 12 h. During the time, the white suspension turned to a clear solution. The reaction mixture was concentrated to *ca.* 1 mL followed by addition of excess Et_2O to induce the precipitation. The precipitate was collected, washed with Et_2O and dried in vacuo to give the product. Off-white solid. Yield: 63%. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.90 (br, 1H), 7.52–6.54 (m, 38H), 3.92 (s, 3H). ^{31}P NMR (162 MHz, CD_2Cl_2): δ –2.0 (br, PPh_3), –144.4 (sep, PF_6^-). ^{19}F NMR (376 MHz, CD_2Cl_2): δ –72.0, –73.9 (PF_6^-). FAB-MS: *m*/*z* 943 ([M – PF_6]$^+$). Anal. calcd (%) for $C_{49}H_{42}BCuF_6N_8P_2S_3$: C 54.02, H 3.89, N 10.29; found C 53.70, H 3.73, N 10.18.

[Cu{(MeIm)Tm^{Ph}}(PCy$_3$)]PF$_6$ (Cu5). This complex was prepared by the same procedure as that for **Cu4** except that PCy_3 (112.2 mg, 0.4 mmol) was used in place of PPh_3. Off-white solid. Yield: 45%. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.90 (br, 1H), 7.53–7.39 (m, 17), 7.04–7.01 (m, 6H), 3.92 (s, 3H), 1.68–1.63 (m, 16H), 1.04–0.90 (m, 17H). ^{31}P NMR (162 MHz, CD_2Cl_2): δ 17.5 (br, PCy_3), –144.3 (sep, PF_6^-). ^{19}F NMR (376 MHz, CD_2Cl_2): δ –72.0, –73.9 (PF_6^-). FAB-MS: *m*/*z* 961 ([M – PF_6]$^+$). Anal. calcd (%) for $C_{49}H_{60}BCuF_6N_8P_2S_3 \cdot H_2O$: C 52.29, H 5.56, N 9.96; found C 52.31, H 5.45, N 9.85.

X-ray Crystal Structure Determinations. Crystals of **Cu1** and **Cu2** were obtained by diffusion of Et_2O into CH_2Cl_2 solutions of these complexes. For **Au1**, a crystal was obtained by diffusion of pentane into a toluene solution of the complex. The X-ray diffraction data were collected on a Bruker X8 Proteum diffractometer. The crystals were kept at 100 K during data collection. The diffraction images were interpreted and the diffraction intensities were integrated by using the program SAINT. Multi-scan SADABS was applied for absorption correction. By

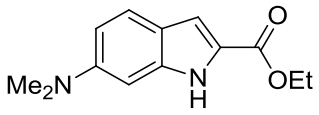
using OLEX2,[6] the structure was solved with the XS[7] structure solution program using direct methods and refined with the shelXL[8] refinement package using least squares minimization. The positions of the H atoms were calculated on the basis of the riding mode with thermal parameters equal to 1.2 times that of the associated C atoms and these positions participated in the calculation of the final R indices. In the final stage of least-squares refinement, all non-hydrogen atoms were refined anisotropically. Crystallographic parameters are summarized in Table S1 and Table S2.

Typical Procedure for Catalytic Aziridination of Alkenes. To a solution of alkene (4 mmol) and catalyst (4 μmol, 1 mol %) in MeCN (3 mL) was added PhI=NTs (0.4 mmol). The reaction mixture was stirred at room temperature for 3 h. Solvent was removed under reduced pressure. The crude mixture was analyzed by ^{1}H NMR spectroscopy using 1,1-diphenylethylene as internal standard. The aziridination products in the reactions were identified by comparison with their spectral data reported in the literature.[9]

Typical Procedure for Catalytic Sulfimidation of Sulfides. To a solution of sulfide (0.4 mmol) and catalyst (4 μmol, 1 mol %) in MeCN (3 mL) was added PhI=NTs (0.4 mmol). The reaction mixture was stirred at room temperature for 0.5 h. Completion of reaction was realized as a clear solution formed upon dissolution of PhI=NTs. Solvent was removed under reduced pressure. The crude mixture was analyzed by ^{1}H NMR spectroscopy using 1,1-diphenylethylene as internal standard. The sulfimidation products in the reactions were identified by comparison with their spectral data reported in the literature.[10]

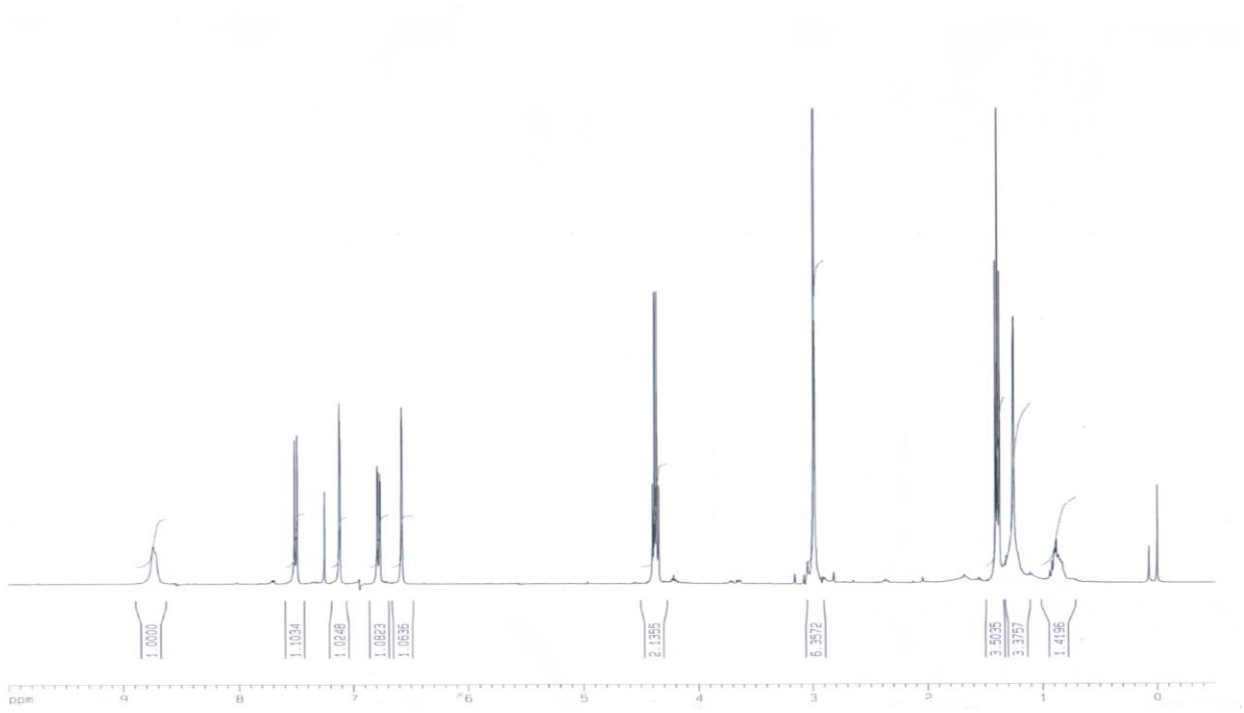
Typical Procedure for Catalytic Intramolecular Amination of Aryl C−H Bond of Vinyl Azides. A mixture of vinyl azide (0.2 mmol), **Cu2** (4 μmol, 2 mol%) and 4 Å molecular sieves (60 mg) in anhydrous 1,2-dichloroethane (1 mL) was refluxed under argon for 2 days. The

mixture was then evaporated to dryness in vacuo. Flash chromatography on silica gel using hexane-ethyl acetate (15∶1 v/v) as eluent gave the corresponding C–H amination products, which were identified by comparison with their spectral data reported in the literature,[5b,11] except for the product depicted below:

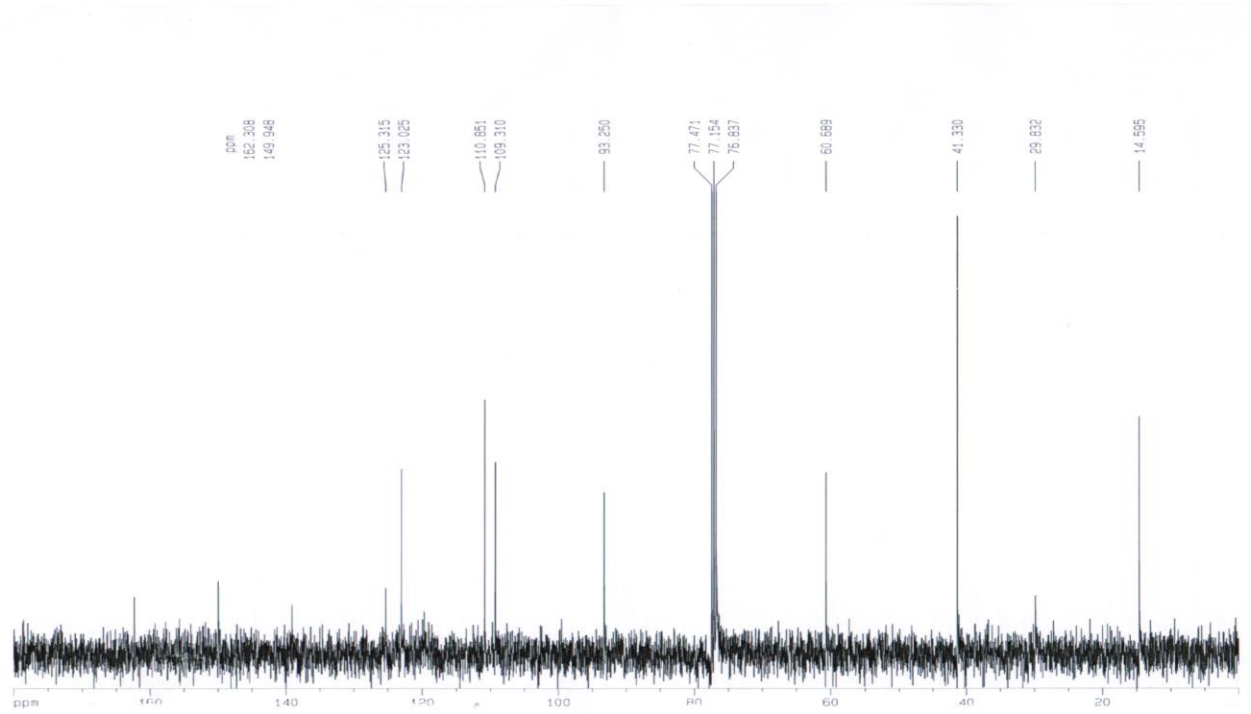


Ethyl 6-(dimethylamino)-1H-indole-2-carboxylate

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.74 (s, 1H), 7.50 (d, *J* = 8.9 Hz, 1H), 7.12 (d, *J* = 1.2 Hz, 1H), 6.78 (dd, *J* = 8.9, 2.2 Hz, 1H), 6.58 (s, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 2.99 (s, 6H), 1.39 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.3, 149.9, 139.1, 125.3, 123.0, 110.9, 109.3, 93.3, 60.7, 41.3, 14.6. HRMS-ESI: *m*/*z* Calcd for $C_{13}H_{17}N_2O_2$ ($[M + H]^+$): 233.1290, found 233.1295.



^{1}H NMR spectrum of ethyl 6-(dimethylamino)-1H-indole-2-carboxylate in $CDCl_3$.



^{13}C NMR spectrum of ethyl 6-(dimethylamino)-1H-indole-2-carboxylate in $CDCl_3$.

Computational Details. Gaussian 09 package[12] was employed to optimize the structures at the M06L level[13] of density function theory (DFT). The vibrational frequency calculations at the same level were carried out to verify that every optimized structure is an energy minima (no imaginary frequency) or a transition state. The 6-31G* Pople basis set[14] was chosen to describe all the atoms except for Cu atom with effective core potential (ECP) type basis set SDD.[15] To further refine the energies, the solvent effect was included by the single point calculations for all the optimized gas-phase structures with self-consistent reactions field (SCRF) based on the polarizable continuum model (PCM) [16] in which acetonitrile was the solvent as in the experimental condition. The functional of M06 [17] was applied; 6-311+G* basis set [18] was employed on all the atoms except for Cu atom with SDD basis set.

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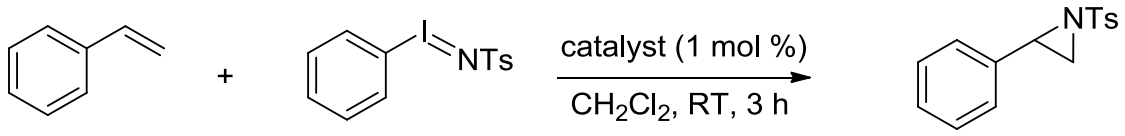
Table S1. Crystallographic Data for Cu1 and Cu2

	Cu1	**Cu2**
chemical formula	$C_{45}H_{37}BCuN_6PS_3$	$C_{45}H_{55}BCuN_6PS_3$
formula weight	863.30	881.45
space group	$R\,\overline{3}$	$P\,\overline{3}$
T (K)	100	100
λ (Å)	1.54178	1.54178
a (Å)	24.3221(10)	14.7346(3)
b (Å)	24.3221(10)	14.7346(3)
c (Å)	36.4934(16)	12.1853(3)
α (°)	90	90
β (°)	90	90
γ (°)	120	120
V (Å^3)	18695.9(17)	2291.10(10)
Z	18	2
D_{calcd} (g cm^{-3})	1.380	1.278
μ (mm^{-1})	2.831	2.568
goodness of fit	1.118	1.057
R	0.0991	0.0948
R_w	0.2925	0.2604

Table S2. Crystallographic Data for Au1

	Au1
chemical formula	$C_{45}H_{37}BAuN_6PS_3$
formula weight	996.73
space group	$P\,\overline{1}$
T (K)	100
λ (Å)	1.54178
a (Å)	9.3602(6)
b (Å)	20.5287(12)
c (Å)	22.3310(14)
α (°)	74.905(4)
β (°)	85.876(5)
γ (°)	89.894(5)
V (Å^3)	4131.5(4)
Z	4
D_{calcd} (g cm^{-3})	1.602
μ (mm^{-1})	8.795
goodness of fit	1.198
R	0.1301
R_w	0.3116

Table S3. Aziridination of Styrene with PhI=NTs Catalyzed by Cu1 as Compared with that Catalyzed by Ag1 and Au1[a]



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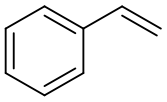
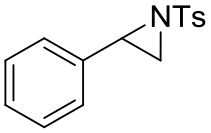
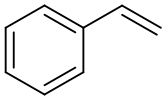
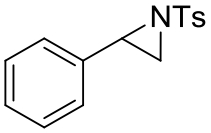
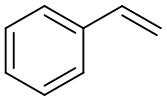
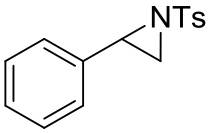
1	**Cu1**			92
2	**Ag1**			<10
3	**Au1**			-[c]

[a] Reaction conditions: catalyst (4 μmol), styrene (4 mmol), PhI=NTs (0.4 mmol), CH_2Cl_2 (3 mL), 3 h, RT, N_2. [b] Determined by ^1H NMR using 1,1-diphenylethene as internal standard. [c] No aziridine product was detected.

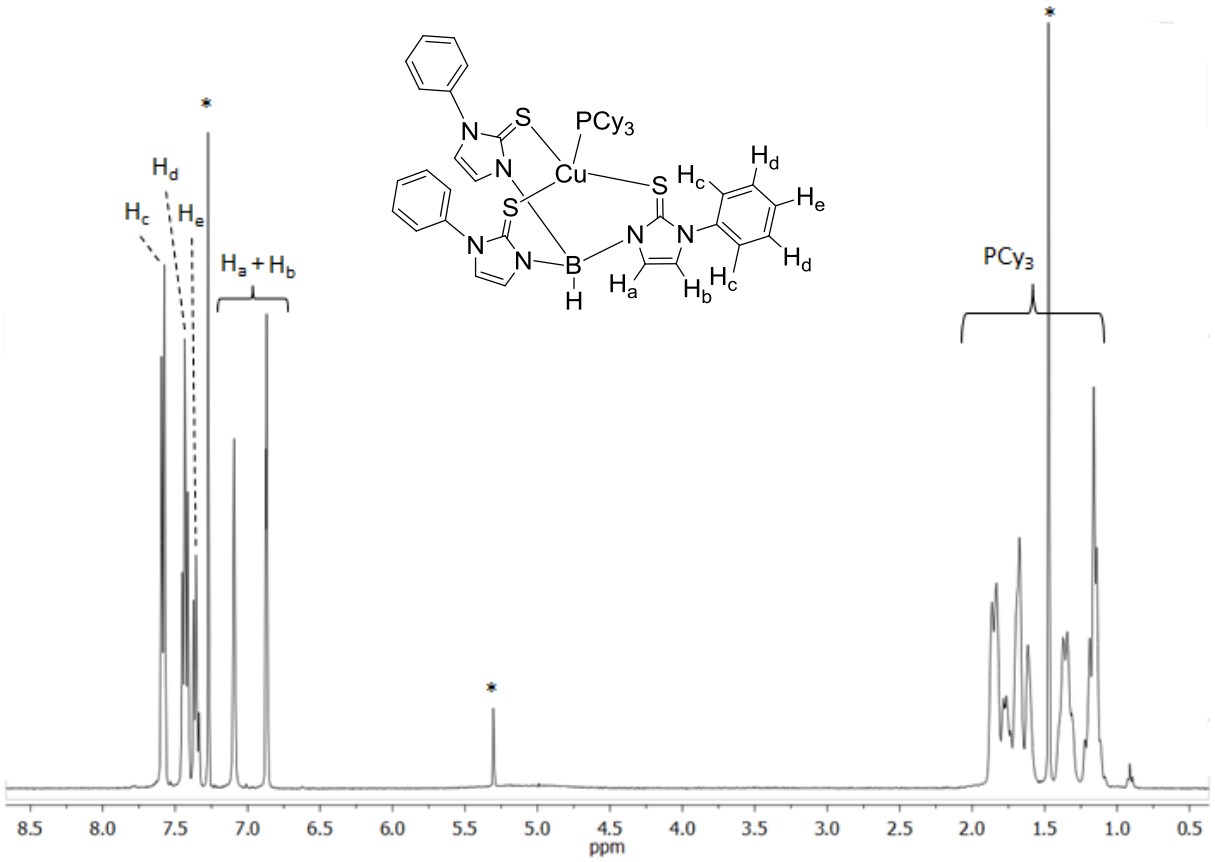


Figure S1. ^{1}H NMR (400 MHz) spectrum of **Cu2** in $CDCl_3$. Asterisks denote the signals of residual solvents ($CHCl_3$, CH_2Cl_2, H_2O).

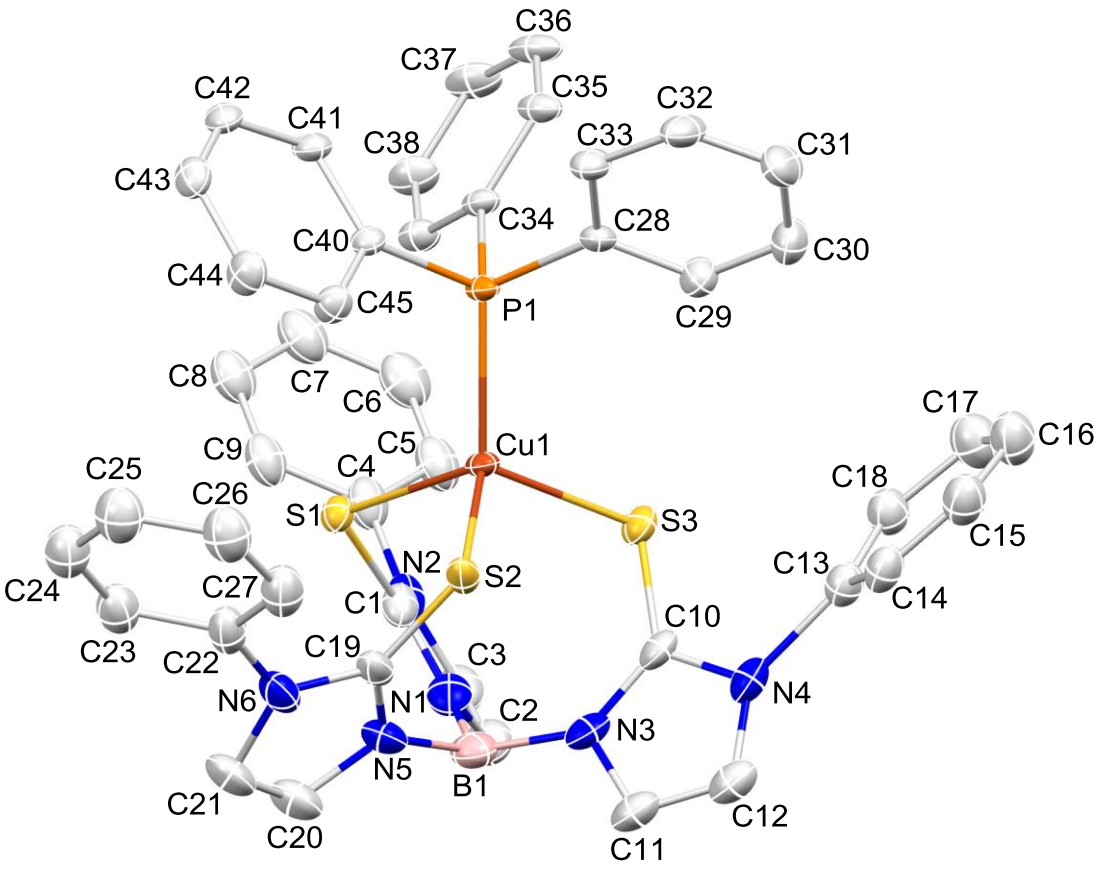


Figure S2. ORTEP drawing for **Cu1** at 30% probability of thermal ellipsoids. Hydrogen atoms are omitted.

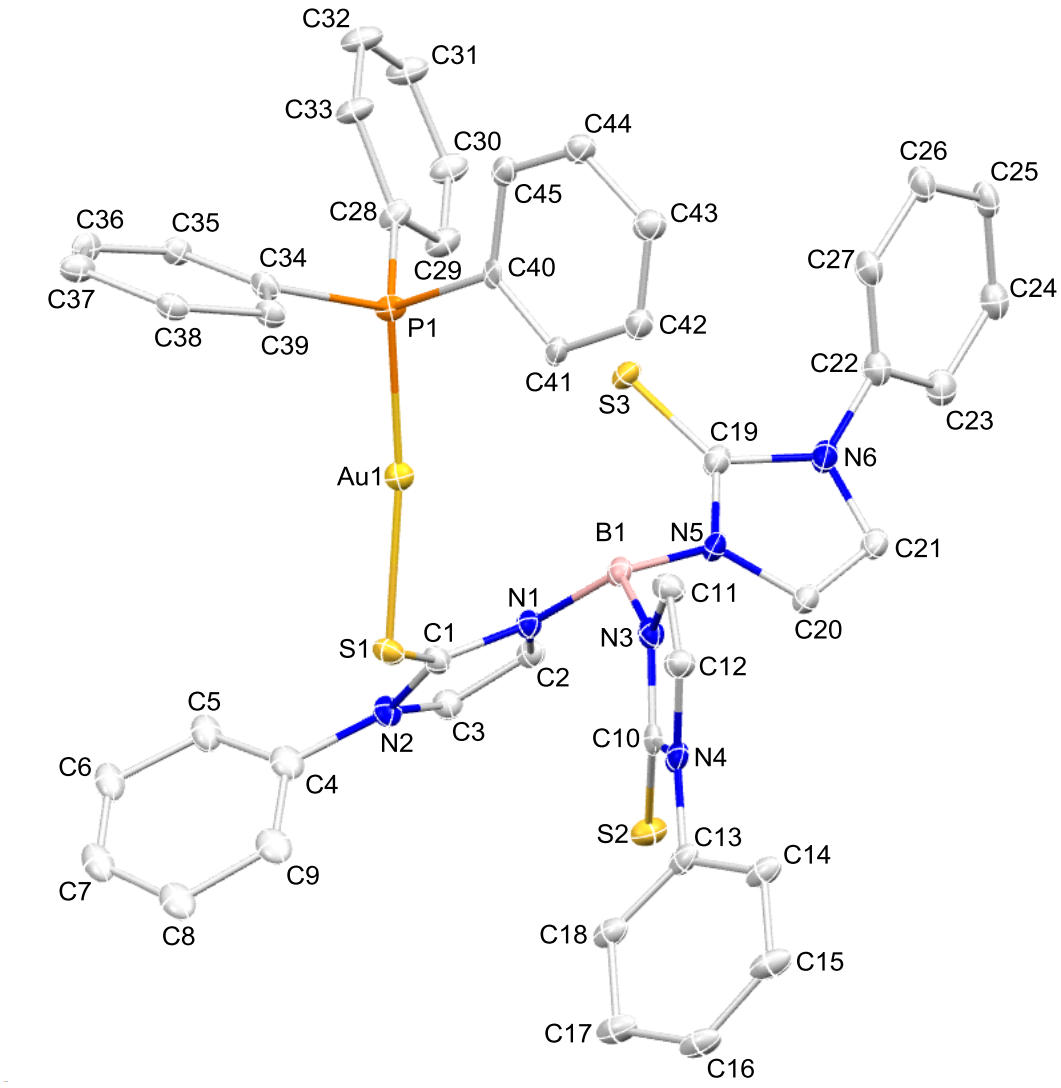


Figure S3. ORTEP drawing for **Au1** at 30% probability of thermal ellipsoids. Hydrogen atoms are omitted. Only one of the two independent molecules in the unit cell is shown.

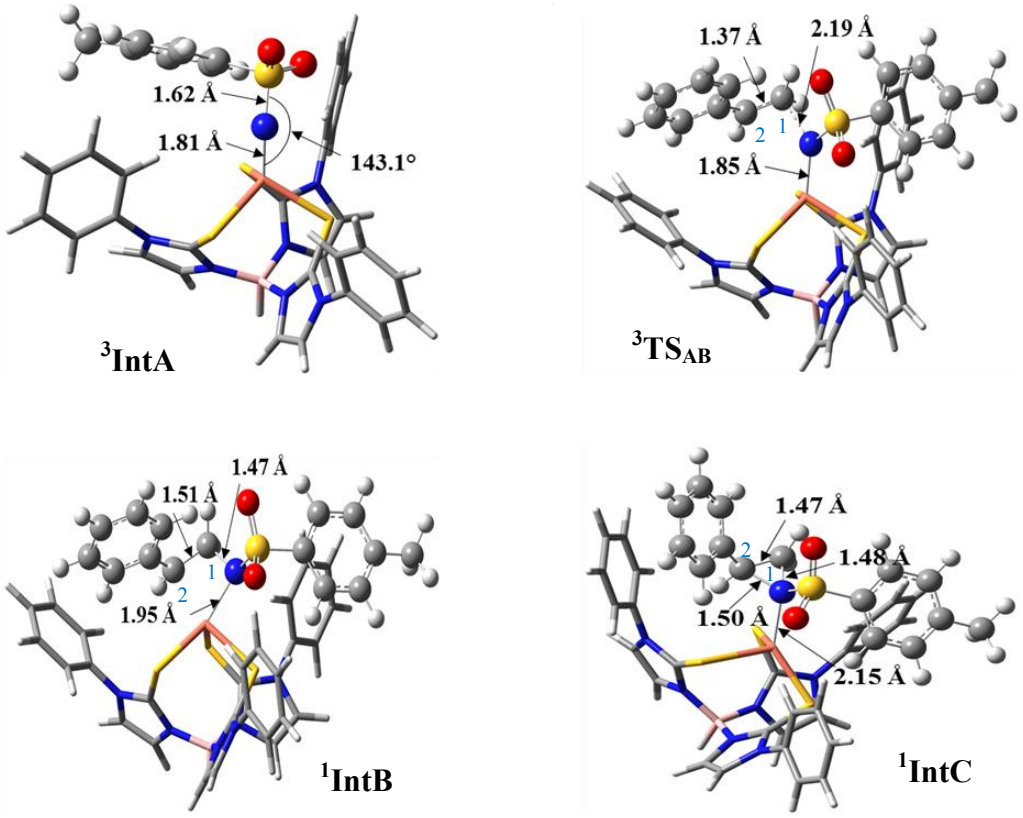


Figure S4. Calculated geometry of ^{3}**IntA**, ^{3}**TS$_{AB}$**, ^{1}**IntB**, and ^{1}**IntC**. For all structures, ball mode represents NTs group and styrene, and tube mode displays Cu(I) with ligand from **Cu2** catalyst. ^{3}**IntA** has a Cu-N-S angle of 143.1°, larger than that in ^{1}**IntA (**129.6°). In ^{3}**TS$_{AB}$**, the spin density on C_2 atom became 0.36, and the C_1-C_2 bond was lengthened to 1.37 Å (cf 1.34 Å in isolated styrene), both indicating the tendency of N-C_1 bond forming and C_1-C_2 double bond breaking. Note that the C_2 atom in **IntC** is chiral; we only took the *S*-product as an example to examine the reaction mechanism.

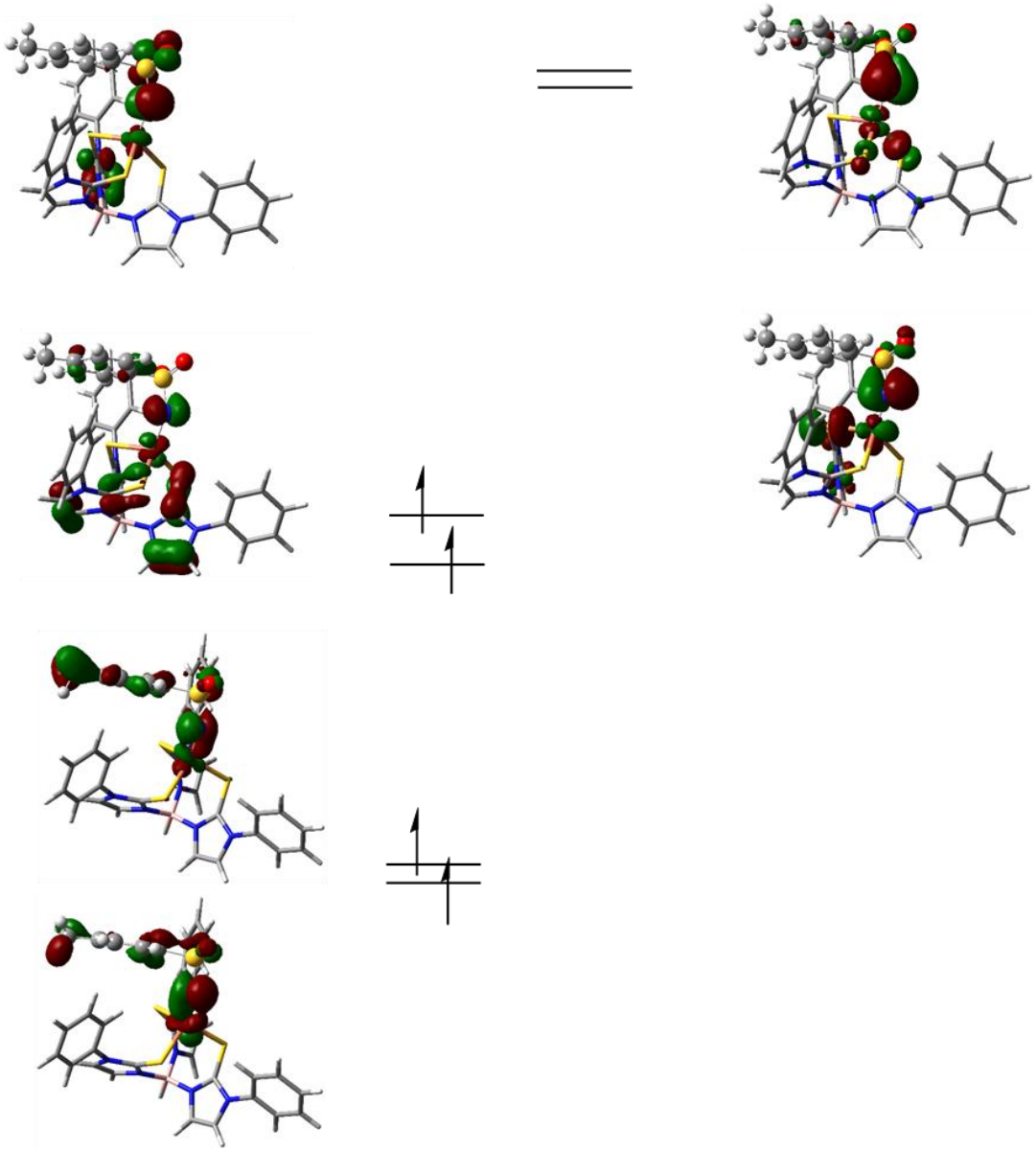
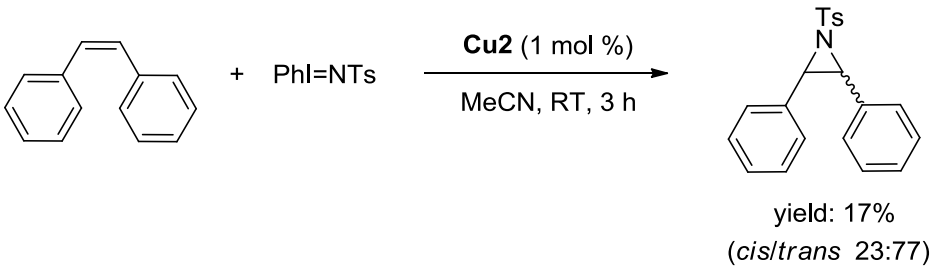


Figure S5. Selected MO diagrams with both spin-up (left panel) and spin-down (right panel) electrons of ^{3}**IntA**.



Scheme S1. Aziridination of *cis*-stilbene with PhI=NTs catalyzed by **Cu2**. Reaction conditions: **Cu2** (4 μmol), *cis*-stilbene (4 mmol), PhI=NTs (0.4 mmol), MeCN (3 mL), 3 h, RT, N_2. The aziridine product was identified by comparison with the spectral data reported in the literature.[9c] The yield and *cis*/*trans* ratio of the aziridine product were determined by NMR spectroscopy with 1,1-diphenylethene as internal standard.

Cartesian Coordinates from DFT Calculations

^{1}IntA

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.007220	8.338670	3.082480
2	16	0	2.137860	8.788110	3.949170
3	7	0	0.954600	9.442440	6.371100
4	5	0	0.289060	8.119090	6.837220
5	1	0	0.441830	8.074460	8.033940
6	7	0	1.883530	11.132180	5.330450
7	6	0	1.364070	11.618340	6.509690
8	1	0	1.440220	12.664820	6.765950
9	6	0	0.786890	10.567520	7.144220
10	1	0	0.255740	10.519310	8.084330
11	6	0	2.156690	11.974950	3.056180
12	1	0	1.313760	11.372910	2.725660
13	6	0	2.577000	11.944580	4.381840
14	6	0	3.644780	12.723730	4.824800
15	1	0	3.960230	12.669220	5.865790
16	6	0	4.304870	13.545540	3.917640
17	1	0	5.141880	14.154720	4.253400
18	6	0	3.903400	13.574130	2.583540
19	1	0	4.428700	14.210720	1.873800
20	6	0	2.835050	12.789440	2.155520
21	1	0	2.515800	12.788820	1.117100
22	16	0	-1.536270	9.804810	4.429390
23	7	0	-1.236560	8.107400	6.591120
24	6	0	-2.002930	8.715020	5.638860
25	7	0	-3.293230	8.281210	5.853090
26	6	0	-3.320310	7.421810	6.938120
27	1	0	-4.239920	6.956340	7.261410
28	6	0	-2.047340	7.315960	7.382710
29	1	0	-1.632160	6.737820	8.196270
30	6	0	-4.460010	8.519650	3.714210
31	1	0	-3.564820	8.191450	3.192790
32	6	0	-4.452610	8.636270	5.103660
33	6	0	-5.590450	9.052310	5.792490
34	1	0	-5.556400	9.150940	6.876360
35	6	0	-6.747820	9.358390	5.083400
36	1	0	-7.635720	9.686900	5.619930
37	6	0	-6.762590	9.255420	3.695420
38	1	0	-7.665250	9.502840	3.140300
39	6	0	-5.619480	8.837300	3.016500

40	1	0	-5.626540	8.753220	1.932050
41	16	0	-0.475020	6.288180	4.014330
42	7	0	1.001090	6.855950	6.280190
43	6	0	0.772700	6.110270	5.169740
44	7	0	1.732220	5.132360	5.146800
45	6	0	2.556850	5.272480	6.250220
46	1	0	3.390600	4.605480	6.413110
47	6	0	2.101180	6.344630	6.939020
48	1	0	2.462100	6.802790	7.848720
49	6	0	1.990230	4.429890	2.817470
50	1	0	1.947130	5.469070	2.496590
51	6	0	1.885120	4.104400	4.168720
52	6	0	1.963180	2.781250	4.598410
53	1	0	1.866310	2.553720	5.658900
54	6	0	2.141070	1.766410	3.663180
55	1	0	2.198850	0.732150	3.995920
56	6	0	2.227990	2.076530	2.308990
57	1	0	2.356380	1.283290	1.575300
58	6	0	2.151980	3.403740	1.893190
59	1	0	2.223420	3.653940	0.836950
60	6	0	1.629660	9.785710	5.240160
61	7	0	-0.241230	9.291490	1.562790
62	16	0	0.728970	9.465380	0.315850
63	8	0	-0.190990	9.277920	-0.826020
64	8	0	1.539850	10.691900	0.383330
65	6	0	1.919120	8.132550	0.204670
66	6	0	3.175770	8.266580	0.796980
67	6	0	1.578830	6.960960	-0.467260
68	6	0	4.079480	7.213320	0.731120
69	1	0	3.434640	9.198890	1.295990
70	6	0	2.505280	5.926470	-0.548120
71	1	0	0.605500	6.884080	-0.947040
72	6	0	3.763400	6.028100	0.055410
73	1	0	5.059830	7.318310	1.196970
74	1	0	2.253220	5.023290	-1.106250
75	6	0	4.746900	4.899590	-0.010280
76	1	0	4.428060	4.125340	-0.717710
77	1	0	5.741530	5.244530	-0.318440
78	1	0	4.869320	4.416050	0.968910

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^{3}IntA

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

1	29	0	-0.274960	8.223380	3.189590
2	16	0	1.965780	8.627080	3.967590
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4	5	0	0.218010	8.088930	6.926580
5	1	0	0.387470	8.054440	8.121560
6	7	0	1.917720	10.993230	5.325080
7	6	0	1.483420	11.524370	6.524360
8	1	0	1.633660	12.567290	6.761850
9	6	0	0.874410	10.518530	7.196580
10	1	0	0.386980	10.510600	8.161380
11	6	0	2.139370	11.743630	3.009820
12	1	0	1.269330	11.157770	2.726290
13	6	0	2.600560	11.747410	4.324230
14	6	0	3.705970	12.508930	4.698600
15	1	0	4.054310	12.484330	5.730220
16	6	0	4.362200	13.274350	3.739570
17	1	0	5.227150	13.869240	4.026230
18	6	0	3.921180	13.264620	2.418400
19	1	0	4.442450	13.856190	1.667990
20	6	0	2.814120	12.498950	2.056680
21	1	0	2.457260	12.477290	1.029640
22	16	0	-1.574390	9.736450	4.457700
23	7	0	-1.317040	8.150400	6.713050
24	6	0	-2.071110	8.728410	5.740400
25	7	0	-3.373940	8.381780	5.999040
26	6	0	-3.424630	7.594930	7.137060
27	1	0	-4.360610	7.200210	7.503510
28	6	0	-2.149370	7.452270	7.565740
29	1	0	-1.745450	6.904380	8.405270
30	6	0	-4.566390	8.489240	3.867350
31	1	0	-3.707410	8.043090	3.372900
32	6	0	-4.524800	8.741760	5.237460
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34	1	0	-5.556430	9.498090	6.966450
35	6	0	-6.765660	9.611910	5.176250
36	1	0	-7.618980	10.052080	5.688320
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43	6	0	0.570910	6.038620	5.270350
44	7	0	1.583550	5.119370	5.157460
45	6	0	2.498390	5.308280	6.180270
46	1	0	3.382390	4.692920	6.259970

47	6	0	2.047020	6.351310	6.912840
48	1	0	2.465700	6.830990	7.786250
49	6	0	1.775430	4.542910	2.791220
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51	6	0	1.738980	4.146010	4.127090
52	6	0	1.905550	2.810280	4.484060
53	1	0	1.863050	2.525530	5.534030
54	6	0	2.104190	1.855780	3.490850
55	1	0	2.229850	0.810420	3.765910
56	6	0	2.129670	2.238230	2.152660
57	1	0	2.276690	1.490240	1.376020
58	6	0	1.965770	3.578760	1.807470
59	1	0	1.990000	3.886970	0.763990
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66	6	0	3.080040	8.354440	0.798270
67	6	0	1.912230	6.843770	-0.698650
68	6	0	4.170370	7.492530	0.800470
69	1	0	3.093860	9.278910	1.372960
70	6	0	3.017240	6.003630	-0.697500
71	1	0	1.025460	6.615120	-1.285900
72	6	0	4.154330	6.302000	0.065460
73	1	0	5.053500	7.747860	1.385940
74	1	0	3.003650	5.094200	-1.299830
75	6	0	5.309370	5.350690	0.112040
76	1	0	5.498550	4.891080	-0.865080
77	1	0	6.230900	5.843990	0.439510
78	1	0	5.114120	4.529480	0.816360

$^{1}TS_{AB}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.181190	9.224150	3.369990
2	16	0	2.306990	8.934890	4.269880
3	7	0	1.301820	9.531220	6.773930
4	5	0	0.301160	8.360660	7.022520
5	1	0	0.390200	8.092860	8.197300
6	7	0	2.683600	11.036920	5.978070
7	6	0	2.290320	11.466260	7.231280

8	1	0	2.640950	12.403720	7.637010
9	6	0	1.434230	10.531980	7.712140
10	1	0	0.888390	10.491420	8.644270
11	6	0	3.264340	11.977540	3.798500
12	1	0	2.337710	11.598060	3.378420
13	6	0	3.586360	11.752040	5.135280
14	6	0	4.773320	12.236260	5.682710
15	1	0	5.011040	12.033020	6.725980
16	6	0	5.652760	12.951920	4.876320
17	1	0	6.582140	13.329650	5.298020
18	6	0	5.352130	13.164880	3.532920
19	1	0	6.048210	13.714020	2.901530
20	6	0	4.162010	12.675250	2.998430
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22	16	0	-0.963970	10.671200	4.753380
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28	6	0	-2.170990	8.132300	7.462190
29	1	0	-1.934570	7.406710	8.227260
30	6	0	-5.075390	9.312920	4.668930
31	1	0	-5.006120	8.233030	4.790440
32	6	0	-4.096070	10.129520	5.234650
33	6	0	-4.132250	11.511990	5.062880
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35	6	0	-5.163830	12.074840	4.318540
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37	6	0	-6.153720	11.269530	3.758810
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39	6	0	-6.107430	9.888760	3.934560
40	1	0	-6.866990	9.252420	3.485510
41	16	0	-1.105830	7.034570	4.129920
42	7	0	0.686700	7.090740	6.234860
43	6	0	0.246210	6.580810	5.042300
44	7	0	1.129440	5.574260	4.713620
45	6	0	2.093110	5.458530	5.698920
46	1	0	2.891940	4.736150	5.617450
47	6	0	1.811920	6.396600	6.631440
48	1	0	2.327590	6.653510	7.546290
49	6	0	1.045680	5.377370	2.276410
50	1	0	0.958050	6.460320	2.178470
51	6	0	1.120400	4.776590	3.532900
52	6	0	1.246670	3.394380	3.662880
53	1	0	1.292070	2.948900	4.655770

54	6	0	1.292760	2.598610	2.522340
55	1	0	1.387820	1.519160	2.623080
56	6	0	1.202290	3.183110	1.261770
57	1	0	1.228410	2.560190	0.369560
58	6	0	1.077650	4.566260	1.146100
59	1	0	1.017200	5.033180	0.164280
60	6	0	2.073920	9.838210	5.699240
61	7	0	0.398650	8.647420	1.640270
62	16	0	1.366040	9.473900	0.638130
63	8	0	0.640110	9.642700	-0.635260
64	8	0	1.976430	10.665490	1.258720
65	6	0	2.708100	8.339720	0.318560
66	6	0	3.831300	8.331080	1.142880
67	6	0	2.559070	7.377920	-0.680660
68	6	0	4.791000	7.336990	0.977090
69	1	0	3.942430	9.101110	1.905310
70	6	0	3.531500	6.400620	-0.841660
71	1	0	1.683990	7.414900	-1.328170
72	6	0	4.652560	6.350670	-0.003670
73	1	0	5.668480	7.325270	1.624150
74	1	0	3.418110	5.651160	-1.626420
75	6	0	5.661730	5.252820	-0.146880
76	1	0	6.593350	5.485180	0.380680
77	1	0	5.281610	4.308120	0.266460
78	1	0	5.908900	5.059000	-1.197750
79	6	0	-1.522170	7.670850	0.544190
80	6	0	-2.413080	8.554010	1.058380
81	1	0	-1.048050	7.820710	-0.423000
82	1	0	-1.307150	6.742550	1.067710
83	1	0	-2.830960	8.333980	2.045970
84	6	0	-2.807480	9.828440	0.501810
85	6	0	-3.608540	10.683070	1.282120
86	6	0	-2.419850	10.264750	-0.780220
87	6	0	-4.009850	11.922610	0.805950
88	1	0	-3.897980	10.360140	2.282030
89	6	0	-2.820710	11.504390	-1.252050
90	1	0	-1.780570	9.633900	-1.391890
91	6	0	-3.619080	12.338090	-0.465580
92	1	0	-4.626030	12.567730	1.431040
93	1	0	-2.504560	11.830670	-2.241370
94	1	0	-3.931240	13.310220	-0.844300

$^3TS_{AB}$

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	29	0	0.242735	9.137629	3.291903
2	16	0	2.445530	8.949849	4.245344
3	7	0	1.356374	9.534899	6.713621
4	5	0	0.388199	8.345778	6.948259
5	1	0	0.461188	8.074678	8.123540
6	7	0	2.709665	11.077223	5.941494
7	6	0	2.265487	11.506242	7.180391
8	1	0	2.573656	12.459104	7.585092
9	6	0	1.428598	10.550638	7.646712
10	1	0	0.857830	10.501376	8.563278
11	6	0	3.324999	12.037094	3.776417
12	1	0	2.420147	11.636929	3.327921
13	6	0	3.614886	11.814557	5.121666
14	6	0	4.772982	12.330039	5.701902
15	1	0	4.986211	12.129746	6.751047
16	6	0	5.654338	13.074018	4.923692
17	1	0	6.560962	13.475304	5.372849
18	6	0	5.383878	13.287096	3.574272
19	1	0	6.079744	13.860678	2.964696
20	6	0	4.222895	12.767031	3.005560
21	1	0	3.999615	12.924195	1.952812
22	16	0	-0.919148	10.613518	4.667293
23	7	0	-1.092696	8.737792	6.695886
24	6	0	-1.669508	9.588418	5.807265
25	7	0	-3.029759	9.457460	5.969545
26	6	0	-3.285085	8.505047	6.944206
27	1	0	-4.294699	8.277503	7.252453
28	6	0	-2.084254	8.072445	7.387257
29	1	0	-1.833632	7.350442	8.151285
30	6	0	-5.108682	9.264388	4.753511
31	1	0	-5.069760	8.189425	4.921944
32	6	0	-4.063334	10.070065	5.208318
33	6	0	-4.067795	11.442914	4.966291
34	1	0	-3.249888	12.059134	5.327743
35	6	0	-5.130821	12.004726	4.267144
36	1	0	-5.131790	13.074828	4.070131
37	6	0	-6.189811	11.212509	3.830001
38	1	0	-7.022937	11.663395	3.293766
39	6	0	-6.175724	9.841282	4.072516
40	1	0	-6.990941	9.212232	3.720453
41	16	0	-0.877378	7.052406	3.986280
42	7	0	0.810967	7.071922	6.175919
43	6	0	0.416362	6.560061	4.975715
44	7	0	1.278379	5.525667	4.696044

45	6	0	2.195613	5.395055	5.725165
46	1	0	2.977160	4.650522	5.687175
47	6	0	1.900377	6.355523	6.630039
48	1	0	2.381834	6.614165	7.562709
49	6	0	1.244802	5.278280	2.263038
50	1	0	1.226487	6.362205	2.153658
51	6	0	1.273161	4.703472	3.533680
52	6	0	1.336087	3.319968	3.691145
53	1	0	1.346513	2.893621	4.693185
54	6	0	1.360183	2.500120	2.567077
55	1	0	1.407839	1.419906	2.689992
56	6	0	1.302097	3.061857	1.294489
57	1	0	1.303856	2.420847	0.414949
58	6	0	1.242442	4.446298	1.148564
59	1	0	1.209264	4.893518	0.157516
60	6	0	2.149330	9.855262	5.655351
61	7	0	0.383355	9.230732	1.445051
62	16	0	1.539692	9.708793	0.403685
63	8	0	0.968284	9.888028	-0.940860
64	8	0	2.268400	10.828093	1.021743
65	6	0	2.685994	8.350131	0.276988
66	6	0	3.745507	8.249319	1.176963
67	6	0	2.492945	7.376734	-0.703590
68	6	0	4.584794	7.142412	1.118316
69	1	0	3.907558	9.040774	1.906690
70	6	0	3.354966	6.289482	-0.762023
71	1	0	1.686479	7.497371	-1.424991
72	6	0	4.395884	6.139370	0.162321
73	1	0	5.407057	7.055697	1.828916
74	1	0	3.213522	5.530235	-1.532628
75	6	0	5.256497	4.914364	0.143024
76	1	0	6.193762	5.064104	0.689994
77	1	0	4.736284	4.067232	0.612792
78	1	0	5.505915	4.605344	-0.879073
79	6	0	-1.220854	8.084075	0.483669
80	6	0	-2.339228	8.714121	0.971597
81	1	0	-0.802013	8.351962	-0.482811
82	1	0	-0.912334	7.128754	0.903931
83	1	0	-2.822312	8.296722	1.860433
84	6	0	-2.869432	9.964775	0.487885
85	6	0	-4.058751	10.481804	1.038282
86	6	0	-2.218539	10.714120	-0.515580
87	6	0	-4.590629	11.682172	0.589151
88	1	0	-4.560344	9.926634	1.831475
89	6	0	-2.753431	11.913651	-0.956897
90	1	0	-1.268851	10.368142	-0.919827

91	6	0	-3.944635	12.401905	-0.415521
92	1	0	-5.512585	12.061970	1.028821
93	1	0	-2.231593	12.481452	-1.725390
94	1	0	-4.359872	13.345101	-0.767328

[1]IntB

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.535550	0.316400	-0.314360
2	16	0	1.628400	0.160470	0.707380
3	7	0	0.802830	0.727910	3.270980
4	5	0	-0.100590	-0.495980	3.584960
5	1	0	0.003620	-0.686500	4.774350
6	7	0	2.066420	2.281450	2.380460
7	6	0	1.745060	2.698850	3.660990
8	1	0	2.090250	3.648410	4.042400
9	6	0	0.960270	1.736780	4.199600
10	1	0	0.488250	1.673330	5.169900
11	6	0	2.560730	3.215260	0.168150
12	1	0	1.644750	2.790240	-0.228950
13	6	0	2.914590	3.017950	1.501700
14	6	0	4.091350	3.560310	2.018040
15	1	0	4.359400	3.376300	3.057440
16	6	0	4.922330	4.308320	1.190540
17	1	0	5.842190	4.729380	1.591860
18	6	0	4.586330	4.497380	-0.147580
19	1	0	5.243350	5.072480	-0.797310
20	6	0	3.410330	3.947970	-0.653440
21	1	0	3.140650	4.081740	-1.698620
22	16	0	-1.574050	1.690040	1.271980
23	7	0	-1.601680	-0.187130	3.330660
24	6	0	-2.227690	0.602200	2.423690
25	7	0	-3.573410	0.368220	2.574240
26	6	0	-3.771280	-0.595620	3.543770
27	1	0	-4.764820	-0.910730	3.826990
28	6	0	-2.543930	-0.928290	4.007060
29	1	0	-2.245040	-1.634910	4.768120
30	6	0	-5.467620	0.113720	1.088350
31	1	0	-5.260570	-0.955320	1.062350
32	6	0	-4.633730	0.952130	1.825840
33	6	0	-4.845920	2.328430	1.861100
34	1	0	-4.176380	2.960520	2.439060
35	6	0	-5.908870	2.867180	1.144300

36	1	0	-6.079110	3.941950	1.164930
37	6	0	-6.750290	2.038860	0.403020
38	1	0	-7.577330	2.468000	-0.159270
39	6	0	-6.529670	0.664090	0.376200
40	1	0	-7.177470	0.016280	-0.210330
41	16	0	-1.463670	-2.067890	0.800420
42	7	0	0.356170	-1.777950	2.865980
43	6	0	-0.070040	-2.374250	1.709440
44	7	0	0.865060	-3.346490	1.422790
45	6	0	1.846620	-3.358090	2.401390
46	1	0	2.683470	-4.038650	2.346190
47	6	0	1.525370	-2.388980	3.285000
48	1	0	2.032350	-2.055180	4.179640
49	6	0	0.783670	-3.617900	-1.000140
50	1	0	0.642120	-2.543940	-1.116390
51	6	0	0.901670	-4.180010	0.270310
52	6	0	1.118490	-5.547210	0.431120
53	1	0	1.198680	-5.965520	1.433590
54	6	0	1.211820	-6.364400	-0.692090
55	1	0	1.379440	-7.432730	-0.567190
56	6	0	1.074960	-5.817720	-1.965450
57	1	0	1.136730	-6.458770	-2.843380
58	6	0	0.858720	-4.448460	-2.112480
59	1	0	0.763590	-4.007990	-3.103510
60	6	0	1.483000	1.059210	2.142430
61	7	0	0.006960	-0.482130	-2.011360
62	16	0	1.097050	0.252290	-3.021970
63	8	0	0.539770	0.385660	-4.379900
64	8	0	1.691950	1.418730	-2.365180
65	6	0	2.350260	-1.012530	-3.138280
66	6	0	3.305550	-1.157410	-2.134720
67	6	0	2.321050	-1.882070	-4.226130
68	6	0	4.214710	-2.205370	-2.215230
69	1	0	3.332960	-0.449860	-1.306410
70	6	0	3.243510	-2.919300	-4.293440
71	1	0	1.583490	-1.728850	-5.011020
72	6	0	4.190520	-3.110650	-3.282550
73	1	0	4.961190	-2.326840	-1.430020
74	1	0	3.225560	-3.600730	-5.144810
75	6	0	5.127420	-4.278010	-3.320490
76	1	0	6.078650	-4.056390	-2.823390
77	1	0	4.691160	-5.144930	-2.804090
78	1	0	5.346360	-4.593510	-4.346920
79	6	0	-1.356190	-0.698920	-2.529270
80	6	0	-2.139690	0.250930	-1.660920
81	1	0	-1.445040	-0.494840	-3.605480

82	1	0	-1.639890	-1.742770	-2.336590
83	1	0	-2.839210	-0.195940	-0.947610
84	6	0	-2.509170	1.576290	-2.123080
85	6	0	-3.570720	2.246420	-1.480440
86	6	0	-1.906250	2.202050	-3.233960
87	6	0	-4.026120	3.472820	-1.937270
88	1	0	-4.042620	1.772430	-0.623390
89	6	0	-2.358970	3.436220	-3.678240
90	1	0	-1.087520	1.715660	-3.759640
91	6	0	-3.417340	4.079330	-3.036010
92	1	0	-4.860290	3.958330	-1.431900
93	1	0	-1.880520	3.900740	-4.538740
94	1	0	-3.767330	5.047060	-3.391980

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^{3}IntB

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.191270	0.287290	-0.133540
2	16	0	2.018300	0.245750	0.830180
3	7	0	0.967030	0.708100	3.336310
4	5	0	0.054680	-0.528240	3.542240
5	1	0	0.151160	-0.833750	4.707150
6	7	0	2.239050	2.327990	2.585100
7	6	0	1.805460	2.699220	3.846150
8	1	0	2.082920	3.650980	4.275170
9	6	0	1.017340	1.696220	4.299160
10	1	0	0.472770	1.593810	5.227360
11	6	0	2.772980	3.354810	0.428200
12	1	0	1.893910	2.898660	-0.016530
13	6	0	3.088130	3.131870	1.767640
14	6	0	4.216070	3.712640	2.345830
15	1	0	4.452860	3.510090	3.389410
16	6	0	5.040230	4.523650	1.572030
17	1	0	5.923280	4.975410	2.020190
18	6	0	4.744570	4.738850	0.228290
19	1	0	5.397190	5.363210	-0.378900
20	6	0	3.614910	4.152400	-0.338350
21	1	0	3.376090	4.307350	-1.388160
22	16	0	-1.346140	1.701240	1.288750
23	7	0	-1.440170	-0.188040	3.313520
24	6	0	-2.052940	0.645120	2.433860
25	7	0	-3.404060	0.468060	2.606250
26	6	0	-3.620550	-0.498600	3.575340

27	1	0	-4.620320	-0.763540	3.885860
28	6	0	-2.402280	-0.893070	4.006900
29	1	0	-2.119660	-1.612170	4.762400
30	6	0	-5.464490	0.224340	1.367790
31	1	0	-5.372890	-0.853580	1.491440
32	6	0	-4.462740	1.059630	1.863070
33	6	0	-4.529210	2.439390	1.682130
34	1	0	-3.742530	3.075760	2.077470
35	6	0	-5.613740	2.980750	1.001240
36	1	0	-5.665050	4.057180	0.851230
37	6	0	-6.629760	2.158290	0.519910
38	1	0	-7.478330	2.592040	-0.006060
39	6	0	-6.552370	0.779730	0.701840
40	1	0	-7.333230	0.129220	0.313180
41	16	0	-1.258370	-1.842050	0.605820
42	7	0	0.521430	-1.756990	2.721230
43	6	0	0.099150	-2.279830	1.534840
44	7	0	1.002290	-3.267310	1.206280
45	6	0	1.973190	-3.350110	2.188140
46	1	0	2.789980	-4.052520	2.110010
47	6	0	1.669960	-2.412180	3.114530
48	1	0	2.185050	-2.129180	4.021750
49	6	0	0.752980	-3.619300	-1.201270
50	1	0	0.670870	-2.543890	-1.343390
51	6	0	0.945390	-4.135290	0.079120
52	6	0	1.109720	-5.505840	0.279050
53	1	0	1.247400	-5.890330	1.288570
54	6	0	1.066840	-6.369130	-0.811230
55	1	0	1.192760	-7.438770	-0.654980
56	6	0	0.838990	-5.867020	-2.089960
57	1	0	0.787070	-6.543960	-2.940710
58	6	0	0.681440	-4.495710	-2.278590
59	1	0	0.515470	-4.094480	-3.275890
60	6	0	1.721520	1.093400	2.272330
61	7	0	-0.032080	0.072110	-2.035940
62	16	0	1.260490	0.534800	-2.948990
63	8	0	0.816260	0.788470	-4.327770
64	8	0	1.968670	1.570510	-2.196960
65	6	0	2.350400	-0.876640	-3.040210
66	6	0	3.316920	-1.068560	-2.053810
67	6	0	2.197740	-1.803710	-4.070070
68	6	0	4.100820	-2.215300	-2.080460
69	1	0	3.460470	-0.306320	-1.290800
70	6	0	3.003540	-2.936660	-4.091540
71	1	0	1.466660	-1.617130	-4.854960
72	6	0	3.948790	-3.174200	-3.088070

73	1	0	4.854310	-2.366590	-1.306880
74	1	0	2.890030	-3.662390	-4.898200
75	6	0	4.747120	-4.440620	-3.071920
76	1	0	5.730350	-4.299450	-2.608910
77	1	0	4.229220	-5.220660	-2.495000
78	1	0	4.901360	-4.840210	-4.080750
79	6	0	-1.130120	-0.652910	-2.703440
80	6	0	-2.437560	-0.106140	-2.228350
81	1	0	-1.025110	-0.539060	-3.793590
82	1	0	-1.070280	-1.729990	-2.475440
83	1	0	-3.038460	-0.709410	-1.543980
84	6	0	-2.909070	1.184950	-2.574710
85	6	0	-4.132670	1.673340	-2.047910
86	6	0	-2.194480	2.030970	-3.465010
87	6	0	-4.619500	2.918270	-2.406890
88	1	0	-4.691160	1.048210	-1.349780
89	6	0	-2.688750	3.277010	-3.809030
90	1	0	-1.246320	1.695350	-3.880680
91	6	0	-3.904270	3.732040	-3.290150
92	1	0	-5.567790	3.264140	-1.996240
93	1	0	-2.120310	3.905830	-4.492910
94	1	0	-4.289980	4.711410	-3.569520

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[1]IntC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.562540	8.738700	3.575640
2	16	0	2.643690	8.529190	4.546660
3	7	0	1.394610	9.290540	6.908240
4	5	0	0.318270	8.190430	7.127060
5	1	0	0.279590	7.979350	8.317380
6	7	0	2.778840	10.776990	6.089390
7	6	0	2.272700	11.300070	7.269030
8	1	0	2.557740	12.283480	7.612970
9	6	0	1.419910	10.375390	7.764200
10	1	0	0.803750	10.389670	8.651890
11	6	0	3.218080	11.696380	3.876170
12	1	0	2.275380	11.278310	3.525810
13	6	0	3.621190	11.500300	5.196700
14	6	0	4.808140	12.049030	5.674260
15	1	0	5.104510	11.874630	6.707520
16	6	0	5.606550	12.801000	4.816020
17	1	0	6.536230	13.230270	5.184750

18	6	0	5.221420	12.991450	3.491950
19	1	0	5.849500	13.576560	2.822590
20	6	0	4.028590	12.439270	3.025240
21	1	0	3.711650	12.591670	1.995230
22	16	0	-0.608720	10.554410	4.738950
23	7	0	-1.096280	8.669720	6.712500
24	6	0	-1.522820	9.529760	5.743670
25	7	0	-2.893460	9.382390	5.680470
26	6	0	-3.300190	8.416900	6.590160
27	1	0	-4.344340	8.168210	6.711850
28	6	0	-2.188000	7.996130	7.228690
29	1	0	-2.060770	7.266920	8.016050
30	6	0	-4.554360	9.077870	3.949970
31	1	0	-4.460160	8.003330	4.102060
32	6	0	-3.760990	9.944030	4.703840
33	6	0	-3.828400	11.322030	4.507170
34	1	0	-3.195720	11.978990	5.097600
35	6	0	-4.700640	11.828520	3.548770
36	1	0	-4.747790	12.903410	3.384350
37	6	0	-5.499130	10.972970	2.793600
38	1	0	-6.167390	11.378360	2.036380
39	6	0	-5.423700	9.597180	2.995330
40	1	0	-6.033660	8.921380	2.398730
41	16	0	-0.822280	6.804520	4.142280
42	7	0	0.711140	6.851290	6.448020
43	6	0	0.402020	6.333300	5.224690
44	7	0	1.267220	5.281150	5.023090
45	6	0	2.089470	5.136300	6.132030
46	1	0	2.855980	4.376120	6.166600
47	6	0	1.738990	6.109130	7.000250
48	1	0	2.141890	6.366150	7.969940
49	6	0	1.533380	5.135160	2.597880
50	1	0	1.498980	6.224000	2.537950
51	6	0	1.405350	4.508410	3.839270
52	6	0	1.474900	3.120740	3.945000
53	1	0	1.362650	2.652770	4.921760
54	6	0	1.667900	2.349790	2.802440
55	1	0	1.720390	1.266140	2.887350
56	6	0	1.779240	2.963870	1.558330
57	1	0	1.920680	2.360970	0.662970
58	6	0	1.710270	4.353370	1.461520
59	1	0	1.807920	4.841140	0.492290
60	6	0	2.239790	9.534540	5.870210
61	7	0	-0.185310	9.045790	1.586570
62	16	0	0.810170	9.975310	0.486470
63	8	0	0.138890	10.146590	-0.800180

64	8	0	1.282180	11.114940	1.263900
65	6	0	2.110170	8.789870	0.280940
66	6	0	3.138410	8.718220	1.218020
67	6	0	2.035470	7.895930	-0.785190
68	6	0	4.082780	7.704870	1.098140
69	1	0	3.191010	9.436020	2.034950
70	6	0	2.999550	6.901880	-0.896770
71	1	0	1.240490	7.996930	-1.521030
72	6	0	4.021090	6.775840	0.053010
73	1	0	4.876500	7.630390	1.841070
74	1	0	2.956860	6.202340	-1.732050
75	6	0	5.001100	5.647500	-0.024730
76	1	0	5.107870	5.267470	-1.046740
77	1	0	5.992620	5.941650	0.336640
78	1	0	4.669620	4.806850	0.601370
79	6	0	-1.118010	8.104390	0.933580
80	6	0	-1.661870	9.286480	1.619010
81	1	0	-1.115990	8.131450	-0.157270
82	1	0	-1.143350	7.120440	1.402430
83	1	0	-1.992280	9.142620	2.652800
84	6	0	-2.309990	10.426450	0.917850
85	6	0	-2.098450	11.728350	1.380650
86	6	0	-3.183170	10.209300	-0.148610
87	6	0	-2.737790	12.798240	0.764300
88	1	0	-1.432890	11.888410	2.229060
89	6	0	-3.832690	11.279870	-0.754880
90	1	0	-3.352870	9.192660	-0.503960
91	6	0	-3.606890	12.577430	-0.302100
92	1	0	-2.558780	13.811090	1.122370
93	1	0	-4.510630	11.100990	-1.588010
94	1	0	-4.105910	13.417020	-0.783670

---

^{3}IntC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.415690	8.753960	3.206140
2	16	0	2.513430	8.712730	4.184110
3	7	0	1.394500	9.319780	6.647090
4	5	0	0.373390	8.175080	6.871230
5	1	0	0.339780	7.989570	8.064550
6	7	0	2.762880	10.842760	5.871710
7	6	0	2.317570	11.287390	7.105110
8	1	0	2.635320	12.239490	7.503690

9	6	0	1.470640	10.342490	7.573290
10	1	0	0.893630	10.303490	8.486090
11	6	0	3.266940	11.882810	3.716290
12	1	0	2.320560	11.519940	3.319630
13	6	0	3.638430	11.590290	5.027830
14	6	0	4.838780	12.060680	5.555660
15	1	0	5.112070	11.809980	6.579520
16	6	0	5.679690	12.831550	4.758010
17	1	0	6.619040	13.199530	5.166100
18	6	0	5.323530	13.118810	3.442900
19	1	0	5.984910	13.717460	2.819450
20	6	0	4.119690	12.644340	2.923950
21	1	0	3.824670	12.856700	1.899140
22	16	0	-0.698420	10.559040	4.573420
23	7	0	-1.063280	8.551210	6.439000
24	6	0	-1.549600	9.453710	5.536590
25	7	0	-2.920660	9.278270	5.524430
26	6	0	-3.264370	8.261720	6.402110
27	1	0	-4.296630	7.990130	6.567150
28	6	0	-2.116520	7.827000	6.964790
29	1	0	-1.944590	7.064950	7.711520
30	6	0	-4.816110	9.100080	4.036480
31	1	0	-4.780690	8.020590	4.178210
32	6	0	-3.865310	9.906360	4.665390
33	6	0	-3.866200	11.286480	4.468770
34	1	0	-3.124360	11.903660	4.965790
35	6	0	-4.818200	11.851670	3.626260
36	1	0	-4.806450	12.926060	3.454760
37	6	0	-5.770580	11.055270	2.997190
38	1	0	-6.501310	11.505870	2.328630
39	6	0	-5.771470	9.678950	3.208570
40	1	0	-6.505410	9.046750	2.712150
41	16	0	-0.531870	6.688620	3.850450
42	7	0	0.845290	6.824010	6.252450
43	6	0	0.582200	6.232930	5.056360
44	7	0	1.385610	5.120440	4.985940
45	6	0	2.135290	5.017230	6.144750
46	1	0	2.845470	4.215630	6.284840
47	6	0	1.799090	6.077330	6.915820
48	1	0	2.156880	6.381940	7.889180
49	6	0	1.821170	4.711380	2.619380
50	1	0	1.953720	5.781480	2.466390
51	6	0	1.502680	4.222780	3.885780
52	6	0	1.347670	2.856870	4.109900
53	1	0	1.088000	2.502570	5.106270
54	6	0	1.508270	1.966460	3.052370

55	1	0	1.384910	0.899020	3.223840
56	6	0	1.813870	2.442940	1.780830
57	1	0	1.933740	1.746650	0.953120
58	6	0	1.969340	3.812080	1.570010
59	1	0	2.216880	4.191980	0.580170
60	6	0	2.191420	9.630480	5.592860
61	7	0	-0.628110	9.068450	1.655360
62	16	0	1.378790	10.501470	0.256350
63	8	0	0.630670	10.427580	-1.027600
64	8	0	2.254290	11.675200	0.554060
65	6	0	2.448360	9.052530	0.283960
66	6	0	3.598190	9.059230	1.069580
67	6	0	2.068650	7.916110	-0.425870
68	6	0	4.382210	7.913010	1.127420
69	1	0	3.873940	9.956320	1.620870
70	6	0	2.873710	6.783800	-0.366410
71	1	0	1.174510	7.940500	-1.044520
72	6	0	4.036170	6.759670	0.413440
73	1	0	5.284540	7.914110	1.738980
74	1	0	2.606100	5.904780	-0.954470
75	6	0	4.883290	5.526960	0.499430
76	1	0	4.679480	4.834770	-0.325740
77	1	0	5.952610	5.767770	0.481440
78	1	0	4.696340	4.978740	1.433560
79	6	0	-1.298540	8.242750	0.686440
80	6	0	-2.049090	9.227330	1.505890
81	1	0	-1.090910	8.491660	-0.359150
82	1	0	-1.385400	7.172650	0.899720
83	1	0	-2.645540	8.814230	2.332030
84	6	0	-2.584970	10.504200	0.948940
85	6	0	-1.915820	11.711280	1.157730
86	6	0	-3.789730	10.509520	0.241550
87	6	0	-2.442460	12.903110	0.668960
88	1	0	-0.976890	11.702530	1.711450
89	6	0	-4.316530	11.699650	-0.250440
90	1	0	-4.315620	9.567660	0.078000
91	6	0	-3.644720	12.901140	-0.034740
92	1	0	-1.907400	13.837220	0.833610
93	1	0	-5.252290	11.689070	-0.808790
94	1	0	-4.052290	13.833110	-0.423840

$^{1}TS_{AD}$

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

1	29	0	0.150100	9.201350	3.375160
2	16	0	2.276860	8.924830	4.277630
3	7	0	1.272520	9.537140	6.779120
4	5	0	0.277000	8.364870	7.039740
5	1	0	0.363580	8.111630	8.217950
6	7	0	2.640530	11.045370	5.964820
7	6	0	2.248020	11.483710	7.215210
8	1	0	2.593320	12.427280	7.611230
9	6	0	1.400510	10.547730	7.707540
10	1	0	0.857960	10.511590	8.641790
11	6	0	3.200110	11.975060	3.774810
12	1	0	2.273910	11.585480	3.362840
13	6	0	3.532220	11.761420	5.111110
14	6	0	4.717980	12.259710	5.648180
15	1	0	4.963470	12.065420	6.691360
16	6	0	5.586080	12.978230	4.832080
17	1	0	6.514440	13.367060	5.245840
18	6	0	5.275390	13.179920	3.489270
19	1	0	5.962270	13.731810	2.850280
20	6	0	4.086600	12.675980	2.965050
21	1	0	3.831420	12.820720	1.917590
22	16	0	-0.990050	10.661040	4.752750
23	7	0	-1.192440	8.788480	6.791880
24	6	0	-1.750590	9.626260	5.881990
25	7	0	-3.110400	9.486350	6.006510
26	6	0	-3.389520	8.533000	6.972450
27	1	0	-4.406910	8.290210	7.241080
28	6	0	-2.198350	8.115310	7.455450
29	1	0	-1.963520	7.392540	8.223720
30	6	0	-5.037280	9.260400	4.563090
31	1	0	-4.940210	8.180160	4.660680
32	6	0	-4.110130	10.089420	5.193700
33	6	0	-4.179770	11.474870	5.057360
34	1	0	-3.447760	12.103290	5.557590
35	6	0	-5.192930	12.028370	4.281320
36	1	0	-5.252840	13.109690	4.173410
37	6	0	-6.127760	11.209480	3.650670
38	1	0	-6.913720	11.650390	3.040720
39	6	0	-6.048850	9.826330	3.793100
40	1	0	-6.767530	9.181340	3.292050
41	16	0	-1.125120	6.998170	4.164680
42	7	0	0.670080	7.088810	6.266320
43	6	0	0.233190	6.565840	5.078010
44	7	0	1.126040	5.566030	4.755140
45	6	0	2.092170	5.466900	5.740090

46	1	0	2.898270	4.752190	5.662440
47	6	0	1.802950	6.408680	6.666320
48	1	0	2.317330	6.677600	7.578430
49	6	0	1.047770	5.360200	2.318570
50	1	0	0.948100	6.441590	2.216110
51	6	0	1.127290	4.764180	3.577080
52	6	0	1.269670	3.383950	3.711270
53	1	0	1.319100	2.941790	4.705440
54	6	0	1.327180	2.585510	2.573000
55	1	0	1.435000	1.507560	2.677040
56	6	0	1.231930	3.165110	1.310540
57	1	0	1.266900	2.539850	0.420230
58	6	0	1.091330	4.546440	1.190600
59	1	0	1.025950	5.010080	0.207430
60	6	0	2.039600	9.839500	5.699200
61	7	0	0.354200	8.595170	1.652140
62	16	0	1.284360	9.443490	0.631280
63	8	0	0.532340	9.607200	-0.627720
64	8	0	1.882430	10.642980	1.249880
65	6	0	2.641670	8.336720	0.284440
66	6	0	3.768480	8.335130	1.104170
67	6	0	2.502260	7.384830	-0.725350
68	6	0	4.742490	7.358300	0.922050
69	1	0	3.870850	9.097030	1.876130
70	6	0	3.488750	6.424180	-0.901990
71	1	0	1.623620	7.415610	-1.368180
72	6	0	4.614350	6.381570	-0.069880
73	1	0	5.622840	7.352110	1.565240
74	1	0	3.383340	5.682710	-1.695380
75	6	0	5.640110	5.301560	-0.230370
76	1	0	6.576530	5.550740	0.280790
77	1	0	5.284270	4.350760	0.190500
78	1	0	5.872120	5.111420	-1.285310
79	6	0	-1.575640	7.602200	0.568240
80	6	0	-2.398410	8.528990	1.118030
81	1	0	-1.124870	7.734890	-0.412710
82	1	0	-1.381200	6.666250	1.086070
83	1	0	-2.771110	8.334710	2.128510
84	6	0	-2.731090	9.828380	0.584020
85	6	0	-3.320550	10.778950	1.438630
86	6	0	-2.455100	10.208080	-0.744700
87	6	0	-3.615180	12.060540	1.000490
88	1	0	-3.518150	10.506450	2.475260
89	6	0	-2.750500	11.481470	-1.197790
90	1	0	-1.984080	9.498220	-1.419430
91	6	0	-3.324210	12.392370	-0.316090

92	1	0	-4.054770	12.802480	1.662230
93	1	0	-2.533670	11.787880	-2.217590
94	9	0	-3.608390	13.631260	-0.755330

$^3TS_{AD}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.242291	9.143559	3.287941
2	16	0	2.441920	8.954391	4.241677
3	7	0	1.351838	9.540587	6.709259
4	5	0	0.383633	8.351500	6.944185
5	1	0	0.455837	8.081732	8.119764
6	7	0	2.705889	11.082373	5.937275
7	6	0	2.261055	11.511970	7.175662
8	1	0	2.569190	12.464914	7.580196
9	6	0	1.423715	10.556673	7.641947
10	1	0	0.852561	10.507877	8.558290
11	6	0	3.323867	12.040799	3.772216
12	1	0	2.419482	11.640411	3.322982
13	6	0	3.612204	11.819047	5.117911
14	6	0	4.769744	12.334595	5.699186
15	1	0	4.981773	12.134916	6.748686
16	6	0	5.652128	13.077886	4.921512
17	1	0	6.558309	13.479270	5.371442
18	6	0	5.383219	13.290242	3.571669
19	1	0	6.079857	13.863350	2.962554
20	6	0	4.222783	12.770096	3.001945
21	1	0	4.000838	12.926787	1.948847
22	16	0	-0.923644	10.618224	4.662339
23	7	0	-1.097421	8.742407	6.690421
24	6	0	-1.674332	9.591788	5.800914
25	7	0	-3.034635	9.458106	5.960913
26	6	0	-3.289741	8.505066	6.935168
27	1	0	-4.299367	8.275683	7.241985
28	6	0	-2.088784	8.075029	7.380179
29	1	0	-1.837931	7.353629	8.144697
30	6	0	-5.111985	9.262293	4.742666
31	1	0	-5.071520	8.187272	4.910434
32	6	0	-4.068139	10.069256	5.198803
33	6	0	-4.074811	11.442392	4.958064
34	1	0	-3.258152	12.059578	5.320767
35	6	0	-5.138934	12.003378	4.259878
36	1	0	-5.142540	13.073990	4.065547

37	6	0	-6.196716	11.209845	3.821733
38	1	0	-7.031760	11.660439	3.288107
39	6	0	-6.180122	9.838206	4.062300
40	1	0	-6.994863	9.208339	3.710512
41	16	0	-0.879374	7.056313	3.981114
42	7	0	0.806179	7.076790	6.173474
43	6	0	0.411784	6.563586	4.973666
44	7	0	1.271888	5.526894	4.697010
45	6	0	2.187727	5.396104	5.727280
46	1	0	2.967367	4.649439	5.691715
47	6	0	1.893574	6.358872	6.630116
48	1	0	2.374183	6.617781	7.563147
49	6	0	1.250111	5.279370	2.264332
50	1	0	1.238401	6.363502	2.155508
51	6	0	1.267210	4.704137	3.534954
52	6	0	1.319713	3.320362	3.692844
53	1	0	1.321019	2.894034	4.694942
54	6	0	1.345230	2.500468	2.568788
55	1	0	1.384610	1.419931	2.691783
56	6	0	1.299798	3.062798	1.295970
57	1	0	1.303343	2.421859	0.416389
58	6	0	1.250175	4.447602	1.149699
59	1	0	1.227072	4.895095	0.158463
60	6	0	2.145437	9.860516	5.651394
61	7	0	0.384421	9.227060	1.440033
62	16	0	1.541033	9.705500	0.401177
63	8	0	0.967576	9.885561	-0.943379
64	8	0	2.269123	10.826238	1.017512
65	6	0	2.689105	8.348933	0.270921
66	6	0	3.747210	8.246608	1.172423
67	6	0	2.498075	7.377692	-0.712168
68	6	0	4.587161	7.140285	1.112582
69	1	0	3.907801	9.036535	1.904156
70	6	0	3.360756	6.290996	-0.771673
71	1	0	1.692601	7.499527	-1.434455
72	6	0	4.400185	6.139242	0.154087
73	1	0	5.408311	7.052322	1.824291
74	1	0	3.220957	5.533521	-1.544312
75	6	0	5.261048	4.914449	0.133673
76	1	0	6.197352	5.063194	0.682528
77	1	0	4.740106	4.066361	0.600884
78	1	0	5.512203	4.607535	-0.888616
79	6	0	-1.208024	8.057844	0.481912
80	6	0	-2.329226	8.678935	0.974526
81	1	0	-0.790451	8.334100	-0.482791
82	1	0	-0.894705	7.101439	0.895852

83	1	0	-2.814311	8.250086	1.856580
84	6	0	-2.855308	9.936327	0.507712
85	6	0	-4.049518	10.446910	1.054305
86	6	0	-2.192408	10.705393	-0.474468
87	6	0	-4.581983	11.653075	0.625718
88	1	0	-4.561720	9.884204	1.834791
89	6	0	-2.713700	11.912739	-0.906468
90	1	0	-1.236063	10.369916	-0.872309
91	6	0	-3.907539	12.367414	-0.356283
92	1	0	-5.504068	12.050539	1.043214
93	1	0	-2.202578	12.514777	-1.653334
94	9	0	-4.419083	13.539267	-0.775413

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[1]IntD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.045120	0.128820	-0.171920
2	16	0	2.048930	-0.214130	0.998410
3	7	0	0.740770	0.534060	3.311250
4	5	0	-0.360680	-0.545640	3.459230
5	1	0	-0.445490	-0.773900	4.643580
6	7	0	2.290480	1.942240	2.660620
7	6	0	1.757470	2.438040	3.839410
8	1	0	2.097150	3.375020	4.255760
9	6	0	0.801400	1.565560	4.230330
10	1	0	0.140140	1.582760	5.085260
11	6	0	3.088770	2.813550	0.529150
12	1	0	2.186100	2.452390	0.044590
13	6	0	3.289610	2.606760	1.892640
14	6	0	4.440440	3.069970	2.527300
15	1	0	4.582360	2.886190	3.591560
16	6	0	5.405420	3.743160	1.783360
17	1	0	6.307050	4.104610	2.274710
18	6	0	5.224740	3.936770	0.415930
19	1	0	5.987630	4.452880	-0.164300
20	6	0	4.068150	3.470010	-0.206660
21	1	0	3.911010	3.611110	-1.274120
22	16	0	-1.194100	1.785040	1.009130
23	7	0	-1.756830	-0.009780	3.039490
24	6	0	-2.135210	0.969160	2.170040
25	7	0	-3.493220	1.151250	2.364820
26	6	0	-3.941740	0.255520	3.326580
27	1	0	-4.967880	0.261170	3.661790

28	6	0	-2.866550	-0.449330	3.734690
29	1	0	-2.774940	-1.219000	4.487230
30	6	0	-5.667310	1.739820	1.487110
31	1	0	-5.971260	0.703760	1.626990
32	6	0	-4.353320	2.115960	1.777280
33	6	0	-3.939100	3.432320	1.574530
34	1	0	-2.921510	3.722480	1.816950
35	6	0	-4.845830	4.361900	1.074550
36	1	0	-4.519120	5.387880	0.916360
37	6	0	-6.160460	3.996740	0.797200
38	1	0	-6.862750	4.731370	0.408880
39	6	0	-6.568160	2.682560	1.007550
40	1	0	-7.588700	2.381560	0.777550
41	16	0	-1.426590	-1.896040	0.449150
42	7	0	0.031500	-1.885250	2.792340
43	6	0	-0.232960	-2.398950	1.559570
44	7	0	0.598670	-3.481430	1.407950
45	6	0	1.367010	-3.641070	2.548080
46	1	0	2.105890	-4.425380	2.620720
47	6	0	1.003760	-2.654100	3.397850
48	1	0	1.358740	-2.411200	4.389520
49	6	0	1.260500	-3.542840	-0.927360
50	1	0	1.348980	-2.455440	-0.906150
51	6	0	0.829590	-4.218300	0.212460
52	6	0	0.723600	-5.606750	0.230350
53	1	0	0.381020	-6.108130	1.134150
54	6	0	1.052980	-6.330010	-0.912420
55	1	0	0.969860	-7.415080	-0.905170
56	6	0	1.485950	-5.666420	-2.058200
57	1	0	1.749080	-6.234580	-2.948620
58	6	0	1.587770	-4.276170	-2.064030
59	1	0	1.941350	-3.750080	-2.950430
60	6	0	1.669160	0.757410	2.338620
61	7	0	0.219050	-0.297470	-2.077430
62	16	0	1.302190	0.549830	-2.959140
63	8	0	0.763460	0.865640	-4.291950
64	8	0	1.792510	1.626150	-2.093050
65	6	0	2.654360	-0.587650	-3.218380
66	6	0	3.594970	-0.780640	-2.205740
67	6	0	2.697770	-1.354920	-4.381260
68	6	0	4.561230	-1.767540	-2.355990
69	1	0	3.560470	-0.154590	-1.313490
70	6	0	3.678050	-2.333550	-4.519030
71	1	0	1.977390	-1.162910	-5.174410
72	6	0	4.610820	-2.568880	-3.503830
73	1	0	5.294240	-1.923380	-1.564060

74	1	0	3.718650	-2.930930	-5.430740
75	6	0	5.611930	-3.676700	-3.623020
76	1	0	6.553580	-3.433390	-3.117810
77	1	0	5.233770	-4.600380	-3.161050
78	1	0	5.839210	-3.911730	-4.668940
79	6	0	-0.521920	-1.306520	-2.810850
80	6	0	-1.913790	-1.468850	-2.365650
81	1	0	-0.568680	-1.001860	-3.875340
82	1	0	-0.020730	-2.289370	-2.805510
83	1	0	-2.293830	-2.487910	-2.296190
84	6	0	-2.832230	-0.431690	-2.130290
85	6	0	-4.162090	-0.766120	-1.747340
86	6	0	-2.523480	0.944540	-2.339410
87	6	0	-5.145550	0.195200	-1.657280
88	1	0	-4.400140	-1.810370	-1.547740
89	6	0	-3.512200	1.906190	-2.267000
90	1	0	-1.509830	1.227500	-2.603900
91	6	0	-4.809990	1.518030	-1.953980
92	1	0	-6.171030	-0.048740	-1.391900
93	1	0	-3.297420	2.954520	-2.455060
94	9	0	-5.779020	2.440460	-1.951160

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^{3}IntD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.116260	0.031720	-0.158270
2	16	0	2.011780	-0.166560	0.982260
3	7	0	0.824660	0.506990	3.386830
4	5	0	-0.236330	-0.612470	3.582790
5	1	0	-0.272150	-0.823920	4.771550
6	7	0	2.326080	1.943720	2.688060
7	6	0	1.851590	2.408350	3.901810
8	1	0	2.207030	3.337620	4.322090
9	6	0	0.922740	1.518640	4.322170
10	1	0	0.307270	1.511220	5.210480
11	6	0	3.062640	2.864390	0.552420
12	1	0	2.145150	2.518690	0.086580
13	6	0	3.303660	2.623440	1.902950
14	6	0	4.474940	3.065380	2.515360
15	1	0	4.648060	2.853810	3.569710
16	6	0	5.420550	3.752420	1.759980
17	1	0	6.337960	4.097950	2.232780
18	6	0	5.200170	3.980160	0.403610

19	1	0	5.947830	4.507210	-0.186360
20	6	0	4.023910	3.533660	-0.195910
21	1	0	3.837090	3.701610	-1.254490
22	16	0	-1.201620	1.618520	1.108340
23	7	0	-1.662640	-0.125710	3.203940
24	6	0	-2.102690	0.786100	2.298140
25	7	0	-3.459960	0.914650	2.494660
26	6	0	-3.854200	0.049650	3.504660
27	1	0	-4.876820	0.021670	3.849270
28	6	0	-2.741500	-0.584410	3.933000
29	1	0	-2.606380	-1.316980	4.715300
30	6	0	-5.658160	1.314220	1.562550
31	1	0	-5.912520	0.278990	1.782640
32	6	0	-4.372120	1.783180	1.832370
33	6	0	-4.021720	3.097720	1.522600
34	1	0	-3.029590	3.467080	1.762450
35	6	0	-4.958490	3.928120	0.918030
36	1	0	-4.677820	4.947630	0.662380
37	6	0	-6.245500	3.470440	0.652150
38	1	0	-6.970290	4.125710	0.174330
39	6	0	-6.594440	2.164620	0.985590
40	1	0	-7.595870	1.793210	0.775240
41	16	0	-1.308070	-1.997110	0.587740
42	7	0	0.186390	-1.936790	2.913790
43	6	0	-0.102920	-2.463840	1.690980
44	7	0	0.771100	-3.509680	1.508090
45	6	0	1.585200	-3.635440	2.620310
46	1	0	2.353560	-4.392850	2.670840
47	6	0	1.218360	-2.658880	3.480530
48	1	0	1.607220	-2.394850	4.454030
49	6	0	1.202700	-3.613280	-0.889830
50	1	0	1.189170	-2.524040	-0.927310
51	6	0	0.962420	-4.267320	0.317840
52	6	0	0.997150	-5.656980	0.399870
53	1	0	0.798610	-6.144340	1.353220
54	6	0	1.276970	-6.403490	-0.741200
55	1	0	1.303930	-7.489630	-0.679940
56	6	0	1.514590	-5.761410	-1.953300
57	1	0	1.734810	-6.345440	-2.845110
58	6	0	1.474650	-4.369500	-2.024910
59	1	0	1.676330	-3.858060	-2.965110
60	6	0	1.694260	0.764500	2.371670
61	7	0	0.072220	-0.197700	-2.057350
62	16	0	1.259710	0.585540	-2.884400
63	8	0	0.768240	0.951920	-4.219750
64	8	0	1.788090	1.616620	-1.988410

65	6	0	2.552070	-0.618900	-3.131870
66	6	0	3.531870	-0.791050	-2.154850
67	6	0	2.532390	-1.426600	-4.268820
68	6	0	4.477160	-1.797900	-2.311410
69	1	0	3.547800	-0.129670	-1.288860
70	6	0	3.492010	-2.422650	-4.413480
71	1	0	1.782590	-1.251330	-5.038130
72	6	0	4.466010	-2.636810	-3.431610
73	1	0	5.242680	-1.936480	-1.547810
74	1	0	3.485810	-3.050250	-5.305350
75	6	0	5.448200	-3.759760	-3.561120
76	1	0	6.389330	-3.541270	-3.044320
77	1	0	5.048860	-4.684110	-3.119150
78	1	0	5.679780	-3.981880	-4.608980
79	6	0	-0.734710	-1.152870	-2.834770
80	6	0	-2.160600	-1.132340	-2.403180
81	1	0	-0.650010	-0.894660	-3.904460
82	1	0	-0.333140	-2.173730	-2.717200
83	1	0	-2.590480	-2.060900	-2.028580
84	6	0	-2.983300	0.018270	-2.428560
85	6	0	-4.305600	-0.047260	-1.917020
86	6	0	-2.548100	1.264970	-2.958550
87	6	0	-5.144570	1.051960	-1.931950
88	1	0	-4.662160	-0.992830	-1.507030
89	6	0	-3.379840	2.371110	-2.959550
90	1	0	-1.545240	1.350720	-3.372450
91	6	0	-4.666470	2.254420	-2.443510
92	1	0	-6.160720	0.999170	-1.550590
93	1	0	-3.047490	3.325850	-3.359640
94	9	0	-5.478950	3.333180	-2.448300

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[1]IntE

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.568270	8.728850	3.572210
2	16	0	2.647300	8.523680	4.547240
3	7	0	1.389970	9.288950	6.903170
4	5	0	0.313440	8.188740	7.120900
5	1	0	0.270190	7.981110	8.311560
6	7	0	2.773860	10.775900	6.084510
7	6	0	2.262860	11.301310	7.261030
8	1	0	2.544930	12.286220	7.603120
9	6	0	1.410460	10.376280	7.756200

10	1	0	0.791910	10.391650	8.642220
11	6	0	3.214260	11.691140	3.869870
12	1	0	2.273220	11.269530	3.519220
13	6	0	3.615830	11.499450	5.191480
14	6	0	4.800210	12.053070	5.669680
15	1	0	5.095380	11.882280	6.703890
16	6	0	5.597670	12.805390	4.810860
17	1	0	6.525380	13.238480	5.180030
18	6	0	5.214190	12.991340	3.485670
19	1	0	5.841520	13.576760	2.815920
20	6	0	4.023830	12.434380	3.018380
21	1	0	3.708120	12.583510	1.987500
22	16	0	-0.604020	10.550520	4.727080
23	7	0	-1.099820	8.666830	6.699580
24	6	0	-1.522630	9.528740	5.731110
25	7	0	-2.893180	9.384740	5.665260
26	6	0	-3.304160	8.419130	6.572910
27	1	0	-4.349120	8.172780	6.692310
28	6	0	-2.193920	7.994950	7.212750
29	1	0	-2.069680	7.263830	7.998790
30	6	0	-4.559810	9.112120	3.933750
31	1	0	-4.469630	8.034960	4.069010
32	6	0	-3.760000	9.962950	4.698010
33	6	0	-3.823130	11.344250	4.524180
34	1	0	-3.186710	11.989250	5.123710
35	6	0	-4.699220	11.869990	3.579950
36	1	0	-4.746460	12.947880	3.436530
37	6	0	-5.504690	11.029630	2.814650
38	1	0	-6.178670	11.449820	2.070570
39	6	0	-5.432170	9.650330	2.992230
40	1	0	-6.048500	8.986790	2.388520
41	16	0	-0.817880	6.796630	4.136450
42	7	0	0.708600	6.848050	6.446700
43	6	0	0.403540	6.327820	5.223420
44	7	0	1.269240	5.275410	5.026530
45	6	0	2.087940	5.132600	6.138360
46	1	0	2.854190	4.372380	6.176940
47	6	0	1.734680	6.106960	7.003720
48	1	0	2.134290	6.365870	7.974260
49	6	0	1.546420	5.127350	2.602810
50	1	0	1.512020	6.216170	2.541970
51	6	0	1.412460	4.501540	3.844010
52	6	0	1.481710	3.114010	3.951300
53	1	0	1.364980	2.646840	4.927910
54	6	0	1.680710	2.342240	2.810340
55	1	0	1.733160	1.258690	2.896380

56	6	0	1.798260	2.955360	1.566310
57	1	0	1.944720	2.351740	0.672260
58	6	0	1.729330	4.344750	1.467980
59	1	0	1.831650	4.831730	0.498820
60	6	0	2.238010	9.531870	5.867170
61	7	0	-0.181110	9.030620	1.580650
62	16	0	0.810530	9.964310	0.481010
63	8	0	0.137740	10.133640	-0.805360
64	8	0	1.275300	11.106380	1.259390
65	6	0	2.115130	8.784540	0.275710
66	6	0	3.141310	8.714140	1.215260
67	6	0	2.044350	7.891360	-0.791340
68	6	0	4.087900	7.702780	1.096430
69	1	0	3.190440	9.431060	2.033220
70	6	0	3.010570	6.899260	-0.901580
71	1	0	1.250780	7.991210	-1.528830
72	6	0	4.030300	6.774480	0.050340
73	1	0	4.880120	7.629200	1.841030
74	1	0	2.971050	6.200340	-1.737480
75	6	0	5.012930	5.648360	-0.025990
76	1	0	5.118570	5.265430	-1.047000
77	1	0	6.004450	5.946160	0.332380
78	1	0	4.685030	4.808910	0.603580
79	6	0	-1.114230	8.090100	0.928270
80	6	0	-1.657870	9.270640	1.617030
81	1	0	-1.113330	8.118260	-0.162580
82	1	0	-1.139000	7.105590	1.395960
83	1	0	-1.984960	9.123890	2.651300
84	6	0	-2.308190	10.410690	0.920360
85	6	0	-2.103470	11.712160	1.389770
86	6	0	-3.179290	10.199120	-0.149250
87	6	0	-2.744630	12.787770	0.788470
88	1	0	-1.438730	11.873710	2.238090
89	6	0	-3.840150	11.263770	-0.751720
90	1	0	-3.345540	9.186470	-0.515840
91	6	0	-3.607240	12.544230	-0.271010
92	1	0	-2.589350	13.807470	1.131950
93	1	0	-4.522520	11.117230	-1.584940
94	9	0	-4.245190	13.582010	-0.845640

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^{3}IntE

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

1	29	0	0.421030	8.749120	3.207310
2	16	0	2.514200	8.714010	4.192620
3	7	0	1.381320	9.316260	6.650460
4	5	0	0.361190	8.169320	6.867960
5	1	0	0.320960	7.983010	8.060840
6	7	0	2.751920	10.842130	5.884500
7	6	0	2.299130	11.284660	7.115930
8	1	0	2.613520	12.236640	7.517490
9	6	0	1.450890	10.338000	7.578270
10	1	0	0.869290	10.297040	8.488040
11	6	0	3.260590	11.886910	3.732790
12	1	0	2.315660	11.523430	3.333280
13	6	0	3.629190	11.592560	5.044750
14	6	0	4.827580	12.063430	5.576440
15	1	0	5.098620	11.811500	6.600570
16	6	0	5.669540	12.836530	4.782020
17	1	0	6.607470	13.204940	5.192970
18	6	0	5.316300	13.125660	3.466530
19	1	0	5.978480	13.726170	2.845770
20	6	0	4.114250	12.650820	2.943810
21	1	0	3.821520	12.865340	1.918790
22	16	0	-0.701430	10.555470	4.568310
23	7	0	-1.073970	8.543500	6.427710
24	6	0	-1.556880	9.448270	5.525920
25	7	0	-2.927780	9.272820	5.507770
26	6	0	-3.274920	8.253680	6.381140
27	1	0	-4.307810	7.981530	6.541380
28	6	0	-2.129190	7.817600	6.947150
29	1	0	-1.960090	7.053260	7.692160
30	6	0	-4.821290	9.109830	4.014920
31	1	0	-4.787540	8.029050	4.146960
32	6	0	-3.870130	9.909040	4.652260
33	6	0	-3.869530	11.290980	4.468940
34	1	0	-3.128000	11.902540	4.973430
35	6	0	-4.821050	11.865550	3.631980
36	1	0	-4.810520	12.942170	3.474040
37	6	0	-5.774220	11.076230	2.995060
38	1	0	-6.506550	11.534260	2.333320
39	6	0	-5.775700	9.697720	3.192290
40	1	0	-6.510810	9.071330	2.690230
41	16	0	-0.525740	6.681760	3.843400
42	7	0	0.840040	6.819980	6.250950
43	6	0	0.586200	6.229620	5.052630
44	7	0	1.397060	5.122720	4.983070
45	6	0	2.142250	5.021920	6.145000
46	1	0	2.857040	4.224710	6.286490

47	6	0	1.795560	6.077950	6.917020
48	1	0	2.147250	6.382650	7.892570
49	6	0	1.840650	4.723350	2.616370
50	1	0	1.963610	5.794970	2.466240
51	6	0	1.524630	4.228680	3.881070
52	6	0	1.381390	2.860870	4.101400
53	1	0	1.123360	2.501480	5.096370
54	6	0	1.551280	1.974780	3.041680
55	1	0	1.437160	0.905850	3.210130
56	6	0	1.854120	2.457280	1.771740
57	1	0	1.980850	1.764210	0.942360
58	6	0	1.997890	3.828260	1.564760
59	1	0	2.242990	4.213260	0.576280
60	6	0	2.183760	9.629520	5.601140
61	7	0	-0.621500	9.059220	1.654610
62	16	0	1.375820	10.510190	0.265790
63	8	0	0.624950	10.440620	-1.016680
64	8	0	2.246630	11.685850	0.569060
65	6	0	2.450010	9.065130	0.286510
66	6	0	3.598240	9.071880	1.074640
67	6	0	2.075950	7.931300	-0.430370
68	6	0	4.386370	7.928370	1.127820
69	1	0	3.869800	9.967030	1.631120
70	6	0	2.885310	6.801770	-0.375540
71	1	0	1.183210	7.955590	-1.051050
72	6	0	4.046290	6.777760	0.406470
73	1	0	5.287560	7.929620	1.741040
74	1	0	2.622150	5.924880	-0.968730
75	6	0	4.898790	5.548380	0.486610
76	1	0	4.691150	4.854810	-0.336390
77	1	0	5.966990	5.793440	0.459660
78	1	0	4.721730	5.000470	1.422780
79	6	0	-1.286910	8.222500	0.691710
80	6	0	-2.044700	9.202820	1.509660
81	1	0	-1.085560	8.468460	-0.355800
82	1	0	-1.362540	7.152540	0.910140
83	1	0	-2.633320	8.787080	2.339950
84	6	0	-2.591530	10.473250	0.950340
85	6	0	-1.936280	11.688170	1.161960
86	6	0	-3.792410	10.469260	0.236590
87	6	0	-2.464490	12.879500	0.675810
88	1	0	-1.000100	11.691560	1.719610
89	6	0	-4.335180	11.649530	-0.260200
90	1	0	-4.310760	9.524880	0.067310
91	6	0	-3.659310	12.838900	-0.027620
92	1	0	-1.961080	13.830990	0.827350

93	1	0	-5.263540	11.660560	-0.826530
94	9	0	-4.181280	13.988420	-0.503590
