General. All manipulations were carried out under an inert atmosphere of dry nitrogen using standard Schlenk techniques or in an inert-atmosphere glove-box. Solvents were dried form the appropriate drying agent, distilled, degassed and stored over 4 Å molecular sieves. ^{1}H and ^{13}C NMR spectra were recorded on Varian 400 and 500 MHz spectrometers. The solution-phase ^{31}P and ^{77}Se spectra were recorded on a Varian 400 MHz spectrometer that was equipped with a X{^{1}H} broadband-observe probe. All spectra were recorded in C_6D_6 at 300 K, unless stated otherwise. The ^{1}H and ^{13}C NMR chemical shifts are were measured relative to residual solvent peaks and reported relative to Me_4Si; ^{31}P and ^{77}Se were externally referenced to H_3PO_4(aq) and Me_2Se, respectively. The data for the X-ray structures were collected at 173 K on a Nonius Kappa CCD diffractometer [λ (Mo, Kα) 0.71073 Å] and refined using the SHELXL-97 software package.[1] [Ge(BDI)(PCy_2)] (**1**) was made according to published procedures.[2]

[CH{$(CH_3)_2$CN-2,6-i$Pr_2C_6H_3$}$_2$GeSeP$(C_6H_{11})_2$], (2). Selenium (0.02 g, 0.291 mmol), finely suspended in toluene, was added dropwise to a solution of β-diketiminate germanium dicyclohexylphosphide (0.20 g, 0.291 mmol) in toluene (5 mL), and the mixture was stirred for 24 hrs at room temperature resulting in the colour changing from purple to orange. The solvent was filtered, concentrated in vacuo and stored at -27°C for 24 hrs yielding [Ge(L)SeP$(C_6H_{10})_2$], (0.05 g, 21%, first crop) as orange crystals. ^{1}H NMR (C_6D_6, 293 K): δ 7.13 (dd, *J* = 7.6 Hz, 2H, m-*H*), 7.08 (t, *J* = 7.6 Hz, 2H, p-*H*), 7.00 (dd, *J* = 7.6 Hz, 2H, m-*H*), 4.65 (s, 1H, γ-C*H*), 3.64 (septet, *J* = 6.8 Hz, 2H, C*H*Me_2), 3.28 (septet, *J* = 6.8 Hz, 2H, C*H*Me_2), 1.61 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$), 1.57-1.54 (br, 4H, Cy-CH_2), 1.50 (s, 6H, NC*Me*), 1.44-1.40 (br, 6H, Cy-CH_2), 1.37 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$), 1.15 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$), 1.10 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$), 1.08-0.96 (br, 10H, Cy-CH_2), 0.67 (br, 2H, Cy-CH_2). ^{13}C{^{1}H} NMR (100.46 MHz, C_6D_6, 293 K): δ 165.2 (N*C*Me), 144.9 (*ipso-C*), 143.9 (*o*-C*),* 140.0 (*o-C*), 126.5 (*p*-C*),* 124.3 (*m-C*), 123.8 (*m-C*), 95.8 (γ-*C*H), 34.9 (Cy-*C*H2), 34.6 (Cy-*C*H2), 29.8 (d, J_{CP} = 18.1 Hz, Cy-*C*H), 29.2 (d, J_{CP} = 7.0 Hz, CH*Me*$_2$), 29.1 (Cy-*C*H2), 28.5 (*C*HMe_2), 27.3 (*C*HMe_2), 27.2 (P*Cy*), 27.2 (P*Cy*), 27.1 (CH*Me*$_2$), 26.7 (P*Cy*), 26.6 (P*Cy*), 26.5 (P*Cy*), 24.9 (P*Cy*), 24.4 (CH*Me*$_2$), 24.2 (CH*Me*$_2$), 22.7 (NC*Me*). ^{31}P{^{1}H} NMR (161.72 MHz, C_6D_6, 293 K): δ 42 (J_{PSe} = 198 Hz). ^{77}Se {^{1}H} NMR (76.19 MHz, C_6D_6, 293 K): -19.3 (J_{SeP} = 198 Hz). IR (Nujol,

cm^{-1}) 1556 (s), 1317 (s), 1172 (s), 1099 (s), 1016 (s), 848 (s), 798 (s), 722 (s), 518 (s). Anal. calc. for $C_{41}H_{63}N_2PSeGe$: C, 64.24; H, 8.28; N, 3.65. Found: C, 65.46; H, 8.00; N, 3.18%.

[CH{(CH$_3$)CN-2,6-^{i}Pr$_2$C$_6$H$_3$}$_2$GeSeP(=Se)(C$_6$H$_{11}$)$_2$], (3).

[(BDI)GePCy$_2$] (**1**) (0.19 g, 0.27 mmol) in toluene (10 mL) was added to an excess of elemental selenium (0.09 g, 1.10 mmol) suspended in toluene (5mL). The mixture was stirred rapidly at room temperature for 20 h, then filtered through a pad of Celite. Volatiles were removed from filtrate under vacuum. The yellow solid residue was washed with cold pentane (3 x ~ 3 mL). Single crystals of [(BDI^{DIPP})GeSeP(Se)Cy$_2$] (**4**) were found along with crystals of [(BDI^{DIPP})Ge(Se)PCy$_2$] (**3**) and separated from a concentrated toluene solution at −30 °C. Yield: 0.15 g, 64% (combined yield with **4**). ^{1}H NMR (399.50 MHz, C$_6$D$_6$, 303K): δ 7.12 (br, 6H, Ar-*H*), 4.68 (s, 1H, γ-C*H*), 3.50 (septet, *J* = 6.8 Hz, 2H, C*H*Me$_2$), 3.31 (septet, *J* = 6.8, 2H, C*H*Me$_2$), 1.74 (br, 2H, Cy-C*H*$_2$), 1.67 (d, *J* = 6.4 Hz, 8H, CH*Me*$_2$ and Cy-C*H*$_2$), 1.59 (d, *J* = 6.4 Hz, 8H, CH*Me*$_2$ and Cy-C*H*$_2$), 1.53 (s, 12H, 287 NC*Me*, Cy-C*H*$_2$), 1.16 (d, *J* = 6.4 Hz, 6H, CH*Me*$_2$), 1.13 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$), 1.03 (br, 6H, Cy-C*H*$_2$, Cy-C*H*). ^{13}C{^{1}H} NMR (100.46 MHz, C$_6$D$_6$, 303K): δ 166.2 (N*C*Me), 146.3 (*ipso*-C), 144.2 (*o*-C), 140.6 (*o*-C), 127.4 (*p*-C), 125.4 (*m*-C), 124.3 (*m*- C), 96.5 (γ-*C*H), 43.1 (d, J_{CP} = 38 Hz, Cy-*C*H), 29.8, 27.1 (*C*HMe$_2$), 26.9, 26.7 (Cy-*C*H$_2$), 26.6, 25.7, 24.9, 23.6 (CH*Me*$_2$), 21.8 (NC*Me*). ^{31}P{^{1}H} NMR (161.72 MHz, C$_6$D$_6$, 303K): δ 63.7 (J_{PSe} = 551 Hz). ^{77}Se NMR (76.19 MHz, C$_6$D$_6$, 303K): δ −18 (d, J_{SeP} = 198 Hz).

[CH{(CH$_3$)CN-2,6-^{i}Pr$_2$C$_6$H$_3$}$_2$Ge(Se)P(C$_6$H$_{11}$)$_2$], (4).

Compound **4** was co-crystallised from the synthesis of [(BDI^{DIPP})GeSeP(Se)Cy$_2$] (**2**). ^{1}H NMR (399.50 MHz, CDCl$_3$, 303K): δ 7.32 (d, J = 4.8 Hz, 3H, Ar-*H*), 7.19 (br, 3H, Ar-*H*), 5.45 (s, 1H, γ-C*H*), 4.01 (septet, J = 6.4 Hz, 2H, C*H*Me$_2$), 3.53 (septet, J = 6.8 Hz, 2H, C*H*Me$_2$), 2.24 (br, 3H, Cy-C*H*$_2$), 1.91 (s, 6H, NC*Me*), 1.45 (d, J 289 = 7.2 Hz, 6H, CH*Me*$_2$), 1.43 (d, J = 6.8 Hz, 6H, CH*Me*$_2$), 1.26–1.35 (br, 6H, Cy-C*H*$_2$), 1.21 (d, J = 6.8 Hz, 6H, CH*Me*$_2$), 1.10–1.14 (br, 3H, Cy-C*H*$_2$), 1.06 (d, J = 6.8 Hz, 6H, CH*Me*$_2$), 0.66–0.87 (br, 14H, Cy-C*H*$_2$). ^{13}C{^{1}H} NMR (100.46 MHz, CDCl$_3$, 303K): δ 167.3 (N*C*Me), 148.1 (ipso-*C*), 144.6 (o-*C*), 139.4 (o-*C*), 128.6 (p-*C*), 126.4 (m-*C*), 124.2 (m-*C*), 98.9 (γ-*C*H), 34.5 (d, J_{CP} = 16 Hz, Cy-*C*H), 34.3 (*C*HMe$_2$), 32.0 (*C*HMe$_2$), 29.7 (CH*Me*$_2$), 29.1, 27.9, 27.7, 27.4, 26.5 (Cy-*C*H$_2$), 25.5, 25.2, 24.4

(CH*Me*$_2$), 21.7 (NC*Me*). $^{31}P\{^1H\}$ NMR (161.72 MHz, $CDCl_3$, 303K): δ 0.7. ^{77}Se NMR (76.19 MHz, $CDCl_3$, 303K): δ −91 (d, J_{SeP} = 12 Hz).

1. G. M. Sheldrick, *SHELXL-97, Program for the Refinement of Crystal Structures*, Göttingen, 1997.
2. E. C. Y. Tam, N. A. Maynard, D. C. Apperley, J. D. Smith, M. P. Coles and J. R. Fulton, *Inorg Chem*, 2012, **51**, 9403.

Computational. All calculations were carried out using the B3LYP[3-6] density functional and the TZVP basis set[7] with the Gaussian 09 suite of programs[8]. All stationary points were confirmed to be minima through the calculation of the force-constants. Energies reported are pure electronic energies (without ZPVE correction) and thermodynamic free energies (ΔG). All energy values are reported in kJ/mol. The Natural Bonding Orbital (NBO) analysis[9,10] carried out is based on the NBO 3.1 implementation included in Gaussian09. The Wiberg bond indices[11] discussed in the manuscript were calculated with the same program.

3. A.D. Becke, *J.Chem.Phys.* 1993, **98** 5648
4. C. Lee, W. Yang, R.G. Parr, *Phys. Rev. B*, 1988, **37**, 785
5. S.H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.* 1980, **58**, 1200
6. P.J. Stephens, F.J. Devlin, C.F. Chabalowski, M.J. Frisch, *J.Phys.Chem.* , 1994, **98**, 11623
7. A. Schaefer, C. Huber, and R. Ahlrichs, *J. Chem. Phys*., 1994, **100**, 5829
8. Gaussian 09, Revision B.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
9. A. E. Reed, R. B. Weinstock, and F. Weinhold, *J. Chem. Phys.*, 1985, **83**, 735
10. A. E. Reed, L. A. Curtiss, and F. Weinhold, *Chem. Rev*., 1988, **88**, 899
11. K. B. Wiberg, *Tetrahedron*, 1968, **24**, 1083

Compound **1**

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

1	32	0	-0.138482	-0.398821	-0.964741
2	15	0	0.043534	1.515084	0.702420
3	7	0	-1.635232	-1.628603	-0.130464
4	7	0	1.307326	-1.777756	-0.260372
5	6	0	-1.492476	-2.948166	-0.203385
6	6	0	-0.270032	-3.599072	-0.413422
7	1	0	-0.324357	-4.675338	-0.483147
8	6	0	1.024809	-3.074048	-0.301421
9	6	0	-2.697659	-3.857559	-0.074861
10	1	0	-3.435719	-3.476095	0.625565
11	1	0	-2.391167	-4.854117	0.236301
12	1	0	-3.190376	-3.946277	-1.046059
13	6	0	2.119489	-4.112166	-0.166273
14	1	0	3.101382	-3.731895	-0.430781
15	1	0	1.885089	-4.971168	-0.795166
16	1	0	2.165408	-4.468386	0.864992
17	6	0	-2.932556	-1.084610	0.170652
18	6	0	-3.248156	-0.764018	1.509584
19	6	0	-4.516166	-0.251563	1.783014
20	1	0	-4.782031	-0.007183	2.803449
21	6	0	-5.445153	-0.044042	0.773888
22	1	0	-6.422894	0.359171	1.009309
23	6	0	-5.117654	-0.355338	-0.535969
24	1	0	-5.848618	-0.189792	-1.317938
25	6	0	-3.868461	-0.883420	-0.867657
26	6	0	-2.266621	-1.005947	2.652492
27	1	0	-1.273774	-1.091653	2.211225
28	6	0	-2.571999	-2.325877	3.385779
29	1	0	-1.852183	-2.485395	4.192560
30	1	0	-2.519781	-3.187817	2.719914
31	1	0	-3.571160	-2.305028	3.828954
32	6	0	-2.216252	0.152439	3.659042
33	1	0	-1.431360	-0.034380	4.395392
34	1	0	-3.155016	0.262174	4.207279
35	1	0	-1.985204	1.095726	3.164933
36	6	0	-3.577312	-1.221637	-2.328608
37	1	0	-2.618082	-1.738100	-2.370743
38	6	0	-4.638781	-2.160014	-2.930768
39	1	0	-4.788924	-3.052606	-2.321181
40	1	0	-4.334058	-2.479346	-3.930162
41	1	0	-5.606333	-1.662709	-3.027943
42	6	0	-3.444527	0.040995	-3.198007
43	1	0	-2.628916	0.678585	-2.856113
44	1	0	-4.364568	0.630251	-3.184966

45	1	0	-3.236789	-0.235709	-4.234612
46	6	0	2.663034	-1.353633	-0.038644
47	6	0	3.149231	-1.217834	1.280481
48	6	0	4.453702	-0.755108	1.458206
49	1	0	4.842451	-0.638899	2.462544
50	6	0	5.268388	-0.453325	0.377524
51	1	0	6.278015	-0.095566	0.540005
52	6	0	4.790193	-0.628298	-0.911957
53	1	0	5.441584	-0.418214	-1.751557
54	6	0	3.492300	-1.082700	-1.150854
55	6	0	2.331054	-1.608571	2.508316
56	1	0	1.362409	-1.967985	2.161152
57	6	0	3.006709	-2.754441	3.285714
58	1	0	2.352733	-3.102322	4.088902
59	1	0	3.942668	-2.425105	3.742974
60	1	0	3.237513	-3.605574	2.643593
61	6	0	2.064972	-0.424137	3.450330
62	1	0	1.500438	-0.761556	4.323430
63	1	0	1.482170	0.354315	2.958201
64	1	0	2.997284	0.016518	3.811879
65	6	0	3.052777	-1.343142	-2.590629
66	1	0	2.000915	-1.627976	-2.574669
67	6	0	3.839958	-2.513186	-3.210964
68	1	0	3.745089	-3.426508	-2.622241
69	1	0	4.903982	-2.277211	-3.289205
70	1	0	3.470947	-2.723898	-4.217647
71	6	0	3.169054	-0.101357	-3.487103
72	1	0	2.801608	-0.329448	-4.490370
73	1	0	4.204278	0.234174	-3.583254
74	1	0	2.581429	0.728896	-3.097351
75	6	0	-1.063003	2.830105	-0.148104
76	1	0	-0.753171	2.927870	-1.194206
77	6	0	-0.908950	4.204901	0.533685
78	1	0	0.126498	4.541659	0.505268
79	1	0	-1.170306	4.102556	1.593155
80	6	0	-1.800728	5.277063	-0.109842
81	1	0	-1.677713	6.225119	0.422880
82	1	0	-1.466086	5.453717	-1.139153
83	6	0	-3.272674	4.859649	-0.123210
84	1	0	-3.878497	5.610579	-0.639221
85	1	0	-3.643614	4.813030	0.907617
86	6	0	-3.442525	3.488716	-0.781506
87	1	0	-3.194945	3.567099	-1.847026
88	1	0	-4.486176	3.165924	-0.727426
89	6	0	-2.543458	2.429575	-0.129659

90	1	0	-2.864387	2.276101	0.905467
91	1	0	-2.689738	1.477417	-0.635504
92	6	0	1.806123	2.153421	0.259903
93	1	0	2.409681	1.244500	0.207572
94	6	0	2.394314	3.000631	1.409109
95	1	0	2.338761	2.442164	2.345169
96	1	0	1.790685	3.900407	1.557509
97	6	0	3.846868	3.415569	1.133511
98	1	0	4.209948	4.051161	1.947284
99	1	0	4.480267	2.521866	1.126461
100	6	0	3.986033	4.139231	-0.209021
101	1	0	3.445895	5.092824	-0.165344
102	1	0	5.034627	4.385194	-0.401925
103	6	0	3.421558	3.289580	-1.351397
104	1	0	4.034878	2.389734	-1.465449
105	1	0	3.485107	3.835209	-2.298255
106	6	0	1.964523	2.882578	-1.085090
107	1	0	1.596320	2.255818	-1.901057
108	1	0	1.349953	3.786532	-1.097284

Compound **2**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	34	0	0.089953	0.881948	0.763944
2	32	0	-0.086893	-0.947932	-0.929161
3	15	0	0.429482	2.530367	-0.826470
4	7	0	-1.765423	-1.970490	-0.225475
5	7	0	1.119384	-2.406717	-0.051318
6	6	0	-1.768623	-3.298267	-0.191472
7	6	0	-0.606304	-4.084092	-0.199323
8	1	0	-0.767870	-5.151882	-0.201300
9	6	0	0.726263	-3.675712	-0.039109
10	6	0	-3.077403	-4.059312	-0.182626
11	1	0	-3.884980	-3.497875	0.278150
12	1	0	-2.964586	-5.014494	0.327249
13	1	0	-3.371798	-4.266366	-1.215423
14	6	0	1.742052	-4.787690	0.114698
15	1	0	2.105685	-5.074537	-0.875972
16	1	0	1.286103	-5.666063	0.567956
17	1	0	2.605527	-4.486831	0.701112
18	6	0	-2.988710	-1.221273	-0.108692
19	6	0	-3.432277	-0.821245	1.171826

20	6	0	-4.610911	-0.081530	1.260368
21	1	0	-4.972700	0.226728	2.232972
22	6	0	-5.327519	0.276172	0.127474
23	1	0	-6.238009	0.856078	0.220238
24	6	0	-4.871720	-0.109876	-1.122024
25	1	0	-5.434722	0.173897	-2.002792
26	6	0	-3.705076	-0.863279	-1.269816
27	6	0	-2.687291	-1.201076	2.447700
28	1	0	-1.682418	-1.508029	2.156110
29	6	0	-3.351639	-2.394020	3.160613
30	1	0	-2.792138	-2.655893	4.062180
31	1	0	-3.394796	-3.280342	2.527312
32	1	0	-4.373467	-2.148078	3.461005
33	6	0	-2.541605	-0.025055	3.425411
34	1	0	-1.895779	-0.313326	4.258255
35	1	0	-3.502802	0.272738	3.850772
36	1	0	-2.095937	0.840503	2.936319
37	6	0	-3.273031	-1.278251	-2.673023
38	1	0	-2.382033	-1.900093	-2.581392
39	6	0	-4.349464	-2.121162	-3.379955
40	1	0	-3.976080	-2.481458	-4.341581
41	1	0	-5.251444	-1.536947	-3.575399
42	1	0	-4.641367	-2.987506	-2.783632
43	6	0	-2.890824	-0.064486	-3.536680
44	1	0	-2.547156	-0.393255	-4.520618
45	1	0	-2.088205	0.513588	-3.077420
46	1	0	-3.744476	0.600982	-3.686233
47	6	0	2.488815	-2.052709	0.216014
48	6	0	2.880578	-1.767643	1.543443
49	6	0	4.209556	-1.416824	1.778000
50	1	0	4.532077	-1.203061	2.788921
51	6	0	5.127749	-1.326290	0.741876
52	1	0	6.154162	-1.046946	0.947557
53	6	0	4.724332	-1.590199	-0.556337
54	1	0	5.444959	-1.513714	-1.361376
55	6	0	3.409230	-1.958476	-0.848729
56	6	0	1.911126	-1.864049	2.717437
57	1	0	0.901900	-1.845728	2.304754
58	6	0	2.031006	-0.679407	3.688268
59	1	0	1.232320	-0.728374	4.432238
60	1	0	1.945031	0.271361	3.163143
61	1	0	2.978727	-0.692177	4.231635
62	6	0	2.077262	-3.188216	3.486558
63	1	0	1.907514	-4.057823	2.851452
64	1	0	1.365485	-3.236999	4.314477

65	1	0	3.083470	-3.271377	3.905502
66	6	0	3.036354	-2.254000	-2.298474
67	1	0	1.996125	-2.580218	-2.319751
68	6	0	3.134936	-0.997626	-3.180313
69	1	0	2.823702	-1.227136	-4.202474
70	1	0	4.159734	-0.620462	-3.219756
71	1	0	2.494833	-0.197516	-2.806892
72	6	0	3.885999	-3.391858	-2.891943
73	1	0	3.532888	-3.643320	-3.894938
74	1	0	3.838606	-4.294373	-2.279934
75	1	0	4.936816	-3.105810	-2.975581
76	6	0	-0.894243	3.812996	-0.368039
77	1	0	-0.623092	4.662648	-1.008983
78	6	0	-0.934633	4.300000	1.086428
79	1	0	-1.135653	3.444924	1.739566
80	1	0	0.036416	4.700883	1.386502
81	6	0	-2.018175	5.367794	1.299654
82	1	0	-1.752445	6.270622	0.736349
83	1	0	-2.047809	5.658259	2.354218
84	6	0	-3.395685	4.877412	0.843817
85	1	0	-3.714960	4.050403	1.488442
86	1	0	-4.138980	5.671476	0.962111
87	6	0	-3.358295	4.394943	-0.609428
88	1	0	-3.158815	5.248938	-1.268174
89	1	0	-4.334386	3.997155	-0.902049
90	6	0	-2.279509	3.324862	-0.822636
91	1	0	-2.546925	2.426381	-0.258346
92	1	0	-2.244642	3.033743	-1.876055
93	6	0	2.016197	3.346976	-0.171636
94	1	0	1.902028	3.526196	0.901963
95	6	0	2.261713	4.693831	-0.877143
96	1	0	2.285155	4.532957	-1.961964
97	1	0	1.441740	5.388626	-0.683008
98	6	0	3.583648	5.338608	-0.434079
99	1	0	3.741361	6.269737	-0.986654
100	1	0	3.509749	5.613803	0.624580
101	6	0	4.773958	4.395352	-0.626888
102	1	0	4.926512	4.221545	-1.698819
103	1	0	5.690375	4.861770	-0.253417
104	6	0	4.531777	3.054170	0.071158
105	1	0	4.502650	3.210254	1.155999
106	1	0	5.362116	2.368675	-0.121022
107	6	0	3.216061	2.409880	-0.382227
108	1	0	3.055503	1.472074	0.151457
109	1	0	3.289345	2.157373	-1.446789

Compound **3**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	34	0	0.259553	0.583560	0.959728
2	34	0	1.244637	1.872769	-2.493737
3	32	0	-0.527075	-1.004392	-0.866455
4	15	0	1.277330	2.165672	-0.363914
5	7	0	-2.466541	-1.347735	-0.170051
6	7	0	0.067614	-2.805506	0.007549
7	6	0	-2.949108	-2.585684	-0.151274
8	6	0	-2.149725	-3.738216	-0.165475
9	1	0	-2.687564	-4.674773	-0.183966
10	6	0	-0.761425	-3.844520	0.002512
11	6	0	-4.443923	-2.826486	-0.158167
12	1	0	-5.006810	-1.988436	0.241522
13	1	0	-4.691335	-3.727848	0.400323
14	1	0	-4.768615	-2.978421	-1.191440
15	6	0	-0.223818	-5.253299	0.138350
16	1	0	0.719029	-5.293122	0.675575
17	1	0	-0.048538	-5.659500	-0.861814
18	1	0	-0.949584	-5.896420	0.633263
19	6	0	-3.335903	-0.206057	-0.046849
20	6	0	-3.625831	0.304581	1.238804
21	6	0	-4.450597	1.424860	1.332682
22	1	0	-4.692384	1.826394	2.308463
23	6	0	-4.964796	2.041403	0.201003
24	1	0	-5.599277	2.914303	0.297962
25	6	0	-4.663644	1.535070	-1.052129
26	1	0	-5.069155	2.019669	-1.931749
27	6	0	-3.854307	0.407171	-1.206462
28	6	0	-3.102994	-0.349172	2.514534
29	1	0	-2.272525	-0.996682	2.230774
30	6	0	-2.564802	0.669338	3.531160
31	1	0	-2.086774	0.146273	4.362826
32	1	0	-3.363210	1.283932	3.953256
33	1	0	-1.825562	1.327965	3.076515
34	6	0	-4.175029	-1.231495	3.181892
35	1	0	-3.772297	-1.700893	4.082967
36	1	0	-4.525185	-2.024850	2.521710
37	1	0	-5.042250	-0.634207	3.474946
38	6	0	-3.598867	-0.122086	-2.614501

39	1	0	-2.976982	-1.014193	-2.532440
40	6	0	-2.831811	0.889715	-3.481741
41	1	0	-2.631065	0.463248	-4.467744
42	1	0	-1.874615	1.163966	-3.036585
43	1	0	-3.411108	1.804605	-3.628785
44	6	0	-4.907608	-0.541440	-3.308794
45	1	0	-4.690938	-0.999941	-4.276604
46	1	0	-5.555883	0.318816	-3.489857
47	1	0	-5.472558	-1.259764	-2.711857
48	6	0	1.470458	-2.975595	0.287322
49	6	0	1.923205	-2.884855	1.623247
50	6	0	3.287373	-3.036027	1.869083
51	1	0	3.653567	-2.978523	2.886097
52	6	0	4.188749	-3.252440	0.836767
53	1	0	5.245120	-3.361947	1.051161
54	6	0	3.731505	-3.326117	-0.468120
55	1	0	4.439826	-3.494685	-1.269887
56	6	0	2.374665	-3.195075	-0.772903
57	6	0	0.970780	-2.668215	2.795381
58	1	0	0.035518	-2.284477	2.386053
59	6	0	0.654067	-3.988566	3.523065
60	1	0	-0.038339	-3.808998	4.349381
61	1	0	1.563210	-4.430684	3.938664
62	1	0	0.198013	-4.724965	2.861489
63	6	0	1.490400	-1.632745	3.804697
64	1	0	1.753029	-0.697084	3.312034
65	1	0	2.366199	-1.996859	4.346680
66	1	0	0.717906	-1.419252	4.547327
67	6	0	1.937499	-3.322701	-2.229026
68	1	0	0.851391	-3.230956	-2.265060
69	6	0	2.298391	-4.700606	-2.813446
70	1	0	1.893434	-4.799466	-3.823409
71	1	0	1.901010	-5.516663	-2.207125
72	1	0	3.380414	-4.835197	-2.878428
73	6	0	2.518719	-2.200259	-3.104762
74	1	0	2.152467	-2.295438	-4.130032
75	1	0	3.609996	-2.248992	-3.137212
76	1	0	2.235620	-1.211989	-2.740480
77	6	0	0.459402	3.791790	0.119689
78	1	0	1.045633	4.522008	-0.449607
79	6	0	0.558263	4.126140	1.616639
80	1	0	0.036385	3.355799	2.192192
81	1	0	1.597953	4.121295	1.951443
82	6	0	-0.067201	5.496609	1.918511
83	1	0	-0.018718	5.689634	2.994064

84	1	0	0.528728	6.279329	1.434537
85	6	0	-1.513635	5.583880	1.424121
86	1	0	-2.133548	4.885667	1.998111
87	1	0	-1.915317	6.584305	1.609135
88	6	0	-1.610479	5.236230	-0.064223
89	1	0	-1.095155	6.005865	-0.650957
90	1	0	-2.654524	5.244891	-0.388920
91	6	0	-0.993927	3.865371	-0.371087
92	1	0	-1.581381	3.084602	0.121054
93	1	0	-1.029784	3.665257	-1.442791
94	6	0	3.028286	2.245246	0.326033
95	1	0	2.891787	2.321421	1.410455
96	6	0	3.788899	3.483558	-0.180249
97	1	0	3.259983	4.401877	0.084589
98	1	0	3.833262	3.447537	-1.272643
99	6	0	5.212774	3.535075	0.393557
100	1	0	5.737692	4.401822	-0.018207
101	1	0	5.161216	3.688773	1.478104
102	6	0	5.992123	2.250150	0.102326
103	1	0	6.152092	2.162745	-0.978378
104	1	0	6.983140	2.297124	0.562984
105	6	0	5.229019	1.019750	0.600086
106	1	0	5.175943	1.043698	1.695136
107	1	0	5.766315	0.104834	0.336191
108	6	0	3.809839	0.958856	0.021164
109	1	0	3.279861	0.093231	0.421091
110	1	0	3.861783	0.828510	-1.063505

Compound **4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	34	0	-0.292657	-0.086157	-2.846000
2	32	0	-0.120914	-0.348534	-0.626059
3	15	0	0.090239	1.544222	0.878640
4	7	0	-1.626845	-1.546869	0.078190
5	7	0	1.291217	-1.726910	-0.161123
6	6	0	-1.506430	-2.866935	-0.051762
7	6	0	-0.306392	-3.522601	-0.352217
8	1	0	-0.390174	-4.589750	-0.495986
9	6	0	0.991810	-3.024100	-0.308433
10	6	0	-2.692871	-3.788063	0.136471
11	1	0	-3.534948	-3.308589	0.623777

12	1	0	-2.394083	-4.660578	0.716567
13	1	0	-3.022079	-4.144955	-0.841947
14	6	0	2.090483	-4.054574	-0.440563
15	1	0	2.325987	-4.182581	-1.499782
16	1	0	1.756599	-5.016329	-0.055916
17	1	0	3.005827	-3.765933	0.067574
18	6	0	-2.898673	-0.987107	0.497934
19	6	0	-3.078078	-0.677179	1.865125
20	6	0	-4.304516	-0.150038	2.269922
21	1	0	-4.460961	0.091640	3.312699
22	6	0	-5.331288	0.065280	1.364380
23	1	0	-6.275637	0.477630	1.699315
24	6	0	-5.145296	-0.257524	0.031424
25	1	0	-5.955327	-0.098163	-0.669026
26	6	0	-3.942119	-0.792267	-0.435824
27	6	0	-2.012056	-0.964841	2.917354
28	1	0	-1.051195	-1.009457	2.406487
29	6	0	-2.251209	-2.332529	3.584816
30	1	0	-1.470009	-2.538532	4.320856
31	1	0	-2.250418	-3.147466	2.860523
32	1	0	-3.212893	-2.348357	4.103890
33	6	0	-1.904257	0.130164	3.987654
34	1	0	-1.053775	-0.074644	4.640675
35	1	0	-2.792580	0.173713	4.621580
36	1	0	-1.748128	1.110287	3.537484
37	6	0	-3.857393	-1.163993	-1.915066
38	1	0	-2.858104	-1.546998	-2.119939
39	6	0	-4.884649	-2.252534	-2.283986
40	1	0	-4.819963	-3.126235	-1.635307
41	1	0	-4.722601	-2.582042	-3.312864
42	1	0	-5.906703	-1.871759	-2.218494
43	6	0	-4.058842	0.051881	-2.835057
44	1	0	-3.975207	-0.259821	-3.878413
45	1	0	-3.298654	0.811496	-2.664706
46	1	0	-5.046111	0.500031	-2.697472
47	6	0	2.653740	-1.347281	0.154900
48	6	0	3.021081	-1.273463	1.519334
49	6	0	4.324461	-0.892293	1.836813
50	1	0	4.622961	-0.831949	2.875669
51	6	0	5.250733	-0.601308	0.847232
52	1	0	6.257506	-0.302671	1.113938
53	6	0	4.886506	-0.712351	-0.483931
54	1	0	5.622894	-0.511023	-1.251739
55	6	0	3.598470	-1.098085	-0.865659
56	6	0	2.074815	-1.669881	2.649457

57	1	0	1.071718	-1.745173	2.231943
58	6	0	2.020766	-0.638646	3.785578
59	1	0	1.310102	-0.964340	4.548316
60	1	0	1.696262	0.336491	3.423210
61	1	0	2.988600	-0.518852	4.276790
62	6	0	2.445652	-3.055787	3.211773
63	1	0	2.439146	-3.824770	2.438568
64	1	0	1.734976	-3.353560	3.986517
65	1	0	3.442655	-3.042080	3.658969
66	6	0	3.319467	-1.290590	-2.353737
67	1	0	2.275591	-1.578760	-2.473665
68	6	0	4.204990	-2.404077	-2.947557
69	1	0	3.902885	-2.608457	-3.977253
70	1	0	4.138124	-3.335445	-2.384421
71	1	0	5.256713	-2.108178	-2.965758
72	6	0	3.516284	-0.000339	-3.163967
73	1	0	3.279241	-0.185213	-4.213730
74	1	0	4.548674	0.354880	-3.110937
75	1	0	2.854232	0.790244	-2.818467
76	6	0	-0.977599	2.852535	-0.008720
77	1	0	-0.595808	2.966801	-1.026230
78	6	0	-0.859378	4.199205	0.735324
79	1	0	-1.186681	4.064039	1.772769
80	1	0	0.176568	4.534002	0.779286
81	6	0	-1.710825	5.293474	0.075046
82	1	0	-1.312988	5.504203	-0.924343
83	1	0	-1.620073	6.221033	0.648287
84	6	0	-3.178425	4.877699	-0.042511
85	1	0	-3.611558	4.793556	0.961387
86	1	0	-3.751295	5.648563	-0.566109
87	6	0	-3.306036	3.534032	-0.763183
88	1	0	-2.990007	3.650079	-1.806065
89	1	0	-4.350584	3.211736	-0.788136
90	6	0	-2.452692	2.445911	-0.098228
91	1	0	-2.550155	1.523475	-0.666226
92	1	0	-2.843192	2.243094	0.904205
93	6	0	1.875461	2.145444	0.497866
94	1	0	2.461926	1.227264	0.437758
95	6	0	2.421944	2.939922	1.704380
96	1	0	1.826699	3.844432	1.859486
97	1	0	2.322091	2.349513	2.617471
98	6	0	3.890348	3.339217	1.500394
99	1	0	4.508053	2.434822	1.487239
100	1	0	4.228680	3.938323	2.351296
101	6	0	4.094202	4.106987	0.191177

102	1	0	3.569908	5.068584	0.248498
103	1	0	5.153869	4.339395	0.050159
104	6	0	3.561379	3.308838	-1.002110
105	1	0	4.162887	2.402714	-1.126456
106	1	0	3.670578	3.885240	-1.925538
107	6	0	2.087617	2.920086	-0.812195
108	1	0	1.736596	2.330566	-1.661123
109	1	0	1.491633	3.836618	-0.806223

Compound **A**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	-0.078518	-0.783021	-0.715385
2	15	0	0.114540	1.678107	0.216325
3	7	0	-1.629786	-1.768496	0.253698
4	7	0	1.337510	-1.889013	0.331391
5	6	0	-1.470875	-3.021123	0.680881
6	6	0	-0.234406	-3.636468	0.899044
7	1	0	-0.283537	-4.656976	1.247432
8	6	0	1.056832	-3.114540	0.771255
9	6	0	-2.676247	-3.914810	0.892030
10	1	0	-3.555050	-3.376377	1.231003
11	1	0	-2.442334	-4.703814	1.604110
12	1	0	-2.930820	-4.389385	-0.059220
13	6	0	2.169589	-4.088442	1.103923
14	1	0	2.375532	-4.700036	0.221843
15	1	0	1.855026	-4.759786	1.901175
16	1	0	3.095449	-3.601955	1.391463
17	6	0	-2.977692	-1.276407	0.070695
18	6	0	-3.635536	-0.646100	1.154016
19	6	0	-4.954489	-0.234971	0.960879
20	1	0	-5.483059	0.244363	1.772937
21	6	0	-5.602709	-0.408390	-0.253756
22	1	0	-6.625319	-0.071760	-0.376082
23	6	0	-4.935378	-1.004280	-1.308937
24	1	0	-5.444713	-1.130882	-2.256288
25	6	0	-3.621640	-1.459610	-1.171405
26	6	0	-2.956173	-0.398619	2.500844
27	1	0	-1.900197	-0.204761	2.303185
28	6	0	-3.042880	-1.606262	3.454512
29	1	0	-2.614902	-1.336366	4.422526
30	1	0	-2.494436	-2.472908	3.090415

31	1	0	-4.082258	-1.903628	3.620639
32	6	0	-3.499454	0.839900	3.227498
33	1	0	-2.848072	1.073468	4.070193
34	1	0	-4.505498	0.674343	3.623158
35	1	0	-3.514642	1.716935	2.581846
36	6	0	-2.965051	-2.141688	-2.369140
37	1	0	-1.982673	-2.500752	-2.061170
38	6	0	-3.766780	-3.362923	-2.854343
39	1	0	-3.951557	-4.074858	-2.048275
40	1	0	-3.220092	-3.882153	-3.645107
41	1	0	-4.736313	-3.070589	-3.263106
42	6	0	-2.744788	-1.158711	-3.531718
43	1	0	-2.238481	-1.658604	-4.361139
44	1	0	-2.128937	-0.312326	-3.225184
45	1	0	-3.693896	-0.767586	-3.905359
46	6	0	2.724116	-1.501547	0.199417
47	6	0	3.369053	-0.857732	1.282252
48	6	0	4.719830	-0.538544	1.137620
49	1	0	5.238389	-0.052556	1.952294
50	6	0	5.413461	-0.818263	-0.031338
51	1	0	6.460451	-0.553220	-0.117751
52	6	0	4.761995	-1.433129	-1.086000
53	1	0	5.309826	-1.649632	-1.994869
54	6	0	3.416493	-1.798862	-0.994335
55	6	0	2.645466	-0.515271	2.584276
56	1	0	1.609784	-0.276764	2.334508
57	6	0	3.225723	0.718986	3.289196
58	1	0	2.540433	1.037207	4.074904
59	1	0	3.346285	1.560881	2.608707
60	1	0	4.192281	0.506321	3.754448
61	6	0	2.622593	-1.688041	3.583783
62	1	0	2.050948	-2.539888	3.220854
63	1	0	2.160194	-1.360990	4.517616
64	1	0	3.636247	-2.028474	3.813223
65	6	0	2.785516	-2.537300	-2.173206
66	1	0	1.763697	-2.802467	-1.901172
67	6	0	3.531201	-3.845634	-2.495719
68	1	0	2.994995	-4.404086	-3.266625
69	1	0	3.628260	-4.487239	-1.618892
70	1	0	4.537523	-3.649781	-2.872074
71	6	0	2.704915	-1.658179	-3.432058
72	1	0	2.232373	-2.209866	-4.248399
73	1	0	3.698003	-1.351183	-3.767891
74	1	0	2.116235	-0.758825	-3.252153
75	6	0	-1.058173	2.640691	-0.932840

76	1	0	-0.800479	2.300270	-1.942995
77	6	0	-0.859468	4.164626	-0.853088
78	1	0	-1.011627	4.480460	0.183137
79	1	0	0.162821	4.435842	-1.114774
80	6	0	-1.827906	4.919521	-1.775711
81	1	0	-1.590020	4.687783	-2.821233
82	1	0	-1.676206	5.996301	-1.655051
83	6	0	-3.286461	4.551147	-1.498922
84	1	0	-3.562278	4.896255	-0.495932
85	1	0	-3.949261	5.065408	-2.201163
86	6	0	-3.487569	3.037031	-1.584476
87	1	0	-3.329610	2.709014	-2.619175
88	1	0	-4.516879	2.771144	-1.329137
89	6	0	-2.524506	2.283679	-0.657615
90	1	0	-2.685942	1.211364	-0.765548
91	1	0	-2.752562	2.530348	0.383001
92	6	0	1.865990	2.117137	-0.416747
93	1	0	2.458007	1.260350	-0.082043
94	6	0	2.490452	3.366361	0.226110
95	1	0	1.930844	4.259243	-0.063166
96	1	0	2.411915	3.302221	1.311629
97	6	0	3.952315	3.529468	-0.211754
98	1	0	4.542449	2.690610	0.174146
99	1	0	4.369428	4.436750	0.235083
100	6	0	4.085575	3.579856	-1.737476
101	1	0	3.600088	4.489058	-2.111921
102	1	0	5.138434	3.648823	-2.026442
103	6	0	3.438692	2.355426	-2.392286
104	1	0	4.004158	1.458125	-2.120313
105	1	0	3.485118	2.438075	-3.482443
106	6	0	1.977122	2.181623	-1.951276
107	1	0	1.558520	1.283474	-2.411790
108	1	0	1.393695	3.025096	-2.330840
109	34	0	-0.161113	2.272969	2.291075

Compound **B**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	34	0	-0.400053	0.853388	0.852598
2	32	0	0.551808	-0.712701	-0.695528
3	15	0	-1.340143	2.371494	-0.652637
4	7	0	-0.462599	-2.415759	-0.445957

5	7	0	2.181438	-1.387023	0.264219
6	6	0	0.224529	-3.560752	-0.538308
7	6	0	1.607615	-3.646895	-0.367308
8	1	0	2.032459	-4.630308	-0.502772
9	6	0	2.495504	-2.675695	0.115742
10	6	0	-0.495521	-4.849042	-0.856017
11	1	0	-1.478441	-4.901520	-0.395233
12	1	0	0.095124	-5.707243	-0.542370
13	1	0	-0.640173	-4.913772	-1.937400
14	6	0	3.877702	-3.177570	0.463707
15	1	0	4.404150	-2.521465	1.149821
16	1	0	4.467691	-3.247659	-0.453392
17	1	0	3.818736	-4.176365	0.893581
18	6	0	-1.910960	-2.438597	-0.341109
19	6	0	-2.483851	-2.567741	0.945755
20	6	0	-3.873077	-2.617708	1.053609
21	1	0	-4.326284	-2.724614	2.030707
22	6	0	-4.687154	-2.536684	-0.065089
23	1	0	-5.764848	-2.575047	0.040375
24	6	0	-4.112565	-2.410334	-1.317004
25	1	0	-4.751374	-2.353472	-2.189185
26	6	0	-2.726278	-2.364927	-1.490571
27	6	0	-1.650619	-2.707930	2.215146
28	1	0	-0.628432	-2.420710	1.972655
29	6	0	-2.133100	-1.782998	3.342747
30	1	0	-1.460112	-1.857012	4.199550
31	1	0	-3.130265	-2.055705	3.694128
32	1	0	-2.156939	-0.743173	3.016910
33	6	0	-1.616017	-4.166736	2.708647
34	1	0	-0.994133	-4.250698	3.603350
35	1	0	-1.210139	-4.844056	1.956575
36	1	0	-2.619375	-4.515931	2.964620
37	6	0	-2.192617	-2.271670	-2.914669
38	1	0	-1.104646	-2.244079	-2.876648
39	6	0	-2.643547	-0.973422	-3.604239
40	1	0	-2.192504	-0.904558	-4.596226
41	1	0	-2.327902	-0.094878	-3.042730
42	1	0	-3.729842	-0.942032	-3.724647
43	6	0	-2.608828	-3.488826	-3.761276
44	1	0	-2.130154	-3.439760	-4.741965
45	1	0	-3.689163	-3.516726	-3.922670
46	1	0	-2.323814	-4.433378	-3.294359
47	6	0	3.107696	-0.465861	0.904352
48	6	0	2.972469	-0.233289	2.292355
49	6	0	3.867163	0.639442	2.910093

50	1	0	3.779585	0.826370	3.971927
51	6	0	4.867394	1.275253	2.192146
52	1	0	5.549562	1.953560	2.690597
53	6	0	4.989334	1.035252	0.835661
54	1	0	5.776451	1.528644	0.279938
55	6	0	4.128657	0.165093	0.160301
56	6	0	1.925933	-0.937686	3.148598
57	1	0	1.128099	-1.270410	2.485255
58	6	0	2.509844	-2.189253	3.830630
59	1	0	1.744203	-2.689571	4.428824
60	1	0	3.332461	-1.918510	4.497215
61	1	0	2.891032	-2.910115	3.106950
62	6	0	1.291830	-0.015059	4.200232
63	1	0	0.911191	0.901015	3.748120
64	1	0	2.001669	0.258446	4.983638
65	1	0	0.458199	-0.523952	4.687170
66	6	0	4.382815	-0.065492	-1.325571
67	1	0	3.610278	-0.728880	-1.712131
68	6	0	5.754682	-0.721664	-1.572810
69	1	0	5.866210	-0.961769	-2.632741
70	1	0	5.883815	-1.642763	-1.003163
71	1	0	6.572639	-0.050907	-1.299045
72	6	0	4.284120	1.241423	-2.129376
73	1	0	4.398420	1.030282	-3.194668
74	1	0	5.066340	1.948581	-1.841500
75	1	0	3.313649	1.715139	-1.993191
76	6	0	-2.983142	2.729272	0.230382
77	1	0	-3.361508	3.577421	-0.356562
78	6	0	-2.941755	3.153339	1.705071
79	1	0	-2.512507	2.339709	2.299316
80	1	0	-2.289268	4.018789	1.841130
81	6	0	-4.344419	3.478056	2.240551
82	1	0	-4.283869	3.734934	3.302319
83	1	0	-4.729315	4.367422	1.727277
84	6	0	-5.315815	2.313093	2.028146
85	1	0	-4.994898	1.461044	2.638773
86	1	0	-6.316415	2.586564	2.375429
87	6	0	-5.359931	1.889290	0.556834
88	1	0	-5.797901	2.699260	-0.038869
89	1	0	-6.014328	1.022042	0.431023
90	6	0	-3.961243	1.561545	0.018075
91	1	0	-3.578266	0.671591	0.526171
92	1	0	-4.018434	1.310477	-1.044010
93	6	0	-0.328503	3.928347	-0.252928
94	1	0	-0.305870	4.077001	0.830990

95	6	0	-0.991496	5.155134	-0.909744
96	1	0	-1.995784	5.313887	-0.510208
97	1	0	-1.107039	4.969425	-1.984355
98	6	0	-0.160472	6.430702	-0.705801
99	1	0	-0.642100	7.266800	-1.221427
100	1	0	-0.151692	6.685657	0.360479
101	6	0	1.279670	6.258613	-1.194991
102	1	0	1.278329	6.127009	-2.283351
103	1	0	1.858536	7.164051	-0.990856
104	6	0	1.939843	5.041886	-0.541002
105	1	0	2.052634	5.225175	0.534199
106	1	0	2.948278	4.896842	-0.938423
107	6	0	1.115459	3.766413	-0.754708
108	1	0	1.592017	2.926807	-0.246253
109	1	0	1.100265	3.516256	-1.821068
110	34	0	0.947996	-0.227905	-2.833672

Cy_2PHSe

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.560705	-0.323454	0.241891
2	6	0	1.628776	-1.817692	-0.118087
3	6	0	2.838140	0.408661	-0.200868
4	1	0	1.460696	-0.220006	1.329131
5	6	0	2.887951	-2.473983	0.468667
6	1	0	1.644417	-1.927551	-1.208579
7	1	0	0.743918	-2.347938	0.240619
8	6	0	4.090634	-0.253356	0.386611
9	1	0	2.901196	0.391559	-1.295717
10	1	0	2.782483	1.457553	0.092253
11	6	0	4.163576	-1.743456	0.040821
12	1	0	2.927556	-3.523392	0.163760
13	1	0	2.816548	-2.469633	1.562319
14	1	0	4.981526	0.265645	0.023267
15	1	0	4.083418	-0.132586	1.475994
16	1	0	5.036162	-2.201843	0.513943
17	1	0	4.299669	-1.857590	-1.041030
18	6	0	-1.444674	-0.500296	0.124344
19	6	0	-2.615033	0.350327	0.637902
20	6	0	-1.908217	-1.451995	-0.993397
21	1	0	-1.065080	-1.098096	0.961303

22	6	0	-3.769329	-0.541273	1.113347
23	1	0	-2.963628	1.008502	-0.163382
24	1	0	-2.279157	1.008268	1.440240
25	6	0	-3.070757	-2.337689	-0.524230
26	1	0	-2.232637	-0.855835	-1.853613
27	1	0	-1.083023	-2.077359	-1.342519
28	6	0	-4.235902	-1.503722	0.016686
29	1	0	-4.600465	0.086564	1.445173
30	1	0	-3.447009	-1.117387	1.989008
31	1	0	-3.405101	-2.970787	-1.350811
32	1	0	-2.712890	-3.014216	0.260729
33	1	0	-5.023990	-2.159814	0.396123
34	1	0	-4.677973	-0.927373	-0.804140
35	15	0	0.035689	0.533843	-0.428053
36	1	0	0.116437	0.217509	-1.812644
37	34	0	-0.046871	2.634874	-0.051846

Cy_2PSeH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.007851	0.447607	0.824818
2	6	0	-1.506728	-0.298608	-0.088194
3	6	0	-1.524906	-1.836436	-0.046609
4	6	0	-2.804171	0.264059	0.518675
5	1	0	-1.445623	0.010746	-1.138245
6	6	0	-2.776407	-2.405340	-0.732666
7	1	0	-1.502889	-2.173642	0.996588
8	1	0	-0.636820	-2.246109	-0.530763
9	6	0	-4.052045	-0.302258	-0.170060
10	1	0	-2.834363	0.009751	1.584764
11	1	0	-2.804228	1.353535	0.455808
12	6	0	-4.066556	-1.832830	-0.140753
13	1	0	-2.771264	-3.496321	-0.653799
14	1	0	-2.734459	-2.170586	-1.802647
15	1	0	-4.949749	0.096335	0.310944
16	1	0	-4.078503	0.041695	-1.210608
17	1	0	-4.934677	-2.217398	-0.683417
18	1	0	-4.170740	-2.173213	0.896253
19	6	0	1.464118	-0.399097	-0.045689
20	6	0	2.687013	0.514566	-0.221237
21	6	0	1.861583	-1.631488	0.796373
22	1	0	1.135186	-0.732162	-1.036821

23	6	0	3.871727	-0.238454	-0.841915
24	1	0	2.983215	0.912484	0.757103
25	1	0	2.430223	1.376503	-0.836809
26	6	0	3.037971	-2.394689	0.172153
27	1	0	2.144937	-1.290731	1.798630
28	1	0	1.015964	-2.307557	0.932697
29	6	0	4.250412	-1.483895	-0.035989
30	1	0	4.729380	0.435212	-0.925352
31	1	0	3.610429	-0.535362	-1.864535
32	1	0	3.303420	-3.243629	0.808801
33	1	0	2.727133	-2.813768	-0.792102
34	1	0	5.055531	-2.030236	-0.535394
35	1	0	4.640888	-1.176706	0.941280
36	1	0	0.183475	3.261817	1.078652
37	34	0	-0.106788	2.548884	-0.173759

$[Cy_2PSe]^-$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.484067	-0.313357	0.091838
2	6	0	1.558862	-1.835425	-0.102683
3	6	0	2.804015	0.338375	-0.343980
4	1	0	1.327294	-0.094101	1.155331
5	6	0	2.781001	-2.457832	0.592798
6	1	0	1.603929	-2.060907	-1.176266
7	1	0	0.654921	-2.315926	0.278823
8	6	0	4.023300	-0.273181	0.357006
9	1	0	2.917556	0.218455	-1.430198
10	1	0	2.743851	1.411261	-0.151523
11	6	0	4.089447	-1.791081	0.157736
12	1	0	2.819425	-3.535695	0.393565
13	1	0	2.668107	-2.345608	1.678264
14	1	0	4.944068	0.195640	-0.009361
15	1	0	3.968437	-0.054065	1.430546
16	1	0	4.936587	-2.218643	0.706867
17	1	0	4.264789	-2.005533	-0.904283
18	6	0	-1.437705	-0.405474	0.015247
19	6	0	-2.646970	0.490242	0.303386
20	6	0	-1.882027	-1.593381	-0.857359
21	1	0	-1.065429	-0.786535	0.976256
22	6	0	-3.795668	-0.288941	0.958103
23	1	0	-2.999792	0.931010	-0.637740
24	1	0	-2.333013	1.331252	0.923631

25	6	0	-3.027793	-2.393025	-0.217704
26	1	0	-2.212024	-1.203673	-1.827977
27	1	0	-1.043706	-2.259551	-1.073645
28	6	0	-4.224587	-1.495447	0.114702
29	1	0	-4.652449	0.373873	1.127316
30	1	0	-3.474370	-0.639571	1.947411
31	1	0	-3.339266	-3.208112	-0.882171
32	1	0	-2.665936	-2.864887	0.704728
33	1	0	-5.003619	-2.070868	0.628764
34	1	0	-4.668915	-1.134919	-0.821606
35	15	0	0.023969	0.539320	-0.833343
36	34	0	0.055717	2.598778	0.089673
