Supplementary Material (ESI) for Chemical Communications

Synthetic, Structural and Theoretical Studies of Amidinate and Guanidinate Stabilised Germanium(I) Dimers

Shaun P. Green, Cameron Jones,* Peter C. Junk, Kai-Alexander Lippert, and Andreas Stasch

SUPPLEMENTARY MATERIAL

Experimental

General. All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity argon. Hexane, THF and toluene were distilled over potassium. ^{1}H and ^{13}C{^{1}H} NMR spectra were recorded on either a Bruker DXP400 spectrometer operating at 400.13 and 100 MHz respectively, or a Jeol Eclipse 300 spectrometer operating at 300.52 and 75.57 MHz respectively and were referenced to the resonances of the solvent used. EI mass spectra and accurate mass EI mass spectra were obtained from the EPSRC National Mass Spectrometric Service at Swansea University. IR spectra were recorded using a Nicolet 510 FT-IR spectrometer as Nujol mulls between NaCl plates. Melting points were determined in sealed glass capillaries under argon and are uncorrected. The microanalysis was performed by Medac Ltd.

Synthesis of [Ge(Piso)Cl] 1: *n*BuLi (0.69 cm^3 of a 1.6 M solution in hexanes, 1.10 mmol) was added to a solution of PisoH (0.45 g, 1.07 mmol) in THF (15 cm^3) at 0 °C, warmed to room temperature and stirred for 3 h. The resultant solution was

added to a solution of $GeCl_2$.dioxane (0.255 g, 1.10 mmol) in THF (20 cm^3) at –80 °C. The mixture was slowly warmed to room temperature and stirred for 2 h. All volatiles were removed *in vacuo*, the residue extracted into hexane (60 cm^3) and filtered. The filtrate was concentrated to *ca.* 15 cm^3 and stored at –30 °C to give colourless blocks of **1**. Further concentration of the supernatant solution gave another crop of **1**. Yield: 0.47 g (83 %). Mp 148 - 150 °C (decomp); ^{1}H NMR (400 MHz, C_6D_6, 298 K): δ 0.99 (s, 9 H, C(CH_3)$_3$), 1.28 (d, $^3J_{HH}$ = 6.8 Hz, 6 H, CH_3), 1.37 (d, $^3J_{HH}$ = 6.8 Hz, 6 H, CH_3), 1.42 (d, $^3J_{HH}$ = 6.8 Hz, 6 H, CH_3), 1.58 (d, $^3J_{HH}$ = 6.8 Hz, 6 H, CH_3), 3.58 (sept, $^3J_{HH}$ = 6.8 Hz, 2 H, C*H*), 4.10 (sept, $^3J_{HH}$ = 6.8 Hz, 2 H, C*H*), 7.10–7.28 (m, 6 H, Ar–H); ^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6, 298 K): δ 21.1, 21.6, 26.65, 26.7 (CH(*C*H$_3$)$_2$), 27.2, 27.5 (*C*H(CH$_3$)$_2$), 28.1 (C(*C*H$_3$)$_3$), 40.6 (*C*(CH$_3$)$_3$), 122.1, 123.3, 125.7, 137.0, 142.9, 145.2 (Ar*C*), 176.9 (backbone *C*N$_2$); MS (EI 70eV), *m*/*z* (%): 420.4 (PisoH$^+$, 12), 377.4 (PisoH$^+$ -Pr^i, 22), 244.3 (PisoH$^+$ -ArNH, 100); IR ν/cm^{-1} (Nujol): 1653, 1616, 1585, 1261, 1170, 969, 933, 891, 846, 800, 767; $C_{29}H_{43}ClGeN_2$ requires C 66.01, H 8.21, N 5.31 %; found C 65.52, H 8.24, N 5.48 %.

Synthesis of [Ge(Giso)Cl] 2: *n*BuLi (0.90 cm^3 of a 1.6 M solution in hexanes, 1.44 mmol) was added to a solution of GisoH (0.645 g, 1.39 mmol) in THF (15 cm^3) at 0 °C, warmed to room temperature and stirred for 3 h. The resultant solution was added to a solution of $GeCl_2$.dioxane (0.36 g, 1.55 mmol) in THF (20 cm^3) at –80 °C. The mixture was slowly warmed to room temperature and stirred for 2 h. All volatiles were removed *in vacuo*, the residue extracted into hexane (60 cm^3) and filtered. The filtrate was concentrated to *ca.* 15 cm^3 and stored at –30 °C to give colourless blocks of **2**. Further concentration of the supernatant solution gave another crop of **2**. Yield: 0.63 g (79 %). Mp 174–175 °C (decomp); ^{1}H NMR (400 MHz, C_6D_6, 298 K): δ 0.91

(d, $^3J_{HH}$ = 6.8 Hz, 12 H, NCH(CH_3)$_2$), 1.33 (d, $^3J_{HH}$ = 6.8 Hz, 6 H, CH(CH_3)$_2$), 1.37 (d, $^3J_{HH}$ = 6.8 Hz, 6 H, CH(CH_3)$_2$), 1.42 (d, $^3J_{HH}$ = 6.8 Hz, 6 H, CH(CH_3)$_2$), 1.62 (d, $^3J_{HH}$ = 6.8 Hz, 6 H, CH(CH_3)$_2$), 3.64 (sept, $^3J_{HH}$ = 6.8 Hz, 2 H, CH(CH$_3$)$_2$), 4.07 (sept, $^3J_{HH}$ = 6.8 Hz, 2 H, CH(CH$_3$)$_2$), 4.18 (sept, $^3J_{HH}$ = 6.8 Hz, 2 H, CH(CH$_3$)$_2$), 7.10-7.29 (m, 6 H, ArH); ^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6, 298 K): δ 23.7, 23.8, 24.5, 28.5 (CH(*C*H$_3$)$_2$), 28.6, 29.3 (*C*H(CH$_3$)$_2$), 30.2 (CH(*C*H$_3$)$_2$), 49.3 (N*C*H(CH$_3$)$_2$), 124.3, 125.3, 127.1, 138.7, 145.2, 147.6 (Ar*C*), 163.3 (backbone *C*N$_3$); IR ν/cm^{-1} (Nujol): 1614 (m), 1582 (m), 1167 (m), 1107 (m), 1054 (m), 873 (m), 801 (m), 758 (s); MS (EI 70eV), *m*/*z* (%): 572.4 (M+H$^+$, 4), 536.4 (M$^+$-Cl, 10), 464.5 (GisoH$^+$, 42); EI Acc. Mass.: on M+H$^+$: calc. for $C_{31}H_{49}N_3Cl1^{74}Ge$: 572.2821, found 572.2837.

Synthesis of [{Ge(Piso)}$_2$] 3: A solution of **1** (0.80 g, 1.52 mmol) in toluene (30 cm^3) was added to a potassium mirror (0.75 g, 19.2 mmol) and stirred for 4 h at room temperature. The mixture was filtered and volatiles removed *in vacuo*. The residue was recrystallised from a hexane/THF mixture (5:1, 20 cm^3) at –30 ° C to form green-red dichromic blocks of **3**. Concentration of the supernatant solution gave a second crop. Yield: 0.13 g (16%). Mp > 300 °C.

Synthesis of [{Ge(Giso)}$_2$] 4: A solution of **2** (0.51 g, 0.89 mmol) in toluene (20 cm^3) was added to a potassium mirror (0.50 g, 12.8 mmol) and stirred for 3 h at room temperature. The mixture was filtered and volatiles removed *in vacuo*. The residue was extracted into hexane (40 cm^3) and the extract cooled to –30^o C yielding lime-green blocks of **4**. Concentration of the supernatant solution gave another crop of **4** at –30 °C. Yield: 60 mg (13%). Mp 200-203 °C (decomp.).

Molecular structures of compounds 2 and 4.

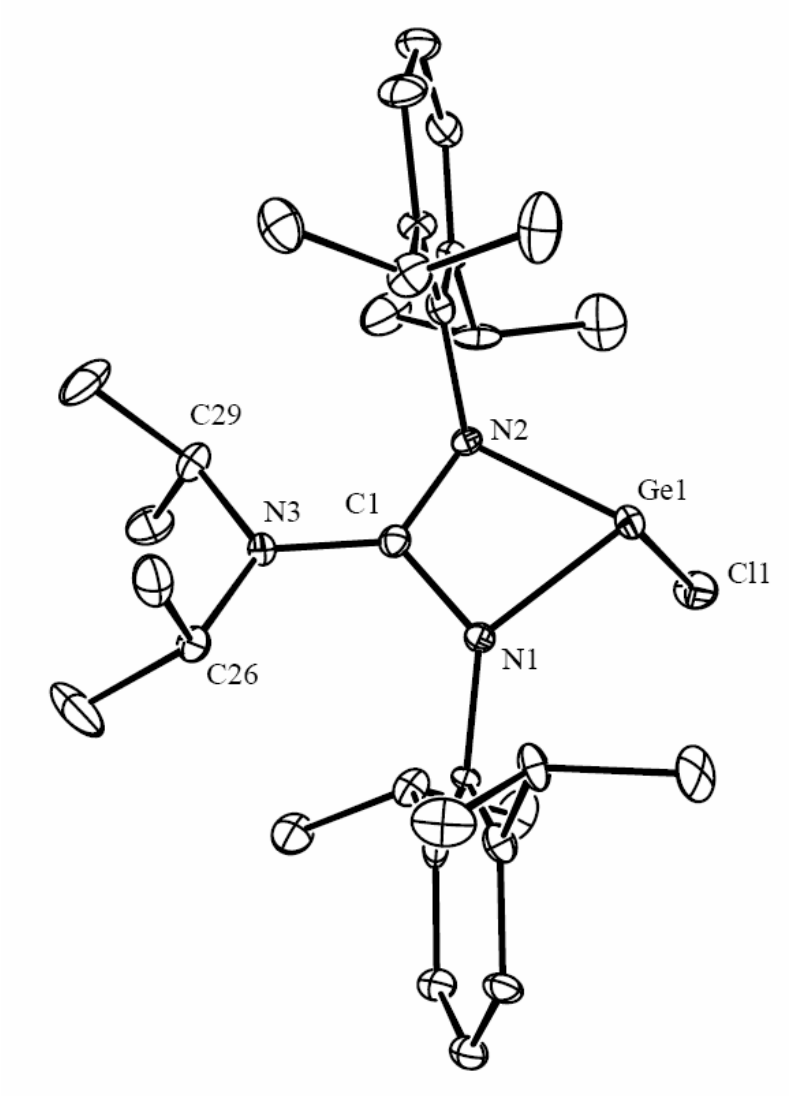

Fig. S1 Molecular structure of **2** (hydrogen atoms omitted, ellipsoids shown at the 25% probability level). Selected bond lengths (Å) and angles (º): Ge(1)-Cl(1) 2.252(4), Ge(1)-N(1) 1.937(5), Ge(1)-N(2) 1.970(5), N(1)-C(1) 1.372(8), C(1)-N(2) 1.327(8), C(1)-N(3) 1.370(5); N(2)-C(1)-N(1) 106.5(3), N(1)-Ge(1)-N(2) 67.22(12), N(1)-Ge(1)-Cl(1) 97.92(17), N(2)-Ge(1)-Cl(1) 98.33(18).

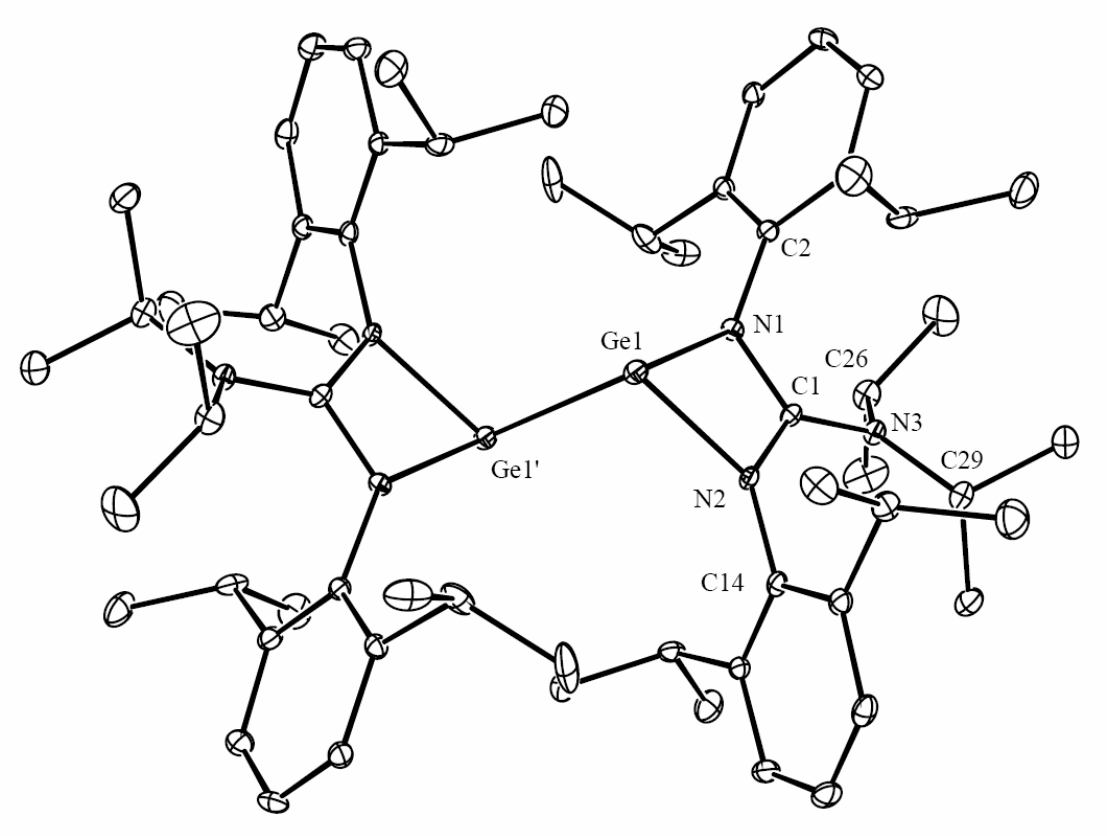

Fig. S2 Molecular structure of **4** (hydrogen atoms omitted, ellipsoids shown at the 25% probability level). Selected bond lengths (Å) and angles (°): Ge(1)-Ge(1)' 2.6721(13), Ge(1)-N(1) 2.056(3), Ge(1)-N(2) 2.043(3), N(1)-C(1) 1.357(5), N(2)-C(1) 1.337(5), N(3)-C(1) 1.371(5); N(2)-Ge(1)-N(1) 63.84(14), N(2)-C(1)-N(1) 107.1(4), N(1)-Ge(1)-Ge(1)' 95.97(10), N(2)-Ge(1)-Ge(1)' 99.47(10). Symmetry operation ': -x+1, -y+2, -z.

Theoretical Studies.

Method. The geometry of the model species [{MeC(NAr')$_2$Ge}$_2$], Ar' = $C_6H_3Me_2$-2,6, was optimised using the Gaussian 98 package[1] employing the methods recommended by Boehme and Frenking.[2] That is the BP86 density functional method,[3] with a 6-31G* basis set on C, N and H,[4] Stuttgart-Dresden ECP/basis sets for Ge,[5] augmented by a d-type polarization function with exponent 0.246 on Ge.[6] Atomic charges, orbital populations and bonding analyses were obtained from the NBO scheme[7] of the optimised structure. To comply with the maximum basis functions allowed by the NBO program, 6-31G basis sets were applied to extra-heterocyclic C and H atoms.

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara,

M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, Pittsburgh PA, **2001**.

2. C. Boehme and G. Frenking, *Chem. Eur. J.*, 1999, **5**, 7.

3. (a) A.D. Becke, *Phys. Rev. A*, 1988, **38**, 3098; (b) J.P. Perdew, *Phys. Rev. A* , 1986, **33**, 8822.

4. (a) R. Ditchfield, W.J. Hehre and J.A. Pople, *J. Chem. Phys.*, 1971, **54**, 724; (b) W.J. Hehre, R. Ditchfield and J.A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257; (c) M.S. Gordon, *Chem. Phys. Lett.*, 1980, **76**, 163; (d) P.C. Hariharan and J.A. Pople, *Theor. Chim. Acta,* 1973, **28**, 213.

5. (a) M. Dolg, U. Wedig, H. Stoll and H. Preuss, *J. Chem. Phys.*, 1987, **86**, 866; (b) A. Bergner, M. Dolg, W. Kuehle, H. Stoll and H. Preuss, *Mol. Phys.*, 1993, **80**, 1431.

6. J. Andzelm, S. Huzinaga, M. Klobukowski, E. Radzio, Y. Sakai and H. Tatekawi, *Gaussian Basis Sets for Molecular Calculations*, Elsevier, Amsterdam, 1984.

7. A. E. Reed, L. A. Curtiss and F. Weinhold, *Chem. Rev*., 1988, **88**, 899.

Cartesian coordinates of the optimised structure of [{MeC(NAr')$_2$Ge}$_2$]

C	-4.32164	-4.13071	-0.63320
C	-4.03105	-4.92112	0.48884
C	-3.20129	-4.41481	1.49526
C	-2.64863	-3.12090	1.40681
C	-2.96054	-2.32307	0.27354
C	-3.79740	-2.83278	-0.76155
C	-1.73513	-2.62714	2.50861
N	-2.39536	-1.02638	0.12815
Ge	-0.87992	-0.02202	-0.99112
N	-2.24557	1.18071	0.12426
C	-2.98732	0.12230	0.50159
C	-4.29367	0.20351	1.24959
C	-4.11999	-1.99349	-1.97845
C	-2.63489	2.54477	0.21524
C	-2.14356	3.36161	1.26849
C	-2.50785	4.72340	1.29333
C	-3.32876	5.27490	0.30354
C	-3.80246	4.46162	-0.73686
C	-3.46729	3.09823	-0.80118
C	-1.24217	2.81594	2.35556
C	-3.98072	2.23527	-1.93249
Ge	0.88997	-0.09430	1.01868
N	2.30810	-1.20215	-0.12711
C	2.77879	-2.53644	-0.26906
C	3.61636	-3.08640	0.74460
C	4.04617	-4.41890	0.62070
C	3.66031	-5.20481	-0.47553
C	2.83011	-4.65815	-1.46041
C	2.37174	-3.32761	-1.37616
C	4.03509	-2.25372	1.93664
C	1.45619	-2.78719	-2.45425
N	2.34733	1.00929	-0.08774
C	2.98799	-0.10126	-0.49615
C	4.28453	-0.11883	-1.26556
C	2.82053	2.34307	-0.21060
C	3.61634	2.90220	0.82741
C	4.03025	4.24282	0.71440
C	3.66965	5.02126	-0.39393
C	2.88220	4.46098	-1.40888
C	2.44252	3.12572	-1.33577
C	4.02130	2.07058	2.02453
C	1.58283	2.54188	-2.43278
H	4.64399	4.67696	1.51314
H	3.99834	6.06415	-0.46469
H	4.69085	-4.84341	1.40001
H	-2.13349	5.35502	2.10856
H	2.59430	5.06645	-2.27683
H	4.00401	-6.24211	-0.55741
H	-3.59776	6.33660	0.33860
H	-2.96686	-5.03059	2.37255
H	2.52203	-5.26964	-2.31767
H	-4.44206	4.88831	-1.51916
H	-4.44787	-5.93102	0.57385
H	-4.96567	-4.52433	-1.42910
H	-3.21218	-1.52479	-2.40072
H	-4.59723	-2.60584	-2.76268

H	-4.81417	-1.16462	-1.73817
H	-1.48620	-1.56118	2.39112
H	-2.19506	-2.76969	3.50389
H	-0.78153	-3.18910	2.51445
H	-4.59212	1.25361	1.39341
H	-5.09048	-0.33082	0.70222
H	-4.20354	-0.27978	2.23907
H	-1.11616	1.72434	2.28007
H	-0.23493	3.27124	2.30079
H	-1.64362	3.04645	3.35980
H	-4.44716	2.85353	-2.71842
H	-3.16736	1.64112	-2.38867
H	-4.74262	1.51001	-1.58652
H	4.53052	-2.87934	2.69868
H	4.74464	-1.45149	1.65517
H	3.16827	-1.75029	2.40337
H	1.30095	-1.70104	-2.35858
H	1.86070	-2.99388	-3.46219
H	0.45980	-3.26717	-2.40579
H	4.69893	0.89809	-1.34960
H	5.02288	-0.77482	-0.77181
H	4.12564	-0.52245	-2.28206
H	4.45716	2.70433	2.81571
H	3.16069	1.52068	2.44741
H	4.77787	1.30802	1.75563
H	1.41364	3.27837	-3.23672
H	2.03656	1.64099	-2.88451
H	0.59235	2.22772	-2.04990

Natural Population Analysis and Natural Electron Configuration for [{MeC(NAr')$_2$Ge}$_2$]

		Natural	Natural Population			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.01666	1.99891	4.00796	0.00979	6.01666
C	2	0.11903	1.99865	3.86850	0.01383	5.88097
C	3	-0.01538	1.99890	4.00676	0.00972	6.01538
C	4	-0.21802	1.99899	4.21023	0.00880	6.21802
C	5	-0.20328	1.99909	4.19466	0.00952	6.20328
C	6	-0.21376	1.99901	4.20604	0.00872	6.21376
N	7	-0.69532	1.99919	5.67857	0.01756	7.69532
C	8	0.48300	1.99890	3.49310	0.02500	5.51700
C	9	-0.78011	1.99917	4.77793	0.00301	6.78011
C	10	-0.72744	1.99922	4.72391	0.00431	6.72744
C	11	-0.72217	1.99921	4.71840	0.00456	6.72217
Ge	12	0.54141	28.00000	3.44545	0.01314	31.45859
N	13	-0.69076	1.99918	5.67457	0.01700	7.69076
C	14	0.12087	1.99866	3.86665	0.01382	5.87913
C	15	-0.01860	1.99891	4.00997	0.00971	6.01860
C	16	-0.21833	1.99899	4.21059	0.00876	6.21833
C	17	-0.20304	1.99909	4.19445	0.00950	6.20304
C	18	-0.21277	1.99900	4.20500	0.00877	6.21277
C	19	-0.01627	1.99892	4.00748	0.00987	6.01627
C	20	-0.72701	1.99922	4.72355	0.00424	6.72701
C	21	-0.73400	1.99922	4.73014	0.00463	6.73400

Ge 22	0.54632	28.00000	3.44068	0.01300	31.45368
N 23	-0.69808	1.99919	5.68137	0.01752	7.69808
C 24	0.11533	1.99864	3.87226	0.01376	5.88467
C 25	-0.01677	1.99891	4.00804	0.00983	6.01677
C 26	-0.21063	1.99901	4.20287	0.00876	6.21063
C 27	-0.20222	1.99910	4.19368	0.00945	6.20222
C 28	-0.21718	1.99899	4.20941	0.00879	6.21718
C 29	-0.01615	1.99890	4.00751	0.00974	6.01615
C 30	-0.73429	1.99921	4.73059	0.00448	6.73429
C 31	-0.72801	1.99922	4.72437	0.00442	6.72801
N 32	-0.69093	1.99919	5.67455	0.01720	7.69093
C 33	0.47824	1.99890	3.49775	0.02511	5.52176
C 34	-0.78024	1.99917	4.77802	0.00304	6.78024
C 35	0.11869	1.99866	3.86882	0.01382	5.88131
C 36	-0.01636	1.99892	4.00759	0.00986	6.01636
C 37	-0.21295	1.99900	4.20517	0.00878	6.21295
C 38	-0.20265	1.99910	4.19414	0.00942	6.20265
C 39	-0.21683	1.99899	4.20903	0.00881	6.21683
C 40	-0.01981	1.99891	4.01127	0.00962	6.01981
C 41	-0.73373	1.99922	4.72988	0.00463	6.73373
C 42	-0.72864	1.99921	4.72533	0.00410	6.72864
H 43	0.21186	0.00000	0.78651	0.00163	0.78814
H 44	0.21173	0.00000	0.78679	0.00148	0.78827
H 45	0.21096	0.00000	0.78739	0.00165	0.78904
H 46	0.21159	0.00000	0.78679	0.00161	0.78841
H 47	0.21147	0.00000	0.78695	0.00157	0.78853
H 48	0.21162	0.00000	0.78693	0.00145	0.78838
H 49	0.21147	0.00000	0.78704	0.00149	0.78853
H 50	0.21123	0.00000	0.78709	0.00168	0.78877
H 51	0.21132	0.00000	0.78700	0.00168	0.78868
H 52	0.21176	0.00000	0.78661	0.00163	0.78824
H 53	0.21134	0.00000	0.78720	0.00145	0.78866
H 54	0.21105	0.00000	0.78726	0.00169	0.78895
H 55	0.25076	0.00000	0.74793	0.00132	0.74924
H 56	0.26145	0.00000	0.73742	0.00113	0.73855
H 57	0.25305	0.00000	0.74568	0.00127	0.74695
H 58	0.25736	0.00000	0.74044	0.00220	0.74264
H 59	0.25464	0.00000	0.74419	0.00116	0.74536
H 60	0.26371	0.00000	0.73499	0.00129	0.73629
H 61	0.27058	0.00000	0.72838	0.00104	0.72942
H 62	0.26763	0.00000	0.73109	0.00129	0.73237
H 63	0.27464	0.00000	0.72431	0.00105	0.72536
H 64	0.25920	0.00000	0.73845	0.00235	0.74080
H 65	0.26334	0.00000	0.73541	0.00125	0.73666
H 66	0.25472	0.00000	0.74412	0.00115	0.74528
H 67	0.24968	0.00000	0.74915	0.00117	0.75032
H 68	0.26897	0.00000	0.72988	0.00116	0.73103
H 69	0.24755	0.00000	0.75116	0.00129	0.75245
H 70	0.24945	0.00000	0.74942	0.00112	0.75055
H 71	0.24552	0.00000	0.75318	0.00130	0.75448
H 72	0.26785	0.00000	0.73093	0.00122	0.73215
H 73	0.25798	0.00000	0.73989	0.00213	0.74202
H 74	0.25463	0.00000	0.74421	0.00116	0.74537
H 75	0.26379	0.00000	0.73492	0.00129	0.73621
H 76	0.27026	0.00000	0.72870	0.00103	0.72974
H 77	0.26529	0.00000	0.73340	0.00131	0.73471
H 78	0.27470	0.00000	0.72424	0.00106	0.72530
H 79	0.24837	0.00000	0.75047	0.00116	0.75163
H 80	0.26758	0.00000	0.73125	0.00117	0.73242
H 81	0.24963	0.00000	0.74897	0.00140	0.75037
H 82	0.24909	0.00000	0.74978	0.00113	0.75091

H 83	0.25570	0.00000	0.74286	0.00144	0.74430
H 84	0.26097	0.00000	0.73673	0.00230	0.73903

Atom No	Natural Electron Configuration
C 1	[core]2s(0.88)2p(3.13)3p(0.01)
C 2	[core]2s(0.82)2p(3.05)3p(0.01)
C 3	[core]2s(0.87)2p(3.13)3p(0.01)
C 4	[core]2s(0.92)2p(3.29)3p(0.01)
C 5	[core]2s(0.92)2p(3.27)3p(0.01)
C 6	[core]2s(0.92)2p(3.29)3p(0.01)
N 7	[core]2s(1.29)2p(4.39)3p(0.01)
C 8	[core]2s(0.80)2p(2.70)3p(0.02)3d(0.01)
C 9	[core]2s(1.12)2p(3.66)
C 10	[core]2s(1.09)2p(3.63)
C 11	[core]2s(1.09)2p(3.62)
Ge 12	[core]4s(1.74)4p(1.70)4d(0.01)
N 13	[core]2s(1.28)2p(4.39)3p(0.01)
C 14	[core]2s(0.82)2p(3.05)3p(0.01)
C 15	[core]2s(0.88)2p(3.13)3p(0.01)
C 16	[core]2s(0.92)2p(3.29)3p(0.01)
C 17	[core]2s(0.92)2p(3.27)3p(0.01)
C 18	[core]2s(0.92)2p(3.29)3p(0.01)
C 19	[core]2s(0.88)2p(3.13)3p(0.01)
C 20	[core]2s(1.09)2p(3.63)
C 21	[core]2s(1.09)2p(3.64)
Ge 22	[core]4s(1.75)4p(1.69)4d(0.01)
N 23	[core]2s(1.29)2p(4.39)3p(0.01)
C 24	[core]2s(0.82)2p(3.05)3p(0.01)
C 25	[core]2s(0.88)2p(3.13)3p(0.01)
C 26	[core]2s(0.92)2p(3.28)3p(0.01)
C 27	[core]2s(0.92)2p(3.27)3p(0.01)
C 28	[core]2s(0.92)2p(3.29)3p(0.01)
C 29	[core]2s(0.87)2p(3.13)3p(0.01)
C 30	[core]2s(1.09)2p(3.64)
C 31	[core]2s(1.09)2p(3.63)
N 32	[core]2s(1.28)2p(4.39)3p(0.01)
C 33	[core]2s(0.80)2p(2.70)3p(0.02)3d(0.01)
C 34	[core]2s(1.12)2p(3.66)
C 35	[core]2s(0.82)2p(3.05)3p(0.01)
C 36	[core]2s(0.88)2p(3.13)3p(0.01)
C 37	[core]2s(0.92)2p(3.29)3p(0.01)
C 38	[core]2s(0.92)2p(3.27)3p(0.01)
C 39	[core]2s(0.92)2p(3.29)3p(0.01)
C 40	[core]2s(0.88)2p(3.14)3p(0.01)
C 41	[core]2s(1.09)2p(3.64)
C 42	[core]2s(1.09)2p(3.63)
H 43	1s(0.79)
H 44	1s(0.79)
H 45	1s(0.79)
H 46	1s(0.79)
H 47	1s(0.79)
H 48	1s(0.79)
H 49	1s(0.79)
H 50	1s(0.79)
H 51	1s(0.79)
H 52	1s(0.79)
H 53	1s(0.79)

```
H 54            1s( 0.79)
H 55            1s( 0.75)
H 56            1s( 0.74)
H 57            1s( 0.75)
H 58            1s( 0.74)
H 59            1s( 0.74)
H 60            1s( 0.73)
H 61            1s( 0.73)
H 62            1s( 0.73)
H 63            1s( 0.72)
H 64            1s( 0.74)
H 65            1s( 0.74)
H 66            1s( 0.74)
H 67            1s( 0.75)
H 68            1s( 0.73)
H 69            1s( 0.75)
H 70            1s( 0.75)
H 71            1s( 0.75)
H 72            1s( 0.73)
H 73            1s( 0.74)
H 74            1s( 0.74)
H 75            1s( 0.73)
H 76            1s( 0.73)
H 77            1s( 0.73)
H 78            1s( 0.72)
H 79            1s( 0.75)
H 80            1s( 0.73)
H 81            1s( 0.75)
H 82            1s( 0.75)
H 83            1s( 0.74)
H 84            1s( 0.74)
```