Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information

Reactions of a Zn(I) complex with group 14 azides – Formation of zinc azide and zinc hexazene complexes

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Experimental Section

Manipulations were performed in a glove box under an Ar-atmosphere or with standard Schlenk techniques. Dry solvents were obtained from a solvent purification system (MBraun) and degassed prior to use. $Mesnacnac_2Zn_2$,[1] PhN_3,[2] and $DippN_3$[3] were prepared according to literature methods. Me_3SnN_3 was prepared by standard reaction of Me_3SnCl with NaN_3, whereas Me_3SiN_3 was commercially available (Acros Organics; Alfa Aesar) and used as received. A Bruker Avance 300 spectrometer was used for NMR spectroscopy. ^1H and $^{13}C\{^1H\}$ NMR spectra were referenced to internal C_6D_5H (^1H: $\delta = 7.154$; ^{13}C: $\delta = 128.0$). IR spectra were recorded on an Alpha-T FT-IR spectrometer with a single reflection ATR sampling module. Melting points were measured in sealed capillaries and were not corrected. Elemental analyses were performed at the *Elementaranalyse Labor* of the University of Duisburg-Essen.

[(Mesnacnac)Zn(μ-N_6Ph_2)Zn(Mesnacnac)] (3)

$Mesnacnac_2Zn_2$ (80 mg, 100 μmol) was dissolved in 15 mL of a mixture of hexane and toluene (8:2) and PhN_3 (30 mg, 250 mmol) was slowly added. The resulting solution was stirred for 12h at ambient temperature, yielding an orange suspension. **3** was isolated as an orange solid by filtration. Crystals of **3** suitable for a single crystal X-ray diffraction study were obtained by recrystallization from a solution in 5 mL of fluorbenzene and storage at 4 °C. Yield: 50 mg (49 %). – M.p. 239 °C. – $C_{64}H_{73}N_{10}Zn_2F$ (1131.05): calcd. C 67.90, H 6.45, N 12.37; found C 65.60, H 6.72, N 10.6. – IR: ν = 3067, 2998, 2962, 2914, 2854, 1592, 1550, 1515, 1483, 1452, 1394, 1348, 1322, 1300, 1258, 1197, 1147, 1018, 953, 855, 804, 751, 726, 687, 632, 596, 567, 520, 504, 463, 388 cm^{-1}. – ^1H NMR (300 MHz, [C_6D_6], 20 °C): $\delta = 1.63$ (s, 12 H, C*CH₃*), 1.95 (s, 12 H, *p*-*CH₃*), 2.16 (s, 12 H, *o*-*CH₃*), 2.17 (s, 12 H, o-*CH₃*), 4.89 (s, 2 H, *CH*), 6.61 (s, 4 H, Mes-*H*), 6.67 (s, 4 H, Mes-*H*), 6.89 (m, 4 H, Ph-*m*-*H*), 7.02 (m, 2 H, Ph-*p*-*H*), 7.45 (d, 4 H, Ph-*o*-*H*). – ^{13}C NMR (125 MHz, [C_6D_6], 20 °C): 18.77 (*o*-*CH₃*), 21.36 (*p*-*C*H_3), 23.31 (*C*CH_3), 94.45 (*γ*–*C*), 120.20 (*p*-Ph), 124.41 (*m*-Ph), 129.38 (*m*-Ar), 131.75 (*o*-Ar), 132.17 (*p*-Ar), 133.44 (*o*-Ph), 144.78 (*i*-Ar), 149.55 (*i*-Ph), 168.58 (*ß*-*C*).

[(Mesnacnac)Zn(μ-N_6Dipp_2)Zn(Mesnacnac)] (4)

$Mesnacnac_2Zn_2$ (80 mg, 100 μmol) was dissolved in 15 mL of a mixture of hexane and toluene (8:2) and $DippN_3$ (30 mg, 250 mmol) was added. The resulting solution was stirred for 12h at ambient temperature, yielding an orange suspension. **4** was isolated as an orange solid by filtration. Yield: 64 mg (53 %). – M.p. 363 °C (decomp.). – $C_{70}H_{104}N_{10}Zn_2$ (1214): calcd. C 69.19, H 8.56, N 11.53; found C 67.53, H 8.21, N 10.48. – IR: ν = 2998, 2962, 2915, 2851, 1523,

1454, 1397, 1260, 1204, 1148, 1017, 857, 838, 784, 748, 632, 575, 567, 503, 389 cm^{-1}. – ^{1}H NMR (300 MHz, [C_6D_6], 20 °C): δ = 1.10 (d, 12 H, CH(CH_3)$_2$), 1.45 (s, 6 H, CCH_3), 1.93 (s, 12 H, *o*-CH_3), 2.33 (s, 6 H, p-CH_3), 3.32 (m, 2 H, CH(CH_3)$_2$), 4.71 (s, 1 H, *CH*), 6.74 (s, 4 H, Mes-*H*), 6.95 (m, 3 H, Dipp-*H*). – ^{13}C NMR (125 MHz, [C_6D_6], 20 °C): 18.81 (*o*-CH_3), 21.30 (*p*-CH_3), 23.33 (CCH_3), 23.87 (CH(CH_3)$_2$), 29.49 (CH(CH_3)$_2$), 94.20 (γ–*C*), 123.46 (*p*-Dipp), 124.67 (*m*-Dipp), 129.41 (*m*-Ar), 131.77 (*o*-Ar), 132.36 (*p*-Ar), 132.65 (*o*-Dipp), 143.69 (*i*-Ar), 146.14 (*i*-Dipp), 167.88 (β-*C*).

Reactions of Mesnacnac$_2$Zn$_2$ with Me$_3$MN$_3$ (M= Si; M= Sn)

Mesnacnac$_2$Zn$_2$ (25 mg, 30 µmol) was dissolved in C_6D_6 in a NMR- tube. After additon of Me_3SiN_3 (7 mg, 60 µmol), the solution was ultrasonically irradiated over night, giving a clear solution that was characterized by ^{1}H NMR spectroscopy without further work-up.

^{1}H-NMR (300 MHz, C_6D_6/ $CDCl_3$, 298 K): δ= 0.04 (s, 18 H, SiCH_3), 1.39 (s, 6 H, CCH_3), 2.01 (s, 12 H, o-CH_3), 2.34 (s, 6 H, p-CH_3), 4.71 (s, 1 H, *CH*), 6.74 (s, 4 H, Ar-*H*). ^{29}Si-NMR (300 MHz, C_6D_6, 298 K): δ= - 22 (*Si*-*Si*) ppm. The resonances agree perfectly with those previously reported for [MesnacnacZnN_3]$_2$ (**2**)[4] and Si_2Me_6.[5]

Mesnacnac$_2$Zn$_2$ (25 mg, 30 µmol) and Me_3SnN_3 (13 mg, 60 µmol) were dissolved in C_6D_6 in a NMR-tube and then ultrasonically irradiated over night, giving a clear solution that was characterized by ^{1}H NMR spectroscopy without further work-up.

^{1}H-NMR (300 MHz, C_6D_6/ $CDCl_3$, 298 K): δ= 0.39 (s, 18 H, SnCH_3), 1.39 (s, 6 H, CCH_3), 2.01 (s, 12 H, o-CH_3), 2.34 (s, 6 H, p-CH_3), 4.71 (s, 1 H, *CH*), 6.74 (s, 4 H, Ar-*H*). The resonances agree perfectly with those previously reported for [MesnacnacZnN_3]$_2$ (**2**)[4] and Sn_2Me_6.[6]

Crystal structure determination

The crystals of **3** were mounted on nylon loops in inert oil. Data were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å) at 180(1) K. The structure was solved by Direct Methods (SHELXS-97)[8] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-97).[9] Absorption corrections was performed semi-empirically from equivalent reflections on basis of multi-scans (Buker AXS APEX2). Hydrogen atoms were refined using a riding model or rigid methyl groups. The fluorobenzene molecule is diorderd over a centre of inversion.

CCDC 959097 (**3**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

References

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Table 1: Crystal structure data of 3

Identification code	sg_510_0m
Empirical formula	$C_{64}H_{72}FN_{10}Zn_2$
Formula weight	1131.05
Density (caculated)	1.249 g · cm^{-1}
F(000)	1190
Temperature	180(1) K
Crystal size	0.250 × 0.170 × 0.050 mm
Crystal colour	pale orange
Crystal description	tablet
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/n$
Unit cell dimensions	
a [Å]	12.8569(9)
b [Å]	17.7885(13)
c [Å]	13.5948(10)
α [°]	90
β [°]	104.691(4)
γ [°]	90
Volume	3007.6(4) $Å^3$
Z	2
Cell measurement reflections used	9552
Cell measurement *θ* min/max	2.52°/32.46°
Diffractometer control software	BRUKER D8 KAPPA APEX 2 (3.0-2009)
Diffractometer measurement device	Bruker D8 KAPPA series II with APEX II area detector system
Diffractometer measurement method	Data collection strategy APEX 2/COSMO
θ range for data collection	1.926°- 33.260°
Completeness to *θ* = 25.242°	100.0%
Index ranges	$-18 \leq h \leq 19$
	$-25 \leq k \leq 27$
	$-20 \leq l \leq 20$
Computing data reduction	BRUKER D8 KAPPA APEX 2 (3.0-2009)
Absorption coefficient	0.848 mm^{-1}

Absorption correction	Semi-empirical from equivalents
Computation absorption correction	BRUKER AXS SMART APEX 2 Vers. 3.0-2009
Max./min. Transmission	0.75/0.68
R_{merg} before/after correction	0.0467/0.0342
Computing structure solution	BRUKER D8 KAPPA APEX 2 (3.0-2009)
Computing structure refinement	SHELXL-2012 (Sheldrick, 2012)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	55228
Independent reflections	11500
R_{int}	0.0277
Data	8564
Restraints	0
Parameter	360
GooF	1.031
Weighting details	$w = 1/[\sigma^2(F_{obs}^2) + (0.0612P)^2 + 0.9651P]$
	where $P = (F_{obs}^2 + 2F_{calc}^2)/3$
R_1 [$I > 2\sigma(I)$]	0.0395
wR_2 [$I > 2\sigma(I)$]	0.1043
R_1 [all data]	0.0618
wR_2 [all data]	0.1178
Largest diff. peak and hole	1.395/-0.282

Table 2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for 3. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
Zn(1)	798(1)	1180(1)	5452(1)	24(1)
N(1)	581(1)	1668(1)	6670(1)	28(1)
N(2)	1051(1)	2060(1)	4708(1)	25(1)
N(3)	1772(1)	278(1)	5579(1)	25(1)
N(4)	1286(1)	-365(1)	5344(1)	27(1)
N(5)	241(1)	-356(1)	5035(1)	26(1)
C(1)	837(2)	2715(1)	7873(2)	48(1)
H(1A)	82	2827	7835	73
H(1B)	1256	3182	7988	73
H(1C)	1118	2366	8435	73

C(2)	924(1)	2362(1)	6886(1)	31(1)
C(3)	1367(1)	2812(1)	6241(1)	32(1)
H(3)	1734	3251	6543	39
C(4)	1338(1)	2699(1)	5210(1)	28(1)
C(5)	1631(2)	3365(1)	4649(1)	40(1)
H(5A)	2210	3224	4334	60
H(5B)	1874	3780	5127	60
H(5C)	1000	3526	4120	60
C(11)	-69(1)	1294(1)	7239(1)	30(1)
C(12)	371(1)	730(1)	7929(1)	37(1)
C(13)	-304(2)	337(1)	8406(1)	43(1)
H(13)	-9	-53	8870	51
C(14)	-1391(2)	498(1)	8223(1)	41(1)
C(15)	-1809(1)	1058(1)	7533(2)	39(1)
H(15)	-2553	1175	7404	47
C(16)	-1172(1)	1457(1)	7020(1)	33(1)
C(17)	1549(2)	543(2)	8156(2)	56(1)
H(17A)	1735	403	7524	84
H(17B)	1706	122	8635	84
H(17C)	1972	982	8455	84
C(18)	-2099(2)	62(1)	8754(2)	57(1)
H(18A)	-2785	325	8671	86
H(18B)	-1740	19	9480	86
H(18C)	-2231	-442	8456	86
C(19)	-1671(2)	2023(1)	6218(2)	46(1)
H(19A)	-1349	2518	6412	68
H(19B)	-2447	2049	6154	68
H(19C)	-1543	1871	5566	68
C(21)	851(1)	2039(1)	3618(1)	26(1)
C(22)	-198(1)	2172(1)	3028(1)	33(1)
C(23)	-408(1)	2122(1)	1975(1)	40(1)
H(23)	-1118	2214	1576	47
C(24)	387(2)	1944(1)	1490(1)	40(1)
C(25)	1413(1)	1804(1)	2094(1)	37(1)
H(25)	1967	1678	1774	44

C(26)	1662(1)	1841(1)	3153(1)	31(1)
C(27)	-1090(1)	2363(1)	3526(1)	46(1)
H(27A)	-1720	2539	3008	69
H(27B)	-846	2758	4033	69
H(27C)	-1282	1914	3858	69
C(28)	155(2)	1918(2)	347(2)	61(1)
H(28A)	-499	1623	74	92
H(28B)	761	1683	149	92
H(28C)	50	2430	75	92
C(29)	2790(1)	1666(1)	3770(2)	47(1)
H(29A)	2822	1145	4011	70
H(29B)	2985	2007	4354	70
H(29C)	3295	1732	3344	70
C(31)	2912(1)	224(1)	5874(1)	26(1)
C(32)	3473(1)	-417(1)	5718(1)	35(1)
H(32)	3093	-851	5417	42
C(33)	4590(1)	-418(1)	6003(2)	42(1)
H(33)	4968	-858	5899	51
C(34)	5154(1)	208(1)	6434(1)	43(1)
H(34)	5918	201	6623	52
C(35)	4606(1)	845(1)	6591(1)	42(1)
H(35)	4992	1278	6889	50
C(36)	3483(1)	854(1)	6312(1)	34(1)
H(36)	3108	1293	6423	41
C(41)	4314(2)	567(2)	10083(2)	70(1)
C(42)	4328(2)	302(2)	9152(2)	72(1)
H(42)	3861	513	8560	87
C(43)	5014(2)	-271(2)	9060(2)	72(1)
H(43)	5021	-459	8407	86
F(1)	3624(4)	1142(2)	10210(4)	102(1)

Table 3: Anisotropic displacement parameters ($Å^2 \times 10^3$) for 3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	26(1)	20(1)	27(1)	-2(1)	9(1)	-1(1)
N(1)	30(1)	28(1)	28(1)	-3(1)	12(1)	-2(1)
N(2)	27(1)	24(1)	26(1)	0(1)	8(1)	-1(1)
N(3)	23(1)	23(1)	30(1)	0(1)	6(1)	-1(1)
N(4)	24(1)	24(1)	32(1)	-1(1)	8(1)	0(1)
N(5)	23(1)	22(1)	34(1)	0(1)	7(1)	2(1)
C(1)	60(1)	50(1)	42(1)	-21(1)	25(1)	-17(1)
C(2)	30(1)	33(1)	31(1)	-8(1)	11(1)	-4(1)
C(3)	35(1)	28(1)	35(1)	-8(1)	12(1)	-10(1)
C(4)	27(1)	24(1)	34(1)	-1(1)	10(1)	-2(1)
C(5)	51(1)	26(1)	48(1)	-1(1)	21(1)	-7(1)
C(11)	32(1)	32(1)	29(1)	-5(1)	14(1)	-4(1)
C(12)	38(1)	45(1)	32(1)	3(1)	14(1)	1(1)
C(13)	53(1)	42(1)	39(1)	5(1)	22(1)	1(1)
C(14)	50(1)	36(1)	45(1)	-8(1)	28(1)	-9(1)
C(15)	35(1)	41(1)	48(1)	-8(1)	21(1)	-4(1)
C(16)	34(1)	32(1)	38(1)	-5(1)	16(1)	0(1)
C(17)	41(1)	83(2)	46(1)	24(1)	13(1)	13(1)
C(18)	68(1)	46(1)	73(1)	1(1)	48(1)	-7(1)
C(19)	38(1)	46(1)	56(1)	6(1)	18(1)	10(1)
C(21)	31(1)	23(1)	27(1)	1(1)	9(1)	0(1)
C(22)	33(1)	33(1)	32(1)	1(1)	8(1)	4(1)
C(23)	41(1)	43(1)	32(1)	2(1)	2(1)	5(1)
C(24)	54(1)	36(1)	28(1)	1(1)	11(1)	0(1)
C(25)	47(1)	32(1)	35(1)	1(1)	19(1)	3(1)
C(26)	33(1)	30(1)	33(1)	2(1)	13(1)	2(1)
C(27)	33(1)	65(1)	40(1)	1(1)	9(1)	12(1)
C(28)	80(2)	73(2)	29(1)	0(1)	12(1)	7(1)
C(29)	33(1)	65(1)	45(1)	2(1)	14(1)	11(1)
C(31)	24(1)	28(1)	26(1)	5(1)	6(1)	0(1)
C(32)	27(1)	31(1)	46(1)	4(1)	9(1)	3(1)
C(33)	29(1)	45(1)	53(1)	9(1)	11(1)	7(1)

C(34)	24(1)	58(1)	45(1)	11(1)	4(1)	-2(1)
C(35)	30(1)	50(1)	41(1)	1(1)	1(1)	-10(1)
C(36)	30(1)	35(1)	35(1)	0(1)	4(1)	-3(1)
C(41)	59(1)	70(2)	88(2)	21(1)	32(1)	-9(1)
C(42)	41(1)	109(2)	60(1)	37(2)	1(1)	-15(1)
C(43)	68(2)	97(2)	52(1)	0(1)	20(1)	-38(2)
F(1)	110(3)	83(3)	127(4)	13(2)	60(3)	-3(2)

Table 4: Bond lengths [Å] for sg_510_0m.

Zn(1)-N(2)	1.9364(12)	C(11)-C(12)	1.392(2)	C(26)-C(29)	1.512(2)
Zn(1)-N(1)	1.9519(12)	C(11)-C(16)	1.404(2)	C(31)-C(36)	1.389(2)
Zn(1)-N(5)#1	1.9801(12)	C(12)-C(13)	1.396(2)	C(31)-C(32)	1.393(2)
Zn(1)-N(3)	2.0166(12)	C(12)-C(17)	1.504(2)	C(32)-C(33)	1.389(2)
N(1)-C(2)	1.319(2)	C(13)-C(14)	1.386(3)	C(33)-C(34)	1.377(3)
N(1)-C(11)	1.4378(18)	C(14)-C(15)	1.379(3)	C(34)-C(35)	1.380(3)
N(2)-C(4)	1.3277(19)	C(14)-C(18)	1.513(2)	C(35)-C(36)	1.396(2)
N(2)-C(21)	1.4389(18)	C(15)-C(16)	1.397(2)	C(41)-C(42)	1.356(4)
N(3)-N(4)	1.3041(17)	C(16)-C(19)	1.503(3)	C(41)-C(43)#2	1.368(4)
N(3)-C(31)	1.4203(17)	C(21)-C(26)	1.395(2)	C(41)-F(1)	1.393(5)
N(4)-N(5)	1.3012(16)	C(21)-C(22)	1.404(2)	C(42)-C(43)	1.374(4)
N(5)-N(5)#1	1.403(2)	C(22)-C(23)	1.390(2)	C(43)-C(41)#2	1.368(4)
N(5)-Zn(1)#1	1.9801(12)	C(22)-C(27)	1.510(2)		
C(1)-C(2)	1.511(2)	C(23)-C(24)	1.387(3)		
C(2)-C(3)	1.409(2)	C(24)-C(25)	1.388(3)		
C(3)-C(4)	1.407(2)	C(24)-C(28)	1.507(2)		
C(4)-C(5)	1.509(2)	C(25)-C(26)	1.395(2)		

#1 -x,-y,-z+1 #2 -x+1,-y,-z+2

Table 5: Bond angles [°] for sg_510_0m.

N(2)-Zn(1)-N(1)	99.33(5)	C(15)-C(14)-C(18)	121.10(18)
N(2)-Zn(1)-N(5)#1	127.80(5)	C(13)-C(14)-C(18)	120.63(19)
N(1)-Zn(1)-N(5)#1	112.56(5)	C(14)-C(15)-C(16)	121.97(16)
N(2)-Zn(1)-N(3)	120.36(5)	C(15)-C(16)-C(11)	118.51(16)
N(1)-Zn(1)-N(3)	120.04(5)	C(15)-C(16)-C(19)	120.45(15)
N(5)#1-Zn(1)-N(3)	77.98(5)	C(11)-C(16)-C(19)	120.99(14)

C(2)-N(1)-C(11)	121.39(12)	C(26)-C(21)-C(22)	120.29(14)
C(2)-N(1)-Zn(1)	119.58(10)	C(26)-C(21)-N(2)	120.96(13)
C(11)-N(1)-Zn(1)	118.57(10)	C(22)-C(21)-N(2)	118.61(12)
C(4)-N(2)-C(21)	120.35(12)	C(23)-C(22)-C(21)	119.00(14)
C(4)-N(2)-Zn(1)	119.03(10)	C(23)-C(22)-C(27)	120.28(14)
C(21)-N(2)-Zn(1)	120.45(9)	C(21)-C(22)-C(27)	120.71(14)
N(4)-N(3)-C(31)	114.01(11)	C(24)-C(23)-C(22)	122.02(15)
N(4)-N(3)-Zn(1)	115.32(8)	C(23)-C(24)-C(25)	117.68(15)
C(31)-N(3)-Zn(1)	130.67(10)	C(23)-C(24)-C(28)	121.34(18)
N(5)-N(4)-N(3)	117.37(11)	C(25)-C(24)-C(28)	120.97(17)
N(4)-N(5)-N(5)#1	115.84(14)	C(24)-C(25)-C(26)	122.47(15)
N(4)-N(5)-Zn(1)#1	130.68(9)	C(21)-C(26)-C(25)	118.51(14)
N(5)#1-N(5)-Zn(1)#1	113.33(11)	C(21)-C(26)-C(29)	121.55(14)
N(1)-C(2)-C(3)	123.92(13)	C(25)-C(26)-C(29)	119.93(14)
N(1)-C(2)-C(1)	119.39(14)	C(36)-C(31)-C(32)	119.16(13)
C(3)-C(2)-C(1)	116.69(14)	C(36)-C(31)-N(3)	117.53(13)
C(4)-C(3)-C(2)	128.76(14)	C(32)-C(31)-N(3)	123.28(13)
N(2)-C(4)-C(3)	124.60(14)	C(33)-C(32)-C(31)	119.87(16)
N(2)-C(4)-C(5)	118.99(14)	C(34)-C(33)-C(32)	120.88(17)
C(3)-C(4)-C(5)	116.39(14)	C(33)-C(34)-C(35)	119.68(15)
C(12)-C(11)-C(16)	120.56(14)	C(34)-C(35)-C(36)	120.07(17)
C(12)-C(11)-N(1)	120.23(14)	C(31)-C(36)-C(35)	120.34(16)
C(16)-C(11)-N(1)	118.95(14)	C(42)-C(41)-C(43)#2	120.4(3)
C(11)-C(12)-C(13)	118.68(16)	C(42)-C(41)-F(1)	122.0(3)
C(11)-C(12)-C(17)	120.93(15)	C(43)#2-C(41)-F(1)	117.6(3)
C(13)-C(12)-C(17)	120.39(17)	C(41)-C(42)-C(43)	120.3(2)
C(14)-C(13)-C(12)	121.99(17)	C(41)#2-C(43)-C(42)	119.3(3)
C(15)-C(14)-C(13)	118.27(15)		

#1 -x,-y,-z+1 #2 -x+1,-y,-z+2

Table 6: Torsion angles [°] for sg_510_0m.

C(31)-N(3)-N(4)-N(5)	-177.84(12)	N(1)-C(2)-C(3)-C(4)	14.1(3)
Zn(1)-N(3)-N(4)-N(5)	1.50(16)	C(1)-C(2)-C(3)-C(4)	-165.20(17)
N(3)-N(4)-N(5)-N(5)#1	1.7(2)	C(21)-N(2)-C(4)-C(3)	168.18(14)
N(3)-N(4)-N(5)-Zn(1)#1	176.78(10)	Zn(1)-N(2)-C(4)-C(3)	-7.08(19)

C(11)-N(1)-C(2)-C(3)	-166.33(15)	C(21)-N(2)-C(4)-C(5)	-10.1(2)
Zn(1)-N(1)-C(2)-C(3)	5.7(2)	Zn(1)-N(2)-C(4)-C(5)	174.63(11)
C(11)-N(1)-C(2)-C(1)	12.9(2)	C(2)-C(3)-C(4)-N(2)	-13.3(3)
Zn(1)-N(1)-C(2)-C(1)	-175.02(13)	C(2)-C(3)-C(4)-C(5)	164.98(16)
C(2)-N(1)-C(11)-C(12)	-106.27(18)	C(21)-C(22)-C(23)-C(24)	0.2(3)
Zn(1)-N(1)-C(11)-C(12)	81.58(17)	C(27)-C(22)-C(23)-C(24)	-179.51(18)
C(2)-N(1)-C(11)-C(16)	79.58(19)	C(22)-C(23)-C(24)-C(25)	0.8(3)
Zn(1)-N(1)-C(11)-C(16)	-92.57(15)	C(22)-C(23)-C(24)-C(28)	-177.88(19)
C(16)-C(11)-C(12)-C(13)	-0.7(2)	C(23)-C(24)-C(25)-C(26)	-0.3(3)
N(1)-C(11)-C(12)-C(13)	-174.79(15)	C(28)-C(24)-C(25)-C(26)	178.38(19)
C(16)-C(11)-C(12)-C(17)	179.01(18)	C(22)-C(21)-C(26)-C(25)	2.1(2)
N(1)-C(11)-C(12)-C(17)	4.9(3)	N(2)-C(21)-C(26)-C(25)	177.71(14)
C(11)-C(12)-C(13)-C(14)	-0.9(3)	C(22)-C(21)-C(26)-C(29)	-177.64(16)
C(17)-C(12)-C(13)-C(14)	179.40(19)	N(2)-C(21)-C(26)-C(29)	-2.0(2)
C(12)-C(13)-C(14)-C(15)	1.1(3)	C(24)-C(25)-C(26)-C(21)	-1.1(3)
C(12)-C(13)-C(14)-C(18)	-179.90(19)	C(24)-C(25)-C(26)-C(29)	178.61(17)
C(13)-C(14)-C(15)-C(16)	0.3(3)	N(4)-N(3)-C(31)-C(36)	-168.43(13)
C(18)-C(14)-C(15)-C(16)	-178.74(18)	Zn(1)-N(3)-C(31)-C(36)	12.35(19)
C(14)-C(15)-C(16)-C(11)	-1.8(3)	N(4)-N(3)-C(31)-C(32)	13.4(2)
C(14)-C(15)-C(16)-C(19)	175.47(17)	Zn(1)-N(3)-C(31)-C(32)	-165.80(12)
C(12)-C(11)-C(16)-C(15)	2.0(2)	C(36)-C(31)-C(32)-C(33)	0.1(2)
N(1)-C(11)-C(16)-C(15)	176.14(14)	N(3)-C(31)-C(32)-C(33)	178.26(15)
C(12)-C(11)-C(16)-C(19)	-175.23(16)	C(31)-C(32)-C(33)-C(34)	-0.4(3)
N(1)-C(11)-C(16)-C(19)	-1.1(2)	C(32)-C(33)-C(34)-C(35)	0.3(3)
C(4)-N(2)-C(21)-C(26)	93.59(17)	C(33)-C(34)-C(35)-C(36)	-0.1(3)
Zn(1)-N(2)-C(21)-C(26)	-91.22(15)	C(32)-C(31)-C(36)-C(35)	0.1(2)
C(4)-N(2)-C(21)-C(22)	-90.72(17)	N(3)-C(31)-C(36)-C(35)	-178.10(14)
Zn(1)-N(2)-C(21)-C(22)	84.47(15)	C(34)-C(35)-C(36)-C(31)	-0.2(3)
C(26)-C(21)-C(22)-C(23)	-1.6(2)	C(43)#2-C(41)-C(42)-C(43)	0.3(4)
N(2)-C(21)-C(22)-C(23)	-177.36(15)	F(1)-C(41)-C(42)-C(43)	-179.4(3)
C(26)-C(21)-C(22)-C(27)	178.03(16)	C(41)-C(42)-C(43)-C(41)#2	-0.3(4)
N(2)-C(21)-C(22)-C(27)	2.3(2)		

#1 -x,-y,-z+1 #2 -x+1,-y,-z+2

Computational Studies

All geometries were fully optimized within the designated symmetry constraints (using tightened convergence criteria and improved integration grids) at the DFT level, employing the BP86 exchange-correlation functional [1] including a third-generation dispersion correction [2] as implemented in the Turbomole V6.3 quantum chemistry program package [3]. A triple-zeta valence quality Gaussian type function basis set termed def2-TZVP [4] was used throughout. The resolution-of-the-identity approximation was employed, making use of an appropriate auxiliary basis set [5]. Atom coordinates, energies, atomic partial charges (NPA,[6]) and Vibrational frequencies of all optimized geometries are given below.

[1] a) A. D. Becke, *Phys. Rev. A* **1988**, *38*, 3098; b) J. P. Perdew, *Phys. Rev. B* **1986**, *33*, 8822.

[2] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104.

[3] a) TURBOMOLE V6.3 2011, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com; b) R. Ahlrichs, M. Bär, M. Häser, H. Horn, C. Kölmel, *Chem. Phys. Letters* **1989**, *162*, 165; c) M. Häser, R. Ahlrichs, *J. Comput. Chem.* **1989**, *10*, 104; d) O. Treutler, R. Ahlrichs, *J. Chem. Phys.* **1995**, *102*, 346; e) M. v. Arnim, R. Ahlrichs, *J. Chem. Phys.* **1999**, *111*, 9183; f) P. Deglmann, F. Furche, R. Ahlrichs, Chem. Phys. Letters 2002, 362, 511; g) P. Deglmann, F. Furche, J. Chem. Phys. 2002, 117, 9535.

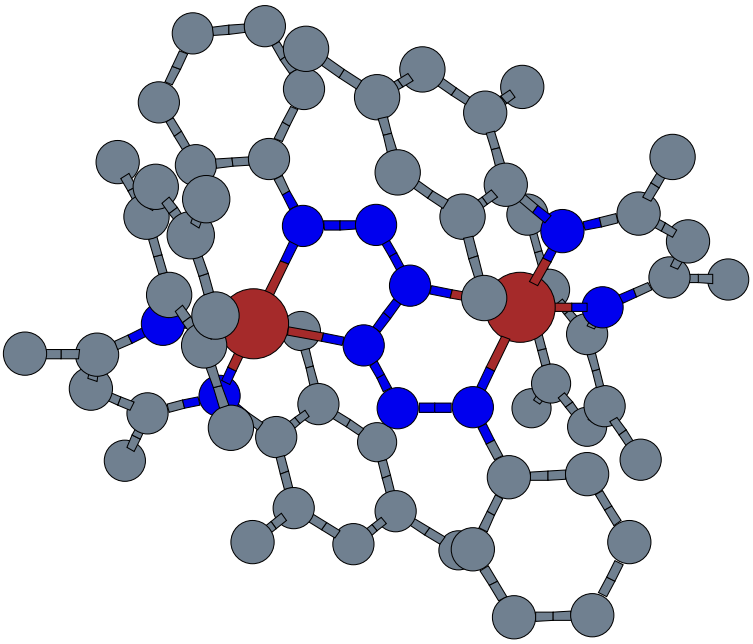
[4] F. Weigend, M. Häser, H. Patzelt, R. Ahlrichs, *Chem. Phys. Letters* **1998**, *294*, 143.

[5] F. Weigend, *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057.

[6] a) A. E. Reed, R. B. Weinstock, F. Weinhold, *J. Chem. Phys.* **1985**, *83*, 735; b) A. E. Reed, L. A. Curtis, F. Weinhold, *Chem Rev.* **1988**, *88*, 899.

Calculated Structures and Frequencies

Compound 3 in C_i Symmetry (H atoms omitted)



Energy (in Hartree) and atomic coordinates (in Å):

Energy = -6359.481170470

Zn	0.9678719	2.0955615	0.4870876
N	0.2833506	2.9253172	2.1349728
N	1.5493131	3.7073919	-0.4441806
N	2.1680266	0.4615787	0.5119964
N	1.5703750	-0.6792130	0.2746621
N	0.2946505	-0.6295218	0.0251182
C	0.1573324	4.7336953	3.7797707
H	-0.9091513	5.0013694	3.7421332
H	0.7239137	5.6323639	4.0509562
H	0.2662514	3.9802756	4.5721841
C	0.6196043	4.1750663	2.4518113
C	1.3553063	5.0249787	1.5944926
H	1.5883000	6.0061709	2.0044252
C	1.6653082	4.8605008	0.2237326
C	2.1113648	6.0870520	-0.5411948
H	3.0837880	5.9257788	-1.0273993
H	2.1802949	6.9625970	0.1133121
H	1.3947224	6.3044912	-1.3477020
C	-0.7871450	2.2296404	2.7663472
C	-0.5271057	1.0728641	3.5267055
C	-1.6087150	0.3133914	3.9914237
H	-1.4064111	-0.5999584	4.5562823
C	-2.9340431	0.6792409	3.7333092
C	-3.1618194	1.8271437	2.9656798

H	-4.1905477	2.1127592	2.7294284
C	-2.1150702	2.5971217	2.4528418
C	0.8923619	0.6599544	3.8100983
H	1.4527802	0.4953608	2.8779132
H	0.9245379	-0.2674451	4.3961639
H	1.4361332	1.4420381	4.3616326
C	-4.0934936	-0.1512526	4.2191816
H	-4.9222108	0.4834543	4.5653063
H	-3.7979724	-0.8140138	5.0421396
H	-4.4827707	-0.7882803	3.4095610
C	-2.3909215	3.7240057	1.4935803
H	-1.9870158	4.6900366	1.8288788
H	-3.4696902	3.8465284	1.3312032
H	-1.9188926	3.5075740	0.5234514
C	1.7436861	3.6405299	-1.8584356
C	0.6073985	3.6657657	-2.6959570
C	0.7846372	3.5391860	-4.0769144
H	-0.0963594	3.5559605	-4.7242359
C	2.0548939	3.4001919	-4.6493571
C	3.1594108	3.3750587	-3.7937574
H	4.1597067	3.2616914	-4.2184411
C	3.0308078	3.4653852	-2.4021378
C	-0.7679544	3.8014679	-2.0994353
H	-1.5262696	3.9493468	-2.8789284
H	-0.8232964	4.6426443	-1.3932299
H	-1.0431079	2.8957030	-1.5340354
C	2.2201292	3.2293731	-6.1382908
H	2.0660684	2.1779359	-6.4336819
H	3.2280141	3.5162509	-6.4679841
H	1.4913375	3.8318690	-6.6987211
C	4.2422945	3.3134920	-1.5212793
H	4.3504382	2.2663940	-1.1973260
H	4.1776371	3.9083801	-0.6018118
H	5.1593031	3.5926701	-2.0570655
C	3.5518616	0.3959923	0.7312364
C	4.3562794	-0.6639521	0.2755191
H	3.8896417	-1.4839131	-0.2672407
C	5.7311804	-0.6308561	0.4988439
H	6.3525158	-1.4503655	0.1333430
C	6.3226304	0.4451963	1.1719558
H	7.4005295	0.4652055	1.3357753
C	5.5209754	1.4982039	1.6247474
H	5.9699031	2.3435976	2.1479423
C	4.1452623	1.4771145	1.4061525
H	3.5108664	2.3001607	1.7445850
N	-2.1680266	-0.4615787	-0.5119964
N	-1.5703750	0.6792130	-0.2746621
N	-0.2946505	0.6295218	-0.0251182
C	-3.5518616	-0.3959923	-0.7312364
C	-4.3562794	0.6639521	-0.2755191
H	-3.8896417	1.4839131	0.2672407

C	-5.7311804	0.6308561	-0.4988439
H	-6.3525158	1.4503655	-0.1333430
C	-6.3226304	-0.4451963	-1.1719558
H	-7.4005295	-0.4652055	-1.3357753
C	-5.5209754	-1.4982039	-1.6247474
H	-5.9699031	-2.3435976	-2.1479423
C	-4.1452623	-1.4771145	-1.4061525
H	-3.5108664	-2.3001607	-1.7445850
Zn	-0.9678719	-2.0955615	-0.4870876
N	-0.2833506	-2.9253172	-2.1349728
N	-1.5493131	-3.7073919	0.4441806
C	-0.1573324	-4.7336953	-3.7797707
H	0.9091513	-5.0013694	-3.7421332
H	-0.7239137	-5.6323639	-4.0509562
H	-0.2662514	-3.9802756	-4.5721841
C	-0.6196043	-4.1750663	-2.4518113
C	-1.3553063	-5.0249787	-1.5944926
H	-1.5883000	-6.0061709	-2.0044252
C	-1.6653082	-4.8605008	-0.2237326
C	-2.1113648	-6.0870520	0.5411948
H	-3.0837880	-5.9257788	1.0273993
H	-2.1802949	-6.9625970	-0.1133121
H	-1.3947224	-6.3044912	1.3477020
C	0.7871450	-2.2296404	-2.7663472
C	0.5271057	-1.0728641	-3.5267055
C	1.6087150	-0.3133914	-3.9914237
H	1.4064111	0.5999584	-4.5562823
C	2.9340431	-0.6792409	-3.7333092
C	3.1618194	-1.8271437	-2.9656798
H	4.1905477	-2.1127592	-2.7294284
C	2.1150702	-2.5971217	-2.4528418
C	-0.8923619	-0.6599544	-3.8100983
H	-1.4527802	-0.4953608	-2.8779132
H	-0.9245379	0.2674451	-4.3961639
H	-1.4361332	-1.4420381	-4.3616326
C	4.0934936	0.1512526	-4.2191816
H	4.9222108	-0.4834543	-4.5653063
H	3.7979724	0.8140138	-5.0421396
H	4.4827707	0.7882803	-3.4095610
C	2.3909215	-3.7240057	-1.4935803
H	1.9870158	-4.6900366	-1.8288788
H	3.4696902	-3.8465284	-1.3312032
H	1.9188926	-3.5075740	-0.5234514
C	-1.7436861	-3.6405299	1.8584356
C	-0.6073985	-3.6657657	2.6959570
C	-0.7846372	-3.5391860	4.0769144
H	0.0963594	-3.5559605	4.7242359
C	-2.0548939	-3.4001919	4.6493571
C	-3.1594108	-3.3750587	3.7937574
H	-4.1597067	-3.2616914	4.2184411
C	-3.0308078	-3.4653852	2.4021378

C	0.7679544	-3.8014679	2.0994353
H	1.5262696	-3.9493468	2.8789284
H	0.8232964	-4.6426443	1.3932299
H	1.0431079	-2.8957030	1.5340354
C	-2.2201292	-3.2293731	6.1382908
H	-2.0660684	-2.1779359	6.4336819
H	-3.2280141	-3.5162509	6.4679841
H	-1.4913375	-3.8318690	6.6987211
C	-4.2422945	-3.3134920	1.5212793
H	-4.3504382	-2.2663940	1.1973260
H	-4.1776371	-3.9083801	0.6018118
H	-5.1593031	-3.5926701	2.0570655

Vibrational frequencies:

mode	symmetry	wave number	IR intensity	selection rules
		cm**(-1)	km/mol	IR RAMAN
1	ag	-2.71	0.00000	NO YES
2		-0.76	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7		0.00	0.00000	- -
8		0.00	0.00000	- -
9	au	16.65	0.04446	YES NO
10	ag	20.12	0.00000	NO YES
11	au	24.50	0.06841	YES NO
12	ag	26.76	0.00000	NO YES
13	au	31.88	0.08252	YES NO
14	ag	33.74	0.00000	NO YES
15	au	35.20	0.24987	YES NO
16	au	39.69	0.27439	YES NO
17	au	43.61	0.14520	YES NO
18	ag	44.16	0.00000	NO YES
19	au	46.68	0.14334	YES NO
20	ag	54.34	0.00000	NO YES
21	au	57.17	0.18114	YES NO
22	ag	59.26	0.00000	NO YES
23	au	62.96	0.21090	YES NO
24	ag	65.47	0.00000	NO YES
25	ag	70.42	0.00000	NO YES
26	au	72.07	0.20676	YES NO
27	ag	72.86	0.00000	NO YES
28	ag	75.33	0.00000	NO YES
29	au	78.44	0.14283	YES NO
30	ag	82.25	0.00000	NO YES

31	au	83.58	2.16252	YES	NO
32	ag	84.69	0.00000	NO	YES
33	ag	87.78	0.00000	NO	YES
34	au	88.86	0.60461	YES	NO
35	au	92.79	0.03219	YES	NO
36	ag	96.80	0.00000	NO	YES
37	au	102.01	0.09965	YES	NO
38	ag	104.08	0.00000	NO	YES
39	au	104.42	1.26819	YES	NO
40	au	107.50	0.54324	YES	NO
41	ag	109.02	0.00000	NO	YES
42	au	116.14	1.12903	YES	NO
43	ag	119.86	0.00000	NO	YES
44	ag	124.45	0.00000	NO	YES
45	au	126.38	2.21278	YES	NO
46	au	127.31	0.79242	YES	NO
47	ag	128.50	0.00000	NO	YES
48	ag	133.98	0.00000	NO	YES
49	au	134.41	1.54215	YES	NO
50	au	136.49	0.67794	YES	NO
51	ag	138.14	0.00000	NO	YES
52	ag	142.37	0.00000	NO	YES
53	au	145.87	1.34164	YES	NO
54	au	157.70	0.55170	YES	NO
55	ag	161.63	0.00000	NO	YES
56	au	165.98	1.32762	YES	NO
57	ag	176.55	0.00000	NO	YES
58	au	177.85	5.61474	YES	NO
59	ag	187.52	0.00000	NO	YES
60	au	188.20	5.50541	YES	NO
61	ag	192.08	0.00000	NO	YES
62	au	195.58	6.26257	YES	NO
63	ag	196.31	0.00000	NO	YES
64	au	197.36	6.04969	YES	NO
65	ag	199.43	0.00000	NO	YES
66	ag	204.92	0.00000	NO	YES
67	au	211.46	4.74399	YES	NO
68	au	213.21	1.37820	YES	NO
69	ag	213.85	0.00000	NO	YES
70	ag	216.65	0.00000	NO	YES
71	au	226.31	8.19336	YES	NO
72	ag	230.35	0.00000	NO	YES
73	au	236.38	0.47975	YES	NO
74	ag	236.52	0.00000	NO	YES
75	au	237.23	0.61077	YES	NO
76	ag	237.65	0.00000	NO	YES
77	au	264.32	7.12618	YES	NO
78	ag	279.32	0.00000	NO	YES
79	au	279.48	0.65579	YES	NO
80	ag	283.96	0.00000	NO	YES
81	au	286.13	1.07367	YES	NO

82	ag	288.72	0.00000	NO	YES
83	au	297.50	10.26866	YES	NO
84	ag	298.52	0.00000	NO	YES
85	au	303.12	7.12964	YES	NO
86	ag	306.57	0.00000	NO	YES
87	au	316.62	27.72439	YES	NO
88	ag	316.66	0.00000	NO	YES
89	au	324.23	0.28173	YES	NO
90	ag	324.81	0.00000	NO	YES
91	au	328.97	7.79171	YES	NO
92	au	347.76	28.88116	YES	NO
93	ag	347.92	0.00000	NO	YES
94	au	372.15	2.41983	YES	NO
95	ag	372.64	0.00000	NO	YES
96	ag	375.05	0.00000	NO	YES
97	au	375.07	3.02128	YES	NO
98	ag	386.11	0.00000	NO	YES
99	au	386.19	7.18674	YES	NO
100	ag	394.36	0.00000	NO	YES
101	au	394.98	0.34055	YES	NO
102	au	406.08	0.33096	YES	NO
103	ag	406.13	0.00000	NO	YES
104	au	426.37	1.07782	YES	NO
105	au	462.62	12.50285	YES	NO
106	au	475.84	0.14190	YES	NO
107	ag	475.89	0.00000	NO	YES
108	au	494.69	2.54428	YES	NO
109	ag	494.80	0.00000	NO	YES
110	ag	495.90	0.00000	NO	YES
111	ag	498.27	0.00000	NO	YES
112	au	498.66	2.24446	YES	NO
113	ag	500.60	0.00000	NO	YES
114	au	500.98	13.41266	YES	NO
115	ag	507.31	0.00000	NO	YES
116	au	507.33	0.93302	YES	NO
117	au	510.92	0.84216	YES	NO
118	ag	511.02	0.00000	NO	YES
119	au	512.80	11.86833	YES	NO
120	ag	519.27	0.00000	NO	YES
121	ag	527.67	0.00000	NO	YES
122	au	527.76	2.46663	YES	NO
123	au	548.85	5.95126	YES	NO
124	ag	550.84	0.00000	NO	YES
125	ag	562.60	0.00000	NO	YES
126	au	564.71	10.36804	YES	NO
127	ag	569.83	0.00000	NO	YES
128	au	569.92	1.57223	YES	NO
129	au	573.65	3.32389	YES	NO
130	ag	574.31	0.00000	NO	YES
131	au	580.42	2.45880	YES	NO
132	ag	580.54	0.00000	NO	YES

133	ag	592.68	0.00000	NO	YES
134	au	592.89	11.01355	YES	NO
135	ag	598.06	0.00000	NO	YES
136	au	607.89	3.73046	YES	NO
137	ag	610.40	0.00000	NO	YES
138	ag	619.32	0.00000	NO	YES
139	au	625.21	4.52841	YES	NO
140	ag	625.23	0.00000	NO	YES
141	ag	630.48	0.00000	NO	YES
142	au	630.57	7.41597	YES	NO
143	au	631.33	10.34676	YES	NO
144	au	651.38	5.03518	YES	NO
145	ag	651.57	0.00000	NO	YES
146	ag	680.52	0.00000	NO	YES
147	au	680.94	54.06956	YES	NO
148	ag	722.57	0.00000	NO	YES
149	au	722.58	4.07576	YES	NO
150	au	725.83	51.97577	YES	NO
151	au	731.74	0.58636	YES	NO
152	ag	731.85	0.00000	NO	YES
153	ag	741.89	0.00000	NO	YES
154	au	742.06	41.29381	YES	NO
155	ag	744.34	0.00000	NO	YES
156	au	746.51	57.44411	YES	NO
157	ag	767.50	0.00000	NO	YES
158	au	809.97	0.76694	YES	NO
159	ag	810.30	0.00000	NO	YES
160	ag	822.97	0.00000	NO	YES
161	au	823.03	2.16126	YES	NO
162	au	829.62	8.63372	YES	NO
163	ag	830.17	0.00000	NO	YES
164	ag	842.36	0.00000	NO	YES
165	au	842.91	52.31015	YES	NO
166	au	846.97	44.48855	YES	NO
167	ag	847.49	0.00000	NO	YES
168	ag	856.02	0.00000	NO	YES
169	au	856.23	0.68858	YES	NO
170	ag	862.59	0.00000	NO	YES
171	au	862.60	11.54709	YES	NO
172	ag	878.10	0.00000	NO	YES
173	au	879.03	5.82274	YES	NO
174	ag	889.61	0.00000	NO	YES
175	au	925.13	0.21008	YES	NO
176	ag	925.18	0.00000	NO	YES
177	au	928.99	0.84512	YES	NO
178	ag	929.07	0.00000	NO	YES
179	au	929.77	5.51413	YES	NO
180	ag	929.98	0.00000	NO	YES
181	au	930.24	1.37288	YES	NO
182	ag	930.51	0.00000	NO	YES
183	ag	932.10	0.00000	NO	YES

184	au	932.37	3.54707	YES	NO
185	ag	932.95	0.00000	NO	YES
186	au	932.95	1.14040	YES	NO
187	au	953.36	100.67938	YES	NO
188	au	956.44	8.78055	YES	NO
189	ag	956.64	0.00000	NO	YES
190	ag	959.35	0.00000	NO	YES
191	au	959.58	3.90875	YES	NO
192	ag	987.90	0.00000	NO	YES
193	au	988.05	4.48098	YES	NO
194	ag	1000.04	0.00000	NO	YES
195	au	1000.16	1.96705	YES	NO
196	ag	1001.48	0.00000	NO	YES
197	au	1001.66	20.08668	YES	NO
198	au	1003.67	21.50636	YES	NO
199	ag	1004.14	0.00000	NO	YES
200	au	1004.81	4.66639	YES	NO
201	ag	1005.13	0.00000	NO	YES
202	ag	1005.51	0.00000	NO	YES
203	au	1005.84	13.25396	YES	NO
204	ag	1008.86	0.00000	NO	YES
205	au	1008.92	10.47132	YES	NO
206	ag	1010.86	0.00000	NO	YES
207	au	1011.17	18.48288	YES	NO
208	ag	1016.82	0.00000	NO	YES
209	au	1016.84	1.39367	YES	NO
210	ag	1018.21	0.00000	NO	YES
211	au	1018.25	4.82790	YES	NO
212	ag	1020.65	0.00000	NO	YES
213	au	1020.70	3.83188	YES	NO
214	ag	1021.46	0.00000	NO	YES
215	au	1021.85	8.68587	YES	NO
216	ag	1022.28	0.00000	NO	YES
217	ag	1022.38	0.00000	NO	YES
218	au	1022.52	8.54785	YES	NO
219	au	1023.43	2.26644	YES	NO
220	ag	1024.02	0.00000	NO	YES
221	au	1024.12	4.12447	YES	NO
222	au	1026.71	0.70562	YES	NO
223	ag	1026.76	0.00000	NO	YES
224	au	1028.23	0.09738	YES	NO
225	ag	1028.41	0.00000	NO	YES
226	ag	1030.25	0.00000	NO	YES
227	au	1030.43	8.06363	YES	NO
228	ag	1041.31	0.00000	NO	YES
229	au	1081.71	8.17486	YES	NO
230	ag	1082.05	0.00000	NO	YES
231	ag	1141.34	0.00000	NO	YES
232	au	1141.38	80.16291	YES	NO
233	ag	1151.78	0.00000	NO	YES
234	au	1152.10	0.33259	YES	NO

235	au	1156.26	0.12749	YES	NO
236	ag	1156.38	0.00000	NO	YES
237	au	1169.97	29.27872	YES	NO
238	ag	1171.06	0.00000	NO	YES
239	ag	1188.65	0.00000	NO	YES
240	au	1189.18	130.53232	YES	NO
241	ag	1197.91	0.00000	NO	YES
242	au	1205.00	339.12650	YES	NO
243	au	1223.47	7.58863	YES	NO
244	ag	1223.77	0.00000	NO	YES
245	au	1240.58	3.49601	YES	NO
246	ag	1240.75	0.00000	NO	YES
247	ag	1241.11	0.00000	NO	YES
248	au	1241.35	1.52346	YES	NO
249	ag	1249.95	0.00000	NO	YES
250	au	1250.23	58.69571	YES	NO
251	au	1261.03	30.04395	YES	NO
252	ag	1261.09	0.00000	NO	YES
253	au	1282.26	722.76410	YES	NO
254	au	1293.82	6.21912	YES	NO
255	ag	1293.87	0.00000	NO	YES
256	au	1294.71	0.73322	YES	NO
257	ag	1294.74	0.00000	NO	YES
258	au	1301.93	293.01962	YES	NO
259	ag	1302.22	0.00000	NO	YES
260	ag	1310.57	0.00000	NO	YES
261	au	1319.72	0.05982	YES	NO
262	ag	1319.77	0.00000	NO	YES
263	ag	1320.04	0.00000	NO	YES
264	au	1320.11	5.35775	YES	NO
265	au	1332.33	227.82138	YES	NO
266	ag	1343.61	0.00000	NO	YES
267	au	1351.35	23.60316	YES	NO
268	ag	1351.41	0.00000	NO	YES
269	au	1353.24	292.89408	YES	NO
270	ag	1354.18	0.00000	NO	YES
271	au	1354.25	38.23296	YES	NO
272	ag	1361.68	0.00000	NO	YES
273	au	1362.12	17.61552	YES	NO
274	ag	1364.30	0.00000	NO	YES
275	au	1364.38	0.14212	YES	NO
276	au	1365.49	6.92968	YES	NO
277	ag	1365.74	0.00000	NO	YES
278	ag	1367.58	0.00000	NO	YES
279	au	1367.63	5.61379	YES	NO
280	ag	1369.64	0.00000	NO	YES
281	au	1370.13	4.59319	YES	NO
282	ag	1373.20	0.00000	NO	YES
283	au	1373.32	8.10017	YES	NO
284	ag	1386.07	0.00000	NO	YES
285	ag	1399.03	0.00000	NO	YES

286	au	1399.33	4.05227	YES	NO
287	au	1400.72	6.74315	YES	NO
288	ag	1400.86	0.00000	NO	YES
289	ag	1403.05	0.00000	NO	YES
290	au	1404.78	325.77885	YES	NO
291	ag	1410.64	0.00000	NO	YES
292	au	1411.29	64.08167	YES	NO
293	ag	1413.34	0.00000	NO	YES
294	au	1413.88	363.49599	YES	NO
295	ag	1423.00	0.00000	NO	YES
296	au	1423.26	96.32134	YES	NO
297	ag	1426.89	0.00000	NO	YES
298	au	1427.09	22.54568	YES	NO
299	au	1428.89	119.54681	YES	NO
300	ag	1429.17	0.00000	NO	YES
301	ag	1430.65	0.00000	NO	YES
302	au	1430.70	3.88739	YES	NO
303	ag	1433.75	0.00000	NO	YES
304	au	1433.93	62.70659	YES	NO
305	ag	1434.85	0.00000	NO	YES
306	au	1434.88	26.23976	YES	NO
307	ag	1435.85	0.00000	NO	YES
308	au	1435.92	13.14167	YES	NO
309	au	1437.27	4.72389	YES	NO
310	ag	1437.98	0.00000	NO	YES
311	au	1440.04	8.67819	YES	NO
312	ag	1440.07	0.00000	NO	YES
313	au	1441.38	23.20132	YES	NO
314	ag	1441.61	0.00000	NO	YES
315	ag	1444.56	0.00000	NO	YES
316	au	1445.35	8.19496	YES	NO
317	ag	1446.99	0.00000	NO	YES
318	au	1448.06	5.58542	YES	NO
319	au	1455.81	16.82613	YES	NO
320	ag	1456.22	0.00000	NO	YES
321	ag	1457.53	0.00000	NO	YES
322	ag	1457.84	0.00000	NO	YES
323	au	1458.20	27.90976	YES	NO
324	au	1461.10	892.92803	YES	NO
325	ag	1469.57	0.00000	NO	YES
326	au	1469.77	33.70723	YES	NO
327	au	1472.91	68.88260	YES	NO
328	ag	1473.18	0.00000	NO	YES
329	au	1478.09	93.33611	YES	NO
330	ag	1479.16	0.00000	NO	YES
331	ag	1508.59	0.00000	NO	YES
332	au	1509.49	541.46526	YES	NO
333	au	1535.43	514.70238	YES	NO
334	ag	1536.46	0.00000	NO	YES
335	au	1565.93	8.54811	YES	NO
336	ag	1566.00	0.00000	NO	YES

337	ag	1567.73	0.00000	NO	YES
338	au	1567.78	3.70321	YES	NO
339	ag	1571.40	0.00000	NO	YES
340	au	1571.76	7.90767	YES	NO
341	au	1591.22	61.06152	YES	NO
342	ag	1591.52	0.00000	NO	YES
343	au	1600.01	20.21775	YES	NO
344	ag	1600.15	0.00000	NO	YES
345	ag	1600.24	0.00000	NO	YES
346	au	1600.34	14.07784	YES	NO
347	ag	2946.46	0.00000	NO	YES
348	au	2946.48	77.01758	YES	NO
349	au	2950.93	25.01695	YES	NO
350	ag	2950.97	0.00000	NO	YES
351	ag	2957.70	0.00000	NO	YES
352	au	2957.78	57.08932	YES	NO
353	ag	2960.53	0.00000	NO	YES
354	au	2960.53	41.65179	YES	NO
355	ag	2965.39	0.00000	NO	YES
356	au	2965.40	13.77110	YES	NO
357	au	2965.74	38.10253	YES	NO
358	ag	2965.76	0.00000	NO	YES
359	ag	2971.21	0.00000	NO	YES
360	au	2971.21	35.96135	YES	NO
361	au	2971.43	22.33218	YES	NO
362	ag	2971.43	0.00000	NO	YES
363	au	3006.18	54.97897	YES	NO
364	ag	3006.20	0.00000	NO	YES
365	ag	3006.94	0.00000	NO	YES
366	au	3006.95	18.22700	YES	NO
367	au	3012.32	44.58058	YES	NO
368	ag	3012.33	0.00000	NO	YES
369	au	3013.57	8.55676	YES	NO
370	ag	3013.58	0.00000	NO	YES
371	au	3019.67	23.26145	YES	NO
372	ag	3019.70	0.00000	NO	YES
373	ag	3022.79	0.00000	NO	YES
374	au	3022.79	32.41928	YES	NO
375	au	3026.15	8.83994	YES	NO
376	ag	3026.15	0.00000	NO	YES
377	ag	3028.70	0.00000	NO	YES
378	au	3028.71	12.82112	YES	NO
379	au	3039.62	20.30426	YES	NO
380	ag	3039.62	0.00000	NO	YES
381	au	3043.59	17.57695	YES	NO
382	ag	3043.60	0.00000	NO	YES
383	ag	3045.08	0.00000	NO	YES
384	au	3045.16	29.42534	YES	NO
385	ag	3046.60	0.00000	NO	YES
386	au	3046.63	27.31976	YES	NO
387	ag	3048.56	0.00000	NO	YES

388	au	3048.58	23.54367	YES	NO
389	ag	3053.08	0.00000	NO	YES
390	au	3053.11	27.02722	YES	NO
391	ag	3061.69	0.00000	NO	YES
392	au	3061.69	35.43361	YES	NO
393	ag	3069.20	0.00000	NO	YES
394	au	3069.21	35.80875	YES	NO
395	au	3071.16	30.45168	YES	NO
396	ag	3071.18	0.00000	NO	YES
397	ag	3073.53	0.00000	NO	YES
398	au	3073.54	29.76702	YES	NO
399	ag	3080.36	0.00000	NO	YES
400	au	3080.38	5.59487	YES	NO
401	ag	3080.58	0.00000	NO	YES
402	au	3080.60	36.44125	YES	NO
403	ag	3085.73	0.00000	NO	YES
404	au	3085.74	20.90143	YES	NO
405	au	3093.51	6.87815	YES	NO
406	ag	3093.56	0.00000	NO	YES
407	au	3105.09	29.11646	YES	NO
408	ag	3105.11	0.00000	NO	YES
409	au	3119.84	26.65766	YES	NO
410	ag	3119.86	0.00000	NO	YES
411	au	3120.74	60.74412	YES	NO
412	ag	3120.80	0.00000	NO	YES
413	au	3142.84	3.05662	YES	NO
414	ag	3143.17	0.00000	NO	YES

Atomic populations according to NPA:

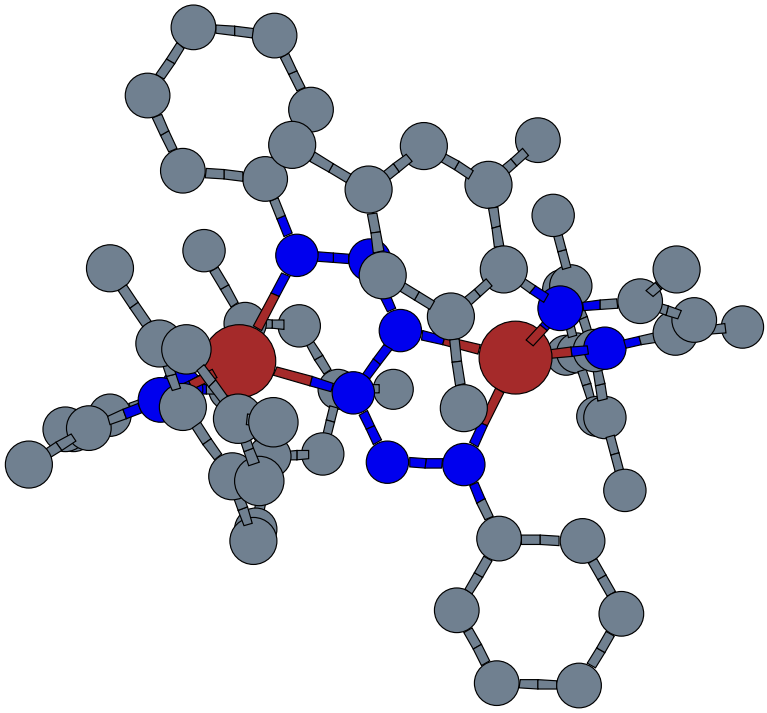
atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 zn	1.61695	6.38940	12.02923	9.96439	0.00003	0.00000
2 n	-0.71898	3.33685	4.37262	0.00851	0.00100	0.00000
3 n	-0.72160	3.33788	4.37449	0.00824	0.00098	0.00000
4 n	-0.50572	3.39326	4.10430	0.00723	0.00094	0.00000
5 n	-0.02250	3.39445	3.61461	0.01230	0.00114	0.00000
6 n	-0.36043	3.40834	3.94450	0.00660	0.00099	0.00000
7 c	-0.67687	3.12126	3.54972	0.00492	0.00096	0.00000
8 h	0.23457	0.76469	0.00074	0.00000	0.00000	0.00000
9 h	0.22580	0.77345	0.00075	0.00000	0.00000	0.00000
10 h	0.23244	0.76687	0.00069	0.00000	0.00000	0.00000
11 c	0.27372	2.88272	2.83731	0.00471	0.00154	0.00000
12 c	-0.40471	2.96880	3.42976	0.00388	0.00227	0.00000
13 h	0.21362	0.78543	0.00095	0.00000	0.00000	0.00000
14 c	0.27164	2.88523	2.83691	0.00467	0.00155	0.00000
15 c	-0.67715	3.12067	3.55056	0.00495	0.00097	0.00000
16 h	0.23427	0.76500	0.00073	0.00000	0.00000	0.00000
17 h	0.22527	0.77398	0.00075	0.00000	0.00000	0.00000

18 h	0.23802	0.76129	0.00070	0.00000	0.00000	0.00000
19 c	0.10677	2.86949	3.01705	0.00499	0.00171	0.00000
20 c	-0.02271	2.91782	3.09926	0.00381	0.00182	0.00000
21 c	-0.20933	2.96695	3.23596	0.00446	0.00196	0.00000
22 h	0.21238	0.78679	0.00083	0.00000	0.00000	0.00000
23 c	-0.01804	2.91622	3.09651	0.00354	0.00176	0.00000
24 c	-0.21559	2.96482	3.24432	0.00442	0.00202	0.00000
25 h	0.20470	0.79448	0.00082	0.00000	0.00000	0.00000
26 c	-0.01929	2.91804	3.09538	0.00399	0.00188	0.00000
27 c	-0.64252	3.10435	3.53286	0.00444	0.00087	0.00000
28 h	0.23170	0.76759	0.00070	0.00000	0.00000	0.00000
29 h	0.22004	0.77922	0.00075	0.00000	0.00000	0.00000
30 h	0.22040	0.77884	0.00075	0.00000	0.00000	0.00000
31 c	-0.63524	3.10591	3.52388	0.00457	0.00088	0.00000
32 h	0.21727	0.78197	0.00076	0.00000	0.00000	0.00000
33 h	0.21867	0.78062	0.00071	0.00000	0.00000	0.00000
34 h	0.22671	0.77257	0.00072	0.00000	0.00000	0.00000
35 c	-0.65009	3.10371	3.54093	0.00456	0.00089	0.00000
36 h	0.21875	0.78048	0.00077	0.00000	0.00000	0.00000
37 h	0.21746	0.78178	0.00076	0.00000	0.00000	0.00000
38 h	0.23618	0.76312	0.00070	0.00000	0.00000	0.00000
39 c	0.10774	2.87068	3.01494	0.00493	0.00171	0.00000
40 c	-0.01995	2.91943	3.09480	0.00385	0.00186	0.00000
41 c	-0.21564	2.96585	3.24350	0.00428	0.00201	0.00000
42 h	0.20618	0.79301	0.00081	0.00000	0.00000	0.00000
43 c	-0.02273	2.91575	3.10155	0.00364	0.00179	0.00000
44 c	-0.21145	2.96507	3.23989	0.00446	0.00203	0.00000
45 h	0.20718	0.79200	0.00082	0.00000	0.00000	0.00000
46 c	-0.02370	2.91799	3.09993	0.00391	0.00187	0.00000
47 c	-0.65206	3.10633	3.54020	0.00464	0.00089	0.00000
48 h	0.22119	0.77805	0.00076	0.00000	0.00000	0.00000
49 h	0.22300	0.77628	0.00072	0.00000	0.00000	0.00000
50 h	0.23866	0.76062	0.00072	0.00000	0.00000	0.00000
51 c	-0.64046	3.10724	3.52797	0.00436	0.00089	0.00000
52 h	0.22096	0.77830	0.00075	0.00000	0.00000	0.00000
53 h	0.21936	0.77993	0.00071	0.00000	0.00000	0.00000
54 h	0.22161	0.77768	0.00071	0.00000	0.00000	0.00000
55 c	-0.65148	3.10475	3.54120	0.00465	0.00088	0.00000
56 h	0.24181	0.75747	0.00072	0.00000	0.00000	0.00000
57 h	0.22474	0.77450	0.00076	0.00000	0.00000	0.00000
58 h	0.22006	0.77916	0.00078	0.00000	0.00000	0.00000
59 c	0.09681	2.88868	3.00817	0.00455	0.00179	0.00000
60 c	-0.23522	2.98320	3.24557	0.00453	0.00192	0.00000
61 h	0.23582	0.76336	0.00082	0.00000	0.00000	0.00000
62 c	-0.20481	2.98254	3.21636	0.00402	0.00189	0.00000
63 h	0.21222	0.78699	0.00079	0.00000	0.00000	0.00000
64 c	-0.22957	2.98409	3.23965	0.00395	0.00188	0.00000
65 h	0.21344	0.78577	0.00079	0.00000	0.00000	0.00000
66 c	-0.20969	2.98127	3.22244	0.00409	0.00189	0.00000
67 h	0.21478	0.78442	0.00080	0.00000	0.00000	0.00000
68 c	-0.22817	2.98105	3.24078	0.00442	0.00191	0.00000

69 h	0.22283	0.77639	0.00078	0.00000	0.00000	0.00000
70 n	-0.50572	3.39326	4.10430	0.00723	0.00094	0.00000
71 n	-0.02250	3.39445	3.61461	0.01230	0.00114	0.00000
72 n	-0.36043	3.40834	3.94450	0.00660	0.00099	0.00000
73 c	0.09681	2.88868	3.00817	0.00455	0.00179	0.00000
74 c	-0.23522	2.98320	3.24557	0.00453	0.00192	0.00000
75 h	0.23582	0.76336	0.00082	0.00000	0.00000	0.00000
76 c	-0.20481	2.98254	3.21636	0.00402	0.00189	0.00000
77 h	0.21222	0.78699	0.00079	0.00000	0.00000	0.00000
78 c	-0.22957	2.98409	3.23965	0.00395	0.00188	0.00000
79 h	0.21344	0.78577	0.00079	0.00000	0.00000	0.00000
80 c	-0.20969	2.98127	3.22244	0.00409	0.00189	0.00000
81 h	0.21478	0.78442	0.00080	0.00000	0.00000	0.00000
82 c	-0.22817	2.98105	3.24078	0.00442	0.00191	0.00000
83 h	0.22283	0.77639	0.00078	0.00000	0.00000	0.00000
84 zn	1.61695	6.38940	12.02923	9.96439	0.00003	0.00000
85 n	-0.71898	3.33685	4.37262	0.00851	0.00100	0.00000
86 n	-0.72160	3.33788	4.37449	0.00824	0.00098	0.00000
87 c	-0.67687	3.12126	3.54972	0.00492	0.00096	0.00000
88 h	0.23457	0.76469	0.00074	0.00000	0.00000	0.00000
89 h	0.22580	0.77345	0.00075	0.00000	0.00000	0.00000
90 h	0.23244	0.76687	0.00069	0.00000	0.00000	0.00000
91 c	0.27372	2.88272	2.83731	0.00471	0.00154	0.00000
92 c	-0.40471	2.96880	3.42976	0.00388	0.00227	0.00000
93 h	0.21362	0.78543	0.00095	0.00000	0.00000	0.00000
94 c	0.27164	2.88523	2.83691	0.00467	0.00155	0.00000
95 c	-0.67715	3.12067	3.55056	0.00495	0.00097	0.00000
96 h	0.23427	0.76500	0.00073	0.00000	0.00000	0.00000
97 h	0.22527	0.77398	0.00075	0.00000	0.00000	0.00000
98 h	0.23802	0.76129	0.00070	0.00000	0.00000	0.00000
99 c	0.10677	2.86949	3.01705	0.00499	0.00171	0.00000
100 c	-0.02271	2.91782	3.09926	0.00381	0.00182	0.00000
101 c	-0.20933	2.96695	3.23596	0.00446	0.00196	0.00000
102 h	0.21238	0.78679	0.00083	0.00000	0.00000	0.00000
103 c	-0.01804	2.91622	3.09651	0.00354	0.00176	0.00000
104 c	-0.21559	2.96482	3.24432	0.00442	0.00202	0.00000
105 h	0.20470	0.79448	0.00082	0.00000	0.00000	0.00000
106 c	-0.01929	2.91804	3.09538	0.00399	0.00188	0.00000
107 c	-0.64252	3.10435	3.53286	0.00444	0.00087	0.00000
108 h	0.23170	0.76759	0.00070	0.00000	0.00000	0.00000
109 h	0.22004	0.77922	0.00075	0.00000	0.00000	0.00000
110 h	0.22040	0.77884	0.00075	0.00000	0.00000	0.00000
111 c	-0.63524	3.10591	3.52388	0.00457	0.00088	0.00000
112 h	0.21727	0.78197	0.00076	0.00000	0.00000	0.00000
113 h	0.21867	0.78062	0.00071	0.00000	0.00000	0.00000
114 h	0.22671	0.77257	0.00072	0.00000	0.00000	0.00000
115 c	-0.65009	3.10371	3.54093	0.00456	0.00089	0.00000
116 h	0.21875	0.78048	0.00077	0.00000	0.00000	0.00000
117 h	0.21746	0.78178	0.00076	0.00000	0.00000	0.00000
118 h	0.23618	0.76312	0.00070	0.00000	0.00000	0.00000
119 c	0.10774	2.87068	3.01494	0.00493	0.00171	0.00000

120 c	-0.01995	2.91943	3.09480	0.00385	0.00186	0.00000
121 c	-0.21564	2.96585	3.24350	0.00428	0.00201	0.00000
122 h	0.20618	0.79301	0.00081	0.00000	0.00000	0.00000
123 c	-0.02273	2.91575	3.10155	0.00364	0.00179	0.00000
124 c	-0.21145	2.96507	3.23989	0.00446	0.00203	0.00000
125 h	0.20718	0.79200	0.00082	0.00000	0.00000	0.00000
126 c	-0.02370	2.91799	3.09993	0.00391	0.00187	0.00000
127 c	-0.65206	3.10633	3.54020	0.00464	0.00089	0.00000
128 h	0.22119	0.77805	0.00076	0.00000	0.00000	0.00000
129 h	0.22300	0.77628	0.00072	0.00000	0.00000	0.00000
130 h	0.23866	0.76062	0.00072	0.00000	0.00000	0.00000
131 c	-0.64046	3.10724	3.52797	0.00436	0.00089	0.00000
132 h	0.22096	0.77830	0.00075	0.00000	0.00000	0.00000
133 h	0.21936	0.77993	0.00071	0.00000	0.00000	0.00000
134 h	0.22161	0.77768	0.00071	0.00000	0.00000	0.00000
135 c	-0.65148	3.10475	3.54120	0.00465	0.00088	0.00000
136 h	0.24181	0.75747	0.00072	0.00000	0.00000	0.00000
137 h	0.22474	0.77450	0.00076	0.00000	0.00000	0.00000
138 h	0.22006	0.77916	0.00078	0.00000	0.00000	0.00000

Compound 3 in C_1 Symmetry (H atoms omitted)



Energy (in Hartree) and atomic coordinates (in Å):

Energy = -6359.483006781

Zn	1.0873017	2.0079650	0.2231119
N	0.2183860	2.7354120	1.8480420
N	1.8805004	3.6572752	-0.4424288
N	2.2123341	0.3648687	0.6037041
N	1.5972450	-0.7746512	0.4191739
N	0.3872537	-0.7293206	-0.0487618
C	0.0261006	4.3362533	3.6855382
H	-1.0359174	4.6019271	3.5770297
H	0.5596764	5.2040212	4.0899871
H	0.0706679	3.5102076	4.4093737
C	0.6059082	3.8972952	2.3598940
C	1.5160770	4.7618740	1.7053610
H	1.7687645	5.6683905	2.2521072
C	1.9903682	4.7152356	0.3755026
C	2.6235858	5.9756715	-0.1731648
H	3.6193638	5.7798288	-0.5943758
H	2.7077867	6.7460009	0.6008852
H	2.0121182	6.3725771	-0.9978177
C	-0.9442725	2.0354437	2.2795126
C	-0.8387159	0.7973178	2.9387784
C	-2.0029038	0.0368389	3.1332931
H	-1.9137869	-0.9380836	3.6180904
C	-3.2590038	0.4868703	2.7202065
C	-3.3365739	1.7320593	2.0840825

H	-4.3067846	2.0858100	1.7274410
C	-2.2022306	2.5006232	1.8268697
C	0.4866515	0.2706341	3.4268525
H	1.3196469	0.9121704	3.1177664
H	0.6715785	-0.7411407	3.0404099
H	0.4960267	0.2001701	4.5253763
C	-4.5049019	-0.3410609	2.8970694
H	-5.2917776	0.2273346	3.4156258
H	-4.3020878	-1.2511862	3.4739648
H	-4.9131735	-0.6377817	1.9174137
C	-2.2946407	3.7431133	0.9824478
H	-1.9216119	4.6426122	1.4939590
H	-3.3314589	3.9326628	0.6757911
H	-1.6798887	3.6254328	0.0770348
C	2.2560631	3.7709515	-1.8166810
C	1.2612647	4.0710297	-2.7679235
C	1.6329190	4.2052380	-4.1100871
H	0.8640111	4.4495916	-4.8478885
C	2.9560188	4.0323106	-4.5307025
C	3.9115126	3.6814806	-3.5692416
H	4.9454319	3.5113342	-3.8817335
C	3.5855306	3.5311313	-2.2162264
C	-0.1726505	4.2133479	-2.3321788
H	-0.8147804	4.5236191	-3.1662769
H	-0.2822348	4.9414909	-1.5151272
H	-0.5559013	3.2521250	-1.9487712
C	3.3311726	4.1483255	-5.9859645
H	2.6321253	4.7960928	-6.5325243
H	3.3136094	3.1599067	-6.4731599
H	4.3444791	4.5554322	-6.1103015
C	4.6171189	3.0923295	-1.2125934
H	4.3786870	2.0910730	-0.8237148
H	4.6565293	3.7518598	-0.3339554
H	5.6177766	3.0546205	-1.6616185
C	3.4992371	0.2756700	1.1557149
C	4.2810044	-0.8940132	1.1202891
H	3.8817619	-1.7849543	0.6374799
C	5.5510638	-0.8940645	1.6932750
H	6.1541218	-1.8030327	1.6571659
C	6.0630422	0.2580743	2.3025393
H	7.0602460	0.2496312	2.7436753
C	5.2862551	1.4203752	2.3356680
H	5.6716254	2.3246429	2.8088767
C	4.0136173	1.4326483	1.7684147
H	3.4019770	2.3382317	1.7920649
N	-2.0772606	-0.5221520	-0.5613035
N	-1.3918256	0.5911556	-0.6490319
N	-0.1178731	0.5239737	-0.3911846
C	-3.4550555	-0.4061780	-0.7923209
C	-4.1254877	0.8244788	-0.9263994
H	-3.5524335	1.7471375	-0.8667055

C	-5.5056292	0.8448485	-1.1117247
H	-6.0169856	1.8047579	-1.2035808
C	-6.2425152	-0.3445398	-1.1711031
H	-7.3236806	-0.3167558	-1.3094521
C	-5.5755065	-1.5677935	-1.0561391
H	-6.1315775	-2.5047455	-1.1099443
C	-4.1946849	-1.5990912	-0.8718581
H	-3.6677807	-2.5527785	-0.7952166
Zn	-0.9817578	-2.2045116	-0.2507432
N	-0.5731938	-3.1120743	-1.9648152
N	-1.2893957	-3.8043225	0.8309547
C	-0.4211446	-5.0040506	-3.5007062
H	0.6324117	-4.8419260	-3.7716238
H	-0.6322580	-6.0786960	-3.5354978
H	-1.0220863	-4.4930611	-4.2673141
C	-0.7159203	-4.4189026	-2.1385770
C	-1.1126513	-5.2928925	-1.0992123
H	-1.1994236	-6.3404253	-1.3808977
C	-1.2863640	-5.0270831	0.2743050
C	-1.4353927	-6.2231644	1.1906293
H	-2.3499558	-6.1606574	1.7964446
H	-1.4503755	-7.1584040	0.6208545
H	-0.5965917	-6.2586214	1.9021376
C	0.0781179	-2.2602212	-2.9027646
C	-0.6664596	-1.4029977	-3.7318134
C	0.0190636	-0.4370774	-4.4827404
H	-0.5600194	0.2376624	-5.1192976
C	1.4069675	-0.2989237	-4.4269917
C	2.1234583	-1.1719454	-3.5950754
H	3.2098253	-1.0704759	-3.5245112
C	1.4879176	-2.1508511	-2.8310079
C	-2.1679669	-1.4980191	-3.8145869
H	-2.5638175	-2.2460299	-3.1187662
H	-2.6407749	-0.5362053	-3.5691966
H	-2.4886834	-1.7728036	-4.8313371
C	2.1272929	0.7497329	-5.2335657
H	2.6493532	0.3004912	-6.0937528
H	1.4333761	1.5087734	-5.6180920
H	2.8786406	1.2717939	-4.6244733
C	2.2690421	-3.0454354	-1.9053425
H	2.2051769	-4.1034365	-2.2037398
H	3.3287580	-2.7602416	-1.8865571
H	1.8779030	-2.9842854	-0.8790717
C	-1.3799310	-3.6629072	2.2506989
C	-0.1953444	-3.5198675	3.0009472
C	-0.2978507	-3.3087454	4.3811643
H	0.6194904	-3.1848937	4.9623887
C	-1.5346209	-3.2537410	5.0332260
C	-2.6919435	-3.4215805	4.2631053
H	-3.6685986	-3.3865861	4.7532311
C	-2.6406664	-3.6107939	2.8773360

C	1.1461449	-3.5944941	2.3218950
H	1.9614809	-3.5826003	3.0564399
H	1.2385989	-4.5056978	1.7120689
H	1.3028939	-2.7450932	1.6374386
C	-1.6237644	-2.9726911	6.5118425
H	-1.7583118	-1.8945001	6.6956647
H	-2.4778875	-3.4904994	6.9704973
H	-0.7109427	-3.2841837	7.0378675
C	-3.9019078	-3.7175152	2.0646645
H	-4.0193439	-2.8325751	1.4229831
H	-3.8963178	-4.5888152	1.3943815
H	-4.7862002	-3.7824210	2.7112286

Vibrational frequencies:

mode	symmetry	wave number	IR intensity	selection rules
		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	13.52	0.00463	YES YES
8	a	19.86	0.00932	YES YES
9	a	22.23	0.03509	YES YES
10	a	23.61	0.03091	YES YES
11	a	25.63	0.09285	YES YES
12	a	31.73	0.00358	YES YES
13	a	33.33	0.04049	YES YES
14	a	37.15	0.13582	YES YES
15	a	40.60	0.40846	YES YES
16	a	42.27	0.01107	YES YES
17	a	44.65	0.05657	YES YES
18	a	47.08	0.18090	YES YES
19	a	47.98	0.14744	YES YES
20	a	52.20	0.06054	YES YES
21	a	54.33	0.03236	YES YES
22	a	57.03	0.08730	YES YES
23	a	57.74	0.04166	YES YES
24	a	62.56	0.10194	YES YES
25	a	67.11	0.09164	YES YES
26	a	67.90	0.43866	YES YES
27	a	73.19	0.05065	YES YES
28	a	75.58	0.03394	YES YES
29	a	79.32	0.33364	YES YES
30	a	81.05	0.03875	YES YES

31	a	83.45	0.36157	YES	YES
32	a	86.40	0.08316	YES	YES
33	a	91.95	0.21611	YES	YES
34	a	92.94	0.18988	YES	YES
35	a	96.70	0.31048	YES	YES
36	a	100.96	0.06919	YES	YES
37	a	102.69	0.65017	YES	YES
38	a	107.00	0.42055	YES	YES
39	a	109.27	0.59026	YES	YES
40	a	116.52	0.19443	YES	YES
41	a	120.04	0.28249	YES	YES
42	a	123.25	0.47028	YES	YES
43	a	126.42	0.23355	YES	YES
44	a	127.46	1.04158	YES	YES
45	a	129.36	0.25874	YES	YES
46	a	132.84	0.58528	YES	YES
47	a	136.30	0.38200	YES	YES
48	a	139.36	0.32831	YES	YES
49	a	140.73	0.66162	YES	YES
50	a	144.78	0.17327	YES	YES
51	a	149.46	0.57195	YES	YES
52	a	153.04	1.83370	YES	YES
53	a	160.19	0.36893	YES	YES
54	a	161.83	1.03776	YES	YES
55	a	166.45	0.19785	YES	YES
56	a	168.50	1.60399	YES	YES
57	a	174.62	0.65206	YES	YES
58	a	180.73	5.19740	YES	YES
59	a	184.19	1.62702	YES	YES
60	a	191.43	2.88109	YES	YES
61	a	194.86	6.85678	YES	YES
62	a	197.30	1.26017	YES	YES
63	a	199.93	0.91392	YES	YES
64	a	204.31	1.04172	YES	YES
65	a	207.81	2.49798	YES	YES
66	a	209.82	3.78042	YES	YES
67	a	213.40	0.55281	YES	YES
68	a	215.66	3.60166	YES	YES
69	a	216.61	1.94424	YES	YES
70	a	220.60	3.24082	YES	YES
71	a	225.95	0.37746	YES	YES
72	a	230.46	0.53592	YES	YES
73	a	231.52	0.11682	YES	YES
74	a	235.40	3.03363	YES	YES
75	a	240.44	0.05629	YES	YES
76	a	242.64	0.46782	YES	YES
77	a	272.70	17.06773	YES	YES
78	a	277.69	0.78030	YES	YES
79	a	278.65	1.97445	YES	YES
80	a	280.30	0.31030	YES	YES
81	a	282.09	0.33037	YES	YES

82	a	286.10	0.78014	YES	YES
83	a	293.54	7.07639	YES	YES
84	a	300.19	0.90521	YES	YES
85	a	301.10	1.15853	YES	YES
86	a	306.48	1.08240	YES	YES
87	a	314.47	14.15289	YES	YES
88	a	318.64	0.97625	YES	YES
89	a	322.25	4.37483	YES	YES
90	a	325.17	0.55604	YES	YES
91	a	330.03	17.42890	YES	YES
92	a	349.90	9.21576	YES	YES
93	a	351.43	16.87578	YES	YES
94	a	373.74	1.02556	YES	YES
95	a	375.95	1.12331	YES	YES
96	a	376.98	1.26756	YES	YES
97	a	381.02	0.71394	YES	YES
98	a	388.20	2.70256	YES	YES
99	a	388.28	7.06621	YES	YES
100	a	393.90	0.73005	YES	YES
101	a	398.64	0.15023	YES	YES
102	a	406.26	0.11625	YES	YES
103	a	413.73	0.13363	YES	YES
104	a	424.59	1.16164	YES	YES
105	a	460.67	13.34901	YES	YES
106	a	476.39	0.10577	YES	YES
107	a	477.29	0.09900	YES	YES
108	a	494.51	0.43908	YES	YES
109	a	496.86	0.10195	YES	YES
110	a	498.76	6.24148	YES	YES
111	a	499.05	0.60160	YES	YES
112	a	500.09	4.64526	YES	YES
113	a	501.30	0.31323	YES	YES
114	a	501.88	2.45049	YES	YES
115	a	503.14	0.81414	YES	YES
116	a	504.90	1.22791	YES	YES
117	a	508.35	0.07083	YES	YES
118	a	509.21	0.16138	YES	YES
119	a	517.16	5.03727	YES	YES
120	a	517.77	6.40754	YES	YES
121	a	527.98	0.79447	YES	YES
122	a	528.64	0.40162	YES	YES
123	a	549.29	3.45857	YES	YES
124	a	551.41	2.74675	YES	YES
125	a	563.04	3.88250	YES	YES
126	a	564.02	4.15133	YES	YES
127	a	570.32	1.02520	YES	YES
128	a	570.46	0.89223	YES	YES
129	a	571.20	0.66272	YES	YES
130	a	574.73	2.60026	YES	YES
131	a	580.07	1.11934	YES	YES
132	a	580.49	0.22984	YES	YES

133	a	593.51	1.53457	YES	YES
134	a	593.80	5.62154	YES	YES
135	a	598.43	0.22880	YES	YES
136	a	606.17	1.95546	YES	YES
137	a	611.96	0.69859	YES	YES
138	a	618.51	0.12887	YES	YES
139	a	625.01	1.49852	YES	YES
140	a	627.21	0.65898	YES	YES
141	a	629.04	2.19095	YES	YES
142	a	630.10	1.83711	YES	YES
143	a	633.03	18.12353	YES	YES
144	a	647.82	1.80335	YES	YES
145	a	650.35	2.78229	YES	YES
146	a	681.52	24.47256	YES	YES
147	a	687.99	28.00251	YES	YES
148	a	720.47	8.30522	YES	YES
149	a	721.24	55.20038	YES	YES
150	a	722.02	2.75245	YES	YES
151	a	731.93	0.72338	YES	YES
152	a	734.59	0.51751	YES	YES
153	a	736.14	16.11176	YES	YES
154	a	740.39	19.94939	YES	YES
155	a	744.09	8.42923	YES	YES
156	a	745.53	51.32002	YES	YES
157	a	765.68	0.28817	YES	YES
158	a	814.33	0.19394	YES	YES
159	a	816.86	0.20638	YES	YES
160	a	819.12	0.34538	YES	YES
161	a	824.58	0.10437	YES	YES
162	a	828.85	4.99715	YES	YES
163	a	829.34	3.06753	YES	YES
164	a	842.04	24.57478	YES	YES
165	a	846.95	13.41469	YES	YES
166	a	847.75	29.59399	YES	YES
167	a	850.11	22.54127	YES	YES
168	a	850.32	1.35397	YES	YES
169	a	855.47	1.55745	YES	YES
170	a	861.17	1.65066	YES	YES
171	a	875.21	0.23089	YES	YES
172	a	878.28	1.24568	YES	YES
173	a	880.69	3.60337	YES	YES
174	a	882.54	2.00083	YES	YES
175	a	924.87	0.93421	YES	YES
176	a	926.12	0.96174	YES	YES
177	a	928.08	0.50633	YES	YES
178	a	928.68	0.65672	YES	YES
179	a	929.43	1.75115	YES	YES
180	a	929.66	0.71112	YES	YES
181	a	929.77	2.48496	YES	YES
182	a	930.77	0.35120	YES	YES
183	a	933.47	1.55820	YES	YES

184	a	933.94	0.61882	YES	YES
185	a	934.79	0.91689	YES	YES
186	a	940.69	0.19851	YES	YES
187	a	949.33	103.42825	YES	YES
188	a	953.57	7.56345	YES	YES
189	a	954.34	5.76005	YES	YES
190	a	957.65	2.91622	YES	YES
191	a	958.88	1.95794	YES	YES
192	a	985.93	1.36812	YES	YES
193	a	987.09	2.41325	YES	YES
194	a	999.72	15.43309	YES	YES
195	a	1000.04	5.30880	YES	YES
196	a	1002.10	6.41664	YES	YES
197	a	1002.26	9.68534	YES	YES
198	a	1003.27	4.72380	YES	YES
199	a	1004.44	10.63003	YES	YES
200	a	1005.59	5.16108	YES	YES
201	a	1005.61	4.40798	YES	YES
202	a	1006.00	10.17739	YES	YES
203	a	1006.23	2.86685	YES	YES
204	a	1010.92	3.19624	YES	YES
205	a	1012.16	6.97573	YES	YES
206	a	1013.02	3.01523	YES	YES
207	a	1014.30	4.15844	YES	YES
208	a	1015.21	1.42484	YES	YES
209	a	1018.22	1.03381	YES	YES
210	a	1019.72	0.87293	YES	YES
211	a	1020.00	2.01893	YES	YES
212	a	1020.67	0.95880	YES	YES
213	a	1021.40	0.80488	YES	YES
214	a	1021.41	4.69928	YES	YES
215	a	1021.86	1.56134	YES	YES
216	a	1022.04	1.03294	YES	YES
217	a	1022.64	1.26395	YES	YES
218	a	1022.72	6.73615	YES	YES
219	a	1023.10	0.87382	YES	YES
220	a	1024.01	0.58241	YES	YES
221	a	1024.23	0.95047	YES	YES
222	a	1026.59	3.47639	YES	YES
223	a	1026.95	0.68025	YES	YES
224	a	1028.71	1.80772	YES	YES
225	a	1029.24	0.57189	YES	YES
226	a	1029.85	5.66293	YES	YES
227	a	1030.60	0.42724	YES	YES
228	a	1036.27	0.44808	YES	YES
229	a	1082.18	4.09848	YES	YES
230	a	1083.17	5.94567	YES	YES
231	a	1139.79	30.81795	YES	YES
232	a	1140.76	37.64899	YES	YES
233	a	1150.18	1.66292	YES	YES
234	a	1150.67	1.04209	YES	YES

235	a	1155.48	0.08798	YES	YES
236	a	1156.27	0.01566	YES	YES
237	a	1169.08	48.33772	YES	YES
238	a	1172.07	5.99250	YES	YES
239	a	1188.28	34.07498	YES	YES
240	a	1189.22	104.79067	YES	YES
241	a	1198.58	23.11160	YES	YES
242	a	1209.46	300.21349	YES	YES
243	a	1224.39	7.90790	YES	YES
244	a	1224.62	2.83280	YES	YES
245	a	1238.19	0.15690	YES	YES
246	a	1238.29	0.97213	YES	YES
247	a	1238.79	1.13304	YES	YES
248	a	1242.49	0.09782	YES	YES
249	a	1247.93	15.37242	YES	YES
250	a	1248.82	70.14664	YES	YES
251	a	1262.96	13.94027	YES	YES
252	a	1264.72	12.01350	YES	YES
253	a	1277.80	635.31831	YES	YES
254	a	1286.88	1.45381	YES	YES
255	a	1287.17	0.91471	YES	YES
256	a	1296.29	2.46387	YES	YES
257	a	1296.43	12.73108	YES	YES
258	a	1297.26	7.89168	YES	YES
259	a	1302.16	355.78250	YES	YES
260	a	1311.40	0.60970	YES	YES
261	a	1318.09	0.70053	YES	YES
262	a	1318.92	0.07842	YES	YES
263	a	1325.88	0.58410	YES	YES
264	a	1328.28	1.92005	YES	YES
265	a	1333.48	183.73405	YES	YES
266	a	1343.68	5.37320	YES	YES
267	a	1350.92	14.36433	YES	YES
268	a	1352.15	11.53635	YES	YES
269	a	1354.34	11.39310	YES	YES
270	a	1355.02	27.55694	YES	YES
271	a	1355.87	270.19144	YES	YES
272	a	1357.07	23.97027	YES	YES
273	a	1358.05	9.00685	YES	YES
274	a	1360.34	0.18126	YES	YES
275	a	1360.93	14.92537	YES	YES
276	a	1363.56	0.74159	YES	YES
277	a	1365.42	2.15298	YES	YES
278	a	1368.24	5.23690	YES	YES
279	a	1369.27	2.26641	YES	YES
280	a	1369.60	8.23978	YES	YES
281	a	1372.00	2.42485	YES	YES
282	a	1372.78	1.11716	YES	YES
283	a	1378.35	1.76083	YES	YES
284	a	1386.87	36.94207	YES	YES
285	a	1399.27	9.39371	YES	YES

286	a	1399.61	26.32196	YES	YES
287	a	1399.88	4.03275	YES	YES
288	a	1402.49	36.41470	YES	YES
289	a	1403.32	19.23280	YES	YES
290	a	1406.04	312.99862	YES	YES
291	a	1411.00	53.45772	YES	YES
292	a	1411.52	40.77699	YES	YES
293	a	1414.71	92.63628	YES	YES
294	a	1416.00	175.66328	YES	YES
295	a	1423.09	19.44252	YES	YES
296	a	1424.04	5.12726	YES	YES
297	a	1424.67	23.58112	YES	YES
298	a	1424.70	5.11536	YES	YES
299	a	1428.60	32.87328	YES	YES
300	a	1429.65	85.41170	YES	YES
301	a	1432.00	38.51948	YES	YES
302	a	1432.53	16.28182	YES	YES
303	a	1433.76	6.86253	YES	YES
304	a	1434.69	9.90397	YES	YES
305	a	1435.27	5.00001	YES	YES
306	a	1435.46	9.49972	YES	YES
307	a	1436.11	7.54372	YES	YES
308	a	1438.97	4.33313	YES	YES
309	a	1439.62	16.66204	YES	YES
310	a	1440.96	15.18187	YES	YES
311	a	1441.41	7.18476	YES	YES
312	a	1441.46	3.44404	YES	YES
313	a	1442.78	10.75807	YES	YES
314	a	1442.90	3.61528	YES	YES
315	a	1443.34	16.08234	YES	YES
316	a	1446.40	1.05160	YES	YES
317	a	1447.51	6.69178	YES	YES
318	a	1447.64	9.38216	YES	YES
319	a	1452.95	12.00447	YES	YES
320	a	1453.68	12.98057	YES	YES
321	a	1457.55	41.75198	YES	YES
322	a	1458.81	31.95913	YES	YES
323	a	1460.33	432.20732	YES	YES
324	a	1462.60	205.37089	YES	YES
325	a	1466.99	130.66623	YES	YES
326	a	1468.09	32.80039	YES	YES
327	a	1473.18	21.69312	YES	YES
328	a	1474.90	20.73034	YES	YES
329	a	1478.92	93.30409	YES	YES
330	a	1479.79	2.02466	YES	YES
331	a	1508.49	277.83629	YES	YES
332	a	1514.76	443.43662	YES	YES
333	a	1541.38	271.48449	YES	YES
334	a	1547.85	226.16358	YES	YES
335	a	1566.16	1.93344	YES	YES
336	a	1567.39	2.32015	YES	YES

337	a	1568.98	8.07998	YES	YES
338	a	1569.03	0.70148	YES	YES
339	a	1571.39	0.14124	YES	YES
340	a	1571.75	8.79876	YES	YES
341	a	1591.14	45.17068	YES	YES
342	a	1592.27	23.63326	YES	YES
343	a	1598.20	9.33456	YES	YES
344	a	1599.00	6.96981	YES	YES
345	a	1600.62	9.38306	YES	YES
346	a	1601.06	14.01880	YES	YES
347	a	2942.27	12.76574	YES	YES
348	a	2948.50	16.93569	YES	YES
349	a	2952.39	48.10970	YES	YES
350	a	2953.06	27.88029	YES	YES
351	a	2953.81	34.60709	YES	YES
352	a	2954.62	36.63950	YES	YES
353	a	2958.48	24.75153	YES	YES
354	a	2961.93	21.23445	YES	YES
355	a	2962.49	22.70454	YES	YES
356	a	2965.91	15.31343	YES	YES
357	a	2968.02	10.09203	YES	YES
358	a	2968.86	21.48890	YES	YES
359	a	2970.95	14.93118	YES	YES
360	a	2971.69	15.10855	YES	YES
361	a	2972.11	14.44238	YES	YES
362	a	2972.76	13.04782	YES	YES
363	a	3000.89	11.87572	YES	YES
364	a	3002.45	9.68720	YES	YES
365	a	3004.22	16.22602	YES	YES
366	a	3010.98	9.67650	YES	YES
367	a	3011.55	22.76426	YES	YES
368	a	3011.95	21.79673	YES	YES
369	a	3013.27	12.56767	YES	YES
370	a	3014.79	8.99222	YES	YES
371	a	3016.64	12.50006	YES	YES
372	a	3021.05	10.40322	YES	YES
373	a	3024.04	6.17142	YES	YES
374	a	3025.00	11.55196	YES	YES
375	a	3025.91	4.40999	YES	YES
376	a	3027.21	4.66228	YES	YES
377	a	3027.73	4.62902	YES	YES
378	a	3028.05	5.47802	YES	YES
379	a	3039.52	9.59742	YES	YES
380	a	3039.84	10.11153	YES	YES
381	a	3043.24	11.50846	YES	YES
382	a	3043.41	8.80037	YES	YES
383	a	3044.13	10.81770	YES	YES
384	a	3045.32	16.61014	YES	YES
385	a	3045.41	16.13518	YES	YES
386	a	3048.69	10.10403	YES	YES
387	a	3048.81	21.02670	YES	YES

388	a	3059.14	6.95305	YES	YES
389	a	3064.44	19.01294	YES	YES
390	a	3065.32	5.95297	YES	YES
391	a	3066.27	5.75633	YES	YES
392	a	3066.56	23.95570	YES	YES
393	a	3069.36	15.12215	YES	YES
394	a	3069.74	17.67310	YES	YES
395	a	3071.45	13.97043	YES	YES
396	a	3072.95	21.99880	YES	YES
397	a	3073.47	18.25270	YES	YES
398	a	3074.77	10.49760	YES	YES
399	a	3075.09	19.24487	YES	YES
400	a	3078.15	12.19241	YES	YES
401	a	3079.81	2.82816	YES	YES
402	a	3080.90	11.96652	YES	YES
403	a	3083.91	8.33077	YES	YES
404	a	3093.42	7.37754	YES	YES
405	a	3093.47	0.19682	YES	YES
406	a	3095.36	1.88996	YES	YES
407	a	3104.43	12.07589	YES	YES
408	a	3105.32	14.74660	YES	YES
409	a	3119.99	30.22139	YES	YES
410	a	3121.48	27.27044	YES	YES
411	a	3122.08	13.75284	YES	YES
412	a	3123.89	14.31470	YES	YES
413	a	3131.40	4.16352	YES	YES
414	a	3145.02	1.23083	YES	YES

Atomic populations according to NPA:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 zn	1.61547	6.39142	12.02915	9.96393	0.00003	0.00000
2 n	-0.71183	3.33627	4.36599	0.00855	0.00103	0.00000
3 n	-0.72897	3.33906	4.38071	0.00825	0.00096	0.00000
4 n	-0.50418	3.39362	4.10243	0.00721	0.00093	0.00000
5 n	-0.03590	3.38874	3.63385	0.01213	0.00119	0.00000
6 n	-0.35147	3.40656	3.93724	0.00670	0.00097	0.00000
7 c	-0.67751	3.12114	3.55054	0.00487	0.00096	0.00000
8 h	0.23542	0.76385	0.00073	0.00000	0.00000	0.00000
9 h	0.22451	0.77474	0.00075	0.00000	0.00000	0.00000
10 h	0.23510	0.76422	0.00068	0.00000	0.00000	0.00000

11 c	0.27600	2.88180	2.83595	0.00471	0.00154	0.00000
12 c	-0.40870	2.96853	3.43401	0.00389	0.00226	0.00000
13 h	0.21432	0.78472	0.00095	0.00000	0.00000	0.00000
14 c	0.26960	2.88555	2.83863	0.00465	0.00156	0.00000
15 c	-0.67636	3.12021	3.55023	0.00496	0.00097	0.00000
16 h	0.23306	0.76620	0.00074	0.00000	0.00000	0.00000
17 h	0.22548	0.77377	0.00075	0.00000	0.00000	0.00000
18 h	0.23775	0.76155	0.00070	0.00000	0.00000	0.00000
19 c	0.10084	2.86935	3.02311	0.00501	0.00169	0.00000
20 c	-0.02735	2.91781	3.10391	0.00386	0.00178	0.00000
21 c	-0.21372	2.96695	3.24031	0.00454	0.00191	0.00000
22 h	0.22292	0.77625	0.00083	0.00000	0.00000	0.00000
23 c	-0.01613	2.91547	3.09527	0.00366	0.00173	0.00000
24 c	-0.20933	2.96433	3.23846	0.00456	0.00199	0.00000
25 h	0.20940	0.78977	0.00082	0.00000	0.00000	0.00000
26 c	-0.02065	2.91774	3.09700	0.00404	0.00187	0.00000
27 c	-0.65355	3.10348	3.54467	0.00455	0.00085	0.00000
28 h	0.23026	0.76902	0.00072	0.00000	0.00000	0.00000
29 h	0.23320	0.76608	0.00072	0.00000	0.00000	0.00000
30 h	0.22293	0.77627	0.00080	0.00000	0.00000	0.00000
31 c	-0.64352	3.10477	3.53330	0.00458	0.00087	0.00000
32 h	0.21903	0.78019	0.00077	0.00000	0.00000	0.00000
33 h	0.22015	0.77914	0.00071	0.00000	0.00000	0.00000
34 h	0.23069	0.76859	0.00071	0.00000	0.00000	0.00000
35 c	-0.64808	3.10345	3.53922	0.00453	0.00089	0.00000
36 h	0.21886	0.78038	0.00076	0.00000	0.00000	0.00000
37 h	0.21782	0.78143	0.00075	0.00000	0.00000	0.00000
38 h	0.23065	0.76865	0.00070	0.00000	0.00000	0.00000
39 c	0.10997	2.87021	3.01313	0.00496	0.00173	0.00000
40 c	-0.02127	2.91912	3.09640	0.00387	0.00188	0.00000
41 c	-0.21514	2.96613	3.24265	0.00432	0.00202	0.00000
42 h	0.20607	0.79311	0.00082	0.00000	0.00000	0.00000
43 c	-0.01398	2.91660	3.09195	0.00364	0.00179	0.00000
44 c	-0.21922	2.96664	3.24625	0.00432	0.00201	0.00000
45 h	0.20692	0.79227	0.00082	0.00000	0.00000	0.00000
46 c	-0.02203	2.91886	3.09740	0.00390	0.00187	0.00000
47 c	-0.64699	3.10704	3.53451	0.00456	0.00089	0.00000
48 h	0.22077	0.77846	0.00076	0.00000	0.00000	0.00000
49 h	0.22463	0.77465	0.00072	0.00000	0.00000	0.00000
50 h	0.23283	0.76648	0.00069	0.00000	0.00000	0.00000
51 c	-0.63936	3.10681	3.52731	0.00435	0.00090	0.00000
52 h	0.21865	0.78064	0.00072	0.00000	0.00000	0.00000
53 h	0.22492	0.77435	0.00073	0.00000	0.00000	0.00000
54 h	0.22000	0.77928	0.00072	0.00000	0.00000	0.00000
55 c	-0.64394	3.10466	3.53387	0.00452	0.00089	0.00000
56 h	0.24009	0.75921	0.00071	0.00000	0.00000	0.00000
57 h	0.22135	0.77789	0.00076	0.00000	0.00000	0.00000
58 h	0.21940	0.77982	0.00078	0.00000	0.00000	0.00000
59 c	0.09867	2.88919	3.00577	0.00459	0.00179	0.00000
60 c	-0.23831	2.98301	3.24896	0.00439	0.00195	0.00000
61 h	0.23017	0.76903	0.00080	0.00000	0.00000	0.00000

62 c	-0.20263	2.98267	3.21407	0.00399	0.00190	0.00000
63 h	0.21261	0.78659	0.00079	0.00000	0.00000	0.00000
64 c	-0.22988	2.98397	3.24009	0.00393	0.00189	0.00000
65 h	0.21316	0.78605	0.00079	0.00000	0.00000	0.00000
66 c	-0.20821	2.98114	3.22109	0.00408	0.00189	0.00000
67 h	0.21418	0.78502	0.00079	0.00000	0.00000	0.00000
68 c	-0.23198	2.98167	3.24392	0.00448	0.00191	0.00000
69 h	0.22628	0.77294	0.00079	0.00000	0.00000	0.00000
70 n	-0.49672	3.39012	4.09847	0.00720	0.00094	0.00000
71 n	-0.01811	3.39205	3.61277	0.01214	0.00115	0.00000
72 n	-0.35316	3.40891	3.93633	0.00698	0.00094	0.00000
73 c	0.10374	2.88756	3.00226	0.00464	0.00180	0.00000
74 c	-0.23603	2.98195	3.24755	0.00462	0.00190	0.00000
75 h	0.23672	0.76244	0.00083	0.00000	0.00000	0.00000
76 c	-0.20642	2.98158	3.21891	0.00405	0.00189	0.00000
77 h	0.21238	0.78682	0.00080	0.00000	0.00000	0.00000
78 c	-0.23226	2.98331	3.24312	0.00396	0.00187	0.00000
79 h	0.21391	0.78529	0.00079	0.00000	0.00000	0.00000
80 c	-0.21200	2.98012	3.22591	0.00409	0.00188	0.00000
81 h	0.21536	0.78385	0.00080	0.00000	0.00000	0.00000
82 c	-0.24167	2.97912	3.25606	0.00459	0.00191	0.00000
83 h	0.22216	0.77703	0.00081	0.00000	0.00000	0.00000
84 zn	1.61583	6.38935	12.02937	9.96542	0.00003	0.00000
85 n	-0.71207	3.33640	4.36606	0.00859	0.00102	0.00000
86 n	-0.73268	3.33974	4.38387	0.00814	0.00093	0.00000
87 c	-0.67738	3.12138	3.55018	0.00486	0.00096	0.00000
88 h	0.23572	0.76356	0.00072	0.00000	0.00000	0.00000
89 h	0.22412	0.77513	0.00075	0.00000	0.00000	0.00000
90 h	0.23522	0.76410	0.00068	0.00000	0.00000	0.00000
91 c	0.27733	2.88140	2.83504	0.00470	0.00154	0.00000
92 c	-0.40132	2.96646	3.42874	0.00382	0.00230	0.00000
93 h	0.21283	0.78622	0.00095	0.00000	0.00000	0.00000
94 c	0.26874	2.88489	2.84017	0.00464	0.00156	0.00000
95 c	-0.67459	3.12001	3.54865	0.00496	0.00097	0.00000
96 h	0.23198	0.76727	0.00075	0.00000	0.00000	0.00000
97 h	0.22564	0.77360	0.00076	0.00000	0.00000	0.00000
98 h	0.23607	0.76323	0.00071	0.00000	0.00000	0.00000
99 c	0.10263	2.86999	3.02070	0.00498	0.00171	0.00000
100 c	-0.02651	2.91756	3.10322	0.00390	0.00183	0.00000
101 c	-0.20797	2.96533	3.23635	0.00427	0.00202	0.00000
102 h	0.20427	0.79493	0.00081	0.00000	0.00000	0.00000
103 c	-0.01495	2.91622	3.09344	0.00354	0.00176	0.00000
104 c	-0.21285	2.96580	3.24073	0.00430	0.00201	0.00000
105 h	0.20549	0.79370	0.00081	0.00000	0.00000	0.00000
106 c	-0.01988	2.91845	3.09562	0.00397	0.00185	0.00000
107 c	-0.65060	3.10503	3.54013	0.00458	0.00086	0.00000
108 h	0.22936	0.76992	0.00072	0.00000	0.00000	0.00000
109 h	0.23281	0.76649	0.00070	0.00000	0.00000	0.00000
110 h	0.22196	0.77725	0.00079	0.00000	0.00000	0.00000
111 c	-0.64273	3.10660	3.53060	0.00465	0.00088	0.00000
112 h	0.21797	0.78123	0.00080	0.00000	0.00000	0.00000

113 h	0.21877	0.78053	0.00070	0.00000	0.00000	0.00000
114 h	0.23180	0.76750	0.00070	0.00000	0.00000	0.00000
115 c	-0.64690	3.10458	3.53689	0.00454	0.00089	0.00000
116 h	0.21657	0.78266	0.00077	0.00000	0.00000	0.00000
117 h	0.21932	0.77993	0.00075	0.00000	0.00000	0.00000
118 h	0.23528	0.76401	0.00072	0.00000	0.00000	0.00000
119 c	0.10727	2.87052	3.01549	0.00498	0.00173	0.00000
120 c	-0.01917	2.91960	3.09379	0.00392	0.00186	0.00000
121 c	-0.21526	2.96682	3.24209	0.00435	0.00201	0.00000
122 h	0.20901	0.79016	0.00082	0.00000	0.00000	0.00000
123 c	-0.02161	2.91682	3.09941	0.00361	0.00176	0.00000
124 c	-0.22377	2.96609	3.25124	0.00445	0.00199	0.00000
125 h	0.20850	0.79067	0.00083	0.00000	0.00000	0.00000
126 c	-0.02154	2.91710	3.09859	0.00397	0.00188	0.00000
127 c	-0.66287	3.10539	3.55201	0.00458	0.00089	0.00000
128 h	0.22165	0.77759	0.00075	0.00000	0.00000	0.00000
129 h	0.22269	0.77658	0.00073	0.00000	0.00000	0.00000
130 h	0.24778	0.75148	0.00074	0.00000	0.00000	0.00000
131 c	-0.63700	3.10734	3.52451	0.00426	0.00089	0.00000
132 h	0.22486	0.77440	0.00074	0.00000	0.00000	0.00000
133 h	0.21920	0.78009	0.00071	0.00000	0.00000	0.00000
134 h	0.21897	0.78032	0.00071	0.00000	0.00000	0.00000
135 c	-0.65206	3.10257	3.54400	0.00460	0.00089	0.00000
136 h	0.24070	0.75858	0.00072	0.00000	0.00000	0.00000
137 h	0.22101	0.77822	0.00076	0.00000	0.00000	0.00000
138 h	0.22050	0.77874	0.00076	0.00000	0.00000	0.00000