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Schulz, Stephan; Gondzik, Sebastian; Schuchmann, Daniella; Westphal, Ulrich; Dobrzycki, Lukasz; Boese, Roland; Harder, Sjoerd

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Supporting Informations

Reactions of Dizincocene with sterically demanding Bis(iminodi(phenyl)phosphorano)methanes

Stephan Schulz, Daniella Schuchmann, Sebastian Gondzik, Lukasz Dobrzycki, Roland Boese and Sjoerd Harder*

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. $H_2C(Ph_2P{=}N\text{-}Dipp)_2$ and $H_2C(Ph_2P{=}N\text{-}TMS)_2$ were prepared according to the literature methods.[1,2] A Bruker Avance 500 spectrometer was used for NMR spectroscopy. ^1H and $^{13}C\{^1H\}$ NMR spectra were referenced to internal C_6D_5H (^1H: δ = 7.154; ^{13}C: δ = 128.0), $^{31}P\{^1H\}$ spectra to external H_3PO_4 ($\delta(^{31}P) = 0$). IR spectra were recorded on a Alpha-T FT-IR spectrometer with a single reflection ATR sampling module. Melting points were measured in sealed capillaries and were not corrected.

$[HC(Ph_2P{=}N\text{-}Ph)_2]_2Zn_2$ (1)

A solution of 0.28 g (0.5 mmol) $H_2C(Ph_2P{=}N\text{-}Ph)_2$ in 25 mL of toluene was added at 0 °C to a solution of 0.10 g (0.25 mmol) $Cp^*_2Zn_2$ in 10 mL of pentane. The solution was stirred for 4 h at 0 °C, yielding a brown precipitate that was isolated by filtration and dried in vacuum. The brown solid was dissolved in CH_2Cl_2/toluene, concentrated and stored at room temperature, yielding colorless crystals after 12 h.

Yield 0.26 g (82.5 %). Anal. Found (calcd) for $C_{74}H_{62}N_4P_4Zn_2$ (1261.97 g/mol): H, 4.87 (4.95); C, 70.29 (70.43); N, 4.37 (4.44). M.p. 135 °C (decomp.). – IR: ν = 3052, 3008, 2961, 2915, 2854, 1588, 1482, 1434, 1256, 1178, 1101, 1028, 1004, 972, 795, 740, 728, 689, 624, 609, 543, 517, 494, 464 cm^{-1}. – ^1H NMR (300 MHz, THF-d_8, 298 K): δ = 6.45 – 7.60 (m, 30H, $C_{Ar}H$). – ^{13}C NMR (300 MHz, THF-d_8, 298 K): δ = 122.9 (*p-Ph_P*), 126.1 (*p-Ph_N*), 128.7 (*m-Ph_P*), 128.9 (*m-Ph_N*) ,129.6 (*o-Ph_P*), 133.5 (*o-Ph_N*) 133.7 (*ipso-Ph_P*), 150.9 (*ipso-Ph_N*). – ^{31}P-NMR (300 MHz, THF-d_8, 298 K): δ = 22.3.

$[HC(Ph_2P{=}N\text{-}TMS)_2]ZnZnCp^*$ (2)

A solution of 0.15 g (0.25 mmol) $H_2C(Ph_2P{=}N\text{-}TMS)_2$ in 15 mL of *n*-pentane was added at -20 °C to a solution of 0.1 g (0.25 mmol) $Cp^*_2Zn_2$ in 15 mL of *n*-pentane, slowly warmed to ambient temperature and stirred for additional 2 h. The solvent was removed in vacuum yielding a white oily solid, which was suspended in *n*-pentane and was stored at -30 °C for 24 h, yielding **2** as colorless solid, which was isolated by filtration and dried in vacuum.

Yield 0.1 g (55.6 %). Anal. Found (calcd) for $C_{41}H_{54}N_2P_2Zn_2$ (767.58 g/mol): H, 7.03 (7.09); C, 64.07 (64.16); N, 3.26 (3.65). M.p. 110 °C (decomp.) – IR: ν = 3057, 2961, 2906, 1590,

1434, 1258, 1067, 1015, 795, 692, 612, 545, 463, 393 cm^{-1}. – ^{1}H-NMR (300 MHz, C_6D_6, 298 K): δ = 0.12 (s, 18H, Si*Me*$_3$), 2.35 (s, 15H, *Cp**), 3.28 (m, 1H, P*CH*P), 7.01 (m, 12H, $C_{Ar}H$), 7.56 (m, 8H, $C_{Ar}H$). – ^{13}C-NMR (125 MHz, C_6D_6, 298 K): δ = 3.6 (Si*Me*$_3$), 10.6 ($C_5(CH_3)_5$), 26.3 (P*C*HP), 108.3 ($C_5(CH_3)_5$, 130.0 (*p*-Ar), 131.4 (*m*-Ar), 131.5 (*o*-Ar), 131.6 (*ipso*-Ar),. – ^{31}P NMR (500 MHz, C_6D_6, 298 K): δ = 24.4.

[HC(Ph$_2$P=N-Dipp)$_2$]ZnZnCp* (3)

A solution of 0.18 g (0.25 mmol) $H_2C(Ph_2P{=}N\text{-}Dipp)_2$ in 10 mL of cyclohexane was added at 0 °C to a solution of 0.1 g (0.25 mmol) $Cp^*_2Zn_2$ in 10 mL of cyclohexane, warmed to ambient temperature and stirred for additional 2 h. The resulting precipitate was isolated by filtration and dried in vacuum, yielding **3** as slightly yellow crystalline solid.

Yield 0.18 g (72.3 %). Anal. Found (calcd) for $C_{59}H_{70}N_2P_2Zn_2$ (999.91 g/mol): H, 7.02 (7.06); C, 70.76 (70.87); N, 2.74 (2.80). M.p. 150 °C (decomp.). – IR: ν = 3054, 2961, 2923, 2850, 1588, 1431, 1258, 1198, 1096, 1012, 981, 862, 786, 743, 692, 598, 529, 508, 385 cm^{-1}. – ^{1}H NMR (500 MHz, C_6D_6, 298 K): δ = 0.81 (d, 12H, CH*CH*$_3$), 1.58 (d, 12H, CH*CH*$_3$), 2.07 (s, 15H, *Cp**), 3.71 (m, 1H, P*CH*P), 3.89 (m, 4H, C*H*CH$_3$), 7.11 (m, 12H, $C_{Ar}H$), 7.16 (m, 6H, $C_{Ar}H$), 7.71 (m, 8H, $C_{Ar}H$). – ^{13}C NMR (500 MHz, C_6D_6, 298 K): δ = 10.5 ($C_5(CH_3)_5$), 22.7 ($CH(CH_3)_2$), 26.5 ($CH(CH_3)_2$), 28.6 (P*C*HP), 108.1 ($C_5(CH_3)_5$), 123.8 (*p*-Ar), 124.0 (*m*-Ar), 130.4 (*p-m*-Ph), 132.8 (*o*-Ph), 136.9 (*ipso-Ph*), 143.6 (*o*-Ar), 146.2 (*ipso-Ar*). – ^{31}P NMR (500 MHz, C_6D_6, 298 K): δ = 27.4.

[HC(Ph$_2$P=N-Ph)$_2$]ZnZnCp* (4)

A solution of 0.14 g (0.25 mmol) $H_2C(Ph_2P{=}N\text{-}Ph)_2$ in 15 mL of toluene was added at 0 °C to a solution of 0.10 g (0.25 mmol) $Cp^*_2Zn_2$ in 15 mL of pentane. The solution was stirred for 6 h at 0 °C. The resulting suspension was concentrated and the resulting brown precipitate was isolated by filtration and dried in vacuum

Yield 0.13 g (62.6 %). Anal. Found (calcd) for $C_{47}H_{46}N_2P_2Zn_2$ (831.59 g/mol): H, 5.52 (5.57); C, 67.82 (67.89); N, 3.34 (3.37). M.p. 105 °C (decomp.). – IR: ν = 3051, 3010, 2959, 2914, 2850, 1592, 1480, 1430, 1257, 1184, 1100, 1022, 1006, 978, 799, 734, 727, 687, 606, 539, 518, 490 cm^{-1}. – ^{1}H NMR (300 MHz, THF-d_8, 298 K): δ = 1.91 (s, 15H, $C_5(CH_3)_5$), 6.56 – 7.44 (m, 30H, $C_{Ar}H$). – ^{13}C NMR (300 MHz, THF-d_8, 298 K): δ = 10.1 ($C_5(CH_3)_5$), 108.4 ($C_5(CH_3)_5$), 123.7 (*p-Ph*$_P$), 127.1 (*p-Ph*$_N$), 129.3 (*m-Ph*$_P$), 129.7 (*m-Ph*$_N$) ,130.1 (*o-Ph*$_P$), 134.3 (*o-Ph*$_N$) 135.9 (*ipso-Ph*$_P$), 139.9 (*ipso-Ph*$_N$).. – ^{31}P NMR (300 MHz, CD_2Cl_2, 298 K): δ = 21.9.

*Single Crystal Structure Determination of **1** and **3***

Data were collected on a Bruker AXS SMART APEX CCD diffractometer (MoK_α radiation, λ = 0.71073 Å). The structure was solved by Direct Methods SHELXL-97[3] and refined by full-matrix least-squares on F^2. A semi-empirical absorption correction was applied. All non-hydrogen atoms were refined anisotropically and hydrogen atoms by a riding model (SHELXL-97, Program for Crystal Structure Refinement)[4].

CCDC 785388 (**1**) and 780366 (**3**) contain 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 data and structure refinement for **1**.

Identification code	sg087_2	
Empirical formula	C95 H86 N4 P4 Zn2	
Formula weight	1538.30	
Temperature	101(2) K	
Wavelength	0.71073 A	
Crystal system, space group	Monoclinic, C2/c	
Unit cell dimensions	a = 30.7145(15) A	alpha = 90 deg.
	b = 9.7542(5) A	beta = 119.1590(10) deg.
	c = 29.716(2) A	gamma = 90 deg.
Volume	7774.6(8) A^3	
Z, Calculated density	4, 1.314 Mg/m^3	
Absorption coefficient	0.750 mm^-1	
F(000)	3216	
Crystal size	0.23 x 0.11 x 0.10 mm	
Theta range for data collection	1.52 to 27.50 deg.	
Limiting indices	-35<=h<=39, -12<=k<=12, -38<=l<=38	
Reflections collected / unique	49120 / 8939 [R(int) = 0.0480]	
Completeness to theta =	27.50 100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.725	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8939 / 118 / 680	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0354, wR2 = 0.0824	
R indices (all data)	R1 = 0.0536, wR2 = 0.0913	
Largest diff. peak and hole	0.578 and -0.295 e.A^-3	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	**y**	**z**	**U(eq)**
Zn(1)	174(1)	1354(1)	2225(1)	23(1)
P(1)	1176(1)	1924(1)	2417(1)	19(1)
P(2)	268(1)	2796(1)	1427(1)	21(1)
N(1)	-112(1)	1700(2)	1454(1)	26(1)
N(2)	862(1)	564(2)	2386(1)	22(1)
C(1)	725(1)	3117(2)	2055(1)	22(1)
C(2)	-598(4)	1152(13)	1092(4)	17(2)
C(3)	-836(4)	1603(9)	580(5)	24(2)
C(4)	-1308(4)	1122(8)	233(3)	30(2)
C(5)	-1551(4)	199(9)	385(4)	31(2)
C(6)	-1320(4)	-262(10)	885(5)	27(2)
C(7)	-844(5)	192(12)	1241(4)	19(2)
C(2A)	-568(4)	1395(13)	1030(5)	20(2)
C(3A)	-795(4)	1937(9)	536(4)	19(2)
C(4A)	-1281(4)	1543(8)	173(3)	24(2)
C(5A)	-1542(4)	612(8)	300(4)	27(2)
C(6A)	-1316(5)	62(10)	794(5)	29(2)
C(7A)	-840(5)	452(12)	1148(4)	21(2)
C(8)	1040(1)	-697(2)	2630(1)	27(1)
C(9)	698(1)	-1775(2)	2498(1)	38(1)
C(10)	850(1)	-3054(2)	2724(1)	54(1)
C(11)	1339(1)	-3298(3)	3081(1)	58(1)
C(12)	1676(1)	-2244(3)	3218(1)	54(1)
C(13)	1533(1)	-949(2)	3000(1)	39(1)
C(14)	1528(1)	2618(2)	3066(1)	24(1)
C(15)	1285(4)	2833(10)	3340(4)	29(3)
C(16)	1530(5)	3316(14)	3850(4)	30(4)
C(17)	2034(5)	3573(11)	4080(4)	34(2)
C(18)	2291(3)	3371(7)	3812(4)	34(2)
C(19)	2038(4)	2907(9)	3304(4)	33(2)
C(14A)	1528(1)	2618(2)	3066(1)	24(1)
C(15A)	1239(4)	3010(11)	3305(4)	18(2)
C(16A)	1476(5)	3337(15)	3817(5)	35(4)
C(17A)	1991(5)	3294(12)	4113(4)	46(3)
C(18A)	2272(3)	2934(10)	3887(3)	65(3)
C(19A)	2047(4)	2571(10)	3370(4)	47(3)
C(20)	1626(1)	1561(2)	2204(1)	22(1)
C(21)	1635(1)	284(2)	1998(1)	25(1)

C(22)	1964(1)	18(2)	1816(1)	29(1)
C(23)	2292(1)	1024(2)	1840(1)	34(1)
C(24)	2282(1)	2310(2)	2035(1)	37(1)
C(25)	1947(1)	2581(2)	2208(1)	32(1)
C(26)	527(1)	2172(2)	1033(1)	24(1)
C(27)	379(1)	919(2)	777(1)	31(1)
C(28)	613(1)	416(2)	508(1)	37(1)
C(29)	992(1)	1138(2)	501(1)	37(1)
C(30)	1143(1)	2377(2)	756(1)	36(1)
C(31)	913(1)	2897(2)	1022(1)	30(1)
C(32)	-81(3)	4317(9)	1141(4)	18(2)
C(33)	-155(2)	4804(7)	671(3)	22(1)
C(34)	-423(2)	5997(7)	460(3)	37(2)
C(35)	-621(3)	6721(7)	718(3)	48(2)
C(36)	-551(3)	6246(9)	1186(3)	42(2)
C(37)	-286(4)	5049(10)	1398(4)	25(2)
C(32A)	25(3)	4551(8)	1174(4)	16(2)
C(33A)	-17(2)	5094(7)	721(3)	23(1)
C(34A)	-243(2)	6351(6)	545(3)	31(1)
C(35A)	-424(2)	7075(6)	817(3)	30(1)
C(36A)	-387(3)	6540(9)	1262(3)	33(2)
C(37A)	-165(4)	5269(11)	1439(4)	28(2)
C(1S)	1031(1)	6906(4)	1311(2)	50(2)
C(2S)	1488(2)	6547(6)	1727(1)	48(4)
C(3S)	1855(1)	5952(6)	1639(1)	42(2)
C(4S)	1764(1)	5705(4)	1142(1)	40(1)
C(5S)	1303(1)	6053(4)	729(1)	43(1)
C(6S)	943(1)	6652(4)	813(1)	43(1)
C(7SA)	630(2)	7570(6)	1358(2)	44(2)
C(7SB)	2147(2)	5135(6)	1040(2)	49(2)
C(1X)	1562(2)	6007(5)	859(2)	56(3)
C(2X)	1940(2)	5602(7)	1335(3)	71(4)
C(3X)	1901(3)	5833(10)	1775(2)	64(4)
C(4X)	1482(3)	6486(9)	1733(2)	72(8)
C(5X)	1098(2)	6898(8)	1257(3)	61(3)
C(6X)	1146(2)	6648(7)	819(2)	54(3)
C(7XA)	1618(3)	5745(8)	418(3)	70(3)
C(7XB)	1440(5)	6677(14)	2184(3)	76(10)
C(1T)	2881(3)	7918(8)	5073(3)	60(5)
C(2T)	2740(3)	7099(9)	4634(3)	48(3)
C(3T)	2284(3)	6415(9)	4424(3)	41(3)

C(4T)	1979(3)	6537(10)	4643(3)	40(6)
C(5T)	2120(3)	7347(12)	5074(4)	59(3)
C(6T)	2576(3)	8039(11)	5292(3)	47(5)
C(7T)	3359(3)	8629(12)	5292(4)	52(3)
C(1U)	2822(3)	8239(9)	5048(4)	38(3)
C(2U)	2754(4)	7949(11)	5463(4)	41(4)
C(3U)	2367(4)	7095(12)	5408(5)	54(4)
C(4U)	2044(4)	6534(11)	4930(5)	61(4)
C(5U)	2111(4)	6820(11)	4510(4)	46(3)
C(6U)	2497(4)	7672(10)	4569(4)	56(3)
C(7U)	3240(4)	9162(11)	5089(4)	51(3)
C(1V)	2271(5)	7172(16)	4905(5)	27(4)
C(2V)	2341(5)	7027(16)	4483(4)	42(4)
C(3V)	2772(6)	7534(17)	4495(5)	32(4)
C(4V)	3133(5)	8187(17)	4937(6)	33(4)
C(5V)	3060(6)	8340(20)	5362(6)	50(15)
C(6V)	2632(7)	7830(20)	5347(5)	29(8)
C(7V)	1809(6)	6650(20)	4903(9)	44(7)

Table 3. Bond lengths [A] and angles [deg] for **1**.

Zn(1)-N(1)	2.0417(16)	C(8)-C(9)	1.400(3)
Zn(1)-N(2)	2.0746(16)	C(9)-C(10)	1.385(3)
Zn(1)-Zn(1)#1	2.3490(5)	C(9)-H(9)	0.9500
Zn(1)-P(2)	2.8909(6)	C(10)-C(11)	1.373(4)
Zn(1)-P(1)	2.8962(5)	C(10)-H(10)	0.9500
P(1)-N(2)	1.6149(16)	C(11)-C(12)	1.372(4)
P(1)-C(1)	1.7249(19)	C(11)-H(11)	0.9500
P(1)-C(20)	1.816(2)	C(12)-C(13)	1.389(3)
P(1)-C(14)	1.8219(19)	C(12)-H(12)	0.9500
P(2)-N(1)	1.6148(18)	C(13)-H(13)	0.9500
P(2)-C(1)	1.7321(19)	C(14)-C(15)	1.363(11)
P(2)-C(32)	1.784(9)	C(14)-C(19)	1.396(11)
P(2)-C(26)	1.811(2)	C(15)-C(16)	1.403(11)
P(2)-C(32A)	1.872(8)	C(15)-H(15)	0.9500
N(1)-C(2A)	1.385(12)	C(16)-C(17)	1.378(12)
N(1)-C(2)	1.451(10)	C(16)-H(16)	0.9500
N(2)-C(8)	1.396(2)	C(17)-C(18)	1.381(12)
C(1)-H(1)	0.88(2)	C(17)-H(17)	0.9500
C(2)-C(3)	1.401(11)	C(18)-C(19)	1.395(11)

C(2)-C(7)	1.403(10)	C(18)-H(18)	0.9500
C(3)-C(4)	1.388(11)	C(19)-H(19)	0.9500
C(3)-H(3)	0.9500	C(15A)-C(16A)	1.367(12)
C(4)-C(5)	1.379(9)	C(15A)-H(15A)	0.9500
C(4)-H(4)	0.9500	C(16A)-C(17A)	1.385(12)
C(5)-C(6)	1.372(10)	C(16A)-H(16A)	0.9500
C(5)-H(5)	0.9500	C(17A)-C(18A)	1.373(11)
C(6)-C(7)	1.395(11)	C(17A)-H(17A)	0.9500
C(6)-H(6)	0.9500	C(18A)-C(19A)	1.389(10)
C(7)-H(7)	0.9500	C(18A)-H(18A)	0.9500
C(2A)-C(3A)	1.388(12)	C(19A)-H(19A)	0.9500
C(2A)-C(7A)	1.397(10)	C(20)-C(21)	1.393(3)
C(3A)-C(4A)	1.402(10)	C(20)-C(25)	1.396(3)
C(3A)-H(3A)	0.9500	C(21)-C(22)	1.386(3)
C(4A)-C(5A)	1.382(8)	C(21)-H(21)	0.9500
C(4A)-H(4A)	0.9500	C(22)-C(23)	1.383(3)
C(5A)-C(6A)	1.388(10)	C(22)-H(22)	0.9500
C(5A)-H(5A)	0.9500	C(23)-C(24)	1.388(3)
C(6A)-C(7A)	1.375(11)	C(23)-H(23)	0.9500
C(6A)-H(6A)	0.9500	C(24)-C(25)	1.382(3)
C(7A)-H(7A)	0.9500	C(24)-H(24)	0.9500
C(8)-C(13)	1.394(3)	C(25)-H(25)	0.9500
C(26)-C(27)	1.393(3)	C(4S)-H(4S)	0.9500
C(26)-C(31)	1.395(3)	C(5S)-C(6S)	1.3760
C(27)-C(28)	1.397(3)	C(5S)-H(5S)	0.9500
C(27)-H(27)	0.9500	C(6S)-H(6S)	0.9500
C(28)-C(29)	1.370(3)	C(7SA)-H(7S1)	0.9800
C(28)-H(28)	0.9500	C(7SA)-H(7S2)	0.9800
C(29)-C(30)	1.381(3)	C(7SA)-H(7S3)	0.9799
C(29)-H(29)	0.9500	C(7SB)-H(7S4)	0.9801
C(30)-C(31)	1.387(3)	C(7SB)-H(7S5)	0.9800
C(30)-H(30)	0.9500	C(7SB)-H(7S6)	0.9801
C(31)-H(31)	0.9500	C(1X)-C(6X)	1.3732
C(32)-C(33)	1.386(11)	C(1X)-C(2X)	1.3811
C(32)-C(37)	1.399(12)	C(1X)-H(1X)	0.9500
C(33)-C(34)	1.387(9)	C(2X)-C(3X)	1.3878
C(33)-H(33)	0.9500	C(2X)-H(2X)	0.9499
C(34)-C(35)	1.385(9)	C(3X)-C(4X)	1.3859
C(34)-H(34)	0.9500	C(3X)-H(3X)	0.9500
C(35)-C(36)	1.379(10)	C(4X)-C(5X)	1.3889
C(35)-H(35)	0.9500	C(4X)-H(4X)	0.9500

C(36)-C(37)	1.387(11)	C(5X)-C(6X)	1.4000
C(36)-H(36)	0.9500	C(5X)-H(5X)	0.9499
C(37)-H(37)	0.9500	C(6X)-H(6X)	0.9500
C(32A)-C(37A)	1.378(12)	C(7XA)-H(7X1)	0.9801
C(32A)-C(33A)	1.392(11)	C(7XA)-H(7X2)	0.9800
C(33A)-C(34A)	1.380(9)	C(7XA)-H(7X3)	0.9800
C(33A)-H(33A)	0.9500	C(7XB)-H(7X4)	0.9800
C(34A)-C(35A)	1.378(9)	C(7XB)-H(7X5)	0.9800
C(34A)-H(34A)	0.9500	C(7XB)-H(7X6)	0.9800
C(35A)-C(36A)	1.375(10)	C(1T)-C(5T)#2	0.506(14)
C(35A)-H(35A)	0.9500	C(1T)-C(4T)#2	0.908(13)
C(36A)-C(37A)	1.389(11)	C(1T)-C(6T)	1.3813
C(36A)-H(36A)	0.9500	C(1T)-C(2T)	1.4052
C(37A)-H(37A)	0.9500	C(1T)-C(7T)	1.4596
C(1S)-C(2S)	1.3887	C(1T)-C(6T)#2	1.591(12)
C(1S)-C(6S)	1.3918	C(1T)-C(3T)#2	1.912(14)
C(1S)-H(1S)	0.9500	C(2T)-C(5T)#2	0.930(14)
C(2S)-C(3S)	1.3986	C(2T)-C(6T)#2	1.101(14)
C(2S)-H(2S)	0.9497	C(2T)-C(3T)	1.3933
C(3S)-C(4S)	1.3866	C(2T)-H(2T)	0.9500
C(3S)-H(3S)	0.9500	C(3T)-C(6T)#2	0.910(11)
C(4S)-C(5S)	1.3909	C(3T)-C(4T)	1.3831
C(3T)-C(1T)#2	1.911(12)	C(1V)-C(6V)	1.3937
C(3T)-H(3T)	0.9499	C(1V)-C(7V)	1.5054
C(4T)-C(1T)#2	0.908(12)	C(2V)-C(3V)	1.3968
C(4T)-C(7T)#2	1.156(15)	C(2V)-H(2V)	0.9499
C(4T)-C(6T)#2	1.349(13)	C(3V)-C(4V)	1.3925
C(4T)-C(5T)	1.3813	C(3V)-H(3V)	0.9500
C(4T)-H(4T)	0.9501	C(4V)-C(5V)	1.3910
C(5T)-C(1T)#2	0.506(12)	C(4V)-H(4V)	0.9501
C(5T)-C(2T)#2	0.930(18)	C(5V)-C(6V)	1.3849
C(5T)-C(6T)	1.3960	C(5V)-H(5V)	0.9501
C(5T)-C(7T)#2	1.642(17)	C(6V)-H(6V)	0.9501
C(5T)-C(6T)#2	1.784(14)	C(7V)-H(7V1)	0.9801
C(5T)-H(5T)	0.9499	C(7V)-H(7V2)	0.9800
C(6T)-C(3T)#2	0.910(12)	C(7V)-H(7V3)	0.9800
C(6T)-C(2T)#2	1.101(15)		
C(6T)-C(4T)#2	1.349(16)	N(1)-Zn(1)-N(2)	98.82(6)
C(6T)-C(1T)#2	1.591(12)	N(1)-Zn(1)-Zn(1)#1	133.46(5)
C(6T)-C(5T)#2	1.784(13)	N(2)-Zn(1)-Zn(1)#1	126.65(5)
C(6T)-C(6T)#2	1.882(12)	N(1)-Zn(1)-P(2)	32.84(5)

C(6T)-H(6T)	0.9499	N(2)-Zn(1)-P(2)	82.66(4)
C(7T)-C(4T)#2	1.156(18)	Zn(1)#1-Zn(1)-P(2)	146.353(13)
C(7T)-C(5T)#2	1.642(13)	N(1)-Zn(1)-P(1)	91.40(5)
C(7T)-H(7T1)	0.9800	N(2)-Zn(1)-P(1)	32.95(4)
C(7T)-H(7T2)	0.9799	Zn(1)#1-Zn(1)-P(1)	131.495(16)
C(7T)-H(7T3)	0.9800	P(2)-Zn(1)-P(1)	63.063(14)
C(1U)-C(2U)	1.3776	N(2)-P(1)-C(1)	104.14(9)
C(1U)-C(6U)	1.3948	N(2)-P(1)-C(20)	110.79(8)
C(1U)-C(7U)	1.5243	C(1)-P(1)-C(20)	115.43(9)
C(2U)-C(3U)	1.3961	N(2)-P(1)-C(14)	113.33(8)
C(2U)-H(2U)	0.9501	C(1)-P(1)-C(14)	106.98(9)
C(3U)-C(4U)	1.3897	C(20)-P(1)-C(14)	106.32(9)
C(3U)-H(3U)	0.9500	C(1)-P(1)-Zn(1)	63.56(7)
C(4U)-C(5U)	1.3876	C(20)-P(1)-Zn(1)	144.19(6)
C(4U)-H(4U)	0.9499	C(14)-P(1)-Zn(1)	107.86(7)
C(5U)-C(6U)	1.3880	N(1)-P(2)-C(1)	106.95(9)
C(5U)-H(5U)	0.9499	N(1)-P(2)-C(32)	107.1(2)
C(6U)-H(6U)	0.9500	C(1)-P(2)-C(32)	110.2(3)
C(7U)-H(7U1)	0.9800	N(1)-P(2)-C(26)	111.45(9)
C(7U)-H(7U2)	0.9800	C(1)-P(2)-C(26)	112.15(9)
C(7U)-H(7U3)	0.9800	C(32)-P(2)-C(26)	108.9(4)
C(1V)-C(2V)	1.3821	N(1)-P(2)-C(32A)	118.0(2)
C(1)-P(2)-C(32A)	102.9(3)	C(5A)-C(4A)-C(3A)	120.8(7)
C(26)-P(2)-C(32A)	105.2(3)	C(5A)-C(4A)-H(4A)	119.6
C(1)-P(2)-Zn(1)	63.67(7)	C(3A)-C(4A)-H(4A)	119.6
C(32)-P(2)-Zn(1)	121.2(3)	C(4A)-C(5A)-C(6A)	118.9(7)
C(26)-P(2)-Zn(1)	128.14(6)	C(4A)-C(5A)-H(5A)	120.5
C(32A)-P(2)-Zn(1)	126.5(3)	C(6A)-C(5A)-H(5A)	120.5
C(2A)-N(1)-P(2)	122.1(5)	C(7A)-C(6A)-C(5A)	120.1(7)
C(2)-N(1)-P(2)	135.6(5)	C(7A)-C(6A)-H(6A)	120.0
C(2A)-N(1)-Zn(1)	132.6(6)	C(5A)-C(6A)-H(6A)	120.0
C(2)-N(1)-Zn(1)	119.7(5)	C(6A)-C(7A)-C(2A)	122.1(7)
P(2)-N(1)-Zn(1)	103.87(8)	C(6A)-C(7A)-H(7A)	118.9
C(8)-N(2)-P(1)	128.49(14)	C(2A)-C(7A)-H(7A)	118.9
C(8)-N(2)-Zn(1)	122.93(13)	C(13)-C(8)-N(2)	124.39(19)
P(1)-N(2)-Zn(1)	102.72(8)	C(13)-C(8)-C(9)	117.8(2)
P(1)-C(1)-P(2)	122.20(11)	N(2)-C(8)-C(9)	117.81(19)
P(1)-C(1)-H(1)	115.4(14)	C(10)-C(9)-C(8)	120.8(2)
P(2)-C(1)-H(1)	117.4(14)	C(10)-C(9)-H(9)	119.6
C(3)-C(2)-C(7)	118.4(7)	C(8)-C(9)-H(9)	119.6
C(3)-C(2)-N(1)	119.6(9)	C(11)-C(10)-C(9)	120.9(2)

C(7)-C(2)-N(1)	122.0(9)	C(11)-C(10)-H(10)	119.5
C(4)-C(3)-C(2)	120.3(7)	C(9)-C(10)-H(10)	119.5
C(4)-C(3)-H(3)	119.8	C(12)-C(11)-C(10)	118.8(2)
C(2)-C(3)-H(3)	119.8	C(12)-C(11)-H(11)	120.6
C(5)-C(4)-C(3)	120.9(7)	C(10)-C(11)-H(11)	120.6
C(5)-C(4)-H(4)	119.6	C(11)-C(12)-C(13)	121.4(3)
C(3)-C(4)-H(4)	119.6	C(11)-C(12)-H(12)	119.3
C(6)-C(5)-C(4)	119.4(7)	C(13)-C(12)-H(12)	119.3
C(6)-C(5)-H(5)	120.3	C(12)-C(13)-C(8)	120.2(2)
C(4)-C(5)-H(5)	120.3	C(12)-C(13)-H(13)	119.9
C(5)-C(6)-C(7)	121.1(7)	C(8)-C(13)-H(13)	119.9
C(5)-C(6)-H(6)	119.5	C(15)-C(14)-C(19)	118.2(7)
C(7)-C(6)-H(6)	119.5	C(15)-C(14)-P(1)	118.2(5)
C(6)-C(7)-C(2)	119.9(7)	C(19)-C(14)-P(1)	123.5(5)
C(6)-C(7)-H(7)	120.0	C(14)-C(15)-C(16)	122.3(8)
C(2)-C(7)-H(7)	120.0	C(14)-C(15)-H(15)	118.8
N(1)-C(2A)-C(3A)	130.2(10)	C(16)-C(15)-H(15)	118.8
N(1)-C(2A)-C(7A)	112.1(10)	C(17)-C(16)-C(15)	118.5(8)
C(3A)-C(2A)-C(7A)	117.6(8)	C(17)-C(16)-H(16)	120.7
C(2A)-C(3A)-C(4A)	120.5(7)	C(15)-C(16)-H(16)	120.7
C(2A)-C(3A)-H(3A)	119.8	C(16)-C(17)-C(18)	120.5(7)
C(4A)-C(3A)-H(3A)	119.8	C(16)-C(17)-H(17)	119.7
C(18)-C(17)-H(17)	119.7	C(28)-C(27)-H(27)	120.0
C(17)-C(18)-C(19)	119.8(8)	C(29)-C(28)-C(27)	120.3(2)
C(17)-C(18)-H(18)	120.1	C(29)-C(28)-H(28)	119.8
C(19)-C(18)-H(18)	120.1	C(27)-C(28)-H(28)	119.8
C(18)-C(19)-C(14)	120.5(8)	C(28)-C(29)-C(30)	120.2(2)
C(18)-C(19)-H(19)	119.7	C(28)-C(29)-H(29)	119.9
C(14)-C(19)-H(19)	119.7	C(30)-C(29)-H(29)	119.9
C(16A)-C(15A)-H(15A)	120.3	C(29)-C(30)-C(31)	120.3(2)
C(15A)-C(16A)-C(17A)	121.6(8)	C(29)-C(30)-H(30)	119.9
C(15A)-C(16A)-H(16A)	119.2	C(31)-C(30)-H(30)	119.9
C(17A)-C(16A)-H(16A)	119.2	C(30)-C(31)-C(26)	120.2(2)
C(18A)-C(17A)-C(16A)	119.4(7)	C(30)-C(31)-H(31)	119.9
C(18A)-C(17A)-H(17A)	120.3	C(26)-C(31)-H(31)	119.9
C(16A)-C(17A)-H(17A)	120.3	C(33)-C(32)-C(37)	118.6(8)
C(17A)-C(18A)-C(19A)	121.0(7)	C(33)-C(32)-P(2)	122.0(8)
C(17A)-C(18A)-H(18A)	119.5	C(37)-C(32)-P(2)	119.4(7)
C(19A)-C(18A)-H(18A)	119.5	C(32)-C(33)-C(34)	120.9(7)
C(18A)-C(19A)-H(19A)	120.0	C(32)-C(33)-H(33)	119.5
C(21)-C(20)-C(25)	118.53(18)	C(34)-C(33)-H(33)	119.5

C(21)-C(20)-P(1)	120.54(14)	C(35)-C(34)-C(33)	120.1(6)
C(25)-C(20)-P(1)	120.79(15)	C(35)-C(34)-H(34)	119.9
C(22)-C(21)-C(20)	120.87(18)	C(33)-C(34)-H(34)	119.9
C(22)-C(21)-H(21)	119.6	C(36)-C(35)-C(34)	119.5(6)
C(20)-C(21)-H(21)	119.6	C(36)-C(35)-H(35)	120.2
C(23)-C(22)-C(21)	119.88(19)	C(34)-C(35)-H(35)	120.2
C(23)-C(22)-H(22)	120.1	C(35)-C(36)-C(37)	120.6(7)
C(21)-C(22)-H(22)	120.1	C(35)-C(36)-H(36)	119.7
C(22)-C(23)-C(24)	120.0(2)	C(37)-C(36)-H(36)	119.7
C(22)-C(23)-H(23)	120.0	C(36)-C(37)-C(32)	120.1(8)
C(24)-C(23)-H(23)	120.0	C(36)-C(37)-H(37)	119.9
C(25)-C(24)-C(23)	120.1(2)	C(32)-C(37)-H(37)	119.9
C(25)-C(24)-H(24)	120.0	C(37A)-C(32A)-C(33A)	119.5(7)
C(23)-C(24)-H(24)	120.0	C(37A)-C(32A)-P(2)	115.6(7)
C(24)-C(25)-C(20)	120.63(19)	C(33A)-C(32A)-P(2)	124.6(7)
C(24)-C(25)-H(25)	119.7	C(34A)-C(33A)-C(32A)	119.8(7)
C(20)-C(25)-H(25)	119.7	C(34A)-C(33A)-H(33A)	120.1
C(27)-C(26)-C(31)	119.09(19)	C(32A)-C(33A)-H(33A)	120.1
C(27)-C(26)-P(2)	121.27(17)	C(35A)-C(34A)-C(33A)	120.3(6)
C(31)-C(26)-P(2)	119.37(15)	C(35A)-C(34A)-H(34A)	119.9
C(26)-C(27)-C(28)	119.9(2)	C(33A)-C(34A)-H(34A)	119.9
C(26)-C(27)-H(27)	120.0	C(36A)-C(35A)-C(34A)	120.2(6)
C(36A)-C(35A)-H(35A)	119.9	C(7T)-C(1T)-C(6T)#2	160.7(5)
C(34A)-C(35A)-H(35A)	119.9	C(5T)#2-C(1T)-C(3T)#2	162.9(18)
C(35A)-C(36A)-C(37A)	119.8(7)	C(2T)-C(1T)-C(3T)#2	147.1(6)
C(35A)-C(36A)-H(36A)	120.1	C(7T)-C(1T)-C(3T)#2	94.7(6)
C(37A)-C(36A)-H(36A)	120.1	C(6T)#2-C(1T)-C(3T)#2	104.5(7)
C(32A)-C(37A)-C(36A)	120.3(8)	C(5T)#2-C(2T)-C(6T)#2	86.4(9)
C(32A)-C(37A)-H(37A)	119.8	C(5T)#2-C(2T)-C(3T)	127.1(8)
C(36A)-C(37A)-H(37A)	119.8	C(6T)#2-C(2T)-C(1T)	77.8(6)
C(2S)-C(1S)-C(6S)	119.4	C(3T)-C(2T)-C(1T)	118.5
C(2S)-C(1S)-H(1S)	120.3	C(6T)#2-C(3T)-C(4T)	68.5(9)
C(6S)-C(1S)-H(1S)	120.3	C(6T)#2-C(3T)-C(2T)	52.1(9)
C(1S)-C(2S)-C(3S)	119.7	C(4T)-C(3T)-C(2T)	120.7
C(4S)-C(3S)-C(2S)	120.6	C(2T)-C(3T)-C(1T)#2	94.4(4)
C(3S)-C(4S)-C(5S)	119.1	C(1T)#2-C(4T)-C(7T)#2	89.2(14)
C(3S)-C(4S)-H(4S)	120.5	C(1T)#2-C(4T)-C(6T)#2	72.5(8)
C(5S)-C(4S)-H(4S)	120.5	C(7T)#2-C(4T)-C(6T)#2	161.7(16)
C(6S)-C(5S)-C(4S)	120.5	C(7T)#2-C(4T)-C(5T)	80.1(12)
C(5S)-C(6S)-C(1S)	120.7	C(6T)#2-C(4T)-C(5T)	81.6(5)
C(6X)-C(1X)-C(2X)	120.1	C(1T)#2-C(4T)-C(3T)	111.4(8)

C(6X)-C(1X)-H(1X)	119.9	C(7T)#2-C(4T)-C(3T)	159.4(12)
C(2X)-C(1X)-H(1X)	119.9	C(5T)-C(4T)-C(3T)	120.5
H(5S)-C(1X)-H(1X)	47.9	C(1T)#2-C(5T)-C(2T)#2	155(2)
C(1X)-C(2X)-C(3X)	120.2	C(2T)#2-C(5T)-C(4T)	171.7(10)
C(4X)-C(3X)-C(2X)	119.5	C(1T)#2-C(5T)-C(6T)	103.4(14)
C(3X)-C(4X)-C(5X)	121.0	C(2T)#2-C(5T)-C(6T)	51.9(10)
C(3X)-C(4X)-H(4X)	119.5	C(4T)-C(5T)-C(6T)	119.8
C(5X)-C(4X)-H(4X)	119.5	C(1T)#2-C(5T)-C(7T)#2	60.3(16)
C(4X)-C(5X)-C(6X)	118.3	C(2T)#2-C(5T)-C(7T)#2	144.3(11)
C(1X)-C(6X)-C(5X)	120.9	C(6T)-C(5T)-C(7T)#2	163.7(8)
C(5T)#2-C(1T)-C(4T)#2	154(2)	C(2T)#2-C(5T)-C(6T)#2	123.3(12)
C(5T)#2-C(1T)-C(6T)	136.8(14)	C(4T)-C(5T)-C(6T)#2	48.4(4)
C(4T)#2-C(1T)-C(6T)	68.7(11)	C(6T)-C(5T)-C(6T)#2	71.4(4)
C(4T)#2-C(1T)-C(2T)	170.5(11)	C(7T)#2-C(5T)-C(6T)#2	92.3(8)
C(6T)-C(1T)-C(2T)	120.8	C(3T)#2-C(6T)-C(2T)#2	87.1(10)
C(5T)#2-C(1T)-C(7T)	102.1(14)	C(3T)#2-C(6T)-C(4T)#2	72.6(10)
C(4T)#2-C(1T)-C(7T)	52.4(11)	C(2T)#2-C(6T)-C(4T)#2	159.7(11)
C(6T)-C(1T)-C(7T)	121.0	C(3T)#2-C(6T)-C(1T)	111.4(13)
C(2T)-C(1T)-C(7T)	118.2	C(2T)#2-C(6T)-C(1T)	161.4(10)
C(5T)#2-C(1T)-C(6T)#2	58.6(12)	C(3T)#2-C(6T)-C(5T)	128.8(13)
C(4T)#2-C(1T)-C(6T)#2	146.9(13)	C(4T)#2-C(6T)-C(5T)	158.6(6)
C(6T)-C(1T)-C(6T)#2	78.2(5)	C(1T)-C(6T)-C(5T)	119.8
C(3T)#2-C(6T)-C(1T)#2	146.8(16)	C(2U)-C(1U)-C(6U)	119.3
C(2T)#2-C(6T)-C(1T)#2	59.7(9)	C(2U)-C(1U)-C(7U)	122.6
C(4T)#2-C(6T)-C(1T)#2	140.6(10)	C(6U)-C(1U)-C(7U)	118.1
C(1T)-C(6T)-C(1T)#2	101.8(4)	C(1U)-C(2U)-C(3U)	120.7
C(3T)#2-C(6T)-C(5T)#2	122.6(14)	C(4U)-C(3U)-C(2U)	119.8
C(2T)#2-C(6T)-C(5T)#2	150.2(11)	C(5U)-C(4U)-C(3U)	119.8
C(4T)#2-C(6T)-C(5T)#2	50.0(5)	C(4U)-C(5U)-C(6U)	120.0
C(5T)-C(6T)-C(5T)#2	108.6(4)	C(5U)-C(6U)-C(1U)	120.5
C(1T)#2-C(6T)-C(5T)#2	90.6(6)	C(2V)-C(1V)-C(6V)	119.7
C(3T)#2-C(6T)-C(6T)#2	167.2(15)	C(2V)-C(1V)-C(7V)	121.7
C(2T)#2-C(6T)-C(6T)#2	105.6(10)	C(6V)-C(1V)-C(7V)	118.6
C(4T)#2-C(6T)-C(6T)#2	94.7(7)	C(1V)-C(2V)-C(3V)	120.4
C(1T)-C(6T)-C(6T)#2	55.8(4)	C(4V)-C(3V)-C(2V)	119.7
C(5T)-C(6T)-C(6T)#2	63.9(4)	C(5V)-C(4V)-C(3V)	119.9
C(1T)#2-C(6T)-C(6T)#2	45.9(3)	C(6V)-C(5V)-C(4V)	120.1
C(4T)#2-C(7T)-C(5T)#2	56.0(5)	C(5V)-C(6V)-C(1V)	120.3

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2 #2 -x+1/2,-y+3/2,-z+1

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **1**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
Zn(1)	19(1)	24(1)	22(1)	0(1)	6(1)	-1(1)
P(1)	19(1)	16(1)	19(1)	0(1)	6(1)	-2(1)
P(2)	23(1)	19(1)	17(1)	0(1)	6(1)	4(1)
N(1)	21(1)	29(1)	19(1)	-3(1)	3(1)	-1(1)
N(2)	20(1)	17(1)	26(1)	2(1)	9(1)	-1(1)
C(1)	24(1)	16(1)	20(1)	-2(1)	6(1)	-2(1)
C(2)	15(3)	21(5)	11(3)	-1(3)	4(3)	-1(3)
C(3)	26(3)	26(4)	25(3)	-1(3)	16(3)	-6(3)
C(4)	30(4)	40(5)	17(3)	-1(3)	8(2)	2(4)
C(5)	20(3)	40(5)	31(5)	-11(4)	10(3)	-6(3)
C(6)	22(3)	26(4)	36(4)	-8(3)	16(3)	-11(3)
C(7)	22(3)	14(4)	22(4)	-1(3)	12(3)	-6(3)
C(2A)	21(3)	15(4)	30(5)	-3(3)	18(3)	-4(2)
C(3A)	15(3)	22(4)	18(3)	1(3)	6(2)	-4(2)
C(4A)	16(3)	31(4)	20(3)	0(3)	5(2)	4(3)
C(5A)	20(3)	34(5)	24(3)	-6(3)	8(2)	-3(3)
C(6A)	30(3)	25(4)	39(5)	-6(3)	22(4)	-11(3)
C(7A)	27(3)	16(5)	20(3)	6(2)	12(3)	-1(3)
C(8)	32(1)	20(1)	37(1)	5(1)	23(1)	2(1)
C(9)	40(1)	25(1)	58(2)	3(1)	31(1)	-2(1)
C(10)	66(2)	22(1)	95(2)	10(1)	57(2)	-1(1)
C(11)	78(2)	32(1)	93(2)	34(1)	63(2)	22(1)
C(12)	51(2)	49(2)	73(2)	39(1)	38(2)	23(1)
C(13)	36(1)	33(1)	48(1)	19(1)	21(1)	6(1)
C(14)	24(1)	21(1)	20(1)	-1(1)	5(1)	-3(1)
C(15)	27(5)	16(3)	30(5)	5(3)	4(3)	-9(3)
C(16)	48(8)	32(7)	10(4)	-4(3)	13(4)	-9(4)
C(17)	36(4)	23(3)	23(3)	4(2)	-1(3)	-13(3)
C(18)	27(3)	26(3)	35(3)	2(2)	3(2)	-6(2)
C(19)	33(4)	21(2)	33(4)	2(2)	6(3)	0(2)
C(14A)	24(1)	21(1)	20(1)	-1(1)	5(1)	-3(1)
C(15A)	23(4)	20(3)	13(3)	1(3)	11(3)	-4(3)
C(16A)	23(5)	35(7)	41(7)	-2(5)	11(4)	-14(4)
C(17A)	40(5)	71(8)	21(4)	-17(4)	10(4)	-6(5)
C(18A)	22(3)	119(10)	33(4)	-30(5)	-1(3)	-2(5)
C(19A)	18(3)	87(8)	29(4)	-22(5)	5(3)	7(4)
C(20)	20(1)	19(1)	23(1)	2(1)	7(1)	-1(1)
C(21)	25(1)	18(1)	28(1)	0(1)	10(1)	-4(1)

C(22)	33(1)	19(1)	34(1)	-1(1)	15(1)	2(1)
C(23)	31(1)	28(1)	49(1)	2(1)	24(1)	3(1)
C(24)	31(1)	25(1)	61(2)	-2(1)	28(1)	-6(1)
C(25)	30(1)	20(1)	47(1)	-4(1)	21(1)	-4(1)
C(26)	27(1)	22(1)	19(1)	1(1)	7(1)	8(1)
C(27)	24(1)	29(1)	30(1)	-7(1)	5(1)	6(1)
C(28)	35(1)	34(1)	31(1)	-10(1)	6(1)	14(1)
C(29)	42(1)	39(1)	30(1)	0(1)	18(1)	17(1)
C(30)	48(1)	30(1)	39(1)	8(1)	29(1)	11(1)
C(31)	42(1)	21(1)	29(1)	3(1)	19(1)	7(1)
C(32)	15(3)	14(3)	20(3)	-4(2)	6(3)	-10(2)
C(33)	20(3)	19(3)	25(2)	0(2)	9(3)	0(2)
C(34)	44(4)	38(4)	28(3)	13(3)	16(3)	16(3)
C(35)	58(5)	40(4)	47(4)	16(3)	26(4)	27(3)
C(36)	51(6)	41(5)	44(5)	10(3)	32(5)	19(4)
C(37)	27(5)	24(3)	27(3)	1(2)	16(3)	4(3)
C(32A)	10(3)	11(3)	22(3)	-1(2)	4(2)	-3(2)
C(33A)	25(4)	20(3)	26(3)	2(2)	14(3)	-2(2)
C(34A)	33(4)	24(3)	34(3)	9(2)	16(3)	4(2)
C(35A)	27(3)	19(3)	36(3)	4(2)	8(3)	6(2)
C(36A)	30(4)	32(4)	32(3)	-5(2)	11(3)	10(3)
C(37A)	23(4)	31(4)	27(3)	4(3)	10(3)	1(3)
C(1S)	63(5)	26(3)	65(5)	-7(3)	34(5)	-13(3)
C(2S)	75(10)	37(6)	34(4)	-1(3)	28(5)	-26(5)
C(3S)	48(4)	27(3)	39(3)	14(2)	12(2)	-8(2)
C(4S)	43(4)	27(3)	42(3)	12(2)	15(3)	6(2)
C(5S)	39(4)	46(3)	37(2)	12(2)	14(3)	1(3)
C(6S)	38(3)	32(2)	52(3)	11(2)	18(3)	0(2)
C(7SA)	59(5)	33(4)	55(5)	-24(4)	38(5)	-25(4)
C(7SB)	35(5)	47(5)	59(5)	-7(4)	18(4)	-4(4)
C(1X)	47(6)	24(3)	87(8)	17(4)	26(6)	5(4)
C(2X)	36(5)	35(4)	110(11)	47(6)	10(6)	8(4)
C(3X)	57(6)	29(5)	72(6)	21(5)	5(5)	-16(4)
C(4X)	53(13)	17(7)	120(14)	1(7)	21(10)	-15(7)
C(5X)	43(6)	27(6)	98(11)	8(6)	23(7)	-1(4)
C(6X)	28(5)	42(5)	68(6)	15(4)	4(4)	6(4)
C(7XA)	88(8)	50(6)	76(7)	10(5)	43(7)	-4(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1**.

	x	**y**	**z**	**U(eq)**
H(1)	809(8)	3980(20)	2143(8)	24(5)
H(3)	-674	2241	469	29
H(4)	-1466	1432	-114	36
H(5)	-1876	-115	147	38
H(6)	-1486	-901	990	32
H(7)	-686	-149	1584	22
H(3A)	-621	2579	442	23
H(4A)	-1431	1922	-164	28
H(5A)	-1872	353	54	33
H(6A)	-1490	-585	886	35
H(7A)	-691	68	1484	25
H(9)	358	-1628	2251	45
H(10)	612	-3772	2631	64
H(11)	1442	-4180	3231	70
H(12)	2014	-2403	3467	65
H(13)	1772	-233	3104	47
H(15)	938	2650	3181	35
H(16)	1351	3461	4032	37
H(17)	2206	3893	4425	41
H(18)	2639	3548	3973	41
H(19)	2214	2786	3118	39
H(15A)	886	3043	3109	22
H(16A)	1283	3599	3974	42
H(17A)	2148	3511	4470	55
H(18A)	2625	2934	4087	77
H(19A)	2247	2290	3222	57
H(21)	1412	-413	1983	30
H(22)	1965	-855	1674	35
H(23)	2524	836	1724	41
H(24)	2505	3004	2049	44
H(25)	1935	3471	2332	38
H(27)	120	407	786	38
H(28)	508	-431	329	45
H(29)	1151	786	320	44
H(30)	1405	2876	749	43
H(31)	1018	3749	1196	36
H(33)	-20	4313	491	26
H(34)	-470	6317	137	45

H(35)	-805	7539	574	58
H(36)	-686	6743	1365	50
H(37)	-243	4726	1719	30
H(33A)	109	4600	533	27
H(34A)	-274	6719	234	37
H(35A)	-574	7947	697	36
H(36A)	-514	7038	1449	40
H(37A)	-144	4893	1744	34
H(1S)	781	7320	1367	60
H(2S)	1552	6705	2069	58
H(3S)	2168	5716	1924	51
H(4S)	2014	5303	1083	47
H(5S)	1235	5875	387	51
H(6S)	630	6896	527	51
H(7S1)	346	7726	1014	66
H(7S2)	747	8451	1536	66
H(7S3)	526	6981	1556	66
H(7S4)	2013	5044	667	73
H(7S5)	2248	4232	1202	73
H(7S6)	2436	5748	1181	73
H(1X)	1589	5842	559	67
H(2X)	2228	5163	1362	85
H(3X)	2159	5546	2102	77
H(4X)	1457	6654	2034	87
H(5X)	810	7338	1229	73
H(6X)	888	6926	490	65
H(7X1)	1942	5311	527	105
H(7X2)	1601	6612	243	105
H(7X3)	1351	5134	181	105
H(7X4)	1127	7150	2094	114
H(7X5)	1721	7231	2433	114
H(7X6)	1444	5784	2337	114
H(2T)	2950	7014	4485	58
H(3T)	2182	5860	4127	49
H(4T)	1671	6060	4497	48
H(5T)	1908	7433	5221	71
H(6T)	2676	8591	5590	56
H(7T1)	3511	8476	5073	78
H(7T2)	3580	8275	5639	78
H(7T3)	3307	9614	5311	78
H(2U)	2974	8333	5791	49

H(3U)	2323	6899	5697	64
H(4U)	1779	5956	4890	73
H(5U)	1893	6434	4183	55
H(6U)	2541	7870	4280	67
H(7U1)	3229	9208	4754	77
H(7U2)	3563	8786	5346	77
H(7U3)	3199	10084	5193	77
H(2V)	2095	6580	4182	50
H(3V)	2819	7435	4204	39
H(4V)	3428	8529	4949	40
H(5V)	3304	8790	5662	60
H(6V)	2585	7925	5638	34
H(7V1)	1831	6832	5238	65
H(7V2)	1780	5655	4840	65
H(7V3)	1515	7107	4631	65

Table 6. Torsion angles [deg] for **1**.

N(1)-Zn(1)-P(1)-N(2)	-104.14(9)	C(26)-P(2)-N(1)-C(2)	-67.7(8)
Zn(1)#1-Zn(1)-P(1)-N(2)	95.77(8)	C(32A)-P(2)-N(1)-C(2)	54.2(9)
P(2)-Zn(1)-P(1)-N(2)	-121.37(8)	Zn(1)-P(2)-N(1)-C(2)	168.9(8)
N(1)-Zn(1)-P(1)-C(1)	49.95(8)	C(1)-P(2)-N(1)-Zn(1)	0.51(11)
N(2)-Zn(1)-P(1)-C(1)	154.09(11)	C(32)-P(2)-N(1)-Zn(1)	-117.6(4)
Zn(1)#1-Zn(1)-P(1)-C(1)	-110.14(7)	C(26)-P(2)-N(1)-Zn(1)	123.42(9)
P(2)-Zn(1)-P(1)-C(1)	32.72(7)	C(32A)-P(2)-N(1)-Zn(1)	-114.7(4)
N(1)-Zn(1)-P(1)-C(20)	-47.55(11)	N(2)-Zn(1)-N(1)-C(2A)	132.5(8)
N(2)-Zn(1)-P(1)-C(20)	56.59(13)	Zn(1)#1-Zn(1)-N(1)-C(2A)	-35.8(8)
Zn(1)#1-Zn(1)-P(1)-C(20)	152.36(10)	P(2)-Zn(1)-N(1)-C(2A)	-166.1(8)
P(2)-Zn(1)-P(1)-C(20)	-64.78(10)	P(1)-Zn(1)-N(1)-C(2A)	164.8(8)
N(1)-Zn(1)-P(1)-C(14)	150.46(8)	N(2)-Zn(1)-N(1)-C(2)	127.5(6)
N(2)-Zn(1)-P(1)-C(14)	-105.39(10)	Zn(1)#1-Zn(1)-N(1)-C(2)	-40.8(6)
Zn(1)#1-Zn(1)-P(1)-C(14)	-9.63(7)	P(2)-Zn(1)-N(1)-C(2)	-171.1(7)
P(2)-Zn(1)-P(1)-C(14)	133.23(6)	P(1)-Zn(1)-N(1)-C(2)	159.8(6)
N(2)-Zn(1)-P(2)-N(1)	118.99(10)	N(2)-Zn(1)-N(1)-P(2)	-61.39(9)
Zn(1)#1-Zn(1)-P(2)-N(1)	-87.79(9)	Zn(1)#1-Zn(1)-N(1)-P(2)	130.29(6)
P(1)-Zn(1)-P(2)-N(1)	146.91(9)	P(1)-Zn(1)-N(1)-P(2)	-29.13(8)
N(1)-Zn(1)-P(2)-C(1)	-179.45(12)	C(1)-P(1)-N(2)-C(8)	-176.87(17)
N(2)-Zn(1)-P(2)-C(1)	-60.46(8)	C(20)-P(1)-N(2)-C(8)	58.42(19)
Zn(1)#1-Zn(1)-P(2)-C(1)	92.76(8)	C(14)-P(1)-N(2)-C(8)	-60.99(19)
P(1)-Zn(1)-P(2)-C(1)	-32.54(7)	Zn(1)-P(1)-N(2)-C(8)	-153.1(2)

N(1)-Zn(1)-P(2)-C(32)	81.8(3)	C(1)-P(1)-N(2)-Zn(1)	-23.79(10)
N(2)-Zn(1)-P(2)-C(32)	-159.2(3)	C(20)-P(1)-N(2)-Zn(1)	-148.50(8)
Zn(1)#1-Zn(1)-P(2)-C(32)	-6.0(3)	C(14)-P(1)-N(2)-Zn(1)	92.09(9)
P(1)-Zn(1)-P(2)-C(32)	-131.3(3)	N(1)-Zn(1)-N(2)-C(8)	-126.16(15)
N(1)-Zn(1)-P(2)-C(26)	-81.05(12)	Zn(1)#1-Zn(1)-N(2)-C(8)	43.28(17)
N(2)-Zn(1)-P(2)-C(26)	37.94(9)	P(2)-Zn(1)-N(2)-C(8)	-154.85(15)
Zn(1)#1-Zn(1)-P(2)-C(26)	-168.83(8)	P(1)-Zn(1)-N(2)-C(8)	155.0(2)
P(1)-Zn(1)-P(2)-C(26)	65.86(8)	N(1)-Zn(1)-N(2)-P(1)	78.81(9)
N(1)-Zn(1)-P(2)-C(32A)	93.8(3)	Zn(1)#1-Zn(1)-N(2)-P(1)	-111.74(6)
N(2)-Zn(1)-P(2)-C(32A)	-147.2(3)	P(2)-Zn(1)-N(2)-P(1)	50.13(7)
Zn(1)#1-Zn(1)-P(2)-C(32A)	6.0(3)	N(2)-P(1)-C(1)-P(2)	-53.55(15)
P(1)-Zn(1)-P(2)-C(32A)	-119.3(3)	C(20)-P(1)-C(1)-P(2)	68.12(15)
C(1)-P(2)-N(1)-C(2A)	168.5(7)	C(14)-P(1)-C(1)-P(2)	-173.81(12)
C(32)-P(2)-N(1)-C(2A)	50.3(8)	Zn(1)-P(1)-C(1)-P(2)	-71.90(11)
C(26)-P(2)-N(1)-C(2A)	-68.6(7)	N(1)-P(2)-C(1)-P(1)	71.67(15)
C(32A)-P(2)-N(1)-C(2A)	53.2(8)	C(32)-P(2)-C(1)-P(1)	-172.3(3)
Zn(1)-P(2)-N(1)-C(2A)	167.9(7)	C(26)-P(2)-C(1)-P(1)	-50.79(16)
C(1)-P(2)-N(1)-C(2)	169.4(8)	C(32A)-P(2)-C(1)-P(1)	-163.4(3)
C(32)-P(2)-N(1)-C(2)	51.3(9)	Zn(1)-P(2)-C(1)-P(1)	72.07(11)
C(2A)-N(1)-C(2)-C(3)	4(4)	C(20)-P(1)-C(14)-C(15)	-172.6(5)
P(2)-N(1)-C(2)-C(3)	0.0(13)	Zn(1)-P(1)-C(14)-C(15)	-3.5(5)
Zn(1)-N(1)-C(2)-C(3)	167.6(5)	N(2)-P(1)-C(14)-C(19)	127.5(4)
C(2A)-N(1)-C(2)-C(7)	-175(6)	C(1)-P(1)-C(14)-C(19)	-118.3(4)
P(2)-N(1)-C(2)-C(7)	-178.9(5)	C(20)-P(1)-C(14)-C(19)	5.6(4)
Zn(1)-N(1)-C(2)-C(7)	-11.3(10)	Zn(1)-P(1)-C(14)-C(19)	174.7(4)
C(7)-C(2)-C(3)-C(4)	1.0(4)	C(19)-C(14)-C(15)-C(16)	-0.7(4)
N(1)-C(2)-C(3)-C(4)	-177.9(11)	P(1)-C(14)-C(15)-C(16)	177.6(3)
C(2)-C(3)-C(4)-C(5)	0.2(4)	C(14)-C(15)-C(16)-C(17)	-0.3(5)
C(3)-C(4)-C(5)-C(6)	-0.9(8)	C(15)-C(16)-C(17)-C(18)	0.6(9)
C(4)-C(5)-C(6)-C(7)	0.2(10)	C(16)-C(17)-C(18)-C(19)	0.2(11)
C(5)-C(6)-C(7)-C(2)	1.1(9)	C(17)-C(18)-C(19)-C(14)	-1.2(10)
C(3)-C(2)-C(7)-C(6)	-1.7(7)	C(15)-C(14)-C(19)-C(18)	1.5(8)
N(1)-C(2)-C(7)-C(6)	177.3(12)	P(1)-C(14)-C(19)-C(18)	-176.7(5)
P(2)-N(1)-C(2A)-C(3A)	-2.6(13)	C(15A)-C(16A)-C(17A)-C(18A)	0.9(10)
Zn(1)-N(1)-C(2A)-C(3A)	161.4(6)	C(16A)-C(17A)-C(18A)-C(19A)	-2.1(13)
C(2)-N(1)-C(2A)-C(7A)	5(5)	N(2)-P(1)-C(20)-C(21)	5.89(18)
P(2)-N(1)-C(2A)-C(7A)	-178.1(4)	C(1)-P(1)-C(20)-C(21)	-112.14(16)
Zn(1)-N(1)-C(2A)-C(7A)	-14.1(11)	C(14)-P(1)-C(20)-C(21)	129.42(16)
N(1)-C(2A)-C(3A)-C(4A)	-175.2(13)	Zn(1)-P(1)-C(20)-C(21)	-32.7(2)
C(7A)-C(2A)-C(3A)-C(4A)	0.1(3)	N(2)-P(1)-C(20)-C(25)	-178.56(16)
C(2A)-C(3A)-C(4A)-C(5A)	0.1(3)	C(1)-P(1)-C(20)-C(25)	63.41(19)

C(3A)-C(4A)-C(5A)-C(6A)	-0.4(6)	C(14)-P(1)-C(20)-C(25)	-55.02(18)
C(4A)-C(5A)-C(6A)-C(7A)	0.5(8)	Zn(1)-P(1)-C(20)-C(25)	142.84(14)
C(5A)-C(6A)-C(7A)-C(2A)	-0.3(8)	C(25)-C(20)-C(21)-C(22)	1.7(3)
N(1)-C(2A)-C(7A)-C(6A)	176.1(11)	P(1)-C(20)-C(21)-C(22)	177.40(15)
C(3A)-C(2A)-C(7A)-C(6A)	0.0(6)	C(20)-C(21)-C(22)-C(23)	0.5(3)
P(1)-N(2)-C(8)-C(13)	7.8(3)	C(21)-C(22)-C(23)-C(24)	-1.7(3)
Zn(1)-N(2)-C(8)-C(13)	-140.48(18)	C(22)-C(23)-C(24)-C(25)	0.6(4)
P(1)-N(2)-C(8)-C(9)	-173.06(16)	C(23)-C(24)-C(25)-C(20)	1.8(4)
Zn(1)-N(2)-C(8)-C(9)	38.7(2)	C(21)-C(20)-C(25)-C(24)	-2.9(3)
C(13)-C(8)-C(9)-C(10)	-1.0(3)	P(1)-C(20)-C(25)-C(24)	-178.53(18)
N(2)-C(8)-C(9)-C(10)	179.8(2)	N(1)-P(2)-C(26)-C(27)	2.82(19)
C(8)-C(9)-C(10)-C(11)	-0.3(4)	C(1)-P(2)-C(26)-C(27)	122.70(17)
C(9)-C(10)-C(11)-C(12)	1.0(4)	C(32)-P(2)-C(26)-C(27)	-115.0(3)
C(10)-C(11)-C(12)-C(13)	-0.5(5)	C(32A)-P(2)-C(26)-C(27)	-126.2(3)
C(11)-C(12)-C(13)-C(8)	-0.7(4)	Zn(1)-P(2)-C(26)-C(27)	49.52(19)
N(2)-C(8)-C(13)-C(12)	-179.4(2)	N(1)-P(2)-C(26)-C(31)	-171.30(15)
C(9)-C(8)-C(13)-C(12)	1.5(3)	C(1)-P(2)-C(26)-C(31)	-51.43(18)
N(2)-P(1)-C(14)-C(15)	-50.7(5)	C(32)-P(2)-C(26)-C(31)	70.8(3)
C(1)-P(1)-C(14)-C(15)	63.5(5)	C(32A)-P(2)-C(26)-C(31)	59.7(3)
Zn(1)-P(2)-C(26)-C(31)	-124.61(14)	C(34A)-C(35A)-C(36A)-C(37A)	0.4(9)
C(31)-C(26)-C(27)-C(28)	-1.0(3)	C(33A)-C(32A)-C(37A)-C(36A)	-1.4(9)
P(2)-C(26)-C(27)-C(28)	-175.12(16)	P(2)-C(32A)-C(37A)-C(36A)	-175.4(6)
C(26)-C(27)-C(28)-C(29)	1.1(3)	C(35A)-C(36A)-C(37A)-C(32A)	0.8(10)
C(27)-C(28)-C(29)-C(30)	-0.6(3)	C(6S)-C(1S)-C(2S)-C(3S)	0.7
C(28)-C(29)-C(30)-C(31)	0.1(3)	C(1S)-C(2S)-C(3S)-C(4S)	-0.7
C(29)-C(30)-C(31)-C(26)	-0.1(3)	C(2S)-C(3S)-C(4S)-C(5S)	-0.2
C(27)-C(26)-C(31)-C(30)	0.5(3)	C(3S)-C(4S)-C(5S)-C(6S)	0.9
P(2)-C(26)-C(31)-C(30)	174.74(16)	C(4S)-C(5S)-C(6S)-C(1S)	-0.8
N(1)-P(2)-C(32)-C(33)	-116.0(4)	C(2S)-C(1S)-C(6S)-C(5S)	0.0
C(1)-P(2)-C(32)-C(33)	128.0(4)	C(6X)-C(1X)-C(2X)-C(3X)	0.4
C(26)-P(2)-C(32)-C(33)	4.6(5)	C(1X)-C(2X)-C(3X)-C(4X)	-0.7
C(32A)-P(2)-C(32)-C(33)	77(3)	C(2X)-C(3X)-C(4X)-C(5X)	0.8
Zn(1)-P(2)-C(32)-C(33)	-161.2(3)	C(3X)-C(4X)-C(5X)-C(6X)	-0.6
N(1)-P(2)-C(32)-C(37)	64.2(5)	C(2X)-C(1X)-C(6X)-C(5X)	-0.2
C(1)-P(2)-C(32)-C(37)	-51.8(5)	C(4X)-C(5X)-C(6X)-C(1X)	0.3
C(26)-P(2)-C(32)-C(37)	-175.2(4)	C(6T)-C(1T)-C(2T)-C(5T)#2	-172(7)
C(32A)-P(2)-C(32)-C(37)	-102(4)	C(7T)-C(1T)-C(2T)-C(5T)#2	8(7)
Zn(1)-P(2)-C(32)-C(37)	19.0(6)	C(6T)#2-C(1T)-C(2T)-C(5T)#2	-171(7)
C(37)-C(32)-C(33)-C(34)	0.5(4)	C(3T)#2-C(1T)-C(2T)-C(5T)#2	-171(8)
P(2)-C(32)-C(33)-C(34)	-179.3(5)	C(5T)#2-C(1T)-C(2T)-C(6T)#2	171(7)
C(32)-C(33)-C(34)-C(35)	0.0(4)	C(6T)-C(1T)-C(2T)-C(6T)#2	-0.7(8)

C(33)-C(34)-C(35)-C(36)	-0.1(8)	C(7T)-C(1T)-C(2T)-C(6T)#2	179.0(8)
C(34)-C(35)-C(36)-C(37)	-0.3(10)	C(3T)#2-C(1T)-C(2T)-C(6T)#2	0.3(17)
C(35)-C(36)-C(37)-C(32)	0.7(11)	C(5T)#2-C(1T)-C(2T)-C(3T)	172(7)
C(33)-C(32)-C(37)-C(36)	-0.8(9)	C(6T)-C(1T)-C(2T)-C(3T)	0.2
P(2)-C(32)-C(37)-C(36)	178.9(6)	C(7T)-C(1T)-C(2T)-C(3T)	179.9
N(1)-P(2)-C(32A)-C(37A)	58.8(6)	C(6T)#2-C(1T)-C(2T)-C(3T)	0.9(8)
C(1)-P(2)-C(32A)-C(37A)	-58.6(5)	C(3T)#2-C(1T)-C(2T)-C(3T)	1.1(17)
C(32)-P(2)-C(32A)-C(37A)	73(3)	C(5T)#2-C(2T)-C(3T)-C(6T)#2	0.2(9)
C(26)-P(2)-C(32A)-C(37A)	-176.2(4)	C(1T)-C(2T)-C(3T)-C(6T)#2	-1.3(12)
Zn(1)-P(2)-C(32A)-C(37A)	8.0(6)	C(5T)#2-C(2T)-C(3T)-C(4T)	1.3(13)
N(1)-P(2)-C(32A)-C(33A)	-114.9(4)	C(6T)#2-C(2T)-C(3T)-C(4T)	1.1(12)
C(1)-P(2)-C(32A)-C(33A)	127.7(4)	C(1T)-C(2T)-C(3T)-C(4T)	-0.2
C(32)-P(2)-C(32A)-C(33A)	-100(4)	C(5T)#2-C(2T)-C(3T)-C(1T)#2	0.9(10)
C(26)-P(2)-C(32A)-C(33A)	10.2(4)	C(6T)#2-C(2T)-C(3T)-C(1T)#2	0.7(9)
Zn(1)-P(2)-C(32A)-C(33A)	-165.6(3)	C(1T)-C(2T)-C(3T)-C(1T)#2	-0.6(5)
C(37A)-C(32A)-C(33A)-C(34A)	0.8(4)	C(6T)#2-C(3T)-C(4T)-C(1T)#2	0.0(7)
P(2)-C(32A)-C(33A)-C(34A)	174.2(5)	C(2T)-C(3T)-C(4T)-C(1T)#2	-0.9(12)
C(32A)-C(33A)-C(34A)-C(35A)	0.5(4)	C(6T)#2-C(3T)-C(4T)-C(7T)#2	-178(5)
C(33A)-C(34A)-C(35A)-C(36A)	-1.1(7)	C(2T)-C(3T)-C(4T)-C(7T)#2	-179(4)
C(1T)#2-C(3T)-C(4T)-C(7T)#2	-178(5)	C(5T)#2-C(1T)-C(6T)-C(1T)#2	-3(2)
C(2T)-C(3T)-C(4T)-C(6T)#2	-0.9(10)	C(4T)#2-C(1T)-C(6T)-C(1T)#2	-178(2)
C(1T)#2-C(3T)-C(4T)-C(6T)#2	0.0(7)	C(2T)-C(1T)-C(6T)-C(1T)#2	0.5(6)
C(6T)#2-C(3T)-C(4T)-C(5T)	1.3(10)	C(7T)-C(1T)-C(6T)-C(1T)#2	-179.2(6)
C(2T)-C(3T)-C(4T)-C(5T)	0.4	C(6T)#2-C(1T)-C(6T)-C(1T)#2	0.0(4)
C(1T)#2-C(3T)-C(4T)-C(5T)	1.3(12)	C(3T)#2-C(1T)-C(6T)-C(1T)#2	-178(3)
C(7T)#2-C(4T)-C(5T)-C(1T)#2	172(8)	C(4T)#2-C(1T)-C(6T)-C(5T)#2	-176(4)
C(6T)#2-C(4T)-C(5T)-C(1T)#2	-7(6)	C(2T)-C(1T)-C(6T)-C(5T)#2	3(3)
C(3T)-C(4T)-C(5T)-C(1T)#2	-8(7)	C(7T)-C(1T)-C(6T)-C(5T)#2	-176(3)
C(1T)#2-C(4T)-C(5T)-C(6T)	7(7)	C(6T)#2-C(1T)-C(6T)-C(5T)#2	3(2)
C(7T)#2-C(4T)-C(5T)-C(6T)	179.1(15)	C(3T)#2-C(1T)-C(6T)-C(5T)#2	-176(4)
C(6T)#2-C(4T)-C(5T)-C(6T)	0.3(7)	C(5T)#2-C(1T)-C(6T)-C(6T)#2	-3(2)
C(3T)-C(4T)-C(5T)-C(6T)	-0.5	C(4T)#2-C(1T)-C(6T)-C(6T)#2	-178.4(19)
C(1T)#2-C(4T)-C(5T)-C(7T)#2	-172(8)	C(2T)-C(1T)-C(6T)-C(6T)#2	0.5(6)
C(6T)#2-C(4T)-C(5T)-C(7T)#2	-179(2)	C(7T)-C(1T)-C(6T)-C(6T)#2	-179.2(6)
C(3T)-C(4T)-C(5T)-C(7T)#2	-179.6(15)	C(3T)#2-C(1T)-C(6T)-C(6T)#2	-178(2)
C(1T)#2-C(4T)-C(5T)-C(6T)#2	7(6)	C(1T)#2-C(5T)-C(6T)-C(3T)#2	-176(4)
C(7T)#2-C(4T)-C(5T)-C(6T)#2	179(2)	C(2T)#2-C(5T)-C(6T)-C(3T)#2	-0.2(9)
C(3T)-C(4T)-C(5T)-C(6T)#2	-0.8(7)	C(4T)-C(5T)-C(6T)-C(3T)#2	-179(3)
C(5T)#2-C(1T)-C(6T)-C(3T)#2	176(4)	C(7T)#2-C(5T)-C(6T)-C(3T)#2	-176(5)
C(4T)#2-C(1T)-C(6T)-C(3T)#2	0.0(10)	C(6T)#2-C(5T)-C(6T)-C(3T)#2	-178(3)
C(2T)-C(1T)-C(6T)-C(3T)#2	179(2)	C(1T)#2-C(5T)-C(6T)-C(2T)#2	-176(4)

C(7T)-C(1T)-C(6T)-C(3T)#2	-1(2)	C(4T)-C(5T)-C(6T)-C(2T)#2	-178(2)
C(6T)#2-C(1T)-C(6T)-C(3T)#2	178(2)	C(7T)#2-C(5T)-C(6T)-C(2T)#2	-176(6)
C(5T)#2-C(1T)-C(6T)-C(2T)#2	-1(5)	C(6T)#2-C(5T)-C(6T)-C(2T)#2	-178(3)
C(4T)#2-C(1T)-C(6T)-C(2T)#2	-177(6)	C(1T)#2-C(5T)-C(6T)-C(4T)#2	1.2(17)
C(2T)-C(1T)-C(6T)-C(2T)#2	2(5)	C(2T)#2-C(5T)-C(6T)-C(4T)#2	178(5)
C(7T)-C(1T)-C(6T)-C(2T)#2	-178(5)	C(4T)-C(5T)-C(6T)-C(4T)#2	-1(3)
C(6T)#2-C(1T)-C(6T)-C(2T)#2	2(5)	C(7T)#2-C(5T)-C(6T)-C(4T)#2	1(4)
C(3T)#2-C(1T)-C(6T)-C(2T)#2	-177(7)	C(6T)#2-C(5T)-C(6T)-C(4T)#2	-1(3)
C(5T)#2-C(1T)-C(6T)-C(4T)#2	176(4)	C(1T)#2-C(5T)-C(6T)-C(1T)	3(2)
C(2T)-C(1T)-C(6T)-C(4T)#2	178.9(16)	C(2T)#2-C(5T)-C(6T)-C(1T)	179(2)
C(7T)-C(1T)-C(6T)-C(4T)#2	-0.8(16)	C(4T)-C(5T)-C(6T)-C(1T)	0.5
C(6T)#2-C(1T)-C(6T)-C(4T)#2	178.4(19)	C(7T)#2-C(5T)-C(6T)-C(1T)	3(4)
C(3T)#2-C(1T)-C(6T)-C(4T)#2	0.0(10)	C(6T)#2-C(5T)-C(6T)-C(1T)	0.7(5)
C(5T)#2-C(1T)-C(6T)-C(5T)	-4(3)	C(2T)#2-C(5T)-C(6T)-C(1T)#2	176(4)
C(4T)#2-C(1T)-C(6T)-C(5T)	-179.2(16)	C(4T)-C(5T)-C(6T)-C(1T)#2	-2(2)
C(2T)-C(1T)-C(6T)-C(5T)	-0.3	C(7T)#2-C(5T)-C(6T)-C(1T)#2	0(3)
C(7T)-C(1T)-C(6T)-C(5T)	180.0	C(6T)#2-C(5T)-C(6T)-C(1T)#2	-1.8(16)
C(6T)#2-C(1T)-C(6T)-C(5T)	-0.8(6)	C(1T)#2-C(5T)-C(6T)-C(5T)#2	1.8(17)
C(3T)#2-C(1T)-C(6T)-C(5T)	-179(2)	C(2T)#2-C(5T)-C(6T)-C(5T)#2	178(3)
C(4T)-C(5T)-C(6T)-C(5T)#2	-0.2(6)	C(7U)-C(1U)-C(2U)-C(3U)	-179.9
C(7T)#2-C(5T)-C(6T)-C(5T)#2	2(4)	C(1U)-C(2U)-C(3U)-C(4U)	-0.1
C(6T)#2-C(5T)-C(6T)-C(5T)#2	0.0(4)	C(2U)-C(3U)-C(4U)-C(5U)	0.3
C(1T)#2-C(5T)-C(6T)-C(6T)#2	1.8(16)	C(3U)-C(4U)-C(5U)-C(6U)	-0.4
C(2T)#2-C(5T)-C(6T)-C(6T)#2	178(3)	C(4U)-C(5U)-C(6U)-C(1U)	0.4
C(4T)-C(5T)-C(6T)-C(6T)#2	-0.2(5)	C(2U)-C(1U)-C(6U)-C(5U)	-0.2
C(7T)#2-C(5T)-C(6T)-C(6T)#2	2(3)	C(7U)-C(1U)-C(6U)-C(5U)	179.8
C(5T)#2-C(1T)-C(7T)-C(4T)#2	-177(4)	C(6V)-C(1V)-C(2V)-C(3V)	0.0
C(6T)-C(1T)-C(7T)-C(4T)#2	0.9(19)	C(7V)-C(1V)-C(2V)-C(3V)	179.6
C(2T)-C(1T)-C(7T)-C(4T)#2	-178.8(19)	C(1V)-C(2V)-C(3V)-C(4V)	0.1
C(6T)#2-C(1T)-C(7T)-C(4T)#2	-177(3)	C(2V)-C(3V)-C(4V)-C(5V)	-0.4
C(3T)#2-C(1T)-C(7T)-C(4T)#2	0.5(11)	C(3V)-C(4V)-C(5V)-C(6V)	0.6
C(4T)#2-C(1T)-C(7T)-C(5T)#2	177(4)	C(4V)-C(5V)-C(6V)-C(1V)	-0.5
C(6T)-C(1T)-C(7T)-C(5T)#2	177.5(19)	C(2V)-C(1V)-C(6V)-C(5V)	0.2
C(2T)-C(1T)-C(7T)-C(5T)#2	-2.2(19)	C(7V)-C(1V)-C(6V)-C(5V)	-179.4
C(6T)#2-C(1T)-C(7T)-C(5T)#2	-0.2(13)		
C(3T)#2-C(1T)-C(7T)-C(5T)#2	177(3)		
C(6U)-C(1U)-C(2U)-C(3U)	0.1		

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2 #2 -x+1/2,-y+3/2,-z+1

X-Ray Crystal Structure of **1**

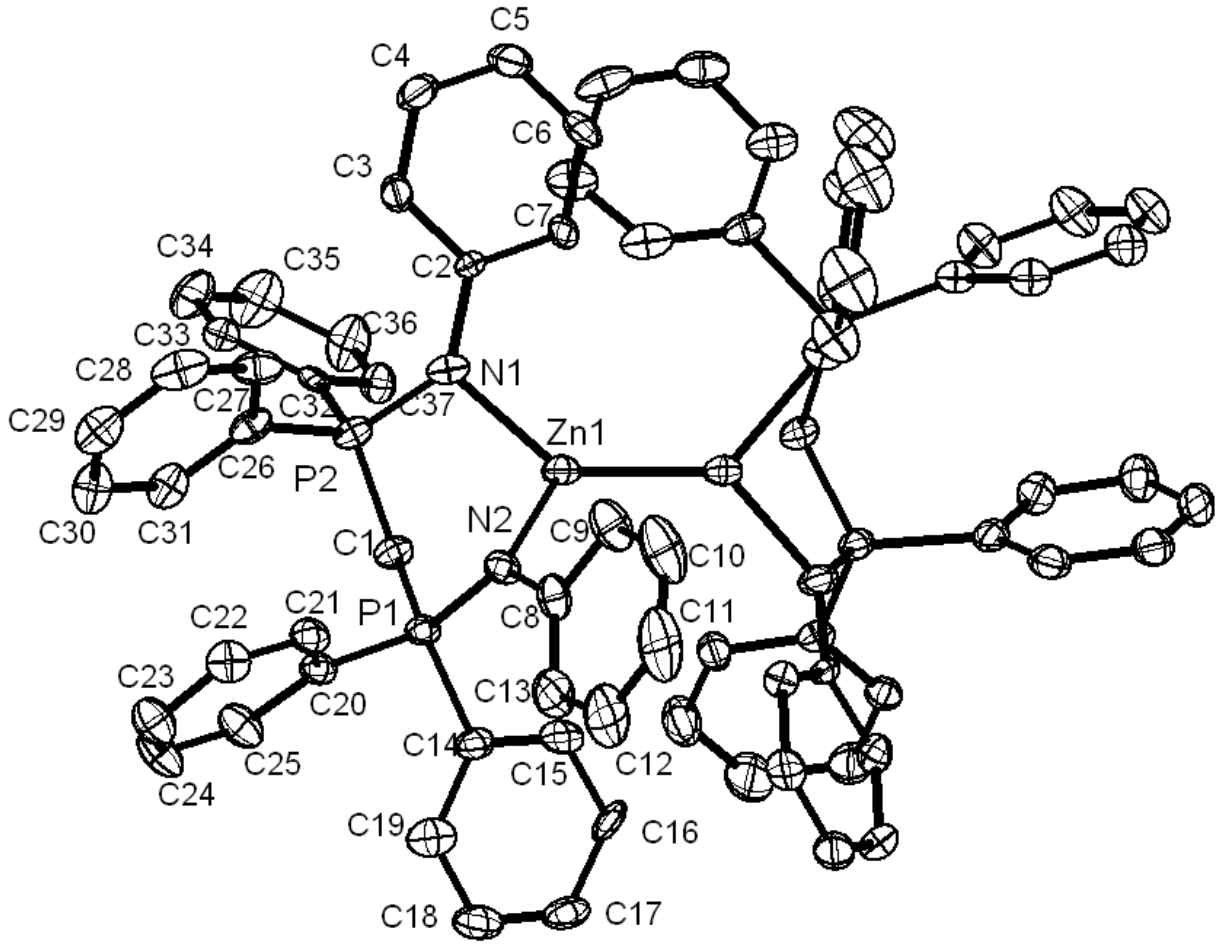


Table 1. Crystal data and structure refinement for **3**.

Empirical formula	C74 H85 N2 P2 Zn2
Formula weight	1195.12
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 12.6320(4) Å alpha = 73.9330(10) deg.
	b = 13.5140(5) Å beta = 89.0060(10) deg.
	c = 21.8795(7) Å gamma = 64.2620(10) deg.
Volume	3210.15(19) $Å^3$
Z, Calculated density	2, 1.236 Mg/m^3
Absorption coefficient	0.840 mm^{-1}
F(000)	1266
Crystal size	0.21 x 0.16 x 0.13 mm
Theta range for data collection	0.98 to 30.70 deg.
Limiting indices	-18<=h<=18, -19<=k<=19, -31<=l<=31
Reflections collected / unique	75343 / 19793 [R(int) = 0.0306]
Completeness to theta = 30.70	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8986 and 0.8433
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	19793 / 27 / 806
Goodness-of-fit on F^2	1.017
Final R indices [I>2sigma(I)]	R1 = 0.0320, wR2 = 0.0776
R indices (all data)	R1 = 0.0458, wR2 = 0.0846
Largest diff. peak and hole	0.556 and -0.317 e. $Å^{-3}$

The complex molecule is located on 2-fold axis of symmetry. In its asymmetric part the moiety exhibits some disorder in the phenyl rings. The disorder was refined as splitting 3 out of 6 phenyl rings into two fragments with the equal occupancies at the 50% level each. These fragments were constraint to have proper geometry and refined as a rigid bodies with ADPs for non-H atoms. All hydrogen atoms in the phenyl rings of the complex molecule were located geometrically and their positions were refined using riding model. Their isotropic thermal parameters were set to be either 1.2 or 1.5 times bigger than U_{eq} of corresponding carbon atoms. The coordinates and isotropic thermal parameter of H(1) atom were free for refinement. The asymmetric part of the unit cell contains one and a half of toluene molecules, severely disordered. All these moieties were refined with series of constraints for distances and angles providing reasonable geometries.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zn(1)	1741(1)	4435(1)	7502(1)	12(1)
Zn(2)	-264(1)	4903(1)	7487(1)	17(1)
P(1)	4303(1)	2886(1)	8359(1)	11(1)
P(2)	3960(1)	4756(1)	7095(1)	12(1)
N(1)	2868(1)	3401(1)	8286(1)	12(1)
N(2)	2634(1)	4993(1)	6859(1)	13(1)
C(1)	4751(1)	3465(1)	7672(1)	14(1)
C(2)	4836(1)	4797(1)	6438(1)	14(1)
C(3)	5582(1)	3784(1)	6299(1)	18(1)
C(4)	6225(1)	3829(1)	5778(1)	21(1)
C(5)	6125(1)	4879(1)	5391(1)	23(1)
C(6)	5384(1)	5884(1)	5526(1)	23(1)
C(7)	4734(1)	5851(1)	6044(1)	19(1)
C(8)	3853(1)	5927(1)	7395(1)	14(1)
C(9)	4887(1)	6027(1)	7513(1)	18(1)
C(10)	4847(1)	6858(1)	7783(1)	22(1)
C(11)	3786(2)	7586(1)	7949(1)	25(1)
C(12)	2762(1)	7493(1)	7837(1)	23(1)
C(13)	2793(1)	6670(1)	7557(1)	17(1)
C(14)	2186(1)	5188(1)	6215(1)	14(1)
C(15)	1553(1)	6327(1)	5805(1)	17(1)
C(16)	994(1)	6502(1)	5212(1)	21(1)
C(17)	1037(1)	5589(1)	5023(1)	22(1)
C(18)	1676(1)	4477(1)	5419(1)	21(1)
C(19)	2269(1)	4255(1)	6012(1)	17(1)
C(20)	1413(1)	7344(1)	6020(1)	21(1)
C(21)	1336(2)	8375(1)	5473(1)	36(1)
C(22)	329(1)	7705(1)	6386(1)	29(1)
C(23)	2962(1)	3011(1)	6421(1)	21(1)
C(24)	3873(1)	2271(1)	6061(1)	26(1)
C(25)	2125(2)	2479(1)	6675(1)	29(1)
C(26)	2231(1)	3232(1)	8826(1)	13(1)
C(27)	1936(1)	2304(1)	8979(1)	15(1)
C(28)	1265(1)	2190(1)	9485(1)	20(1)
C(29)	899(1)	2958(1)	9840(1)	22(1)
C(30)	1170(1)	3881(1)	9678(1)	21(1)
C(31)	1804(1)	4057(1)	9164(1)	16(1)
C(32)	2304(1)	1431(1)	8610(1)	17(1)
C(33)	3102(1)	209(1)	9045(1)	24(1)

C(34)	1231(1)	1438(1)	8284(1)	23(1)
C(35)	1936(1)	5164(1)	8960(1)	18(1)
C(36)	2372(1)	5429(1)	9518(1)	25(1)
C(37)	749(1)	6183(1)	8628(1)	22(1)
C(38)	5112(1)	1332(1)	8487(1)	16(1)
C(39)	4907(1)	921(1)	8002(1)	19(1)
C(40)	5478(1)	-241(1)	8055(1)	25(1)
C(41)	6282(2)	-1012(1)	8590(1)	30(1)
C(42)	6515(1)	-619(1)	9066(1)	28(1)
C(43)	5932(1)	553(1)	9016(1)	21(1)
C(44)	4796(1)	3058(1)	9084(1)	14(1)
C(45)	4617(1)	2512(1)	9694(1)	16(1)
C(46)	5018(1)	2659(1)	10235(1)	19(1)
C(47)	5599(1)	3340(1)	10176(1)	21(1)
C(48)	5774(1)	3889(1)	9573(1)	21(1)
C(49)	5372(1)	3749(1)	9029(1)	17(1)
C(50)	-1856(1)	4703(1)	7180(1)	21(1)
C(51)	-1802(1)	4528(1)	7854(1)	21(1)
C(52)	-1965(1)	5568(1)	7968(1)	22(1)
C(53)	-2128(1)	6396(1)	7362(1)	21(1)
C(54)	-2063(1)	5859(1)	6877(1)	20(1)
C(55)	-1744(2)	3824(2)	6855(1)	33(1)
C(56)	-1708(1)	3467(2)	8357(1)	31(1)
C(57)	-2009(1)	5748(2)	8619(1)	31(1)
C(58)	-2380(2)	7630(1)	7248(1)	31(1)
C(59)	-2198(2)	6431(2)	6164(1)	29(1)
C(1A)	8020(2)	486(2)	7531(1)	51(1)
C(2A)	9084(2)	547(2)	7561(1)	51(1)
C(3A)	9631(2)	687(2)	7013(1)	42(1)
C(4A)	9123(2)	754(2)	6443(1)	37(1)
C(5A)	8072(2)	676(2)	6417(1)	39(1)
C(6A)	7523(2)	535(2)	6963(1)	43(1)
C(1B)	4265(12)	-1233(11)	5894(6)	58(4)
C(2B)	4180(11)	-750(11)	5249(6)	59(3)
C(3B)	3261(10)	239(10)	4871(4)	44(2)
C(4B)	2351(2)	801(2)	5182(1)	46(1)
C(5B)	2423(9)	337(9)	5830(4)	52(3)
C(6B)	3336(12)	-671(11)	6207(7)	49(3)
C(1D)	4028(11)	-1085(9)	6045(5)	47(3)
C(2D)	4286(13)	-916(13)	5423(5)	57(3)
C(3D)	3392(10)	68(12)	5015(4)	50(3)
C(4D)	2351(2)	801(2)	5182(1)	46(1)

C(5D)	2127(9)	570(9)	5811(3)	33(2)
C(6D)	3008(13)	-377(12)	6233(7)	51(3)
C(1C)	10845(9)	-514(10)	10408(4)	81(5)
C(2C)	9793(10)	461(8)	10359(4)	84(3)
C(3C)	8943(9)	871(8)	9845(5)	59(2)
C(4C)	9138(8)	297(10)	9386(5)	63(3)
C(5C)	10159(8)	-702(7)	9452(4)	85(3)
C(6C)	11007(9)	-1114(8)	9965(5)	102(5)

Table 3. Bond lengths [Å] and angles [deg] for **3**.

Zn(1)-N(2)	1.9794(11)	C(11)-C(12)	1.385(2)
Zn(1)-N(1)	1.9886(10)	C(11)-H(11)	0.9500
Zn(1)-Zn(2)	2.3272(2)	C(12)-C(13)	1.3975(19)
Zn(2)-C(50)	2.2786(14)	C(12)-H(12)	0.9500
Zn(2)-C(54)	2.2839(13)	C(13)-H(13)	0.9500
Zn(2)-C(51)	2.2918(14)	C(14)-C(19)	1.4114(18)
Zn(2)-C(53)	2.2987(14)	C(14)-C(15)	1.4154(18)
Zn(2)-C(52)	2.3018(14)	C(15)-C(16)	1.3986(18)
P(1)-N(1)	1.6277(11)	C(15)-C(20)	1.5122(19)
P(1)-C(1)	1.7018(13)	C(16)-C(17)	1.386(2)
P(1)-C(44)	1.8235(13)	C(16)-H(16)	0.9500
P(1)-C(38)	1.8307(13)	C(17)-C(18)	1.382(2)
P(2)-N(2)	1.6266(11)	C(17)-H(17)	0.9500
P(2)-C(1)	1.7163(13)	C(18)-C(19)	1.3984(18)
P(2)-C(2)	1.8043(13)	C(18)-H(18)	0.9500
P(2)-C(8)	1.8272(13)	C(19)-C(23)	1.5203(19)
N(1)-C(26)	1.4385(16)	C(20)-C(21)	1.532(2)
N(2)-C(14)	1.4376(16)	C(20)-C(22)	1.534(2)
C(1)-H(1)	0.9500	C(20)-H(20)	1.0000
C(2)-C(3)	1.3971(19)	C(21)-H(21A)	0.9800
C(2)-C(7)	1.3980(18)	C(21)-H(21B)	0.9800
C(3)-C(4)	1.3911(19)	C(21)-H(21C)	0.9800
C(3)-H(3)	0.9500	C(22)-H(22A)	0.9800
C(4)-C(5)	1.388(2)	C(22)-H(22B)	0.9800
C(4)-H(4)	0.9500	C(22)-H(22C)	0.9800
C(5)-C(6)	1.384(2)	C(23)-C(24)	1.534(2)
C(5)-H(5)	0.9500	C(23)-C(25)	1.536(2)
C(6)-C(7)	1.3901(19)	C(23)-H(23)	1.0000
C(6)-H(6)	0.9500	C(24)-H(24A)	0.9800
C(7)-H(7)	0.9500	C(24)-H(24B)	0.9800

C(8)-C(13)	1.3925(19)	C(24)-H(24C)	0.9800
C(8)-C(9)	1.4050(18)	C(25)-H(25A)	0.9800
C(9)-C(10)	1.3890(19)	C(25)-H(25B)	0.9800
C(9)-H(9)	0.9500	C(25)-H(25C)	0.9800
C(10)-C(11)	1.389(2)	C(26)-C(27)	1.4117(18)
C(10)-H(10)	0.9500	C(26)-C(31)	1.4163(18)
C(27)-C(28)	1.3971(18)	C(42)-H(42)	0.9500
C(27)-C(32)	1.5159(18)	C(43)-H(43)	0.9500
C(28)-C(29)	1.383(2)	C(44)-C(49)	1.3932(18)
C(28)-H(28)	0.9500	C(44)-C(45)	1.4031(18)
C(29)-C(30)	1.386(2)	C(45)-C(46)	1.3907(18)
C(29)-H(29)	0.9500	C(45)-H(45)	0.9500
C(30)-C(31)	1.3957(19)	C(46)-C(47)	1.386(2)
C(30)-H(30)	0.9500	C(46)-H(46)	0.9500
C(31)-C(35)	1.5205(19)	C(47)-C(48)	1.389(2)
C(32)-C(34)	1.537(2)	C(47)-H(47)	0.9500
C(32)-C(33)	1.5380(19)	C(48)-C(49)	1.3930(18)
C(32)-H(32)	1.0000	C(48)-H(48)	0.9500
C(33)-H(33A)	0.9800	C(49)-H(49)	0.9500
C(33)-H(33B)	0.9800	C(50)-C(54)	1.424(2)
C(33)-H(33C)	0.9800	C(50)-C(51)	1.426(2)
C(34)-H(34A)	0.9800	C(50)-C(55)	1.501(2)
C(34)-H(34B)	0.9800	C(51)-C(52)	1.422(2)
C(34)-H(34C)	0.9800	C(51)-C(56)	1.504(2)
C(35)-C(36)	1.5336(19)	C(52)-C(53)	1.428(2)
C(35)-C(37)	1.5381(19)	C(52)-C(57)	1.506(2)
C(35)-H(35)	1.0000	C(53)-C(54)	1.425(2)
C(36)-H(36A)	0.9800	C(53)-C(58)	1.502(2)
C(36)-H(36B)	0.9800	C(54)-C(59)	1.512(2)
C(36)-H(36C)	0.9800	C(55)-H(55A)	0.9800
C(37)-H(37A)	0.9800	C(55)-H(55B)	0.9800
C(37)-H(37B)	0.9800	C(55)-H(55C)	0.9800
C(37)-H(37C)	0.9800	C(56)-H(56A)	0.9800
C(38)-C(43)	1.3940(19)	C(56)-H(56B)	0.9800
C(38)-C(39)	1.4008(19)	C(56)-H(56C)	0.9800
C(39)-C(40)	1.3845(19)	C(57)-H(57A)	0.9800
C(39)-H(39)	0.9500	C(57)-H(57B)	0.9800
C(40)-C(41)	1.389(2)	C(57)-H(57C)	0.9800
C(40)-H(40)	0.9500	C(58)-H(58A)	0.9800
C(41)-C(42)	1.381(3)	C(58)-H(58B)	0.9800
C(41)-H(41)	0.9500	C(58)-H(58C)	0.9800
C(42)-C(43)	1.400(2)	C(59)-H(59A)	0.9800

C(59)-H(59B)	0.9800	C(1C)-C(6C)	1.386(7)
C(59)-H(59C)	0.9800	C(1C)-H(1C)	0.9500
C(1A)-C(6A)	1.375(3)	C(2C)-C(3C)	1.381(7)
C(1A)-C(2A)	1.386(3)	C(2C)-H(2C)	0.9500
C(1A)-H(1A1)	0.9500	C(3C)-C(4C)	1.389(7)
C(2A)-C(3A)	1.383(3)	C(3C)-H(3C)	0.9500
C(2A)-H(2A)	0.9500	C(4C)-C(5C)	1.375(7)
C(3A)-C(4A)	1.374(3)	C(4C)-H(4C)	0.9500
C(3A)-H(3A)	0.9500	C(5C)-C(6C)	1.378(7)
C(4A)-C(5A)	1.381(3)	C(5C)-H(5C)	0.9500
C(4A)-H(4A)	0.9500	C(6C)-H(6C)	0.9500
C(5A)-C(6A)	1.379(3)	N(2)-Zn(1)-N(1)	107.47(4)
C(5A)-H(5A)	0.9500	N(2)-Zn(1)-Zn(2)	131.41(3)
C(6A)-H(6A)	0.9500	N(1)-Zn(1)-Zn(2)	120.91(3)
C(1B)-C(2B)	1.365(8)	C(50)-Zn(2)-C(54)	36.39(5)
C(1B)-C(6B)	1.383(8)	C(50)-Zn(2)-C(51)	36.35(5)
C(1B)-H(1B1)	0.9500	C(54)-Zn(2)-C(51)	60.41(5)
C(2B)-C(3B)	1.375(8)	C(50)-Zn(2)-C(53)	60.58(5)
C(2B)-H(2B)	0.9500	C(54)-Zn(2)-C(53)	36.24(5)
C(3B)-C(4B)	1.364(8)	C(51)-Zn(2)-C(53)	60.27(5)
C(3B)-H(3B)	0.9500	C(50)-Zn(2)-C(52)	60.52(5)
C(4B)-C(5B)	1.368(8)	C(54)-Zn(2)-C(52)	60.37(5)
C(4B)-H(4B)	0.9500	C(51)-Zn(2)-C(52)	36.07(6)
C(5B)-C(6B)	1.383(8)	C(53)-Zn(2)-C(52)	36.16(5)
C(5B)-H(5B)	0.9500	C(50)-Zn(2)-Zn(1)	150.30(4)
C(6B)-H(6B)	0.9500	C(54)-Zn(2)-Zn(1)	145.57(4)
C(1D)-C(6D)	1.368(8)	C(51)-Zn(2)-Zn(1)	152.00(4)
C(1D)-C(2D)	1.375(8)	C(53)-Zn(2)-Zn(1)	144.07(4)
C(1D)-H(1D)	0.9500	C(52)-Zn(2)-Zn(1)	147.71(4)
C(2D)-C(3D)	1.384(8)	N(1)-P(1)-C(1)	110.43(6)
C(2D)-H(2D)	0.9500	N(1)-P(1)-C(44)	109.05(6)
C(3D)-H(3D)	0.9500	C(1)-P(1)-C(44)	115.51(6)
C(5D)-C(6D)	1.369(8)	N(1)-P(1)-C(38)	115.06(6)
C(5D)-H(5D)	0.9500	C(1)-P(1)-C(38)	103.83(6)
C(6D)-H(6D)	0.9500	C(44)-P(1)-C(38)	102.87(6)
C(1C)-C(2C)	1.385(7)	N(2)-P(2)-C(1)	114.56(6)
N(2)-P(2)-C(2)	111.60(6)	C(10)-C(9)-H(9)	119.8
C(1)-P(2)-C(2)	106.99(6)	C(8)-C(9)-H(9)	119.8
N(2)-P(2)-C(8)	108.92(6)	C(9)-C(10)-C(11)	120.25(13)
C(1)-P(2)-C(8)	109.31(6)	C(9)-C(10)-H(10)	119.9
C(2)-P(2)-C(8)	105.01(6)	C(11)-C(10)-H(10)	119.9
C(26)-N(1)-P(1)	122.33(8)	C(12)-C(11)-C(10)	119.88(13)

C(26)-N(1)-Zn(1)	110.19(8)	C(12)-C(11)-H(11)	120.1
P(1)-N(1)-Zn(1)	127.25(6)	C(10)-C(11)-H(11)	120.1
C(14)-N(2)-P(2)	126.02(9)	C(11)-C(12)-C(13)	120.20(14)
C(14)-N(2)-Zn(1)	112.18(8)	C(11)-C(12)-H(12)	119.9
P(2)-N(2)-Zn(1)	118.01(6)	C(13)-C(12)-H(12)	119.9
P(1)-C(1)-P(2)	128.02(8)	C(8)-C(13)-C(12)	120.41(13)
P(1)-C(1)-H(1)	116.0	C(8)-C(13)-H(13)	119.8
P(2)-C(1)-H(1)	116.0	C(12)-C(13)-H(13)	119.8
C(3)-C(2)-C(7)	119.35(12)	C(19)-C(14)-C(15)	119.69(11)
C(3)-C(2)-P(2)	120.54(10)	C(19)-C(14)-N(2)	120.11(11)
C(7)-C(2)-P(2)	120.06(10)	C(15)-C(14)-N(2)	119.88(11)
C(4)-C(3)-C(2)	120.07(13)	C(16)-C(15)-C(14)	118.90(13)
C(4)-C(3)-H(3)	120.0	C(16)-C(15)-C(20)	120.22(12)
C(2)-C(3)-H(3)	120.0	C(14)-C(15)-C(20)	120.76(11)
C(5)-C(4)-C(3)	120.28(14)	C(17)-C(16)-C(15)	121.40(13)
C(5)-C(4)-H(4)	119.9	C(17)-C(16)-H(16)	119.3
C(3)-C(4)-H(4)	119.9	C(15)-C(16)-H(16)	119.3
C(6)-C(5)-C(4)	119.83(13)	C(18)-C(17)-C(16)	119.45(12)
C(6)-C(5)-H(5)	120.1	C(18)-C(17)-H(17)	120.3
C(4)-C(5)-H(5)	120.1	C(16)-C(17)-H(17)	120.3
C(5)-C(6)-C(7)	120.45(13)	C(17)-C(18)-C(19)	121.34(13)
C(5)-C(6)-H(6)	119.8	C(17)-C(18)-H(18)	119.3
C(7)-C(6)-H(6)	119.8	C(19)-C(18)-H(18)	119.3
C(6)-C(7)-C(2)	120.02(13)	C(18)-C(19)-C(14)	119.15(13)
C(6)-C(7)-H(7)	120.0	C(18)-C(19)-C(23)	118.52(12)
C(2)-C(7)-H(7)	120.0	C(14)-C(19)-C(23)	122.32(11)
C(13)-C(8)-C(9)	118.90(12)	C(15)-C(20)-C(21)	113.78(13)
C(13)-C(8)-P(2)	121.84(10)	C(15)-C(20)-C(22)	109.88(12)
C(9)-C(8)-P(2)	119.09(10)	C(21)-C(20)-C(22)	110.42(13)
C(10)-C(9)-C(8)	120.36(13)	C(15)-C(20)-H(20)	107.5
C(21)-C(20)-H(20)	107.5	C(28)-C(27)-C(32)	118.43(12)
C(22)-C(20)-H(20)	107.5	C(26)-C(27)-C(32)	122.54(11)
C(20)-C(21)-H(21A)	109.5	C(29)-C(28)-C(27)	121.32(13)
C(20)-C(21)-H(21B)	109.5	C(29)-C(28)-H(28)	119.3
H(21A)-C(21)-H(21B)	109.5	C(27)-C(28)-H(28)	119.3
C(20)-C(21)-H(21C)	109.5	C(28)-C(29)-C(30)	119.37(13)
H(21A)-C(21)-H(21C)	109.5	C(28)-C(29)-H(29)	120.3
H(21B)-C(21)-H(21C)	109.5	C(30)-C(29)-H(29)	120.3
C(20)-C(22)-H(22A)	109.5	C(29)-C(30)-C(31)	121.65(13)
C(20)-C(22)-H(22B)	109.5	C(29)-C(30)-H(30)	119.2
H(22A)-C(22)-H(22B)	109.5	C(31)-C(30)-H(30)	119.2
C(20)-C(22)-H(22C)	109.5	C(30)-C(31)-C(26)	118.56(12)

H(22A)-C(22)-H(22C)	109.5	C(30)-C(31)-C(35)	118.89(12)
H(22B)-C(22)-H(22C)	109.5	C(26)-C(31)-C(35)	122.41(11)
C(19)-C(23)-C(24)	112.32(12)	C(27)-C(32)-C(34)	112.06(11)
C(19)-C(23)-C(25)	110.95(13)	C(27)-C(32)-C(33)	111.41(11)
C(24)-C(23)-C(25)	110.04(12)	C(34)-C(32)-C(33)	109.55(11)
C(19)-C(23)-H(23)	107.8	C(27)-C(32)-H(32)	107.9
C(24)-C(23)-H(23)	107.8	C(34)-C(32)-H(32)	107.9
C(25)-C(23)-H(23)	107.8	C(33)-C(32)-H(32)	107.9
C(23)-C(24)-H(24A)	109.5	C(32)-C(33)-H(33A)	109.5
C(23)-C(24)-H(24B)	109.5	C(32)-C(33)-H(33B)	109.5
H(24A)-C(24)-H(24B)	109.5	H(33A)-C(33)-H(33B)	109.5
C(23)-C(24)-H(24C)	109.5	C(32)-C(33)-H(33C)	109.5
H(24A)-C(24)-H(24C)	109.5	H(33A)-C(33)-H(33C)	109.5
H(24B)-C(24)-H(24C)	109.5	H(33B)-C(33)-H(33C)	109.5
C(23)-C(25)-H(25A)	109.5	C(32)-C(34)-H(34A)	109.5
C(23)-C(25)-H(25B)	109.5	C(32)-C(34)-H(34B)	109.5
H(25A)-C(25)-H(25B)	109.5	H(34A)-C(34)-H(34B)	109.5
C(23)-C(25)-H(25C)	109.5	C(32)-C(34)-H(34C)	109.5
H(25A)-C(25)-H(25C)	109.5	H(34A)-C(34)-H(34C)	109.5
H(25B)-C(25)-H(25C)	109.5	H(34B)-C(34)-H(34C)	109.5
C(27)-C(26)-C(31)	119.92(11)	C(31)-C(35)-C(36)	113.41(12)
C(27)-C(26)-N(1)	119.98(11)	C(31)-C(35)-C(37)	109.93(11)
C(31)-C(26)-N(1)	119.84(11)	C(36)-C(35)-C(37)	109.05(11)
C(28)-C(27)-C(26)	119.02(12)	C(31)-C(35)-H(35)	108.1
C(36)-C(35)-H(35)	108.1	C(46)-C(45)-H(45)	120.0
C(37)-C(35)-H(35)	108.1	C(44)-C(45)-H(45)	120.0
C(35)-C(36)-H(36A)	109.5	C(47)-C(46)-C(45)	120.41(13)
C(35)-C(36)-H(36B)	109.5	C(47)-C(46)-H(46)	119.8
H(36A)-C(36)-H(36B)	109.5	C(45)-C(46)-H(46)	119.8
C(35)-C(36)-H(36C)	109.5	C(46)-C(47)-C(48)	119.95(12)
H(36A)-C(36)-H(36C)	109.5	C(46)-C(47)-H(47)	120.0
H(36B)-C(36)-H(36C)	109.5	C(48)-C(47)-H(47)	120.0
C(35)-C(37)-H(37A)	109.5	C(47)-C(48)-C(49)	119.96(13)
C(35)-C(37)-H(37B)	109.5	C(47)-C(48)-H(48)	120.0
H(37A)-C(37)-H(37B)	109.5	C(49)-C(48)-H(48)	120.0
C(35)-C(37)-H(37C)	109.5	C(48)-C(49)-C(44)	120.54(12)
H(37A)-C(37)-H(37C)	109.5	C(48)-C(49)-H(49)	119.7
H(37B)-C(37)-H(37C)	109.5	C(44)-C(49)-H(49)	119.7
C(43)-C(38)-C(39)	118.66(12)	C(54)-C(50)-C(51)	107.73(13)
C(43)-C(38)-P(1)	124.73(11)	C(54)-C(50)-C(55)	126.73(14)
C(39)-C(38)-P(1)	116.57(10)	C(51)-C(50)-C(55)	125.52(14)
C(40)-C(39)-C(38)	120.85(14)	C(54)-C(50)-Zn(2)	72.01(8)

C(40)-C(39)-H(39)	119.6	C(51)-C(50)-Zn(2)	72.33(8)
C(38)-C(39)-H(39)	119.6	C(55)-C(50)-Zn(2)	122.36(11)
C(39)-C(40)-C(41)	119.95(15)	C(52)-C(51)-C(50)	108.28(13)
C(39)-C(40)-H(40)	120.0	C(52)-C(51)-C(56)	125.40(14)
C(41)-C(40)-H(40)	120.0	C(50)-C(51)-C(56)	126.08(15)
C(42)-C(41)-C(40)	120.06(14)	C(52)-C(51)-Zn(2)	72.35(8)
C(42)-C(41)-H(41)	120.0	C(50)-C(51)-Zn(2)	71.32(8)
C(40)-C(41)-H(41)	120.0	C(56)-C(51)-Zn(2)	126.58(10)
C(41)-C(42)-C(43)	120.17(14)	C(51)-C(52)-C(53)	107.93(13)
C(41)-C(42)-H(42)	119.9	C(51)-C(52)-C(57)	124.62(14)
C(43)-C(42)-H(42)	119.9	C(53)-C(52)-C(57)	127.40(15)
C(38)-C(43)-C(42)	120.28(14)	C(51)-C(52)-Zn(2)	71.58(8)
C(38)-C(43)-H(43)	119.9	C(53)-C(52)-Zn(2)	71.80(8)
C(42)-C(43)-H(43)	119.9	C(57)-C(52)-Zn(2)	124.44(10)
C(49)-C(44)-C(45)	119.11(12)	C(54)-C(53)-C(52)	107.84(13)
C(49)-C(44)-P(1)	118.91(10)	C(54)-C(53)-C(58)	125.58(13)
C(45)-C(44)-P(1)	121.98(10)	C(52)-C(53)-C(58)	126.52(14)
C(46)-C(45)-C(44)	120.02(12)	C(54)-C(53)-Zn(2)	71.32(8)
C(52)-C(53)-Zn(2)	72.04(8)	H(59A)-C(59)-H(59C)	109.5
C(58)-C(53)-Zn(2)	124.28(11)	H(59B)-C(59)-H(59C)	109.5
C(50)-C(54)-C(53)	108.22(12)	C(6A)-C(1A)-C(2A)	120.2(2)
C(50)-C(54)-C(59)	126.34(14)	C(6A)-C(1A)-H(1A1)	119.9
C(53)-C(54)-C(59)	125.43(14)	C(2A)-C(1A)-H(1A1)	119.9
C(50)-C(54)-Zn(2)	71.60(8)	C(3A)-C(2A)-C(1A)	119.7(2)
C(53)-C(54)-Zn(2)	72.44(8)	C(3A)-C(2A)-H(2A)	120.1
C(59)-C(54)-Zn(2)	122.06(10)	C(1A)-C(2A)-H(2A)	120.1
C(50)-C(55)-H(55A)	109.5	C(4A)-C(3A)-C(2A)	119.9(2)
C(50)-C(55)-H(55B)	109.5	C(4A)-C(3A)-H(3A)	120.0
H(55A)-C(55)-H(55B)	109.5	C(2A)-C(3A)-H(3A)	120.0
C(50)-C(55)-H(55C)	109.5	C(3A)-C(4A)-C(5A)	120.12(18)
H(55A)-C(55)-H(55C)	109.5	C(3A)-C(4A)-H(4A)	119.9
H(55B)-C(55)-H(55C)	109.5	C(5A)-C(4A)-H(4A)	119.9
C(51)-C(56)-H(56A)	109.5	C(6A)-C(5A)-C(4A)	120.23(19)
C(51)-C(56)-H(56B)	109.5	C(6A)-C(5A)-H(5A)	119.9
H(56A)-C(56)-H(56B)	109.5	C(4A)-C(5A)-H(5A)	119.9
C(51)-C(56)-H(56C)	109.5	C(1A)-C(6A)-C(5A)	119.7(2)
H(56A)-C(56)-H(56C)	109.5	C(1A)-C(6A)-H(6A)	120.1
H(56B)-C(56)-H(56C)	109.5	C(5A)-C(6A)-H(6A)	120.1
C(52)-C(57)-H(57A)	109.5	C(2B)-C(1B)-C(6B)	117.1(12)
C(52)-C(57)-H(57B)	109.5	C(2B)-C(1B)-H(1B1)	121.5
H(57A)-C(57)-H(57B)	109.5	C(6B)-C(1B)-H(1B1)	121.5
C(52)-C(57)-H(57C)	109.5	C(1B)-C(2B)-C(3B)	127.0(11)

H(57A)-C(57)-H(57C)	109.5	C(1B)-C(2B)-H(2B)	116.5
H(57B)-C(57)-H(57C)	109.5	C(3B)-C(2B)-H(2B)	116.5
C(53)-C(58)-H(58A)	109.5	C(4B)-C(3B)-C(2B)	115.9(8)
C(53)-C(58)-H(58B)	109.5	C(4B)-C(3B)-H(3B)	122.1
H(58A)-C(58)-H(58B)	109.5	C(2B)-C(3B)-H(3B)	122.1
C(53)-C(58)-H(58C)	109.5	C(3B)-C(4B)-C(5B)	118.1(6)
H(58A)-C(58)-H(58C)	109.5	C(3B)-C(4B)-H(4B)	121.0
H(58B)-C(58)-H(58C)	109.5	C(5B)-C(4B)-H(4B)	121.0
C(54)-C(59)-H(59A)	109.5	C(4B)-C(5B)-C(6B)	126.1(9)
C(54)-C(59)-H(59B)	109.5	C(4B)-C(5B)-H(5B)	117.0
H(59A)-C(59)-H(59B)	109.5	C(6B)-C(5B)-H(5B)	117.0
C(54)-C(59)-H(59C)	109.5	C(1B)-C(6B)-C(5B)	115.9(12)
C(1B)-C(6B)-H(6B)	122.1	C(3C)-C(2C)-C(1C)	119.6(5)
C(5B)-C(6B)-H(6B)	122.1	C(3C)-C(2C)-H(2C)	120.2
C(6D)-C(1D)-C(2D)	124.1(11)	C(1C)-C(2C)-H(2C)	120.2
C(6D)-C(1D)-H(1D)	118.0	C(2C)-C(3C)-C(4C)	120.0(5)
C(2D)-C(1D)-H(1D)	118.0	C(2C)-C(3C)-H(3C)	120.0
C(1D)-C(2D)-C(3D)	111.3(11)	C(4C)-C(3C)-H(3C)	120.0
C(1D)-C(2D)-H(2D)	124.4	C(5C)-C(4C)-C(3C)	120.3(5)
C(3D)-C(2D)-H(2D)	124.4	C(5C)-C(4C)-H(4C)	119.9
C(2D)-C(3D)-H(3D)	116.7	C(3C)-C(4C)-H(4C)	119.9
C(6D)-C(5D)-H(5D)	122.2	C(4C)-C(5C)-C(6C)	119.9(5)
C(1D)-C(6D)-C(5D)	122.8(13)	C(4C)-C(5C)-H(5C)	120.1
C(1D)-C(6D)-H(6D)	118.6	C(6C)-C(5C)-H(5C)	120.1
C(5D)-C(6D)-H(6D)	118.6	C(5C)-C(6C)-C(1C)	120.1(5)
C(2C)-C(1C)-C(6C)	120.0(5)	C(5C)-C(6C)-H(6C)	119.9
C(2C)-C(1C)-H(1C)	120.0	C(1C)-C(6C)-H(6C)	119.9
C(6C)-C(1C)-H(1C)	120.0		

Symmetry transformations use d to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **3**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zn(1)	10(1)	15(1)	11(1)	-4(1)	2(1)	-6(1)
Zn(2)	11(1)	22(1)	19(1)	-7(1)	2(1)	-7(1)
P(1)	10(1)	12(1)	11(1)	-3(1)	2(1)	-4(1)
P(2)	11(1)	14(1)	10(1)	-3(1)	2(1)	-6(1)
N(1)	11(1)	14(1)	11(1)	-3(1)	2(1)	-5(1)
N(2)	12(1)	18(1)	11(1)	-3(1)	1(1)	-8(1)
C(1)	12(1)	15(1)	12(1)	-2(1)	3(1)	-5(1)
C(2)	13(1)	21(1)	11(1)	-4(1)	2(1)	-10(1)
C(3)	15(1)	23(1)	14(1)	-4(1)	2(1)	-8(1)
C(4)	15(1)	31(1)	17(1)	-9(1)	3(1)	-8(1)
C(5)	18(1)	42(1)	14(1)	-9(1)	5(1)	-18(1)
C(6)	28(1)	33(1)	15(1)	-3(1)	3(1)	-22(1)
C(7)	21(1)	22(1)	15(1)	-5(1)	4(1)	-13(1)
C(8)	16(1)	15(1)	12(1)	-3(1)	1(1)	-8(1)
C(9)	16(1)	21(1)	18(1)	-5(1)	0(1)	-9(1)
C(10)	25(1)	27(1)	21(1)	-7(1)	-2(1)	-16(1)
C(11)	34(1)	24(1)	22(1)	-11(1)	3(1)	-17(1)
C(12)	25(1)	21(1)	24(1)	-11(1)	6(1)	-10(1)
C(13)	17(1)	18(1)	18(1)	-6(1)	2(1)	-9(1)
C(14)	13(1)	20(1)	12(1)	-4(1)	2(1)	-10(1)
C(15)	15(1)	20(1)	15(1)	-2(1)	0(1)	-9(1)
C(16)	17(1)	27(1)	15(1)	-1(1)	-1(1)	-10(1)
C(17)	20(1)	36(1)	13(1)	-6(1)	1(1)	-16(1)
C(18)	25(1)	32(1)	16(1)	-10(1)	5(1)	-19(1)
C(19)	18(1)	22(1)	14(1)	-5(1)	4(1)	-13(1)
C(20)	22(1)	17(1)	20(1)	0(1)	-5(1)	-9(1)
C(21)	51(1)	26(1)	29(1)	5(1)	-10(1)	-23(1)
C(22)	23(1)	23(1)	33(1)	-9(1)	-1(1)	-4(1)
C(23)	30(1)	20(1)	16(1)	-7(1)	4(1)	-15(1)
C(24)	27(1)	27(1)	26(1)	-11(1)	7(1)	-14(1)
C(25)	43(1)	25(1)	30(1)	-13(1)	18(1)	-22(1)
C(26)	10(1)	17(1)	10(1)	-3(1)	2(1)	-5(1)
C(27)	12(1)	17(1)	13(1)	-3(1)	2(1)	-6(1)
C(28)	17(1)	21(1)	17(1)	-1(1)	4(1)	-9(1)
C(29)	18(1)	28(1)	15(1)	-3(1)	7(1)	-7(1)
C(30)	16(1)	25(1)	16(1)	-9(1)	4(1)	-5(1)
C(31)	12(1)	19(1)	15(1)	-6(1)	2(1)	-5(1)
C(32)	17(1)	16(1)	17(1)	-4(1)	5(1)	-9(1)
C(33)	23(1)	17(1)	27(1)	-4(1)	5(1)	-8(1)

C(34)	24(1)	27(1)	24(1)	-8(1)	4(1)	-15(1)
C(35)	16(1)	19(1)	20(1)	-11(1)	4(1)	-7(1)
C(36)	20(1)	26(1)	30(1)	-15(1)	-2(1)	-6(1)
C(37)	21(1)	20(1)	22(1)	-9(1)	1(1)	-7(1)
C(38)	14(1)	14(1)	17(1)	-4(1)	6(1)	-5(1)
C(39)	20(1)	17(1)	20(1)	-6(1)	6(1)	-8(1)
C(40)	29(1)	20(1)	32(1)	-14(1)	15(1)	-12(1)
C(41)	30(1)	13(1)	40(1)	-6(1)	17(1)	-3(1)
C(42)	23(1)	18(1)	28(1)	1(1)	5(1)	-1(1)
C(43)	18(1)	19(1)	20(1)	-1(1)	3(1)	-4(1)
C(44)	11(1)	15(1)	13(1)	-4(1)	1(1)	-4(1)
C(45)	16(1)	16(1)	15(1)	-3(1)	2(1)	-6(1)
C(46)	20(1)	20(1)	12(1)	-3(1)	0(1)	-6(1)
C(47)	21(1)	26(1)	16(1)	-7(1)	-2(1)	-9(1)
C(48)	21(1)	24(1)	21(1)	-7(1)	0(1)	-13(1)
C(49)	16(1)	20(1)	15(1)	-4(1)	1(1)	-8(1)
C(50)	14(1)	29(1)	22(1)	-5(1)	0(1)	-11(1)
C(51)	11(1)	28(1)	20(1)	-1(1)	2(1)	-8(1)
C(52)	12(1)	28(1)	19(1)	-5(1)	4(1)	-3(1)
C(53)	12(1)	24(1)	20(1)	-5(1)	4(1)	-3(1)
C(54)	12(1)	28(1)	16(1)	-3(1)	0(1)	-7(1)
C(55)	31(1)	41(1)	35(1)	-13(1)	-2(1)	-23(1)
C(56)	20(1)	35(1)	31(1)	3(1)	6(1)	-12(1)
C(57)	23(1)	39(1)	21(1)	-10(1)	7(1)	-4(1)
C(58)	27(1)	24(1)	33(1)	-9(1)	8(1)	-3(1)
C(59)	26(1)	35(1)	18(1)	-1(1)	-3(1)	-11(1)
C(1A)	62(1)	61(1)	44(1)	-19(1)	24(1)	-39(1)
C(2A)	67(2)	68(2)	37(1)	-19(1)	11(1)	-46(1)
C(3A)	43(1)	46(1)	46(1)	-15(1)	12(1)	-28(1)
C(4A)	44(1)	30(1)	37(1)	-10(1)	13(1)	-15(1)
C(5A)	41(1)	30(1)	40(1)	-8(1)	-1(1)	-12(1)
C(6A)	38(1)	37(1)	55(1)	-11(1)	9(1)	-19(1)
C(1B)	39(3)	26(3)	108(10)	-14(5)	3(5)	-16(2)
C(2B)	55(6)	36(4)	98(8)	-30(5)	38(6)	-26(4)
C(3B)	80(5)	50(4)	14(4)	0(3)	5(3)	-45(3)
C(4B)	47(1)	39(1)	55(1)	-3(1)	-10(1)	-28(1)
C(5B)	36(5)	53(5)	99(7)	-55(5)	34(4)	-29(4)
C(6B)	85(8)	52(8)	29(3)	-5(4)	2(4)	-50(6)
C(1D)	66(9)	26(4)	43(4)	-1(3)	-15(4)	-20(5)
C(2D)	64(5)	43(5)	63(6)	-8(4)	-6(4)	-27(4)
C(3D)	81(5)	67(6)	13(4)	5(4)	-1(3)	-52(4)
C(4D)	47(1)	39(1)	55(1)	-3(1)	-10(1)	-28(1)

C(5D)	38(4)	35(3)	42(3)	-20(2)	13(2)	-26(3)
C(6D)	84(7)	45(6)	37(3)	-7(4)	-6(4)	-44(5)
C(1C)	77(8)	104(12)	55(9)	32(6)	-5(6)	-68(8)
C(2C)	141(9)	91(7)	69(5)	-20(5)	48(6)	-98(7)
C(3C)	66(4)	45(4)	66(6)	-5(4)	35(4)	-35(3)
C(4C)	56(4)	77(5)	51(6)	7(4)	19(3)	-41(4)
C(5C)	121(8)	63(4)	96(7)	-27(4)	77(6)	-63(5)
C(6C)	46(4)	58(6)	143(11)	48(6)	31(6)	-18(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **3**.

x	y	z	U(eq)	
H(1)	5536	3017	7598	16
H(3)	5651	3064	6561	21
H(4)	6733	3139	5686	25
H(5)	6564	4907	5035	27
H(6)	5319	6602	5262	28
H(7)	4221	6545	6130	22
H(9)	5617	5524	7407	22
H(10)	5547	6929	7854	27
H(11)	3764	8146	8140	29
H(12)	2037	7991	7950	27
H(13)	2086	6616	7477	21
H(16)	576	7263	4932	25
H(17)	629	5726	4624	27
H(18)	1714	3852	5286	25
H(20)	2127	7085	6326	25
H(21A)	2011	8123	5230	54
H(21B)	1348	8962	5651	54
H(21C)	598	8701	5189	54
H(22A)	-393	8032	6089	43
H(22B)	312	8282	6581	43
H(22C)	374	7030	6723	43
H(23)	3401	3005	6799	25
H(24A)	3462	2232	5699	38
H(24B)	4336	1493	6351	38
H(24C)	4404	2616	5901	38
H(25A)	1592	2917	6936	44
H(25B)	2591	1678	6936	44

H(25C)	1659	2502	6313	44
H(28)	1055	1572	9586	23
H(29)	465	2854	10191	27
H(30)	919	4406	9924	25
H(32)	2769	1642	8268	20
H(33A)	2663	-21	9383	35
H(33B)	3802	199	9238	35
H(33C)	3350	-330	8789	35
H(34A)	1506	896	8031	35
H(34B)	729	2214	8003	35
H(34C)	775	1207	8611	35
H(35)	2526	5087	8644	21
H(36A)	1787	5545	9824	38
H(36B)	2477	6128	9353	38
H(36C)	3128	4783	9732	38
H(37A)	498	6049	8250	32
H(37B)	841	6893	8497	32
H(37C)	149	6257	8926	32
H(39)	4369	1445	7632	23
H(40)	5321	-511	7727	30
H(41)	6671	-1809	8627	36
H(42)	7072	-1147	9428	34
H(43)	6096	819	9345	26
H(45)	4221	2041	9738	20
H(46)	4893	2289	10648	23
H(47)	5877	3432	10547	25
H(48)	6168	4360	9532	25
H(49)	5491	4127	8618	21
H(55A)	-1780	4148	6391	49
H(55B)	-2393	3612	6945	49
H(55C)	-985	3138	7016	49
H(56A)	-1130	3269	8718	47
H(56B)	-1451	2827	8173	47
H(56C)	-2482	3616	8508	47
H(57A)	-2801	5919	8749	46
H(57B)	-1834	6394	8601	46
H(57C)	-1422	5048	8931	46
H(58A)	-2017	7872	6873	47
H(58B)	-2050	7708	7625	47
H(58C)	-3238	8116	7173	47
H(59A)	-1518	6588	6056	43
H(59B)	-2927	7156	6042	43

H(59C)	-2234	5920	5932	43
H(1A1)	7632	410	7905	61
H(2A)	9436	493	7956	61
H(3A)	10357	736	7030	50
H(4A)	9497	855	6065	45
H(5A)	7725	720	6023	47
H(6A)	6804	472	6946	52
H(1B1)	4935	-1925	6117	70
H(2B)	4824	-1140	5038	71
H(3B)	3260	515	4422	53
H(4B)	1686	1494	4956	56
H(5B)	1788	745	6040	62
H(6B)	3325	-960	6655	59
H(1D)	4592	-1735	6365	56
H(2D)	4988	-1411	5290	68
H(3D)	3507	257	4576	60
H(4D)	1791	1462	4866	56
H(5D)	1407	1037	5943	40
H(6D)	2908	-549	6675	61
H(1C)	11455	-770	10744	97
H(2C)	9658	846	10677	101
H(3C)	8224	1545	9805	70
H(4C)	8565	595	9024	76
H(5C)	10278	-1107	9145	102
H(6C)	11706	-1812	10016	123

Table 6. Torsion angles [deg] for **3**.

N(2)-Zn(1)-Zn(2)-C(50)	80.63(9)	N(2)-P(2)-C(2)-C(3)	-94.35(11)
N(1)-Zn(1)-Zn(2)-C(50)	-105.27(8)	C(1)-P(2)-C(2)-C(3)	31.70(12)
N(2)-Zn(1)-Zn(2)-C(54)	9.07(8)	C(8)-P(2)-C(2)-C(3)	147.79(10)
N(1)-Zn(1)-Zn(2)-C(54)	-176.84(8)	N(2)-P(2)-C(2)-C(7)	82.81(11)
N(2)-Zn(1)-Zn(2)-C(51)	161.13(9)	C(1)-P(2)-C(2)-C(7)	-151.14(10)
N(1)-Zn(1)-Zn(2)-C(51)	-24.77(9)	C(8)-P(2)-C(2)-C(7)	-35.04(12)
N(2)-Zn(1)-Zn(2)-C(53)	-56.23(8)	C(7)-C(2)-C(3)-C(4)	0.66(19)
N(1)-Zn(1)-Zn(2)-C(53)	117.87(7)	P(2)-C(2)-C(3)-C(4)	177.84(10)
N(2)-Zn(1)-Zn(2)-C(52)	-123.15(8)	C(2)-C(3)-C(4)-C(5)	-0.2(2)
N(1)-Zn(1)-Zn(2)-C(52)	50.95(8)	C(3)-C(4)-C(5)-C(6)	0.0(2)
C(1)-P(1)-N(1)-C(26)	-168.16(10)	C(4)-C(5)-C(6)-C(7)	-0.3(2)

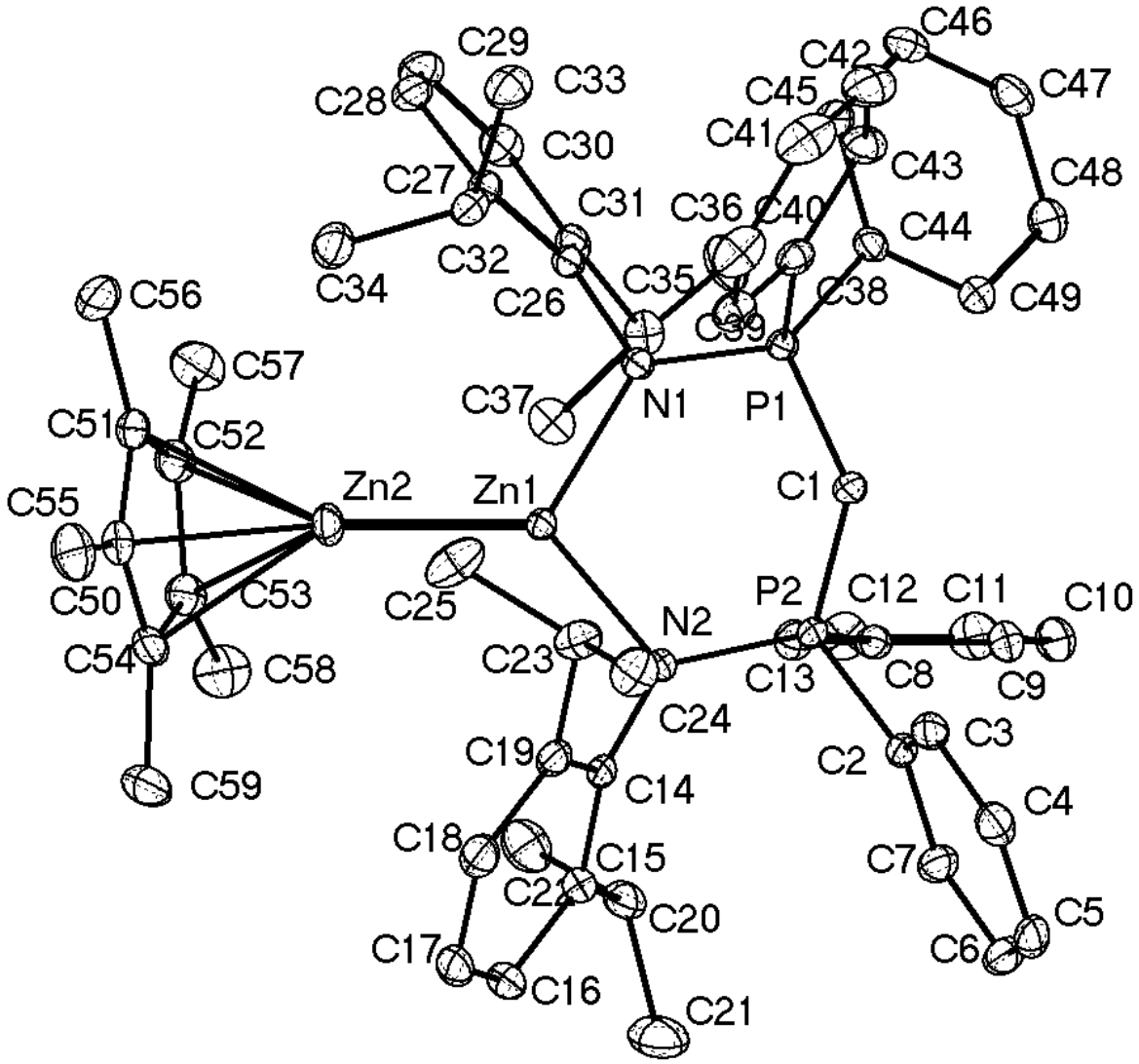
C(44)-P(1)-N(1)-C(26)	-40.21(11)	C(5)-C(6)-C(7)-C(2)	0.7(2)
C(38)-P(1)-N(1)-C(26)	74.72(11)	C(3)-C(2)-C(7)-C(6)	-0.89(19)
C(1)-P(1)-N(1)-Zn(1)	5.87(9)	P(2)-C(2)-C(7)-C(6)	-178.09(10)
C(44)-P(1)-N(1)-Zn(1)	133.82(7)	N(2)-P(2)-C(8)-C(13)	16.94(12)
C(38)-P(1)-N(1)-Zn(1)	-111.25(8)	C(1)-P(2)-C(8)-C(13)	-108.91(11)
N(2)-Zn(1)-N(1)-C(26)	163.37(8)	C(2)-P(2)-C(8)-C(13)	136.60(11)
Zn(2)-Zn(1)-N(1)-C(26)	-11.99(9)	N(2)-P(2)-C(8)-C(9)	-168.01(10)
N(2)-Zn(1)-N(1)-P(1)	-11.26(9)	C(1)-P(2)-C(8)-C(9)	66.13(12)
Zn(2)-Zn(1)-N(1)-P(1)	173.38(5)	C(2)-P(2)-C(8)-C(9)	-48.36(12)
C(1)-P(2)-N(2)-C(14)	-120.40(11)	C(13)-C(8)-C(9)-C(10)	-0.3(2)
C(2)-P(2)-N(2)-C(14)	1.37(13)	P(2)-C(8)-C(9)-C(10)	-175.49(11)
C(8)-P(2)-N(2)-C(14)	116.85(11)	C(8)-C(9)-C(10)-C(11)	1.1(2)
C(1)-P(2)-N(2)-Zn(1)	35.86(9)	C(9)-C(10)-C(11)-C(12)	-1.0(2)
C(2)-P(2)-N(2)-Zn(1)	157.63(6)	C(10)-C(11)-C(12)-C(13)	0.1(2)
C(8)-P(2)-N(2)-Zn(1)	-86.88(7)	C(9)-C(8)-C(13)-C(12)	-0.6(2)
N(1)-Zn(1)-N(2)-C(14)	148.06(8)	P(2)-C(8)-C(13)-C(12)	174.49(11)
Zn(2)-Zn(1)-N(2)-C(14)	-37.25(10)	C(11)-C(12)-C(13)-C(8)	0.7(2)
N(1)-Zn(1)-N(2)-P(2)	-11.36(8)	P(2)-N(2)-C(14)-C(19)	92.08(14)
Zn(2)-Zn(1)-N(2)-P(2)	163.33(4)	Zn(1)-N(2)-C(14)-C(19)	-65.35(14)
N(1)-P(1)-C(1)-P(2)	24.71(11)	P(2)-N(2)-C(14)-C(15)	-94.44(14)
C(44)-P(1)-C(1)-P(2)	-99.60(10)	Zn(1)-N(2)-C(14)-C(15)	108.13(11)
C(38)-P(1)-C(1)-P(2)	148.58(9)	C(19)-C(14)-C(15)-C(16)	1.72(19)
N(2)-P(2)-C(1)-P(1)	-48.13(11)	N(2)-C(14)-C(15)-C(16)	-171.80(12)
C(2)-P(2)-C(1)-P(1)	-172.38(9)	C(19)-C(14)-C(15)-C(20)	177.79(12)
C(8)-P(2)-C(1)-P(1)	74.41(10)	N(2)-C(14)-C(15)-C(20)	4.27(19)
C(14)-C(15)-C(16)-C(17)	0.8(2)	C(28)-C(27)-C(32)-C(34)	61.05(16)
C(20)-C(15)-C(16)-C(17)	-175.27(13)	C(26)-C(27)-C(32)-C(34)	-118.01(13)
C(15)-C(16)-C(17)-C(18)	-2.1(2)	C(28)-C(27)-C(32)-C(33)	-62.09(16)
C(16)-C(17)-C(18)-C(19)	0.9(2)	C(26)-C(27)-C(32)-C(33)	118.85(13)
C(17)-C(18)-C(19)-C(14)	1.6(2)	C(30)-C(31)-C(35)-C(36)	50.23(17)
C(17)-C(18)-C(19)-C(23)	-179.66(13)	C(26)-C(31)-C(35)-C(36)	-134.12(13)
C(15)-C(14)-C(19)-C(18)	-2.90(19)	C(30)-C(31)-C(35)-C(37)	-72.13(15)
N(2)-C(14)-C(19)-C(18)	170.60(12)	C(26)-C(31)-C(35)-C(37)	103.51(14)
C(15)-C(14)-C(19)-C(23)	178.41(12)	N(1)-P(1)-C(38)-C(43)	-121.20(12)
N(2)-C(14)-C(19)-C(23)	-8.09(19)	C(1)-P(1)-C(38)-C(43)	118.00(12)
C(16)-C(15)-C(20)-C(21)	-34.97(19)	C(44)-P(1)-C(38)-C(43)	-2.75(13)
C(14)-C(15)-C(20)-C(21)	149.01(14)	N(1)-P(1)-C(38)-C(39)	60.98(12)
C(16)-C(15)-C(20)-C(22)	89.40(15)	C(1)-P(1)-C(38)-C(39)	-59.81(11)
C(14)-C(15)-C(20)-C(22)	-86.61(15)	C(44)-P(1)-C(38)-C(39)	179.44(10)
C(18)-C(19)-C(23)-C(24)	54.90(17)	C(43)-C(38)-C(39)-C(40)	2.0(2)
C(14)-C(19)-C(23)-C(24)	-126.40(14)	P(1)-C(38)-C(39)-C(40)	179.94(11)
C(18)-C(19)-C(23)-C(25)	-68.73(16)	C(38)-C(39)-C(40)-C(41)	-1.1(2)

C(14)-C(19)-C(23)-C(25)	109.98(14)	C(39)-C(40)-C(41)-C(42)	-0.3(2)
P(1)-N(1)-C(26)-C(27)	-94.09(13)	C(40)-C(41)-C(42)-C(43)	0.8(2)
Zn(1)-N(1)-C(26)-C(27)	90.97(12)	C(39)-C(38)-C(43)-C(42)	-1.5(2)
P(1)-N(1)-C(26)-C(31)	91.84(13)	P(1)-C(38)-C(43)-C(42)	-179.23(11)
Zn(1)-N(1)-C(26)-C(31)	-83.10(12)	C(41)-C(42)-C(43)-C(38)	0.1(2)
C(31)-C(26)-C(27)-C(28)	-2.70(18)	N(1)-P(1)-C(44)-C(49)	-117.62(11)
N(1)-C(26)-C(27)-C(28)	-176.76(11)	C(1)-P(1)-C(44)-C(49)	7.41(13)
C(31)-C(26)-C(27)-C(32)	176.36(11)	C(38)-P(1)-C(44)-C(49)	119.79(11)
N(1)-C(26)-C(27)-C(32)	2.30(18)	N(1)-P(1)-C(44)-C(45)	62.67(12)
C(26)-C(27)-C(28)-C(29)	-0.8(2)	C(1)-P(1)-C(44)-C(45)	-172.30(10)
C(32)-C(27)-C(28)-C(29)	-179.89(12)	C(38)-P(1)-C(44)-C(45)	-59.92(12)
C(27)-C(28)-C(29)-C(30)	2.1(2)	C(49)-C(44)-C(45)-C(46)	-0.33(19)
C(28)-C(29)-C(30)-C(31)	0.1(2)	P(1)-C(44)-C(45)-C(46)	179.38(10)
C(29)-C(30)-C(31)-C(26)	-3.5(2)	C(44)-C(45)-C(46)-C(47)	-0.2(2)
C(29)-C(30)-C(31)-C(35)	172.30(13)	C(45)-C(46)-C(47)-C(48)	0.6(2)
C(27)-C(26)-C(31)-C(30)	4.78(18)	C(46)-C(47)-C(48)-C(49)	-0.4(2)
N(1)-C(26)-C(31)-C(30)	178.85(11)	C(47)-C(48)-C(49)-C(44)	-0.2(2)
C(27)-C(26)-C(31)-C(35)	-170.88(12)	C(45)-C(44)-C(49)-C(48)	0.5(2)
N(1)-C(26)-C(31)-C(35)	3.19(18)	P(1)-C(44)-C(49)-C(48)	-179.20(11)
C(51)-Zn(2)-C(50)-C(54)	116.08(13)	Zn(2)-C(51)-C(52)-C(53)	63.02(10)
C(53)-Zn(2)-C(50)-C(54)	37.29(8)	C(50)-C(51)-C(52)-C(57)	177.69(13)
C(52)-Zn(2)-C(50)-C(54)	79.04(9)	C(56)-C(51)-C(52)-C(57)	3.1(2)
Zn(1)-Zn(2)-C(50)-C(54)	-115.28(9)	Zn(2)-C(51)-C(52)-C(57)	-119.64(14)
C(54)-Zn(2)-C(50)-C(51)	-116.08(13)	C(50)-C(51)-C(52)-Zn(2)	-62.67(10)
C(53)-Zn(2)-C(50)-C(51)	-78.79(9)	C(56)-C(51)-C(52)-Zn(2)	122.76(14)
C(52)-Zn(2)-C(50)-C(51)	-37.03(8)	C(50)-Zn(2)-C(52)-C(51)	37.33(8)
Zn(1)-Zn(2)-C(50)-C(51)	128.64(8)	C(54)-Zn(2)-C(52)-C(51)	79.40(9)
C(54)-Zn(2)-C(50)-C(55)	122.59(16)	C(53)-Zn(2)-C(52)-C(51)	116.80(12)
C(51)-Zn(2)-C(50)-C(55)	-121.33(16)	Zn(1)-Zn(2)-C(52)-C(51)	-129.40(8)
C(53)-Zn(2)-C(50)-C(55)	159.88(14)	C(50)-Zn(2)-C(52)-C(53)	-79.48(9)
C(52)-Zn(2)-C(50)-C(55)	-158.37(14)	C(54)-Zn(2)-C(52)-C(53)	-37.41(9)
Zn(1)-Zn(2)-C(50)-C(55)	7.31(18)	C(51)-Zn(2)-C(52)-C(53)	-116.80(12)
C(54)-C(50)-C(51)-C(52)	-0.42(15)	Zn(1)-Zn(2)-C(52)-C(53)	113.79(9)
C(55)-C(50)-C(51)-C(52)	-179.10(14)	C(50)-Zn(2)-C(52)-C(57)	157.17(15)
Zn(2)-C(50)-C(51)-C(52)	63.33(10)	C(54)-Zn(2)-C(52)-C(57)	-160.76(16)
C(54)-C(50)-C(51)-C(56)	174.10(13)	C(51)-Zn(2)-C(52)-C(57)	119.85(17)
C(55)-C(50)-C(51)-C(56)	-4.6(2)	C(53)-Zn(2)-C(52)-C(57)	-123.35(18)
Zn(2)-C(50)-C(51)-C(56)	-122.14(14)	Zn(1)-Zn(2)-C(52)-C(57)	-9.56(18)
C(54)-C(50)-C(51)-Zn(2)	-63.76(9)	C(51)-C(52)-C(53)-C(54)	-0.14(16)
C(55)-C(50)-C(51)-Zn(2)	117.57(15)	C(57)-C(52)-C(53)-C(54)	-177.39(14)
C(50)-Zn(2)-C(51)-C(52)	-117.07(12)	Zn(2)-C(52)-C(53)-C(54)	62.73(10)
C(54)-Zn(2)-C(51)-C(52)	-79.28(9)	C(51)-C(52)-C(53)-C(58)	177.34(14)

C(53)-Zn(2)-C(51)-C(52)	-37.33(8)	C(57)-C(52)-C(53)-C(58)	0.1(2)
Zn(1)-Zn(2)-C(51)-C(52)	118.45(9)	Zn(2)-C(52)-C(53)-C(58)	-119.78(15)
C(54)-Zn(2)-C(51)-C(50)	37.79(9)	C(51)-C(52)-C(53)-Zn(2)	-62.88(10)
C(53)-Zn(2)-C(51)-C(50)	79.73(9)	C(57)-C(52)-C(53)-Zn(2)	119.87(15)
C(52)-Zn(2)-C(51)-C(50)	117.07(12)	C(50)-Zn(2)-C(53)-C(54)	-37.44(8)
Zn(1)-Zn(2)-C(51)-C(50)	-124.48(9)	C(51)-Zn(2)-C(53)-C(54)	-79.48(9)
C(50)-Zn(2)-C(51)-C(56)	121.55(18)	C(52)-Zn(2)-C(53)-C(54)	-116.72(13)
C(54)-Zn(2)-C(51)-C(56)	159.33(16)	Zn(1)-Zn(2)-C(53)-C(54)	119.68(8)
C(53)-Zn(2)-C(51)-C(56)	-158.72(16)	C(50)-Zn(2)-C(53)-C(52)	79.28(10)
C(52)-Zn(2)-C(51)-C(56)	-121.39(17)	C(54)-Zn(2)-C(53)-C(52)	116.72(13)
Zn(1)-Zn(2)-C(51)-C(56)	-2.9(2)	C(51)-Zn(2)-C(53)-C(52)	37.24(9)
C(50)-C(51)-C(52)-C(53)	0.35(16)	Zn(1)-Zn(2)-C(53)-C(52)	-123.61(8)
C(56)-C(51)-C(52)-C(53)	-174.22(13)	C(50)-Zn(2)-C(53)-C(58)	-158.29(14)
C(54)-Zn(2)-C(53)-C(58)	-120.85(16)	Zn(1)-Zn(2)-C(54)-C(53)	-115.61(8)
C(51)-Zn(2)-C(53)-C(58)	159.67(15)	C(50)-Zn(2)-C(54)-C(59)	-121.91(16)
C(52)-Zn(2)-C(53)-C(58)	122.43(17)	C(51)-Zn(2)-C(54)-C(59)	-159.67(15)
Zn(1)-Zn(2)-C(53)-C(58)	-1.18(16)	C(53)-Zn(2)-C(54)-C(59)	121.29(16)
C(51)-C(50)-C(54)-C(53)	0.33(15)	C(52)-Zn(2)-C(54)-C(59)	158.61(15)
C(55)-C(50)-C(54)-C(53)	178.99(14)	Zn(1)-Zn(2)-C(54)-C(59)	5.68(17)
Zn(2)-C(50)-C(54)-C(53)	-63.63(10)	C(6A)-C(1A)-C(2A)-C(3A)	1.6(4)
C(51)-C(50)-C(54)-C(59)	-179.31(13)	C(1A)-C(2A)-C(3A)-C(4A)	-0.6(3)
C(55)-C(50)-C(54)-C(59)	-0.7(2)	C(2A)-C(3A)-C(4A)-C(5A)	-0.3(3)
Zn(2)-C(50)-C(54)-C(59)	116.73(14)	C(3A)-C(4A)-C(5A)-C(6A)	0.3(3)
C(51)-C(50)-C(54)-Zn(2)	63.96(9)	C(2A)-C(1A)-C(6A)-C(5A)	-1.7(3)
C(55)-C(50)-C(54)-Zn(2)	-117.38(15)	C(4A)-C(5A)-C(6A)-C(1A)	0.8(3)
C(52)-C(53)-C(54)-C(50)	-0.12(16)	C(6B)-C(1B)-C(2B)-C(3B)	0(3)
C(58)-C(53)-C(54)-C(50)	-177.63(14)	C(1B)-C(2B)-C(3B)-C(4B)	1(3)
Zn(2)-C(53)-C(54)-C(50)	63.09(10)	C(2B)-C(3B)-C(4B)-C(5B)	0(2)
C(52)-C(53)-C(54)-C(59)	179.53(13)	C(3B)-C(4B)-C(5B)-C(6B)	-1(2)
C(58)-C(53)-C(54)-C(59)	2.0(2)	C(2B)-C(1B)-C(6B)-C(5B)	-1(2)
Zn(2)-C(53)-C(54)-C(59)	-117.26(14)	C(4B)-C(5B)-C(6B)-C(1B)	2(3)
C(52)-C(53)-C(54)-Zn(2)	-63.20(10)	C(6D)-C(1D)-C(2D)-C(3D)	1(3)
C(58)-C(53)-C(54)-Zn(2)	119.28(15)	C(2D)-C(1D)-C(6D)-C(5D)	1(3)
C(51)-Zn(2)-C(54)-C(50)	-37.76(8)	C(6C)-C(1C)-C(2C)-C(3C)	-4.2(16)
C(53)-Zn(2)-C(54)-C(50)	-116.80(12)	C(1C)-C(2C)-C(3C)-C(4C)	0.9(16)
C(52)-Zn(2)-C(54)-C(50)	-79.48(9)	C(2C)-C(3C)-C(4C)-C(5C)	2(2)
Zn(1)-Zn(2)-C(54)-C(50)	127.60(8)	C(3C)-C(4C)-C(5C)-C(6C)	-2.1(19)
C(50)-Zn(2)-C(54)-C(53)	116.80(12)	C(4C)-C(5C)-C(6C)-C(1C)	-1.2(16)
C(51)-Zn(2)-C(54)-C(53)	79.04(9)	C(2C)-C(1C)-C(6C)-C(5C)	4.4(18)
C(52)-Zn(2)-C(54)-C(53)	37.32(8)		

Symmetry transformations use d to generate equivalent atoms:

X-Ray Crystal Structure of **3**



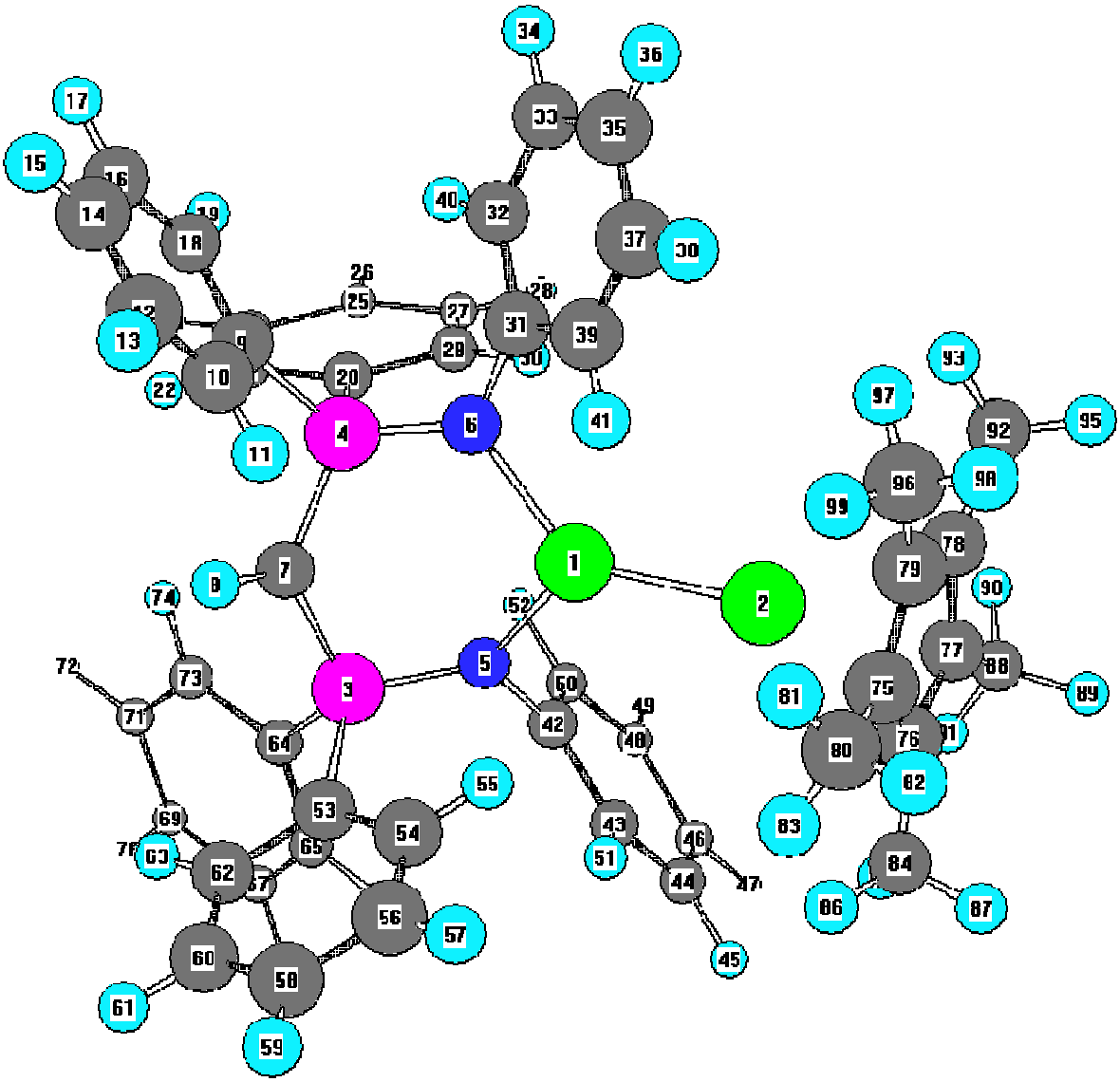
Computational Studies

DFT calculations were carried out with the Gaussian09 suite of programs (Gaussian 09, Revision A.02, 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, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.). The molecular structure and energy of **3** was obtained by performing a complete energy optimization of all geometric parameters at the b3lyp/svp level (input keywords "# b3lyp/svp opt"). A population analysis was carried out with the NBO module as implemented in Gaussian03. The final molecular structure and lists of the final atomic coordinates and energies, selected bond distances, and NBO atomic populations of **3** is given below.

The structures of three heteroleptic and two homoleptic complexes of the types LZn-ZnCp* (L1 **4**, L2 **2**, L3 **3**) and LZn-ZnL (L1 **1**, L2 **5**) were calculated and the structural parameters are given in the following tables. The central Zn-Zn bond length and NBO's are given below.

L =	**LZn-ZnCp***			**LZn-ZnL**	
	Zn-Zn	NBO ZnCp*	NBO Zn(L)	Zn-Zn	NBO Zn
L^1	2,369	0,57	0,76	2,396	0,65/0,68
L^2	2,376	0,55	0,79	2,438	0,68/0,72
L^3	2,381	0,57	0,76	-	-

Calculated Structure and Atom Numbering Scheme of 4



HF=-6167.785034 8

Optimized Parameters (Angstroms and Degrees) Compound 4

Name	Definition	Value	[1]		Definition	Value	[1]
R1	R(1,2)	2.3692	0.0	R34	R(21,23)	1.3961	0.0
R2	R(1,5)	2.0444	0.0	R35	R(23,24)	1.0931	0.0
R3	R(1,6)	2.0223	0.0	R36	R(23,25)	1.3999	0.0
R4	R(2,75)	2.3352	0.0	R37	R(25,26)	1.0931	0.0
R5	R(2,76)	2.3317	0.0	R38	R(25,27)	1.3968	0.0
R6	R(2,77)	2.3263	0.0	R39	R(27,28)	1.0929	0.0
R7	R(2,78)	2.3266	0.0	R40	R(27,29)	1.3993	0.0
R8	R(2,79)	2.333	0.0	R41	R(29,30)	1.0918	0.0
R9	R(3,5)	1.6448	0.0	R42	R(31,32)	1.4118	0.0
R10	R(3,7)	1.7233	0.0	R43	R(31,39)	1.4133	0.0
R11	R(3,53)	1.8489	0.0	R44	R(32,33)	1.398	0.0
R12	R(3,64)	1.8455	0.0	R45	R(32,40)	1.0906	0.0
R13	R(4,6)	1.6626	0.0	R46	R(33,34)	1.0938	0.0
R14	R(4,7)	1.7293	0.0	R47	R(33,35)	1.3963	0.0
R15	R(4,9)	1.8358	0.0	R48	R(35,36)	1.0927	0.0
R16	R(4,20)	1.8447	0.0	R49	R(35,37)	1.3995	0.0
R17	R(5,42)	1.4217	0.0	R50	R(37,38)	1.0937	0.0
R18	R(6,31)	1.4122	0.0	R51	R(37,39)	1.3943	0.0
R19	R(7,8)	1.0909	0.0	R52	R(39,41)	1.0914	0.0
R20	R(9,10)	1.4067	0.0	R53	R(42,43)	1.4082	0.0
R21	R(9,18)	1.4026	0.0	R54	R(42,50)	1.4076	0.0
R22	R(10,11)	1.0925	0.0	R55	R(43,44)	1.398	0.0
R23	R(10,12)	1.3959	0.0	R56	R(43,51)	1.0915	0.0
R24	R(12,13)	1.0929	0.0	R57	R(44,45)	1.0936	0.0
R25	R(12,14)	1.3986	0.0	R58	R(44,46)	1.3986	0.0
R26	R(14,15)	1.093	0.0	R59	R(46,47)	1.0929	0.0
R27	R(14,16)	1.3969	0.0	R60	R(46,48)	1.3985	0.0
R28	R(16,17)	1.0929	0.0	R61	R(48,49)	1.0935	0.0
R29	R(16,18)	1.3984	0.0	R62	R(48,50)	1.3969	0.0
R30	R(18,19)	1.0912	0.0	R63	R(50,52)	1.0922	0.0
R31	R(20,21)	1.4063	0.0	R64	R(53,54)	1.4042	0.0
R32	R(20,29)	1.4026	0.0	R65	R(53,62)	1.4042	0.0
R33	R(21,22)	1.0929	0.0	R66	R(54,55)	1.0935	0.0
R67	R(54,56)	1.3971	0.0	R89	R(76,77)	1.434	0.0

R68	R(56,57)	1.0931	0.0	R90	R(76,84)	1.5035	0.0
R69	R(56,58)	1.3988	0.0	R91	R(77,78)	1.4347	0.0
R70	R(58,59)	1.0931	0.0	R92	R(77,88)	1.5038	0.0
R71	R(58,60)	1.3978	0.0	R93	R(78,79)	1.434	0.0
R72	R(60,61)	1.0932	0.0	R94	R(78,92)	1.5039	0.0
R73	R(60,62)	1.3985	0.0	R95	R(79,96)	1.5036	0.0
R74	R(62,63)	1.0927	0.0	R96	R(80,81)	1.1013	0.0
R75	R(64,65)	1.4071	0.0	R97	R(80,82)	1.1061	0.0
R76	R(64,73)	1.4017	0.0	R98	R(80,83)	1.1015	0.0
R77	R(65,66)	1.0919	0.0	R99	R(84,85)	1.1011	0.0
R78	R(65,67)	1.3962	0.0	R100	R(84,86)	1.1014	0.0
R79	R(67,68)	1.093	0.0	R101	R(84,87)	1.1061	0.0
R80	R(67,69)	1.3995	0.0	R102	R(88,89)	1.106	0.0
R81	R(69,70)	1.0932	0.0	R103	R(88,90)	1.1009	0.0
R82	R(69,71)	1.397	0.0	R104	R(88,91)	1.1012	0.0
R83	R(71,72)	1.0932	0.0	R105	R(92,93)	1.1012	0.0
R84	R(71,73)	1.3988	0.0	R106	R(92,94)	1.101	0.0
R85	R(73,74)	1.0915	0.0	R107	R(92,95)	1.106	0.0
R86	R(75,76)	1.4344	0.0	R108	R(96,97)	1.1013	0.0
R87	R(75,79)	1.4342	0.0	R109	R(96,98)	1.1061	0.0
R88	R(75,80)	1.5038	0.0	R110	R(96,99)	1.1013	0.0

[1] = Derivative Info -DE/DX =

Standard Orientation of 4

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
1	30	0	0.811717	0.243544	-0.010996
2	30	0	3.176091	0.097157	-0.050074
3	15	0	-1.756626	-1.504984	0.737279
4	15	0	-2.046441	1.485321	0.116446
5	7	0	-0.431759	-1.364735	-0.227241
6	7	0	-0.424006	1.843115	0.053153
7	6	0	-2.396294	0.066170	1.040606
8	1	0	-2.867136	0.230164	2.010850
9	6	0	-2.938946	2.853371	0.954228

10	6	0	-2.646880	3.064472	2.313940
11	1	0	-1.922294	2.422703	2.820508
12	6	0	-3.270015	4.095737	3.018730
13	1	0	-3.035662	4.248201	4.075272
14	6	0	-4.183767	4.935271	2.373462
15	1	0	-4.669626	5.744035	2.925285
16	6	0	-4.465447	4.742733	1.018914
17	1	0	-5.169581	5.402321	0.505434
18	6	0	-3.843866	3.709869	0.310166
19	1	0	-4.066678	3.579068	-0.749955
20	6	0	-2.708960	1.339932	-1.599027
21	6	0	-4.081057	1.133353	-1.827705
22	1	0	-4.772829	1.091899	-0.982596
23	6	0	-4.567847	0.976840	-3.126745
24	1	0	-5.637419	0.823691	-3.292258
25	6	0	-3.686633	1.004491	-4.214087
26	1	0	-4.067099	0.873731	-5.230411
27	6	0	-2.320192	1.195055	-3.995792
28	1	0	-1.626011	1.212159	-4.839759
29	6	0	-1.834028	1.367205	-2.694967
30	1	0	-0.766329	1.517969	-2.523627
31	6	0	0.093805	3.145137	-0.122963
32	6	0	-0.486508	4.119360	-0.963997
33	6	0	0.077034	5.392243	-1.093039
34	1	0	-0.402084	6.122188	-1.751788
35	6	0	1.241565	5.732472	-0.401928
36	1	0	1.681801	6.726839	-0.508442
37	6	0	1.832708	4.776492	0.431970
38	1	0	2.740855	5.021951	0.989857
39	6	0	1.267629	3.509817	0.574578
40	1	0	-1.384031	3.880782	-1.535858
41	1	0	1.728571	2.776298	1.238350
42	6	0	0.064443	-2.424348	-1.034865
43	6	0	1.019836	-3.338349	-0.550167
44	6	0	1.530282	-4.345316	-1.374639
45	1	0	2.268687	-5.046082	-0.975093

46	6	0	1.103900	-4.458167	-2.701884
47	1	0	1.505266	-5.244912	-3.345631
48	6	0	0.162975	-3.549901	-3.197396
49	1	0	-0.175812	-3.623970	-4.234491
50	6	0	-0.349201	-2.543608	-2.375004
51	1	0	1.361091	-3.249813	0.482834
52	1	0	-1.082868	-1.831126	-2.758544
53	6	0	-1.376316	-2.257918	2.382535
54	6	0	-0.089629	-2.101847	2.922791
55	1	0	0.686139	-1.597332	2.340188
56	6	0	0.207956	-2.592173	4.196739
57	1	0	1.214965	-2.469463	4.603781
58	6	0	-0.779327	-3.238634	4.947686
59	1	0	-0.546353	-3.622461	5.944308
60	6	0	-2.063732	-3.395271	4.418798
61	1	0	-2.838266	-3.901430	5.000963
62	6	0	-2.361014	-2.911416	3.140829
63	1	0	-3.365108	-3.050320	2.732871
64	6	0	-2.964608	-2.700531	0.018058
65	6	0	-2.637337	-4.058453	-0.151574
66	1	0	-1.654286	-4.430939	0.143519
67	6	0	-3.567284	-4.944034	-0.699581
68	1	0	-3.300551	-5.995736	-0.831412
69	6	0	-4.835312	-4.488503	-1.077850
70	1	0	-5.562306	-5.184978	-1.503990
71	6	0	-5.170767	-3.143551	-0.904279
72	1	0	-6.162284	-2.783635	-1.191377
73	6	0	-4.238961	-2.254401	-0.358628
74	1	0	-4.493515	-1.203347	-0.210802
75	6	0	5.179011	-0.134428	1.128058
76	6	0	5.090487	-1.212756	0.186270
77	6	0	5.094235	-0.650899	-1.133042
78	6	0	5.185634	0.775312	-1.006642
79	6	0	5.238809	1.094090	0.390482
80	6	0	5.301582	-0.274428	2.620337
81	1	0	4.886240	0.595249	3.153343

82	1	0	6.357378	-0.367587	2.936627
83	1	0	4.778326	-1.167858	2.996141
84	6	0	5.097824	-2.680010	0.514510
85	1	0	4.536386	-3.268354	-0.227883
86	1	0	4.650716	-2.885256	1.499982
87	1	0	6.125268	-3.089032	0.539246
88	6	0	5.103167	-1.430025	-2.419276
89	1	0	6.127462	-1.734124	-2.705085
90	1	0	4.699506	-0.841945	-3.257819
91	1	0	4.502173	-2.350215	-2.350372
92	6	0	5.310920	1.760276	-2.136167
93	1	0	4.845234	2.728387	-1.894085
94	1	0	4.835147	1.391877	-3.058158
95	1	0	6.369443	1.965704	-2.382471
96	6	0	5.429002	2.468908	0.968843
97	1	0	4.935057	3.242584	0.360384
98	1	0	6.498942	2.742566	1.029948
99	1	0	5.022341	2.546985	1.989332

Summary of Natural Population Analysis: Natural Population of 4

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
Zn	1	0.76114	17.99725	11.23771	0.00390	29.23886
Zn	2	0.56209	17.99801	11.43447	0.00543	29.43791
P	3	1.82204	9.99700	3.09487	0.08610	13.17796
P	4	1.80275	9.99702	3.11653	0.08370	13.19725
N	5	-1.18952	1.99937	6.17867	0.01148	8.18952
N	6	-1.17018	1.99936	6.15827	0.01254	8.17018
C	7	-1.35892	1.99884	5.34715	0.01294	7.35892
H	8	0.28367	0.00000	0.71382	0.00251	0.71633
C	9	-0.36034	1.99882	4.33709	0.02443	6.36034
C	10	-0.19207	1.99890	4.17643	0.01674	6.19207
H	11	0.23678	0.00000	0.75979	0.00344	0.76322
C	12	-0.21170	1.99893	4.19724	0.01554	6.21170
H	13	0.22733	0.00000	0.77000	0.00267	0.77267

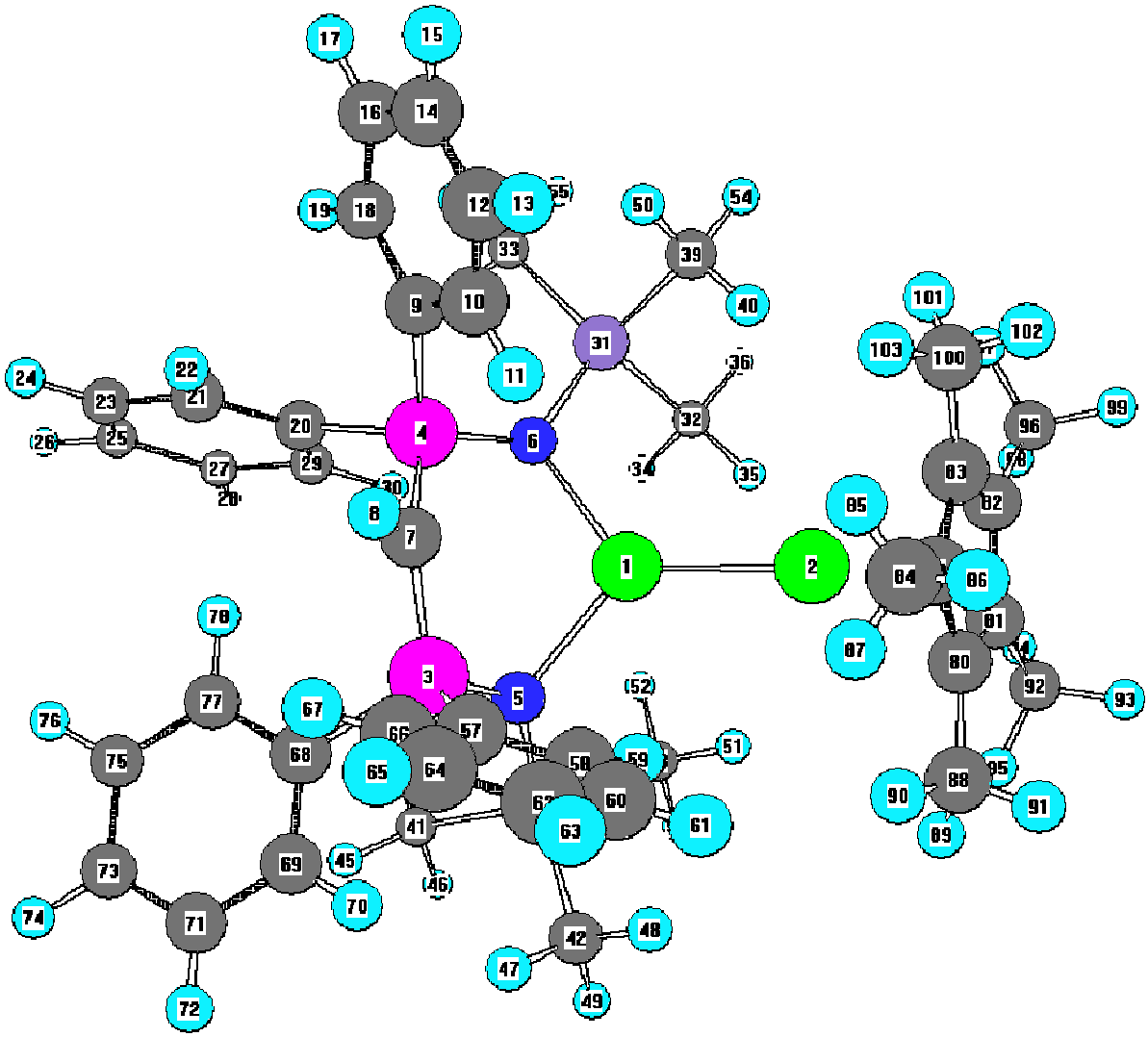
C	14	-0.20448	1.99893	4.19051	0.01504	6.20448
H	15	0.22546	0.00000	0.77188	0.00266	0.77454
C	16	-0.21361	1.99892	4.19913	0.01555	6.21361
H	17	0.22599	0.00000	0.77134	0.00267	0.77401
C	18	-0.19897	1.99888	4.18346	0.01664	6.19897
H	19	0.23321	0.00000	0.76383	0.00296	0.76679
C	20	-0.38359	1.99879	4.35696	0.02784	6.38359
C	21	-0.20788	1.99888	4.19167	0.01732	6.20788
H	22	0.23228	0.00000	0.76469	0.00304	0.76772
C	23	-0.21755	1.99891	4.20303	0.01561	6.21755
H	24	0.22590	0.00000	0.77140	0.00270	0.77410
C	25	-0.20522	1.99893	4.19114	0.01515	6.20522
H	26	0.22585	0.00000	0.77149	0.00265	0.77415
C	27	-0.21553	1.99891	4.20103	0.01559	6.21553
H	28	0.22891	0.00000	0.76844	0.00265	0.77109
C	29	-0.19886	1.99887	4.18143	0.01856	6.19886
H	30	0.23974	0.00000	0.75604	0.00422	0.76026
C	31	0.18583	1.99885	3.79361	0.02170	5.81417
C	32	-0.26953	1.99889	4.25566	0.01498	6.26953
C	33	-0.20901	1.99893	4.19491	0.01517	6.20901
H	34	0.21768	0.00000	0.77949	0.00284	0.78232
C	35	-0.25037	1.99892	4.23605	0.01539	6.25037
H	36	0.21831	0.00000	0.77900	0.00269	0.78169
C	37	-0.21523	1.99893	4.20118	0.01512	6.21523
H	38	0.21965	0.00000	0.77751	0.00284	0.78035
C	39	-0.24347	1.99889	4.22893	0.01565	6.24347
H	40	0.21686	0.00000	0.77974	0.00340	0.78314
H	41	0.22211	0.00000	0.77359	0.00430	0.77789
C	42	0.16818	1.99881	3.81003	0.02298	5.83182
C	43	-0.24290	1.99884	4.22828	0.01578	6.24290
C	44	-0.22106	1.99893	4.20697	0.01516	6.22106
H	45	0.22198	0.00000	0.77522	0.00280	0.77802
C	46	-0.23783	1.99893	4.22373	0.01517	6.23783
H	47	0.22052	0.00000	0.77679	0.00269	0.77948
C	48	-0.21469	1.99893	4.20078	0.01498	6.21469
H	49	0.22053	0.00000	0.77665	0.00281	0.77947

C	50	-0.23049	1.99884	4.21565	0.01600	6.23049
H	51	0.22656	0.00000	0.77021	0.00323	0.77344
H	52	0.22916	0.00000	0.76746	0.00338	0.77084
C	53	-0.37643	1.99880	4.34836	0.02927	6.37643
C	54	-0.19905	1.99888	4.18247	0.01770	6.19905
H	55	0.22680	0.00000	0.76832	0.00488	0.77320
C	56	-0.21483	1.99892	4.20033	0.01558	6.21483
H	57	0.22678	0.00000	0.77053	0.00269	0.77322
C	58	-0.20891	1.99893	4.19489	0.01509	6.20891
H	59	0.22487	0.00000	0.77246	0.00266	0.77513
C	60	-0.21518	1.99893	4.20060	0.01565	6.21518
H	61	0.22548	0.00000	0.77182	0.00270	0.77452
C	62	-0.20420	1.99889	4.18890	0.01641	6.20420
H	63	0.23321	0.00000	0.76394	0.00285	0.76679
C	64	-0.38946	1.99880	4.36296	0.02770	6.38946
C	65	-0.19212	1.99889	4.17574	0.01749	6.19212
H	66	0.23702	0.00000	0.75989	0.00309	0.76298
C	67	-0.21514	1.99892	4.20062	0.01561	6.21514
H	68	0.22641	0.00000	0.77089	0.00270	0.77359
C	69	-0.20657	1.99893	4.19257	0.01506	6.20657
H	70	0.22371	0.00000	0.77361	0.00268	0.77629
C	71	-0.22048	1.99892	4.20598	0.01559	6.22048
H	72	0.22325	0.00000	0.77401	0.00274	0.77675
C	73	-0.19283	1.99887	4.17721	0.01675	6.19283
H	74	0.23612	0.00000	0.76047	0.00341	0.76388
C	75	-0.16460	1.99883	4.14135	0.02442	6.16460
C	76	-0.16485	1.99883	4.14141	0.02461	6.16485
C	77	-0.16260	1.99883	4.13924	0.02453	6.16260
C	78	-0.16324	1.99883	4.13991	0.02450	6.16324
C	79	-0.16422	1.99883	4.14080	0.02459	6.16422
C	80	-0.62807	1.99919	4.61934	0.00953	6.62807
H	81	0.21826	0.00000	0.77931	0.00243	0.78174
H	82	0.21803	0.00000	0.77854	0.00343	0.78197
H	83	0.21633	0.00000	0.78124	0.00243	0.78367
C	84	-0.62845	1.99919	4.61972	0.00954	6.62845
H	85	0.22016	0.00000	0.77712	0.00272	0.77984

H	86	0.21596	0.00000	0.78162	0.00242	0.78404
H	87	0.21711	0.00000	0.77948	0.00341	0.78289
C	88	-0.62970	1.99919	4.62086	0.00965	6.62970
H	89	0.21638	0.00000	0.78028	0.00335	0.78362
H	90	0.21921	0.00000	0.77840	0.00239	0.78079
H	91	0.22325	0.00000	0.77424	0.00252	0.77675
C	92	-0.62965	1.99919	4.62082	0.00964	6.62965
H	93	0.22259	0.00000	0.77492	0.00249	0.77741
H	94	0.21898	0.00000	0.77863	0.00239	0.78102
H	95	0.21699	0.00000	0.77964	0.00337	0.78301
C	96	-0.62976	1.99919	4.62100	0.00957	6.62976
H	97	0.22136	0.00000	0.77597	0.00267	0.77864
H	98	0.21740	0.00000	0.77921	0.00339	0.78260
H	99	0.21718	0.00000	0.78042	0.00240	0.78282

* Total * 0.00000 153.93702 276.91094 1.15204 432.00000

Calculated Structure and Atom Numbering Scheme of 2



HF=-6523.098

Optimized Parameters (Angstroms and Degrees) Compound 2

Name	Definition	Value	[1]		Definition	Value	[1]
R1	R(1,2)	2.3759	0.0	R41	R(23,24)	1.0932	0.0
R2	R(1,5)	2.0695	0.0	R42	R(23,25)	1.4001	0.0
R3	R(1,6)	2.0578	0.0	R43	R(25,26)	1.0931	0.0
R4	R(1,43)	3.3387	0.0	R44	R(25,27)	1.3972	0.0
R5	R(1,51)	3.0801	0.0	R45	R(27,28)	1.0931	0.0
R6	R(2,43)	4.273	0.0	R46	R(27,29)	1.399	0.0
R7	R(2,51)	3.4102	0.0	R47	R(29,30)	1.0915	0.0
R8	R(2,79)	2.3425	0.0	R48	R(31,32)	1.8907	0.0
R9	R(2,80)	2.3385	0.0	R49	R(31,33)	1.8953	0.0
R10	R(2,81)	2.3361	0.0	R50	R(31,39)	1.8915	0.0
R11	R(2,82)	2.3406	0.0	R51	R(31,40)	2.4995	0.0
R12	R(2,83)	2.3455	0.0	R52	R(31,50)	2.5121	0.0
R13	R(3,5)	1.6261	0.0	R53	R(31,54)	2.511	0.0
R14	R(3,7)	1.7351	0.0	R54	R(32,33)	3.0628	0.0
R15	R(3,56)	3.1067	0.0	R55	R(32,34)	1.1027	0.0
R16	R(3,57)	1.8462	0.0	R56	R(32,35)	1.1022	0.0
R17	R(3,68)	1.8506	0.0	R57	R(32,36)	1.1031	0.0
R18	R(4,6)	1.6305	0.0	R58	R(33,34)	3.2845	0.0
R19	R(4,7)	1.7423	0.0	R59	R(33,37)	1.1013	0.0
R20	R(4,9)	1.8474	0.0	R60	R(33,38)	1.1013	0.0
R21	R(4,20)	1.851	0.0	R61	R(33,55)	1.1037	0.0
R22	R(5,56)	1.7563	0.0	R62	R(39,40)	1.102	0.0
R23	R(6,31)	1.7607	0.0	R63	R(39,50)	1.1022	0.0
R24	R(7,8)	1.0926	0.0	R64	R(39,54)	1.1034	0.0
R25	R(9,10)	1.4065	0.0	R65	R(41,44)	1.1024	0.0
R26	R(9,18)	1.4048	0.0	R66	R(41,45)	1.1008	0.0
R27	R(9,37)	3.4858	0.0	R67	R(41,46)	1.1037	0.0
R28	R(10,11)	1.0922	0.0	R68	R(41,56)	1.8928	0.0
R29	R(10,12)	1.3966	0.0	R69	R(42,47)	1.1018	0.0
R30	R(12,13)	1.093	0.0	R70	R(42,48)	1.1025	0.0
R31	R(12,14)	1.3987	0.0	R71	R(42,49)	1.1035	0.0
R32	R(14,15)	1.0931	0.0	R72	R(42,56)	1.8951	0.0
R33	R(14,16)	1.3973	0.0	R73	R(43,51)	1.102	0.0
R34	R(16,17)	1.093	0.0	R74	R(43,52)	1.1029	0.0
R35	R(16,18)	1.3986	0.0	R75	R(43,53)	1.1031	0.0
R36	R(18,19)	1.0915	0.0	R76	R(43,56)	1.8909	0.0
R37	R(20,21)	1.407	0.0	R77	R(57,58)	1.402	0.0
R38	R(20,29)	1.4031	0.0	R78	R(57,66)	1.4054	0.0
R39	R(21,22)	1.093	0.0	R79	R(58,59)	1.0921	0.0
R40	R(21,23)	1.3968	0.0	R80	R(58,60)	1.399	0.0

R81	R(60,61)	1.0931	0.0	R103	R(80,88)	1.5039	0.0
R82	R(60,62)	1.3975	0.0	R104	R(81,82)	1.4343	0.0
R83	R(62,63)	1.0931	0.0	R105	R(81,92)	1.5041	0.0
R84	R(62,64)	1.3993	0.0	R106	R(82,83)	1.4338	0.0
R85	R(64,65)	1.0932	0.0	R107	R(82,96)	1.5039	0.0
R86	R(64,66)	1.397	0.0	R108	R(83,100)	1.504	0.0
R87	R(66,67)	1.0935	0.0	R109	R(84,85)	1.101	0.0
R88	R(68,69)	1.4063	0.0	R110	R(84,86)	1.1061	0.0
R89	R(68,77)	1.4031	0.0	R111	R(84,87)	1.1012	0.0
R90	R(69,70)	1.0924	0.0	R112	R(88,89)	1.1013	0.0
R91	R(69,71)	1.3974	0.0	R113	R(88,90)	1.1015	0.0
R92	R(71,72)	1.0932	0.0	R114	R(88,91)	1.1061	0.0
R93	R(71,73)	1.3988	0.0	R115	R(92,93)	1.1061	0.0
R94	R(73,74)	1.0932	0.0	R116	R(92,94)	1.1013	0.0
R95	R(73,75)	1.3979	0.0	R117	R(92,95)	1.1012	0.0
R96	R(75,76)	1.093	0.0	R118	R(96,97)	1.1011	0.0
R97	R(75,77)	1.3978	0.0	R119	R(96,98)	1.1011	0.0
R98	R(77,78)	1.0905	0.0	R120	R(96,99)	1.106	0.0
R99	R(79,80)	1.434	0.0	R121	R(100,101)	1.1011	0.0
R100	R(79,83)	1.4337	0.0	R122	R(100,102)	1.106	0.0
R101	R(79,84)	1.5037	0.0	R123	R(100,103)	1.1011	0.0
R102	R(80,81)	1.4342	0.0				

[1] = Derivative Info -DE/DX =

Standard Orientation of 2

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
1	30	0	0.726440	0.069592	-0.576360
2	30	0	3.084408	-0.038346	-0.305954
3	15	0	-1.493961	-1.558643	0.548252
4	15	0	-1.681705	1.563260	0.420043
5	7	0	-0.610846	-1.491534	-0.815551
6	7	0	-0.499497	1.718340	-0.692173
7	6	0	-1.626937	0.026961	1.240058
8	1	0	-1.900930	0.058419	2.297300
9	6	0	-1.552312	2.815061	1.772483
10	6	0	-0.646798	2.572970	2.821195
11	1	0	-0.103492	1.626034	2.853885
12	6	0	-0.433578	3.534594	3.811355
13	1	0	0.270995	3.330235	4.621624

14	6	0	-1.113716	4.755853	3.764096
15	1	0	-0.944823	5.508792	4.538297
16	6	0	-2.006515	5.011157	2.719922
17	1	0	-2.538978	5.964606	2.673538
18	6	0	-2.223562	4.048337	1.729025
19	1	0	-2.924064	4.264787	0.920423
20	6	0	-3.319268	1.879064	-0.382871
21	6	0	-4.484638	2.076374	0.380506
22	1	0	-4.423256	2.132945	1.470352
23	6	0	-5.730036	2.191551	-0.241329
24	1	0	-6.625872	2.354446	0.363743
25	6	0	-5.832433	2.092990	-1.634153
26	1	0	-6.807715	2.180395	-2.119949
27	6	0	-4.683045	1.878459	-2.399116
28	1	0	-4.756336	1.792190	-3.486356
29	6	0	-3.434108	1.774776	-1.777332
30	1	0	-2.534180	1.598590	-2.369280
31	14	0	0.188421	3.147031	-1.457451
32	6	0	1.037652	2.574341	-3.046670
33	6	0	-1.086867	4.470800	-1.919410
34	1	0	0.315421	2.136348	-3.755594
35	1	0	1.807407	1.814430	-2.834884
36	1	0	1.533543	3.420602	-3.551364
37	1	0	-1.609225	4.875627	-1.038481
38	1	0	-1.848800	4.098290	-2.621872
39	6	0	1.477310	3.950262	-0.329873
40	1	0	2.247805	3.216621	-0.042602
41	6	0	-2.260138	-2.480721	-3.169847
42	6	0	-0.030502	-4.238311	-1.981836
43	6	0	0.666071	-1.638374	-3.444476
44	1	0	-2.638526	-1.457305	-3.327434
45	1	0	-3.025413	-3.037486	-2.607611
46	1	0	-2.154720	-2.959002	-4.158880
47	1	0	-0.722888	-4.778771	-1.316731
48	1	0	0.971454	-4.274297	-1.523264
49	1	0	0.015628	-4.795946	-2.932971
50	1	0	1.017403	4.334223	0.595310
51	1	0	1.670257	-1.590326	-2.993161
52	1	0	0.367966	-0.609897	-3.708624
53	1	0	0.746006	-2.210972	-4.383974
54	1	0	1.978214	4.794244	-0.834165
55	1	0	-0.566469	5.313811	-2.405892

56	14	0	-0.586902	-2.452332	-2.285539
57	6	0	-0.702856	-2.591973	1.857773
58	6	0	0.631639	-2.994330	1.706939
59	1	0	1.173352	-2.722041	0.798561
60	6	0	1.266882	-3.725956	2.716053
61	1	0	2.305840	-4.039618	2.585604
62	6	0	0.576951	-4.054937	3.885994
63	1	0	1.074400	-4.626292	4.674008
64	6	0	-0.753755	-3.652599	4.045252
65	1	0	-1.298323	-3.908817	4.957895
66	6	0	-1.391985	-2.928293	3.035483
67	1	0	-2.436470	-2.631589	3.164928
68	6	0	-3.100824	-2.435517	0.276254
69	6	0	-3.178949	-3.839406	0.302714
70	1	0	-2.293435	-4.433580	0.539490
71	6	0	-4.387734	-4.488389	0.037495
72	1	0	-4.434309	-5.580276	0.062231
73	6	0	-5.535194	-3.743211	-0.253659
74	1	0	-6.481004	-4.251372	-0.459200
75	6	0	-5.468969	-2.347019	-0.272185
76	1	0	-6.362088	-1.756473	-0.491638
77	6	0	-4.260467	-1.697373	-0.005148
78	1	0	-4.218376	-0.607731	-0.011739
79	6	0	4.878238	-0.484488	1.132918
80	6	0	5.001260	-1.344267	-0.008083
81	6	0	5.202939	-0.520126	-1.164386
82	6	0	5.206929	0.848962	-0.736972
83	6	0	5.007362	0.870546	0.682757
84	6	0	4.745308	-0.929959	2.562983
85	1	0	4.235519	-0.176102	3.182682
86	1	0	5.731894	-1.113271	3.028169
87	1	0	4.169972	-1.864512	2.654220
88	6	0	5.031406	-2.847577	0.019802
89	1	0	4.656121	-3.287689	-0.917354
90	1	0	4.421132	-3.256972	0.840300
91	1	0	6.058042	-3.232802	0.164739
92	6	0	5.483773	-1.008598	-2.559003
93	1	0	6.567357	-1.149047	-2.730923
94	1	0	5.129580	-0.301042	-3.324960
95	1	0	5.001837	-1.977442	-2.763297
96	6	0	5.487288	2.043434	-1.606638
97	1	0	4.984319	2.950474	-1.236950

98	1	0	5.153175	1.886026	-2.644001
99	1	0	6.568667	2.271530	-1.649838
100	6	0	5.040067	2.092809	1.558600
101	1	0	4.670572	2.987606	1.034015
102	1	0	6.066815	2.322640	1.899516
103	1	0	4.424334	1.969412	2.463067

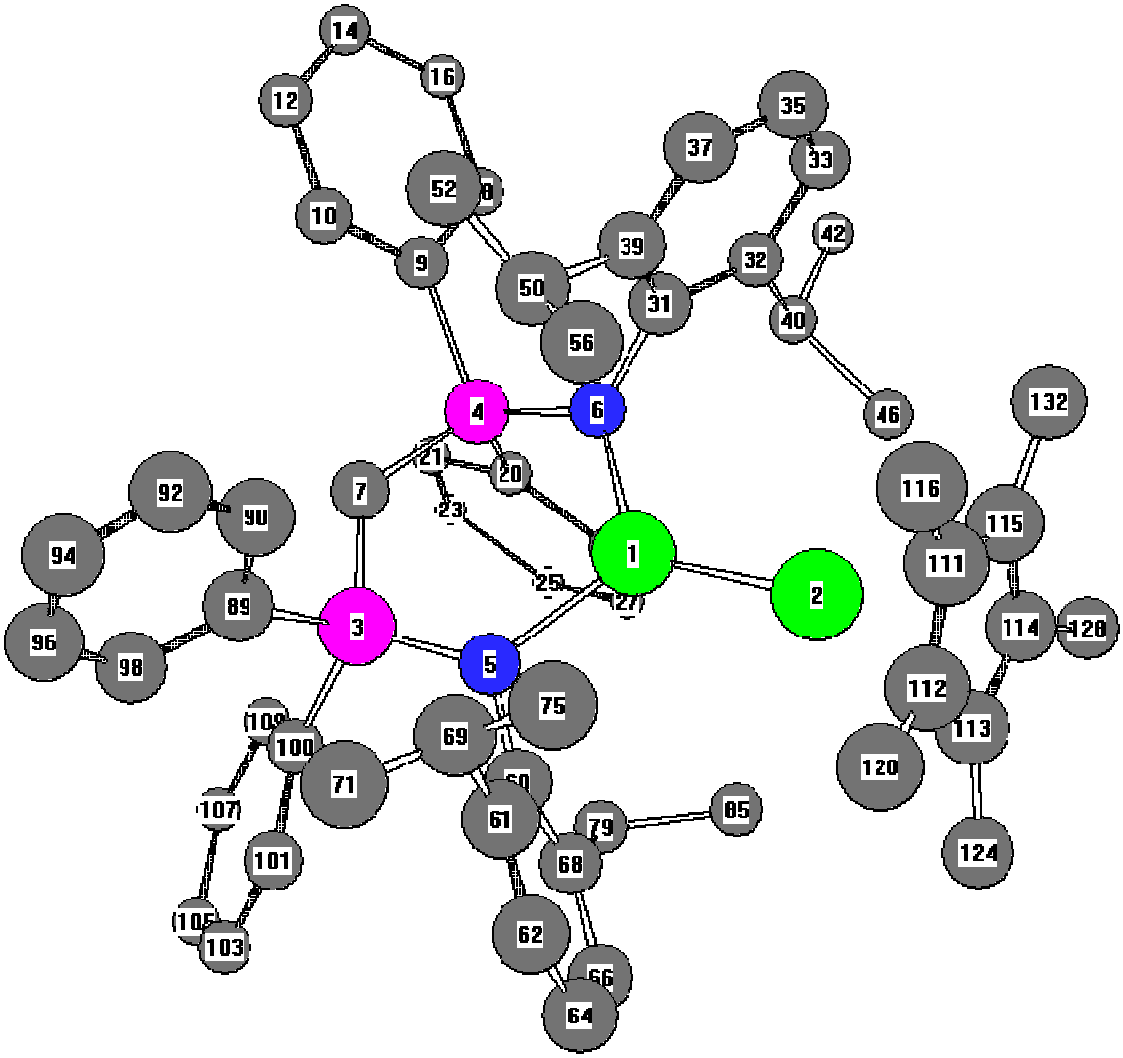
Summary of Natural Population Analysis: Natural Population of 2

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
Zn	1	0.79065	17.99711	11.20795	0.00429	29.20935
Zn	2	0.55214	17.99798	11.44424	0.00564	29.44786
P	3	1.83559	9.99707	3.08389	0.08345	13.16441
P	4	1.83079	9.99707	3.08915	0.08299	13.16921
N	5	-1.60826	1.99947	6.60197	0.00683	8.60826
N	6	-1.60711	1.99948	6.60054	0.00709	8.60711
C	7	-1.37375	1.99890	5.36198	0.01287	7.37375
H	8	0.27928	0.00000	0.71806	0.00267	0.72072
C	9	-0.37307	1.99882	4.34903	0.02522	6.37307
C	10	-0.19510	1.99890	4.17892	0.01728	6.19510
H	11	0.24179	0.00000	0.75460	0.00360	0.75821
C	12	-0.21445	1.99892	4.20004	0.01549	6.21445
H	13	0.22718	0.00000	0.77015	0.00268	0.77282
C	14	-0.20677	1.99893	4.19272	0.01511	6.20677
H	15	0.22549	0.00000	0.77184	0.00266	0.77451
C	16	-0.21608	1.99892	4.20151	0.01565	6.21608
H	17	0.22641	0.00000	0.77091	0.00268	0.77359
C	18	-0.21032	1.99890	4.19450	0.01692	6.21032
H	19	0.23441	0.00000	0.76255	0.00304	0.76559
C	20	-0.38560	1.99879	4.35983	0.02697	6.38560
C	21	-0.21370	1.99887	4.19806	0.01677	6.21370
H	22	0.23298	0.00000	0.76409	0.00294	0.76702
C	23	-0.22016	1.99892	4.20552	0.01573	6.22016
H	24	0.22604	0.00000	0.77126	0.00271	0.77396
C	25	-0.21332	1.99893	4.19914	0.01525	6.21332
H	26	0.22512	0.00000	0.77222	0.00266	0.77488
C	27	-0.21419	1.99892	4.19972	0.01555	6.21419
H	28	0.22705	0.00000	0.77028	0.00267	0.77295
C	29	-0.20189	1.99888	4.18498	0.01804	6.20189
H	30	0.23981	0.00000	0.75627	0.00392	0.76019

Si	31	1.89467	9.99767	2.05989	0.04777	12.10533
C	32	-1.16035	1.99914	5.14807	0.01313	7.16035
C	33	-1.15854	1.99913	5.14626	0.01314	7.15854
H	34	0.23566	0.00000	0.76230	0.00203	0.76434
H	35	0.23851	0.00000	0.75837	0.00312	0.76149
H	36	0.23979	0.00000	0.75843	0.00179	0.76021
H	37	0.23367	0.00000	0.76427	0.00206	0.76633
H	38	0.23767	0.00000	0.76040	0.00193	0.76233
C	39	-1.16274	1.99912	5.14985	0.01378	7.16274
H	40	0.23792	0.00000	0.75898	0.00310	0.76208
C	41	-1.16029	1.99913	5.14789	0.01328	7.16029
C	42	-1.16136	1.99913	5.14830	0.01393	7.16136
C	43	-1.16465	1.99917	5.15276	0.01272	7.16465
H	44	0.23716	0.00000	0.76061	0.00223	0.76284
H	45	0.24055	0.00000	0.75686	0.00259	0.75945
H	46	0.23576	0.00000	0.76235	0.00189	0.76424
H	47	0.23242	0.00000	0.76555	0.00203	0.76758
H	48	0.23744	0.00000	0.76055	0.00201	0.76256
H	49	0.23749	0.00000	0.76061	0.00191	0.76251
H	50	0.23998	0.00000	0.75781	0.00220	0.76002
H	51	0.23956	0.00000	0.75733	0.00311	0.76044
H	52	0.23645	0.00000	0.76121	0.00234	0.76355
H	53	0.24148	0.00000	0.75674	0.00178	0.75852
H	54	0.23503	0.00000	0.76312	0.00185	0.76497
H	55	0.24014	0.00000	0.75796	0.00190	0.75986
Si	56	1.90546	9.99766	2.04992	0.04695	12.09454
C	57	-0.37534	1.99881	4.34752	0.02901	6.37534
C	58	-0.19765	1.99887	4.18102	0.01776	6.19765
H	59	0.23626	0.00000	0.75850	0.00524	0.76374
C	60	-0.21588	1.99892	4.20136	0.01561	6.21588
H	61	0.22501	0.00000	0.77227	0.00271	0.77499
C	62	-0.21073	1.99893	4.19667	0.01513	6.21073
H	63	0.22432	0.00000	0.77302	0.00267	0.77568
C	64	-0.21693	1.99892	4.20233	0.01568	6.21693
H	65	0.22471	0.00000	0.77259	0.00270	0.77529
C	66	-0.20735	1.99889	4.19197	0.01649	6.20735
H	67	0.22992	0.00000	0.76740	0.00268	0.77008
C	68	-0.38421	1.99881	4.35841	0.02699	6.38421
C	69	-0.20857	1.99890	4.19268	0.01699	6.20857
H	70	0.23283	0.00000	0.76413	0.00304	0.76717
C	71	-0.21823	1.99891	4.20360	0.01571	6.21823
H	72	0.22591	0.00000	0.77138	0.00271	0.77409

C	73	-0.20959	1.99893	4.19557	0.01509	6.20959
H	74	0.22423	0.00000	0.77309	0.00267	0.77577
C	75	-0.21565	1.99892	4.20116	0.01557	6.21565
H	76	0.22575	0.00000	0.77146	0.00278	0.77425
C	77	-0.18618	1.99886	4.17029	0.01703	6.18618
H	78	0.23145	0.00000	0.76275	0.00580	0.76855
C	79	-0.16236	1.99883	4.13919	0.02434	6.16236
C	80	-0.16511	1.99883	4.14172	0.02456	6.16511
C	81	-0.16450	1.99883	4.14123	0.02445	6.16450
C	82	-0.16304	1.99883	4.13971	0.02450	6.16304
C	83	-0.16184	1.99883	4.13866	0.02436	6.16184
C	84	-0.62751	1.99919	4.61875	0.00957	6.62751
H	85	0.21949	0.00000	0.77809	0.00242	0.78051
H	86	0.21705	0.00000	0.77957	0.00338	0.78295
H	87	0.21677	0.00000	0.78061	0.00261	0.78323
C	88	-0.62722	1.99919	4.61852	0.00951	6.62722
H	89	0.21932	0.00000	0.77826	0.00242	0.78068
H	90	0.21415	0.00000	0.78334	0.00251	0.78585
H	91	0.21830	0.00000	0.77830	0.00340	0.78170
C	92	-0.62940	1.99919	4.62069	0.00951	6.62940
H	93	0.21781	0.00000	0.77878	0.00341	0.78219
H	94	0.22014	0.00000	0.77747	0.00239	0.77986
H	95	0.21886	0.00000	0.77874	0.00240	0.78114
C	96	-0.62926	1.99919	4.62058	0.00949	6.62926
H	97	0.22014	0.00000	0.77742	0.00245	0.77986
H	98	0.21951	0.00000	0.77809	0.00240	0.78049
H	99	0.21753	0.00000	0.77910	0.00337	0.78247
C	100	-0.62905	1.99919	4.62040	0.00946	6.62905
H	101	0.22031	0.00000	0.77721	0.00247	0.77969
H	102	0.21758	0.00000	0.77908	0.00335	0.78242
H	103	0.21843	0.00000	0.77915	0.00242	0.78157

Calculated Structure and Atom Numbering Scheme of 3



HF=-6639.1865474

Optimized Parameters (Angstroms and Degrees) Compound 3'

	Definition	Value	[1]		Definition	Value	[1]
R1	R(1,2)	2.3809	0.0	R31	R(20,21)	1.4072	0.0
R2	R(1,5)	2.0477	0.0	R32	R(20,29)	1.4022	0.0
R3	R(1,6)	2.0419	0.0	R33	R(21,22)	1.0931	0.0
R4	R(2,111)	2.3351	0.0	R34	R(21,23)	1.3962	0.0
R5	R(2,112)	2.345	0.0	R35	R(23,24)	1.0932	0.0
R6	R(2,113)	2.349	0.0	R36	R(23,25)	1.3996	0.0
R7	R(2,114)	2.351	0.0	R37	R(25,26)	1.093	0.0
R8	R(2,115)	2.3388	0.0	R38	R(25,27)	1.3966	0.0
R9	R(3,5)	1.6573	0.0	R39	R(27,28)	1.093	0.0
R10	R(3,7)	1.7216	0.0	R40	R(27,29)	1.3997	0.0
R11	R(3,89)	1.8642	0.0	R41	R(29,30)	1.0909	0.0
R12	R(3,100)	1.8519	0.0	R42	R(31,32)	1.4259	0.0
R13	R(4,6)	1.6529	0.0	R43	R(31,39)	1.4259	0.0
R14	R(4,7)	1.7313	0.0	R44	R(32,33)	1.4018	0.0
R15	R(4,9)	1.8374	0.0	R45	R(32,40)	1.5243	0.0
R16	R(4,20)	1.857	0.0	R46	R(33,34)	1.0919	0.0
R17	R(5,60)	1.4376	0.0	R47	R(33,35)	1.3928	0.0
R18	R(6,31)	1.4367	0.0	R48	R(35,36)	1.0931	0.0
R19	R(7,8)	1.0912	0.0	R49	R(35,37)	1.3908	0.0
R20	R(9,10)	1.404	0.0	R50	R(37,38)	1.093	0.0
R21	R(9,18)	1.4056	0.0	R51	R(37,39)	1.403	0.0
R22	R(10,11)	1.0911	0.0	R52	R(39,50)	1.5271	0.0
R23	R(10,12)	1.398	0.0	R53	R(40,41)	1.0953	0.0
R24	R(12,13)	1.0929	0.0	R54	R(40,42)	1.5366	0.0
R25	R(12,14)	1.3973	0.0	R55	R(40,46)	1.5388	0.0
R26	R(14,15)	1.093	0.0	R56	R(42,43)	1.1018	0.0
R27	R(14,16)	1.3981	0.0	R57	R(42,44)	1.1022	0.0
R28	R(16,17)	1.0928	0.0	R58	R(42,45)	1.1021	0.0
R29	R(16,18)	1.3965	0.0	R59	R(46,47)	1.1027	0.0
R30	R(18,19)	1.0913	0.0	R60	R(46,48)	1.1031	0.0
R61	R(46,49)	1.1003	0.0	R91	R(79,80)	1.0981	0.0
R62	R(50,51)	1.0997	0.0	R92	R(79,81)	1.5372	0.0
R63	R(50,52)	1.5391	0.0	R93	R(79,85)	1.5411	0.0

R64	R(50,56)	1.5405	0.0	R94	R(81,82)	1.1025	0.0
R65	R(52,53)	1.1024	0.0	R95	R(81,83)	1.1022	0.0
R66	R(52,54)	1.1031	0.0	R96	R(81,84)	1.0988	0.0
R67	R(52,55)	1.0997	0.0	R97	R(85,86)	1.1011	0.0
R68	R(56,57)	1.101	0.0	R98	R(85,87)	1.1026	0.0
R69	R(56,58)	1.1032	0.0	R99	R(85,88)	1.1025	0.0
R70	R(56,59)	1.1025	0.0	R100	R(89,90)	1.4072	0.0
R71	R(60,61)	1.4252	0.0	R101	R(89,98)	1.4032	0.0
R72	R(60,68)	1.4267	0.0	R102	R(90,91)	1.0915	0.0
R73	R(61,62)	1.403	0.0	R103	R(90,92)	1.3947	0.0
R74	R(61,69)	1.5258	0.0	R104	R(92,93)	1.0931	0.0
R75	R(62,63)	1.0932	0.0	R105	R(92,94)	1.4002	0.0
R76	R(62,64)	1.3923	0.0	R106	R(94,95)	1.0931	0.0
R77	R(64,65)	1.0932	0.0	R107	R(94,96)	1.3952	0.0
R78	R(64,66)	1.3925	0.0	R108	R(96,97)	1.0931	0.0
R79	R(66,67)	1.0928	0.0	R109	R(96,98)	1.401	0.0
R80	R(66,68)	1.4023	0.0	R110	R(98,99)	1.09	0.0
R81	R(68,79)	1.5275	0.0	R111	R(100,101)	1.4081	0.0
R82	R(69,70)	1.0948	0.0	R112	R(100,109)	1.4029	0.0
R83	R(69,71)	1.5374	0.0	R113	R(101,102)	1.0914	0.0
R84	R(69,75)	1.5388	0.0	R114	R(101,103)	1.3972	0.0
R85	R(71,72)	1.1025	0.0	R115	R(103,104)	1.093	0.0
R86	R(71,73)	1.1006	0.0	R116	R(103,105)	1.3992	0.0
R87	R(71,74)	1.102	0.0	R117	R(105,106)	1.0932	0.0
R88	R(75,76)	1.103	0.0	R118	R(105,107)	1.3971	0.0
R89	R(75,77)	1.1002	0.0	R119	R(107,108)	1.093	0.0
R90	R(75,78)	1.1023	0.0	R120	R(107,109)	1.3987	0.0
R121	R(109,110)	1.0921	0.0	A5	A(1,2,112)	151.3651	0.0
R122	R(111,112)	1.4357	0.0	A6	A(1,2,113)	148.6794	0.0
R123	R(111,115)	1.4342	0.0	A7	A(1,2,114)	146.0601	0.0
R124	R(111,116)	1.5039	0.0	A8	A(1,2,115)	146.7549	0.0
R125	R(112,113)	1.4326	0.0	A9	A(111,2,113)	59.3942	0.0
R126	R(112,120)	1.5033	0.0	A10	A(111,2,114)	59.3613	0.0
R127	R(113,114)	1.4344	0.0	A11	A(112,2,114)	59.2092	0.0
R128	R(113,124)	1.5038	0.0	A12	A(112,2,115)	59.412	0.0
R129	R(114,115)	1.434	0.0	A13	A(113,2,115)	59.343	0.0

R130	R(114,128)	1.5037	0.0	A14	A(5,3,7)	110.8624	0.0
R131	R(115,132)	1.5039	0.0	A15	A(5,3,89)	116.7129	0.0
R132	R(116,117)	1.1012	0.0	A16	A(5,3,100)	109.8462	0.0
R133	R(116,118)	1.1061	0.0	A17	A(7,3,89)	102.5867	0.0
R134	R(116,119)	1.1009	0.0	A18	A(7,3,100)	114.2763	0.0
R135	R(120,121)	1.1012	0.0	A19	A(89,3,100)	102.3191	0.0
R136	R(120,122)	1.1	0.0	A20	A(6,4,7)	114.0095	0.0
R137	R(120,123)	1.1062	0.0	A21	A(6,4,9)	112.1495	0.0
R138	R(124,125)	1.1062	0.0	A22	A(6,4,20)	109.9121	0.0
R139	R(124,126)	1.1006	0.0	A23	A(7,4,9)	106.8159	0.0
R140	R(124,127)	1.1013	0.0	A24	A(7,4,20)	109.67	0.0
R141	R(128,129)	1.1003	0.0	A25	A(9,4,20)	103.7491	0.0
R142	R(128,130)	1.1011	0.0	A26	A(1,5,3)	124.923	0.0
R143	R(128,131)	1.106	0.0	A27	A(1,5,60)	112.4844	0.0
R144	R(132,133)	1.1006	0.0	A28	A(3,5,60)	122.4476	0.0
R145	R(132,134)	1.1062	0.0	A29	A(1,6,4)	117.8117	0.0
R146	R(132,135)	1.101	0.0	A30	A(1,6,31)	114.615	0.0
A1	A(2,1,5)	125.8608	0.0	A31	A(4,6,31)	124.8658	0.0
A2	A(2,1,6)	125.7326	0.0	A32	A(3,7,4)	131.011	0.0
A3	A(5,1,6)	108.2802	0.0	A33	A(3,7,8)	113.3517	0.0
A4	A(1,2,111)	150.019	0.0	A34	A(4,7,8)	115.2572	0.0
A35	A(4,9,10)	121.3863	0.0	A65	A(25,27,28)	120.1174	0.0
A36	A(4,9,18)	119.6419	0.0	A66	A(25,27,29)	120.2702	0.0
A37	A(10,9,18)	118.9122	0.0	A67	A(28,27,29)	119.6105	0.0
A38	A(9,10,11)	119.9478	0.0	A68	A(20,29,27)	120.6489	0.0
A39	A(9,10,12)	120.4435	0.0	A69	A(20,29,30)	119.7086	0.0
A40	A(11,10,12)	119.6077	0.0	A70	A(27,29,30)	119.6393	0.0
A41	A(10,12,13)	119.6125	0.0	A71	A(6,31,32)	121.1408	0.0
A42	A(10,12,14)	120.2259	0.0	A72	A(6,31,39)	119.9445	0.0
A43	A(13,12,14)	120.1612	0.0	A73	A(32,31,39)	118.8191	0.0
A44	A(12,14,15)	120.1464	0.0	A74	A(31,32,33)	119.4455	0.0
A45	A(12,14,16)	119.7272	0.0	A75	A(31,32,40)	121.5783	0.0
A46	A(15,14,16)	120.1263	0.0	A76	A(33,32,40)	118.9389	0.0
A47	A(14,16,17)	120.2038	0.0	A77	A(32,33,34)	119.3073	0.0
A48	A(14,16,18)	120.1357	0.0	A78	A(32,33,35)	121.6379	0.0
A49	A(17,16,18)	119.6605	0.0	A79	A(34,33,35)	119.0538	0.0

A50	A(9,18,16)	120.5522	0.0	A80	A(33,35,36)	120.4547	0.0
A51	A(9,18,19)	120.1623	0.0	A81	A(33,35,37)	119.0233	0.0
A52	A(16,18,19)	119.2821	0.0	A82	A(36,35,37)	120.5218	0.0
A53	A(4,20,21)	119.4803	0.0	A83	A(35,37,38)	119.2134	0.0
A54	A(4,20,29)	121.6386	0.0	A84	A(35,37,39)	121.6375	0.0
A55	A(21,20,29)	118.6201	0.0	A85	A(38,37,39)	119.1489	0.0
A56	A(20,21,22)	119.9896	0.0	A86	A(31,39,37)	119.4328	0.0
A57	A(20,21,23)	120.7419	0.0	A87	A(31,39,50)	122.7253	0.0
A58	A(22,21,23)	119.2681	0.0	A88	A(37,39,50)	117.8343	0.0
A59	A(21,23,24)	119.7369	0.0	A89	A(32,40,41)	106.9203	0.0
A60	A(21,23,25)	120.1477	0.0	A90	A(32,40,42)	114.2219	0.0
A61	A(24,23,25)	120.1153	0.0	A91	A(32,40,46)	110.9392	0.0
A62	A(23,25,26)	120.2045	0.0	A92	A(41,40,42)	106.8832	0.0
A63	A(23,25,27)	119.5638	0.0	A93	A(41,40,46)	106.9096	0.0
A64	A(26,25,27)	120.2317	0.0	A94	A(42,40,46)	110.5538	0.0
A95	A(40,42,43)	111.8496	0.0	A125	A(5,60,61)	120.7118	0.0
A96	A(40,42,44)	110.0345	0.0	A126	A(5,60,68)	120.0861	0.0
A97	A(40,42,45)	112.3622	0.0	A127	A(61,60,68)	119.0781	0.0
A98	A(43,42,44)	107.9997	0.0	A128	A(60,61,62)	119.2747	0.0
A99	A(43,42,45)	107.4759	0.0	A129	A(60,61,69)	122.5248	0.0
A100	A(44,42,45)	106.8912	0.0	A130	A(62,61,69)	118.157	0.0
A101	A(40,46,47)	110.6213	0.0	A131	A(61,62,63)	119.1301	0.0
A102	A(40,46,48)	111.0918	0.0	A132	A(61,62,64)	121.627	0.0
A103	A(40,46,49)	111.3973	0.0	A133	A(63,62,64)	119.2393	0.0
A104	A(47,46,48)	107.7863	0.0	A134	A(62,64,65)	120.4739	0.0
A105	A(47,46,49)	107.4402	0.0	A135	A(62,64,66)	119.0604	0.0
A106	A(48,46,49)	108.3513	0.0	A136	A(65,64,66)	120.4597	0.0
A107	A(39,50,51)	107.0461	0.0	A137	A(64,66,67)	119.1716	0.0
A108	A(39,50,52)	112.5292	0.0	A138	A(64,66,68)	121.6761	0.0
A109	A(39,50,56)	111.5688	0.0	A139	A(67,66,68)	119.1519	0.0
A110	A(51,50,52)	107.2888	0.0	A140	A(60,68,66)	119.2234	0.0
A111	A(51,50,56)	107.7773	0.0	A141	A(60,68,79)	122.6023	0.0
A112	A(52,50,56)	110.3666	0.0	A142	A(66,68,79)	118.1102	0.0
A113	A(50,52,53)	111.7253	0.0	A143	A(61,69,70)	106.9934	0.0
A114	A(50,52,54)	110.5138	0.0	A144	A(61,69,71)	112.8524	0.0
A115	A(50,52,55)	111.6274	0.0	A145	A(61,69,75)	111.3562	0.0

A116	A(53,52,54)	107.1039	0.0	A146	A(70,69,71)	107.6343	0.0
A117	A(53,52,55)	107.6073	0.0	A147	A(70,69,75)	106.8236	0.0
A118	A(54,52,55)	108.0664	0.0	A148	A(71,69,75)	110.8474	0.0
A119	A(50,56,57)	111.3998	0.0	A149	A(69,71,72)	111.7848	0.0
A120	A(50,56,58)	110.9747	0.0	A150	A(69,71,73)	111.641	0.0
A121	A(50,56,59)	111.2516	0.0	A151	A(69,71,74)	110.4456	0.0
A122	A(57,56,58)	108.0031	0.0	A152	A(72,71,73)	107.8175	0.0
A123	A(57,56,59)	107.4514	0.0	A153	A(72,71,74)	107.3552	0.0
A124	A(58,56,59)	107.583	0.0	A154	A(73,71,74)	107.5961	0.0
A155	A(69,75,76)	110.5795	0.0	A185	A(90,92,93)	119.7791	0.0
A156	A(69,75,77)	111.0225	0.0	A186	A(90,92,94)	120.0583	0.0
A157	A(69,75,78)	111.6551	0.0	A187	A(93,92,94)	120.1607	0.0
A158	A(76,75,77)	108.0713	0.0	A188	A(92,94,95)	120.1844	0.0
A159	A(76,75,78)	107.6467	0.0	A189	A(92,94,96)	119.5744	0.0
A160	A(77,75,78)	107.7112	0.0	A190	A(95,94,96)	120.2396	0.0
A161	A(68,79,80)	107.3118	0.0	A191	A(94,96,97)	120.1601	0.0
A162	A(68,79,81)	113.6182	0.0	A192	A(94,96,98)	120.3179	0.0
A163	A(68,79,85)	110.4605	0.0	A193	A(97,96,98)	119.5216	0.0
A164	A(80,79,81)	107.2682	0.0	A194	A(89,98,96)	120.6278	0.0
A165	A(80,79,85)	107.5872	0.0	A195	A(89,98,99)	120.4218	0.0
A166	A(81,79,85)	110.3224	0.0	A196	A(96,98,99)	118.9446	0.0
A167	A(79,81,82)	111.8782	0.0	A197	A(3,100,101)	122.1241	0.0
A168	A(79,81,83)	110.0638	0.0	A198	A(3,100,109)	118.9792	0.0
A169	A(79,81,84)	111.7207	0.0	A199	A(101,100,109)	118.8857	0.0
A170	A(82,81,83)	107.1896	0.0	A200	A(100,101,102)	120.4853	0.0
A171	A(82,81,84)	107.9365	0.0	A201	A(100,101,103)	120.3906	0.0
A172	A(83,81,84)	107.8584	0.0	A202	A(102,101,103)	119.1239	0.0
A173	A(79,85,86)	111.4725	0.0	A203	A(101,103,104)	119.6112	0.0
A174	A(79,85,87)	110.9354	0.0	A204	A(101,103,105)	120.2437	0.0
A175	A(79,85,88)	111.0876	0.0	A205	A(104,103,105)	120.1445	0.0
A176	A(86,85,87)	108.3267	0.0	A206	A(103,105,106)	120.0807	0.0
A177	A(86,85,88)	107.2766	0.0	A207	A(103,105,107)	119.7358	0.0
A178	A(87,85,88)	107.5705	0.0	A208	A(106,105,107)	120.1833	0.0
A179	A(3,89,90)	117.1205	0.0	A209	A(105,107,108)	120.1976	0.0
A180	A(3,89,98)	124.2586	0.0	A210	A(105,107,109)	120.1061	0.0
A181	A(90,89,98)	118.4449	0.0	A211	A(108,107,109)	119.6962	0.0

A182	A(89,90,91)	119.4103	0.0	A212	A(100,109,107)	120.6347	0.0
A183	A(89,90,92)	120.966	0.0	A213	A(100,109,110)	119.1701	0.0
A184	A(91,90,92)	119.6177	0.0	A214	A(107,109,110)	120.1952	0.0
A215	A(2,111,116)	125.1787	0.0	A245	A(121,120,123)	106.8733	0.0
A216	A(112,111,115)	107.9529	0.0	A246	A(122,120,123)	106.8885	0.0
A217	A(112,111,116)	126.1861	0.0	A247	A(113,124,125)	111.6233	0.0
A218	A(115,111,116)	125.6346	0.0	A248	A(113,124,126)	111.8453	0.0
A219	A(2,112,120)	126.7698	0.0	A249	A(113,124,127)	112.0583	0.0
A220	A(111,112,113)	108.0075	0.0	A250	A(125,124,126)	106.8543	0.0
A221	A(111,112,120)	126.3824	0.0	A251	A(125,124,127)	106.9807	0.0
A222	A(113,112,120)	125.2699	0.0	A252	A(126,124,127)	107.1623	0.0
A223	A(2,113,124)	125.3667	0.0	A253	A(114,128,129)	112.0305	0.0
A224	A(112,113,114)	108.0301	0.0	A254	A(114,128,130)	112.0723	0.0
A225	A(112,113,124)	125.4325	0.0	A255	A(114,128,131)	111.488	0.0
A226	A(114,113,124)	126.3346	0.0	A256	A(129,128,130)	107.2391	0.0
A227	A(2,114,128)	126.0603	0.0	A257	A(129,128,131)	106.8906	0.0
A228	A(113,114,115)	108.0044	0.0	A258	A(130,128,131)	106.7965	0.0
A229	A(113,114,128)	125.8489	0.0	A259	A(115,132,133)	111.9939	0.0
A230	A(115,114,128)	125.9198	0.0	A260	A(115,132,134)	111.6283	0.0
A231	A(2,115,132)	124.7918	0.0	A261	A(115,132,135)	112.0807	0.0
A232	A(111,115,114)	108.0028	0.0	A262	A(133,132,134)	106.9066	0.0
A233	A(111,115,132)	125.62	0.0	A263	A(133,132,135)	106.9533	0.0
A234	A(114,115,132)	126.2043	0.0	A264	A(134,132,135)	106.9474	0.0
A235	A(111,116,117)	111.9507	0.0	D1	D(5,1,2,111)	-105.1828	0.0
A236	A(111,116,118)	111.6039	0.0	D2	D(5,1,2,112)	-27.6144	0.0
A237	A(111,116,119)	112.0536	0.0	D3	D(5,1,2,113)	47.5188	0.0
A238	A(117,116,118)	106.7995	0.0	D4	D(5,1,2,114)	116.3079	0.0
A239	A(117,116,119)	107.2421	0.0	D5	D(5,1,2,115)	-176.6081	0.0
A240	A(118,116,119)	106.8665	0.0	D6	D(6,1,2,111)	79.3889	0.0
A241	A(112,120,121)	112.1873	0.0	D7	D(6,1,2,112)	156.9573	0.0
A242	A(112,120,122)	112.0337	0.0	D8	D(6,1,2,113)	-127.9095	0.0
A243	A(112,120,123)	111.2303	0.0	D9	D(6,1,2,114)	-59.1204	0.0
A244	A(121,120,122)	107.3128	0.0	D10	D(6,1,2,115)	7.9636	0.0
D11	D(2,1,5,3)	169.6466	0.0	D41	D(5,3,7,8)	-165.4902	0.0
D12	D(2,1,5,60)	-14.656	0.0	D42	D(89,3,7,4)	147.3607	0.0
D13	D(6,1,5,3)	-14.2607	0.0	D43	D(89,3,7,8)	-40.1802	0.0

D14	D(6,1,5,60)	161.4367	0.0	D44	D(100,3,7,4)	-102.7307	0.0
D15	D(2,1,6,4)	167.0635	0.0	D45	D(100,3,7,8)	69.7284	0.0
D16	D(2,1,6,31)	-30.6491	0.0	D46	D(5,3,89,90)	61.7374	0.0
D17	D(5,1,6,4)	-9.0355	0.0	D47	D(5,3,89,98)	-123.1722	0.0
D18	D(5,1,6,31)	153.2519	0.0	D48	D(7,3,89,90)	-59.6522	0.0
D19	D(1,2,111,116)	4.3701	0.0	D49	D(7,3,89,98)	115.4382	0.0
D20	D(113,2,111,116)	-159.5491	0.0	D50	D(100,3,89,90)	-178.3344	0.0
D21	D(114,2,111,116)	158.9086	0.0	D51	D(100,3,89,98)	-3.244	0.0
D22	D(1,2,112,120)	-1.075	0.0	D52	D(5,3,100,101)	61.6559	0.0
D23	D(114,2,112,120)	-158.5717	0.0	D53	D(5,3,100,109)	-119.5648	0.0
D24	D(115,2,112,120)	159.7742	0.0	D54	D(7,3,100,101)	-173.0253	0.0
D25	D(1,2,113,124)	-5.9993	0.0	D55	D(7,3,100,109)	5.754	0.0
D26	D(111,2,113,124)	158.558	0.0	D56	D(89,3,100,101)	-62.9543	0.0
D27	D(115,2,113,124)	-159.6581	0.0	D57	D(89,3,100,109)	115.825	0.0
D28	D(1,2,114,128)	-1.7342	0.0	D58	D(7,4,6,1)	33.036	0.0
D29	D(111,2,114,128)	-159.1045	0.0	D59	D(7,4,6,31)	-127.2632	0.0
D30	D(112,2,114,128)	159.0872	0.0	D60	D(9,4,6,1)	154.5865	0.0
D31	D(1,2,115,132)	4.488	0.0	D61	D(9,4,6,31)	-5.7127	0.0
D32	D(112,2,115,132)	-158.8474	0.0	D62	D(20,4,6,1)	-90.5551	0.0
D33	D(113,2,115,132)	159.6071	0.0	D63	D(20,4,6,31)	109.1457	0.0
D34	D(7,3,5,1)	9.4316	0.0	D64	D(6,4,7,3)	-45.9541	0.0
D35	D(7,3,5,60)	-165.8565	0.0	D65	D(6,4,7,8)	141.7015	0.0
D36	D(89,3,5,1)	-107.4954	0.0	D66	D(9,4,7,3)	-170.4113	0.0
D37	D(89,3,5,60)	77.2164	0.0	D67	D(9,4,7,8)	17.2444	0.0
D38	D(100,3,5,1)	136.6835	0.0	D68	D(20,4,7,3)	77.7679	0.0
D39	D(100,3,5,60)	-38.6046	0.0	D69	D(20,4,7,8)	-94.5764	0.0
D40	D(5,3,7,4)	22.0507	0.0	D70	D(6,4,9,10)	-102.3301	0.0
D71	D(6,4,9,18)	74.831	0.0	D101	D(11,10,12,14)	179.0162	0.0
D72	D(7,4,9,10)	23.2581	0.0	D102	D(10,12,14,15)	-179.806	0.0
D73	D(7,4,9,18)	-159.5808	0.0	D103	D(10,12,14,16)	0.1709	0.0
D74	D(20,4,9,10)	139.1044	0.0	D104	D(13,12,14,15)	-0.037	0.0
D75	D(20,4,9,18)	-43.7345	0.0	D105	D(13,12,14,16)	179.94	0.0
D76	D(6,4,20,21)	-163.3967	0.0	D106	D(12,14,16,17)	-179.8678	0.0
D77	D(6,4,20,29)	22.5548	0.0	D107	D(12,14,16,18)	0.2097	0.0
D78	D(7,4,20,21)	70.5127	0.0	D108	D(15,14,16,17)	0.1092	0.0
D79	D(7,4,20,29)	-103.5358	0.0	D109	D(15,14,16,18)	-179.8133	0.0

D80	D(9,4,20,21)	-43.3002	0.0	D110	D(14,16,18,9)	-0.1502	0.0
D81	D(9,4,20,29)	142.6513	0.0	D111	D(14,16,18,19)	179.1791	0.0
D82	D(1,5,60,61)	94.5268	0.0	D112	D(17,16,18,9)	179.9269	0.0
D83	D(1,5,60,68)	-81.388	0.0	D113	D(17,16,18,19)	-0.7437	0.0
D84	D(3,5,60,61)	-89.6533	0.0	D114	D(4,20,21,22)	5.0579	0.0
D85	D(3,5,60,68)	94.4318	0.0	D115	D(4,20,21,23)	-175.1699	0.0
D86	D(1,6,31,32)	107.3222	0.0	D116	D(29,20,21,22)	179.2862	0.0
D87	D(1,6,31,39)	-69.0804	0.0	D117	D(29,20,21,23)	-0.9415	0.0
D88	D(4,6,31,32)	-91.8235	0.0	D118	D(4,20,29,27)	174.4609	0.0
D89	D(4,6,31,39)	91.7739	0.0	D119	D(4,20,29,30)	-6.191	0.0
D90	D(4,9,10,11)	-1.7816	0.0	D120	D(21,20,29,27)	0.3628	0.0
D91	D(4,9,10,12)	177.8481	0.0	D121	D(21,20,29,30)	179.7109	0.0
D92	D(18,9,10,11)	-178.9629	0.0	D122	D(20,21,23,24)	-179.1498	0.0
D93	D(18,9,10,12)	0.6668	0.0	D123	D(20,21,23,25)	0.7985	0.0
D94	D(4,9,18,16)	-177.5173	0.0	D124	D(22,21,23,24)	0.624	0.0
D95	D(4,9,18,19)	3.1593	0.0	D125	D(22,21,23,25)	-179.4277	0.0
D96	D(10,9,18,16)	-0.2858	0.0	D126	D(21,23,25,26)	179.9764	0.0
D97	D(10,9,18,19)	-179.6093	0.0	D127	D(21,23,25,27)	-0.0614	0.0
D98	D(9,10,12,13)	179.6148	0.0	D128	D(24,23,25,26)	-0.0754	0.0
D99	D(9,10,12,14)	-0.6148	0.0	D129	D(24,23,25,27)	179.8867	0.0
D100	D(11,10,12,13)	-0.7542	0.0	D130	D(23,25,27,28)	179.9925	0.0
D131	D(23,25,27,29)	-0.514	0.0	D161	D(33,35,37,39)	-0.0535	0.0
D132	D(26,25,27,28)	-0.0453	0.0	D162	D(36,35,37,38)	0.0099	0.0
D133	D(26,25,27,29)	179.4482	0.0	D163	D(36,35,37,39)	179.8369	0.0
D134	D(25,27,29,20)	0.3606	0.0	D164	D(35,37,39,31)	0.5674	0.0
D135	D(25,27,29,30)	-178.9878	0.0	D165	D(35,37,39,50)	179.5913	0.0
D136	D(28,27,29,20)	179.8568	0.0	D166	D(38,37,39,31)	-179.6054	0.0
D137	D(28,27,29,30)	0.5083	0.0	D167	D(38,37,39,50)	-0.5815	0.0
D138	D(6,31,32,33)	-176.0835	0.0	D168	D(31,39,50,51)	-7.5284	0.0
D139	D(6,31,32,40)	1.6726	0.0	D169	D(31,39,50,52)	-125.1552	0.0
D140	D(39,31,32,33)	0.3588	0.0	D170	D(31,39,50,56)	110.1556	0.0
D141	D(39,31,32,40)	178.1148	0.0	D171	D(37,39,50,51)	173.4821	0.0
D142	D(6,31,39,37)	175.7759	0.0	D172	D(37,39,50,52)	55.8553	0.0
D143	D(6,31,39,50)	-3.1981	0.0	D173	D(37,39,50,56)	-68.8339	0.0
D144	D(32,31,39,37)	-0.71	0.0	D174	D(32,40,42,43)	-50.9034	0.0
D145	D(32,31,39,50)	-179.684	0.0	D175	D(32,40,42,44)	-170.9425	0.0

D146	D(31,32,33,34)	179.798	0.0	D176	D(32,40,42,45)	70.0819	0.0
D147	D(31,32,33,35)	0.1557	0.0	D177	D(41,40,42,43)	67.1342	0.0
D148	D(40,32,33,34)	1.9824	0.0	D178	D(41,40,42,44)	-52.9049	0.0
D149	D(40,32,33,35)	-177.6599	0.0	D179	D(41,40,42,45)	-171.8805	0.0
D150	D(31,32,40,41)	26.2205	0.0	D180	D(46,40,42,43)	-176.8622	0.0
D151	D(31,32,40,42)	144.237	0.0	D181	D(46,40,42,44)	63.0988	0.0
D152	D(31,32,40,46)	-90.0063	0.0	D182	D(46,40,42,45)	-55.8769	0.0
D153	D(33,32,40,41)	-156.0123	0.0	D183	D(32,40,46,47)	-65.2496	0.0
D154	D(33,32,40,42)	-37.9959	0.0	D184	D(32,40,46,48)	175.0837	0.0
D155	D(33,32,40,46)	87.7609	0.0	D185	D(32,40,46,49)	54.182	0.0
D156	D(32,33,35,36)	179.7952	0.0	D186	D(41,40,46,47)	178.517	0.0
D157	D(32,33,35,37)	-0.3143	0.0	D187	D(41,40,46,48)	58.8502	0.0
D158	D(34,33,35,36)	0.152	0.0	D188	D(41,40,46,49)	-62.0514	0.0
D159	D(34,33,35,37)	-179.9574	0.0	D189	D(42,40,46,47)	62.5298	0.0
D160	D(33,35,37,38)	-179.8806	0.0	D190	D(42,40,46,48)	-57.137	0.0
D191	D(42,40,46,49)	-178.0386	0.0	D221	D(69,61,62,64)	-176.6689	0.0
D192	D(39,50,52,53)	-67.3737	0.0	D222	D(60,61,69,70)	6.611	0.0
D193	D(39,50,52,54)	173.4751	0.0	D223	D(60,61,69,71)	124.8107	0.0
D194	D(39,50,52,55)	53.1744	0.0	D224	D(60,61,69,75)	-109.7771	0.0
D195	D(51,50,52,53)	175.1431	0.0	D225	D(62,61,69,70)	-175.8068	0.0
D196	D(51,50,52,54)	55.992	0.0	D226	D(62,61,69,71)	-57.6071	0.0
D197	D(51,50,52,55)	-64.3087	0.0	D227	D(62,61,69,75)	67.8051	0.0
D198	D(56,50,52,53)	57.973	0.0	D228	D(61,62,64,65)	-179.8921	0.0
D199	D(56,50,52,54)	-61.1782	0.0	D229	D(61,62,64,66)	0.9998	0.0
D200	D(56,50,52,55)	178.5211	0.0	D230	D(63,62,64,65)	0.7938	0.0
D201	D(39,50,56,57)	-56.1065	0.0	D231	D(63,62,64,66)	-178.3143	0.0
D202	D(39,50,56,58)	-176.4873	0.0	D232	D(62,64,66,67)	178.4585	0.0
D203	D(39,50,56,59)	63.7624	0.0	D233	D(62,64,66,68)	-1.3011	0.0
D204	D(51,50,56,57)	61.1363	0.0	D234	D(65,64,66,67)	-0.6497	0.0
D205	D(51,50,56,58)	-59.2445	0.0	D235	D(65,64,66,68)	179.5907	0.0
D206	D(51,50,56,59)	-178.9948	0.0	D236	D(64,66,68,60)	-0.402	0.0
D207	D(52,50,56,57)	178.0039	0.0	D237	D(64,66,68,79)	176.7644	0.0
D208	D(52,50,56,58)	57.6231	0.0	D238	D(67,66,68,60)	179.8384	0.0
D209	D(52,50,56,59)	-62.1273	0.0	D239	D(67,66,68,79)	-2.9953	0.0
D210	D(5,60,61,62)	-178.6273	0.0	D240	D(60,68,79,80)	-12.1995	0.0
D211	D(5,60,61,69)	-1.0711	0.0	D241	D(60,68,79,81)	-130.6012	0.0

D212	D(68,60,61,62)	-2.6718	0.0	D242	D(60,68,79,85)	104.8073	0.0
D213	D(68,60,61,69)	174.8844	0.0	D243	D(66,68,79,80)	170.7362	0.0
D214	D(5,60,68,66)	178.3654	0.0	D244	D(66,68,79,81)	52.3345	0.0
D215	D(5,60,68,79)	1.3324	0.0	D245	D(66,68,79,85)	-72.257	0.0
D216	D(61,60,68,66)	2.384	0.0	D246	D(61,69,71,72)	65.0177	0.0
D217	D(61,60,68,79)	-174.649	0.0	D247	D(61,69,71,73)	-55.8513	0.0
D218	D(60,61,62,63)	-179.6911	0.0	D248	D(61,69,71,74)	-175.5215	0.0
D219	D(60,61,62,64)	0.9941	0.0	D249	D(70,69,71,72)	-177.1582	0.0
D220	D(69,61,62,63)	2.6459	0.0	D250	D(70,69,71,73)	61.9728	0.0
D251	D(70,69,71,74)	-57.6973	0.0	D281	D(81,79,85,88)	-63.7389	0.0
D252	D(75,69,71,72)	-60.6693	0.0	D282	D(3,89,90,91)	-2.4835	0.0
D253	D(75,69,71,73)	178.4617	0.0	D283	D(3,89,90,92)	176.6244	0.0
D254	D(75,69,71,74)	58.7915	0.0	D284	D(98,89,90,91)	-177.8692	0.0
D255	D(61,69,75,76)	176.2393	0.0	D285	D(98,89,90,92)	1.2387	0.0
D256	D(61,69,75,77)	56.2877	0.0	D286	D(3,89,98,96)	-175.8135	0.0
D257	D(61,69,75,78)	-63.9276	0.0	D287	D(3,89,98,99)	3.2954	0.0
D258	D(70,69,75,76)	59.7474	0.0	D288	D(90,89,98,96)	-0.7834	0.0
D259	D(70,69,75,77)	-60.2042	0.0	D289	D(90,89,98,99)	178.3254	0.0
D260	D(70,69,75,78)	179.5806	0.0	D290	D(89,90,92,93)	179.6728	0.0
D261	D(71,69,75,76)	-57.2404	0.0	D291	D(89,90,92,94)	-0.8255	0.0
D262	D(71,69,75,77)	-177.1921	0.0	D292	D(91,90,92,93)	-1.2212	0.0
D263	D(71,69,75,78)	62.5927	0.0	D293	D(91,90,92,94)	178.2805	0.0
D264	D(68,79,81,82)	-66.8478	0.0	D294	D(90,92,94,95)	-179.6172	0.0
D265	D(68,79,81,83)	174.0932	0.0	D295	D(90,92,94,96)	-0.0645	0.0
D266	D(68,79,81,84)	54.2964	0.0	D296	D(93,92,94,95)	-0.1174	0.0
D267	D(80,79,81,82)	174.7254	0.0	D297	D(93,92,94,96)	179.4353	0.0
D268	D(80,79,81,83)	55.6665	0.0	D298	D(92,94,96,97)	-179.2454	0.0
D269	D(80,79,81,84)	-64.1304	0.0	D299	D(92,94,96,98)	0.5139	0.0
D270	D(85,79,81,82)	57.818	0.0	D300	D(95,94,96,97)	0.307	0.0
D271	D(85,79,81,83)	-61.2409	0.0	D301	D(95,94,96,98)	-179.9336	0.0
D272	D(85,79,81,84)	178.9622	0.0	D302	D(94,96,98,89)	-0.0817	0.0
D273	D(68,79,85,86)	-56.8704	0.0	D303	D(94,96,98,99)	-179.2035	0.0
D274	D(68,79,85,87)	-177.6846	0.0	D304	D(97,96,98,89)	179.6792	0.0
D275	D(68,79,85,88)	62.7154	0.0	D305	D(97,96,98,99)	0.5574	0.0
D276	D(80,79,85,86)	59.966	0.0	D306	D(3,100,101,102)	-1.6313	0.0
D277	D(80,79,85,87)	-60.8482	0.0	D307	D(3,100,101,103)	178.2062	0.0

D278	D(80,79,85,88)	179.5518	0.0	D308	D(109,100,101,102)	179.5882	0.0
D279	D(81,79,85,86)	176.6753	0.0	D309	D(109,100,101,103)	-0.5742	0.0
D280	D(81,79,85,87)	55.8611	0.0	D310	D(3,100,109,107)	-178.5676	0.0
D311	D(3,100,109,110)	1.4569	0.0	D341	D(112,111,116,117)	-151.5804	0.0
D312	D(101,100,109,107)	0.2517	0.0	D342	D(112,111,116,118)	88.7658	0.0
D313	D(101,100,109,110)	-179.7237	0.0	D343	D(112,111,116,119)	-31.0444	0.0
D314	D(100,101,103,104)	-179.9222	0.0	D344	D(115,111,116,117)	34.5549	0.0
D315	D(100,101,103,105)	0.3577	0.0	D345	D(115,111,116,118)	-85.0989	0.0
D316	D(102,101,103,104)	-0.0825	0.0	D346	D(115,111,116,119)	155.0908	0.0
D317	D(102,101,103,105)	-179.8025	0.0	D347	D(111,112,113,114)	0.4685	0.0
D318	D(101,103,105,106)	179.9843	0.0	D348	D(111,112,113,124)	175.5546	0.0
D319	D(101,103,105,107)	0.1891	0.0	D349	D(120,112,113,114)	-173.1773	0.0
D320	D(104,103,105,106)	0.2658	0.0	D350	D(120,112,113,124)	1.9089	0.0
D321	D(104,103,105,107)	-179.5294	0.0	D351	D(2,112,120,121)	53.2289	0.0
D322	D(103,105,107,108)	179.6299	0.0	D352	D(2,112,120,122)	-67.5523	0.0
D323	D(103,105,107,109)	-0.5113	0.0	D353	D(2,112,120,123)	172.8806	0.0
D324	D(106,105,107,108)	-0.1651	0.0	D354	D(111,112,120,121)	146.9698	0.0
D325	D(106,105,107,109)	179.6937	0.0	D355	D(111,112,120,122)	26.1885	0.0
D326	D(105,107,109,100)	0.2897	0.0	D356	D(111,112,120,123)	-93.3785	0.0
D327	D(105,107,109,110)	-179.7351	0.0	D357	D(113,112,120,121)	-40.5425	0.0
D328	D(108,107,109,100)	-179.8508	0.0	D358	D(113,112,120,122)	-161.3237	0.0
D329	D(108,107,109,110)	0.1244	0.0	D359	D(113,112,120,123)	79.1093	0.0
D330	D(115,111,112,113)	-0.2879	0.0	D360	D(112,113,114,115)	-0.4703	0.0
D331	D(115,111,112,120)	173.2677	0.0	D361	D(112,113,114,128)	174.3058	0.0
D332	D(116,111,112,113)	-175.049	0.0	D362	D(124,113,114,115)	-175.5	0.0
D333	D(116,111,112,120)	-1.4933	0.0	D363	D(124,113,114,128)	-0.7239	0.0
D334	D(112,111,115,114)	-0.0027	0.0	D364	D(2,113,124,125)	-173.0779	0.0
D335	D(112,111,115,132)	-175.4569	0.0	D365	D(2,113,124,126)	67.2571	0.0
D336	D(116,111,115,114)	174.7949	0.0	D366	D(2,113,124,127)	-53.1048	0.0
D337	D(116,111,115,132)	-0.6593	0.0	D367	D(112,113,124,125)	-80.6809	0.0
D338	D(2,111,116,117)	-58.1346	0.0	D368	D(112,113,124,126)	159.6541	0.0
D339	D(2,111,116,118)	-177.7884	0.0	D369	D(112,113,124,127)	39.2922	0.0
D340	D(2,111,116,119)	62.4013	0.0	D370	D(114,113,124,125)	93.5159	0.0
D371	D(114,113,124,126)	-26.149	0.0	D384	D(115,114,128,130)	-153.5403	0.0
D372	D(114,113,124,127)	-146.5109	0.0	D385	D(115,114,128,131)	86.8064	0.0
D373	D(113,114,115,111)	0.2919	0.0	D386	D(2,115,132,133)	-64.9235	0.0

D374	D(113,114,115,132)	175.7124	0.0	D387	D(2,115,132,134)	175.2392	0.0
D375	D(128,114,115,111)	-174.4794	0.0	D388	D(2,115,132,135)	55.2898	0.0
D376	D(128,114,115,132)	0.941	0.0	D389	D(111,115,132,133)	-156.9079	0.0
D377	D(2,114,128,129)	59.8496	0.0	D390	D(111,115,132,134)	83.2549	0.0
D378	D(2,114,128,130)	-60.7521	0.0	D391	D(111,115,132,135)	-36.6946	0.0
D379	D(2,114,128,131)	179.5946	0.0	D392	D(114,115,132,133)	28.4521	0.0
D380	D(113,114,128,129)	153.1995	0.0	D393	D(114,115,132,134)	-91.3852	0.0
D381	D(113,114,128,130)	32.5978	0.0	D394	D(114,115,132,135)	148.6653	0.0
D382	D(113,114,128,131)	-87.0555	0.0	D384	D(115,114,128,130)	-153.5403	0.0
D383	D(115,114,128,129)	-32.9385	0.0				

[1] = Derivative Info -DE/DX =

Standard Orientation of 3

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
1	30	0	0.764133	-0.094033	0.066474
2	30	0	3.081368	-0.623492	-0.070460
3	15	0	-2.355149	-1.074932	0.431756
4	15	0	-1.664411	1.929183	-0.177560
5	7	0	-0.775290	-1.444073	0.093388
6	7	0	-0.032839	1.785754	0.045098
7	6	0	-2.584994	0.629865	0.501812
8	1	0	-3.530898	0.920219	0.961830
9	6	0	-2.327797	3.483948	0.542512
10	6	0	-3.014051	3.487978	1.767365
11	1	0	-3.187791	2.550230	2.297488
12	6	0	-3.471454	4.688308	2.319104
13	1	0	-4.009667	4.675011	3.270214
14	6	0	-3.238041	5.898868	1.661366
15	1	0	-3.593467	6.836879	2.095481
16	6	0	-2.547483	5.905468	0.445757
17	1	0	-2.358764	6.847909	-0.074187
18	6	0	-2.096695	4.706759	-0.110996
19	1	0	-1.570983	4.726721	-1.067078

20	6	0	-2.044352	2.084281	-1.988637
21	6	0	-3.304119	2.563067	-2.393401
22	1	0	-4.019399	2.917966	-1.646879
23	6	0	-3.654657	2.596113	-3.744486
24	1	0	-4.632476	2.984361	-4.041677
25	6	0	-2.757618	2.135118	-4.714901
26	1	0	-3.031210	2.160203	-5.772757
27	6	0	-1.510591	1.643720	-4.322558
28	1	0	-0.803138	1.281316	-5.072782
29	6	0	-1.154867	1.621913	-2.969005
30	1	0	-0.171767	1.251275	-2.675474
31	6	0	0.810658	2.799861	0.614517
32	6	0	1.466915	3.761202	-0.209147
33	6	0	2.346536	4.683240	0.374873
34	1	0	2.850376	5.416230	-0.258396
35	6	0	2.600785	4.684022	1.744232
36	1	0	3.293022	5.409877	2.178817
37	6	0	1.959349	3.749509	2.550150
38	1	0	2.155091	3.748606	3.625472
39	6	0	1.064025	2.809600	2.017715
40	6	0	1.274966	3.780721	-1.721143
41	1	0	0.294750	3.335890	-1.923820
42	6	0	1.262090	5.188516	-2.336876
43	1	0	0.558829	5.857639	-1.815648
44	1	0	0.960046	5.134880	-3.395514
45	1	0	2.254766	5.666628	-2.310923
46	6	0	2.321551	2.894991	-2.419850
47	1	0	3.335181	3.304764	-2.276335
48	1	0	2.131949	2.837294	-3.504984
49	1	0	2.318418	1.872720	-2.012783
50	6	0	0.415676	1.817345	2.980625
51	1	0	-0.331126	1.250955	2.405404
52	6	0	-0.327810	2.514615	4.133766
53	1	0	0.367725	3.036838	4.811040
54	1	0	-0.878845	1.776508	4.740733
55	1	0	-1.049135	3.256391	3.761135

56	6	0	1.443230	0.812506	3.535183
57	1	0	1.960606	0.277775	2.723592
58	1	0	0.954133	0.062786	4.179910
59	1	0	2.212724	1.320371	4.139649
60	6	0	-0.360606	-2.758932	-0.313788
61	6	0	0.021882	-3.733552	0.653175
62	6	0	0.449227	-4.998052	0.220833
63	1	0	0.737209	-5.745540	0.964744
64	6	0	0.528696	-5.318848	-1.131645
65	1	0	0.862578	-6.310747	-1.447483
66	6	0	0.194811	-4.352290	-2.076799
67	1	0	0.280860	-4.593920	-3.139046
68	6	0	-0.244377	-3.074903	-1.700221
69	6	0	0.038319	-3.441088	2.150589
70	1	0	-0.396682	-2.445680	2.286991
71	6	0	-0.808638	-4.434699	2.962318
72	1	0	-0.398845	-5.457019	2.913421
73	1	0	-1.848009	-4.470934	2.602207
74	1	0	-0.834024	-4.141157	4.024244
75	6	0	1.476791	-3.376662	2.693199
76	1	0	1.476442	-3.098785	3.760642
77	1	0	2.071826	-2.630064	2.146375
78	1	0	1.990254	-4.347713	2.600849
79	6	0	-0.516917	-2.053500	-2.802776
80	1	0	-1.004154	-1.188453	-2.333648
81	6	0	-1.461346	-2.569396	-3.900471
82	1	0	-1.004541	-3.384340	-4.485790
83	1	0	-1.701248	-1.756816	-4.605512
84	1	0	-2.406335	-2.942109	-3.481707
85	6	0	0.806367	-1.563365	-3.422130
86	1	0	1.474423	-1.135058	-2.658765
87	1	0	0.620797	-0.795070	-4.190892
88	1	0	1.349616	-2.392540	-3.904604
89	6	0	-3.013394	-1.641719	2.081232
90	6	0	-2.392351	-1.122763	3.232385
91	1	0	-1.537592	-0.452615	3.124341

92	6	0	-2.864622	-1.437684	4.506390
93	1	0	-2.364073	-1.027976	5.387567
94	6	0	-3.982650	-2.267557	4.654618
95	1	0	-4.358302	-2.510642	5.651931
96	6	0	-4.619268	-2.774210	3.521208
97	1	0	-5.500201	-3.412914	3.625482
98	6	0	-4.138356	-2.464826	2.242203
99	1	0	-4.660695	-2.862022	1.371894
100	6	0	-3.473410	-1.945614	-0.760227
101	6	0	-3.528031	-3.350012	-0.846428
102	1	0	-2.882705	-3.968657	-0.220418
103	6	0	-4.412380	-3.969924	-1.732960
104	1	0	-4.445108	-5.061002	-1.788544
105	6	0	-5.247471	-3.199379	-2.549502
106	1	0	-5.938169	-3.687159	-3.242324
107	6	0	-5.191566	-1.805164	-2.478502
108	1	0	-5.836179	-1.195857	-3.117212
109	6	0	-4.311792	-1.182786	-1.586884
110	1	0	-4.269989	-0.093122	-1.527104
111	6	0	5.175135	-0.817853	0.944867
112	6	0	4.887596	-2.070851	0.305777
113	6	0	4.804233	-1.839320	-1.105552
114	6	0	5.050759	-0.446267	-1.342239
115	6	0	5.275735	0.185641	-0.074795
116	6	0	5.450859	-0.610370	2.408622
117	1	0	5.154137	0.395362	2.744870
118	1	0	6.526931	-0.720265	2.639927
119	1	0	4.913150	-1.336587	3.037557
120	6	0	4.837371	-3.419197	0.968717
121	1	0	4.090512	-4.082764	0.505542
122	1	0	4.590402	-3.344362	2.037987
123	1	0	5.812891	-3.936113	0.899628
124	6	0	4.612388	-2.900798	-2.153314
125	1	0	5.563449	-3.411228	-2.395386
126	1	0	4.226452	-2.481706	-3.095024
127	1	0	3.903371	-3.678616	-1.829086

128	6	0	5.178339	0.209002	-2.689682
129	1	0	4.897638	1.272464	-2.659688
130	1	0	4.542418	-0.275110	-3.447084
131	1	0	6.217026	0.161322	-3.066657
132	6	0	5.660930	1.622641	0.145450
133	1	0	5.290316	2.276570	-0.658457
134	1	0	6.759211	1.749272	0.182533
135	1	0	5.260136	2.018232	1.091523

Summary of Natural Population Analysis: Natural Population of 3

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
Zn	1	0.76170	17.99727	11.23571	0.00533	29.23830
Zn	2	0.57419	17.99800	11.42131	0.00651	29.42581
P	3	1.82342	9.99695	3.09630	0.08333	13.17658
P	4	1.82735	9.99692	3.09272	0.08301	13.17265
N	5	-1.18585	1.99941	6.17637	0.01008	8.18585
N	6	-1.20390	1.99939	6.19439	0.01013	8.20390
C	7	-1.38537	1.99883	5.37353	0.01301	7.38537
H	8	0.28408	0.00000	0.71311	0.00281	0.71592
C	9	-0.37106	1.99880	4.34870	0.02356	6.37106
C	10	-0.19924	1.99888	4.18282	0.01753	6.19924
H	11	0.23961	0.00000	0.75719	0.00320	0.76039
C	12	-0.21631	1.99891	4.20194	0.01546	6.21631
H	13	0.22785	0.00000	0.76950	0.00265	0.77215
C	14	-0.20151	1.99893	4.18745	0.01513	6.20151
H	15	0.22627	0.00000	0.77108	0.00265	0.77373
C	16	-0.21172	1.99892	4.19727	0.01553	6.21172
H	17	0.22807	0.00000	0.76928	0.00265	0.77193
C	18	-0.18945	1.99890	4.17314	0.01741	6.18945
H	19	0.23326	0.00000	0.76317	0.00357	0.76674
C	20	-0.37511	1.99878	4.34762	0.02870	6.37511
C	21	-0.21115	1.99887	4.19541	0.01686	6.21115
H	22	0.23153	0.00000	0.76550	0.00297	0.76847

C	23	-0.21699	1.99892	4.20244	0.01564	6.21699
H	24	0.22525	0.00000	0.77205	0.00270	0.77475
C	25	-0.21137	1.99893	4.19717	0.01527	6.21137
H	26	0.22519	0.00000	0.77216	0.00265	0.77481
C	27	-0.21344	1.99891	4.19894	0.01560	6.21344
H	28	0.22722	0.00000	0.77012	0.00266	0.77278
C	29	-0.21505	1.99887	4.19696	0.01922	6.21505
H	30	0.23491	0.00000	0.76056	0.00453	0.76509
C	31	0.18647	1.99869	3.79128	0.02356	5.81353
C	32	-0.03646	1.99878	4.01764	0.02005	6.03646
C	33	-0.22359	1.99888	4.20968	0.01503	6.22359
H	34	0.21703	0.00000	0.77987	0.00311	0.78297
C	35	-0.21534	1.99890	4.20054	0.01590	6.21534
H	36	0.21867	0.00000	0.77853	0.00279	0.78133
C	37	-0.22250	1.99888	4.20823	0.01539	6.22250
H	38	0.21558	0.00000	0.78133	0.00309	0.78442
C	39	-0.03592	1.99879	4.01714	0.01999	6.03592
C	40	-0.24949	1.99893	4.23619	0.01437	6.24949
H	41	0.22935	0.00000	0.76372	0.00693	0.77065
C	42	-0.62288	1.99924	4.61354	0.01011	6.62288
H	43	0.21336	0.00000	0.78407	0.00256	0.78664
H	44	0.21787	0.00000	0.77961	0.00252	0.78213
H	45	0.20821	0.00000	0.78910	0.00270	0.79179
C	46	-0.61718	1.99920	4.60793	0.01005	6.61718
H	47	0.21092	0.00000	0.78639	0.00269	0.78908
H	48	0.21048	0.00000	0.78684	0.00268	0.78952
H	49	0.21846	0.00000	0.77690	0.00463	0.78154
C	50	-0.25966	1.99896	4.24611	0.01458	6.25966
H	51	0.22806	0.00000	0.76538	0.00656	0.77194
C	52	-0.61348	1.99922	4.60405	0.01021	6.61348
H	53	0.20783	0.00000	0.78958	0.00259	0.79217
H	54	0.20841	0.00000	0.78894	0.00264	0.79159
H	55	0.21923	0.00000	0.77794	0.00283	0.78077
C	56	-0.61779	1.99921	4.60851	0.01007	6.61779
H	57	0.21513	0.00000	0.78063	0.00424	0.78487
H	58	0.20924	0.00000	0.78818	0.00258	0.79076

H	59	0.21208	0.00000	0.78535	0.00256	0.78792
C	60	0.17312	1.99869	3.80527	0.02292	5.82688
C	61	-0.03769	1.99877	4.01864	0.02029	6.03769
C	62	-0.22492	1.99888	4.21080	0.01524	6.22492
H	63	0.21769	0.00000	0.77925	0.00306	0.78231
C	64	-0.21800	1.99890	4.20315	0.01596	6.21800
H	65	0.21944	0.00000	0.77776	0.00280	0.78056
C	66	-0.22271	1.99887	4.20853	0.01531	6.22271
H	67	0.21747	0.00000	0.77946	0.00307	0.78253
C	68	-0.03300	1.99878	4.01375	0.02046	6.03300
C	69	-0.25187	1.99893	4.23782	0.01511	6.25187
H	70	0.23228	0.00000	0.76086	0.00686	0.76772
C	71	-0.61604	1.99922	4.60658	0.01025	6.61604
H	72	0.20522	0.00000	0.79218	0.00261	0.79478
H	73	0.21579	0.00000	0.78142	0.00279	0.78421
H	74	0.21529	0.00000	0.78215	0.00256	0.78471
C	75	-0.61355	1.99921	4.60417	0.01018	6.61355
H	76	0.21089	0.00000	0.78654	0.00257	0.78911
H	77	0.21623	0.00000	0.77914	0.00463	0.78377
H	78	0.20787	0.00000	0.78950	0.00263	0.79213
C	79	-0.25369	1.99895	4.23968	0.01506	6.25369
H	80	0.23035	0.00000	0.76314	0.00651	0.76965
C	81	-0.61296	1.99921	4.60346	0.01029	6.61296
H	82	0.20278	0.00000	0.79462	0.00261	0.79722
H	83	0.21399	0.00000	0.78350	0.00251	0.78601
H	84	0.21957	0.00000	0.77648	0.00395	0.78043
C	85	-0.61649	1.99920	4.60729	0.00999	6.61649
H	86	0.21316	0.00000	0.78230	0.00453	0.78684
H	87	0.20603	0.00000	0.79119	0.00279	0.79397
H	88	0.21306	0.00000	0.78434	0.00260	0.78694
C	89	-0.37248	1.99880	4.34426	0.02942	6.37248
C	90	-0.19485	1.99888	4.17809	0.01788	6.19485
H	91	0.23040	0.00000	0.76545	0.00415	0.76960
C	92	-0.21919	1.99891	4.20472	0.01557	6.21919
H	93	0.22629	0.00000	0.77101	0.00270	0.77371
C	94	-0.20559	1.99893	4.19149	0.01517	6.20559

H	95	0.22495	0.00000	0.77239	0.00266	0.77505
C	96	-0.21715	1.99892	4.20263	0.01560	6.21715
H	97	0.22560	0.00000	0.77169	0.00270	0.77440
C	98	-0.20379	1.99887	4.18829	0.01663	6.20379
H	99	0.23576	0.00000	0.76098	0.00326	0.76424
C	100	-0.38858	1.99881	4.36137	0.02841	6.38858
C	101	-0.21010	1.99889	4.19311	0.01810	6.21010
H	102	0.24079	0.00000	0.75591	0.00330	0.75921
C	103	-0.21893	1.99890	4.20438	0.01566	6.21893
H	104	0.22841	0.00000	0.76890	0.00269	0.77159
C	105	-0.20964	1.99892	4.19562	0.01510	6.20964
H	106	0.22513	0.00000	0.77219	0.00268	0.77487
C	107	-0.21794	1.99892	4.20342	0.01561	6.21794
H	108	0.22543	0.00000	0.77180	0.00277	0.77457
C	109	-0.19200	1.99886	4.17634	0.01680	6.19200
H	110	0.23718	0.00000	0.75896	0.00386	0.76282
C	111	-0.16496	1.99883	4.14138	0.02475	6.16496
C	112	-0.16209	1.99882	4.13866	0.02461	6.16209
C	113	-0.16192	1.99882	4.13873	0.02437	6.16192
C	114	-0.15998	1.99882	4.13678	0.02438	6.15998
C	115	-0.16435	1.99882	4.14109	0.02444	6.16435
C	116	-0.62930	1.99919	4.62056	0.00955	6.62930
H	117	0.22084	0.00000	0.77665	0.00251	0.77916
H	118	0.21709	0.00000	0.77955	0.00337	0.78291
H	119	0.21898	0.00000	0.77864	0.00239	0.78102
C	120	-0.63085	1.99919	4.62182	0.00985	6.63085
H	121	0.22365	0.00000	0.77379	0.00256	0.77635
H	122	0.21854	0.00000	0.77890	0.00256	0.78146
H	123	0.21707	0.00000	0.77955	0.00338	0.78293
C	124	-0.63053	1.99919	4.62168	0.00966	6.63053
H	125	0.21597	0.00000	0.78064	0.00339	0.78403
H	126	0.21790	0.00000	0.77964	0.00245	0.78210
H	127	0.22463	0.00000	0.77285	0.00252	0.77537
C	128	-0.62746	1.99918	4.61879	0.00949	6.62746
H	129	0.21849	0.00000	0.77875	0.00276	0.78151
H	130	0.21835	0.00000	0.77926	0.00239	0.78165

H	131	0.21736	0.00000	0.77931	0.00333	0.78264
C	132	-0.62911	1.99919	4.62015	0.00978	6.62911
H	133	0.21934	0.00000	0.77821	0.00245	0.78066
H	134	0.21534	0.00000	0.78130	0.00337	0.78466
H	135	0.22353	0.00000	0.77397	0.00250	0.77647

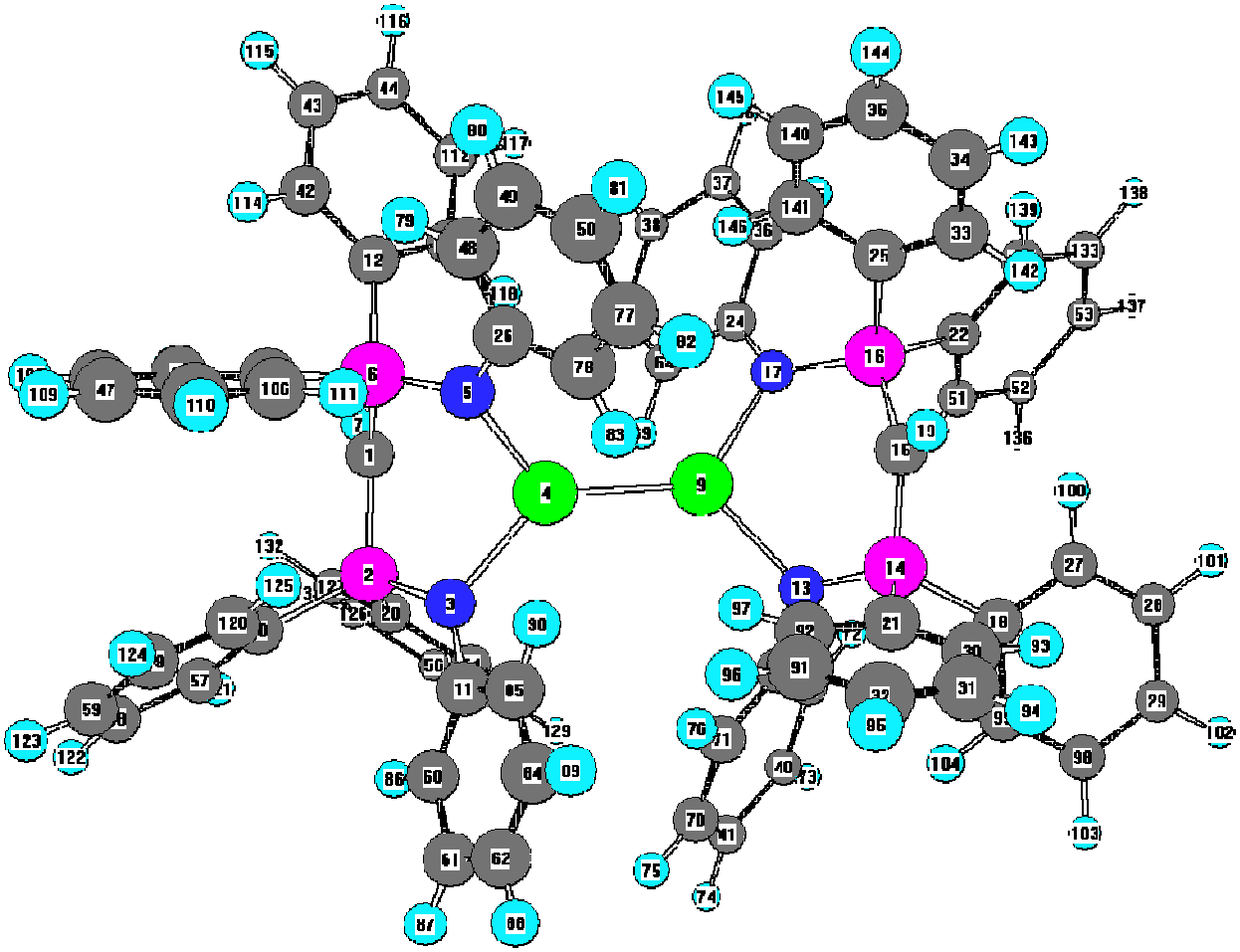
Total 0.00000 177.92533 348.67363 1.40104 528.00000

Natural Population of 3

Core	177.92533 (99.9580% of 178)
Valence	348.67363 (99.6210% of 350)
Natural Minimal Basis	526.59896 (99.7347% of 528)
Natural Rydberg Basis	1.40104 (0.2653% of 528)

Atom	No	Natural Electron Configuration
Zn	1	[core] 4S(0.84) 3d(9.95) 4p(0.45)
Zn	2	[core] 4S(1.00) 3d(9.94) 4p(0.47) 5S(0.01)
P	3	[core] 3S(0.91) 3p(2.19) 3d(0.06) 4p(0.02)
P	4	[core] 3S(0.90) 3p(2.19) 3d(0.06) 4p(0.02)
N	5	[core] 2S(1.41) 2p(4.77) 3p(0.01)
N	6	[core] 2S(1.40) 2p(4.80) 3p(0.01)
C	7	[core] 2S(1.13) 2p(4.25) 3p(0.01)
H	8	1S(0.71)
C	9	[core] 2S(0.95) 2p(3.40) 3p(0.02)
C	10	[core] 2S(0.93) 2p(3.25) 3p(0.01)

Calculated Structure and Atom Numbering Scheme of 1



HF=-7997.5154371

Optimized Parameters (Angstroms and Degrees) Compound 1

Name	Definition	Value	[1]		Definition	Value	[1]
R1	R(1,2)	1.736	0.0	R41	R(21,92)	1.4041	0.0
R2	R(1,6)	1.7402	0.0	R42	R(22,51)	1.4069	0.0
R3	R(1,7)	1.0908	0.0	R43	R(22,134)	1.4034	0.0
R4	R(2,3)	1.6393	0.0	R44	R(23,39)	1.4102	0.0
R5	R(2,10)	1.8481	0.0	R45	R(23,71)	1.4108	0.0
R6	R(2,20)	1.8396	0.0	R46	R(24,36)	1.4151	0.0
R7	R(3,4)	2.0992	0.0	R47	R(24,64)	1.4165	0.0
R8	R(3,11)	1.3967	0.0	R48	R(25,33)	1.4066	0.0
R9	R(4,5)	2.1019	0.0	R49	R(25,141)	1.4029	0.0
R10	R(4,9)	2.3964	0.0	R50	R(26,48)	1.4158	0.0
R11	R(5,6)	1.6457	0.0	R51	R(26,78)	1.4167	0.0
R12	R(5,26)	1.3967	0.0	R52	R(27,28)	1.3989	0.0
R13	R(6,8)	1.8436	0.0	R53	R(27,100)	1.0919	0.0
R14	R(6,12)	1.8427	0.0	R54	R(28,29)	1.3973	0.0
R15	R(8,45)	1.406	0.0	R55	R(28,101)	1.0931	0.0
R16	R(8,106)	1.4034	0.0	R56	R(29,98)	1.3995	0.0
R17	R(9,13)	2.0843	0.0	R57	R(29,102)	1.0933	0.0
R18	R(9,17)	2.0805	0.0	R58	R(30,31)	1.3985	0.0
R19	R(10,57)	1.4044	0.0	R59	R(30,93)	1.0923	0.0
R20	R(10,120)	1.4066	0.0	R60	R(31,32)	1.3978	0.0
R21	R(11,60)	1.4139	0.0	R61	R(31,94)	1.0932	0.0
R22	R(11,85)	1.4152	0.0	R62	R(32,91)	1.3987	0.0
R23	R(12,42)	1.4036	0.0	R63	R(32,95)	1.0932	0.0
R24	R(12,113)	1.4064	0.0	R64	R(33,34)	1.397	0.0
R25	R(13,14)	1.6347	0.0	R65	R(33,142)	1.0929	0.0
R26	R(13,23)	1.4131	0.0	R66	R(34,35)	1.3993	0.0
R27	R(14,15)	1.73	0.0	R67	R(34,143)	1.0932	0.0
R28	R(14,18)	1.8445	0.0	R68	R(35,140)	1.397	0.0
R29	R(14,21)	1.8471	0.0	R69	R(35,144)	1.0931	0.0
R30	R(15,16)	1.7335	0.0	R70	R(36,37)	1.3969	0.0
R31	R(15,19)	1.0909	0.0	R71	R(36,65)	1.0907	0.0
R32	R(16,17)	1.6456	0.0	R72	R(37,38)	1.398	0.0
R33	R(16,22)	1.8511	0.0	R73	R(37,66)	1.0939	0.0
R34	R(16,25)	1.8393	0.0	R74	R(38,63)	1.4	0.0
R35	R(17,24)	1.3987	0.0	R75	R(38,67)	1.0927	0.0
R36	R(18,27)	1.4025	0.0	R76	R(39,40)	1.397	0.0
R37	R(18,99)	1.4074	0.0	R77	R(39,72)	1.0921	0.0
R38	R(20,54)	1.4031	0.0	R78	R(40,41)	1.3994	0.0
R39	R(20,127)	1.4068	0.0	R79	R(40,73)	1.0938	0.0
R40	R(21,30)	1.4038	0.0	R80	R(41,70)	1.3993	0.0

R81	R(41,74)	1.0932	0.0	R122	R(61,87)	1.0939	0.0
R82	R(42,43)	1.3986	0.0	R123	R(62,84)	1.3995	0.0
R83	R(42,114)	1.0915	0.0	R124	R(62,88)	1.0925	0.0
R84	R(43,44)	1.3976	0.0	R125	R(63,64)	1.394	0.0
R85	R(43,115)	1.0931	0.0	R126	R(63,68)	1.0937	0.0
R86	R(44,112)	1.3988	0.0	R127	R(64,69)	1.0927	0.0
R87	R(44,116)	1.0932	0.0	R128	R(70,71)	1.3977	0.0
R88	R(45,46)	1.396	0.0	R129	R(70,75)	1.0933	0.0
R89	R(45,107)	1.0931	0.0	R130	R(71,76)	1.0913	0.0
R90	R(46,47)	1.3995	0.0	R131	R(77,78)	1.3931	0.0
R91	R(46,108)	1.093	0.0	R132	R(77,82)	1.0937	0.0
R92	R(47,105)	1.3973	0.0	R133	R(78,83)	1.0925	0.0
R93	R(47,109)	1.0932	0.0	R134	R(84,85)	1.3945	0.0
R94	R(48,49)	1.3972	0.0	R135	R(84,89)	1.0938	0.0
R95	R(48,79)	1.0904	0.0	R136	R(85,90)	1.0931	0.0
R96	R(49,50)	1.3973	0.0	R137	R(91,92)	1.3968	0.0
R97	R(49,80)	1.094	0.0	R138	R(91,96)	1.0927	0.0
R98	R(50,77)	1.3999	0.0	R139	R(92,97)	1.0932	0.0
R99	R(50,81)	1.0926	0.0	R140	R(98,99)	1.3965	0.0
R100	R(51,52)	1.3954	0.0	R141	R(98,103)	1.0931	0.0
R101	R(51,135)	1.0927	0.0	R142	R(99,104)	1.0922	0.0
R102	R(52,53)	1.3993	0.0	R143	R(105,106)	1.3993	0.0
R103	R(52,136)	1.093	0.0	R144	R(105,110)	1.093	0.0
R104	R(53,133)	1.3968	0.0	R145	R(106,111)	1.0906	0.0
R105	R(53,137)	1.0931	0.0	R146	R(112,113)	1.3968	0.0
R106	R(54,55)	1.3991	0.0	R147	R(112,117)	1.0926	0.0
R107	R(54,128)	1.0917	0.0	R148	R(113,118)	1.0925	0.0
R108	R(55,56)	1.397	0.0	R149	R(119,120)	1.3954	0.0
R109	R(55,129)	1.0926	0.0	R150	R(119,124)	1.0927	0.0
R110	R(56,126)	1.3996	0.0	R151	R(120,125)	1.0916	0.0
R111	R(56,130)	1.0932	0.0	R152	R(121,132)	2.4994	0.0
R112	R(57,58)	1.3989	0.0	R153	R(126,127)	1.3969	0.0
R113	R(57,121)	1.091	0.0	R154	R(126,131)	1.0932	0.0
R114	R(58,59)	1.3968	0.0	R155	R(127,132)	1.0932	0.0
R115	R(58,122)	1.0932	0.0	R156	R(133,134)	1.3994	0.0
R116	R(59,119)	1.3988	0.0	R157	R(133,138)	1.0932	0.0
R117	R(59,123)	1.0931	0.0	R158	R(134,139)	1.0911	0.0
R118	R(60,61)	1.397	0.0	R159	R(140,141)	1.3986	0.0
R119	R(60,76)	3.8682	0.0	R160	R(140,145)	1.0924	0.0
R120	R(60,86)	1.0912	0.0	R161	R(141,146)	1.0918	0.0
R121	R(61,62)	1.3977	0.0				

[1] = Derivative Info -DE/DX =

Standard Orientation of 1

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
1	6	0	-3.499490	0.411103	-1.211921
2	15	0	-3.595666	-1.308834	-0.996596
3	7	0	-2.617935	-1.671522	0.268174
4	30	0	-1.212767	-0.114752	0.361689
5	7	0	-2.429677	1.428992	1.105987
6	15	0	-3.622731	1.657927	-0.004226
7	1	0	-3.505921	0.765038	-2.243636
8	6	0	-5.274976	1.720436	0.811190
9	30	0	1.137405	-0.097994	-0.106639
10	6	0	-5.265410	-2.030373	-0.669954
11	6	0	-2.559898	-2.856435	1.005388
12	6	0	-3.432826	3.231882	-0.943473
13	7	0	2.551565	-1.629176	-0.103867
14	15	0	3.743769	-1.316460	0.969905
15	6	0	3.841531	0.397669	1.182506
16	15	0	3.671344	1.667848	0.015125
17	7	0	2.317955	1.425971	-0.889149
18	6	0	5.310887	-2.164960	0.494171
19	1	0	4.054946	0.732273	2.198614
20	6	0	-3.040614	-1.986296	-2.614367
21	6	0	3.412080	-1.981951	2.660732
22	6	0	5.081424	1.861814	-1.168345
23	6	0	2.295497	-2.864652	-0.740271
24	6	0	1.979197	2.093831	-2.070529
25	6	0	3.603501	3.186781	1.050064
26	6	0	-2.044249	2.291531	2.134632
27	6	0	6.466810	-1.415516	0.231392
28	6	0	7.656449	-2.052483	-0.137440
29	6	0	7.701354	-3.445016	-0.243147
30	6	0	4.443226	-2.374472	3.528696
31	6	0	4.147964	-2.805085	4.826058
32	6	0	2.821639	-2.851592	5.264765
33	6	0	4.660480	3.552411	1.903120
34	6	0	4.536958	4.663299	2.741064
35	6	0	3.354910	5.412123	2.743545
36	6	0	2.461312	3.372752	-2.437194
37	6	0	2.071176	3.978581	-3.633936
38	6	0	1.177333	3.346217	-4.503142

39	6	0	2.912252	-3.185424	-1.967209
40	6	0	2.617883	-4.378038	-2.632426
41	6	0	1.690618	-5.278384	-2.095962
42	6	0	-4.390241	4.257998	-0.967342
43	6	0	-4.145356	5.432898	-1.685541
44	6	0	-2.944301	5.594433	-2.381645
45	6	0	-6.437925	1.763664	0.022206
46	6	0	-7.699829	1.759004	0.619276
47	6	0	-7.815011	1.693473	2.012538
48	6	0	-2.588206	3.579088	2.360105
49	6	0	-2.142611	4.379254	3.415209
50	6	0	-1.140216	3.936873	4.282352
51	6	0	5.201889	0.882068	-2.170779
52	6	0	6.250994	0.930497	-3.089527
53	6	0	7.194654	1.961642	-3.025067
54	6	0	-1.876502	-2.768644	-2.653155
55	6	0	-1.381737	-3.238221	-3.874761
56	6	0	-2.042135	-2.925344	-5.065424
57	6	0	-5.991648	-2.778239	-1.610974
58	6	0	-7.259728	-3.277240	-1.294756
59	6	0	-7.814505	-3.041668	-0.034694
60	6	0	-2.967235	-4.123151	0.527339
61	6	0	-2.855516	-5.265380	1.323902
62	6	0	-2.328487	-5.191583	2.616374
63	6	0	0.680728	2.085329	-4.151782
64	6	0	1.076229	1.469231	-2.965456
65	1	0	3.148164	3.905271	-1.778239
66	1	0	2.473907	4.964176	-3.885097
67	1	0	0.877152	3.823028	-5.439338
68	1	0	-0.017702	1.566111	-4.814177
69	1	0	0.686442	0.479003	-2.717236
70	6	0	1.059535	-4.968069	-0.886249
71	6	0	1.356995	-3.778238	-0.215799
72	1	0	3.630735	-2.480922	-2.391548
73	1	0	3.116739	-4.604301	-3.579184
74	1	0	1.461333	-6.212296	-2.615794
75	1	0	0.325209	-5.653920	-0.455356
76	1	0	0.852075	-3.542024	0.722390
77	6	0	-0.587136	2.668146	4.071961
78	6	0	-1.029751	1.862249	3.025410
79	1	0	-3.367656	3.965531	1.702843
80	1	0	-2.591584	5.366935	3.556083

81	1	0	-0.796720	4.566092	5.106870
82	1	0	0.201107	2.296982	4.733047
83	1	0	-0.581165	0.877888	2.872780
84	6	0	-1.922236	-3.945050	3.106009
85	6	0	-2.040133	-2.798923	2.320410
86	1	0	-3.371503	-4.218329	-0.481742
87	1	0	-3.183754	-6.228167	0.921598
88	1	0	-2.240186	-6.088304	3.234176
89	1	0	-1.519044	-3.862049	4.119390
90	1	0	-1.749053	-1.825054	2.722628
91	6	0	1.789561	-2.462975	4.404386
92	6	0	2.082454	-2.028275	3.109624
93	1	0	5.482414	-2.347715	3.193199
94	1	0	4.957921	-3.108202	5.494763
95	1	0	2.591330	-3.192914	6.277439
96	1	0	0.750567	-2.500403	4.740615
97	1	0	1.275014	-1.721450	2.439618
98	6	0	6.554716	-4.201436	0.024736
99	6	0	5.365997	-3.567636	0.392873
100	1	0	6.429990	-0.328019	0.322149
101	1	0	8.549946	-1.456361	-0.340149
102	1	0	8.631144	-3.943682	-0.529656
103	1	0	6.586031	-5.291342	-0.052146
104	1	0	4.480588	-4.170547	0.606168
105	6	0	-6.664581	1.627098	2.802772
106	6	0	-5.398577	1.639795	2.206817
107	1	0	-6.354502	1.781885	-1.067527
108	1	0	-8.596706	1.792893	-0.004528
109	1	0	-8.803069	1.685326	2.480200
110	1	0	-6.748584	1.564889	3.890791
111	1	0	-4.504950	1.580115	2.829165
112	6	0	-1.981492	4.580095	-2.355270
113	6	0	-2.221243	3.407168	-1.635722
114	1	0	-5.329564	4.149488	-0.422145
115	1	0	-4.898390	6.225203	-1.697846
116	1	0	-2.756017	6.513905	-2.942212
117	1	0	-1.036917	4.693457	-2.892523
118	1	0	-1.457586	2.626161	-1.613780
119	6	0	-7.093174	-2.308094	0.913072
120	6	0	-5.828407	-1.808601	0.599870
121	1	0	-5.567497	-2.990448	-2.593486
122	1	0	-7.811005	-3.860206	-2.037288

123	1	0	-8.804007	-3.435256	0.212133
124	1	0	-7.514514	-2.125646	1.904675
125	1	0	-5.269684	-1.247956	1.351552
126	6	0	-3.196849	-2.134949	-5.036234
127	6	0	-3.693602	-1.664858	-3.818256
128	1	0	-1.342634	-2.999003	-1.729167
129	1	0	-0.471637	-3.842710	-3.885250
130	1	0	-1.654195	-3.290516	-6.019971
131	1	0	-3.710574	-1.879575	-5.966785
132	1	0	-4.589505	-1.038445	-3.810138
133	6	0	7.077075	2.945747	-2.040769
134	6	0	6.025128	2.899437	-1.119057
135	1	0	4.459512	0.082711	-2.233557
136	1	0	6.328825	0.162644	-3.863448
137	1	0	8.014621	2.001606	-3.746821
138	1	0	7.802166	3.762461	-1.991988
139	1	0	5.938697	3.689228	-0.371202
140	6	0	2.294643	5.043360	1.911989
141	6	0	2.416672	3.934536	1.068429
142	1	0	5.579842	2.961902	1.926248
143	1	0	5.363547	4.940555	3.400530
144	1	0	3.257696	6.277856	3.403832
145	1	0	1.360057	5.608799	1.927029
146	1	0	1.579395	3.634121	0.435385

Summary of Natural Population Analysis: Natural Population of 1

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-1.36335	1.99892	5.35028	0.01415	7.36335
P	2	1.80241	9.99704	3.11432	0.08622	13.19759
N	3	-1.13624	1.99933	6.12484	0.01207	8.13624
Zn	4	0.65226	17.99776	11.34550	0.00448	29.34774
N	5	-1.12548	1.99933	6.11383	0.01232	8.12548
P	6	1.80089	9.99704	3.11676	0.08531	13.19911
H	7	0.28599	0.00000	0.71129	0.00272	0.71401
C	8	-0.38867	1.99880	4.36287	0.02701	6.38867
Zn	9	0.68014	17.99761	11.31810	0.00415	29.31986
C	10	-0.37868	1.99880	4.35262	0.02726	6.37868
C	11	0.19227	1.99885	3.78627	0.02260	5.80773
C	12	-0.37658	1.99882	4.35144	0.02631	6.37658

N	13	-1.17325	1.99934	6.16181	0.01210	8.17325
P	14	1.81602	9.99697	3.10004	0.08696	13.18398
C	15	-1.36499	1.99888	5.35315	0.01297	7.36499
P	16	1.80553	9.99705	3.11218	0.08525	13.19447
N	17	-1.13839	1.99934	6.12705	0.01201	8.13839
C	18	-0.39160	1.99880	4.36505	0.02775	6.39160
H	19	0.28597	0.00000	0.71140	0.00263	0.71403
C	20	-0.37928	1.99882	4.35274	0.02773	6.37928
C	21	-0.37729	1.99880	4.34909	0.02940	6.37729
C	22	-0.37671	1.99879	4.35039	0.02753	6.37671
C	23	0.17194	1.99881	3.80614	0.02311	5.82806
C	24	0.19193	1.99886	3.78699	0.02221	5.80807
C	25	-0.37707	1.99882	4.35131	0.02694	6.37707
C	26	0.18910	1.99886	3.78961	0.02243	5.81090
C	27	-0.19669	1.99887	4.18065	0.01718	6.19669
C	28	-0.21936	1.99892	4.20479	0.01565	6.21936
C	29	-0.20967	1.99893	4.19567	0.01506	6.20967
C	30	-0.20262	1.99888	4.18731	0.01643	6.20262
C	31	-0.21798	1.99893	4.20342	0.01563	6.21798
C	32	-0.20785	1.99893	4.19385	0.01506	6.20785
C	33	-0.21783	1.99889	4.20224	0.01670	6.21783
C	34	-0.21786	1.99892	4.20324	0.01570	6.21786
C	35	-0.20713	1.99893	4.19317	0.01503	6.20713
C	36	-0.27274	1.99890	4.25896	0.01488	6.27274
C	37	-0.21204	1.99893	4.19780	0.01531	6.21204
C	38	-0.26817	1.99891	4.25343	0.01583	6.26817
C	39	-0.23688	1.99885	4.22171	0.01632	6.23688
C	40	-0.22270	1.99892	4.20872	0.01506	6.22270
C	41	-0.25241	1.99892	4.23803	0.01547	6.25241
C	42	-0.20870	1.99887	4.19339	0.01644	6.20870
C	43	-0.21793	1.99892	4.20334	0.01567	6.21793
C	44	-0.20714	1.99893	4.19321	0.01500	6.20714
C	45	-0.20191	1.99888	4.18604	0.01699	6.20191
C	46	-0.21698	1.99891	4.20230	0.01576	6.21698
C	47	-0.20801	1.99893	4.19388	0.01520	6.20801
C	48	-0.28085	1.99890	4.26769	0.01425	6.28085
C	49	-0.21103	1.99894	4.19682	0.01528	6.21103
C	50	-0.26527	1.99892	4.25069	0.01566	6.26527
C	51	-0.19494	1.99888	4.17849	0.01756	6.19494
C	52	-0.21041	1.99892	4.19588	0.01561	6.21041
C	53	-0.21204	1.99893	4.19799	0.01512	6.21204
C	54	-0.19379	1.99887	4.17699	0.01793	6.19379

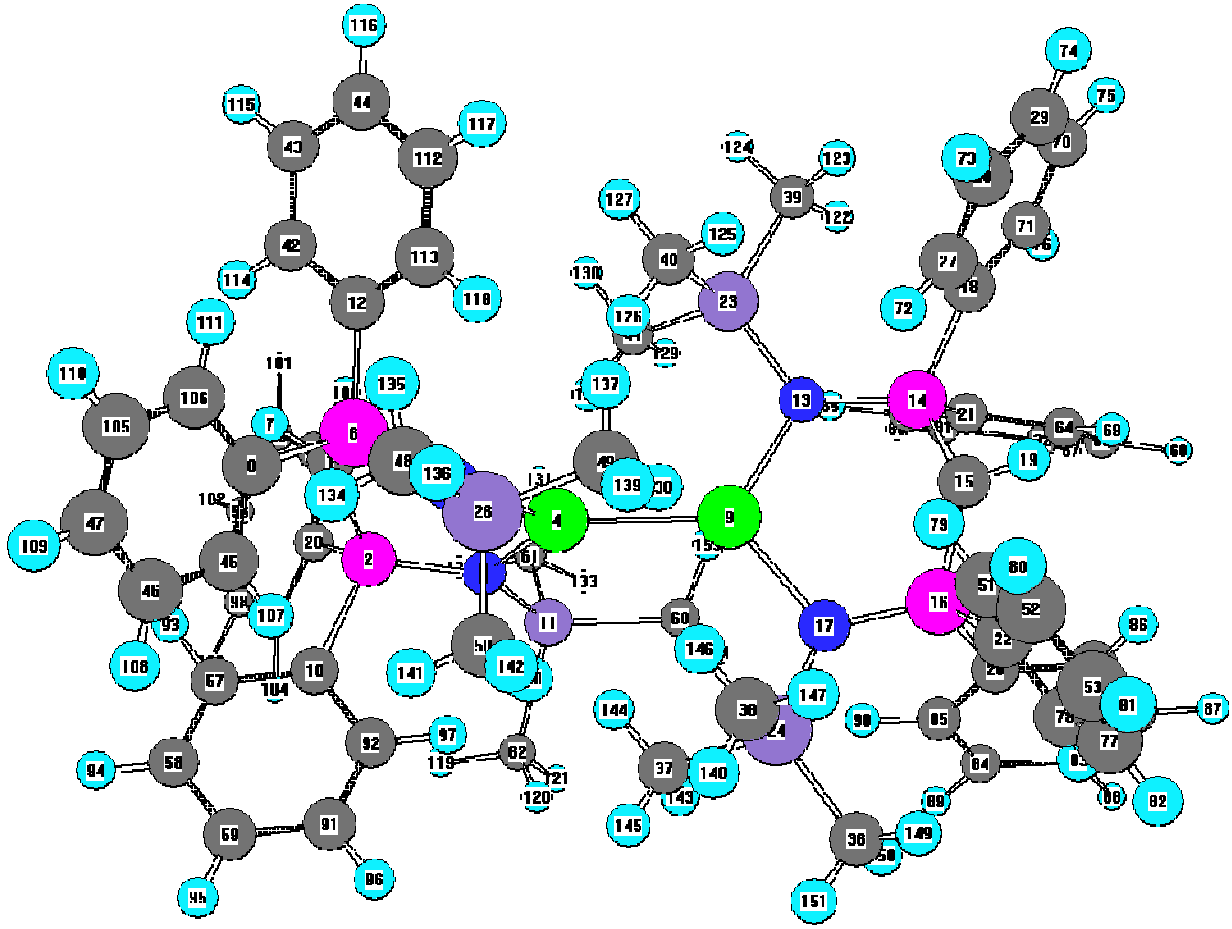
C	55	-0.20736	1.99892	4.19273	0.01572	6.20736
C	56	-0.20841	1.99893	4.19446	0.01501	6.20841
C	57	-0.20575	1.99888	4.19065	0.01622	6.20575
C	58	-0.21762	1.99893	4.20306	0.01563	6.21762
C	59	-0.20968	1.99893	4.19566	0.01509	6.20968
C	60	-0.26914	1.99890	4.25553	0.01472	6.26914
C	61	-0.21082	1.99893	4.19666	0.01523	6.21082
C	62	-0.25768	1.99892	4.24323	0.01553	6.25768
C	63	-0.21444	1.99893	4.19995	0.01556	6.21444
C	64	-0.25484	1.99889	4.24018	0.01578	6.25484
H	65	0.21921	0.00000	0.77733	0.00346	0.78079
H	66	0.21835	0.00000	0.77882	0.00284	0.78165
H	67	0.21834	0.00000	0.77898	0.00267	0.78166
H	68	0.22095	0.00000	0.77620	0.00285	0.77905
H	69	0.21806	0.00000	0.77826	0.00368	0.78194
C	70	-0.22077	1.99893	4.20630	0.01555	6.22077
C	71	-0.24004	1.99884	4.22561	0.01559	6.24004
H	72	0.22336	0.00000	0.77356	0.00308	0.77664
H	73	0.21935	0.00000	0.77783	0.00282	0.78065
H	74	0.21940	0.00000	0.77792	0.00269	0.78060
H	75	0.22695	0.00000	0.77014	0.00291	0.77305
H	76	0.23320	0.00000	0.76329	0.00351	0.76680
C	77	-0.20999	1.99893	4.19574	0.01531	6.20999
C	78	-0.25183	1.99890	4.23703	0.01589	6.25183
H	79	0.21695	0.00000	0.77942	0.00363	0.78305
H	80	0.21674	0.00000	0.78040	0.00286	0.78326
H	81	0.21655	0.00000	0.78074	0.00271	0.78345
H	82	0.21983	0.00000	0.77734	0.00283	0.78017
H	83	0.21377	0.00000	0.78263	0.00360	0.78623
C	84	-0.21467	1.99893	4.20063	0.01511	6.21467
C	85	-0.25346	1.99889	4.23885	0.01572	6.25346
H	86	0.21930	0.00000	0.77734	0.00336	0.78070
H	87	0.21857	0.00000	0.77860	0.00283	0.78143
H	88	0.21818	0.00000	0.77913	0.00269	0.78182
H	89	0.21569	0.00000	0.78143	0.00288	0.78431
H	90	0.21681	0.00000	0.77976	0.00344	0.78319
C	91	-0.21370	1.99892	4.19919	0.01558	6.21370
C	92	-0.19363	1.99888	4.17684	0.01791	6.19363
H	93	0.23285	0.00000	0.76420	0.00295	0.76715
H	94	0.22411	0.00000	0.77318	0.00271	0.77589
H	95	0.22356	0.00000	0.77377	0.00267	0.77644
H	96	0.22452	0.00000	0.77258	0.00291	0.77548

H	97	0.23200	0.00000	0.76298	0.00501	0.76800
C	98	-0.21649	1.99892	4.20197	0.01560	6.21649
C	99	-0.19592	1.99889	4.17963	0.01739	6.19592
H	100	0.23831	0.00000	0.75796	0.00373	0.76169
H	101	0.22503	0.00000	0.77224	0.00273	0.77497
H	102	0.22305	0.00000	0.77427	0.00268	0.77695
H	103	0.22590	0.00000	0.77140	0.00270	0.77410
H	104	0.23834	0.00000	0.75868	0.00298	0.76166
C	105	-0.21768	1.99892	4.20313	0.01562	6.21768
C	106	-0.19483	1.99887	4.17813	0.01782	6.19483
H	107	0.23384	0.00000	0.76313	0.00303	0.76616
H	108	0.22620	0.00000	0.77110	0.00270	0.77380
H	109	0.22456	0.00000	0.77277	0.00267	0.77544
H	110	0.22753	0.00000	0.76979	0.00268	0.77247
H	111	0.24660	0.00000	0.75005	0.00335	0.75340
C	112	-0.20778	1.99892	4.19310	0.01577	6.20778
C	113	-0.18832	1.99889	4.17193	0.01750	6.18832
H	114	0.23300	0.00000	0.76397	0.00302	0.76700
H	115	0.22414	0.00000	0.77316	0.00270	0.77586
H	116	0.22367	0.00000	0.77366	0.00267	0.77633
H	117	0.23711	0.00000	0.75976	0.00314	0.76289
H	118	0.24224	0.00000	0.75337	0.00439	0.75776
C	119	-0.20985	1.99892	4.19534	0.01559	6.20985
C	120	-0.18891	1.99889	4.17172	0.01830	6.18891
H	121	0.23088	0.00000	0.76606	0.00305	0.76912
H	122	0.22366	0.00000	0.77362	0.00272	0.77634
H	123	0.22302	0.00000	0.77431	0.00268	0.77698
H	124	0.22651	0.00000	0.77074	0.00275	0.77349
H	125	0.23594	0.00000	0.75978	0.00428	0.76406
C	126	-0.21748	1.99892	4.20282	0.01574	6.21748
C	127	-0.21858	1.99889	4.20303	0.01665	6.21858
H	128	0.24621	0.00000	0.74944	0.00435	0.75379
H	129	0.23498	0.00000	0.76205	0.00297	0.76502
H	130	0.22452	0.00000	0.77282	0.00267	0.77548
H	131	0.22518	0.00000	0.77212	0.00270	0.77482
H	132	0.23035	0.00000	0.76680	0.00284	0.76965
C	133	-0.21664	1.99893	4.20207	0.01565	6.21664
C	134	-0.20857	1.99887	4.19327	0.01643	6.20857
H	135	0.23478	0.00000	0.76041	0.00480	0.76522
H	136	0.22633	0.00000	0.77098	0.00269	0.77367
H	137	0.22345	0.00000	0.77388	0.00267	0.77655
H	138	0.22386	0.00000	0.77343	0.00271	0.77614

H	139	0.23062	0.00000	0.76639	0.00299	0.76938
C	140	-0.20655	1.99892	4.19193	0.01570	6.20655
C	141	-0.19025	1.99888	4.17334	0.01803	6.19025
H	142	0.23099	0.00000	0.76609	0.00292	0.76901
H	143	0.22495	0.00000	0.77235	0.00270	0.77505
H	144	0.22443	0.00000	0.77289	0.00268	0.77557
H	145	0.23287	0.00000	0.76437	0.00276	0.76713
H	146	0.24611	0.00000	0.75004	0.00384	0.75389

* Total * 0.00000 231.89889 420.21823 1.88287 654.00000

Calculated Structure and Atom Numbering Scheme of 5



HF=-8708.106859

Optimized Parameters (Angstroms and Degrees) Compound 5

Name	Definition	Value	[1]		Definition	Value	[1]
R1	R(1,2)	1.7288	0.0	R41	R(20,54)	1.4061	0.0
R2	R(1,6)	1.7258	0.0	R42	R(20,99)	1.4042	0.0
R3	R(1,7)	1.0909	0.0	R43	R(21,30)	1.4019	0.0
R4	R(2,3)	1.6422	0.0	R44	R(21,64)	1.4059	0.0
R5	R(2,10)	1.8556	0.0	R45	R(22,51)	1.407	0.0
R6	R(2,20)	1.8475	0.0	R46	R(22,78)	1.4037	0.0
R7	R(3,4)	2.1123	0.0	R47	R(23,39)	1.899	0.0
R8	R(3,11)	1.7709	0.0	R48	R(23,40)	1.889	0.0
R9	R(4,5)	2.113	0.0	R49	R(23,41)	1.8928	0.0
R10	R(4,9)	2.4363	0.0	R50	R(24,36)	1.8991	0.0
R11	R(5,6)	1.632	0.0	R51	R(24,37)	1.8934	0.0
R12	R(5,26)	1.7718	0.0	R52	R(24,38)	1.8918	0.0
R13	R(6,8)	1.8595	0.0	R53	R(24,140)	3.7316	0.0
R14	R(6,12)	1.8505	0.0	R54	R(25,33)	1.4068	0.0
R15	R(8,45)	1.4072	0.0	R55	R(25,85)	1.4018	0.0
R16	R(8,106)	1.4039	0.0	R56	R(26,38)	4.6522	0.0
R17	R(9,13)	2.1002	0.0	R57	R(26,48)	1.897	0.0
R18	R(9,17)	2.1002	0.0	R58	R(26,49)	1.8936	0.0
R19	R(9,153)	2.8156	0.0	R59	R(26,50)	1.891	0.0
R20	R(10,57)	1.4069	0.0	R60	R(26,146)	3.6283	0.0
R21	R(10,92)	1.402	0.0	R61	R(26,148)	4.9044	0.0
R22	R(11,60)	1.8896	0.0	R62	R(27,28)	1.3964	0.0
R23	R(11,61)	1.8984	0.0	R63	R(27,72)	1.0924	0.0
R24	R(11,62)	1.8999	0.0	R64	R(28,29)	1.3993	0.0
R25	R(12,42)	1.4069	0.0	R65	R(28,73)	1.0932	0.0
R26	R(12,113)	1.4006	0.0	R66	R(29,70)	1.3971	0.0
R27	R(13,14)	1.6347	0.0	R67	R(29,74)	1.0932	0.0
R28	R(13,23)	1.7697	0.0	R68	R(30,31)	1.3995	0.0
R29	R(13,153)	3.1223	0.0	R69	R(30,65)	1.0908	0.0
R30	R(14,15)	1.7285	0.0	R70	R(31,32)	1.3966	0.0
R31	R(14,18)	1.849	0.0	R71	R(31,66)	1.0932	0.0
R32	R(14,21)	1.8551	0.0	R72	R(32,63)	1.3997	0.0
R33	R(15,16)	1.7279	0.0	R73	R(32,67)	1.0932	0.0
R34	R(15,19)	1.091	0.0	R74	R(33,34)	1.3958	0.0
R35	R(16,17)	1.6423	0.0	R75	R(33,86)	1.0933	0.0
R36	R(16,22)	1.8513	0.0	R76	R(34,35)	1.4	0.0
R37	R(16,25)	1.8546	0.0	R77	R(34,87)	1.0934	0.0
R38	R(17,24)	1.7738	0.0	R78	R(35,84)	1.3963	0.0
R39	R(18,27)	1.4065	0.0	R79	R(35,88)	1.0932	0.0
R40	R(18,71)	1.4025	0.0	R80	R(36,149)	1.0992	0.0

R81	R(36,150)	1.1011	0.0	R123	R(51,72)	4.2962	0.0
R82	R(36,151)	1.1041	0.0	R124	R(51,79)	1.0922	0.0
R83	R(37,143)	1.102	0.0	R125	R(52,53)	1.3988	0.0
R84	R(37,144)	1.099	0.0	R126	R(52,80)	1.0931	0.0
R85	R(37,145)	1.1032	0.0	R127	R(53,77)	1.3971	0.0
R86	R(38,49)	4.0076	0.0	R128	R(53,81)	1.0932	0.0
R87	R(38,146)	1.0997	0.0	R129	R(54,55)	1.3964	0.0
R88	R(38,147)	1.1019	0.0	R130	R(54,100)	1.0921	0.0
R89	R(38,148)	1.1032	0.0	R131	R(54,132)	2.9516	0.0
R90	R(39,122)	1.1018	0.0	R132	R(55,56)	1.3987	0.0
R91	R(39,123)	1.0995	0.0	R133	R(55,101)	1.0931	0.0
R92	R(39,124)	1.1041	0.0	R134	R(56,98)	1.3976	0.0
R93	R(40,125)	1.1026	0.0	R135	R(56,102)	1.0931	0.0
R94	R(40,126)	1.1004	0.0	R136	R(57,58)	1.3955	0.0
R95	R(40,127)	1.1023	0.0	R137	R(57,93)	1.093	0.0
R96	R(41,128)	1.0995	0.0	R138	R(58,59)	1.4008	0.0
R97	R(41,129)	1.1028	0.0	R139	R(58,94)	1.0932	0.0
R98	R(41,130)	1.1035	0.0	R140	R(59,91)	1.3968	0.0
R99	R(41,131)	3.1766	0.0	R141	R(59,95)	1.0932	0.0
R100	R(42,43)	1.3961	0.0	R142	R(60,152)	1.0979	0.0
R101	R(42,114)	1.0927	0.0	R143	R(60,153)	1.1005	0.0
R102	R(43,44)	1.3999	0.0	R144	R(60,154)	1.1042	0.0
R103	R(43,115)	1.0932	0.0	R145	R(61,129)	3.5838	0.0
R104	R(44,112)	1.3961	0.0	R146	R(61,131)	1.1016	0.0
R105	R(44,116)	1.0931	0.0	R147	R(61,132)	1.0991	0.0
R106	R(45,46)	1.3956	0.0	R148	R(61,133)	1.1041	0.0
R107	R(45,107)	1.0913	0.0	R149	R(62,119)	1.1014	0.0
R108	R(46,47)	1.3999	0.0	R150	R(62,120)	1.1021	0.0
R109	R(46,108)	1.093	0.0	R151	R(62,121)	1.1038	0.0
R110	R(47,105)	1.3963	0.0	R152	R(63,64)	1.396	0.0
R111	R(47,109)	1.0932	0.0	R153	R(63,68)	1.0932	0.0
R112	R(48,134)	1.0992	0.0	R154	R(64,69)	1.0931	0.0
R113	R(48,135)	1.1018	0.0	R155	R(65,76)	4.0574	0.0
R114	R(48,136)	1.1042	0.0	R156	R(70,71)	1.3991	0.0
R115	R(49,137)	1.1027	0.0	R157	R(70,75)	1.0931	0.0
R116	R(49,138)	1.0993	0.0	R158	R(71,76)	1.0911	0.0
R117	R(49,139)	1.1031	0.0	R159	R(71,123)	2.8444	0.0
R118	R(49,146)	2.9201	0.0	R160	R(77,78)	1.3991	0.0
R119	R(50,140)	1.1008	0.0	R161	R(77,82)	1.0931	0.0
R120	R(50,141)	1.1021	0.0	R162	R(78,83)	1.0909	0.0
R121	R(50,142)	1.1029	0.0	R163	R(83,86)	2.6213	0.0
R122	R(51,52)	1.3966	0.0	R123	R(51,72)	4.2962	0.0

R164	R(84,85)	1.3996	0.0	R173	R(98,103)	1.0931	0.0
R165	R(84,89)	1.0932	0.0	R174	R(99,104)	1.0914	0.0
R166	R(85,90)	1.0908	0.0	R175	R(105,106)	1.3996	0.0
R167	R(90,143)	2.9884	0.0	R176	R(105,110)	1.0933	0.0
R168	R(91,92)	1.4002	0.0	R177	R(106,111)	1.0909	0.0
R169	R(91,96)	1.0931	0.0	R178	R(111,114)	2.8918	0.0
R170	R(92,97)	1.0907	0.0	R179	R(112,113)	1.3999	0.0
R171	R(93,104)	2.7994	0.0	R180	R(112,117)	1.0929	0.0
R172	R(98,99)	1.3983	0.0	R181	R(113,118)	1.0906	0.0

[1] = Derivative Info -DE/DX =

Standard Orientation of 5

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
1	6	0	4.352123	0.487665	0.855958
2	15	0	3.807316	-1.094009	1.292266
3	7	0	2.179486	-1.299429	1.223476
4	30	0	1.216184	-0.070356	-0.198985
5	7	0	2.716134	0.847793	-1.370264
6	15	0	4.083874	1.333667	-0.624202
7	1	0	5.159045	0.879858	1.476473
8	6	0	5.545183	1.181201	-1.764030
9	30	0	-1.215941	0.026320	-0.303361
10	6	0	4.610869	-2.412192	0.262648
11	14	0	1.254119	-2.382094	2.275860
12	6	0	4.086410	3.134532	-0.198298
13	7	0	-2.239654	1.341955	0.974193
14	15	0	-3.870125	1.400578	0.871920
15	6	0	-4.500088	0.676380	-0.565596
16	15	0	-4.159287	-0.894888	-1.198430
17	7	0	-2.557392	-1.240363	-1.306884
18	6	0	-4.557926	3.115030	0.791231
19	1	0	-5.403853	1.143744	-0.959367
20	6	0	4.523278	-1.337858	2.977823
21	6	0	-4.599763	0.666248	2.411368
22	6	0	-5.036050	-0.874401	-2.828864
23	14	0	-1.195232	2.499527	1.811436
24	14	0	-1.874995	-2.408913	-2.453630

25	6	0	-4.993099	-2.223796	-0.209374
26	14	0	2.302398	0.995300	-3.086775
27	6	0	-4.217519	3.883307	-0.336712
28	6	0	-4.686428	5.191582	-0.472734
29	6	0	-5.503831	5.750152	0.516144
30	6	0	-3.788632	0.268890	3.483509
31	6	0	-4.350002	-0.315866	4.624399
32	6	0	-5.730908	-0.507705	4.706470
33	6	0	-6.389033	-2.215271	-0.034940
34	6	0	-7.011973	-3.169240	0.771373
35	6	0	-6.246389	-4.132496	1.439217
36	6	0	-3.012248	-3.868551	-2.881200
37	6	0	-0.315183	-3.217905	-1.748259
38	6	0	-1.455352	-1.557299	-4.089967
39	6	0	-2.105081	3.657121	3.010692
40	6	0	-0.327137	3.586599	0.533528
41	6	0	0.102441	1.620082	2.872294
42	6	0	5.041385	3.672506	0.683781
43	6	0	5.025958	5.030534	1.007113
44	6	0	4.052927	5.873255	0.456903
45	6	0	5.843256	-0.093766	-2.279632
46	6	0	6.936753	-0.284257	-3.125553
47	6	0	7.760329	0.795472	-3.465621
48	6	0	3.466852	2.070897	-4.128681
49	6	0	0.593156	1.788760	-3.272402
50	6	0	2.283621	-0.732020	-3.856215
51	6	0	-4.774740	0.214863	-3.680214
52	6	0	-5.374997	0.295068	-4.938660
53	6	0	-6.245027	-0.713064	-5.366939
54	6	0	4.471084	-0.270193	3.891393
55	6	0	4.950301	-0.426093	5.193670
56	6	0	5.477941	-1.653696	5.607025
57	6	0	6.010462	-2.555826	0.260029
58	6	0	6.628187	-3.493764	-0.568313
59	6	0	5.857684	-4.285474	-1.429563
60	6	0	-0.602781	-2.246985	1.952710
61	6	0	1.450540	-2.002942	4.125636
62	6	0	1.708706	-4.209651	2.025011
63	6	0	-6.549196	-0.125085	3.637218
64	6	0	-5.986099	0.447894	2.495544
65	1	0	-2.708652	0.406141	3.416058
66	1	0	-3.702755	-0.624436	5.449561

67	1	0	-6.170525	-0.963402	5.597625
68	1	0	-7.629401	-0.284894	3.689544
69	1	0	-6.628407	0.720766	1.654186
70	6	0	-5.845173	4.994722	1.640737
71	6	0	-5.372585	3.685283	1.780221
72	1	0	-3.583695	3.446045	-1.111595
73	1	0	-4.413715	5.777631	-1.354360
74	1	0	-5.872404	6.773822	0.409863
75	1	0	-6.480948	5.425613	2.418591
76	1	0	-5.638299	3.112271	2.669924
77	6	0	-6.507350	-1.801570	-4.531357
78	6	0	-5.905060	-1.884145	-3.271274
79	1	0	-4.097903	1.003928	-3.345205
80	1	0	-5.162229	1.148464	-5.587803
81	1	0	-6.716457	-0.650438	-6.351228
82	1	0	-7.184605	-2.594450	-4.859293
83	1	0	-6.116875	-2.743986	-2.634154
84	6	0	-4.857429	-4.131314	1.296568
85	6	0	-4.235383	-3.184368	0.474806
86	1	0	-6.995447	-1.451721	-0.529554
87	1	0	-8.099088	-3.156771	0.887391
88	1	0	-6.733602	-4.875408	2.076150
89	1	0	-4.250497	-4.870032	1.826639
90	1	0	-3.149386	-3.175424	0.372999
91	6	0	4.469310	-4.133515	-1.452075
92	6	0	3.848847	-3.207272	-0.604991
93	1	0	6.623236	-1.921010	0.905206
94	1	0	7.716029	-3.600903	-0.551431
95	1	0	6.341625	-5.015432	-2.083853
96	1	0	3.861230	-4.741445	-2.127049
97	1	0	2.764439	-3.091218	-0.619278
98	6	0	5.523709	-2.724352	4.709897
99	6	0	5.049474	-2.568065	3.403749
100	1	0	4.043869	0.684414	3.577069
101	1	0	4.904730	0.413763	5.891903
102	1	0	5.849698	-1.776309	6.627659
103	1	0	5.932370	-3.687871	5.025310
104	1	0	5.094804	-3.413178	2.714669
105	6	0	7.478271	2.064059	-2.954992
106	6	0	6.377320	2.256849	-2.112531
107	1	0	5.214894	-0.947030	-2.018704
108	1	0	7.148288	-1.282351	-3.517595

109	1	0	8.618360	0.646363	-4.126377
110	1	0	8.113438	2.914617	-3.216703
111	1	0	6.164987	3.259254	-1.738229
112	6	0	3.096789	5.347440	-0.413953
113	6	0	3.113680	3.985674	-0.737848
114	1	0	5.809872	3.031495	1.122665
115	1	0	5.775620	5.433402	1.693332
116	1	0	4.039757	6.936094	0.711987
117	1	0	2.326502	5.994761	-0.840688
118	1	0	2.351273	3.578540	-1.403031
119	1	0	2.778198	-4.410284	2.195627
120	1	0	1.465424	-4.552650	1.006334
121	1	0	1.137979	-4.834916	2.733247
122	1	0	-2.751566	3.118873	3.722314
123	1	0	-2.718163	4.412472	2.498397
124	1	0	-1.342734	4.194004	3.602036
125	1	0	-1.065263	4.172967	-0.038340
126	1	0	0.237275	2.966089	-0.178693
127	1	0	0.377753	4.289668	1.006791
128	1	0	0.734447	0.920591	2.306524
129	1	0	-0.368560	1.054509	3.693607
130	1	0	0.766127	2.374230	3.329000
131	1	0	1.305962	-0.930840	4.333563
132	1	0	2.426431	-2.299176	4.535472
133	1	0	0.674580	-2.559897	4.679395
134	1	0	4.448752	1.607816	-4.301144
135	1	0	3.634210	3.068901	-3.692953
136	1	0	2.987829	2.218242	-5.112605
137	1	0	0.593256	2.833158	-2.918709
138	1	0	-0.169426	1.244989	-2.696868
139	1	0	0.291485	1.794070	-4.333484
140	1	0	1.619720	-1.415160	-3.304594
141	1	0	3.296079	-1.167100	-3.842980
142	1	0	1.940769	-0.704074	-4.904071
143	1	0	-0.561452	-3.911058	-0.927663
144	1	0	0.403992	-2.482140	-1.361945
145	1	0	0.179524	-3.803516	-2.541547
146	1	0	-0.792662	-0.691460	-3.946922
147	1	0	-2.372960	-1.197153	-4.582348
148	1	0	-0.954670	-2.256629	-4.780834
149	1	0	-3.883051	-3.576134	-3.484910
150	1	0	-3.374198	-4.405937	-1.990845

151	1	0	-2.423705	-4.583332	-3.482704
152	1	0	-0.880329	-2.481747	0.916691
153	1	0	-1.002392	-1.251011	2.196737
154	1	0	-1.112294	-2.974384	2.608788

Summary of Natural Population Analysis: Natural Population of 5

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-1.36406	1.99884	5.35276	0.01246	7.36406
P	2	1.82128	9.99701	3.09806	0.08365	13.17872
N	3	-1.60082	1.99949	6.59391	0.00742	8.60082
Zn	4	0.67990	17.99743	11.31817	0.00450	29.32010
N	5	-1.59740	1.99948	6.59085	0.00707	8.59740
P	6	1.84518	9.99702	3.07472	0.08309	13.15482
H	7	0.27230	0.00000	0.72500	0.00270	0.72770
C	8	-0.37667	1.99881	4.34834	0.02952	6.37667
Zn	9	0.71818	17.99744	11.28024	0.00414	29.28182
C	10	-0.38613	1.99880	4.35887	0.02846	6.38613
Si	11	1.89660	9.99763	2.05774	0.04804	12.10340
C	12	-0.36895	1.99881	4.34153	0.02861	6.36895
N	13	-1.60422	1.99948	6.59742	0.00731	8.60422
P	14	1.83031	9.99701	3.08943	0.08325	13.16969
C	15	-1.37901	1.99885	5.36737	0.01279	7.37901
P	16	1.82313	9.99700	3.09682	0.08304	13.17687
N	17	-1.59715	1.99949	6.59037	0.00729	8.59715
C	18	-0.36599	1.99883	4.34056	0.02661	6.36599
H	19	0.28484	0.00000	0.71251	0.00265	0.71516
C	20	-0.36783	1.99884	4.34425	0.02474	6.36783
C	21	-0.38075	1.99880	4.35256	0.02939	6.38075
C	22	-0.36814	1.99882	4.34365	0.02568	6.36814
Si	23	1.88565	9.99766	2.06780	0.04888	12.11435
Si	24	1.89009	9.99766	2.06376	0.04849	12.10991
C	25	-0.37874	1.99881	4.35090	0.02904	6.37874
Si	26	1.88641	9.99765	2.06832	0.04762	12.11359
C	27	-0.19887	1.99889	4.18259	0.01739	6.19887
C	28	-0.21927	1.99892	4.20478	0.01557	6.21927
C	29	-0.20991	1.99893	4.19584	0.01514	6.20991
C	30	-0.19711	1.99887	4.18050	0.01774	6.19711
C	31	-0.21657	1.99892	4.20207	0.01558	6.21657
C	32	-0.21021	1.99893	4.19615	0.01513	6.21021

C	33	-0.20899	1.99888	4.19287	0.01724	6.20899
C	34	-0.21966	1.99891	4.20506	0.01569	6.21966
C	35	-0.21099	1.99893	4.19687	0.01519	6.21099
C	36	-1.16084	1.99913	5.14800	0.01372	7.16084
C	37	-1.16039	1.99913	5.14828	0.01297	7.16039
C	38	-1.16084	1.99910	5.14782	0.01392	7.16084
C	39	-1.16131	1.99913	5.14866	0.01352	7.16131
C	40	-1.16156	1.99910	5.14864	0.01381	7.16156
C	41	-1.15893	1.99912	5.14625	0.01356	7.15893
C	42	-0.20548	1.99889	4.19008	0.01652	6.20548
C	43	-0.21844	1.99892	4.20384	0.01568	6.21844
C	44	-0.21299	1.99893	4.19891	0.01515	6.21299
C	45	-0.19842	1.99888	4.18159	0.01794	6.19842
C	46	-0.21757	1.99891	4.20307	0.01558	6.21757
C	47	-0.21547	1.99893	4.20135	0.01519	6.21547
C	48	-1.16022	1.99913	5.14780	0.01329	7.16022
C	49	-1.15777	1.99913	5.14528	0.01336	7.15777
C	50	-1.15959	1.99911	5.14674	0.01374	7.15959
C	51	-0.19654	1.99889	4.18002	0.01762	6.19654
C	52	-0.21859	1.99892	4.20417	0.01551	6.21859
C	53	-0.20722	1.99893	4.19311	0.01518	6.20722
C	54	-0.19727	1.99889	4.18060	0.01778	6.19727
C	55	-0.21535	1.99892	4.20096	0.01547	6.21535
C	56	-0.20890	1.99893	4.19486	0.01511	6.20890
C	57	-0.20448	1.99888	4.18846	0.01713	6.20448
C	58	-0.22222	1.99892	4.20740	0.01590	6.22222
C	59	-0.21649	1.99893	4.20235	0.01521	6.21649
C	60	-1.16352	1.99914	5.15140	0.01298	7.16352
C	61	-1.15922	1.99912	5.14600	0.01409	7.15922
C	62	-1.16102	1.99913	5.14731	0.01458	7.16102
C	63	-0.21833	1.99891	4.20374	0.01568	6.21833
C	64	-0.20436	1.99888	4.18804	0.01744	6.20436
H	65	0.23052	0.00000	0.76565	0.00384	0.76948
H	66	0.22435	0.00000	0.77293	0.00272	0.77565
H	67	0.22237	0.00000	0.77495	0.00268	0.77763
H	68	0.22295	0.00000	0.77430	0.00275	0.77705
H	69	0.23008	0.00000	0.76669	0.00323	0.76992
C	70	-0.21771	1.99892	4.20326	0.01554	6.21771
C	71	-0.20238	1.99887	4.18642	0.01709	6.20238
H	72	0.23832	0.00000	0.75793	0.00375	0.76168
H	73	0.22499	0.00000	0.77231	0.00270	0.77501
H	74	0.22365	0.00000	0.77367	0.00268	0.77635

H	75	0.22477	0.00000	0.77253	0.00270	0.77523
H	76	0.23609	0.00000	0.76081	0.00310	0.76391
C	77	-0.21814	1.99891	4.20365	0.01558	6.21814
C	78	-0.21087	1.99888	4.19463	0.01736	6.21087
H	79	0.24175	0.00000	0.75468	0.00357	0.75825
H	80	0.22582	0.00000	0.77149	0.00269	0.77418
H	81	0.22410	0.00000	0.77322	0.00268	0.77590
H	82	0.22540	0.00000	0.77191	0.00269	0.77460
H	83	0.23854	0.00000	0.75843	0.00303	0.76146
C	84	-0.21451	1.99892	4.20000	0.01560	6.21451
C	85	-0.19959	1.99888	4.18266	0.01806	6.19959
H	86	0.22844	0.00000	0.76842	0.00313	0.77156
H	87	0.22251	0.00000	0.77475	0.00274	0.77749
H	88	0.22230	0.00000	0.77502	0.00268	0.77770
H	89	0.22418	0.00000	0.77310	0.00272	0.77582
H	90	0.23458	0.00000	0.76126	0.00416	0.76542
C	91	-0.21816	1.99891	4.20361	0.01564	6.21816
C	92	-0.20283	1.99886	4.18488	0.01908	6.20283
H	93	0.23307	0.00000	0.76392	0.00301	0.76693
H	94	0.22487	0.00000	0.77241	0.00272	0.77513
H	95	0.22338	0.00000	0.77394	0.00267	0.77662
H	96	0.22614	0.00000	0.77113	0.00273	0.77386
H	97	0.23609	0.00000	0.75896	0.00495	0.76391
C	98	-0.21800	1.99891	4.20346	0.01562	6.21800
C	99	-0.20707	1.99889	4.19139	0.01680	6.20707
H	100	0.24321	0.00000	0.75349	0.00330	0.75679
H	101	0.22565	0.00000	0.77166	0.00270	0.77435
H	102	0.22437	0.00000	0.77295	0.00268	0.77563
H	103	0.22580	0.00000	0.77151	0.00270	0.77420
H	104	0.23555	0.00000	0.76140	0.00305	0.76445
C	105	-0.21718	1.99892	4.20266	0.01560	6.21718
C	106	-0.20966	1.99888	4.19394	0.01684	6.20966
H	107	0.23161	0.00000	0.76293	0.00546	0.76839
H	108	0.22522	0.00000	0.77200	0.00278	0.77478
H	109	0.22235	0.00000	0.77496	0.00269	0.77765
H	110	0.22307	0.00000	0.77420	0.00273	0.77693
H	111	0.23233	0.00000	0.76438	0.00329	0.76767
C	112	-0.21489	1.99892	4.20030	0.01567	6.21489
C	113	-0.19849	1.99887	4.18185	0.01776	6.19849
H	114	0.22676	0.00000	0.77049	0.00275	0.77324
H	115	0.22428	0.00000	0.77301	0.00271	0.77572
H	116	0.22380	0.00000	0.77352	0.00267	0.77620

H	117	0.22671	0.00000	0.77061	0.00268	0.77329
H	118	0.23005	0.00000	0.76613	0.00382	0.76995
H	119	0.23319	0.00000	0.76482	0.00199	0.76681
H	120	0.23549	0.00000	0.76259	0.00192	0.76451
H	121	0.23578	0.00000	0.76224	0.00198	0.76422
H	122	0.23650	0.00000	0.76154	0.00196	0.76350
H	123	0.24016	0.00000	0.75727	0.00257	0.75984
H	124	0.23893	0.00000	0.75907	0.00200	0.76107
H	125	0.23503	0.00000	0.76288	0.00209	0.76497
H	126	0.23534	0.00000	0.76096	0.00369	0.76466
H	127	0.23752	0.00000	0.76054	0.00194	0.76248
H	128	0.23430	0.00000	0.76146	0.00424	0.76570
H	129	0.23199	0.00000	0.76607	0.00194	0.76801
H	130	0.23917	0.00000	0.75887	0.00196	0.76083
H	131	0.23962	0.00000	0.75838	0.00200	0.76038
H	132	0.23686	0.00000	0.76015	0.00299	0.76314
H	133	0.23394	0.00000	0.76407	0.00199	0.76606
H	134	0.24336	0.00000	0.75403	0.00261	0.75664
H	135	0.23686	0.00000	0.76118	0.00196	0.76314
H	136	0.23899	0.00000	0.75905	0.00196	0.76101
H	137	0.23433	0.00000	0.76377	0.00191	0.76567
H	138	0.23277	0.00000	0.76387	0.00336	0.76723
H	139	0.23756	0.00000	0.76058	0.00185	0.76244
H	140	0.23458	0.00000	0.76272	0.00270	0.76542
H	141	0.23834	0.00000	0.75952	0.00215	0.76166
H	142	0.23764	0.00000	0.76053	0.00182	0.76236
H	143	0.23724	0.00000	0.76070	0.00206	0.76276
H	144	0.22748	0.00000	0.76910	0.00342	0.77252
H	145	0.24011	0.00000	0.75801	0.00188	0.75989
H	146	0.23586	0.00000	0.76111	0.00303	0.76414
H	147	0.23960	0.00000	0.75820	0.00220	0.76040
H	148	0.23539	0.00000	0.76273	0.00187	0.76461
H	149	0.23676	0.00000	0.76103	0.00221	0.76324
H	150	0.23853	0.00000	0.75958	0.00189	0.76147
H	151	0.23899	0.00000	0.75901	0.00200	0.76101
H	152	0.23217	0.00000	0.76416	0.00367	0.76783
H	153	0.23622	0.00000	0.75993	0.00385	0.76378
H	154	0.23973	0.00000	0.75808	0.00220	0.76027

* Total * 0.00000 247.90530 404.25553 1.83917 654.00000

Natural Population

Core	247.90530 (99.9618% of 248)
Valence	404.25553 (99.5703% of 406)
Natural Minimal Basis	652.16083 (99.7188% of 654)
Natural Rydberg Basis	1.83917 (0.2812% of 654)