Supplementary Material (ESI) for Chemical Communications

SUPPLEMENTARY MATERIAL

Convenient Synthesis and Crystal Structure of a Monomeric Zinc Hydride Complex with a Three-Fold Coordinated Metal Center

Jan Spielmann, Dirk Piesik, Bernd Wittkamp, Georg Jansen and Sjoerd Harder*

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1) Preparations

All experiments were carried out under argon using standard Schlenk-techniques and freshly dried degassed solvents. The following starting materials have been prepared according to literature: (DIPP-nacnac)ZnCl[1] and $NH_2(i\text{Pr})BH_3$[2] (DIPP-nacnac = $CH\{(CMe)(2,6\text{-}i\text{Pr}_2C_6H_3N)\}_2$).

Preparation of KNH(iPr)BH$_3$. A solution of $KN(SiMe_3)_2$ (1.36 g, 6.81 mmol) and $NH_2(i\text{Pr})BH_3$ (0.50 g, 6.85 mmol) in toluene (20 mL) was stirred for one hour. The formed colourless precipitate was separated by centrifugation, washed with 10 mL of hexane, and dried under vacuo. Yield: 0.55 g, 4.95 mmol, 72%. Elemental analysis (%) calcd for $C_3H_{11}BKN$ (M_r = 111.05): C 32.45, H 9.99; found C 32.16, H 9.87. $^1H\{^{11}B\}$ NMR (300 MHz, [THF-d_8], 20 °C): δ = –0.71, (m , 1H, NH), 0.92 (d, $^3J(H,H)$ = 6.0 Hz, 6H, *i*Pr), 1.42 (d, $^3J(H,H)$ = 4.3 Hz, 3H, BH_3), 2.58 (sept, $^3J(H,H)$ = 6.0 Hz, 1H, *i*Pr). ^{11}B NMR (160 MHz, [THF-d_8], 20 °C): δ = –18.9 (q, $^1J(B,H)$ = 82.1 Hz). ^{13}C NMR (75 MHz, [THF-d_8], 20 °C): 26.8 (*i*Pr-Me), 51.5 (*i*Pr-CH).

Preparation of (DIPP-nacnac)ZnH (Method A). A solution of $KNH(i\text{Pr})BH_3$ (139 mg, 1.25 mmol) in 20 mL of THF was added to a solution of (DIPP-nacnac)ZnCl (612 mg, 1.18 mmol) in 20 mL of THF and the solution was stirred for one hour. Then the solvents were removed under vacuo and the residue was extracted with 20 mL of toluene. The insoluble precipitate (KCl) was filtered off and the solution was concentrated to a volume of about 5 mL. Slow cooling to –30 °C gave colourless crystals of (DIPP-nacnac)ZnH. Yield: 406 mg, 0.84 mmol, 71%. Mp. 211 °C. Elemental analysis (%) calcd for $C_{29}H_{42}N_2Zn$ (M_r = 484.05): C 71.96, H 8.75; found C 71.89, H 8.94. ^1H NMR (300 MHz, [benzene-d_6], 20 °C): δ = 1.11 (d, $^3J(H,H)$ = 6.9 Hz, 12H, *i*Pr), 1.27 (d, $^3J(H,H)$ = 6.9 Hz, 12H, *i*Pr), 1.68 (s, 6H, Me backbone), 3.18 (sept, $^3J(H,H)$ = 6.9 Hz, 4H, *i*Pr), 4.39 (s, 1H, ZnH), 5.02 (s, 1H, H backbone), 7.12 (m, 6H, aryl). ^{13}C NMR (75 MHz, [benzene-d_6], 20 °C): 23.2 (*i*Pr-Me), 23.5 (Me backbone), 24.8 (*i*Pr-Me), 28.4 (*i*Pr-CH), 96.0 (backbone), 123.9 (aryl), 126.2 (aryl), 141.8 (aryl), 144.6 (aryl), 168.1 (backbone *C*Me).

Preparation of (DIPP-nacnac)ZnH (Method B). A suspension of CaH_2 (250 mg, 5.94 mmol) and (DIPP-nacnac)ZnCl (439 mg, 0.847 mmol) in 8 mL of THF was stirred for two hours. The mother liquor was separated by centrifugation. Removal of the solvent under vacuo gave pure (DIPP-nacnac)ZnH in quantitative yield. Analyses of the material correponds to the results given above.

2) Crystal structure determination

The crystal has been measured at –150 °C on a Siemens SMART CCD diffractometer. Crystal data are listed in the manuscript. The structure has been solved and refined using the programs SHELXS-97 and SHELXL-97, respectively.[3] Geometry calculations have been performed with PLATON.[4] All hydrogen atoms have been located in the difference Fourier map and could be isotropically refined. Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 724884. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)1223-336-033; E-mail: deposit@ccdc.cam.ac.uk).

3) DFT Calculations

All geometries were fully optimized within the designated symmetry constraints (using tight convergence criteria) at the density functional theory level. The Turbomole V 5.10 program package has been employed throughout [5]. Geometries for all compounds, i.e., the monomeric systems (Mes-nacnac)ZnH and (DIPP-nacnac)ZnH and their respective dimers, have been optimized employing the B97-D functional which includes an empirical correction for dispersion interactions.[6] Use of a method which takes dispersion interactions into account seems mandatory for the case at hand due to the small size of the dimerization energies and the possibility of stabilization of the dimer through CH-π interactions between the ligands. The TZV2P Gaussian type function basis set used in these calculations consists of a triple-zeta valence quality set[7] and the polarization functions of Dunning's cc-pVTZ set[8] for all atoms, discarding the d polarization function for hydrogen and the f polarization functions for the remaining atoms. In the framework of B97-D calculations this basis set is expected to be large enough to allow for the neglect of counterpoise corrections of the basis set superposition error.[6] This level of theory has also been employed to verify that the optimized structures were minima through numerical frequency analyses which make use of analytical gradients in a central differences formula, and to determine atomic charges by Natural Population Analysis (NPA).[9] Note that all computations were carried out in the framework of the efficient "resolution-of-the-identity" (RI) approximation using the appropriate TZVP auxiliary basis set.[10] For pre-optimizations of the investigated structures we have also used smaller basis sets, i.e. SV(P) and TZVP, and the corresponding auxiliary basis sets of the Turbomole basis set library.[11]

Energies and Zero-Point-Energies (Hartree) at various levels of theory

(Mes-nacnac)ZnH (C_{2v})			**[(Mes-nacnac)ZnH]$_2$ (D_2)**	
Level	Energy	ZPE	Energy	ZPE
SV(P)	-2704.075824508	0.4032788	-5408.195288058	0.8107447
TZVP	-2705.330853050	0.4030850*	-5410.696746674	0.8100204
TZV2P	-2705.351742716	0.4040046	-5410.738663814	0.8116307

(DIPP-nacnac)ZnH (C_{2v})			**[(DIPP-nacnac)ZnH]$_2$ (D_2)**	
Level	Energy	ZPE	Energy	ZPE
SV(P)	-3018.115358183	0.6256140	-6036.263783630	1.2606831
TZVP	-3019.727329698	0.6259274	-6039.478908384	1.2613901
TZV2P	-3019.755179731	0.6267459	-6039.535405469	1.2630700

* one imaginary frequency

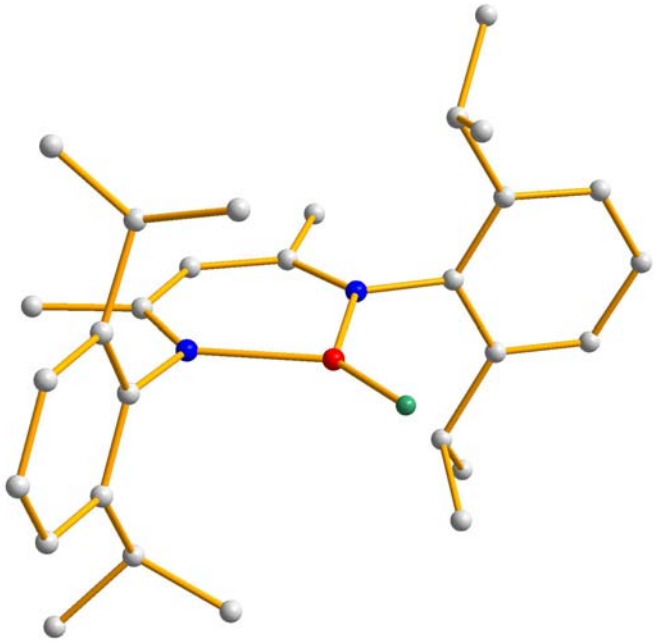
Dimerization energies (kcal/mol) at various levels of theory

2 (Mes-nacnac)ZnH (C_{2v}) →	**[(Mes-nacnac)ZnH]$_2$ (D_2)**		
level	ΔE	ΔZPE	ΔE (incl. ZPE)
SV(P)	-27.38	+2.63	-24.76
TZVP	-21.99	+2.42	-19.57
TZV2P	-22.07	+2.27	-19.80

2 (DIPP-nacnac)ZnH (C_{2v}) →	**[(DIPP-nacnac)ZnH]$_2$ (D_2)**		
level	ΔE	ΔZPE	ΔE (incl. ZPE)
SV(P)	-20.75	+5.93	-14.82
TZVP	-15.22	+5.98	-9.23
TZV2P	-15.72	+6.01	-9.71

XYZ-coordinates (Å) and NPA charges for the B97-D/TZV2P optimized species:

(DIPP-nacnac)ZnH (C_{2v})



Zn	0.0000000	0.0000000	-0.8049586
N	0.0000000	1.4716015	0.5429800
N	0.0000000	-1.4716015	0.5429800
C	0.0000000	2.4787384	2.7790476
C	0.0000000	1.2723646	1.8628527
C	0.0000000	0.0000000	2.4652957
C	0.0000000	-1.2723646	1.8628527
C	0.0000000	-2.4787384	2.7790476
C	0.0000000	2.8096156	0.0327604
C	-1.2302750	3.4433803	-0.2424440
C	-1.2061770	4.7180906	-0.8204115
C	0.0000000	5.3536258	-1.1111177
C	1.2061770	4.7180906	-0.8204115
C	1.2302750	3.4433803	-0.2424440
C	-2.5495629	2.7331984	0.0256243
C	-3.6424231	3.6625008	0.5788983
C	-3.0353474	2.0294855	-1.2575809
C	2.5495629	2.7331984	0.0256243
C	3.6424231	3.6625008	0.5788983
C	3.0353474	2.0294855	-1.2575809
C	0.0000000	-2.8096156	0.0327604
C	1.2302750	-3.4433803	-0.2424440
C	1.2061770	-4.7180906	-0.8204115
C	0.0000000	-5.3536258	-1.1111177
C	-1.2061770	-4.7180906	-0.8204115
C	-1.2302750	-3.4433803	-0.2424440
C	2.5495629	-2.7331984	0.0256243
C	3.0353474	-2.0294855	-1.2575809
C	3.6424231	-3.6625008	0.5788983
C	-2.5495629	-2.7331984	0.0256243
C	-3.6424231	-3.6625008	0.5788983
C	-3.0353474	-2.0294855	-1.2575809
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H	0.8783389	3.1040433	2.5804362
H	0.0000000	2.1782331	3.8294750
H	0.0000000	0.0000000	3.5489304
H	0.0000000	-2.1782331	3.8294750
H	0.8783389	-3.1040433	2.5804362
H	-0.8783389	-3.1040433	2.5804362
H	-2.1430641	5.2193036	-1.0461083
H	0.0000000	6.3433025	-1.5609286
H	2.1430641	5.2193036	-1.0461083
H	-2.3684052	1.9585702	0.7771305
H	-4.5299992	3.0747628	0.8423564
H	-3.9476538	4.4087515	-0.1639791
H	-3.2971341	4.1936954	1.4738298
H	-3.9519534	1.4589110	-1.0621175
H	-2.2741879	1.3447733	-1.6494651
H	-3.2468724	2.7731232	-2.0360280
H	2.3684052	1.9585702	0.7771305
H	4.5299992	3.0747628	0.8423564
H	3.9476538	4.4087515	-0.1639791
H	3.2971341	4.1936954	1.4738298
H	3.2468724	2.7731232	-2.0360280

H	3.9519534	1.4589110	-1.0621175
H	2.2741879	1.3447733	-1.6494651
H	2.1430641	-5.2193036	-1.0461083
H	0.0000000	-6.3433025	-1.5609286
H	-2.1430641	-5.2193036	-1.0461083
H	2.3684052	-1.9585702	0.7771305
H	2.2741879	-1.3447733	-1.6494651
H	3.9519534	-1.4589110	-1.0621175
H	3.2468724	-2.7731232	-2.0360280
H	4.5299992	-3.0747628	0.8423564
H	3.9476538	-4.4087515	-0.1639791
H	3.2971341	-4.1936954	1.4738298
H	-2.3684052	-1.9585702	0.7771305
H	-4.5299992	-3.0747628	0.8423564
H	-3.9476538	-4.4087515	-0.1639791
H	-3.2971341	-4.1936954	1.4738298
H	-2.2741879	-1.3447733	-1.6494651
H	-3.9519534	-1.4589110	-1.0621175
H	-3.2468724	-2.7731232	-2.0360280
H	0.0000000	0.0000000	-2.3525951

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
1	zn	1.35514	17.99761	10.60842	0.03883	28.64486
2	n	-0.73584	1.99935	5.69979	0.03669	7.73584
3	n	-0.73584	1.99935	5.69979	0.03669	7.73584
4	c	-0.65266	1.99937	4.64330	0.00998	6.65266
5	c	0.27787	1.99915	3.70067	0.02231	5.72213
6	c	-0.39093	1.99900	4.37585	0.01608	6.39093
7	c	0.27787	1.99915	3.70067	0.02231	5.72213
8	c	-0.65266	1.99937	4.64330	0.00998	6.65266
9	c	0.12211	1.99880	3.85485	0.02425	5.87789
10	c	-0.01888	1.99894	4.00082	0.01912	6.01888
11	c	-0.21013	1.99908	4.19687	0.01418	6.21013
12	c	-0.20303	1.99919	4.18898	0.01486	6.20303
13	c	-0.21013	1.99908	4.19687	0.01418	6.21013
14	c	-0.01888	1.99894	4.00082	0.01912	6.01888
15	c	-0.23660	1.99936	4.22329	0.01395	6.23660
16	c	-0.58489	1.99944	4.57683	0.00862	6.58489
17	c	-0.58282	1.99942	4.57471	0.00869	6.58282
18	c	-0.23660	1.99936	4.22329	0.01395	6.23660
19	c	-0.58489	1.99944	4.57683	0.00862	6.58489
20	c	-0.58282	1.99942	4.57471	0.00869	6.58282
21	c	0.12211	1.99880	3.85485	0.02425	5.87789
22	c	-0.01888	1.99894	4.00082	0.01912	6.01888
23	c	-0.21013	1.99908	4.19687	0.01418	6.21013
24	c	-0.20303	1.99919	4.18898	0.01486	6.20303
25	c	-0.21013	1.99908	4.19687	0.01418	6.21013
26	c	-0.01888	1.99894	4.00082	0.01912	6.01888
27	c	-0.23660	1.99936	4.22329	0.01395	6.23660
28	c	-0.58282	1.99942	4.57471	0.00869	6.58282
29	c	-0.58489	1.99944	4.57683	0.00862	6.58489
30	c	-0.23660	1.99936	4.22329	0.01395	6.23660
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36	h	0.20734	0.00000	0.79076	0.00190	0.79266
37	h	0.21682	0.00000	0.78201	0.00117	0.78318
38	h	0.22777	0.00000	0.77047	0.00176	0.77223
39	h	0.22777	0.00000	0.77047	0.00176	0.77223
40	h	0.20449	0.00000	0.79353	0.00198	0.79551
41	h	0.20547	0.00000	0.79290	0.00163	0.79453
42	h	0.20449	0.00000	0.79353	0.00198	0.79551
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44	h	0.20470	0.00000	0.79398	0.00132	0.79530
45	h	0.19524	0.00000	0.80314	0.00162	0.80476
46	h	0.20446	0.00000	0.79414	0.00140	0.79554
47	h	0.20005	0.00000	0.79838	0.00157	0.79995
48	h	0.20826	0.00000	0.78962	0.00212	0.79174
49	h	0.20101	0.00000	0.79738	0.00161	0.79899
50	h	0.21000	0.00000	0.78756	0.00244	0.79000
51	h	0.20470	0.00000	0.79398	0.00132	0.79530
52	h	0.19524	0.00000	0.80314	0.00162	0.80476
53	h	0.20446	0.00000	0.79414	0.00140	0.79554
54	h	0.20101	0.00000	0.79738	0.00161	0.79899
55	h	0.20005	0.00000	0.79838	0.00157	0.79995
56	h	0.20826	0.00000	0.78962	0.00212	0.79174
57	h	0.20449	0.00000	0.79353	0.00198	0.79551
58	h	0.20547	0.00000	0.79290	0.00163	0.79453
59	h	0.20449	0.00000	0.79353	0.00198	0.79551
60	h	0.21000	0.00000	0.78756	0.00244	0.79000
61	h	0.20826	0.00000	0.78962	0.00212	0.79174
62	h	0.20005	0.00000	0.79838	0.00157	0.79995
63	h	0.20101	0.00000	0.79738	0.00161	0.79899
64	h	0.20470	0.00000	0.79398	0.00132	0.79530
65	h	0.19524	0.00000	0.80314	0.00162	0.80476
66	h	0.20446	0.00000	0.79414	0.00140	0.79554
67	h	0.21000	0.00000	0.78756	0.00244	0.79000
68	h	0.20470	0.00000	0.79398	0.00132	0.79530
69	h	0.19524	0.00000	0.80314	0.00162	0.80476
70	h	0.20446	0.00000	0.79414	0.00140	0.79554
71	h	0.20826	0.00000	0.78962	0.00212	0.79174
72	h	0.20005	0.00000	0.79838	0.00157	0.79995
73	h	0.20101	0.00000	0.79738	0.00161	0.79899
74	h	-0.52365	0.00000	1.51217	0.01148	1.52365
* Total *		0.00000	79.97333	179.41506	0.61162	260.00000

(Mes-nacnac)ZnH (C_{2v})

Zn	0.0000000	0.0000000	-0.9266443
N	0.0000000	1.4707830	0.4242610
N	0.0000000	-1.4707830	0.4242610
C	0.0000000	2.4796984	2.6608455
C	0.0000000	1.2723664	1.7440227
C	0.0000000	0.0000000	2.3470006
C	0.0000000	-1.2723664	1.7440227
C	0.0000000	-2.4796984	2.6608455
C	0.0000000	2.8042812	-0.0869560
C	-1.2263151	3.4363079	-0.3650518
C	-1.2072817	4.7288161	-0.9019448
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C	1.2263151	3.4363079	-0.3650518
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H	-2.5785016	1.7851881	-0.6740641
C	2.5255946	2.7187429	-0.0975336
H	3.3800450	3.3461197	-0.3707103
H	2.5785016	1.7851881	-0.6740641
C	0.0000000	-2.8042812	-0.0869560
C	1.2263151	-3.4363079	-0.3650518
C	1.2072817	-4.7288161	-0.9019448
C	0.0000000	-5.3774045	-1.1659864
C	-1.2072817	-4.7288161	-0.9019448
C	-1.2263151	-3.4363079	-0.3650518
C	2.5255946	-2.7187429	-0.0975336
H	2.5785016	-1.7851881	-0.6740641
H	3.3800450	-3.3461197	-0.3707103
C	-2.5255946	-2.7187429	-0.0975336
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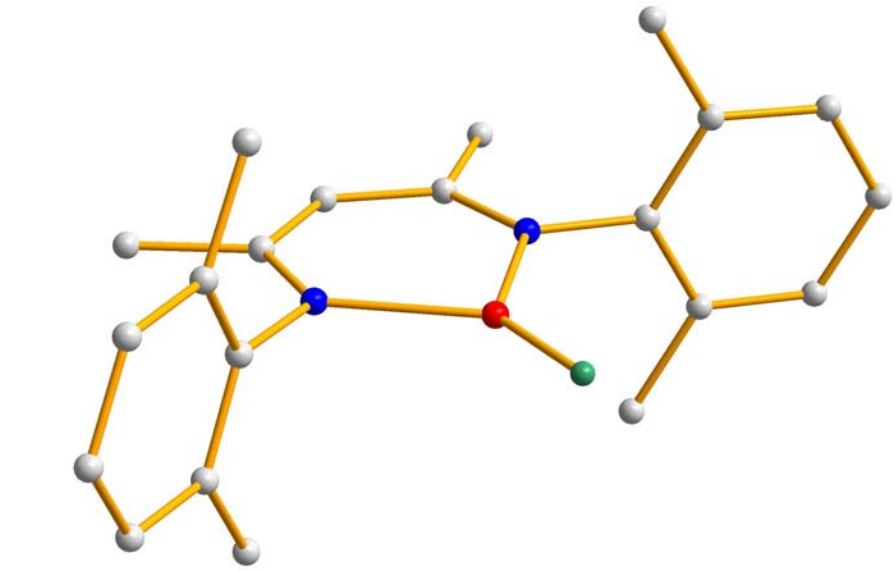
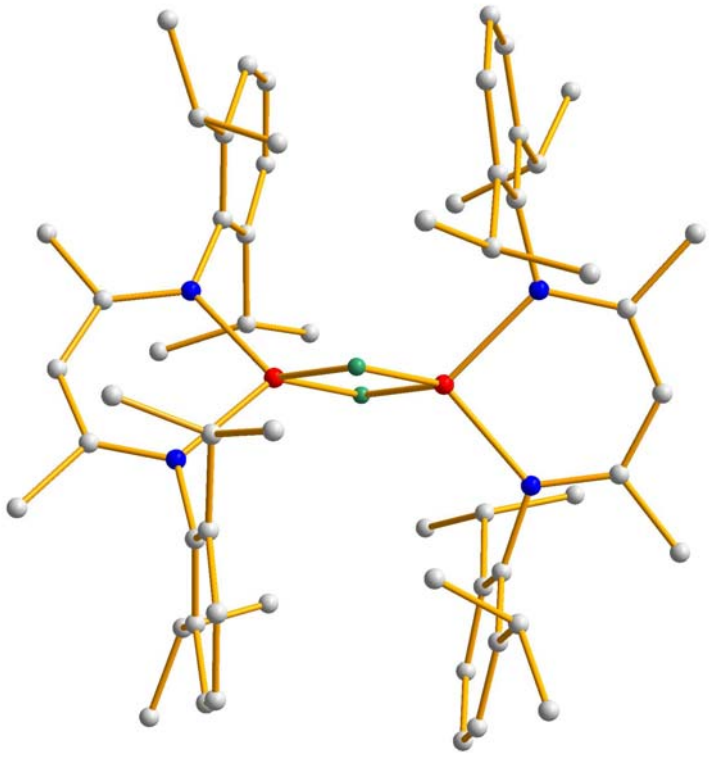


Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
1	zn	1.33854	17.99771	10.62326	0.04049	28.66146
2	n	-0.72728	1.99934	5.68989	0.03805	7.72728
3	n	-0.72728	1.99934	5.68989	0.03805	7.72728
4	c	-0.65233	1.99938	4.64296	0.00999	6.65233
5	c	0.27717	1.99916	3.70175	0.02193	5.72283
6	c	-0.38743	1.99901	4.37261	0.01580	6.38743
7	c	0.27717	1.99916	3.70175	0.02193	5.72283
8	c	-0.65233	1.99938	4.64296	0.00999	6.65233
9	c	0.12513	1.99879	3.85257	0.02352	5.87487
10	c	-0.03151	1.99899	4.01717	0.01535	6.03151
11	c	-0.20373	1.99911	4.19026	0.01436	6.20373
12	c	-0.20591	1.99919	4.19198	0.01474	6.20591
13	c	-0.20373	1.99911	4.19027	0.01436	6.20373
14	c	-0.03151	1.99899	4.01717	0.01535	6.03151
15	c	-0.61381	1.99941	4.60489	0.00952	6.61381
16	h	0.21217	0.00000	0.78654	0.00129	0.78783
17	h	0.21576	0.00000	0.78218	0.00205	0.78424
18	c	-0.61381	1.99941	4.60489	0.00952	6.61381
19	h	0.21217	0.00000	0.78654	0.00129	0.78783
20	h	0.21576	0.00000	0.78218	0.00205	0.78424
21	c	0.12513	1.99879	3.85257	0.02352	5.87487
22	c	-0.03151	1.99899	4.01717	0.01535	6.03151
23	c	-0.20373	1.99911	4.19026	0.01436	6.20373
24	c	-0.20591	1.99919	4.19198	0.01474	6.20591
25	c	-0.20373	1.99911	4.19027	0.01436	6.20373
26	c	-0.03151	1.99899	4.01717	0.01535	6.03151
27	c	-0.61381	1.99941	4.60489	0.00952	6.61381
28	h	0.21576	0.00000	0.78218	0.00205	0.78424
29	h	0.21217	0.00000	0.78654	0.00129	0.78783
30	c	-0.61381	1.99941	4.60489	0.00952	6.61381
31	h	0.21217	0.00000	0.78654	0.00129	0.78783
32	h	0.21576	0.00000	0.78218	0.00205	0.78424
33	h	0.22641	0.00000	0.77192	0.00167	0.77359
34	h	0.22641	0.00000	0.77192	0.00167	0.77359
35	h	0.21690	0.00000	0.78192	0.00118	0.78310
36	h	0.20632	0.00000	0.79179	0.00189	0.79368
37	h	0.21690	0.00000	0.78192	0.00118	0.78310
38	h	0.22641	0.00000	0.77192	0.00167	0.77359
39	h	0.22641	0.00000	0.77192	0.00167	0.77359
40	h	0.20313	0.00000	0.79509	0.00179	0.79687
41	h	0.20708	0.00000	0.79132	0.00159	0.79292
42	h	0.20313	0.00000	0.79509	0.00179	0.79687
43	h	0.21251	0.00000	0.78567	0.00183	0.78749
44	h	0.21251	0.00000	0.78567	0.00183	0.78749
45	h	0.20313	0.00000	0.79509	0.00179	0.79687
46	h	0.20708	0.00000	0.79132	0.00159	0.79292
47	h	0.20313	0.00000	0.79509	0.00179	0.79687
48	h	0.21251	0.00000	0.78567	0.00183	0.78749
49	h	0.21251	0.00000	0.78567	0.00183	0.78749
50	h	-0.52262	0.00000	1.51215	0.01047	1.52262
* Total *		0.00000	63.97846	131.53946	0.48208	196.00000

[(DIPP-nacnac)ZnH]$_2$, (D_2)



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C	2.2622274	-0.9404532	-4.9246115
C	1.1772959	-0.4910478	-3.9571950
C	0.0000000	0.0000000	-4.5459461
C	-1.1772959	0.4910478	-3.9571950
C	-2.2622274	0.9404532	-4.9246115
C	2.6434956	-1.1595808	-2.2498782
C	3.8041106	-0.3543405	-2.2407000
C	5.0337118	-0.9686059	-1.9765582
C	5.1176596	-2.3432770	-1.7582528
C	3.9599465	-3.1176294	-1.7511075
C	2.7019929	-2.5423447	-1.9712488
C	3.7020883	1.1372784	-2.5337175
C	5.0158732	1.7718147	-3.0136048
C	3.1822421	1.8843716	-1.2959540
C	1.4326471	-3.3865856	-1.9396440
C	1.0128862	-3.8659296	-3.3440330
C	1.5356296	-4.5953759	-0.9975618
C	-2.6434956	1.1595808	-2.2498782
C	-3.8041106	0.3543405	-2.2407000
C	-5.0337118	0.9686059	-1.9765582
C	-5.1176596	2.3432770	-1.7582528
C	-3.9599465	3.1176294	-1.7511075
C	-2.7019929	2.5423447	-1.9712488
C	-3.7020883	-1.1372784	-2.5337175
C	-3.1822421	-1.8843716	-1.2959540
C	-5.0158732	-1.7718147	-3.0136048
C	-1.4326471	3.3865856	-1.9396440
C	-1.0128862	3.8659296	-3.3440330
C	-1.5356296	4.5953759	-0.9975618
H	3.1376652	-0.2865735	-4.8469454
H	2.6046795	-1.9518676	-4.6879549
H	1.8958290	-0.9172599	-5.9535619
H	0.0000000	0.0000000	-5.6288421
H	-1.8958290	0.9172599	-5.9535619
H	-3.1376652	0.2865735	-4.8469454
H	-2.6046795	1.9518676	-4.6879549
H	5.9404590	-0.3724753	-1.9658698
H	6.0841445	-2.8073955	-1.5780181
H	4.0361188	-4.1815597	-1.5517074
H	2.9649375	1.2714837	-3.3320513
H	4.8306232	2.8094106	-3.3142915
H	5.7646377	1.7877196	-2.2121266
H	5.4389662	1.2298741	-3.8679804
H	3.0992456	2.9587329	-1.5029038
H	2.1983149	1.5233533	-0.9857746
H	3.8696279	1.7460490	-0.4599087
H	0.6324191	-2.7420902	-1.5582899
H	0.1249119	-4.5063648	-3.2672010
H	1.8188266	-4.4523199	-3.8042342
H	0.7692095	-3.0292192	-4.0026556
H	2.2573457	-5.3334306	-1.3685338
H	0.5614503	-5.0895254	-0.9376196
H	1.8379111	-4.2904928	0.0099169
H	-5.9404590	0.3724753	-1.9658698

H	-6.0841445	2.8073955	-1.5780181
H	-4.0361188	4.1815597	-1.5517074
H	-2.9649375	-1.2714837	-3.3320513
H	-2.1983149	-1.5233533	-0.9857746
H	-3.0992456	-2.9587329	-1.5029038
H	-3.8696279	-1.7460490	-0.4599087
H	-4.8306232	-2.8094106	-3.3142915
H	-5.7646377	-1.7877196	-2.2121266
H	-5.4389662	-1.2298741	-3.8679804
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H	-0.1249119	4.5063648	-3.2672010
H	-1.8188266	4.4523199	-3.8042342
H	-0.7692095	3.0292192	-4.0026556
H	-1.8379111	4.2904928	0.0099169
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N	1.3904617	0.5829305	2.6399414
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C	2.2622274	0.9404532	4.9246115
C	1.1772959	0.4910478	3.9571950
C	0.0000000	0.0000000	4.5459461
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C	-2.2622274	-0.9404532	4.9246115
C	2.6434956	1.1595808	2.2498782
C	2.7019929	2.5423447	1.9712488
C	3.9599465	3.1176294	1.7511075
C	5.1176596	2.3432770	1.7582528
C	5.0337118	0.9686059	1.9765582
C	3.8041106	0.3543405	2.2407000
C	1.4326471	3.3865856	1.9396440
C	1.0128862	3.8659296	3.3440330
C	1.5356296	4.5953759	0.9975618
C	3.7020883	-1.1372784	2.5337175
C	5.0158732	-1.7718147	3.0136048
C	3.1822421	-1.8843716	1.2959540
C	-2.6434956	-1.1595808	2.2498782
C	-2.7019929	-2.5423447	1.9712488
C	-3.9599465	-3.1176294	1.7511075
C	-5.1176596	-2.3432770	1.7582528
C	-5.0337118	-0.9686059	1.9765582
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C	-1.4326471	-3.3865856	1.9396440
C	-1.5356296	-4.5953759	0.9975618
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C	-3.7020883	1.1372784	2.5337175
C	-5.0158732	1.7718147	3.0136048
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H	2.6046795	1.9518676	4.6879549
H	3.1376652	0.2865735	4.8469454
H	1.8958290	0.9172599	5.9535619
H	0.0000000	0.0000000	5.6288421
H	-1.8958290	-0.9172599	5.9535619
H	-2.6046795	-1.9518676	4.6879549
H	-3.1376652	-0.2865735	4.8469454
H	4.0361188	4.1815597	1.5517074
H	6.0841445	2.8073955	1.5780181
H	5.9404590	0.3724753	1.9658698

H	0.6324191	2.7420902	1.5582899
H	0.1249119	4.5063648	3.2672010
H	1.8188266	4.4523199	3.8042342
H	0.7692095	3.0292192	4.0026556
H	0.5614503	5.0895254	0.9376196
H	1.8379111	4.2904928	-0.0099169
H	2.2573457	5.3334306	1.3685338
H	2.9649375	-1.2714837	3.3320513
H	4.8306232	-2.8094106	3.3142915
H	5.7646377	-1.7877196	2.2121266
H	5.4389662	-1.2298741	3.8679804
H	3.8696279	-1.7460490	0.4599087
H	3.0992456	-2.9587329	1.5029038
H	2.1983149	-1.5233533	0.9857746
H	-4.0361188	-4.1815597	1.5517074
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H	-5.9404590	-0.3724753	1.9658698
H	-0.6324191	-2.7420902	1.5582899
H	-1.8379111	-4.2904928	-0.0099169
H	-0.5614503	-5.0895254	0.9376196
H	-2.2573457	-5.3334306	1.3685338
H	-0.1249119	-4.5063648	3.2672010
H	-1.8188266	-4.4523199	3.8042342
H	-0.7692095	-3.0292192	4.0026556
H	-2.9649375	1.2714837	3.3320513
H	-4.8306232	2.8094106	3.3142915
H	-5.7646377	1.7877196	2.2121266
H	-5.4389662	1.2298741	3.8679804
H	-2.1983149	1.5233533	0.9857746
H	-3.0992456	2.9587329	1.5029038
H	-3.8696279	1.7460490	0.4599087
H	0.0000000	1.2469812	0.0000000

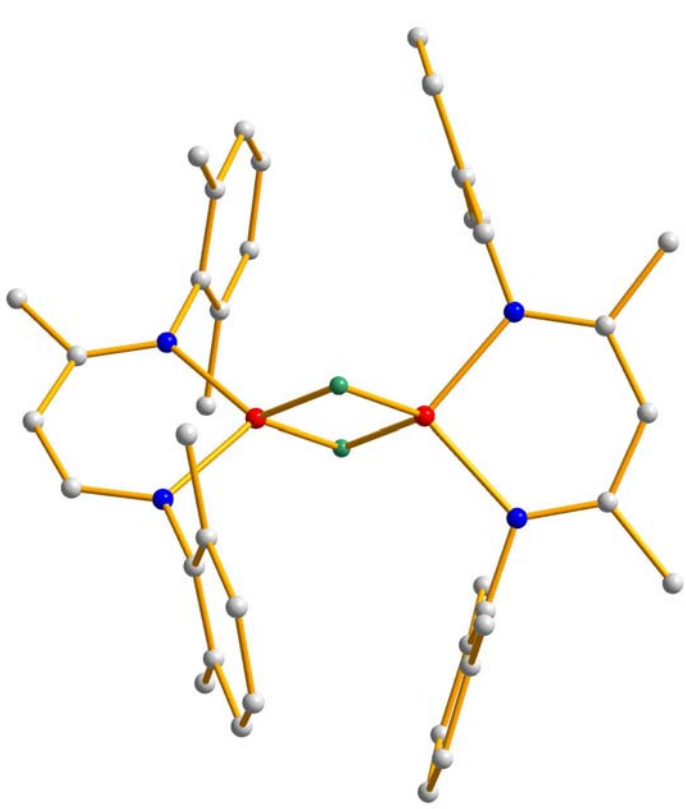
Summary of Natural Population Analysis:

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
1	zn	1.51785	17.99755	10.43232	0.05227	28.48215
2	n	-0.73112	1.99934	5.69717	0.03461	7.73112
3	n	-0.73112	1.99934	5.69717	0.03461	7.73112
4	c	-0.65754	1.99936	4.64798	0.01020	6.65754
5	c	0.27800	1.99913	3.70083	0.02203	5.72200
6	c	-0.40292	1.99898	4.38680	0.01715	6.40292
7	c	0.27800	1.99913	3.70083	0.02203	5.72200
8	c	-0.65754	1.99936	4.64798	0.01020	6.65754
9	c	0.13044	1.99878	3.84660	0.02418	5.86956
10	c	-0.01359	1.99893	3.99566	0.01900	6.01359
11	c	-0.21782	1.99907	4.20420	0.01455	6.21782
12	c	-0.21176	1.99918	4.19710	0.01549	6.21176
13	c	-0.21657	1.99907	4.20290	0.01461	6.21657
14	c	-0.00941	1.99892	3.99013	0.02035	6.00941
15	c	-0.24138	1.99936	4.22764	0.01437	6.24138
16	c	-0.58980	1.99944	4.58161	0.00874	6.58980
17	c	-0.58419	1.99941	4.57503	0.00974	6.58419
18	c	-0.24729	1.99936	4.23191	0.01603	6.24729
19	c	-0.58324	1.99941	4.57522	0.00860	6.58324
20	c	-0.59056	1.99944	4.58223	0.00890	6.59056
21	c	0.13044	1.99878	3.84660	0.02418	5.86956
22	c	-0.01359	1.99893	3.99566	0.01900	6.01359
23	c	-0.21782	1.99907	4.20420	0.01455	6.21782
24	c	-0.21176	1.99918	4.19710	0.01549	6.21176

25	c	-0.21657	1.99907	4.20290	0.01461	6.21657
26	c	-0.00941	1.99892	3.99013	0.02035	6.00941
27	c	-0.24138	1.99936	4.22764	0.01437	6.24138
28	c	-0.58419	1.99941	4.57503	0.00974	6.58419
29	c	-0.58980	1.99944	4.58161	0.00874	6.58980
30	c	-0.24729	1.99936	4.23191	0.01603	6.24729
31	c	-0.58324	1.99941	4.57522	0.00860	6.58324
32	c	-0.59056	1.99944	4.58223	0.00890	6.59056
33	h	0.22659	0.00000	0.77155	0.00187	0.77341
34	h	0.23197	0.00000	0.76624	0.00179	0.76803
35	h	0.21622	0.00000	0.78258	0.00120	0.78378
36	h	0.20665	0.00000	0.79135	0.00200	0.79335
37	h	0.21622	0.00000	0.78258	0.00120	0.78378
38	h	0.22659	0.00000	0.77155	0.00187	0.77341
39	h	0.23197	0.00000	0.76624	0.00179	0.76803
40	h	0.20864	0.00000	0.78944	0.00192	0.79136
41	h	0.20581	0.00000	0.79249	0.00170	0.79419
42	h	0.20756	0.00000	0.79049	0.00196	0.79244
43	h	0.20806	0.00000	0.78925	0.00269	0.79194
44	h	0.20665	0.00000	0.79206	0.00129	0.79335
45	h	0.19728	0.00000	0.80102	0.00170	0.80272
46	h	0.20368	0.00000	0.79489	0.00143	0.79632
47	h	0.19690	0.00000	0.80158	0.00152	0.80310
48	h	0.20037	0.00000	0.79616	0.00348	0.79963
49	h	0.21905	0.00000	0.77842	0.00253	0.78095
50	h	0.21910	0.00000	0.77439	0.00651	0.78090
51	h	0.20175	0.00000	0.79683	0.00142	0.79825
52	h	0.19600	0.00000	0.80238	0.00162	0.80400
53	h	0.21048	0.00000	0.78794	0.00158	0.78952
54	h	0.19288	0.00000	0.80555	0.00157	0.80712
55	h	0.20850	0.00000	0.79008	0.00143	0.79150
56	h	0.20896	0.00000	0.78954	0.00150	0.79104
57	h	0.20864	0.00000	0.78944	0.00192	0.79136
58	h	0.20581	0.00000	0.79249	0.00170	0.79419
59	h	0.20756	0.00000	0.79049	0.00196	0.79244
60	h	0.20806	0.00000	0.78925	0.00269	0.79194
61	h	0.20037	0.00000	0.79616	0.00348	0.79963
62	h	0.19690	0.00000	0.80158	0.00152	0.80310
63	h	0.21905	0.00000	0.77842	0.00253	0.78095
64	h	0.20665	0.00000	0.79206	0.00129	0.79335
65	h	0.19728	0.00000	0.80102	0.00170	0.80272
66	h	0.20368	0.00000	0.79489	0.00143	0.79632
67	h	0.21910	0.00000	0.77439	0.00651	0.78090
68	h	0.20175	0.00000	0.79683	0.00142	0.79825
69	h	0.19600	0.00000	0.80238	0.00162	0.80400
70	h	0.21048	0.00000	0.78794	0.00158	0.78952
71	h	0.20896	0.00000	0.78954	0.00150	0.79104
72	h	0.20850	0.00000	0.79008	0.00143	0.79150
73	h	0.19288	0.00000	0.80555	0.00157	0.80712
74	h	-0.68281	0.00000	1.66603	0.01678	1.68281
75	zn	1.51785	17.99755	10.43232	0.05227	28.48215
76	n	-0.73112	1.99934	5.69717	0.03461	7.73112
77	n	-0.73112	1.99934	5.69717	0.03461	7.73112
78	c	-0.65754	1.99936	4.64798	0.01020	6.65754
79	c	0.27800	1.99913	3.70083	0.02203	5.72200
80	c	-0.40292	1.99898	4.38680	0.01715	6.40292
81	c	0.27800	1.99913	3.70083	0.02203	5.72200
82	c	-0.65754	1.99936	4.64798	0.01020	6.65754
83	c	0.13044	1.99878	3.84660	0.02418	5.86956
84	c	-0.00941	1.99892	3.99013	0.02035	6.00941
85	c	-0.21657	1.99907	4.20290	0.01461	6.21657
86	c	-0.21176	1.99918	4.19710	0.01549	6.21176
87	c	-0.21782	1.99907	4.20420	0.01455	6.21782

88	c	-0.01359	1.99893	3.99566	0.01900	6.01359
89	c	-0.24729	1.99936	4.23191	0.01603	6.24729
90	c	-0.58324	1.99941	4.57522	0.00860	6.58324
91	c	-0.59056	1.99944	4.58223	0.00890	6.59056
92	c	-0.24138	1.99936	4.22764	0.01437	6.24138
93	c	-0.58980	1.99944	4.58161	0.00874	6.58980
94	c	-0.58419	1.99941	4.57503	0.00974	6.58419
95	c	0.13044	1.99878	3.84660	0.02418	5.86956
96	c	-0.00941	1.99892	3.99013	0.02035	6.00941
97	c	-0.21657	1.99907	4.20290	0.01461	6.21657
98	c	-0.21176	1.99918	4.19710	0.01549	6.21176
99	c	-0.21782	1.99907	4.20420	0.01455	6.21782
100	c	-0.01359	1.99893	3.99566	0.01900	6.01359
101	c	-0.24729	1.99936	4.23191	0.01603	6.24729
102	c	-0.59056	1.99944	4.58223	0.00890	6.59056
103	c	-0.58324	1.99941	4.57522	0.00860	6.58324
104	c	-0.24138	1.99936	4.22764	0.01437	6.24138
105	c	-0.58980	1.99944	4.58161	0.00874	6.58980
106	c	-0.58419	1.99941	4.57503	0.00974	6.58419
107	h	0.23197	0.00000	0.76624	0.00179	0.76803
108	h	0.22659	0.00000	0.77155	0.00187	0.77341
109	h	0.21622	0.00000	0.78258	0.00120	0.78378
110	h	0.20665	0.00000	0.79135	0.00200	0.79335
111	h	0.21622	0.00000	0.78258	0.00120	0.78378
112	h	0.23197	0.00000	0.76624	0.00179	0.76803
113	h	0.22659	0.00000	0.77155	0.00187	0.77341
114	h	0.20756	0.00000	0.79049	0.00196	0.79244
115	h	0.20581	0.00000	0.79249	0.00170	0.79419
116	h	0.20864	0.00000	0.78944	0.00192	0.79136
117	h	0.21910	0.00000	0.77439	0.00651	0.78090
118	h	0.20175	0.00000	0.79683	0.00142	0.79825
119	h	0.19600	0.00000	0.80238	0.00162	0.80400
120	h	0.21048	0.00000	0.78794	0.00158	0.78952
121	h	0.20850	0.00000	0.79008	0.00143	0.79150
122	h	0.20896	0.00000	0.78954	0.00150	0.79104
123	h	0.19288	0.00000	0.80555	0.00157	0.80712
124	h	0.20806	0.00000	0.78925	0.00269	0.79194
125	h	0.20665	0.00000	0.79206	0.00129	0.79335
126	h	0.19728	0.00000	0.80102	0.00170	0.80272
127	h	0.20368	0.00000	0.79489	0.00143	0.79632
128	h	0.21905	0.00000	0.77842	0.00253	0.78095
129	h	0.19690	0.00000	0.80158	0.00152	0.80310
130	h	0.20037	0.00000	0.79616	0.00348	0.79963
131	h	0.20756	0.00000	0.79049	0.00196	0.79244
132	h	0.20581	0.00000	0.79249	0.00170	0.79419
133	h	0.20864	0.00000	0.78944	0.00192	0.79136
134	h	0.21910	0.00000	0.77439	0.00651	0.78090
135	h	0.20896	0.00000	0.78954	0.00150	0.79104
136	h	0.20850	0.00000	0.79008	0.00143	0.79150
137	h	0.19288	0.00000	0.80555	0.00157	0.80712
138	h	0.20175	0.00000	0.79683	0.00142	0.79825
139	h	0.19600	0.00000	0.80238	0.00162	0.80400
140	h	0.21048	0.00000	0.78794	0.00158	0.78952
141	h	0.20806	0.00000	0.78925	0.00269	0.79194
142	h	0.20665	0.00000	0.79206	0.00129	0.79335
143	h	0.19728	0.00000	0.80102	0.00170	0.80272
144	h	0.20368	0.00000	0.79489	0.00143	0.79632
145	h	0.20037	0.00000	0.79616	0.00348	0.79963
146	h	0.19690	0.00000	0.80158	0.00152	0.80310
147	h	0.21905	0.00000	0.77842	0.00253	0.78095
148	h	-0.68281	0.00000	1.66603	0.01678	1.68281
* Total *		0.00000	159.94590	358.74929	1.30482	520.00000

[(Mes-nacnac)ZnH]$_2$, (D_2)



Zn	1.2232418	0.0000000	0.0000000
N	2.5430918	1.4071409	0.5051168
C	3.8586123	1.1934642	0.4532849
C	4.4548466	0.0000000	0.0000000
C	4.7912957	2.2981064	0.9132083
C	2.0682155	2.6284055	1.0704713
C	1.8269261	3.7344374	0.2370360
C	1.4113302	4.9343406	0.8249550
C	1.2039140	5.0265355	2.2007736
C	1.4052629	3.9060593	3.0086241
C	1.8424459	2.6954189	2.4598126
C	2.0148492	3.6158436	-1.2533593
C	2.0850241	1.4848990	3.3254482
H	5.5383556	0.0000000	0.0000000
H	4.6015684	3.2177923	0.3481320
H	5.8371131	2.0070841	0.7899037
H	4.6069696	2.5364691	1.9673221
H	1.2398934	5.7967967	0.1869640
H	0.8773688	5.9650514	2.6418773
H	1.2307606	3.9661486	4.0807781
H	1.8142695	4.5707431	-1.7468233
H	1.3274804	2.8674746	-1.6678657
H	3.0316119	3.2886621	-1.5041948
H	1.8090319	1.6896705	4.3650966
H	3.1392332	1.1791701	3.2986180
H	1.4998247	0.6309204	2.9611052
H	0.0000000	0.0000000	-1.2771098
Zn	-1.2232418	0.0000000	0.0000000
N	-2.5430918	-1.4071409	0.5051168
C	-3.8586123	-1.1934642	0.4532849
C	-4.4548466	0.0000000	0.0000000
C	-4.7912957	-2.2981064	0.9132083
C	-2.0682155	-2.6284055	1.0704713
C	-1.8269261	-3.7344374	0.2370360
C	-1.4113302	-4.9343406	0.8249550
C	-1.2039140	-5.0265355	2.2007736
C	-1.4052629	-3.9060593	3.0086241
C	-1.8424459	-2.6954189	2.4598126
C	-2.0148492	-3.6158436	-1.2533593
C	-2.0850241	-1.4848990	3.3254482
H	-5.5383556	0.0000000	0.0000000
H	-4.6015684	-3.2177923	0.3481320
H	-5.8371131	-2.0070841	0.7899037
H	-4.6069696	-2.5364691	1.9673221
H	-1.2398934	-5.7967967	0.1869640
H	-0.8773688	-5.9650514	2.6418773
H	-1.2307606	-3.9661486	4.0807781
H	-1.8142695	-4.5707431	-1.7468233
H	-1.3274804	-2.8674746	-1.6678657
H	-3.0316119	-3.2886621	-1.5041948
H	-1.8090319	-1.6896705	4.3650966
H	-3.1392332	-1.1791701	3.2986180
H	-1.4998247	-0.6309204	2.9611052
N	2.5430918	-1.4071409	-0.5051168
C	3.8586123	-1.1934642	-0.4532849
C	4.7912957	-2.2981064	-0.9132083
C	2.0682155	-2.6284055	-1.0704713

C	1.8269261	-3.7344374	-0.2370360
C	1.4113302	-4.9343406	-0.8249550
C	1.2039140	-5.0265355	-2.2007736
C	1.4052629	-3.9060593	-3.0086241
C	1.8424459	-2.6954189	-2.4598126
C	2.0148492	-3.6158436	1.2533593
C	2.0850241	-1.4848990	-3.3254482
H	4.6015684	-3.2177923	-0.3481320
H	5.8371131	-2.0070841	-0.7899037
H	4.6069696	-2.5364691	-1.9673221
H	1.2398934	-5.7967967	-0.1869640
H	0.8773688	-5.9650514	-2.6418773
H	1.2307606	-3.9661486	-4.0807781
H	1.8142695	-4.5707431	1.7468233
H	1.3274804	-2.8674746	1.6678657
H	3.0316119	-3.2886621	1.5041948
H	1.8090319	-1.6896705	-4.3650966
H	3.1392332	-1.1791701	-3.2986180
H	1.4998247	-0.6309204	-2.9611052
H	0.0000000	0.0000000	1.2771098
N	-2.5430918	1.4071409	-0.5051168
C	-3.8586123	1.1934642	-0.4532849
C	-4.7912957	2.2981064	-0.9132083
C	-2.0682155	2.6284055	-1.0704713
C	-1.8269261	3.7344374	-0.2370360
C	-1.4113302	4.9343406	-0.8249550
C	-1.2039140	5.0265355	-2.2007736
C	-1.4052629	3.9060593	-3.0086241
C	-1.8424459	2.6954189	-2.4598126
C	-2.0148492	3.6158436	1.2533593
C	-2.0850241	1.4848990	-3.3254482
H	-4.6015684	3.2177923	-0.3481320
H	-5.8371131	2.0070841	-0.7899037
H	-4.6069696	2.5364691	-1.9673221
H	-1.2398934	5.7967967	-0.1869640
H	-0.8773688	5.9650514	-2.6418773
H	-1.2307606	3.9661486	-4.0807781
H	-1.8142695	4.5707431	1.7468233
H	-1.3274804	2.8674746	1.6678657
H	-3.0316119	3.2886621	1.5041948
H	-1.8090319	1.6896705	-4.3650966
H	-3.1392332	1.1791701	-3.2986180
H	-1.4998247	0.6309204	-2.9611052

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
1	zn	1.49151	17.99747	10.44998	0.06104	28.50849
2	n	-0.72554	1.99934	5.69056	0.03564	7.72554
3	c	0.27968	1.99915	3.69995	0.02122	5.72032
4	c	-0.39892	1.99901	4.38354	0.01637	6.39892
5	c	-0.65143	1.99938	4.64207	0.00999	6.65143
6	c	0.12309	1.99878	3.85377	0.02436	5.87691
7	c	-0.02641	1.99897	4.01088	0.01656	6.02641
8	c	-0.20302	1.99909	4.18911	0.01482	6.20302
9	c	-0.21352	1.99918	4.19931	0.01503	6.21352
10	c	-0.21016	1.99910	4.19649	0.01457	6.21016

11	c	-0.02932	1.99899	4.01422	0.01611	6.02932
12	c	-0.61873	1.99940	4.60931	0.01002	6.61873
13	c	-0.62053	1.99940	4.61126	0.00988	6.62053
14	h	0.20547	0.00000	0.79258	0.00194	0.79453
15	h	0.22590	0.00000	0.77240	0.00170	0.77410
16	h	0.21599	0.00000	0.78283	0.00118	0.78401
17	h	0.22640	0.00000	0.77188	0.00172	0.77360
18	h	0.20482	0.00000	0.79322	0.00197	0.79518
19	h	0.20496	0.00000	0.79335	0.00169	0.79504
20	h	0.20257	0.00000	0.79558	0.00185	0.79743
21	h	0.21394	0.00000	0.78460	0.00146	0.78606
22	h	0.22693	0.00000	0.77092	0.00214	0.77307
23	h	0.21169	0.00000	0.78654	0.00177	0.78831
24	h	0.20895	0.00000	0.78973	0.00132	0.79105
25	h	0.21182	0.00000	0.78625	0.00193	0.78818
26	h	0.22663	0.00000	0.76990	0.00347	0.77337
27	h	-0.66750	0.00000	1.64956	0.01794	1.66750
28	zn	1.49151	17.99747	10.44998	0.06104	28.50849
29	n	-0.72554	1.99934	5.69056	0.03564	7.72554
30	c	0.27968	1.99915	3.69995	0.02122	5.72032
31	c	-0.39892	1.99901	4.38354	0.01637	6.39892
32	c	-0.65143	1.99938	4.64207	0.00999	6.65143
33	c	0.12309	1.99878	3.85377	0.02436	5.87691
34	c	-0.02641	1.99897	4.01088	0.01656	6.02641
35	c	-0.20302	1.99909	4.18911	0.01482	6.20302
36	c	-0.21352	1.99918	4.19931	0.01503	6.21352
37	c	-0.21016	1.99910	4.19649	0.01457	6.21016
38	c	-0.02932	1.99899	4.01422	0.01611	6.02932
39	c	-0.61873	1.99940	4.60931	0.01002	6.61873
40	c	-0.62053	1.99940	4.61126	0.00988	6.62053
41	h	0.20547	0.00000	0.79258	0.00194	0.79453
42	h	0.22590	0.00000	0.77240	0.00170	0.77410
43	h	0.21599	0.00000	0.78283	0.00118	0.78401
44	h	0.22640	0.00000	0.77188	0.00172	0.77360
45	h	0.20482	0.00000	0.79322	0.00197	0.79518
46	h	0.20496	0.00000	0.79335	0.00169	0.79504
47	h	0.20257	0.00000	0.79558	0.00185	0.79743
48	h	0.21394	0.00000	0.78460	0.00146	0.78606
49	h	0.22693	0.00000	0.77092	0.00214	0.77307
50	h	0.21169	0.00000	0.78654	0.00177	0.78831
51	h	0.20895	0.00000	0.78973	0.00132	0.79105
52	h	0.21182	0.00000	0.78625	0.00193	0.78818
53	h	0.22663	0.00000	0.76990	0.00347	0.77337
54	n	-0.72554	1.99934	5.69056	0.03564	7.72554
55	c	0.27968	1.99915	3.69995	0.02122	5.72032
56	c	-0.65143	1.99938	4.64207	0.00999	6.65143
57	c	0.12309	1.99878	3.85377	0.02436	5.87691
58	c	-0.02641	1.99897	4.01088	0.01656	6.02641
59	c	-0.20302	1.99909	4.18911	0.01482	6.20302
60	c	-0.21352	1.99918	4.19931	0.01503	6.21352
61	c	-0.21016	1.99910	4.19649	0.01457	6.21016
62	c	-0.02932	1.99899	4.01421	0.01611	6.02932
63	c	-0.61873	1.99940	4.60931	0.01002	6.61873
64	c	-0.62053	1.99940	4.61126	0.00988	6.62053
65	h	0.22590	0.00000	0.77240	0.00170	0.77410
66	h	0.21599	0.00000	0.78283	0.00118	0.78401
67	h	0.22640	0.00000	0.77188	0.00172	0.77360
68	h	0.20482	0.00000	0.79322	0.00197	0.79518
69	h	0.20496	0.00000	0.79335	0.00169	0.79504
70	h	0.20257	0.00000	0.79558	0.00185	0.79743
71	h	0.21394	0.00000	0.78460	0.00146	0.78606
72	h	0.22693	0.00000	0.77092	0.00214	0.77307
73	h	0.21169	0.00000	0.78654	0.00177	0.78831

74	h	0.20895	0.00000	0.78973	0.00132	0.79105
75	h	0.21182	0.00000	0.78625	0.00193	0.78818
76	h	0.22663	0.00000	0.76990	0.00347	0.77337
77	h	-0.66750	0.00000	1.64956	0.01794	1.66750
78	n	-0.72554	1.99934	5.69056	0.03564	7.72554
79	c	0.27968	1.99915	3.69995	0.02122	5.72032
80	c	-0.65143	1.99938	4.64207	0.00999	6.65143
81	c	0.12309	1.99878	3.85377	0.02436	5.87691
82	c	-0.02641	1.99897	4.01088	0.01656	6.02641
83	c	-0.20302	1.99909	4.18911	0.01482	6.20302
84	c	-0.21352	1.99918	4.19931	0.01503	6.21352
85	c	-0.21016	1.99910	4.19649	0.01457	6.21016
86	c	-0.02932	1.99899	4.01422	0.01611	6.02932
87	c	-0.61873	1.99940	4.60931	0.01002	6.61873
88	c	-0.62053	1.99940	4.61126	0.00988	6.62053
89	h	0.22590	0.00000	0.77240	0.00170	0.77410
90	h	0.21599	0.00000	0.78283	0.00118	0.78401
91	h	0.22640	0.00000	0.77188	0.00172	0.77360
92	h	0.20482	0.00000	0.79322	0.00197	0.79518
93	h	0.20496	0.00000	0.79335	0.00169	0.79504
94	h	0.20257	0.00000	0.79558	0.00185	0.79743
95	h	0.21394	0.00000	0.78460	0.00146	0.78606
96	h	0.22693	0.00000	0.77092	0.00214	0.77307
97	h	0.21169	0.00000	0.78654	0.00177	0.78831
98	h	0.20895	0.00000	0.78973	0.00132	0.79105
99	h	0.21182	0.00000	0.78625	0.00193	0.78818
100	h	0.22663	0.00000	0.76990	0.00347	0.77337
* Total *		0.00000	127.95609	263.00774	1.03617	392.00000

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[11] The basis sets and auxiliary basis sets are available in the link of the "Downloads" "Quantum Chemistry" area at "www.cosmologic.de"