Synthesis, molecular and electronic structure, and reactions of a Zn–Hg–Zn bonded complex

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SUPPORTING INFORMATION

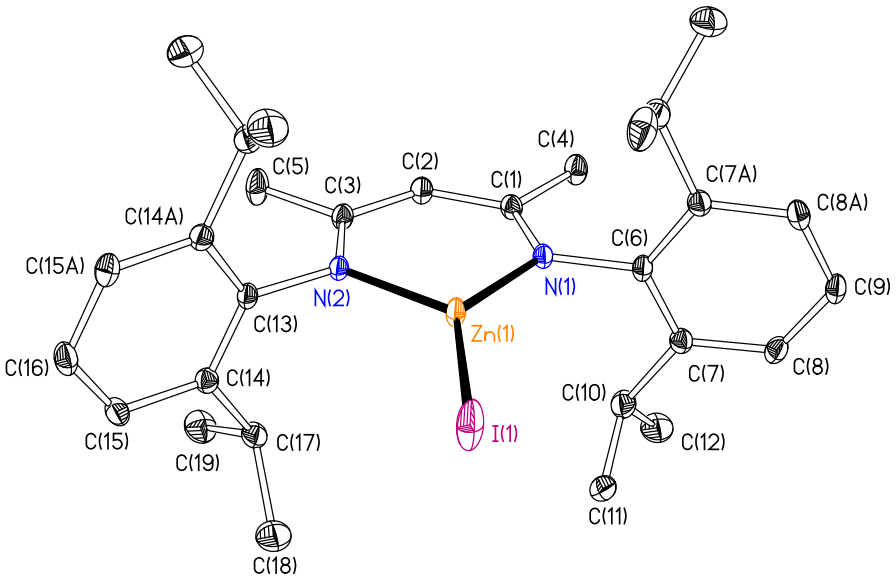
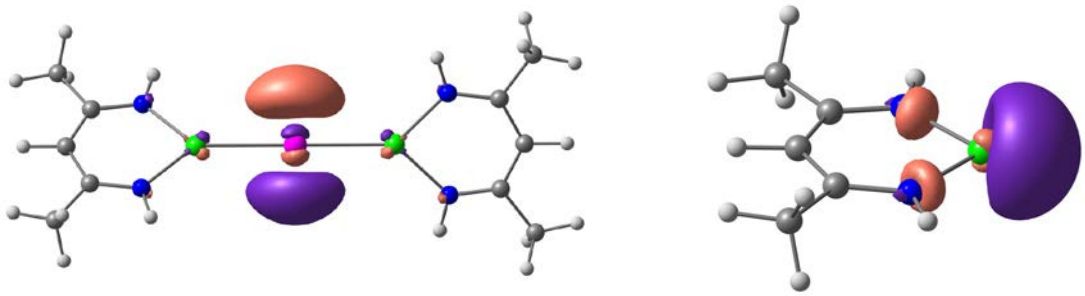


Figure S1. Displacement ellipsoid plot (20% probability) of ($^{Ar'}$NacNac)ZnI (**3**). H atoms omitted for clarity. Atoms carrying the suffix "A" are related to their counterparts by the symmetry operator *x*, y, ½-*z*. Selected distances (Å) and angles (°): Zn(1)-I(1) 2.4528(7), Zn(1)-N(1) 1.917(3), Zn(1)-N(2) 1.927(3), N(1)-Zn(1)-N(2) 101.07(15), N(1)-Zn(1)-I(1) 134.45(11), N(2)-Zn(1)-I(1) 124.48(11).



(a) **(b)**

Figure S2. (a) Isosurface (0.06 au) for LUMO+2 of {(^{H}NacNac)Zn}$_2$Hg (**II**) (-1.25 eV); (b) Isosurface (0.06 au) for the α-SHOMO of (^{H}NacNac)Zn (**III**) (-3.50 eV). Zn, Hg, C and N atoms are shown in green, magenta, grey and blue, respectively.

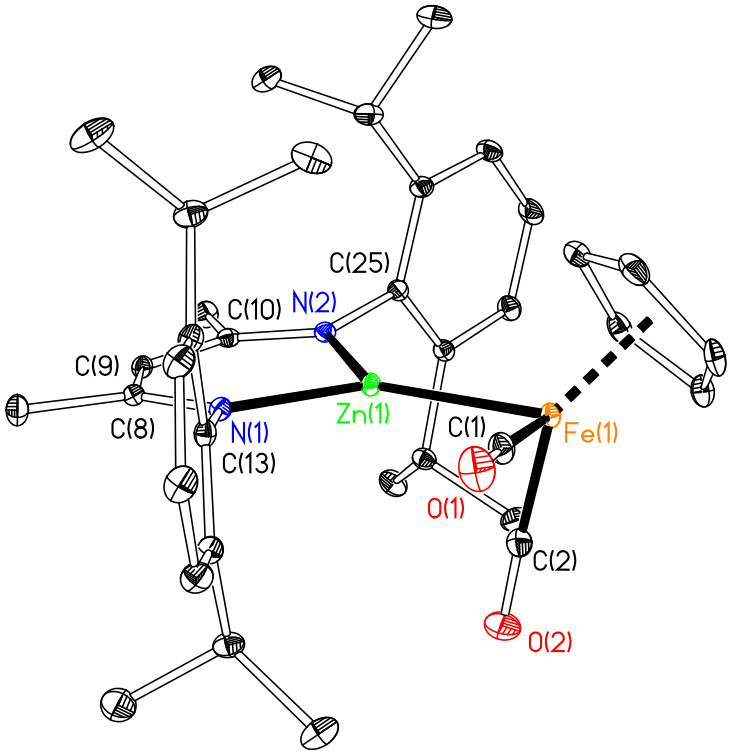


Figure S3. Displacement ellipsoid plot (20% probability) of ($^{Ar'}$NacNac)ZnFp (**4**). H atoms omitted for clarity. Selected distances (Å) and angles (°): Zn(1)-Fe(1) 2.37135(18), Zn(1)-N(1) 1.9807(8), Zn(1)-N(2) 1.9907(8), N(1)-Zn(1)-N(2) 96.40(3), N(1)-Zn(1)-Fe(1) 132.09(2), N(2)-Zn(1)-Fe(1) 131.50(2).

Experimental Details

General methods and instrumentation. All manipulations were carried out using standard Schlenk line or dry-box techniques under an atmosphere of argon or dinitrogen. Solvents were degassed by sparging with dinitrogen and dried by passing through a column of the appropriate drying agent.[1] Toluene and THF were refluxed over sodium and potassium, respectively, and distilled. NMR spectra were recorded in C_6D_6 which was dried over potassium, distilled under reduced pressure and stored under dinitrogen in Teflon valve ampoules. NMR samples were prepared under dinitrogen in 5 mm Wilmad 507-PP tubes fitted with J. Young Teflon valves. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Ascend 400 at ambient temperature and referenced internally to residual protio-solvent (^{1}H) or solvent (^{13}C) resonances and are reported relative to tetramethylsilane (δ = 0 ppm). Assignments were confirmed using two-dimensional ^{1}H-^{1}H and ^{13}C-^{1}H NMR correlation experiments. Chemical shifts are quoted in δ (ppm) and coupling constants in Hz. IR spectra were recorded on a Thermo Scientific Nicolet iS5 FTIR spectrometer. Samples were prepared in a dry-box as Nujol mulls between NaCl plates. The data are quoted in

wavenumbers (cm^{-1}). Elemental analyses were carried out by the Elemental Analysis Service at London Metropolitan University.

Starting materials. H($^{Ar'}$NacNac),[2] FpI[3] and KFp[4] were prepared according to published procedures. All other reagents were purchased from Sigma Aldrich.

($^{Ar'}$NacNac)ZnI (3). To a solution of H($^{Ar'}$NacNac) (3.07 g, 7.32 mmol) in THF (20 mL) was added $KN(SiMe_3)_2$ (1.53 g, 7.69 mmol) in THF (20 mL). The solution was stirred at RT for 2 h then added to a suspension of ZnI_2 (2.34 g, 7.32 mmol) in THF (20 mL). The white suspension was stirred for 16 h at RT. Volatiles were removed under reduced pressure to give an off-white solid, which was extracted with hot toluene (2 x 25 mL) to give a pale yellow solution. Volatiles were removed under reduced pressure to give an off-white solid. The solid was washed with pentane (2 x 5 mL) and dried *in vacuo* to afford **3·0.25(THF)** as a white solid. Yield: 3.14 g (68%). ^{1}H NMR (C_6D_6, 400.1 MHz): δ 7.15-7.08 (6H, m, ArH), 4.98 (1 H, s, NC(Me)C<u>H</u>), 3.59 (1 H, m, OCH_2), 3.11 (4 H, sept, ^3J = 6.9 Hz, C<u>H</u>Me_2), 1.67 (s, 6 H, Me), 1.41 (1 H, m, $OCH_2C\underline{H}_2$), 1.36 (12 H, d, ^3J = 6.9 Hz, CH<u>Me</u>$_2$), 1.13 (12 H, d, ^3J = 6.9 Hz, CH<u>Me</u>$_2$). ^{13}C{^{1}H} NMR (C_6D_6, 100.6 MHz): δ 169.9 (CN), 142.8 (1-C_6H_3), 141.9 (2,6-C_6H_3), 126.9 (4-C_6H_3), 124.2 (3,5-C_6H_3), 96.2 (NC(Me)<u>C</u>H), 68.4 (OCH_2), 28.8 (<u>C</u>HMe_2), 25.8 ($OCH_2\underline{C}H_2$), 24.9 (CH<u>Me</u>$_2$), 23.8 (Me), 23.6 (CH<u>Me</u>$_2$). EI-HRMS: m/z found (calc. for $C_{30}H_{43}IN_2Zn$, $[M]^+$) 608.1606 (608.1602). IR (NaCl plates, Nujol mull, cm^{-1}): 1931 (w), 1865 (w), 1630 (w), 1583 (w), 1555 (w), 1529 (s), 1318 (m), 1268 (m), 1252 (m), 1233 (w), 1178 (s), 1101 (w), 1055 (w), 1031 (m), 967 (w), 934 (w), 869 (w), 797 (s), 775 (w), 636 (w). Anal. Found (calcd. for $C_{30}H_{43}IN_2O_{0.25}Zn$): C, 57.28 (57.38); H, 7.05 (6.90); N, 4.55 (4.46)%.

{($^{Ar'}$NacNac)Zn}$_2$Hg (1). To a stirring potassium amalgam (0.125 g, 3.18 mmol K; 8 mL Hg) was added a suspension of ($^{Ar'}$NacNac)ZnI·0.25(THF) (**3·0.25(THF)**, 0.400 g, 0.637 mmol) in hexanes (20 mL). After 2 h a pale yellow solution had formed above the amalgam with grey precipitate. The mixture was stirred for a further 48 h. The yellow solution was filtered away from the amalgam and the amalgam washed with hexanes (2 x 10 mL). Volatiles were removed from the combined yellow solution under reduced pressure to give a yellow-orange solid. The solid was dried *in vacuo* to afford **1** as a yellow solid. Yield: 283 mg (76%). ^{1}H NMR (C_6D_6, 400.1 MHz): δ 7.15 (t overlapping with solvent, ^3J = 6.4 Hz, ArH), 7.10 (8 H, d, ^3J = 6.4 Hz, 3,5-C_6H_3), 4.87 (2 H, s, NC(Me)C<u>H</u>), 3.10 (8 H, sept, ^3J = 6.9 Hz, C<u>H</u>Me_2), 1.68 (12 H, s, Me), 1.17 (24 H, d, ^3J = 6.9, CH<u>Me</u>$_2$), 1.12 (24 H, d, ^3J = 6.9, CH<u>Me</u>$_2$). ^{13}C{^{1}H} NMR (C_6D_6, 100.6 MHz): δ 166.2 (CN), 145.0 (1-C_6H_3), 141.7 (2,6-C_6H_3), 125.4 (4-C_6H_3), 123.5 (3,5-C_6H_3), 95.3 (NC(Me)<u>C</u>H), 28.7 (<u>C</u>HMe_2), 24.7 (CH<u>Me</u>$_2$), 24.0 (Me), 23.8 (CH<u>Me</u>$_2$). EI-MS: m/z = 1166 (3%) [{($^{Ar'}$NacNac)Zn}$_2$Hg]$^+$, 481 (90%) [($^{Ar'}$NacNac)Zn]$^+$. IR (NaCl plates, Nujol mull, cm^{-1}): 1914 (w), 1865 (w), 1790 (w), 1622 (m), 1557 (s), 1518 (s), 1488 (s, sh), 1455 (s, br), 1403 (s, br), 1321 (s), 1261 (s), 1230 (m), 1174

(m), 1100 (s), 1055 (m), 1024 (s), 961 (w), 935 (m), 902 (w), 855 (m), 842 (m), 793 (s), 758 (s), 748 (s), 702 (w), 631 (w). Anal. Found (calcd. for $C_{58}H_{82}HgN_4Zn$): C, 59.86 (59.71); H, 7.27 (7.08); N, 4.86 (4.80)%.

The ^{199}Hg NMR spectrum (Tol-d_8, 90.0 MHz) for complex **1** at room temperature and -80 ^{o}C gave no detectable signal in the range *ca.* +1000 to -1500 ppm. DFT calculations predicted the chemical shifts (relative to Me_2Hg) to be -855 and -181 ppm for **1** and **1-fixed**, respectively. The calculated enthalpy difference between **1** and **1-fixed** (3.6 kJ mol^{-1}) implies that both species would be present in solution (ratio *ca*. 4:1). The absence of an observable signal is attributable to a rapid dynamic equilibrium between these two isomers in solution which cannot be 'frozen' out.

Reaction of {($^{Ar'}$NacNac)Zn}$_2$Hg (1) with I_2. To a yellow solution of {($^{Ar'}$NacNac)Zn}$_2$Hg (**1**, 0.200 mg, 0.171 mmol) in C_6H_6 (5 mL) was added a purple solution of I_2 (43.5 mg, 0.171 mmol) in C_6H_6 (10 mL), immediately forming a grey precipitate. The mixture was stirred at RT for 1 h to give a colourless solution with grey precipitate. The solution was filtered and the residue further extracted with C_6H_6 (2 x 3 mL). Volatiles were removed from the combined solution under reduced pressure to give a white solid. The solid was dried *in vacuo*. ^{1}H NMR analysis of the solid confirmed the product as ($^{Ar'}$NacNac)ZnI (**3**). Yield: 205 mg (98%).

NMR tube-scale reaction of {($^{Ar'}$NacNac)Zn}$_2$Hg (1) with FpI. To an orange solution of {($^{Ar'}$NacNac)Zn}$_2$Hg (**1**, 15.0 mg, 0.129 μmol) and 2,4-dimethoxybenzene internal standard (3.6 mg, 0.257 μmol) in C_6D_6 (0.2 mL) was added a black solution of FpI (3.9 mg, 0.129 μmol) in C_6D_6 (0.3 mL), forming a yellow solution and grey precipitate. ^{1}H NMR analysis after 5 min showed full conversion to ($^{Ar'}$NacNac)ZnI (**3**) and ($^{Ar'}$NacNac)ZnFp (**4**) in a 1:1 ratio.

Indpendent synthesis of ($^{Ar'}$NacNac)ZnFp (4). To ($^{Ar'}$NacNac)ZnI·0.25(THF) (**3·0.25(THF)**, 0.500 g, 0.796 mmol) and KFp (172 mg, 0.796 mmol) was added THF (20 mL) to give a red-brown suspension. The suspension was stirred for 16 h at RT. Volatiles were removed under reduced pressure to give a brown solid, which was extracted with C_6H_6 (2 x 10 mL) to give a red-brown solution. Volatiles were removed under reduced pressure and the resultant off-white solid (**4**) dried *in vacuo*. Yield: 380 mg (72%). ^{1}H NMR (C_6D_6, 400.1 MHz): δ 7.17-7.10 (m overlapping with solvent, ArH), 5.05 (1 H, s, NC(Me)C<u>H</u>), 3.94 (5 H, s, Cp), 3.34 (4 H, sept, ^3J = 6.9 Hz, C<u>H</u>Me$_2$), 1.72 (6 H, s, Me), 1.34 (12 H, d, ^3J = 6.9 Hz, CH<u>Me</u>$_2$), 1.15 (12 H, d, ^3J = 6.9 Hz, CH<u>Me</u>$_2$). ^{13}C{^{1}H} NMR (C_6D_6, 100.6 MHz): δ 217.8 (CO), 167.7 (CN), 145.9 (1-C_6H_3), 142.3 (2,6-C_6H_3), 126.4 (4-C_6H_3), 124.2 (3,5-C_6H_3), 96.2 (NC(Me)<u>C</u>H), 79.1 (Cp), 28.7 (<u>C</u>HMe$_2$), 24.4 (Me), 24.3 (CH<u>Me</u>$_2$), 24.3 (CH<u>Me</u>$_2$). EI-MS: m/z = 481 (100%) [($^{Ar'}$NacNac)Zn]$^+$. IR (NaCl plates, Nujol mull, cm^{-1}): 1962 (s, ν(CO)), 1895 (s, ν(CO)), 1545 (m), 1526 (s), 1439 (s), 1340 (s), 1316 (m), 1264 (m), 1178 (m), 1100 (w), 1054 (w), 1013 (w), 935 (w), 835 (w), 838 (w), 825 (w), 796 (m), 761 (m), 722 (w),

652 (m), 588 (m). Anal. Found (calcd. for $C_{36}H_{46}FeN_2O_2Zn$): C, 65.42 (65.51); H, 7.16 (7.03); N, 4.20 (4.24)%.

NMR tube-scale reaction of {($^{Ar'}$NacNac)Zn}$_2$Hg (1) with 2 FpI. To an orange solution of {($^{Ar'}$NacNac)Zn}$_2$Hg (**1**, 15.0 mg, 0.129 μmol) and 2,4-dimethoxybenzene internal standard (3.6 mg, 0.257 μmol) in C_6D_6 (0.2 mL) was added a black solution of FpI (7.8 mg, 0.257 μmol) in C_6D_6 (0.3 mL), forming a yellow solution and grey precipitate. ^{1}H NMR analysis after 5 min showed full conversion of {($^{Ar'}$NacNac)Zn}$_2$Hg (**1**) to ($^{Ar'}$NacNac)ZnI (**3**, greater than 90% yield) and less than 10% formation of ($^{Ar'}$NacNac)ZnFp (**4**) relative to the internal standard. The other major product (represented by a singlet at 4.08 ppm) was $HgFp_2$ (singlet at 4.08 ppm confirmed by comparison with an independently-prepared sample in C_6D_6), and this was accompanied by a small amount (less than 3%) of Fp_2. The resonances for Fp_2 grew in intensity over the course of 24 h with concomitant decomposition of $HgFp_2$.

Reaction of {($^{Ar'}$NacNac)Zn}$_2$Hg (1) with Fp$_2$. To a yellow solution of {($^{Ar'}$NacNac)Zn}$_2$Hg (**1**, 0.245 mg, 0.210 mmol) in toluene (10 mL) at -78 °C was added a red-brown solution of Fp_2 (0.372 mg, 0.105 mmol) in toluene (10 mL) at -78 °C to give a red-brown solution. The solution was stirred at -78 °C for 10 min then allowed to warm to RT over 1 h. The solution was stirred at RT for a further 2 h, giving an opaque brown solution. Volatiles were removed under reduced pressure to give a light brown solid, which was extracted with C_6H_6 (2 x 5 mL) to give a dark yellow solution, leaving a grey residue. Volatiles were removed from the solution under reduced pressure and the resultant solid dried *in vacuo* to afford a light brown solid. ^{1}H NMR analysis showed a set of signals consistent with ($^{Ar'}$NacNac)ZnFp (**4**, 42% by integration) accompanied by other unidentified $^{Ar'}$NacNac signals. Further attempts to purify the sample resulted in decomposition.

Computational Details

Gradient corrected density functional theory calculations were carried out using the PBE functional,[5, 6] as implemented in the Gaussian 09 Rev D.01 (G09) quantum chemistry code.[7] The cc-pVDZ basis set of Dunning *et al.* was used for all atoms, except Hg and I. For Hg a relativistic pseudopotential plus (8s7p6d2f)/[6s5p3d2f] valence contraction was employed.[8] For I a relativistic pseudopotential plus (4s5p)/[2s3p] valence contraction was employed.[9] The ultrafine grid was employed and the SCF convergence criterion set to 10^{-6} in all cases. For geometry optimisations, the default convergence criteria were used or decreased maxstep specified where convergence could not otherwise be achieved. All frequency calculations were performed at optimised geometries. For optimisations where the geometry was unconstrained, no imaginary frequencies were observed.

Bond dissociation enthalpies were calculated from frequency calculations in G09 at optimised geometries (SCF total energies modified with zero point energies and thermal corrections to 298.15 K). Molecular orbital contributions were calculated in G09 using Mulliken population analysis. Atoms-in-molecules analyses were performed with the AIMALL program (Version 14.04.17),[10] using wavefunction or formatted checkpoint files from G09 as input. Electron densities, Laplacians and energy densities were all calculated at bond critical points. Partial atomic charges and bond delocalisation indices were also calculated.

References

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DFT (PBE) converged Cartesian coordinates and total energies (H)

{($^{Ar'}$NacNac)Zn}$_2$Hg (1) (-6187.55810430) optimised using maxstep=15

Zn	-2.124816	1.234733	-0.534353
Hg	0.000000	0.000000	0.000000
N	-3.709171	2.388420	-0.250638
N	-2.580882	0.835718	-2.480015
C	-4.634943	2.664904	-1.194708
C	-4.599063	2.165675	-2.517872
C	-3.647416	1.308784	-3.132392
C	-5.791795	3.567938	-0.819143
C	-3.856722	0.920765	-4.580596
C	-3.823789	2.935000	1.070122
C	-4.483997	2.183320	2.080289
C	-4.495067	2.690513	3.392974
C	-3.869319	3.904085	3.706988
C	-3.208556	4.625534	2.704112
C	-3.170071	4.159655	1.376661
C	-5.095768	0.821002	1.766246
C	-4.125378	-0.298056	2.194688
C	-6.487838	0.622455	2.386009
C	-2.377706	4.910687	0.310441
C	-0.875137	4.598562	0.459923
C	-2.638336	6.425127	0.314518
C	-1.608767	-0.031341	-3.069600
C	-0.416912	0.528388	-3.610359
C	0.647165	-0.336283	-3.929630
C	0.551251	-1.718600	-3.726966
C	-0.639321	-2.257999	-3.224588
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C	0.183019	2.422780	-5.198543
C	-2.996000	-2.050475	-2.276209
C	-2.715438	-2.562339	-0.849300
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H	-6.480124	3.720968	-1.669596
H	-6.362111	3.141488	0.031633
H	-5.422639	4.555636	-0.474109
H	-3.928407	-0.182050	-4.678719
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H	-5.206826	0.753931	0.664777
H	-3.982045	-0.294868	3.296060
H	-4.509700	-1.296371	1.898624
H	-3.125137	-0.160703	1.730333
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H	-6.450798	0.599827	3.495078
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H	-0.486766	4.984875	1.426157
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H	-3.719625	6.651963	0.217553
H	-2.275697	6.907591	1.245997
H	1.583882	0.085610	-4.323507
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H	0.799282	3.708582	-2.810043
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Zn	2.124816	-1.234733	0.534353
N	3.709171	-2.388420	0.250638
N	2.580882	-0.835718	2.480015
C	4.634943	-2.664904	1.194708
C	4.599063	-2.165675	2.517872
C	3.647416	-1.308784	3.132392
C	5.791795	-3.567938	0.819143
C	3.856722	-0.920765	4.580596
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C	4.483997	-2.183320	-2.080289
C	4.495067	-2.690513	-3.392974
C	3.869319	-3.904085	-3.706988
C	3.208556	-4.625534	-2.704112
C	3.170071	-4.159655	-1.376661
C	5.095768	-0.821002	-1.766246
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C	-0.551251	1.718600	3.726966
C	0.639321	2.257999	3.224588
C	1.732967	1.437697	2.888322

C	0.255423	-2.037404	3.775173
C	-0.711968	-2.605782	2.719233
C	-0.183019	-2.422780	5.198543
C	2.996000	2.050475	2.276209
C	2.715438	2.562339	0.849300
C	3.583627	3.159367	3.162348
H	5.428435	-2.486088	3.161011
H	6.480124	-3.720968	1.669596
H	6.362111	-3.141488	-0.031633
H	5.422639	-4.555636	0.474109
H	3.928407	0.182050	4.678719
H	2.984492	-1.228158	5.193502
H	4.769970	-1.377529	5.003351
H	4.999179	-2.120567	-4.187582
H	3.890676	-4.285500	-4.738591
H	2.705631	-5.570192	-2.959341
H	5.206826	-0.753931	-0.664777
H	3.982045	0.294868	-3.296060
H	4.509700	1.296371	-1.898624
H	3.125137	0.160703	-1.730333
H	6.922718	0.342817	-2.055476
H	7.184401	-1.432925	-2.089418
H	6.450798	-0.599827	-3.495078
H	2.697059	-4.518291	0.676482
H	0.689782	-3.503062	-0.443024
H	0.286531	-5.061705	0.359273
H	0.486766	-4.984875	-1.426157
H	2.108264	-6.909891	0.530586
H	3.719625	-6.651963	-0.217553
H	2.275697	-6.907591	-1.245997
H	-1.583882	-0.085610	4.323507
H	-1.408856	2.372105	3.943613
H	0.712316	3.344222	3.065165
H	1.247198	-2.499098	3.592612
H	-1.726724	-2.169117	2.825557
H	-0.799282	-3.708582	2.810043
H	-0.356452	-2.373674	1.692973
H	-0.216422	-3.525973	5.311031
H	0.514615	-2.019280	5.960483
H	-1.196102	-2.036069	5.435434
H	3.746814	1.243846	2.194719
H	3.638385	2.970695	0.387342
H	2.342548	1.741276	0.201254
H	1.946208	3.362265	0.848065
H	2.895969	4.026159	3.250617
H	4.535277	3.534790	2.733041
H	3.789504	2.791536	4.188212

{($^{Ar'}$NacNac)Zn}$_2$Hg (1-fixed) (-6187.55629409) optimised using maxstep=15

Zn	-2.495364	-0.484000	-0.480000
Hg	-0.006000	0.060000	-0.805000

N	-3.854058	1.422147	-0.325957
N	-3.853316	-1.423460	0.326259
C	-5.185119	1.250234	-0.267294
C	-5.794263	-0.981000	0.941000
C	-5.184539	-1.251961	0.268822
C	-6.085522	2.445499	-0.498708
C	-6.084326	-2.447503	0.501281
C	-3.262673	2.680929	-0.667844
C	-2.718642	3.498898	0.359850
C	-2.028972	4.669987	-0.008303
C	-1.871325	5.027003	-1.351858
C	-2.386021	4.195786	-2.356316
C	-3.074859	3.010901	-2.040505
C	-2.824046	3.107908	1.831304
C	-1.432379	2.816491	2.425464
C	-3.576217	4.167578	2.655756
C	-3.506750	2.043496	-3.140229
C	-2.322012	1.128429	-3.515440
C	-4.084594	2.739493	-4.381778
C	-3.261257	-2.681876	0.668422
C	-2.717444	-3.500123	-0.359194
C	-2.027152	-4.670792	0.009127
C	-1.868729	-5.027173	1.352756
C	-2.383219	-4.195704	2.357114
C	-3.072616	-3.011177	2.041151
C	-2.823730	-3.109785	-1.830771
C	-1.432492	-2.817730	-2.425631
C	-3.575619	-4.170252	-2.654486
C	-3.504132	-2.043377	3.140668
C	-2.319436	-1.127801	3.514704
C	-4.080977	-2.738950	4.382920
H	-6.891597	-0.001144	0.001380
H	-7.150949	2.186263	-0.362543
H	-5.821640	3.268095	0.197100
H	-5.945971	2.852712	-1.521247
H	-5.943913	-2.854348	1.523856
H	-5.820602	-3.270219	-0.194470
H	-7.149956	-2.188714	0.365789
H	-1.594395	5.307305	0.776485
H	-1.331891	5.947760	-1.619610
H	-2.231932	4.465691	-3.411363
H	-3.411646	2.167590	1.879259
H	-0.779002	3.713055	2.410036
H	-1.517105	2.469119	3.476448
H	-0.913575	2.024947	1.844291
H	-3.688087	3.837471	3.709153
H	-4.589298	4.356030	2.245449
H	-3.033837	5.136167	2.665508
H	-4.301325	1.391431	-2.724014
H	-1.926724	0.595104	-2.623464
H	-2.625180	0.366599	-4.263883
H	-1.484176	1.721173	-3.939331

H	-4.471432	1.987371	-5.099044
H	-4.917504	3.421705	-4.115636
H	-3.319102	3.336050	-4.920221
H	-1.592709	-5.308280	-0.775597
H	-1.328821	-5.947612	1.620641
H	-2.228499	-4.465097	3.412199
H	-3.411957	-2.169835	-1.878827
H	-0.778512	-3.713858	-2.410017
H	-1.517855	-2.470891	-3.476751
H	-0.913989	-2.025561	-1.845009
H	-3.688172	-3.840609	-3.707966
H	-4.588404	-4.359168	-2.243633
H	-3.032643	-5.138515	-2.664127
H	-4.299165	-1.391756	2.724645
H	-2.622395	-0.365634	4.262869
H	-1.924764	-0.594882	2.622233
H	-1.481222	-1.720084	3.938468
H	-3.314958	-3.335012	4.921160
H	-4.467575	-1.986603	5.173000
H	-4.913856	-3.421546	4.117658
Zn	2.495347	0.332000	-0.265000
N	3.853872	-1.422282	-0.326178
N	3.853461	1.423326	0.326051
C	5.185017	-1.250369	-0.268193
C	5.794242	0.810000	-0.088000
C	5.184599	1.251798	0.268047
C	6.085263	-2.445644	-0.500224
C	6.084555	2.447279	0.500100
C	3.262328	-2.680987	-0.668190
C	3.073931	-3.010593	-2.040878
C	2.384950	-4.195404	-2.356696
C	1.870697	-5.026893	-1.352236
C	2.028933	-4.670253	-0.008650
C	2.718758	-3.499264	0.359527
C	3.505339	-2.042911	-3.140550
C	2.320342	-1.127997	-3.515288
C	4.082965	-2.738616	-4.382371
C	2.824735	-3.108587	1.831033
C	1.433328	-2.816491	2.425469
C	3.576499	-4.168782	2.655193
C	3.261604	2.681835	0.668123
C	3.073421	3.011438	2.040827
C	2.384282	4.196109	2.356770
C	1.869601	5.027451	1.352404
C	2.027552	4.670757	0.008803
C	2.717554	3.499906	-0.359483
C	3.505195	2.043826	3.140400
C	2.320585	1.128312	3.514870
C	4.082334	2.739587	4.382410
C	2.823338	3.109290	-1.831014
C	1.431860	2.817779	-2.425571
C	3.575519	4.169295	-2.655038

H	6.891576	0.992000	-0.104000
H	7.150780	-2.186433	-0.364669
H	5.945093	-2.852795	-1.522713
H	5.821763	-3.268278	0.195706
H	5.820658	3.269987	-0.195572
H	5.944543	2.854171	1.522700
H	7.150108	2.188406	0.364233
H	2.230382	-4.465010	-3.411752
H	1.331147	-5.947574	-1.625000
H	1.594704	-5.307792	0.776150
H	4.299920	-1.390785	-2.724430
H	1.482489	-1.720808	-3.939052
H	2.623187	-0.365996	-4.263682
H	1.925217	-0.594882	-2.623115
H	4.469449	-1.986317	-5.099642
H	4.916087	-3.420710	-4.116576
H	3.317427	-3.335246	-4.920668
H	3.412873	-2.168586	1.878991
H	0.914905	-2.024523	1.844527
H	1.518394	-2.469398	3.476518
H	0.779449	-3.712685	2.409900
H	3.688814	-3.838824	3.708594
H	4.589380	-4.357760	2.244608
H	3.033578	-5.137071	2.665017
H	2.229922	4.465740	3.411845
H	1.329931	5.948039	1.620263
H	1.592982	5.308161	-0.775920
H	4.300121	1.392134	2.724305
H	1.482464	1.720671	3.938715
H	2.623712	0.366281	4.263110
H	1.925711	0.595227	2.622587
H	4.469157	1.987350	5.099556
H	4.915107	3.422187	4.116841
H	3.316430	3.335678	4.920778
H	3.411119	2.169077	-1.879059
H	1.516892	2.470708	-3.476638
H	0.913075	2.025968	-1.844728
H	0.778301	3.714215	-2.410051
H	3.032981	5.137800	-2.664660
H	3.687675	3.839476	-3.708500
H	4.588482	4.357806	-2.244458

($^{Ar'}$NacNac)$_2$Zn$_2$ (2) (-6034.00819496) optimised using maxstep=15

Zn	-0.927285	-0.732045	-0.227238
Zn	0.927232	0.732826	-0.225966
N	-1.215656	-2.562220	0.603924
N	-2.591155	-0.856119	-1.385049
N	2.591554	0.859523	-1.382515
N	1.215309	2.560862	0.610081
C	-1.952131	-3.508041	0.452000
C	-2.637933	-3.291934	-1.223894

H	-3.067176	-4.189039	-1.687396
C	-2.990808	-2.068293	-1.834162
C	-2.101957	-4.867265	0.650989
H	-2.545135	-4.753867	1.662043
H	-1.120782	-5.359430	0.801076
H	-2.749483	-5.531940	0.051633
C	-3.868356	-2.139984	-3.070390
H	-4.771417	-1.506822	-2.979512
H	-4.177963	-3.178228	-3.287646
H	-3.304572	-1.749084	-3.943648
C	-0.592550	-2.835403	1.867282
C	0.648618	-3.528130	1.916848
C	1.256647	-3.725890	3.170824
H	2.218967	-4.256814	3.222140
C	0.669265	-3.250531	4.348902
H	1.161430	-3.416443	5.318537
C	-0.540733	-2.549857	4.283533
H	-0.992427	-2.160530	5.207870
C	-1.189464	-2.328376	3.054611
C	1.369376	-3.972862	0.648586
H	0.655002	-3.893298	-0.195385
C	2.530738	-3.007514	0.358032
H	2.164451	-1.964044	0.274436
H	3.045648	-3.261541	-0.589457
H	3.287000	-3.036629	1.176596
C	1.863390	-5.428083	0.705903
H	1.040913	-6.136794	0.933628
H	2.647678	-5.568232	1.478512
H	2.308394	-5.719931	-0.267138
C	-2.469676	-1.502624	3.368000
H	-2.935336	-1.685955	2.010255
C	-3.496651	-1.903580	4.071011
H	-3.731734	-2.986239	4.023381
H	-4.440712	-1.339108	3.927657
H	-3.138603	-1.679646	5.097398
C	-2.125724	-0.003209	3.085353
H	-3.035994	0.624449	3.008158
H	-1.431069	0.303978	2.273609
H	-1.620446	0.239895	4.042616
C	-3.374276	0.285035	-1.764204
C	-2.938424	1.185350	-2.771742
C	-3.775571	2.262170	-3.124948
H	-3.449522	2.957763	-3.913169
C	-5.011198	2.461219	-2.500584
H	-5.657936	3.297936	-2.802974
C	-5.403612	1.603489	-1.465027
H	-6.355757	1.785454	-0.945161
C	-4.596159	0.524273	-1.063442
C	-5.016236	-0.341433	0.124500
H	-4.106316	-0.880725	0.459131
C	-5.519940	0.503860	1.307883
H	-5.664739	-0.138098	2.200830

H	-6.497043	0.983610	1.091257
H	-4.800319	1.303647	1.570421
C	-6.069510	-1.400388	-0.254311
H	-5.687172	-2.117642	-1.004852
H	-6.980908	-0.920533	-0.669787
H	-6.370934	-1.983513	0.640558
C	-1.588246	1.034109	-3.460474
H	-1.128596	0.103198	-3.071440
C	-1.731946	0.896980	-4.986231
H	-2.353917	0.020379	-5.259067
H	-0.739066	0.777931	-5.464516
H	-2.207286	1.794309	-5.433848
C	-0.654585	2.203391	-3.094530
H	-0.509402	2.267438	-1.996145
H	-1.066407	3.176389	-3.434004
H	0.344882	2.078439	-3.559428
C	1.952090	3.508059	0.009356
C	2.638234	3.295002	-1.215388
H	3.067558	4.193281	-1.676561
C	2.991325	2.072914	-1.828572
C	2.102205	4.865458	0.663541
H	2.547570	4.749274	1.673336
H	1.121053	5.356486	0.817201
H	2.748153	5.532345	0.064945
C	3.868959	2.147667	-3.064580
H	4.771055	1.512834	-2.976005
H	4.180069	3.186212	-3.278246
H	3.304389	1.760811	-3.939218
C	3.374710	-0.280785	-1.764222
C	4.596416	-0.521859	-1.063695
C	5.403738	-1.600342	-1.467546
H	6.355653	-1.783780	-0.947776
C	5.011457	-2.455549	-2.505246
H	5.658134	-3.291678	-2.809359
C	3.776119	-2.254742	-3.129570
H	3.450223	-2.948303	-3.919626
C	2.939064	-1.178609	-2.774083
C	1.589205	-1.025392	-3.463023
H	1.129622	-0.095242	-3.072035
C	0.655062	-2.195266	-3.100208
H	0.509376	-2.261860	-2.002044
H	1.066769	-3.167561	-3.441845
H	-0.344158	-2.068941	-3.565233
C	1.733582	-0.884714	-4.988386
H	2.356081	-0.007764	-5.258902
H	0.740950	-0.764074	-5.466785
H	2.208657	-1.781219	-5.437941
C	5.016394	0.341111	0.126228
H	4.106424	0.879585	0.462129
C	6.069513	1.401106	-0.250277
H	5.686947	2.120094	-0.999027
H	6.980874	0.922291	-0.667045

H	6.371045	1.982124	0.645939
C	5.520372	-0.506725	1.307674
H	5.664628	0.133203	2.202164
H	6.497835	-0.985343	1.090061
H	4.801195	-1.307569	1.568206
C	0.591982	2.830650	1.873994
C	-0.649159	3.523330	1.925154
C	-1.257427	3.717787	3.179551
H	-2.219712	4.248672	3.232097
C	-0.670279	3.239279	4.356485
H	-1.162622	3.402659	5.326458
C	0.539672	2.538679	4.289464
H	0.991170	2.146856	5.212837
C	1.188609	2.320407	3.060081
C	-1.369586	3.971670	0.657951
H	-0.655117	3.894014	-0.186104
C	-1.862925	5.426955	0.719050
H	-1.040087	6.134702	0.948420
H	-2.647016	5.565492	1.492149
H	-2.307927	5.721493	-0.253176
C	-2.531319	3.007572	0.364711
H	-2.165454	1.964167	0.278535
H	-3.045900	3.264188	-0.582259
H	-3.280809	3.034950	1.183132
C	2.468728	1.494659	3.003900
H	2.934265	1.679999	2.014091
C	3.495883	1.893340	4.075231
H	3.731259	2.976023	4.029598
H	4.439788	1.328882	3.930792
H	3.137802	1.667595	5.101206
C	2.124677	-0.004900	3.085740
H	3.034887	-0.632453	3.006910
H	1.429787	-0.310221	2.273522
H	1.619699	-0.250103	4.042615

($^{Ar'}$NacNac)ZnI (3) (-3028.48051043)

Zn	0.011794	0.136948	-0.194131
I	-0.049218	0.542966	-2.653916
N	-1.474706	-0.092387	1.049287
N	1.506217	-0.044518	1.044694
C	-1.263855	-0.254211	2.371205
C	0.020458	-0.272881	2.966695
C	1.301231	-0.202119	2.369253
C	-2.460366	-0.432161	3.279319
C	2.505589	-0.328149	3.275959
C	-2.809375	-0.132445	0.514751
C	-3.300985	-1.354412	-0.015819
C	-4.583636	-1.358052	-0.595728
C	-5.353939	-0.191426	-0.659330
C	-2.470950	-2.635846	0.009865
C	-2.141390	-3.115083	-1.416379

C	-3.157156	-3.745847	0.826873
C	2.840256	-0.081798	0.507889
C	3.402016	-1.339822	0.155776
C	4.673617	-1.352266	-0.444912
C	5.370883	-0.162164	-0.691286
C	2.624522	-2.637289	0.369299
C	1.879479	-3.031872	-0.921103
C	3.501050	-3.793599	0.876164
H	0.023995	-0.394552	4.056759
H	-3.081216	-1.287425	2.944716
H	-2.150713	-0.598687	4.326213
H	3.194287	0.528884	3.135581
H	3.091832	-1.235542	3.023896
H	-4.982844	-2.295157	-1.012111
H	-6.352783	-0.214214	-1.119111
H	-1.511000	-2.400498	0.512703
H	-3.061422	-3.393937	-1.971151
H	-1.625539	-2.324635	-1.997712
H	-1.483333	-4.008073	-1.385121
H	-2.515302	-4.649534	0.874053
H	-4.123738	-4.046065	0.371150
H	-3.365264	-3.420035	1.866370
H	5.126512	-2.312518	-0.731156
H	6.363342	-0.193811	-1.164163
H	1.854904	-2.443947	1.144616
H	1.260314	-3.939018	-0.760867
H	1.212189	-2.219600	-1.276724
H	2.596328	-3.241703	-1.742043
H	2.871547	-4.673575	1.119212
H	4.237946	-4.122899	0.114683
H	4.063867	-3.510280	1.788863
C	-3.570868	1.064808	0.448066
C	-4.845158	1.007879	-0.145523
C	-3.010651	2.393573	0.949048
C	-2.540788	3.256927	-0.238423
C	-4.003080	3.162929	1.837222
C	3.530136	1.133515	0.264829
C	4.800605	1.065653	-0.338701
C	2.923503	2.487077	0.623745
C	2.634228	3.318475	-0.640164
C	3.807679	3.267734	1.613355
H	-3.120163	0.458227	3.238152
H	2.206307	-0.382438	4.337650
H	-5.449260	1.924700	-0.212553
H	-2.117005	2.168581	1.566295
H	-3.394106	3.518170	-0.898633
H	-1.796165	2.720826	-0.861414
H	-2.081625	4.202242	0.118377
H	-3.524153	4.073316	2.251744
H	-4.896674	3.494015	1.268614
H	-4.358253	2.544563	2.686944
H	5.351073	1.997093	-0.539085

H	1.953182	2.292066	1.125387
H	2.141234	4.276196	-0.373429
H	1.973192	2.769744	-1.340453
H	3.571136	3.561372	-1.183707
H	3.317556	4.218628	1.906928
H	4.790503	3.524425	1.165969
H	4.004122	2.685031	2.536493

{($^{Ar'}$NacNac)Zn}Hg (I) (-3170.50889834) optimised using maxstep=15

Zn	0.224706	0.522000	-0.036232
Hg	-1.088244	-0.021428	-2.451038
N	1.882369	0.009037	1.082623
N	-1.056687	0.013549	1.511433
C	1.865347	0.019897	2.430815
C	0.683943	0.027091	3.210161
C	-0.670956	0.024307	2.799583
C	3.187630	0.024674	3.169780
C	-1.735180	0.033923	3.876500
C	3.133835	0.002913	0.381688
C	3.716248	-1.239118	0.011015
C	4.900859	-1.218960	-0.748449
C	5.493876	-0.013000	-1.133329
C	4.902607	1.205387	-0.766379
C	3.718047	1.238505	-0.007313
C	3.036377	-2.557382	0.371690
C	2.157008	-3.032449	-0.802251
C	4.020681	-3.654286	0.806256
C	3.040036	2.562886	0.334016
C	2.158684	3.020362	-0.845424
C	4.026106	3.665632	0.749350
C	-2.444085	0.010479	1.154277
C	-3.099991	1.247055	0.906918
C	-4.414944	1.215600	0.406596
C	-5.069244	0.001640	0.162690
C	-4.415108	-1.207787	0.428640
C	-3.100143	-1.230305	0.929392
C	-2.384557	2.576980	1.131581
C	-1.885695	3.157071	-0.205467
C	-3.248875	3.596533	1.892024
C	-2.384630	-2.555954	1.177866
C	-1.883189	-3.158370	-0.148302
C	-3.249746	-3.562930	1.953960
H	0.842440	0.035998	4.295673
H	3.039413	0.033430	4.264502
H	3.793120	-0.863512	2.896043
H	3.794709	0.907346	2.882110
H	-2.394661	-0.853009	3.781969
H	-2.394956	0.918747	3.765767
H	-1.290761	0.043197	4.887943
H	5.367351	-2.168959	-1.047532
H	6.420307	-0.015052	-1.726168

H	5.370512	2.150153	-1.079464
H	2.359714	-2.358121	1.228182
H	2.776258	-3.245417	-1.698653
H	1.598083	-3.953929	-0.537062
H	1.416154	-2.253819	-1.089774
H	3.467805	-4.550143	1.154901
H	4.674875	-3.310279	1.633044
H	4.675316	-3.981925	-0.027812
H	2.364903	2.377693	1.194868
H	1.416542	2.238049	-1.119344
H	1.601087	3.946364	-0.593504
H	2.776298	3.218768	-1.746283
H	3.474649	4.567196	1.085291
H	4.681896	3.333994	1.579915
H	4.679077	3.979820	-0.091163
H	-4.936211	2.161869	0.199127
H	-6.094849	-0.001901	-0.234353
H	-4.936521	-2.157584	0.238398
H	-1.488886	2.370657	1.752557
H	-2.733021	3.362986	-0.892144
H	-1.328926	4.104045	-0.046886
H	-1.206480	2.444310	-0.720430
H	-2.659486	4.507936	2.120296
H	-3.621895	3.179061	2.849404
H	-4.130705	3.917873	1.299885
H	-1.490101	-2.338713	1.796766
H	-1.326340	-4.102301	0.027236
H	-1.203322	-2.454177	-0.674088
H	-2.729219	-3.376181	-0.832899
H	-4.130226	-3.894973	1.365731
H	-2.660202	-4.469907	2.198833
H	-3.624846	-3.129454	2.903378

{(^{H}NacNac)Zn}$_2$Hg (II) (-4322.16957028)

Zn	2.562982	0.150000	-0.234000
Hg	0.001000	0.055000	-0.471000
N	3.949453	-1.209974	-0.770069
N	3.949156	1.210138	0.770235
C	5.278316	-1.067711	-0.679024
C	5.909031	-0.102000	0.717000
C	5.278098	1.067655	0.680031
C	6.156108	-2.111836	-1.342851
C	6.155623	2.111742	1.344313
H	7.006440	-0.210000	0.001082
H	7.233924	-1.901622	-1.211847
H	5.945190	-3.117422	-0.921949
H	5.941990	-2.160753	-2.431235
H	5.940811	2.160807	2.432563
H	5.945102	3.117315	0.923144
H	7.233500	1.901361	1.213998
Zn	-2.562981	-0.090000	-0.292000

N	-3.949553	1.209979	-0.770036
N	-3.949059	-1.210229	0.770114
C	-5.278403	1.067617	-0.678963
C	-5.909040	-0.058000	0.778000
C	-5.278018	-1.067802	0.680010
C	-6.156302	2.111652	-1.342807
C	-6.155428	-2.111883	1.344439
H	-7.006447	-0.006000	0.001199
H	-7.234096	1.901665	-1.211273
H	-5.942633	2.160107	-2.431302
H	-5.945038	3.117368	-0.922387
H	-5.944347	-3.117602	0.923906
H	-5.941064	-2.160280	2.432807
H	-7.233328	-1.901972	1.213563
H	-3.690315	-2.049517	1.304304
H	-3.691129	2.049141	-1.304541
H	3.690963	-2.049098	-1.304584
H	3.690486	2.049428	1.304462

{(^{H}NacNac)Zn}$_2$Hg (II-fixed) (-4322.16255129) optimised using maxstep=5

Zn	-2.168716	1.255861	-0.558056
Hg	0.000000	0.000000	0.000000
N	-3.738621	2.396296	-0.287272
N	-2.612526	0.853677	-2.486054
C	-4.665409	2.674845	-1.220909
C	-4.642160	2.181435	-2.544050
C	-3.678325	1.325871	-3.138769
C	-5.812595	3.582046	-0.818783
C	-3.875455	0.931305	-4.590645
H	-5.470895	2.498700	-3.189899
H	-6.523180	3.755154	-1.648062
H	-6.373310	3.141295	0.032321
H	-5.426168	4.566945	-0.481617
H	-3.952297	-0.172502	-4.682036
H	-3.002278	1.250013	-5.197768
H	-4.785451	1.378953	-5.032011
Zn	2.168716	-1.255861	0.558056
N	3.738621	-2.396296	0.287272
N	2.612526	-0.853677	2.486054
C	4.665409	-2.674845	1.220909
C	4.642160	-2.181435	2.544050
C	3.678325	-1.325871	3.138769
C	5.812595	-3.582046	0.818783
C	3.875455	-0.931305	4.590645
H	5.470895	-2.498700	3.189899
H	6.523180	-3.755154	1.648062
H	6.373310	-3.141295	-0.032321
H	5.426168	-4.566945	0.481617
H	3.952297	0.172502	4.682036
H	3.002278	-1.250013	5.197768
H	4.785451	-1.378953	5.032011

H	-3.943076	2.855527	0.608146
H	-2.025958	0.250345	-3.076382
H	2.025958	-0.250345	3.076382
H	3.943076	-2.855527	-0.608146

(^{H}NacNac)Zn (III) (-2084.26083145) optimised using maxstep=5

Zn	-1.724599	0.038000	0.004000
N	-0.370038	-1.456996	-0.182000
N	-0.369965	1.457017	0.164000
C	0.957177	-1.270537	-0.122000
C	1.579492	-0.033000	-0.010000
C	0.957234	1.270498	0.105000
C	1.844874	-2.500454	0.113000
C	1.844990	2.500367	-0.097000
H	2.676780	-0.054000	-0.008000
H	2.920322	-2.243321	-0.001539
H	1.635976	-3.126709	-0.892476
H	1.638283	-3.124602	0.894729
H	1.638345	3.124615	-0.894628
H	1.636208	3.126543	0.892575
H	2.920423	2.243174	0.001430
H	-0.625415	2.452092	0.218000
H	-0.625534	-2.452061	-0.224000

($^{Ar'}$NacNac)Zn (IV) (-3016.93797292) optimised using maxstep=5

Zn	-0.032000	0.073000	-0.829724
N	-1.497116	0.012000	0.520435
N	1.497133	0.053000	0.520418
C	-1.283083	-0.003000	1.850352
C	0.007000	0.123000	2.447652
C	1.283091	0.183000	1.850300
C	-2.481410	-0.168000	2.777608
C	2.481401	0.416000	2.777581
C	-2.838082	-0.057000	0.013202
C	-3.473512	1.238612	-0.272310
C	-4.756961	1.211954	-0.848911
C	-5.397337	-0.157000	-1.135365
C	-4.756711	-1.212205	-0.849247
C	-3.473274	-1.238756	-0.272634
C	-2.755921	2.561119	-0.014775
C	-2.062700	3.043865	-1.303877
C	-3.672894	3.649998	0.563842
C	-2.755491	-2.561204	-0.015371
C	-2.062634	-3.043870	-1.304695
C	-3.672220	-3.650150	0.563514
C	2.838091	0.019000	0.013205
C	3.473440	-1.238681	-0.272287
C	4.756877	-1.212134	-0.848872
C	5.397351	-0.089000	-1.135350

C	4.756817	1.212014	-0.849265
C	3.473369	1.238671	-0.272658
C	2.755760	-2.561127	-0.014713
C	2.062500	-3.043848	-1.303799
C	3.672650	-3.650067	0.563916
C	2.755677	2.561191	-0.015433
C	2.062831	3.043843	-1.304776
C	3.672491	3.650093	0.563409
H	0.038000	0.165000	3.544667
H	-2.172114	-0.265000	3.838210
H	-3.122693	0.885317	2.590413
H	-3.122585	-0.885686	2.590211
H	3.122466	0.886025	2.590257
H	3.122799	-0.884962	2.590334
H	2.172090	0.412000	3.838172
H	-5.265088	2.159467	-1.080571
H	-6.400759	-0.192000	-1.585910
H	-5.264635	-2.159757	-1.081166
H	-1.958919	2.365621	0.731889
H	-2.808375	3.250085	-2.173000
H	-1.480934	3.971652	-1.122175
H	-1.363748	2.272750	-1.696915
H	-3.080661	4.548929	0.830477
H	-4.196064	3.299389	1.476735
H	-4.445567	3.975164	-0.163487
H	-1.958283	-2.365660	0.731053
H	-1.363836	-2.272703	-1.697897
H	-1.480775	-3.971634	-1.123198
H	-2.808528	-3.250099	-2.100681
H	-3.079869	-4.549080	0.829887
H	-4.195070	-3.299606	1.476610
H	-4.445148	-3.975288	-0.163553
H	5.264927	-2.159682	-1.080505
H	6.400774	-0.133000	-1.585882
H	5.264808	2.159533	-1.081207
H	1.958787	-2.365568	0.731955
H	2.808158	-3.250114	-2.099987
H	1.480690	-3.971603	-1.122094
H	1.363592	-2.272706	-1.696846
H	3.080341	-4.548935	0.830574
H	4.195848	-3.299479	1.476792
H	4.445287	-3.975319	-0.163405
H	1.958461	2.365731	0.731009
H	1.481051	3.971670	-1.123324
H	1.363965	2.272703	-1.697915
H	2.808734	3.249972	-2.100782
H	4.445444	3.975155	-0.163668
H	3.080198	4.549068	0.829757
H	4.195311	3.299530	1.476516

(^{H}NacNac)$_2$Zn$_2$ (V) (-4168.62982683) optimised using maxstep=5

Zn	1.186957	-0.003000	-0.004000
Zn	-1.186957	0.018000	-0.001000
N	2.579977	-1.011958	1.010141
N	2.579967	1.011889	-1.010177
N	-2.579972	1.011901	1.010172
N	-2.579972	-1.011954	-1.010139
C	3.908745	-0.895027	0.893394
C	4.541685	-0.046000	-0.041000
H	5.639135	-0.062000	-0.046000
C	3.908771	0.894962	-0.893452
C	4.784507	-1.771834	1.768796
H	4.570432	-2.844524	1.577876
H	4.571460	-1.581537	2.841807
H	5.862844	-1.598514	1.594753
C	4.784495	1.771934	-1.768730
H	4.570459	1.582841	-2.841758
H	5.862842	1.597662	-1.595680
H	4.571365	2.844603	-1.576587
C	-3.908741	-0.895037	-0.893385
C	-4.541685	-0.063000	0.054000
H	-5.639135	-0.092000	0.068000
C	-3.908775	0.894957	0.893456
C	-4.784499	-1.771843	-1.768793
H	-4.570330	-2.844531	-1.577976
H	-4.571542	-1.581442	-2.841804
H	-5.862836	-1.598616	-1.594661
C	-4.784503	1.771930	1.768728
H	-4.570409	1.582906	2.841757
H	-5.862849	1.597596	1.595736
H	-4.571435	2.844600	1.576518
H	2.319499	1.715736	-1.712785
H	2.319531	-1.715790	1.712743
H	-2.319522	-1.715782	-1.712742
H	-2.319508	1.715755	1.712773

{(^{H}NacNac)Zn}Hg (VI) (-2237.82520438) optimised using maxstep=5

Zn	0.469802	0.010000	-0.068183
Hg	-2.273380	0.001000	0.016131
N	1.820186	-1.450890	-0.025722
N	1.820215	1.450902	-0.025757
C	3.148234	-1.269138	0.013870
C	3.771726	-0.010000	0.032462
C	3.148251	1.269128	0.013857
C	4.031786	-2.501059	0.039874
C	4.031828	2.501026	0.039897
H	4.868477	-0.019000	0.065278
H	5.107235	-2.246817	0.076278
H	3.792876	-3.128240	0.924221
H	3.852270	-3.123165	-0.861964
H	3.793026	3.128105	0.924344
H	3.852227	3.123244	-0.861844

H	5.107275	2.246762	0.076155
H	1.564583	-2.445999	-0.033428
H	1.564630	2.446010	-0.033490

FpI (-1694.83692976)

C	0.483122	1.345754	-1.286513
I	-1.867395	-0.318672	0.214000
Fe	0.754319	0.168271	-0.135000
O	0.359814	2.118821	2.148560
O	0.358204	2.118640	-2.148708
C	2.633739	-0.368031	0.715756
C	0.484015	1.345969	1.286213
C	2.633633	-0.368167	-0.716197
C	1.088785	-1.940732	-0.037000
C	1.671362	-1.347481	-1.162826
C	1.671498	-1.347401	1.162588
H	3.252837	0.268701	-1.357767
H	1.415484	-1.580855	-2.201459
H	0.281631	-2.680224	0.143000
H	1.415572	-1.580872	2.201148
H	3.253051	0.268667	1.357370

Hg (-153.550010010)

Hg	0.000000	0.000000	0.000000

HgI_2 (-176.463352027)

Hg	0.000000	0.000000	0.000000
I	0.000000	0.000000	2.633683
I	0.000000	0.000000	-2.633683

It was not possible to perform a successful frequency calculation for $HgFp_2$ with empericaldispersion=gd3 due limitations of the G09 software. The sum of the electronic and thermal enthalpies for $HgFp_2$ was calculated by taking the total SCF energy (-3520.33247326 au) for the geometry optimised structure of $HgFp_2$ with dispersion correction and adding the thermal correction to the enthalpies (0.222189 au) obtained from a single point frequency calculation at the same geometry without dispersion correction.

$HgFp_2$ using dispersion correction (-3520.33247326) optimised using maxstep=5
$HgFp_2$ without dispersion correction (-3520.30519323) non-optimised geometry

Hg	0.000000	0.000000	-0.015200
Fe	0.000000	2.574162	0.580000
O	1.998515	2.425857	-2.129526
O	1.998353	2.425626	2.129777
C	1.197900	2.457315	-1.271289
C	1.197791	2.457164	1.271478

C	-1.011729	4.270953	0.713184
H	-0.565532	5.033829	1.359881
C	-1.692500	3.076335	1.158116
H	-1.852995	2.777728	2.199313
C	-2.124899	2.351922	-0.560000
H	-2.704010	1.422286	-0.014400
C	-1.691899	3.076486	-1.158093
H	-1.852794	2.778015	-2.199341
C	-1.011659	4.271044	-0.712947
H	-0.565403	5.034300	-1.359503
Fe	0.000000	-2.574162	0.580000
O	-1.998515	-2.425857	-2.129526
O	-1.998353	-2.425626	2.129777
C	-1.197900	-2.457315	-1.271289
C	-1.197791	-2.457164	1.271478
C	1.011729	-4.270953	0.713184
H	0.565532	-5.033829	1.359881
C	1.692500	-3.076335	1.158116
H	1.852995	-2.777728	2.199313
C	2.124899	-2.351922	-0.560000
H	2.704010	-1.422286	-0.014400
C	1.691899	-3.076486	-1.158093
H	1.852794	-2.778015	-2.199341
C	1.011659	-4.271044	-0.712947
H	0.565403	-5.034300	-1.359503