Carbodiimides as Catalysts for the Reduction of a Cadmium Hydride Complex

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General. All manipulations were carried out under dry nitrogen using standard Schlenk-line and cannula techniques, or in an inert atmosphere glovebox. Solvents were dried using a PureSolv system (Innovative Technologies) and stored over 4 Å sieves. All other reagents were either distilled prior to use and stored over 4 Å sieves or used as received. Celite 545 (ROTH) was used as the "celite" filtering agent The ^{1}H and ^{13}C spectra were recorded in either C_6D_6 at 298 K, using a Varian INOVA system at 300 MHz (^{1}H) or 75 MHz (^{13}C). Proton and carbon chemical shifts were referenced internally to residual solvent resonances. The ^{113}Cd spectra was obtained on a 400MHz JNM-ECZ400S NMR using a Royal probe. Repeated combustion analysis on compounds **1** and **2** were unsuccessful.

[CH{(CH$_3$)CN-2,6-*i*Pr$_2$C$_6$H$_3$}$_2$CdH], [(BDI)CdH] (1). 238 μL of LiHBEt$_3$ in THF (0.0252 g, 0.238 mmol) was added drop-wise to a slurry of [(BDI)CdCl] (0.150 g, 0.265 mmol) in 4 mL of toluene at -30 °C. The mixture was allowed to stir for 1 minute where it was filtered through celite to remove black precipitate and the volatiles were removed in *vacuo*. Solid was re-dissolved and crystalized from hexane or diethyl ether to give [(BDI)CdH] as small colourless cubic crystals (0.0944 g, 74.6%). The product was stable at room temperature but decomposed above 126 °C. ^{1}H NMR (299.74 MHz, C$_6$D$_6$, 298 K): δ 7.11 (s, 6H, Ar*H*), 5.63 (br, 1H, Cd*H*), 4.91 (s, 1H, γ-C*H*), 3.29 (septet, J = 6.7 Hz, 4H, C*H*Me$_2$), 1.70 (s, 6H, NC*Me*), 1.23 (d, J = 6.8 Hz, 12H, CH*Me*$_2$), 1.16 (d, J = 6.7 Hz, 12H, CH*Me*$_2$). ^{13}C{^{1}H} NMR (150.76 MHz, C$_6$D$_6$, 298 K): δ 168.14 (N*C*Me), 146.42 (*ipso*-*C*), 141.10 (*o*-*C*), 125.76 (*p*-*C*), 124.00 (*m*-*C*), 94.71 (γ-*C*), 28.21 (*C*HMe$_2$), 24.79 (CH*Me*$_2$), 24.10 (CH*Me*$_2$), 23.30 (NC*Me*). ^{113}Cd{^{1}H} NMR (C$_6$D$_6$): δ 650 (unable to observe Cd-H coupling). IR (Nujol): ν(Cd-H) 1734 cm^{-1}.

[CH{(CH$_3$)CN-2,6-*i*Pr$_2$C$_6$H$_3$}$_2$Cd]$_2$, [(BDI)Cd]$_2$ (2). A hexane solution (5 mL) of dicyclohexylcarbodiimide (0.019 g, 0.094 mmol) in hexane (5 mL) was added to a hexane solution (5 mL) of **1** (0.050 g, 0.094 mmol). The colourless reaction was stirred for 16 hours. Volatiles were removed *in vacuo* from the colourless and transparent solution. The resulting residue was re-dissolved into hexane (2 mL) and kept at -30 °C. Colourless cubic crystals suitable for X-ray diffraction were grown within 24 hours (0.078 g, 78%). ^{1}H NMR (299.74 MHz, C$_6$D$_6$, 298 K): δ 7.04 (s, 6H, Ar*H*), 4.78 (s, 1H, γ-C*H*), 3.12 (septet, J = 6.9 Hz, 4H, C*H*Me$_2$), 1.57 (s, 6H, NC*Me*), 1.16 (d, J = 6.7 Hz, 12H, CH*Me*$_2$), 0.92 (d, J = 7.0 Hz, 12H, CH*Me*$_2$). ^{13}C{^{1}H} NMR (150.76 MHz, C$_6$D$_6$, 298 K): δ 166.74 (N*C*Me), 147.79 (*ipso*-*C*), 141.06 (*o*-*C*), 125.02 (*p*-*C*), 123.88 (*m*-*C*), 95.04 (γ-*C*), 28.24 (*C*HMe$_2$), 24.94 (CH*Me*$_2$), 24.63 (CH*Me*$_2$), 23.06 (N*C*Me). A ^{113}Cd NMR signal was not observed.

Crystal-Structure Data. Crystals were mounted on an Agilent SuperNova diffractometer fitted with an Atlas detector. Data was collected at 120.01(10) K using Mo-Kα radiation at 0.71073 A. The structures were refined with SHELXL-97.

Table S1. Data Collection Parameters for **1** and **2**

	[(BDI)CdH] (**1**)	$[(BDI)Cd]_2$
Empirical formula	$C_{29}H_{42}CdN_2$	$C_{58}H_{82}Cd_2N_4$
Formula weight	531.04	1060.07
Crystal system	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/c$
a/Å	12.5364(4)	14.4118(4)
b/Å	15.9813(3)	14.2417(4)
c/Å	14.0907(4)	26.8111(8)
α/°	90	90
β/°	105.609(3)	94.817(3)
γ/°	90	90
Volume/Å^3	2718.94(12)	5483.5(3)
Z	4	4
ρ_{calc}g/cm^3	1.297	1.284
μ/mm^{-1}	0.821	0.814
F(000)	1112.0	2216.0
Crystal size/mm^3	0.23 × 0.2 × 0.04	0.23 × 0.2 × 0.04
2Θ range for data collection/°	5.688 to 70.548	5.396 to 54.998
Reflections collected	35828	60496
Independent reflections	11367 [R_{int} = 0.0347, R_{sigma} = 0.0389]	12588 [R_{int} = 0.0470, R_{sigma} = 0.0364]
Data/restraints/parameters	11367/0/303	12588/0/597
Goodness-of-fit on F^2	1.079	1.117
Final R indexes [I>=2σ (I)]	R_1 = 0.0330, wR_2 = 0.0772	R_1 = 0.0352, wR_2 = 0.0746
Final R indexes [all data]	R_1 = 0.0489, wR_2 = 0.0874	R_1 = 0.0471, wR_2 = 0.0812
Largest diff. peak/hole/e Å^{-3}	1.17/-0.81	0.89/-0.71

Figure S1. ORTEP diagram of **1**. Ellipsoids shown at 30%.

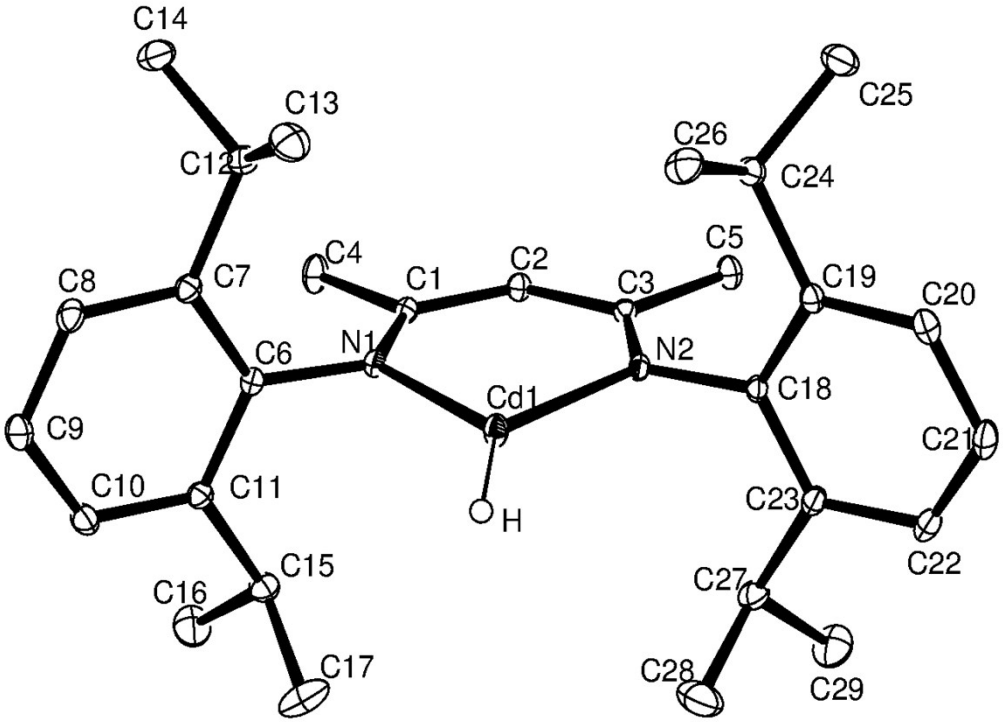
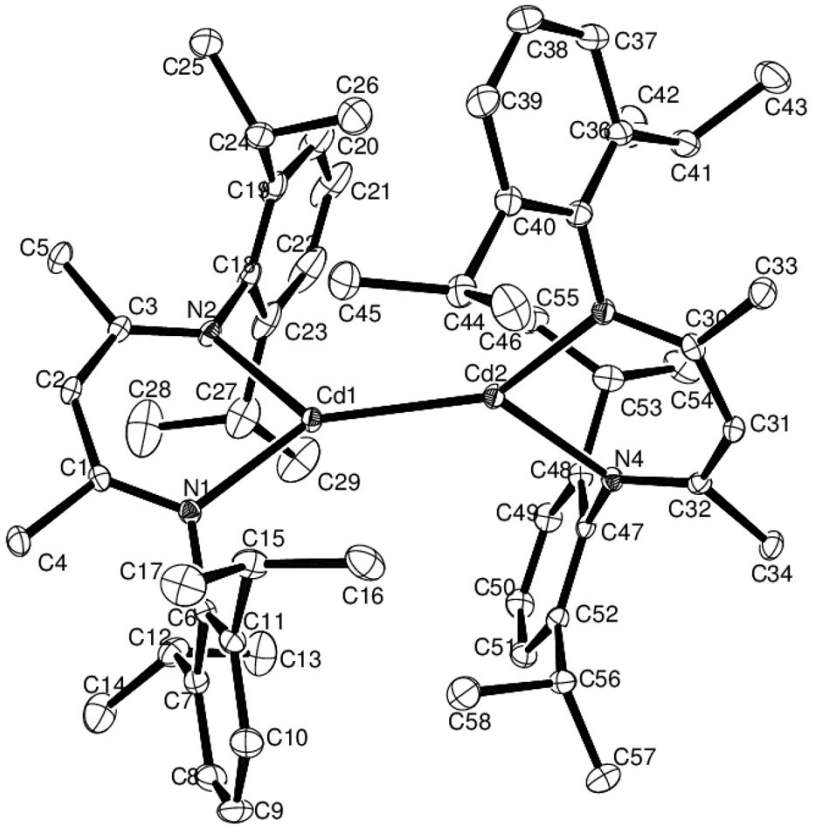


Figure S2. ORTEP diagram of **2**. Ellipsoids shown at 30%.



Computational Methods

All structural optimisations were carried out with the Gaussian 09 suite of programs (Revision D.01)[2] using the density functional method (DFT). with the the PBE0 hybrid functional[3] and the balanced, polarised def2-TZVP basis-set[4] of triple-ζ quality. Grimme's empirical dispersion correction[5] (D3) with Becke-Johnston damping[6] (BJ) was applied. We refer to the resulting computational model as PBE0-D3(BJ)/def2-TZVP. Frequency calculations at the same level of theory were employed to ensure that the obtained structures are minima on the potential energy surface.

The bonding was analysed using the Natural Bond Orbital (NBO) approach[7-13] using the NBO 6.0 program[14, 15] and Wiberg Bond Indices (WBI) were computed[16].

Natural Bond Orbitals (NBOs)[7-13] are orbitals that have been localised to one or two (or, in the case of multiple center bonds or strong delocalisation, more) nuclei with the additional condition to maximise the density (i.e. the occupation) of these orbitals. Hence, NBOs are the molecular orbital analogue of finding the Lewis structure, *i.e.* assigning electron pairs to atoms (as either "core electrons" or "lone pairs") and bonds in optimally compact form.

Table S2: Wiberg Bond Indices for the Cd-H and Zn-H bonds as well as for the Cd-Cd and Zn-Zn bonds in the investigated complexes of different symmetry. The lowest energy structures are indicated in bold.

Bond	Symmetry	Bond Length (Å)	WBI
Cd-H	**C_{2v}**	**1.675**	**0.6570**
Zn-H	**C_{2v}**	**1.551**	**0.6108**
Cd-Cd	**D_2**	**2.675**	**0.6856**
Cd-Cd	D_{2d}	2.681	0.7056
Cd-Cd	D_{2h}	2.772	0.7018
Zn-Zn	**D_{2d}**	**2.525**	**0.7100**
Zn-Zn	D_{2h}	2.666	0.7084

Table S3. Reaction energies for the formation of Cd-Cd and Zn-Zn from Cd-H and Zn-H in a reaction: 2 M-H → H_2 + M-M. All energies in kJ mol^{-1}

	ΔE_{0K}	ΔH
Cd-Cd	−142.33	−138.27
Zn-Zn	−14.50	−18.19

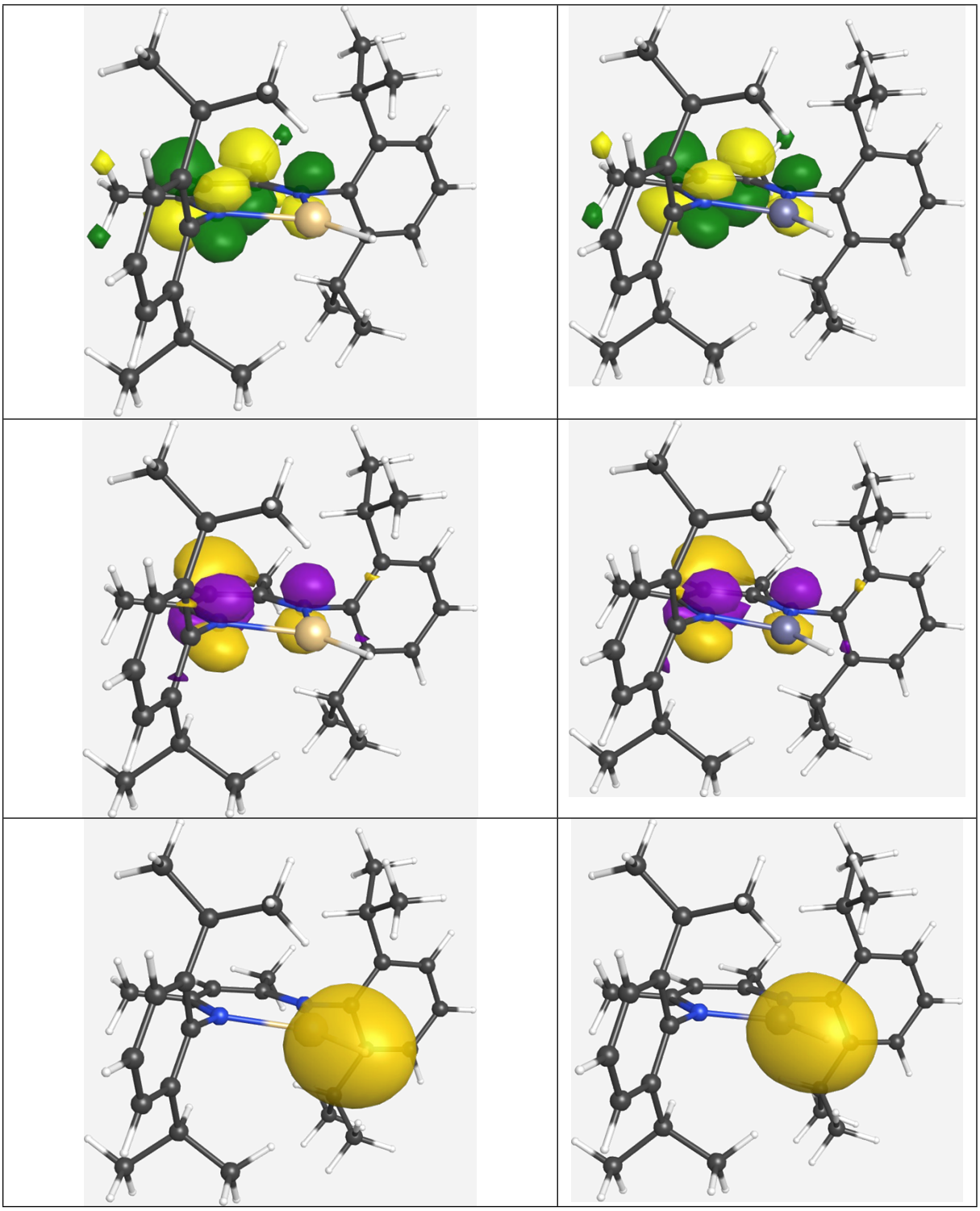


Figure S3. Plots of the Canonical LUMO (top), HOMO (middle) and the Natural Bonding Orbital that describes the M-H bond (bottom) for [(BDI)CdH] (**1**, left) and [(BDI)ZnH] (right).

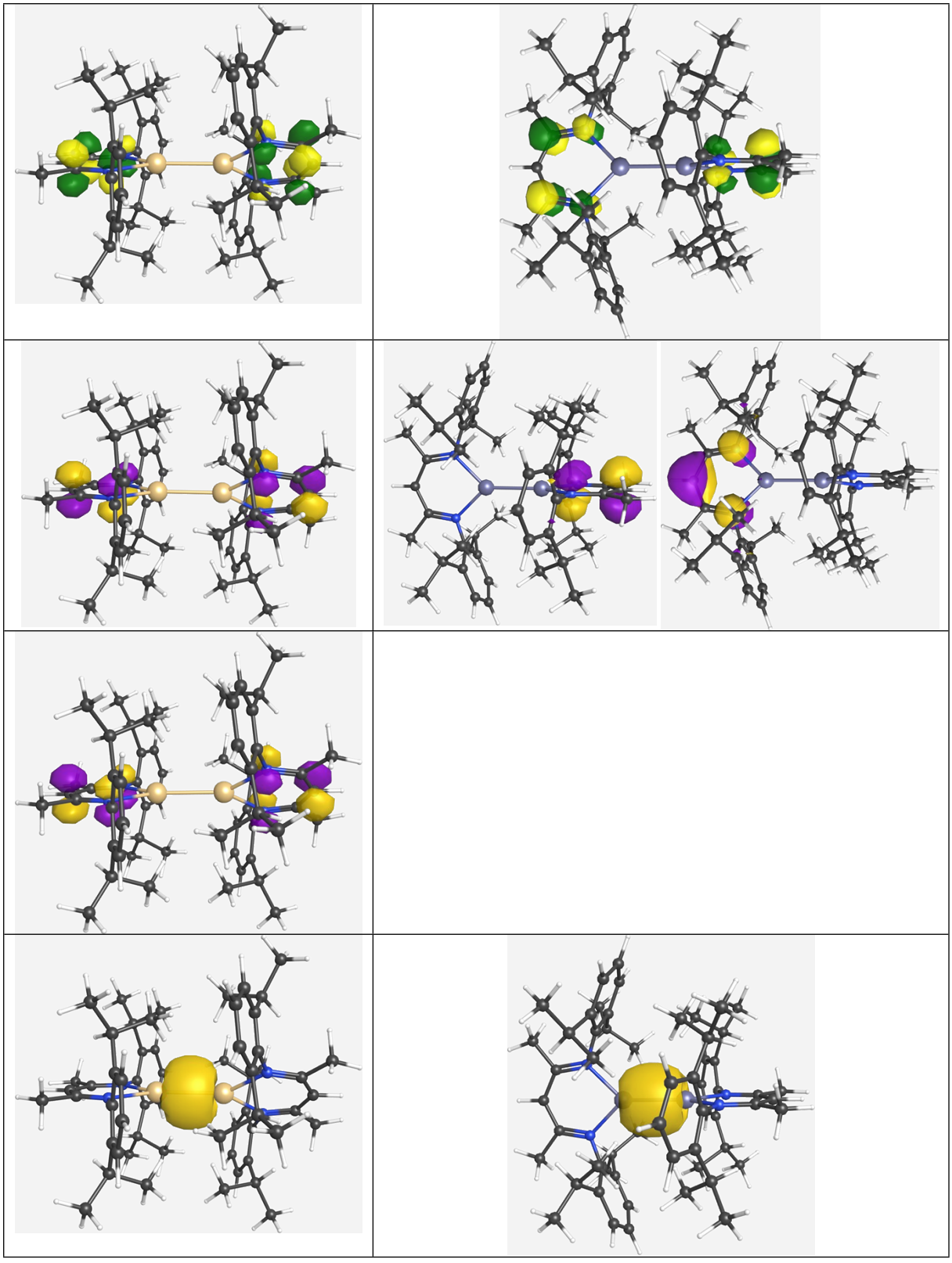


Figure S2 Plots of the Canonical LUMO (top), HOMO (second from the top, note that the LUMO of $[(BDI)Zn]_2$ compound is doubly degenerate), the HOMO-1 of the **2** compound (second from the bottom, left column) and the Natural Bonding Orbital that describes the metal-metal bond (bottom) for $[(BDI)Cd]_2$ (**2**, left) and $[(BDI)Zn]_2$ (right).

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Cartesian Coordinates

[(BDI)CdH] (**1**) (C_{2v})

C	-3.120337	-2.250978	1.216110
H	-3.356305	-3.071091	1.899640
H	-4.039047	-1.688416	1.029498
H	-2.416405	-1.592816	1.732115
C	-2.536559	-2.788928	-0.088846
C	-1.220525	-3.487604	0.168856
C	0.000000	-2.850449	-0.102169
N	0.000000	-1.513740	-0.576087
Cd	0.000000	0.000000	1.003255
N	0.000000	1.513740	-0.576087
C	0.000000	1.273050	-1.873740
C	0.000000	0.000000	-2.458928
C	0.000000	-1.273050	-1.873740
C	0.000000	-2.443650	-2.818004
H	0.874770	-3.075002	-2.644807
H	0.000000	-2.114084	-3.854788
H	-0.874770	-3.075002	-2.644807
H	0.000000	0.000000	-3.539549
C	0.000000	2.443650	-2.818004
H	-0.874770	3.075002	-2.644807
H	0.000000	2.114084	-3.854788
H	0.874770	3.075002	-2.644807
C	0.000000	2.850449	-0.102169
C	-1.220525	3.487604	0.168856
C	-1.196424	4.763164	0.719982
H	-2.131478	5.266328	0.939258
C	0.000000	5.400761	0.996793
H	0.000000	6.395122	1.428175
C	1.196424	4.763164	0.719982
H	2.131478	5.266328	0.939258
C	1.220525	3.487604	0.168856
C	2.536559	2.788928	-0.088846
H	2.331517	1.932705	-0.735582
C	3.120337	2.250978	1.216110
H	3.356305	3.071091	1.899640
H	4.039047	1.688416	1.029498
H	2.416405	1.592816	1.732115
C	3.545568	3.675996	-0.808389

H	3.132281	4.080029	-1.735416
H	4.442583	3.103469	-1.056992
H	3.859027	4.519418	-0.188318
C	-2.536559	2.788928	-0.088846
H	-2.331517	1.932705	-0.735582
C	-3.545568	3.675996	-0.808389
H	-3.859027	4.519418	-0.188318
H	-4.442583	3.103469	-1.056992
H	-3.132281	4.080029	-1.735416
C	-3.120337	2.250978	1.216110
H	-2.416405	1.592816	1.732115
H	-4.039047	1.688416	1.029498
H	-3.356305	3.071091	1.899640
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C	1.196424	-4.763164	0.719982
C	0.000000	-5.400761	0.996793
C	-1.196424	-4.763164	0.719982
H	-2.131478	-5.266328	0.939258
H	0.000000	-6.395122	1.428175
H	2.131478	-5.266328	0.939258
C	2.536559	-2.788928	-0.088846
H	2.331517	-1.932705	-0.735582
C	3.545568	-3.675996	-0.808389
H	3.859027	-4.519418	-0.188318
H	4.442583	-3.103469	-1.056992
H	3.132281	-4.080029	-1.735416
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H	4.039047	-1.688416	1.029498
H	3.356305	-3.071091	1.899640
H	-2.331517	-1.932705	-0.735582
C	-3.545568	-3.675996	-0.808389
H	-4.442583	-3.103469	-1.056992
H	-3.859027	-4.519418	-0.188318
H	-3.132281	-4.080029	-1.735416

[(BDI)ZnH] (C_{2v})

Zn	0.000000	0.000000	0.793949
N	0.000000	1.463281	-0.519070

N	0.000000	-1.463281	-0.519070
C	0.000000	-1.263418	-1.826615
C	0.000000	1.263418	-1.826615
C	0.000000	0.000000	-2.428632
H	0.000000	0.000000	-3.509155
C	3.067201	2.089207	1.297509
H	3.293205	2.863266	2.036024
H	3.983158	1.524182	1.104855
H	2.335464	1.413750	1.747528
C	0.000000	2.455269	-2.739317
H	-0.874756	3.082142	-2.550166
H	0.000000	2.150287	-3.783664
H	0.874756	3.082142	-2.550166
C	0.000000	-2.455269	-2.739317
H	0.874756	-3.082142	-2.550166
H	0.000000	-2.150287	-3.783664
H	-0.874756	-3.082142	-2.550166
C	0.000000	2.788761	-0.006677
C	1.221047	3.417398	0.275240
C	1.196943	4.683885	0.847209
H	2.131305	5.183711	1.075441
C	0.000000	5.316071	1.133577
H	0.000000	6.303403	1.580931
C	-1.196943	4.683885	0.847209
H	-2.131305	5.183711	1.075441
C	-1.221047	3.417398	0.275240
C	2.534654	2.717078	0.010690
H	2.338202	1.905127	-0.693643
C	3.579074	3.628057	-0.622314
H	4.469091	3.052381	-0.887876
H	3.896969	4.418840	0.061499
H	3.198532	4.104038	-1.529107
C	-2.534654	2.717078	0.010690
H	-2.338202	1.905127	-0.693643
C	-3.579074	3.628057	-0.622314
H	-3.896969	4.418840	0.061499
H	-4.469091	3.052381	-0.887876
H	-3.198532	4.104038	-1.529107
C	-3.067201	2.089207	1.297509
H	-2.335464	1.413750	1.747528
H	-3.983158	1.524182	1.104855

H	-3.293205	2.863266	2.036024
C	0.000000	-2.788761	-0.006677
C	1.221047	-3.417398	0.275240
C	1.196943	-4.683885	0.847209
H	2.131305	-5.183711	1.075441
C	0.000000	-5.316071	1.133577
H	0.000000	-6.303403	1.580931
C	-1.196943	-4.683885	0.847209
H	-2.131305	-5.183711	1.075441
C	-1.221047	-3.417398	0.275240
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H	3.198532	-4.104038	-1.529107
C	3.067201	-2.089207	1.297509
H	2.335464	-1.413750	1.747528
H	3.983158	-1.524182	1.104855
H	3.293205	-2.863266	2.036024
C	-2.534654	-2.717078	0.010690
H	-2.338202	-1.905127	-0.693643
C	-3.067201	-2.089207	1.297509
H	-3.293205	-2.863266	2.036024
H	-3.983158	-1.524182	1.104855
H	-2.335464	-1.413750	1.747528
C	-3.579074	-3.628057	-0.622314
H	-3.198532	-4.104038	-1.529107
H	-4.469091	-3.052381	-0.887876
H	-3.896969	-4.418840	0.061499
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[(BDI)Cd]$_2$ (**2**) (D_2)

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N	-1.435215	-0.547166	-2.968789
C	-1.195761	-0.442067	-4.263795
C	1.195761	0.442067	-4.263795
C	0.000000	0.000000	-4.841695
H	0.000000	0.000000	-5.922106

C	3.015132	-2.066241	-1.276101
H	3.767665	-2.010321	-0.488624
H	2.789342	-3.119533	-1.463577
H	2.112064	-1.594134	-0.881798
C	2.284380	0.823892	-5.232811
H	2.568205	1.870909	-5.103536
H	1.964654	0.669397	-6.261124
H	3.186746	0.236076	-5.048678
C	-2.284380	-0.823892	-5.232811
H	-2.568205	-1.870909	-5.103536
H	-1.964654	-0.669397	-6.261124
H	-3.186746	-0.236076	-5.048678
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C	3.737291	0.094634	-2.315744
C	4.968323	0.572023	-1.880872
H	5.769123	-0.127961	-1.674793
C	5.195314	1.928692	-1.728793
H	6.164904	2.284491	-1.398931
C	4.183090	2.830905	-2.007858
H	4.372289	3.892336	-1.898066
C	2.929728	2.397387	-2.422626
C	3.507417	-1.382450	-2.545514
H	2.716971	-1.470256	-3.295588
C	4.735824	-2.101164	-3.088858
H	4.475400	-3.125238	-3.367014
H	5.532336	-2.162900	-2.343042
H	5.138984	-1.599948	-3.972029
C	1.820684	3.384504	-2.710979
H	1.123452	2.897902	-3.397499
C	2.309020	4.661807	-3.381131
H	2.923601	5.265873	-2.708891
H	1.456922	5.277308	-3.679425
H	2.901763	4.445834	-4.273100
C	1.046184	3.706298	-1.437027
H	0.663066	2.798492	-0.965761
H	0.196857	4.361351	-1.648016
H	1.690692	4.203926	-0.707682
C	-2.709911	-1.018007	-2.565128
C	-2.929728	-2.397387	-2.422626
C	-4.183090	-2.830905	-2.007858
H	-4.372289	-3.892336	-1.898066

C	-5.195314	-1.928692	-1.728793
H	-6.164904	-2.284491	-1.398931
C	-4.968323	-0.572023	-1.880872
H	-5.769123	0.127961	-1.674793
C	-3.737291	-0.094634	-2.315744
C	-1.820684	-3.384504	-2.710979
H	-1.123452	-2.897902	-3.397499
C	-2.309020	-4.661807	-3.381131
H	-2.923601	-5.265873	-2.708891
H	-1.456922	-5.277308	-3.679425
H	-2.901763	-4.445834	-4.273100
C	-1.046184	-3.706298	-1.437027
H	-0.663066	-2.798492	-0.965761
H	-0.196857	-4.361351	-1.648016
H	-1.690692	-4.203926	-0.707682
C	-3.507417	1.382450	-2.545514
H	-2.716971	1.470256	-3.295588
C	-3.015132	2.066241	-1.276101
H	-3.767665	2.010321	-0.488624
H	-2.789342	3.119533	-1.463577
H	-2.112064	1.594134	-0.881798
C	-4.735824	2.101164	-3.088858
H	-5.138984	1.599948	-3.972029
H	-4.475400	3.125238	-3.367014
H	-5.532336	2.162900	-2.343042
Cd	0.000000	0.000000	1.337261
N	1.435215	-0.547166	2.968789
N	-1.435215	0.547166	2.968789
C	1.195761	-0.442067	4.263795
C	2.709911	-1.018007	2.565128
C	-1.195761	0.442067	4.263795
C	-2.709911	1.018007	2.565128
C	0.000000	0.000000	4.841695
C	2.284380	-0.823892	5.232811
C	3.737291	-0.094634	2.315744
C	2.929728	-2.397387	2.422626
C	-2.284380	0.823892	5.232811
C	-2.929728	2.397387	2.422626
C	-3.737291	0.094634	2.315744
H	0.000000	0.000000	5.922106
H	2.568205	-1.870909	5.103536

H	1.964654	-0.669397	6.261124
H	3.186746	-0.236076	5.048678
C	4.968323	-0.572023	1.880872
C	3.507417	1.382450	2.545514
C	4.183090	-2.830905	2.007858
C	1.820684	-3.384504	2.710979
H	-2.568205	1.870909	5.103536
H	-1.964654	0.669397	6.261124
H	-3.186746	0.236076	5.048678
C	-4.183090	2.830905	2.007858
C	-1.820684	3.384504	2.710979
C	-4.968323	0.572023	1.880872
C	-3.507417	-1.382450	2.545514
H	5.769123	0.127961	1.674793
C	5.195314	-1.928692	1.728793
C	3.015132	2.066241	1.276101
H	2.716971	1.470256	3.295588
C	4.735824	2.101164	3.088858
H	4.372289	-3.892336	1.898066
H	1.123452	-2.897902	3.397499
C	2.309020	-4.661807	3.381131
C	1.046184	-3.706298	1.437027
H	-4.372289	3.892336	1.898066
C	-5.195314	1.928692	1.728793
H	-1.123452	2.897902	3.397499
C	-2.309020	4.661807	3.381131
C	-1.046184	3.706298	1.437027
H	-5.769123	-0.127961	1.674793
H	-2.716971	-1.470256	3.295588
C	-3.015132	-2.066241	1.276101
C	-4.735824	-2.101164	3.088858
H	6.164904	-2.284491	1.398931
H	3.767665	2.010321	0.488624
H	2.789342	3.119533	1.463577
H	2.112064	1.594134	0.881798
H	4.475400	3.125238	3.367014
H	5.532336	2.162900	2.343042
H	5.138984	1.599948	3.972029
H	2.923601	-5.265873	2.708891
H	1.456922	-5.277308	3.679425
H	2.901763	-4.445834	4.273100

H	0.663066	-2.798492	0.965761
H	0.196857	-4.361351	1.648016
H	1.690692	-4.203926	0.707682
H	-6.164904	2.284491	1.398931
H	-2.923601	5.265873	2.708891
H	-1.456922	5.277308	3.679425
H	-2.901763	4.445834	4.273100
H	-0.663066	2.798492	0.965761
H	-0.196857	4.361351	1.648016
H	-1.690692	4.203926	0.707682
H	-3.767665	-2.010321	0.488624
H	-2.789342	-3.119533	1.463577
H	-2.112064	-1.594134	0.881798
H	-5.138984	-1.599948	3.972029
H	-4.475400	-3.125238	3.367014
H	-5.532336	-2.162900	2.343042

[(BDI)Cd]$_2$ (**2**) (D_{2d})

Cd	0.000000	0.000000	1.340306
N	0.000000	1.489733	3.014428
N	0.000000	-1.489733	3.014428
C	0.000000	-1.265467	4.313595
C	0.000000	1.265467	4.313595
C	0.000000	0.000000	4.910118
H	0.000000	0.000000	5.990716
C	-3.243973	2.070078	1.580303
H	-3.644217	2.768958	0.844643
H	-4.081267	1.489735	1.975939
H	-2.584473	1.382610	1.045541
C	0.000000	2.445524	5.248112
H	0.875054	3.075671	5.072317
H	0.000000	2.123632	6.287569
H	-0.875054	3.075671	5.072317
C	0.000000	-2.445524	5.248112
H	-0.875054	-3.075671	5.072317
H	0.000000	-2.123632	6.287569
H	0.875054	-3.075671	5.072317
C	0.000000	2.815537	2.526569
C	-1.224115	3.447019	2.255021
C	-1.199072	4.676424	1.607925
H	-2.131662	5.178643	1.376172

C	0.000000	5.277242	1.262055
H	0.000000	6.231473	0.747731
C	1.199072	4.676424	1.607925
H	2.131662	5.178643	1.376172
C	1.224115	3.447019	2.255021
C	-2.523889	2.809395	2.702147
H	-2.264529	2.062261	3.455055
C	-3.461124	3.814911	3.361168
H	-4.333969	3.302467	3.773456
H	-3.827005	4.555727	2.645631
H	-2.965750	4.352978	4.172768
C	2.523889	2.809395	2.702147
H	2.264529	2.062261	3.455055
C	3.461124	3.814911	3.361168
H	3.827005	4.555727	2.645631
H	4.333969	3.302467	3.773456
H	2.965750	4.352978	4.172768
C	3.243973	2.070078	1.580303
H	2.584473	1.382610	1.045541
H	4.081267	1.489735	1.975939
H	3.644217	2.768958	0.844643
C	0.000000	-2.815537	2.526569
C	-1.224115	-3.447019	2.255021
C	-1.199072	-4.676424	1.607925
H	-2.131662	-5.178643	1.376172
C	0.000000	-5.277242	1.262055
H	0.000000	-6.231473	0.747731
C	1.199072	-4.676424	1.607925
H	2.131662	-5.178643	1.376172
C	1.224115	-3.447019	2.255021
C	-2.523889	-2.809395	2.702147
H	-2.264529	-2.062261	3.455055
C	-3.461124	-3.814911	3.361168
H	-3.827005	-4.555727	2.645631
H	-4.333969	-3.302467	3.773456
H	-2.965750	-4.352978	4.172768
C	-3.243973	-2.070078	1.580303
H	-2.584473	-1.382610	1.045541
H	-4.081267	-1.489735	1.975939
H	-3.644217	-2.768958	0.844643
C	2.523889	-2.809395	2.702147

H	2.264529	-2.062261	3.455055
C	3.243973	-2.070078	1.580303
H	3.644217	-2.768958	0.844643
H	4.081267	-1.489735	1.975939
H	2.584473	-1.382610	1.045541
C	3.461124	-3.814911	3.361168
H	2.965750	-4.352978	4.172768
H	4.333969	-3.302467	3.773456
H	3.827005	-4.555727	2.645631
Cd	0.000000	0.000000	-1.340306
N	-1.489733	0.000000	-3.014428
N	1.489733	0.000000	-3.014428
C	-1.265467	0.000000	-4.313595
C	-2.815537	0.000000	-2.526569
C	1.265467	0.000000	-4.313595
C	2.815537	0.000000	-2.526569
C	0.000000	0.000000	-4.910118
C	-2.445524	0.000000	-5.248112
C	-3.447019	1.224115	-2.255021
C	-3.447019	-1.224115	-2.255021
C	2.445524	0.000000	-5.248112
C	3.447019	1.224115	-2.255021
C	3.447019	-1.224115	-2.255021
H	0.000000	0.000000	-5.990716
H	-3.075671	-0.875054	-5.072317
H	-2.123632	0.000000	-6.287569
H	-3.075671	0.875054	-5.072317
C	-4.676424	1.199072	-1.607925
C	-2.809395	2.523889	-2.702147
C	-4.676424	-1.199072	-1.607925
C	-2.809395	-2.523889	-2.702147
H	3.075671	0.875054	-5.072317
H	2.123632	0.000000	-6.287569
H	3.075671	-0.875054	-5.072317
C	4.676424	1.199072	-1.607925
C	2.809395	2.523889	-2.702147
C	4.676424	-1.199072	-1.607925
C	2.809395	-2.523889	-2.702147
H	-5.178643	2.131662	-1.376172
C	-5.277242	0.000000	-1.262055
C	-2.070078	3.243973	-1.580303

H	-2.062261	2.264529	-3.455055
C	-3.814911	3.461124	-3.361168
H	-5.178643	-2.131662	-1.376172
H	-2.062261	-2.264529	-3.455055
C	-3.814911	-3.461124	-3.361168
C	-2.070078	-3.243973	-1.580303
H	5.178643	2.131662	-1.376172
C	5.277242	0.000000	-1.262055
H	2.062261	2.264529	-3.455055
C	3.814911	3.461124	-3.361168
C	2.070078	3.243973	-1.580303
H	5.178643	-2.131662	-1.376172
H	2.062261	-2.264529	-3.455055
C	2.070078	-3.243973	-1.580303
C	3.814911	-3.461124	-3.361168
H	-6.231473	0.000000	-0.747731
H	-2.768958	3.644217	-0.844643
H	-1.489735	4.081267	-1.975939
H	-1.382610	2.584473	-1.045541
H	-3.302467	4.333969	-3.773456
H	-4.555727	3.827005	-2.645631
H	-4.352978	2.965750	-4.172768
H	-4.555727	-3.827005	-2.645631
H	-3.302467	-4.333969	-3.773456
H	-4.352978	-2.965750	-4.172768
H	-1.382610	-2.584473	-1.045541
H	-1.489735	-4.081267	-1.975939
H	-2.768958	-3.644217	-0.844643
H	6.231473	0.000000	-0.747731
H	4.555727	3.827005	-2.645631
H	3.302467	4.333969	-3.773456
H	4.352978	2.965750	-4.172768
H	1.382610	2.584473	-1.045541
H	1.489735	4.081267	-1.975939
H	2.768958	3.644217	-0.844643
H	2.768958	-3.644217	-0.844643
H	1.489735	-4.081267	-1.975939
H	1.382610	-2.584473	-1.045541
H	4.352978	-2.965750	-4.172768
H	3.302467	-4.333969	-3.773456
H	4.555727	-3.827005	-2.645631

[(BDI)Cd]$_2$ (**2**) (D_{2h})

Cd	0.000000	1.385760	0.000000
N	-1.509940	3.094026	0.000000
N	1.509940	3.094026	0.000000
C	1.265872	4.392745	0.000000
C	-1.265872	4.392745	0.000000
C	0.000000	4.982241	0.000000
H	0.000000	6.062454	0.000000
C	-2.217917	1.731909	3.233724
H	-2.978999	1.026979	3.570945
H	-1.654316	2.067821	4.108332
H	-1.534880	1.188994	2.576559
C	-2.427892	5.352867	0.000000
H	-3.063172	5.194702	-0.874055
H	-2.079498	6.383586	0.000000
H	-3.063172	5.194702	0.874055
C	2.427892	5.352867	0.000000
H	3.063172	5.194702	0.874055
H	2.079498	6.383586	0.000000
H	3.063172	5.194702	-0.874055
C	-2.866572	2.687882	0.000000
C	-3.529022	2.495753	1.221572
C	-4.820982	1.985308	1.198062
H	-5.347273	1.815999	2.130667
C	-5.456127	1.709354	0.000000
H	-6.461963	1.306874	0.000000
C	-4.820982	1.985308	-1.198062
H	-5.347273	1.815999	-2.130667
C	-3.529022	2.495753	-1.221572
C	-2.866671	2.907486	2.519451
H	-2.066711	3.604695	2.261820
C	-3.824078	3.635760	3.455618
H	-3.280691	4.026612	4.319527
H	-4.603710	2.970849	3.835809
H	-4.316299	4.472758	2.954951
C	-2.866671	2.907486	-2.519451
H	-2.066711	3.604695	-2.261820
C	-3.824078	3.635760	-3.455618
H	-4.603710	2.970849	-3.835809
H	-3.280691	4.026612	-4.319527

H	-4.316299	4.472758	-2.954951
C	-2.217917	1.731909	-3.233724
H	-1.534880	1.188994	-2.576559
H	-1.654316	2.067821	-4.108332
H	-2.978999	1.026979	-3.570945
C	2.866572	2.687882	0.000000
C	3.529022	2.495753	1.221572
C	4.820982	1.985308	1.198062
H	5.347273	1.815999	2.130667
C	5.456127	1.709354	0.000000
H	6.461963	1.306874	0.000000
C	4.820982	1.985308	-1.198062
H	5.347273	1.815999	-2.130667
C	3.529022	2.495753	-1.221572
C	2.866671	2.907486	2.519451
H	2.066711	3.604695	2.261820
C	3.824078	3.635760	3.455618
H	4.603710	2.970849	3.835809
H	3.280691	4.026612	4.319527
H	4.316299	4.472758	2.954951
C	2.217917	1.731909	3.233724
H	1.534880	1.188994	2.576559
H	1.654316	2.067821	4.108332
H	2.978999	1.026979	3.570945
C	2.866671	2.907486	-2.519451
H	2.066711	3.604695	-2.261820
C	2.217917	1.731909	-3.233724
H	2.978999	1.026979	-3.570945
H	1.654316	2.067821	-4.108332
H	1.534880	1.188994	-2.576559
C	3.824078	3.635760	-3.455618
H	4.316299	4.472758	-2.954951
H	3.280691	4.026612	-4.319527
H	4.603710	2.970849	-3.835809
Cd	0.000000	-1.385760	0.000000
N	1.509940	-3.094026	0.000000
N	-1.509940	-3.094026	0.000000
C	1.265872	-4.392745	0.000000
C	2.866572	-2.687882	0.000000
C	-1.265872	-4.392745	0.000000
C	-2.866572	-2.687882	0.000000

C	0.000000	-4.982241	0.000000
C	2.427892	-5.352867	0.000000
C	3.529022	-2.495753	1.221572
C	3.529022	-2.495753	-1.221572
C	-2.427892	-5.352867	0.000000
C	-3.529022	-2.495753	1.221572
C	-3.529022	-2.495753	-1.221572
H	0.000000	-6.062454	0.000000
H	3.063172	-5.194702	-0.874055
H	2.079498	-6.383586	0.000000
H	3.063172	-5.194702	0.874055
C	4.820982	-1.985308	1.198062
C	2.866671	-2.907486	2.519451
C	4.820982	-1.985308	-1.198062
C	2.866671	-2.907486	-2.519451
H	-3.063172	-5.194702	0.874055
H	-2.079498	-6.383586	0.000000
H	-3.063172	-5.194702	-0.874055
C	-4.820982	-1.985308	1.198062
C	-2.866671	-2.907486	2.519451
C	-4.820982	-1.985308	-1.198062
C	-2.866671	-2.907486	-2.519451
H	5.347273	-1.815999	2.130667
C	5.456127	-1.709354	0.000000
C	2.217917	-1.731909	3.233724
H	2.066711	-3.604695	2.261820
C	3.824078	-3.635760	3.455618
H	5.347273	-1.815999	-2.130667
H	2.066711	-3.604695	-2.261820
C	3.824078	-3.635760	-3.455618
C	2.217917	-1.731909	-3.233724
H	-5.347273	-1.815999	2.130667
C	-5.456127	-1.709354	0.000000
H	-2.066711	-3.604695	2.261820
C	-3.824078	-3.635760	3.455618
C	-2.217917	-1.731909	3.233724
H	-5.347273	-1.815999	-2.130667
H	-2.066711	-3.604695	-2.261820
C	-2.217917	-1.731909	-3.233724
C	-3.824078	-3.635760	-3.455618
H	6.461963	-1.306874	0.000000

H	2.978999	-1.026979	3.570945
H	1.654316	-2.067821	4.108332
H	1.534880	-1.188994	2.576559
H	3.280691	-4.026612	4.319527
H	4.603710	-2.970849	3.835809
H	4.316299	-4.472758	2.954951
H	4.603710	-2.970849	-3.835809
H	3.280691	-4.026612	-4.319527
H	4.316299	-4.472758	-2.954951
H	1.534880	-1.188994	-2.576559
H	1.654316	-2.067821	-4.108332
H	2.978999	-1.026979	-3.570945
H	-6.461963	-1.306874	0.000000
H	-4.603710	-2.970849	3.835809
H	-3.280691	-4.026612	4.319527
H	-4.316299	-4.472758	2.954951
H	-1.534880	-1.188994	2.576559
H	-1.654316	-2.067821	4.108332
H	-2.978999	-1.026979	3.570945
H	-2.978999	-1.026979	-3.570945
H	-1.654316	-2.067821	-4.108332
H	-1.534880	-1.188994	-2.576559
H	-4.316299	-4.472758	-2.954951
H	-3.280691	-4.026612	-4.319527
H	-4.603710	-2.970849	-3.835809

$[(BDI)Zn]_2$ (D_{2d})

Zn	0.000000	0.000000	1.262588
N	1.450112	0.000000	2.717770
N	-1.450112	0.000000	2.717770
C	-1.253608	0.000000	4.026863
C	1.253608	0.000000	4.026863
C	0.000000	0.000000	4.637004
H	0.000000	0.000000	5.717105
C	1.928199	3.179867	1.470066
H	2.538250	3.638405	0.692695
H	1.317571	3.968602	1.915721
H	1.256551	2.473100	0.978544
C	2.439744	0.000000	4.954566
H	3.071565	-0.873880	4.782728
H	2.115096	0.000000	5.993157

H	3.071565	0.873880	4.782728
C	-2.439744	0.000000	4.954566
H	-3.071565	0.873880	4.782728
H	-2.115096	0.000000	5.993157
H	-3.071565	-0.873880	4.782728
C	2.794381	0.000000	2.269076
C	3.449683	1.224915	2.071110
C	4.732858	1.199152	1.538038
H	5.262728	2.129172	1.368691
C	5.358313	0.000000	1.241183
H	6.356341	0.000000	0.817896
C	4.732858	-1.199152	1.538038
H	5.262728	-2.129172	1.368691
C	3.449683	-1.224915	2.071110
C	2.796226	2.514626	2.530225
H	2.125622	2.244508	3.349173
C	3.802009	3.514812	3.085941
H	3.276405	4.362824	3.531636
H	4.451433	3.914494	2.302674
H	4.438675	3.065864	3.852071
C	2.796226	-2.514626	2.530225
H	2.125622	-2.244508	3.349173
C	3.802009	-3.514812	3.085941
H	4.451433	-3.914494	2.302674
H	3.276405	-4.362824	3.531636
H	4.438675	-3.065864	3.852071
C	1.928199	-3.179867	1.470066
H	1.256551	-2.473100	0.978544
H	1.317571	-3.968602	1.915721
H	2.538250	-3.638405	0.692695
C	-2.794381	0.000000	2.269076
C	-3.449683	1.224915	2.071110
C	-4.732858	1.199152	1.538038
H	-5.262728	2.129172	1.368691
C	-5.358313	0.000000	1.241183
H	-6.356341	0.000000	0.817896
C	-4.732858	-1.199152	1.538038
H	-5.262728	-2.129172	1.368691
C	-3.449683	-1.224915	2.071110
C	-2.796226	2.514626	2.530225
H	-2.125622	2.244508	3.349173

C	-3.802009	3.514812	3.085941
H	-4.451433	3.914494	2.302674
H	-3.276405	4.362824	3.531636
H	-4.438675	3.065864	3.852071
C	-1.928199	3.179867	1.470066
H	-1.256551	2.473100	0.978544
H	-1.317571	3.968602	1.915721
H	-2.538250	3.638405	0.692695
C	-2.796226	-2.514626	2.530225
H	-2.125622	-2.244508	3.349173
C	-1.928199	-3.179867	1.470066
H	-2.538250	-3.638405	0.692695
H	-1.317571	-3.968602	1.915721
H	-1.256551	-2.473100	0.978544
C	-3.802009	-3.514812	3.085941
H	-4.438675	-3.065864	3.852071
H	-3.276405	-4.362824	3.531636
H	-4.451433	-3.914494	2.302674
Zn	0.000000	0.000000	-1.262588
N	0.000000	1.450112	-2.717770
N	0.000000	-1.450112	-2.717770
C	0.000000	1.253608	-4.026863
C	0.000000	2.794381	-2.269076
C	0.000000	-1.253608	-4.026863
C	0.000000	-2.794381	-2.269076
C	0.000000	0.000000	-4.637004
C	0.000000	2.439744	-4.954566
C	1.224915	3.449683	-2.071110
C	-1.224915	3.449683	-2.071110
C	0.000000	-2.439744	-4.954566
C	1.224915	-3.449683	-2.071110
C	-1.224915	-3.449683	-2.071110
H	0.000000	0.000000	-5.717105
H	-0.873880	3.071565	-4.782728
H	0.000000	2.115096	-5.993157
H	0.873880	3.071565	-4.782728
C	1.199152	4.732858	-1.538038
C	2.514626	2.796226	-2.530225
C	-1.199152	4.732858	-1.538038
C	-2.514626	2.796226	-2.530225
H	0.873880	-3.071565	-4.782728

H	0.000000	-2.115096	-5.993157
H	-0.873880	-3.071565	-4.782728
C	1.199152	-4.732858	-1.538038
C	2.514626	-2.796226	-2.530225
C	-1.199152	-4.732858	-1.538038
C	-2.514626	-2.796226	-2.530225
H	2.129172	5.262728	-1.368691
C	0.000000	5.358313	-1.241183
C	3.179867	1.928199	-1.470066
H	2.244508	2.125622	-3.349173
C	3.514812	3.802009	-3.085941
H	-2.129172	5.262728	-1.368691
H	-2.244508	2.125622	-3.349173
C	-3.514812	3.802009	-3.085941
C	-3.179867	1.928199	-1.470066
H	2.129172	-5.262728	-1.368691
C	0.000000	-5.358313	-1.241183
H	2.244508	-2.125622	-3.349173
C	3.514812	-3.802009	-3.085941
C	3.179867	-1.928199	-1.470066
H	-2.129172	-5.262728	-1.368691
H	-2.244508	-2.125622	-3.349173
C	-3.179867	-1.928199	-1.470066
C	-3.514812	-3.802009	-3.085941
H	0.000000	6.356341	-0.817896
H	3.638405	2.538250	-0.692695
H	3.968602	1.317571	-1.915721
H	2.473100	1.256551	-0.978544
H	4.362824	3.276405	-3.531636
H	3.914494	4.451433	-2.302674
H	3.065864	4.438675	-3.852071
H	-3.914494	4.451433	-2.302674
H	-4.362824	3.276405	-3.531636
H	-3.065864	4.438675	-3.852071
H	-2.473100	1.256551	-0.978544
H	-3.968602	1.317571	-1.915721
H	-3.638405	2.538250	-0.692695
H	0.000000	-6.356341	-0.817896
H	3.914494	-4.451433	-2.302674
H	4.362824	-3.276405	-3.531636
H	3.065864	-4.438675	-3.852071

H	2.473100	-1.256551	-0.978544
H	3.968602	-1.317571	-1.915721
H	3.638405	-2.538250	-0.692695
H	-3.638405	-2.538250	-0.692695
H	-3.968602	-1.317571	-1.915721
H	-2.473100	-1.256551	-0.978544
H	-3.065864	-4.438675	-3.852071
H	-4.362824	-3.276405	-3.531636
H	-3.914494	-4.451433	-2.302674

$[(BDI)Zn]_2$ (D_{2h})

Zn	0.000000	1.332887	0.000000
N	-1.460136	2.834006	0.000000
N	1.460136	2.834006	0.000000
C	1.252185	4.143985	0.000000
C	-1.252185	4.143985	0.000000
C	0.000000	4.750874	0.000000
H	0.000000	5.830563	0.000000
C	-2.036547	1.697089	3.207782
H	-2.708378	0.956589	3.639550
H	-1.437973	2.122453	4.017628
H	-1.363374	1.179368	2.521936
C	-2.424551	5.093410	0.000000
H	-3.061020	4.938432	-0.872782
H	-2.076452	6.124294	0.000000
H	-3.061020	4.938432	0.872782
C	2.424551	5.093410	0.000000
H	3.061020	4.938432	0.872782
H	2.076452	6.124294	0.000000
H	3.061020	4.938432	-0.872782
C	-2.825591	2.445478	0.000000
C	-3.499149	2.312315	1.223292
C	-4.818648	1.877594	1.198885
H	-5.362045	1.756896	2.128586
C	-5.464782	1.633571	0.000000
H	-6.493367	1.293353	0.000000
C	-4.818648	1.877594	-1.198885
H	-5.362045	1.756896	-2.128586
C	-3.499149	2.312315	-1.223292
C	-2.836141	2.780264	2.504639
H	-2.120285	3.553849	2.218947

C	-3.821519	3.418415	3.475661
H	-3.281316	3.870344	4.311173
H	-4.510506	2.681998	3.897311
H	-4.418098	4.196471	2.993527
C	-2.836141	2.780264	-2.504639
H	-2.120285	3.553849	-2.218947
C	-3.821519	3.418415	-3.475661
H	-4.510506	2.681998	-3.897311
H	-3.281316	3.870344	-4.311173
H	-4.418098	4.196471	-2.993527
C	-2.036547	1.697089	-3.207782
H	-1.363374	1.179368	-2.521936
H	-1.437973	2.122453	-4.017628
H	-2.708378	0.956589	-3.639550
C	2.825591	2.445478	0.000000
C	3.499149	2.312315	1.223292
C	4.818648	1.877594	1.198885
H	5.362045	1.756896	2.128586
C	5.464782	1.633571	0.000000
H	6.493367	1.293353	0.000000
C	4.818648	1.877594	-1.198885
H	5.362045	1.756896	-2.128586
C	3.499149	2.312315	-1.223292
C	2.836141	2.780264	2.504639
H	2.120285	3.553849	2.218947
C	3.821519	3.418415	3.475661
H	4.510506	2.681998	3.897311
H	3.281316	3.870344	4.311173
H	4.418098	4.196471	2.993527
C	2.036547	1.697089	3.207782
H	1.363374	1.179368	2.521936
H	1.437973	2.122453	4.017628
H	2.708378	0.956589	3.639550
C	2.836141	2.780264	-2.504639
H	2.120285	3.553849	-2.218947
C	2.036547	1.697089	-3.207782
H	2.708378	0.956589	-3.639550
H	1.437973	2.122453	-4.017628
H	1.363374	1.179368	-2.521936
C	3.821519	3.418415	-3.475661
H	4.418098	4.196471	-2.993527

H	3.281316	3.870344	-4.311173
H	4.510506	2.681998	-3.897311
Zn	0.000000	-1.332887	0.000000
N	1.460136	-2.834006	0.000000
N	-1.460136	-2.834006	0.000000
C	1.252185	-4.143985	0.000000
C	2.825591	-2.445478	0.000000
C	-1.252185	-4.143985	0.000000
C	-2.825591	-2.445478	0.000000
C	0.000000	-4.750874	0.000000
C	2.424551	-5.093410	0.000000
C	3.499149	-2.312315	1.223292
C	3.499149	-2.312315	-1.223292
C	-2.424551	-5.093410	0.000000
C	-3.499149	-2.312315	1.223292
C	-3.499149	-2.312315	-1.223292
H	0.000000	-5.830563	0.000000
H	3.061020	-4.938432	-0.872782
H	2.076452	-6.124294	0.000000
H	3.061020	-4.938432	0.872782
C	4.818648	-1.877594	1.198885
C	2.836141	-2.780264	2.504639
C	4.818648	-1.877594	-1.198885
C	2.836141	-2.780264	-2.504639
H	-3.061020	-4.938432	0.872782
H	-2.076452	-6.124294	0.000000
H	-3.061020	-4.938432	-0.872782
C	-4.818648	-1.877594	1.198885
C	-2.836141	-2.780264	2.504639
C	-4.818648	-1.877594	-1.198885
C	-2.836141	-2.780264	-2.504639
H	5.362045	-1.756896	2.128586
C	5.464782	-1.633571	0.000000
C	2.036547	-1.697089	3.207782
H	2.120285	-3.553849	2.218947
C	3.821519	-3.418415	3.475661
H	5.362045	-1.756896	-2.128586
H	2.120285	-3.553849	-2.218947
C	3.821519	-3.418415	-3.475661
C	2.036547	-1.697089	-3.207782
H	-5.362045	-1.756896	2.128586

C	-5.464782	-1.633571	0.000000
H	-2.120285	-3.553849	2.218947
C	-3.821519	-3.418415	3.475661
C	-2.036547	-1.697089	3.207782
H	-5.362045	-1.756896	-2.128586
H	-2.120285	-3.553849	-2.218947
C	-2.036547	-1.697089	-3.207782
C	-3.821519	-3.418415	-3.475661
H	6.493367	-1.293353	0.000000
H	2.708378	-0.956589	3.639550
H	1.437973	-2.122453	4.017628
H	1.363374	-1.179368	2.521936
H	3.281316	-3.870344	4.311173
H	4.510506	-2.681998	3.897311
H	4.418098	-4.196471	2.993527
H	4.510506	-2.681998	-3.897311
H	3.281316	-3.870344	-4.311173
H	4.418098	-4.196471	-2.993527
H	1.363374	-1.179368	-2.521936
H	1.437973	-2.122453	-4.017628
H	2.708378	-0.956589	-3.639550
H	-6.493367	-1.293353	0.000000
H	-4.510506	-2.681998	3.897311
H	-3.281316	-3.870344	4.311173
H	-4.418098	-4.196471	2.993527
H	-1.363374	-1.179368	2.521936
H	-1.437973	-2.122453	4.017628
H	-2.708378	-0.956589	3.639550
H	-2.708378	-0.956589	-3.639550
H	-1.437973	-2.122453	-4.017628
H	-1.363374	-1.179368	-2.521936
H	-4.418098	-4.196471	-2.993527
H	-3.281316	-3.870344	-4.311173
H	-4.510506	-2.681998	-3.897311

H_2

H	0.000000	0.000000	0.126898
H	0.000000	0.000000	0.873102