Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information

Differentiating intramolecular spodium bonds from coordination bonds in two polynuclear zinc(II) Schiff base complexes

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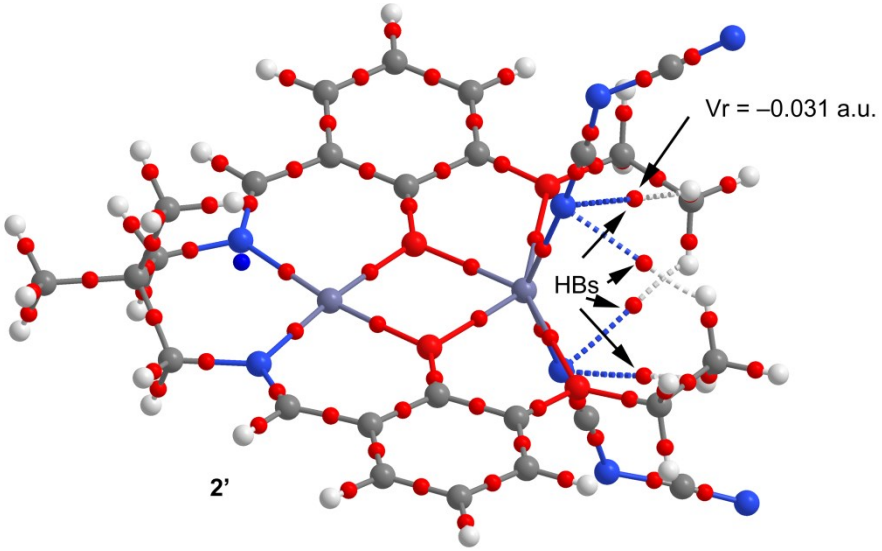

Figure S1. Hydrogen bonds interaction in **2'**

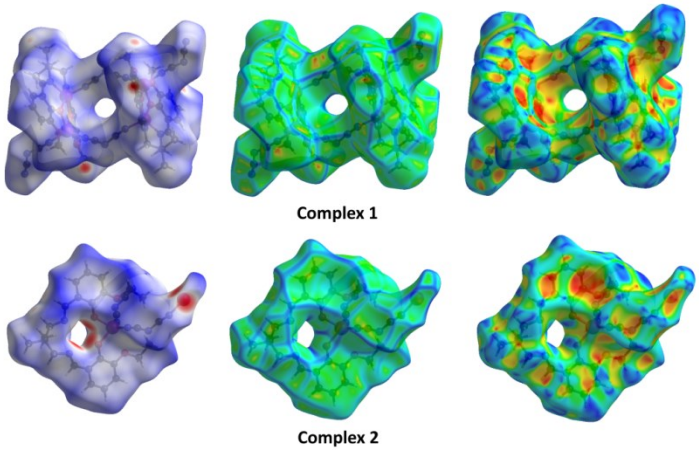

Figure S2. Hirshfeld surfaces mapped over d_{norm} (left), curvedness (middle) and shape index (right) for complexes **1**(top) and **2**(bottom).

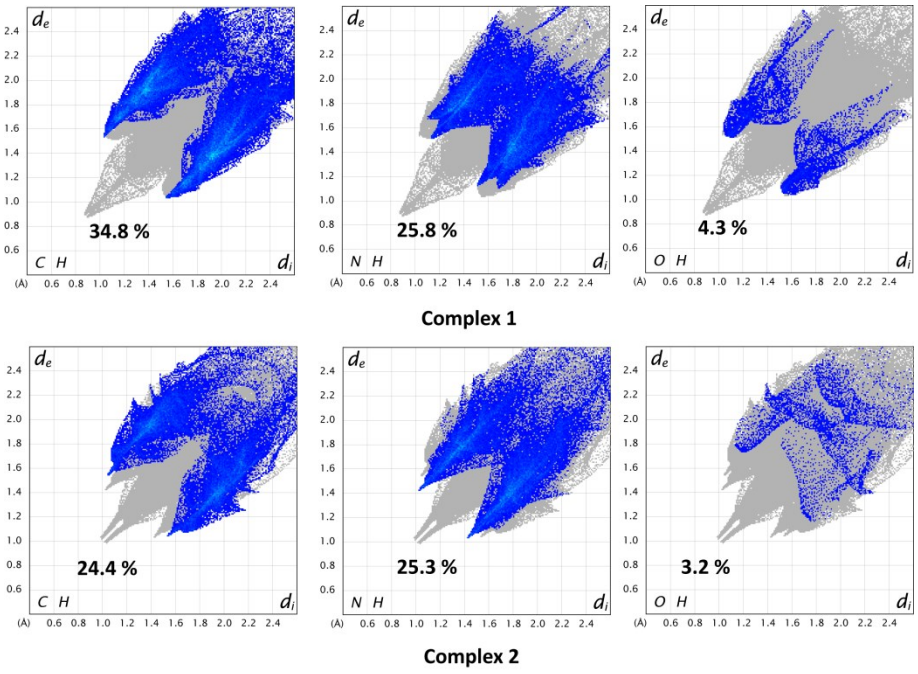

Figure S3. Fingerprint plot: Resolved into C···H/H···C, N···H/H···N and O···H/H···O contacts contributed to the total Hirshfeld Surface area of complexes **1** and **2**.

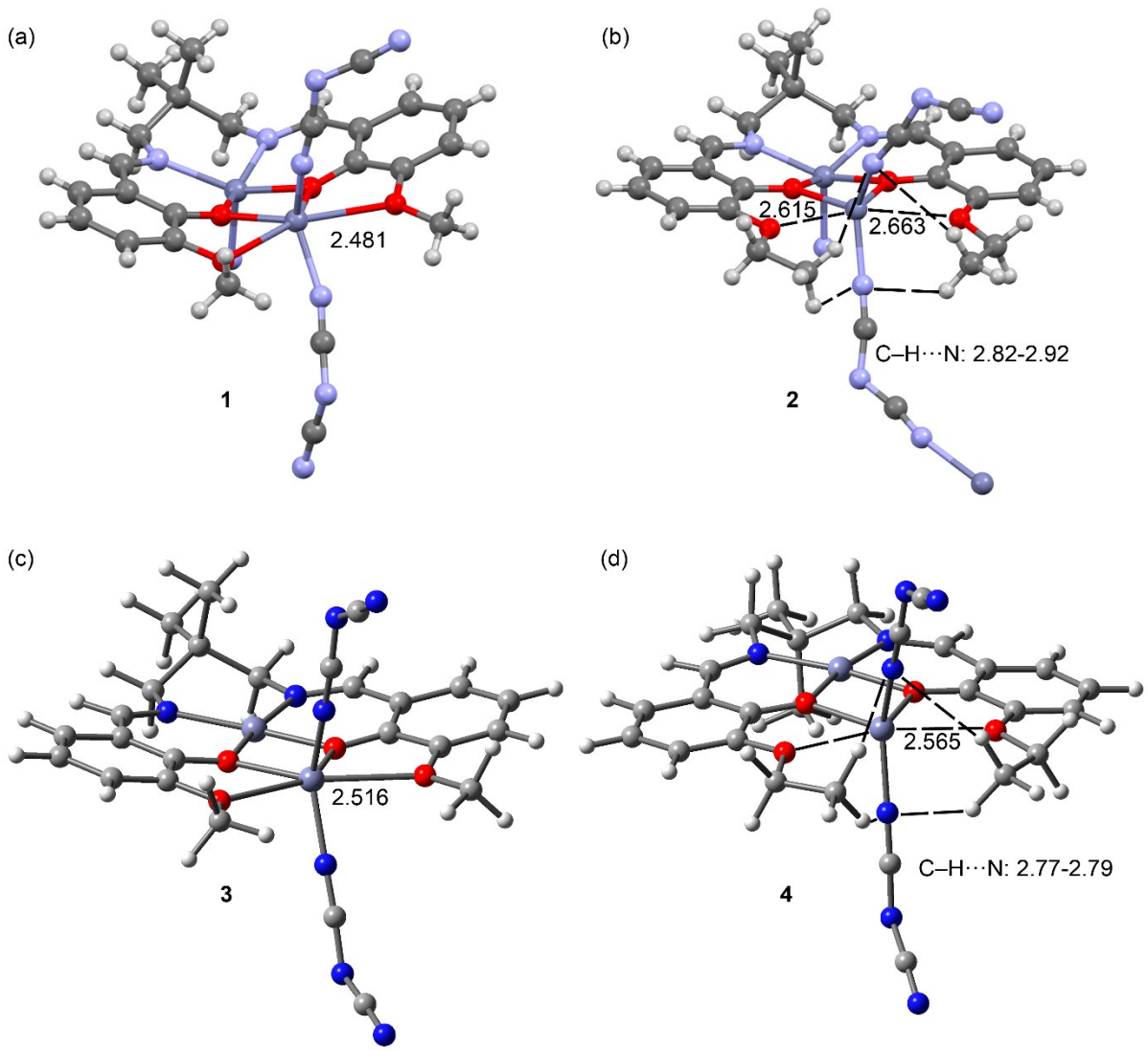

Figure S4: Experimental and theoretical geometries of 1 (a,c) and 2 (b,d). Distances in Å.

Table S1. Selected bond angles (°) of complexes 1 and 2.

Complex	1	2
O(1)–Zn(1)–O(2)	75.5(2)	76.1(3)
O(1)–Zn(1)–N(5)	105.9(3)	102.0(3)
O(1)–Zn(1)–N(1)	88.8(2)	88.4(3)
O(1)–Zn(1)–N(2)	154.6(3)	152.9(2)
O(2)–Zn(1)–N(1)	146.6(3)	152.8(3)
O(2)–Zn(1)–N(2)	87.6(2)	88.6(2)
O(2)–Zn(1)–N(5)	109.6(3)	105.5(3)

N(1)–Zn(1)–N(5)	102.9(3)	99.7(3)
N(1)–Zn(1)–N(2)	95.5(2)	95.9(2)
N(2)–Zn(1)–N(5)	97.5(3)	103.6(3)
O(1)–Zn(2)–O(2)	76.8(3)	78.1(3)
O(1)–Zn(2)–O(3)	67.8(2)	68.2(2)
O(1)–Zn(2)–O(4)	146.7(2)	145.9(2)
O(1)–Zn(2)–N(3)	107.9(3)	110.6(3)
O(1)–Zn(2)–N(4)	112.1(3)	109.7(3)
O(2)–Zn(2)–O(3)	144.6(2)	146.1(2)
O(2)–Zn(2)–O(4)	69.8(2)	67.9(2)
O(2)–Zn(2)–N(3)	110.0(3)	115.5(3)
O(2)–Zn(2)–N(4)	114.1(3)	109.9(3)
O(3)–Zn(2)–O(4)	145.3(2)	145.8(2)
O(3)–Zn(2)–N(3)	84.4(3)	80.8(3)
O(3)–Zn(2)–N(4)	77.9(2)	79.7(3)
O(4)–Zn(2)–N(3)	84.2(3)	85.2(3)
O(4)–Zn(2)–N(4)	82.3(3)	82.6(3)
N(3)–Zn(2)–N(4)	125.3(3)	123.8(3)

Table S2. Electron charge density (ρ), its Laplacian ($\nabla^2\rho$), kinetic (V), Lagrangian (G) and total (H) energy densities at the bond CPs labelled in Figure 4 for complexes 1 and 2 in a.u.

CP	ρ(r)	$\nabla^2\rho(r)$	V(r)	G(r)	H(r)
Complex 1					
a	0.0785	0.3378	–0.1147	0.0996	–0.0151
b	0.0756	0.3168	–0.1070	0.0931	–0.0139
c	0.0683	0.3550	–0.1062	0.0975	–0.0087

d	0.0676	0.3498	–0.1045	0.0960	–0.0085
e	0.0734	0.3939	–0.1194	0.1089	–0.0105
f	0.0710	0.3818	–0.1140	0.1047	–0.0093
g	0.0920	0.4452	–0.1537	0.1325	–0.0212
h	0.0905	0.4409	–0.1504	0.1303	–0.0201
i	0.0244	0.0962	–0.0241	0.0241	0.0000
j	0.0213	0.0794	–0.0199	0.0199	0.0000
Complex 2					
a	0.0822	0.3586	–0.1232	0.1064	–0.0168
b	0.0760	0.3216	–0.1084	0.0944	–0.0140
c	0.0681	0.3500	–0.1052	0.0964	–0.0088
d	0.0696	0.3613	–0.1090	0.0997	–0.0093
e	0.0760	0.4162	–0.1264	0.1152	–0.0112
f	0.0738	0.4010	–0.1210	0.1106	–0.0104
g	0.0910	0.4350	–0.1498	0.1293	–0.0205
h	0.0894	0.4340	–0.1481	0.1283	–0.0208
i	0.0170	0.0595	–0.0149	0.0149	0.0000
j	0.0185	0.0667	–0.0167	0.0167	0.0000

IR and UV-Vis Spectra and magnetic moment

The characteristic imines (C=N) stretching vibration of the synthesized complexes were located within the range 1580-1621 cm^{-1}.[1]Dicyanamide complexes displayed strong bands at ~ 2327 cm^{-1} and 2298 cm^{-1} in complex **1**; 2346 cm^{-1} and 2266 cm^{-1} in complex **2**.[2] Such spectral values are due to the bridging mode of ν(dca). The IR spectra were extensively compared with previously reported Zn (II)-complexes concerning the bridging mode of dicyanamide co-ligands.[3-5]The electronic spectra of both complexes show bands at ~270 and ~370 nm, which may be assigned as $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions, respectively.[6] The absence

of any d-d transition is in accordance with the presence of d^{10} configuration of zinc(II).[7] Room temperature magnetic susceptibility measurements show that both complexes are diamagnetic, as anticipated for zinc(II) complexes.

Hirshfeld analysis

Hirshfeld surface study[8–10] leads us to understand the different intermolecular interactions that were carried out for both complexes **1** and **2** with the help of Crystal Explorer software.[11] Two-dimentional fingerprint plots[12–14] were obtained and two types of distances (d_e and d_i) are obtained for each point on the Hirshfeldisosurface. d_e is defined as the distance between the surface and the nearest nucleus external to the surface whereas d_i is just the opposite of d_e i.e. the distance between the surface and the nearest nucleus internal to the surface. Another three dimensional term (d_{norm}) is also important as far as Hirshfeld surface analysis is concerned. It is nothing but a normalized contact distance. d_e and d_i are normalised by the van der Waals radius of the atom (r_i^{vdW} and r_e^{vdW}) and the summation of these two quantities result in normalized contact distance (d_{norm}) according to the following equation:

$$d_{norm} = \frac{(d_i - r_i^{vdw})}{r_i^{vdw}} + \frac{(d_e - r_e^{vdw})}{r_e^{vdw}}$$

Three types of Hirshfeld surfaces of the complex were achieved on mapping over d_{norm}, curvedness and shape index (Figure **S1**). Curvedness is actually a function of the root mean square of the curvature of the surface and thus defining the shape of the crystal. On the other hand shape index is a qualitative measurement of the shape and very sensitive to a slight change in the shape of the surface, particularly in a region where the curvedness is

very low. Figure **S2** clearly depicts three types of regions i.e. red, blue and white which are defined by d_{norm} values.

On analyzing the 2D Fingerprint plots (Figure **S2**),it is found that the proportion of the Hirshfeld surface for C···H interaction in **1** (34.8%) is considerably higher than that in **2 (**24.4%**)**.The Hirshfeld surface proportion of H···N/N···H interaction is, on the other hand, is comparable (25.8% for complex**1**and 25.3%for complex**2**. The O···H/H···O interaction is around 4.3% for complex**1** which is also slightly greater thanthat for complex **2** (3.2%).

CartesianCoordinates

$Zn(dca)_2$

Zn	-0.5213713	0.0483826	0.0000000
N	-0.8609402	-4.1259880	0.0000000
C	-0.0333586	-5.1433856	0.0000000
C	-0.7085018	-2.9068655	0.0000000
N	0.6354453	-6.0861879	0.0000000
N	-0.7033123	-1.7225076	0.0000000
N	-0.0506760	4.2098461	0.0000000
C	0.9491408	5.0580363	0.0000000
C	-0.1319338	2.9842630	0.0000000
N	1.7778470	5.8639858	0.0000000
N	-0.3523392	1.8204209	0.0000000

1'

Zn	2.0031065	0.2902218	0.0000000
O	0.3031543	0.4477893	1.2707529
O	2.6036876	0.2440500	2.4437055
C	-2.1987519	0.2680719	2.7564249
H	-3.0087677	0.1818666	3.4886895
N	-2.5435269	0.4736885	1.5294002
N	-2.5435269	0.4736885	-1.5294002
C	0.2922268	0.2440693	2.5612951
C	0.3825812	-0.2209708	5.3395333
H	0.4331156	-0.4024873	6.4052770
C	-0.8233930	-0.0921347	4.7103439
H	-1.7477032	-0.1672325	5.2726161
C	1.5304595	0.1162226	3.2429324
C	-0.8932088	0.1409646	3.3175661
C	-0.8233930	-0.0921347	-4.7103439
H	-1.7477032	-0.1672325	-5.2726161
C	1.5304595	0.1162226	-3.2429324
C	1.5678598	-0.1167989	-4.5991921
H	2.5209551	-0.2206817	-5.1014510
O	2.6036876	0.2440500	-2.4437055
O	0.3031543	0.4477893	-1.2707529
C	1.5678598	-0.1167989	4.5991921
H	2.5209551	-0.2206817	5.1014510
C	-0.8932088	0.1409646	-3.3175661
C	-2.1987519	0.2680719	-2.7564249

H	-3.0087677	0.1818666	-3.4886895
C	3.8968731	0.0798362	2.9879420
H	4.0219625	-0.9261125	3.3991777
H	4.0939157	0.8294598	3.7595944
C	-3.9663479	0.6197074	1.2648246
H	-4.1919855	1.6893387	1.1728124
H	-4.5360114	0.2453435	2.1243334
C	0.2922268	0.2440693	-2.5612951
C	0.3825812	-0.2209708	-5.3395333
H	0.4331156	-0.4024873	-6.4052770
C	3.8968731	0.0798362	-2.9879420
H	4.0939157	0.8294598	-3.7595944
H	4.0219625	-0.9261125	-3.3991777
C	-3.9663479	0.6197074	-1.2648246
H	-4.5360114	0.2453435	-2.1243334
H	-4.1919855	1.6893387	-1.1728124
C	-4.4677587	-0.0868570	0.0000000
C	-5.9902454	0.0444635	0.0000000
H	-6.4210909	-0.4347661	0.8818230
H	-6.3018815	1.0929709	0.0000000
H	-6.4210909	-0.4347661	-0.8818230
C	-4.0787626	-1.5595162	0.0000000
H	-4.4779020	-2.0628195	0.8838499
H	-4.4779020	-2.0628195	-0.8838499
H	-2.9964467	-1.7066426	0.0000000
Zn	-1.2205883	0.5040019	0.0000000

N	2.8354215	-3.9696157	0.0000000
C	3.9730602	-4.6251447	0.0000000
C	2.7039866	-2.7166384	0.0000000
N	4.9282664	-5.2822858	0.0000000
N	2.4567264	-1.5713970	0.0000000
N	4.2823727	3.9772474	0.0000000
C	5.5849135	4.1431922	0.0000000
C	3.6854537	2.8678198	0.0000000
N	6.7206589	4.3768201	0.0000000
N	3.0276321	1.8987308	0.0000000
H	4.5889405	0.2249098	2.1617637
H	4.5889405	0.2249098	-2.1617637

1'a

Zn	2.2154523	0.1743833	0.0000000
O	0.6210695	0.3939183	1.2725497
C	-1.8772422	0.3383749	2.7714962
H	-2.6873755	0.2853763	3.5066372
N	-2.2218346	0.4725535	1.5352310
N	-2.2218346	0.4725535	-1.5352310
C	0.6294042	0.2933367	2.5867140
C	0.6945300	0.0588546	5.4066238
C	-0.5078991	0.1366093	4.7388859
H	-1.4245153	0.1064407	5.3179929

C	1.8366969	0.2159409	3.2833067
C	-0.5685150	0.2561375	3.3399125
C	-0.5078991	0.1366093	-4.7388859
H	-1.4245153	0.1064407	-5.3179929
C	1.8366969	0.2159409	-3.2833067
C	1.8761570	0.1015110	-4.6574488
H	2.8408875	0.0451340	-5.1446599
O	0.6210695	0.3939183	-1.2725497
C	1.8761570	0.1015110	4.6574488
H	2.8408875	0.0451340	5.1446599
C	-0.5685150	0.2561375	-3.3399125
C	-1.8772422	0.3383749	-2.7714962
H	-2.6873755	0.2853763	-3.5066372
C	-3.6476722	0.5868952	1.2648703
H	-3.8959932	1.6512616	1.1698463
H	-4.2114264	0.2020154	2.1232995
C	0.6294042	0.2933367	-2.5867140
C	0.6945300	0.0588546	-5.4066238
C	-3.6476722	0.5868952	-1.2648703
H	-4.2114264	0.2020154	-2.1232995
H	-3.8959932	1.6512616	-1.1698463
C	-4.1299071	-0.1324983	0.0000000
C	-5.6553903	-0.0383315	0.0000000
H	-6.0742635	-0.5279539	0.8818216
H	-5.9927409	1.0022413	0.0000000
H	-6.0742635	-0.5279539	-0.8818216

C	-3.7071269	-1.5959801	0.0000000
H	-4.0945922	-2.1080885	0.8839246
H	-4.0945922	-2.1080885	-0.8839246
H	-2.6219089	-1.7211729	0.0000000
Zn	-0.9031864	0.4744436	0.0000000
N	3.0737346	-4.0457561	0.0000000
C	4.1801956	-4.7524288	0.0000000
C	2.9694254	-2.7951606	0.0000000
N	5.1000939	-5.4570177	0.0000000
N	2.7407261	-1.6440836	0.0000000
N	4.5447203	3.7968689	0.0000000
C	5.8360936	4.0337692	0.0000000
C	3.9754975	2.6793899	0.0000000
N	6.9542299	4.3380403	0.0000000
N	3.3281891	1.7001162	0.0000000
H	2.7641113	0.2519516	-2.7224357
H	2.7641113	0.2519516	2.7224357
O	0.6408811	-0.0511177	-6.7536004
O	0.6408811	-0.0511177	6.7536004
C	1.8578569	-0.1573413	7.4570476
H	1.5919066	-0.2463462	8.5085235
H	2.4218005	-1.0461991	7.1536208
H	2.4819790	0.7323239	7.3198374
C	1.8578569	-0.1573413	-7.4570476
H	2.4218005	-1.0461991	-7.1536208
H	1.5919066	-0.2463462	-8.5085235

H	2.4819790	0.7323239	-7.3198374

2'

Zn	1.5701321	0.1644807	0.0000000
O	-0.1156304	0.2947378	1.2772997
O	2.1976347	0.0877003	2.4862408
C	-2.6158903	0.3121233	2.7646022
H	-3.4277794	0.2855300	3.4994215
N	-2.9571280	0.4599431	1.5283636
N	-2.9571280	0.4599431	-1.5283636
C	-0.1256836	0.1904047	2.5792802
C	-0.0626032	-0.0574678	5.3878577
H	-0.0200537	-0.1540009	6.4650090
C	-1.2612364	0.0570588	4.7435136
H	-2.1901798	0.0549882	5.3031608
C	1.1074345	0.0712393	3.2746299
C	-1.3158083	0.1850415	3.3369973
C	-1.2612364	0.0570588	-4.7435136
H	-2.1901798	0.0549882	-5.3031608
C	1.1074345	0.0712393	-3.2746299
C	1.1263629	-0.0499788	-4.6475580
H	2.0712464	-0.1410946	-5.1662905
O	2.1976347	0.0877003	-2.4862408

O	-0.1156304	0.2947378	-1.2772997
C	1.1263629	-0.0499788	4.6475580
H	2.0712464	-0.1410946	5.1662905
C	4.5201850	-0.0714306	2.0018251
H	5.5093124	-0.1951238	2.4457410
H	4.3515577	-0.8905649	1.3023437
H	4.5028616	0.8711588	1.4544777
C	-1.3158083	0.1850415	-3.3369973
C	-2.6158903	0.3121233	-2.7646022
H	-3.4277794	0.2855300	-3.4994215
C	3.4789327	-0.0796666	3.0874320
H	3.4914742	-1.0284382	3.6363875
H	3.6463391	0.7369736	3.7990944
C	-4.3785626	0.6241893	1.2629315
H	-4.5912468	1.6963722	1.1685988
H	-4.9525981	0.2588463	2.1232822
C	-0.1256836	0.1904047	-2.5792802
C	4.5201850	-0.0714306	-2.0018251
H	5.5093124	-0.1951238	-2.4457410
H	4.5028616	0.8711588	-1.4544777
H	4.3515577	-0.8905649	-1.3023437
C	-0.0626032	-0.0574678	-5.3878577
H	-0.0200537	-0.1540009	-6.4650090
C	3.4789327	-0.0796666	-3.0874320
H	3.6463391	0.7369736	-3.7990944
H	3.4914742	-1.0284382	-3.6363875

C	-4.3785626	0.6241893	-1.2629315
H	-4.9525981	0.2588463	-2.1232822
H	-4.5912468	1.6963722	-1.1685988
C	-4.8886275	-0.0776899	0.0000000
C	-6.4095003	0.0713584	0.0000000
H	-6.8457860	-0.4028675	0.8818707
H	-6.7088492	1.1234192	0.0000000
H	-6.8457860	-0.4028675	-0.8818707
C	-4.5186701	-1.5554045	0.0000000
H	-4.9242923	-2.0532683	0.8839513
H	-4.9242923	-2.0532683	-0.8839513
H	-3.4386122	-1.7180505	0.0000000
Zn	-1.6325694	0.4183420	0.0000000
N	2.3886112	-4.0929738	0.0000000
C	3.5300443	-4.7429458	0.0000000
C	2.2636933	-2.8390698	0.0000000
N	4.4910307	-5.3915668	0.0000000
N	2.0350789	-1.6903168	0.0000000
N	3.3302269	4.1274149	0.0000000
C	4.6077142	4.4355604	0.0000000
C	2.8759759	2.9513223	0.0000000
N	5.7122387	4.7881165	0.0000000
N	2.3543575	1.9031929	0.0000000

2'a

Zn	2.0944496	0.2195387	0.0000000
O	0.5013672	0.4419432	1.2726539
C	-1.9972196	0.3697904	2.7706152
H	-2.8074443	0.3115692	3.5053350
N	-2.3420667	0.5087732	1.5347986
N	-2.3420667	0.5087732	-1.5347986
C	0.5093291	0.3344641	2.5865156
C	0.5738541	0.0820113	5.4063262
C	-0.6280383	0.1600466	4.7372405
H	-1.5450438	0.1227137	5.3153861
C	1.7163163	0.2578675	3.2835228
C	-0.6886821	0.2882251	3.3388916
C	-0.6280383	0.1600466	-4.7372405
H	-1.5450438	0.1227137	-5.3153861
C	1.7163163	0.2578675	-3.2835228
C	1.7557618	0.1345442	-4.6569250
H	2.7205948	0.0789149	-5.1436768
O	0.5013672	0.4419432	-1.2726539
C	1.7557618	0.1345442	4.6569250
H	2.7205948	0.0789149	5.1436768
C	-0.6886821	0.2882251	-3.3388916
C	-1.9972196	0.3697904	-2.7706152
H	-2.8074443	0.3115692	-3.5053350
C	-3.7679315	0.6217456	1.2648157
H	-4.0174633	1.6858590	1.1699094

H	-4.3312122	0.2362494	2.1233226
C	0.5093291	0.3344641	-2.5865156
C	0.5738541	0.0820113	-5.4063262
C	-3.7679315	0.6217456	-1.2648157
H	-4.3312122	0.2362494	-2.1233226
H	-4.0174633	1.6858590	-1.1699094
C	-4.2496387	-0.0980660	0.0000000
C	-5.7751910	-0.0054935	0.0000000
H	-6.1935945	-0.4955168	0.8818295
H	-6.1135478	1.0347586	0.0000000
H	-6.1935945	-0.4955168	-0.8818295
C	-3.8250341	-1.5609860	0.0000000
H	-4.2118479	-2.0736276	0.8839163
H	-4.2118479	-2.0736276	-0.8839163
H	-2.7396533	-1.6844359	0.0000000
Zn	-1.0233863	0.5173807	0.0000000
N	2.9263113	-4.0059290	0.0000000
C	4.0270025	-4.7214951	0.0000000
C	2.8323670	-2.7543153	0.0000000
N	4.9409687	-5.4339307	0.0000000
N	2.6132962	-1.6015731	0.0000000
N	4.4181895	3.8447744	0.0000000
C	5.7081559	4.0889478	0.0000000
C	3.8549768	2.7241145	0.0000000
N	6.8243593	4.4002681	0.0000000
N	3.2131830	1.7411729	0.0000000

H	2.6438894	0.3013719	-2.7233841
H	2.6438894	0.3013719	2.7233841
O	0.5192354	-0.0374684	-6.7513878
O	0.5192354	-0.0374684	6.7513878
C	1.7371744	-0.1489451	7.4685879
H	2.2974111	-1.0238514	7.1145332
H	2.3539855	0.7418870	7.2948045
C	1.7371744	-0.1489451	-7.4685879
H	2.2974111	-1.0238514	-7.1145332
H	2.3539855	0.7418870	-7.2948045
C	1.3967322	-0.2865523	8.9288957
H	2.3114581	-0.3764131	9.5176183
H	0.8439175	0.5867081	9.2790934
H	0.7861129	-1.1746753	9.0995334
C	1.3967322	-0.2865523	-8.9288957
H	0.8439175	0.5867081	-9.2790934
H	2.3114581	-0.3764131	-9.5176183
H	0.7861129	-1.1746753	-9.0995334

ZnL^1

O	1.1489382	0.3025799	1.3459645
O	3.4446612	0.1082809	2.5747208
C	-1.3703506	0.2538569	2.7662561
H	-2.2040275	0.2173428	3.4784280

N	-1.6804722	0.4280215	1.5202839
N	-1.6804722	0.4280215	-1.5202839
C	1.1065265	0.1648897	2.6123206
C	1.1290404	-0.1619719	5.4348810
H	1.1588121	-0.2874346	6.5099356
C	-0.0585202	-0.0519705	4.7760212
H	-0.9971285	-0.0853850	5.3203228
C	2.3400371	0.0491313	3.3442984
C	-0.0943912	0.1150854	3.3696715
C	-0.0585202	-0.0519705	-4.7760212
H	-0.9971285	-0.0853850	-5.3203228
C	2.3400371	0.0491313	-3.3442984
C	2.3354757	-0.1094113	-4.7085099
H	3.2718214	-0.1971955	-5.2450633
O	3.4446612	0.1082809	-2.5747208
O	1.1489382	0.3025799	-1.3459645
C	2.3354757	-0.1094113	4.7085099
H	3.2718214	-0.1971955	5.2450633
C	-0.0943912	0.1150854	-3.3696715
C	-1.3703506	0.2538569	-2.7662561
H	-2.2040275	0.2173428	-3.4784280
C	4.6894696	0.0032029	3.2114088
H	4.7998321	-0.9571417	3.7300682
H	4.8463194	0.8152238	3.9319536
C	-3.0954448	0.6191731	1.2562929
H	-3.2924846	1.6947799	1.1550327

H	-3.6792151	0.2713476	2.1192861
C	1.1065265	0.1648897	-2.6123206
C	1.1290404	-0.1619719	-5.4348810
H	1.1588121	-0.2874346	-6.5099356
C	4.6894696	0.0032029	-3.2114088
H	4.8463194	0.8152238	-3.9319536
H	4.7998321	-0.9571417	-3.7300682
C	-3.0954448	0.6191731	-1.2562929
H	-3.6792151	0.2713476	-2.1192861
H	-3.2924846	1.6947799	-1.1550327
C	-3.6239743	-0.0746696	0.0000000
C	-5.1413667	0.1005996	0.0000000
H	-5.5866287	-0.3646901	0.8826466
H	-5.4205789	1.1584877	0.0000000
H	-5.5866287	-0.3646901	-0.8826466
C	-3.2776315	-1.5573439	0.0000000
H	-3.6901085	-2.0488621	0.8849154
H	-3.6901085	-2.0488621	-0.8849154
H	-2.1992671	-1.7255263	0.0000000
Zn	-0.2613013	0.3947467	0.0000000
H	5.4398984	0.0730001	-2.4254328
H	5.4398984	0.0730001	2.4254328

ZnL^2

O	0.5130190	0.3031873	1.3419725
O	2.8084551	0.0939210	2.5566664
C	-2.0027522	0.2525113	2.7671624
H	-2.8354818	0.2153067	3.4804452
N	-2.3145856	0.4280987	1.5215518
N	-2.3145856	0.4280987	-1.5215518
C	0.4734217	0.1607949	2.6077722
C	0.5053736	-0.1756573	5.4272787
H	0.5385176	-0.3045716	6.5018601
C	-0.6846794	-0.0598020	4.7737118
H	-1.6211023	-0.0923865	5.3218283
C	1.7099772	0.0375544	3.3334038
C	-0.7256325	0.1116955	3.3678794
C	-0.6846794	-0.0598020	-4.7737118
H	-1.6211023	-0.0923865	-5.3218283
C	1.7099772	0.0375544	-3.3334038
C	1.7100623	-0.1254244	-4.6972647
H	2.6479605	-0.2185818	-5.2301844
O	2.8084551	0.0939210	-2.5566664
O	0.5130190	0.3031873	-1.3419725
C	1.7100623	-0.1254244	4.6972647
H	2.6479605	-0.2185818	5.2301844
C	5.1128917	0.0568646	2.0851842
H	6.1134207	-0.0304311	2.5141422
H	4.9706131	-0.7454020	1.3595619

H	5.0391204	1.0089670	1.5572060
C	-0.7256325	0.1116955	-3.3678794
C	-2.0027522	0.2525113	-2.7671624
H	-2.8354818	0.2153067	-3.4804452
C	4.0707014	-0.0260584	3.1708130
H	4.1389443	-0.9835982	3.7057719
H	4.2082925	0.7770995	3.9080989
C	-3.7294168	0.6187679	1.2571566
H	-3.9270603	1.6942966	1.1562114
H	-4.3135417	0.2701548	2.1196252
C	0.4734217	0.1607949	-2.6077722
C	5.1128917	0.0568646	-2.0851842
H	6.1134207	-0.0304311	-2.5141422
H	5.0391204	1.0089670	-1.5572060
H	4.9706131	-0.7454020	-1.3595619
C	0.5053736	-0.1756573	-5.4272787
H	0.5385176	-0.3045716	-6.5018601
C	4.0707014	-0.0260584	-3.1708130
H	4.2082925	0.7770995	-3.9080989
H	4.1389443	-0.9835982	-3.7057719
C	-3.7294168	0.6187679	-1.2571566
H	-4.3135417	0.2701548	-2.1196252
H	-3.9270603	1.6942966	-1.1562114
C	-4.2572454	-0.0749476	0.0000000
C	-5.7747573	0.0995315	0.0000000
H	-6.2197721	-0.3659490	0.8826632

H	-6.0545070	1.1572837	0.0000000
H	-6.2197721	-0.3659490	-0.8826632
C	-3.9103271	-1.5575079	0.0000000
H	-4.3225680	-2.0491303	0.8849663
H	-4.3225680	-2.0491303	-0.8849663
H	-2.8319017	-1.7252853	0.0000000
Zn	-0.8996185	0.3964706	0.0000000

ZnL^{1a}

O	1.5430453	0.3371718	1.3403548
C	-0.9886473	0.3212950	2.7717391
H	-1.8219329	0.2958349	3.4848382
N	-1.2957175	0.4718384	1.5232411
N	-1.2957175	0.4718384	-1.5232411
C	1.5015803	0.2211656	2.6178871
C	1.5153815	-0.0509143	5.4551072
C	0.3293449	0.0561375	4.7744873
H	-0.5979887	0.0386907	5.3383929
C	2.7038869	0.1084198	3.3544060
C	0.2925199	0.1942420	3.3723435
C	0.3293449	0.0561375	-4.7744873
H	-0.5979887	0.0386907	-5.3383929
C	2.7038869	0.1084198	-3.3544060
C	2.7142896	-0.0229190	-4.7220473

H	3.6675684	-0.1050539	-5.2298143
O	1.5430453	0.3371718	-1.3403548
C	2.7142896	-0.0229190	4.7220473
H	3.6675684	-0.1050539	5.2298143
C	0.2925199	0.1942420	-3.3723435
C	-0.9886473	0.3212950	-2.7717391
H	-1.8219329	0.2958349	-3.4848382
C	-2.7120001	0.6512866	1.2557677
H	-2.9162579	1.7252225	1.1517995
H	-3.2948014	0.3011224	2.1183217
C	1.5015803	0.2211656	-2.6178871
C	1.5153815	-0.0509143	-5.4551072
C	-2.7120001	0.6512866	-1.2557677
H	-3.2948014	0.3011224	-2.1183217
H	-2.9162579	1.7252225	-1.1517995
C	-3.2324911	-0.0488535	0.0000000
C	-4.7518062	0.1099964	0.0000000
H	-5.1919377	-0.3601239	0.8826238
H	-5.0425608	1.1647713	0.0000000
H	-5.1919377	-0.3601239	-0.8826238
C	-2.8706330	-1.5278646	0.0000000
H	-3.2780583	-2.0235909	0.8848800
H	-3.2780583	-2.0235909	-0.8848800
H	-1.7906395	-1.6853886	0.0000000
Zn	0.1361173	0.4301680	0.0000000
H	3.6304529	0.1278730	-2.7932558

H	3.6304529	0.1278730	2.7932558
O	1.4454401	-0.1737325	-6.8116467
O	1.4454401	-0.1737325	6.8116467
C	2.6499716	-0.3062406	7.5193295
H	3.2051374	-1.2024226	7.2163758
H	3.2962308	0.5709786	7.3947928
C	2.6499716	-0.3062406	-7.5193295
H	3.2051374	-1.2024226	-7.2163758
H	3.2962308	0.5709786	-7.3947928
H	2.3784988	-0.3976954	8.5702260
H	2.3784988	-0.3976954	-8.5702260

ZnL^{2a}

O	1.3176951	0.3298392	1.3399860
C	-1.2124161	0.3596538	2.7736048
H	-2.0454739	0.3474597	3.4873487
N	-1.5195051	0.4969776	1.5234707
N	-1.5195051	0.4969776	-1.5234707
C	1.2763343	0.2348882	2.6193459
C	1.2904085	0.0098863	5.4617877
C	0.1052153	0.1170273	4.7795340
H	-0.8218283	0.1180007	5.3442257
C	2.4780148	0.1209791	3.3566921
C	0.0680018	0.2323279	3.3752078

C	0.1052153	0.1170273	-4.7795340
H	-0.8218283	0.1180007	-5.3442257
C	2.4780148	0.1209791	-3.3566921
C	2.4888398	0.0127179	-4.7262939
H	3.4419005	-0.0709494	-5.2339850
O	1.3176951	0.3298392	-1.3399860
C	2.4888398	0.0127179	4.7262939
H	3.4419005	-0.0709494	5.2339850
C	0.0680018	0.2323279	-3.3752078
C	-1.2124161	0.3596538	-2.7736048
H	-2.0454739	0.3474597	-3.4873487
C	-2.9354681	0.6790605	1.2555697
H	-3.1380901	1.7532886	1.1511018
H	-3.5190473	0.3302022	2.1181019
C	1.2763343	0.2348882	-2.6193459
C	1.2904085	0.0098863	-5.4617877
C	-2.9354681	0.6790605	-1.2555697
H	-3.5190473	0.3302022	-2.1181019
H	-3.1380901	1.7532886	-1.1511018
C	-3.4570252	-0.0205067	0.0000000
C	-4.9761006	0.1406951	0.0000000
H	-5.4169611	-0.3287578	0.8826278
H	-5.2652392	1.1959131	0.0000000
H	-5.4169611	-0.3287578	-0.8826278
C	-3.0979563	-1.5002136	0.0000000
H	-3.5063656	-1.9951289	0.8848783

H	-3.5063656	-1.9951289	-0.8848783
H	-2.0183641	-1.6601873	0.0000000
Zn	-0.0885404	0.4380972	0.0000000
H	3.4042026	0.1210752	-2.7944951
H	3.4042026	0.1210752	2.7944951
O	1.2200217	-0.0878215	-6.8195705
O	1.2200217	-0.0878215	6.8195705
C	2.4227944	-0.2260242	7.5424365
H	2.9603548	-1.1263101	7.2138823
H	3.0765917	0.6376092	7.3596071
C	2.4227944	-0.2260242	-7.5424365
H	2.9603548	-1.1263101	-7.2138823
H	3.0765917	0.6376092	-7.3596071
C	2.0701737	-0.3224919	9.0046564
H	2.9760863	-0.4340550	9.6039430
H	1.5457503	0.5768089	9.3326081
H	1.4243828	-1.1831623	9.1874217
C	2.0701737	-0.3224919	-9.0046564
H	1.5457503	0.5768089	-9.3326081
H	2.9760863	-0.4340550	-9.6039430
H	1.4243828	-1.1831623	-9.1874217

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