SUPPORTING INFORMATION

The Building Blocks of Metallothioneins: Heterometallic Zn^{2+} and Cd^{2+} Clusters from First-Principles Calculations

Kasper P. Jensen* and Martin Rykær

Technical University of Denmark, DTU Chemistry, Building 206, DK-2800 Kongens Lyngby, Denmark

Table S1. The effect of COSMO dielectricity constants on the M-S bond lengths of thiolate complexes (Data used in Figure 3).

ε	$Cd(SCH_3)_4^{2-}$	$Zn(SCH_3)_4^{2-}$
1	2.639	2.420
4	2.610	2.401
6	2.603	2.392
8	2.603	2.392
10	2.600	2.390
16	2.598	2.388
80	2.594	2.385

Table S2. Optimized Non-Screened equilibrium bond lengths of all studied isomers of $Cd_xZn_{4-x}S_{11}^{3-}$ (pm).

Metal	Sulfur	Distance	Mode	Metal	Sulfur	Distance	Mode
Cd_4							
1	2	267.319	b	10	2	264.684	b
cd	3	256.675	t	cd	9	262.288	b
	4	264.958	b		11	256.576	t
	5	257.554	t		12	261.722	b
6	4	263.696	b	13	8	267.317	b
cd	7	257.596	t	cd	12	266.656	b
	8	261.576	b		14	255.492	t
	9	263.077	b		15	257.137	t
Cd_3Zn	**Isomer 1**						
1	2	245.895	b	10	2	266.015	b
zn	3	235.945	t	cd	9	262.870	b
	4	245.477	b		11	256.432	t
	5	237.781	t		12	260.064	b
6	4	260.916	b	13	8	267.408	b
cd	7	257.476	t	cd	12	267.010	b
	8	263.430	b		14	255.537	t
	9	264.107	b		15	257.624	t
Cd_3Zn	**Isomer 2**						
1	2	267.055	b	10	2	265.854	b
cd	3	256.660	t	cd	9	262.567	b
	4	264.853	b		11	256.307	t
	5	257.934	t		12	260.882	b
6	4	263.940	b	13	8	246.272	b
cd	7	257.521	t	zn	12	245.400	b
	8	260.952	b		14	235.392	t
	9	262.947	b		15	236.767	t
Cd_3Zn	**Isomer 3**						
1	2	267.270	b	10	2	264.221	b
cd	3	257.247	t	cd	9	261.412	b
	4	265.592	b		11	256.625	t
	5	258.243	t		12	261.904	b
6	4	243.374	b	13	8	266.654	b
zn	7	237.057	t	cd	12	266.875	b
	8	241.694	b		14	255.707	t
	9	241.091	b		15	257.445	t
Cd_3Zn	**Isomer 4**						
1	2	266.906	b	10	2	244.765	b
cd	3	256.747	t	zn	9	241.838	b

	4	265.619	b		11	236.167	t
	5	258.664	t		12	240.393	b
6	4	262.924	b	13	8	267.645	b
cd	7	258.306	t	cd	12	265.993	b
	8	261.512	b		14	255.705	t
	9	262.7	b		15	257.296	t
Cd_2Zn_2	**Isomer 1**						
1	2	245.545	b	10	2	266.892	b
zn	3	236.114	t	cd	9	262.771	b
	4	245.616	b		11	256.377	t
	5	238.009	t		12	259.435	b
6	4	261.571	b	13	8	246.239	b
cd	7	257.624	t	zn	12	245.291	b
	8	263.154	b		14	235.38	t
	9	264.339	b		15	237.519	t
Cd_2Zn_2	**Isomer 2**						
1	2	245.778	b	10	2	266.317	b
zn	3	236.232	t	cd	9	262.398	b
	4	244.428	b		11	256.823	t
	5	237.813	t		12	260.712	b
6	4	241.331	b	13	8	266.689	b
zn	7	237.333	t	cd	12	267.157	b
	8	242.646	b		14	256.067	t
	9	242.103	b		15	257.757	t
Cd_2Zn_2	**Isomer 3**						
1	2	245.78	b	10	2	244.481	b
zn	3	235.564	t	zn	9	241.459	b
	4	245.516	b		11	236.593	t
	5	238.437	t		12	240.091	b
6	4	260.868	b	13	8	267.728	b
cd	7	258.499	t	cd	12	266.835	b
	8	261.825	b		14	256.063	t
	9	263.763	b		15	257.632	t
Cd_2Zn_2	**Isomer 4**						
1	2	266.376	b	10	2	245.783	b
cd	3	256.757	t	zn	9	241.879	b
	4	265.54	b		11	235.589	t
	5	259.102	t		12	239.363	b
6	4	263.188	b	13	8	246.481	b
cd	7	258.226	t	zn	12	244.573	b
	8	260.781	b		14	235.45	t
	9	262.832	b		15	237.024	t
Cd_2Zn_2	**Isomer 5**						
1	2	267.008	b	10	2	263.505	b
cd	3	257.011	t	cd	9	260.593	b

	4	265.484	b		11	256.568	t
	5	257.175	t		12	262.533	b
6	4	243.141	b	13	8	245.365	b
zn	7	236.143	t	zn	12	246.183	b
	8	241.084	b		14	235.797	t
	9	241.839	b		15	236.875	t
Cd_2Zn_2	**Isomer 6**						
1	2	266.77	b	10	2	244.835	b
cd	3	256.059	t	zn	9	240.943	b
	4	265.196	b		11	236.342	t
	5	259.194	t		12	239.679	b
6	4	242.295	b	13	8	267.111	b
zn	7	237.278	t	cd	12	266.99	b
	8	242.51	b		14	256.079	t
	9	242.259	b		15	258.107	t
$CdZn_3$	**Isomer 1**						
1	2	245.531	b	10	2	245.68	b
zn	3	236.292	t	zn	9	241.537	b
	4	245.236	b		11	236.181	t
	5	238.144	t		12	239.514	b
6	4	260.822	b	13	8	246.588	b
cd	7	257.679	t	zn	12	245.122	b
	8	262.913	b		14	235.564	t
	9	263.429	b		15	237.751	t
$CdZn_3$	**Isomer 2**						
1	2	267.006	b	10	2	244.926	b
Cd	3	257.172	t	zn	9	240.895	b
	4	264.699	b		11	236.647	t
	5	259.766	t		12	240.046	b
6	4	243.417	b	13	8	244.862	b
zn	7	237.322	t	zn	12	246.082	b
	8	240.788	b		14	235.921	t
	9	241.128	b		15	236.946	t
$CdZn_3$	**Isomer 3**						
1	2	244.952	b	10	2	262.764	b
zn	3	237.304	t	cd	9	261.592	b
	4	245.488	b		11	256.948	t
	5	237.189	t		12	263.1	b
6	4	242.832	b	13	8	245.456	b
zn	7	236.546	t	zn	12	245.593	b
	8	241.814	b		14	235.809	t
	9	241.342	b		15	237.187	t
$CdZn_3$	**Isomer 4**						
1	2	244.887	b	10	2	241.035	b

zn	3	237.409	t	zn	9	239.951	b
	4	246.125	b		11	236.589	t
	5	236.988	t		12	243.284	b
6	4	242.109	b	13	8	266.04	b
zn	7	236.721	t	cd	12	267.101	b
	8	242.635	b		14	256.652	t
	9	240.533	b		15	257.873	t
Zn_4							
1	2	245.619	b	10	2	245.005	b
zn	3	236.488	t	zn	9	241.241	b
	4	244.335	b		11	236.449	t
	5	238.03	t		12	239.094	b
6	4	241.161	b	13	8	246.1	b
zn	7	237.539	t	zn	12	244.939	b
	8	242.54	b		14	236.075	t
	9	241.706	b		15	237.886	t

Table S3. Optimized Screened equilibrium bond lengths of all studied isomers of $Cd_xZn_{4-x}S_{11}^{3-}$ (pm). Screened with Cosmo model, ε = 10.

Metal	Sulfur	Distance	Mode	Metal	Sulfur	Distance	Mode
Cd_4							
1	2	264.286	b	10	2	260.339	b
cd	3	255.472	t	cd	9	260.709	b
	4	264.804	b		11	253.508	t
	5	253.882	t		12	261.191	b
6	4	261.685	b	13	8	264.906	b
cd	7	253.953	t	cd	12	264.491	b
	8	260.779	b		14	253.382	t
	9	260.580	b		15	254.905	t
Cd_3Zn	**Isomer 1**						
1	2	243.215	b	10	2	262.747	b
zn	3	234.662	t	cd	9	261.138	b
	4	243.646	b		11	254.152	t
	5	235.275	t		12	258.567	b
6	4	259.198	b	13	8	264.928	b
cd	7	254.007	t	cd	12	264.681	b
	8	262.035	b		14	253.368	t
	9	261.216	b		15	255.395	t
Cd_3Zn	**Isomer 2**						
1	2	265.879	b	10	2	261.444	b
cd	3	255.535	t	cd	9	261.061	b
	4	264.101	b		11	255.133	t
	5	254.305	t		12	260.466	b
6	4	261.924	b	13	8	242.041	b
cd	7	253.206	t	zn	12	244.988	b
	8	260.085	b		14	233.517	t
	9	260.794	b		15	235.260	t
Cd_3Zn	**Isomer 3**						
1	2	264.737	b	10	2	260.303	b
cd	3	255.42	t	cd	9	260.571	b
	4	264.073	b		11	254.963	t
	5	254.146	t		12	261.516	b
6	4	240.241	b	13	8	262.668	b
zn	7	233.485	t	cd	12	265.804	b
	8	239.783	b		14	253.153	t
	9	240.203	b		15	255.461	t

Cd_3Zn	**Isomer 4**						
1	2	263.351	b	10	2	244.765	b
cd	3	255.246	t	zn	9	241.838	b
	4	264.135	b		11	236.167	t
	5	255.196	t		12	240.393	b
6	4	261.012	b	13	8	265.162	b
cd	7	254.916	t	cd	12	264.081	b
	8	260.127	b		14	253.238	t
	9	260.024	b		15	254.762	t
Cd_2Zn_2	**Isomer 1**						
1	2	242.975	b	10	2	263.051	b
zn	3	234.806	t	cd	9	261.276	b
	4	243.712	b		11	253.969	t
	5	235.457	t		12	258.151	b
6	4	259.468	b	13	8	244.107	b
cd	7	254.1	t	zn	12	243.129	b
	8	261.249	b		14	233.751	t
	9	261.324	b		15	235.423	t
Cd_2Zn_2	**Isomer 2**						
1	2	243.665	b	10	2	262.748	b
zn	3	234.675	t	cd	9	261.367	b
	4	241.719	b		11	254.213	t
	5	234.858	t		12	258.175	b
6	4	239.498	b	13	8	264.177	b
zn	7	234.28	t	cd	12	264.561	b
	8	241.506	b		14	253.94	t
	9	240.120	b		15	255.383	t
Cd_2Zn_2	**Isomer 3**						
1	2	242.777	b	10	2	241.560	b
zn	3	234.502	t	zn	9	240.056	b
	4	244.167	b		11	234.819	t
	5	235.670	t		12	238.763	b
6	4	259.508	b	13	8	264.821	b
cd	7	254.803	t	cd	12	264.275	b
	8	260.525	b		14	253.178	t
	9	260.429	b		15	255.154	t
Cd_2Zn_2	**Isomer 4**						
1	2	262.506	b	10	2	242.803	b
cd	3	255.286	t	zn	9	240.525	b
	4	264.581	b		11	233.934	t
	5	255.970	t		12	238.247	b
6	4	261.525	b	13	8	243.998	b
cd	7	254.590	t	zn	12	242.692	b
	8	259.572	b		14	233.179	t
	9	260.006	b		15	235.056	t

Cd_2Zn_2	**Isomer 5**						
1	2	263.452	b	10	2	260.647	b
cd	3	255.658	t	cd	9	260.069	b
	4	264.177	b		11	254.100	t
	5	254.261	t		12	261.454	b
6	4	240.775	b	13	8	241.994	b
zn	7	233.487	t	zn	12	244.952	b
	8	239.747	b		14	233.541	t
	9	239.993	b		15	235.703	t
Cd_2Zn_2	**Isomer 6**						
1	2	263.446	b	10	2	241.845	b
cd	3	254.473	t	zn	9	240.099	b
	4	263.381	b		11	234.257	t
	5	255.492	t		12	238.055	b
6	4	240.155	b	13	8	264.212	b
zn	7	234.519	t	cd	12	263.901	b
	8	240.613	b		14	253.566	t
	9	240.044	b		15	255.468	t
$CdZn_3$	**Isomer 1**						
1	2	242.865	b	10	2	241.940	b
zn	3	234.911	t	zn	9	240.135	b
	4	243.355	b		11	234.75	t
	5	235.539	t		12	238.314	b
6	4	259.222	b	13	8	243.931	b
cd	7	254.097	t	zn	12	242.791	b
	8	261.126	b		14	233.744	t
	9	260.894	b		15	235.664	t
$CdZn_3$	**Isomer 2**						
1	2	263.078	b	10	2	242.747	b
Cd	3	255.502	t	zn	9	239.874	b
	4	263.775	b		11	234.663	t
	5	256.198	t		12	238.007	b
6	4	241.695	b	13	8	242.874	b
zn	7	234.568	t	zn	12	243.724	b
	8	239.424	b		14	233.716	t
	9	239.240	b		15	235.146	t
$CdZn_3$	**Isomer 3**						
1	2	242.587	b	10	2	260.021	b
zn	3	236.05	t	cd	9	259.627	b
	4	243.767	b		11	254.093	t
	5	234.900	t		12	261.426	b
6	4	240.259	b	13	8	241.625	b
zn	7	233.515	t	zn	12	244.783	b
	8	239.906	b		14	233.579	t
	9	239.952	b		15	235.703	t

$CdZn_3$	**Isomer 4**						
1	2	242.029	b	10	2	239.850	b
zn	3	236.236	t	zn	9	239.016	b
	4	243.667	b		11	234.103	t
	5	234.702	t		12	240.897	b
6	4	240.827	b	13	8	264.320	b
zn	7	234.151	t	cd	12	264.930	b
	8	240.794	b		14	253.465	t
	9	239.066	b		15	254.916	t
Zn_4							
1	2	242.614	b	10	2	241.723	b
zn	3	235.000	t	zn	9	240.056	b
	4	243.173	b		11	234.530	t
	5	235.585	t		12	237.734	b
6	4	239.628	b	13	8	243.749	b
zn	7	234.737	t	zn	12	242.030	b
	8	240.729	b		14	234.138	t
	9	239.765	b		15	235.725	t

Table S4. Optimized equilibrium bond lengths of all studied isomers of $Cd_yZn_{3-y}S_9^{3-}$ (pm). Screened with Cosmo model, ε = 10.

Metal	Sulfur	Distance	Mode	Metal	Sulfur	Distance	Mode	Metal	Sulfur	Distance	Mode
Cd_3											
1	2	261.647	b	6	2	262.412	b	10	3	263.599	b
	3	264.109	b		7	264.371	b		7	263.749	b
	4	256.914	t		8	257.282	t		11	255.908	t
	5	254.701	t		9	253.540	t		12	255.268	t
Cd_2Zn		**isomer**	**1**								
1	2	264.378	b	6	2	263.233	b	10	3	242.325	b
cd	3	261.084	b	cd	7	262.295	b	zn	7	243.481	b
	4	258.122	t		8	255.893	t		11	235.040	t
	5	253.632	t		9	257.080	t		12	234.552	t
Cd_2Zn		**isomer**	**2**								
1	2	261.245	b	6	2	242.084	b	10	3	264.326	b
cd	3	265.750	b	zn	7	241.940	b	cd	7	262.514	b
	4	257.650	t		8	236.578	t		11	256.483	t
	5	253.660	t		9	235.299	t		12	254.623	t
Cd_2Zn		**isomer**	**3**								
1	2	242.355	b	6	2	261.122	b	10	3	263.241	b
zn	3	243.237	b		7	263.471	b		7	264.101	b
	4	236.014	t		8	256.804	t		11	255.788	t
	5	233.655	t		9	255.926	t		12	255.202	t
$CdZn_2$		**isomer**	**1**								
1	2	241.770	b	6	2	240.619	b	10	3	262.596	b
zn	3	240.778	b	zn	7	243.018	b	cd	7	264.175	b
	4	236.261	t		8	237.493	t		11	257.045	t
	5	235.820	t		9	234.181	t		12	254.661	t
$CdZn_2$		**isomer**	**2**								
1	2	243.176	b	6	2	261.501	b	10	3	242.063	b
zn	3	241.772	b	cd	7	262.861	b	zn	7	244.430	b
	4	236.780	t		8	256.972	t		11	234.860	t
	5	233.608	t		9	256.671	t		12	235.319	t
$CdZn_2$		**isomer**	**3**								
1	2	261.935	b	6	2	241.329	b	10	3	243.389	b
cd	3	262.417	b	zn	7	242.241	b	zn	7	241.342	b
	4	257.229	t		8	235.867	t		11	236.816	t
	5	255.357	t		9	236.304	t		12	234.160	t
Zn_3											
1	2	240.589	b	6	2	241.375	b	10	3	243.309	b
	3	242.486	b		7	241.526	b		7	241.867	b
	4	238.214	t		8	236.478	t		11	235.860	t
	5	234.458	t		9	236.489	t		12	235.112	t

TABLE S5. Average Equilibrium bond lengths (Å) of geometry-optimized clusters without Screening.

Cluster	*Isomer*	*Cd-S^t_{av}*	*Zn-S^t_{av}*	*Cd-S^b_{av}*	*Zn-S^b_{av}*
Cd_4	1	2.57	---	2.64	---
Cd_3Zn	1	2.57	2.37	2.64	2.46
	2	2.57	2.36	2.64	2.46
	3	2.57	2.37	2.65	2.42
	4	2.57	2.36	2.65	2.42
Cd_2Zn_2	1	2.57	2.37	2.63	2.46
	2	2.57	2.37	2.65	2.43
	3	2.57	2.37	2.64	2.43
	4	2.58	2.36	2.64	2.44
	5	2.57	2.36	2.64	2.44
	6	2.57	2.37	2.67	2.42
$CdZn_3$	1	2.58	2.37	2.62	2.44
	2	2.58	2.37	2.66	2.43
	3	2.57	2.37	2.62	2.44
	4	2.57	2.37	2.67	2.43
Zn_4	1	---	2.37	---	2.43
Cd_3	1	2.59	---	2.66	---
Cd_2Zn	1	2.60	2.36	2.65	2.46
	2	2.59	2.39	2.67	2.44
	3	2.59	2.38	2.66	2.45
$CdZn_2$	1	2.58	2.39	2.68	2.44
	2	2.61	2.38	2.65	2.45
	3	2.60	2.38	2.65	2.45
Zn_3	1	---	2.39	---	2.45
average		*2.58*	*2.37*	*2.65*	*2.44*

TABLE S6. Optimized equilibrium S-M-S angles of all studied isomers. Screened with Cosmo model, ε = 10.

Cd_4

2	1	3	102.7	4	6	7	105.2	2	10	9	115.3	8	13	12	106.6
2	1	4	110.2	4	6	8	106.1	2	10	11	112.8	8	13	14	110.1
2	1	5	109.1	4	6	9	113.2	2	10	12	103.6	8	13	15	107.3
3	1	4	105.4	7	6	8	112.7	9	10	11	107.3	12	13	14	110.7
3	1	5	120.9	7	6	9	111.1	9	10	12	107.9	12	13	15	107.9
4	1	5	108.3	8	6	9	108.6	11	10	12	109.7	14	13	15	114.1
	Cd				Cd				Cd				Cd		

Cd_3Zn Isomer 1

2	1	3	112.8	4	6	7	112.4	2	10	9	103.9	8	13	12	102.9
2	1	4	108.9	4	6	8	102.1	2	10	11	103.8	8	13	14	110.3
2	1	5	108.8	4	6	9	116.4	2	10	12	114.8	8	13	15	111.0
3	1	4	104.1	7	6	8	111.4	9	10	11	118.2	12	13	14	114.1
3	1	5	110.0	7	6	9	107.2	9	10	12	108.5	12	13	15	104.1
4	1	5	112.3	8	6	9	107.2	11	10	12	108.0	14	13	15	113.9
	Zn				Cd				Cd				Cd		

Cd_3Zn Isomer 2

2	1	3	102.6	4	6	7	107.2	2	10	9	110.8	8	13	12	107.3
2	1	4	112.8	4	6	8	104.0	2	10	11	110.4	8	13	14	114.7
2	1	5	109.6	4	6	9	113.4	2	10	12	108.1	8	13	15	106.4
3	1	4	104.6	7	6	8	113.4	9	10	11	111.4	12	13	14	112.0
3	1	5	120.4	7	6	9	111.4	9	10	12	109.8	12	13	15	109.1
4	1	5	106.9	8	6	9	107.3	11	10	12	106.2	14	13	15	112.5
	Cd				Cd				Cd				Zn		

Cd_3Zn Isomer 3

2	1	3	105.4	4	6	7	107.3	2	10	9	111.1	8	13	12	98.8
2	1	4	111.4	4	6	8	103.1	2	10	11	111.6	8	13	14	118.6
2	1	5	110.5	4	6	9	114.2	2	10	12	108.5	8	13	15	104.7
3	1	4	106.5	7	6	8	115.1	9	10	11	112.2	12	13	14	111.3
3	1	5	114.1	7	6	9	109.9	9	10	12	107.4	12	13	15	110.4
4	1	5	108.9	8	6	9	107.4	11	10	12	106.0	14	13	15	112.3
	Cd				Zn				Cd				Cd		

Cd_3Zn Isomer 4

2	1	3	107.8	4	6	7	107.1	2	10	9	107.9	8	13	12	105.3
2	1	4	113.9	4	6	8	105.5	2	10	11	108.5	8	13	14	109.4
2	1	5	107.1	4	6	9	112.4	2	10	12	108.2	8	13	15	109.0
3	1	4	106.7	7	6	8	109.2	9	10	11	112.5	12	13	14	113.7
3	1	5	113.1	7	6	9	108.7	9	10	12	110.9	12	13	15	103.4
4	1	5	108.4	8	6	9	113.7	11	10	12	108.7	14	13	15	115.4
	Cd				Cd				Zn				Cd		

Zn_4

2	1	3	113.2	4	6	7	110.1	2	10	9	105.0	8	13	12	104.1
2	1	4	108.5	4	6	8	102.4	2	10	11	105.8	8	13	14	113.3
2	1	5	108.6	4	6	9	115.4	2	10	12	112.0	8	13	15	108.6
3	1	4	104.7	7	6	8	113.2	9	10	11	116.3	12	13	14	111.4
3	1	5	108.8	7	6	9	107.6	9	10	12	107.9	12	13	15	106.4
4	1	5	113.0	8	6	9	108.2	11	10	12	109.8	14	13	15	112.4
	Zn				Zn				Zn				Zn		

Cd_2Zn_2 Isomer 1

2	1	3	112.6	4	6	7	111.3	2	10	9	102.9	8	13	12	104.3
2	1	4	109.0	4	6	8	102.0	2	10	11	103.5	8	13	14	112.4
2	1	5	108.9	4	6	9	116.8	2	10	12	115.4	8	13	15	108.9
3	1	4	104.6	7	6	8	113.0	9	10	11	118.1	12	13	14	111.5
3	1	5	109.6	7	6	9	106.8	9	10	12	107.7	12	13	15	106.6
4	1	5	112.2	8	6	9	107.1	11	10	12	109.4	14	13	15	112.7
	Zn				Cd				Cd				Zn		

Cd_2Zn_2 Isomer 2

2	1	3	112.0	4	6	7	111.8	2	10	9	101.5	8	13	12	106.7
2	1	4	105.4	4	6	8	98.8	2	10	11	104.4	8	13	14	110.0
2	1	5	110.2	4	6	9	116.8	2	10	12	117.0	8	13	15	109.4
3	1	4	106.2	7	6	8	114.0	9	10	11	118.0	12	13	14	110.5
3	1	5	110.5	7	6	9	108.3	9	10	12	108.1	12	13	15	105.6
4	1	5	112.5	8	6	9	107.0	11	10	12	108.3	14	13	15	114.3
	Zn				Zn				Cd				Cd		

Cd_2Zn_2 Isomer 3

2	1	3	113.2	4	6	7	108.9	2	10	9	105.5	8	13	12	104.8
2	1	4	109.6	4	6	8	104.4	2	10	11	105.2	8	13	14	111.2
2	1	5	108.2	4	6	9	116.3	2	10	12	112.7	8	13	15	108.6
3	1	4	106.0	7	6	8	111.2	9	10	11	115.3	12	13	14	112.3
3	1	5	109.9	7	6	9	106.7	9	10	12	109.8	12	13	15	105.9
4	1	5	110.0	8	6	9	109.3	11	10	12	108.3	14	13	15	113.5
	Zn				Cd				Zn				Cd		

Cd_2Zn_2 Isomer 4

2	1	3	109.3	4	6	7	107.8	2	10	9	107.0	8	13	12	103.4
2	1	4	112.9	4	6	8	105.0	2	10	11	107.6	8	13	14	112.8
2	1	5	107.0	4	6	9	112.5	2	10	12	107.9	8	13	15	108.5
3	1	4	108.4	7	6	8	110.3	9	10	11	112.9	12	13	14	112.2
3	1	5	110.1	7	6	9	108.9	9	10	12	110.6	12	13	15	106.5
4	1	5	109.1	8	6	9	112.3	11	10	12	110.6	14	13	15	112.9
	Cd				Cd				Zn				Zn		

Cd_2Zn_2 Isomer 5

2	1	3	105.2	4	6	7	106.7	2	10	9	116.0	8	13	12	102.3
2	1	4	111.3	4	6	8	104.1	2	10	11	108.8	8	13	14	114.7
2	1	5	108.1	4	6	9	114.3	2	10	12	107.6	8	13	15	106.4
3	1	4	105.6	7	6	8	115.4	9	10	11	108.3	12	13	14	112.4
3	1	5	116.9	7	6	9	111.0	9	10	12	105.2	12	13	15	108.9
4	1	5	109.6	8	6	9	105.4	11	10	12	111.0	14	13	15	111.5
	Cd				Zn				Cd				Zn		

Cd_2Zn_2 Isomer 6

2	1	3	110.9	4	6	7	110.5	2	10	9	105.0	8	13	12	101.6
2	1	4	109.2	4	6	8	101.2	2	10	11	105.5	8	13	14	111.3
2	1	5	107.1	4	6	9	115.5	2	10	12	112.6	8	13	15	110.4
3	1	4	107.4	7	6	8	112.7	9	10	11	116.1	12	13	14	115.3
3	1	5	111.0	7	6	9	107.4	9	10	12	108.3	12	13	15	104.1
4	1	5	111.3	8	6	9	109.5	11	10	12	109.4	14	13	15	113.3
	Cd				Zn				Zn				Cd		

$CdZn_3$ Isomer 1

2	1	3	113.1	4	6	7	111.7	2	10	9	105.5	8	13	12	104.1
2	1	4	108.1	4	6	8	101.4	2	10	11	105.2	8	13	14	112.3
2	1	5	108.5	4	6	9	117.1	2	10	12	113.4	8	13	15	109.1
3	1	4	105.6	7	6	8	113.3	9	10	11	116.2	12	13	14	113.4
3	1	5	109.6	7	6	9	106.2	9	10	12	107.1	12	13	15	105.5
4	1	5	112.0	8	6	9	107.2	11	10	12	109.5	14	13	15	112.1
	Zn				Cd				Zn				Zn		

$CdZn_3$ Isomer 2

2	1	3	108.3	4	6	7	106.1	2	10	9	109.3	8	13	12	103.7
2	1	4	113.7	4	6	8	104.8	2	10	11	108.3	8	13	14	112.9
2	1	5	107.0	4	6	9	113.7	2	10	12	108.4	8	13	15	108.7
3	1	4	107.5	7	6	8	113.6	9	10	11	112.4	12	13	14	112.8
3	1	5	111.2	7	6	9	109.1	9	10	12	108.4	12	13	15	106.0
4	1	5	109.1	8	6	9	109.6	11	10	12	110.1	14	13	15	112.5
	Cd				Zn				Zn				Zn		

$CdZn_3$ Isomer 3

2	1	3	106.6	4	6	7	108.2	2	10	9	114.9	8	13	12	102.0
2	1	4	111.1	4	6	8	103.4	2	10	11	109.2	8	13	14	114.4
2	1	5	109.4	4	6	9	113.2	2	10	12	108.8	8	13	15	106.4
3	1	4	104.3	7	6	8	114.9	9	10	11	108.5	12	13	14	112.9
3	1	5	113.7	7	6	9	110.5	9	10	12	106.3	12	13	15	108.9
4	1	5	111.7	8	6	9	106.3	11	10	12	109.7	14	13	15	111.6
	Zn				Zn				Cd				Zn		

$CdZn_3$ Isomer 4

2	1	3	107.0	4	6	7	106.6	2	10	9	115.8	8	13	12	105.5
2	1	4	108.4	4	6	8	105.4	2	10	11	110.0	8	13	14	110.6
2	1	5	110.7	4	6	9	113.3	2	10	12	105.4	8	13	15	107.9
3	1	4	104.5	7	6	8	112.8	9	10	11	107.5	12	13	14	111.3
3	1	5	113.8	7	6	9	110.3	9	10	12	107.4	12	13	15	107.6
4	1	5	112.1	8	6	9	108.4	11	10	12	110.7	14	13	15	113.5
	Zn				Zn				Zn				Cd		

Cd_3

2	1	3	112.5	2	6	7	111.9	3	10	7	115.5
2	1	4	104.9	2	6	8	106.0	3	10	11	106.6
2	1	5	111.3	2	6	9	111.9	3	10	12	106.1
3	1	4	105.7	7	6	8	104.5	7	10	11	105.5
3	1	5	109.3	7	6	9	109.2	7	10	12	109.5
4	1	5	113.0	8	6	9	113.1	11	10	12	114.0
	Cd				Cd				Cd		

Cd_2Zn Isomer 1

2	1	3	98.3	2	6	7	110.4	3	10	7	103.0
2	1	4	109.6	2	6	8	105.5	3	10	11	111.2
2	1	5	111.5	2	6	9	112.1	3	10	12	109.8
3	1	4	105.4	7	6	8	117.9	7	10	11	109.5
3	1	5	123.5	7	6	9	103.1	7	10	12	112.1
4	1	5	107.7	8	6	9	107.9	11	10	12	111.0
	Cd				Cd				Zn		

Cd_2Zn Isomer 2

2	1	3	105.3	2	6	7	112.4	3	10	7	108.9
2	1	4	106.2	2	6	8	106.3	3	10	11	107.3
2	1	5	115.8	2	6	9	108.0	3	10	12	112.5
3	1	4	108.5	7	6	8	112.6	7	10	11	106.3
3	1	5	109.1	7	6	9	105.8	7	10	12	112.9
4	1	5	111.6	8	6	9	111.9	11	10	12	108.5
	Cd				Zn				Cd		

Cd_2Zn Isomer 3

2	1	3	109.1	2	6	7	113.9	3	10	7	111.4
2	1	4	105.6	2	6	8	109.6	3	10	11	107.5
2	1	5	111.7	2	6	9	108.5	3	10	12	111.7
3	1	4	105.4	7	6	8	108.1	7	10	11	108.7
3	1	5	111.6	7	6	9	106.6	7	10	12	106.5
4	1	5	113.2	8	6	9	110.2	11	10	12	111.1
	Zn				Cd				Cd		

$CdZn_2$ Isomer 1

2	1	3	114.4	2	6	7	114.4	3	10	7	109.5
2	1	4	106.4	2	6	8	104.5	3	10	11	107.2
2	1	5	107.3	2	6	9	112.4	3	10	12	112.3
3	1	4	109.0	7	6	8	105.5	7	10	11	104.7
3	1	5	107.2	7	6	9	105.1	7	10	12	112.7
4	1	5	112.6	8	6	9	115.2	11	10	12	109.9
	Zn				Zn				Cd		

$CdZn_2$ Isomer 2

2	1	3	102.7	2	6	7	112.8	3	10	7	107.0
2	1	4	109.0	2	6	8	110.4	3	10	11	111.4
2	1	5	111.2	2	6	9	106.1	3	10	12	108.3
3	1	4	102.8	7	6	8	108.2	7	10	11	109.7
3	1	5	120.0	7	6	9	109.8	7	10	12	109.6
4	1	5	110.3	8	6	9	109.5	11	10	12	110.8
	Zn				Cd				Zn		

$CdZn_2$ Isomer 3

2	1	3	114.6	2	6	7	112.3	3	10	7	107.4
2	1	4	103.8	2	6	8	107.4	3	10	11	109.5
2	1	5	111.1	2	6	9	107.8	3	10	12	110.7
3	1	4	110.9	7	6	8	114.3	7	10	11	107.1
3	1	5	107.3	7	6	9	103.5	7	10	12	114.8
4	1	5	109.0	8	6	9	111.5	11	10	12	107.4
	Cd				Zn				Zn		

Zn_3

2	1	3	107.7	2	6	7	110.6	3	10	7	107.6
2	1	4	103.9	2	6	8	107.7	3	10	11	111.3
2	1	5	115.7	2	6	9	107.9	3	10	12	108.4
3	1	4	110.6	7	6	8	114.1	7	10	11	108.0
3	1	5	108.4	7	6	9	105.9	7	10	12	113.6
4	1	5	110.6	8	6	9	110.6	11	10	12	108.1
	Zn				Zn				Zn		

TABLE S7. Mean Absolute Deviation (MAD) of cluster S-M-S angles from ideal (109.5º).

Cd_4

2	1	3	6.8	4	6	7	4.3	2	10	9	5.8	8	13	12	2.9
2	1	4	0.7	4	6	8	3.4	2	10	11	3.3	8	13	14	0.6
2	1	5	0.4	4	6	9	3.7	2	10	12	5.9	8	13	15	2.2
3	1	4	4.1	7	6	8	3.2	9	10	11	2.2	12	13	14	1.2
3	1	5	11.4	7	6	9	1.6	9	10	12	1.6	12	13	15	1.6
4	1	5	1.2	8	6	9	0.9	11	10	12	0.2	14	13	15	4.6
	Cd	***MAD***	***4.1***		Cd	***MAD***	***2.9***		Cd	***MAD***	***3.2***		Cd	***MAD***	***2.2***

Cd_3Zn Isomer 1

2	1	3	3.3	4	6	7	2.9	2	10	9	5.6	8	13	12	6.6
2	1	4	0.6	4	6	8	7.4	2	10	11	5.7	8	13	14	0.8
2	1	5	0.7	4	6	9	6.9	2	10	12	5.3	8	13	15	1.5
3	1	4	5.4	7	6	8	1.9	9	10	11	8.7	12	13	14	4.6
3	1	5	0.5	7	6	9	2.3	9	10	12	1.0	12	13	15	5.4
4	1	5	2.8	8	6	9	2.3	11	10	12	1.5	14	13	15	4.4
	Zn	***MAD***	***2.2***		Cd	***MAD***	***4.0***		Cd	***MAD***	***4.6***		Cd	***MAD***	***3.9***

Cd_3Zn Isomer 2

2	1	3	6.9	4	6	7	2.3	2	10	9	1.3	8	13	12	2.2
2	1	4	3.3	4	6	8	5.5	2	10	11	0.9	8	13	14	5.2
2	1	5	0.1	4	6	9	3.9	2	10	12	1.4	8	13	15	3.1
3	1	4	4.9	7	6	8	3.9	9	10	11	1.9	12	13	14	2.5
3	1	5	10.9	7	6	9	1.9	9	10	12	0.3	12	13	15	0.4
4	1	5	2.6	8	6	9	2.2	11	10	12	3.3	14	13	15	3.0
	Cd	***MAD***	***4.8***		Cd	***MAD***	***3.3***		Cd	***MAD***	***1.5***		Zn	***MAD***	***2.7***

Cd_3Zn Isomer 3

2	1	3	4.1	4	6	7	2.2	2	10	9	1.6	8	13	12	10.7
2	1	4	1.9	4	6	8	6.4	2	10	11	2.1	8	13	14	9.1
2	1	5	1.0	4	6	9	4.7	2	10	12	1.0	8	13	15	4.8
3	1	4	3.0	7	6	8	5.6	9	10	11	2.7	12	13	14	1.8
3	1	5	4.6	7	6	9	0.4	9	10	12	2.1	12	13	15	0.9
4	1	5	0.6	8	6	9	2.1	11	10	12	3.5	14	13	15	2.8
	Cd	***MAD***	***2.5***		Zn	***MAD***	***3.6***		Cd	***MAD***	***2.2***		Cd	***MAD***	***5.0***

Cd_3Zn Isomer 4

2	1	3	1.7	4	6	7	2.4	2	10	9	1.6	8	13	12	4.2
2	1	4	4.4	4	6	8	4.0	2	10	11	1.0	8	13	14	0.1
2	1	5	2.4	4	6	9	2.9	2	10	12	1.3	8	13	15	0.5
3	1	4	2.8	7	6	8	0.3	9	10	11	3.0	12	13	14	4.2
3	1	5	3.6	7	6	9	0.8	9	10	12	1.4	12	13	15	6.1
4	1	5	1.1	8	6	9	4.2	11	10	12	0.8	14	13	15	5.9
	Cd	***MAD***	***2.7***		Cd	***MAD***	***2.4***		Zn	***MAD***	***1.5***		Cd	***MAD***	***3.5***

Zn_4

2	1	3	3.7	4	6	7	0.6	2	10	9	4.5	8	13	12	5.4
2	1	4	1.0	4	6	8	7.1	2	10	11	3.7	8	13	14	3.8
2	1	5	0.9	4	6	9	5.9	2	10	12	2.5	8	13	15	0.9
3	1	4	4.8	7	6	8	3.7	9	10	11	6.8	12	13	14	1.9
3	1	5	0.7	7	6	9	1.9	9	10	12	1.6	12	13	15	3.1
4	1	5	3.5	8	6	9	1.3	11	10	12	0.3	14	13	15	2.9
		MAD	***2.4***			***MAD***	***3.4***			***MAD***	***3.2***			***MAD***	***3.0***

Cd_2Zn_2 Isomer 1

2	1	3	3.1	4	6	7	1.8	2	10	9	6.6	8	13	12	5.2
2	1	4	0.5	4	6	8	7.5	2	10	11	6.0	8	13	14	2.9
2	1	5	0.6	4	6	9	7.3	2	10	12	5.9	8	13	15	0.6
3	1	4	4.9	7	6	8	3.5	9	10	11	8.6	12	13	14	2.0
3	1	5	0.1	7	6	9	2.7	9	10	12	1.8	12	13	15	2.9
4	1	5	2.7	8	6	9	2.4	11	10	12	0.1	14	13	15	3.2
	Zn	***MAD***	***2.0***		Cd	***MAD***	***4.2***		Cd	***MAD***	***4.8***		Zn	***MAD***	***2.8***

Cd_2Zn_2 Isomer 2

2	1	3	2.5	4	6	7	2.3	2	10	9	8.0	8	13	12	2.8
2	1	4	4.1	4	6	8	10.7	2	10	11	5.1	8	13	14	0.5
2	1	5	0.7	4	6	9	7.3	2	10	12	7.5	8	13	15	0.1
3	1	4	3.3	7	6	8	4.5	9	10	11	8.5	12	13	14	1.0
3	1	5	1.0	7	6	9	1.2	9	10	12	1.4	12	13	15	3.9
4	1	5	3.0	8	6	9	2.5	11	10	12	1.2	14	13	15	4.8
	Zn	***MAD***	***2.4***		Zn	***MAD***	***4.8***		Cd	***MAD***	***5.3***		Cd	***MAD***	***2.2***

Cd_2Zn_2 Isomer 3

2	1	3	3.7	4	6	7	0.6	2	10	9	4.0	8	13	12	4.7
2	1	4	0.1	4	6	8	5.1	2	10	11	4.3	8	13	14	1.7
2	1	5	1.3	4	6	9	6.8	2	10	12	3.2	8	13	15	0.9
3	1	4	3.5	7	6	8	1.7	9	10	11	5.8	12	13	14	2.8
3	1	5	0.4	7	6	9	2.8	9	10	12	0.3	12	13	15	3.6
4	1	5	0.5	8	6	9	0.2	11	10	12	1.2	14	13	15	4.0
	Zn	***MAD***	***1.6***		Cd	***MAD***	***2.9***		Zn	***MAD***	***3.1***		Cd	***MAD***	***3.0***

Cd_2Zn_2 Isomer 4

2	1	3	0.2	4	6	7	1.7	2	10	9	2.5	8	13	12	6.1
2	1	4	3.4	4	6	8	4.5	2	10	11	1.9	8	13	14	3.3
2	1	5	2.5	4	6	9	3.0	2	10	12	1.6	8	13	15	1.0
3	1	4	1.1	7	6	8	0.8	9	10	11	3.4	12	13	14	2.7
3	1	5	0.6	7	6	9	0.6	9	10	12	1.1	12	13	15	3.0
4	1	5	0.4	8	6	9	2.8	11	10	12	1.1	14	13	15	3.4
	Cd	***MAD***	***1.4***		Cd	***MAD***	***2.2***		Zn	***MAD***	***1.9***		Zn	***MAD***	***3.3***

Cd_2Zn_2 Isomer 5

2	1	3	4.3	4	6	7	2.8	2	10	9	6.5	8	13	12	7.2
2	1	4	1.8	4	6	8	5.4	2	10	11	0.7	8	13	14	5.2
2	1	5	1.4	4	6	9	4.8	2	10	12	1.9	8	13	15	3.1
3	1	4	3.9	7	6	8	5.9	9	10	11	1.2	12	13	14	2.9
3	1	5	7.4	7	6	9	1.5	9	10	12	4.3	12	13	15	0.6
4	1	5	0.1	8	6	9	4.1	11	10	12	1.5	14	13	15	2.0
	Cd	***MAD***	***3.2***		Zn	***MAD***	***4.1***		Cd	***MAD***	***2.7***		Zn	***MAD***	***3.5***

Cd_2Zn_2 Isomer 6

2	1	3	1.4	4	6	7	1.0	2	10	9	4.5	8	13	12	7.9
2	1	4	0.3	4	6	8	8.3	2	10	11	4.0	8	13	14	1.8
2	1	5	2.4	4	6	9	6.0	2	10	12	3.1	8	13	15	0.9
3	1	4	2.1	7	6	8	3.2	9	10	11	6.6	12	13	14	5.8
3	1	5	1.5	7	6	9	2.1	9	10	12	1.2	12	13	15	5.4
4	1	5	1.8	8	6	9	0.0	11	10	12	0.1	14	13	15	3.8
	Cd	***MAD***	***1.6***		Zn	***MAD***	***3.4***		Zn	***MAD***	***3.3***		Cd	***MAD***	***4.3***

$CdZn_3$ Isomer 1

2	1	3	3.6	4	6	7	2.2	2	10	9	4.0	8	13	12	5.4
2	1	4	1.4	4	6	8	8.1	2	10	11	4.3	8	13	14	2.8
2	1	5	1.0	4	6	9	7.6	2	10	12	3.9	8	13	15	0.4
3	1	4	3.9	7	6	8	3.8	9	10	11	6.7	12	13	14	3.9
3	1	5	0.1	7	6	9	3.3	9	10	12	2.4	12	13	15	4.0
4	1	5	2.5	8	6	9	2.3	11	10	12	0.0	14	13	15	2.6
	Zn	***MAD***	***2.1***		Cd	***MAD***	***4.6***		Zn	***MAD***	***3.6***		Zn	***MAD***	***3.2***

$CdZn_3$ Isomer 2

2	1	3	1.2	4	6	7	3.4	2	10	9	0.2	8	13	12	5.8
2	1	4	4.2	4	6	8	4.7	2	10	11	1.2	8	13	14	3.4
2	1	5	2.5	4	6	9	4.2	2	10	12	1.1	8	13	15	0.8
3	1	4	2.0	7	6	8	4.1	9	10	11	2.9	12	13	14	3.3
3	1	5	1.7	7	6	9	0.4	9	10	12	1.1	12	13	15	3.5
4	1	5	0.4	8	6	9	0.1	11	10	12	0.6	14	13	15	3.0
	Cd	***MAD***	***2.0***		Zn	***MAD***	***2.8***		Zn	***MAD***	***1.2***		Zn	***MAD***	***3.3***

$CdZn_3$ Isomer 3

2	1	3	2.9	4	6	7	1.3	2	10	9	5.4	8	13	12	7.5
2	1	4	1.6	4	6	8	6.1	2	10	11	0.3	8	13	14	4.9
2	1	5	0.1	4	6	9	3.7	2	10	12	0.7	8	13	15	3.1
3	1	4	5.2	7	6	8	5.4	9	10	11	1.0	12	13	14	3.4
3	1	5	4.2	7	6	9	1.0	9	10	12	3.2	12	13	15	0.6
4	1	5	2.2	8	6	9	3.2	11	10	12	0.2	14	13	15	2.1
	Zn	***MAD***	***2.7***		Zn	***MAD***	***3.5***		Cd	***MAD***	***1.8***		Zn	***MAD***	***3.6***

$CdZn_3$ Isomer 4

2	1	3	2.5	4	6	7	2.9	2	10	9	6.3	8	13	12	4.0
2	1	4	1.1	4	6	8	4.1	2	10	11	0.5	8	13	14	1.1
2	1	5	1.2	4	6	9	3.8	2	10	12	4.1	8	13	15	1.6
3	1	4	5.0	7	6	8	3.3	9	10	11	2.0	12	13	14	1.8
3	1	5	4.3	7	6	9	0.8	9	10	12	2.1	12	13	15	1.9
4	1	5	2.6	8	6	9	1.1	11	10	12	1.2	14	13	15	4.0
	Zn	***MAD***	***2.8***		Zn	***MAD***	***2.7***		Zn	***MAD***	***2.7***		Cd	***MAD***	***2.4***

Cd_3

2	1	3	3.0	2	6	7	2.4	3	10	7	6.0
2	1	4	4.6	2	6	8	3.5	3	10	11	2.9
2	1	5	1.8	2	6	9	2.4	3	10	12	3.4
3	1	4	3.8	7	6	8	5.0	7	10	11	4.0
3	1	5	0.2	7	6	9	0.3	7	10	12	0.0
4	1	5	3.5	8	6	9	3.6	11	10	12	4.5
	Cd	***MAD***	***2.8***		Cd	***MAD***	***2.9***		Cd	***MAD***	***3.5***

Cd_2Zn Isomer 1

2	1	3	11.2	2	6	7	0.9	3	10	7	6.5
2	1	4	0.1	2	6	8	4.0	3	10	11	1.7
2	1	5	2.0	2	6	9	2.6	3	10	12	0.3
3	1	4	4.1	7	6	8	8.4	7	10	11	0.0
3	1	5	14.0	7	6	9	6.4	7	10	12	2.6
4	1	5	1.8	8	6	9	1.6	11	10	12	1.5
	Cd	***MAD***	***5.5***		Cd	***MAD***	***4.0***		Zn	***MAD***	***2.1***

Cd_2Zn Isomer 2

2	1	3	4.2	2	6	7	2.9	3	10	7	0.6
2	1	4	3.3	2	6	8	3.2	3	10	11	2.2
2	1	5	6.3	2	6	9	1.5	3	10	12	3.0
3	1	4	1.0	7	6	8	3.1	7	10	11	3.2
3	1	5	0.4	7	6	9	3.7	7	10	12	3.4
4	1	5	2.1	8	6	9	2.4	11	10	12	1.0
	Cd	***MAD***	***2.9***		Zn	***MAD***	***2.8***		Cd	***MAD***	***2.2***

Cd_2Zn Isomer 3

2	1	3	0.4	2	6	7	4.4	3	10	7	1.9
2	1	4	3.9	2	6	8	0.1	3	10	11	2.0
2	1	5	2.2	2	6	9	1.0	3	10	12	2.2
3	1	4	4.1	7	6	8	1.4	7	10	11	0.8
3	1	5	2.1	7	6	9	2.9	7	10	12	3.0
4	1	5	3.7	8	6	9	0.7	11	10	12	1.6
	Zn	***MAD***	***2.7***		Cd	***MAD***	***1.8***		Cd	***MAD***	***1.9***

$CdZn_2$ Isomer 1

2	1	3	4.9	2	6	7	4.9	3	10	7	0.0
2	1	4	3.1	2	6	8	5.0	3	10	11	2.3
2	1	5	2.2	2	6	9	2.9	3	10	12	2.8
3	1	4	0.5	7	6	8	4.0	7	10	11	4.8
3	1	5	2.3	7	6	9	4.4	7	10	12	3.2
4	1	5	3.1	8	6	9	5.7	11	10	12	0.4
	Zn	***MAD***	***2.7***		Zn	***MAD***	***4.5***		Cd	***MAD***	***2.3***

$CdZn_2$ Isomer 2

2	1	3	6.8	2	6	7	3.3	3	10	7	2.5
2	1	4	0.5	2	6	8	0.9	3	10	11	1.9
2	1	5	1.7	2	6	9	3.4	3	10	12	1.2
3	1	4	6.7	7	6	8	1.3	7	10	11	0.2
3	1	5	10.5	7	6	9	0.3	7	10	12	0.1
4	1	5	0.8	8	6	9	0.0	11	10	12	1.3
	Zn	***MAD***	***4.5***		Cd	***MAD***	***1.5***		Zn	***MAD***	***1.2***

$CdZn_2$ Isomer 3

2	1	3	5.1	2	6	7	2.8	3	10	7	2.1
2	1	4	5.7	2	6	8	2.1	3	10	11	0.0
2	1	5	1.6	2	6	9	1.7	3	10	12	1.2
3	1	4	1.4	7	6	8	4.8	7	10	11	2.4
3	1	5	2.2	7	6	9	6.0	7	10	12	5.3
4	1	5	0.5	8	6	9	2.0	11	10	12	2.1
	Cd	***MAD***	***2.8***		Zn	***MAD***	***3.2***		Zn	***MAD***	***2.2***

Zn_3

2	1	3	1.8	2	6	7	1.1	3	10	7	1.9
2	1	4	5.6	2	6	8	1.8	3	10	11	1.8
2	1	5	6.2	2	6	9	1.6	3	10	12	1.1
3	1	4	1.1	7	6	8	4.6	7	10	11	1.5
3	1	5	1.1	7	6	9	3.6	7	10	12	4.1
4	1	5	1.1	8	6	9	1.1	11	10	12	1.4
	Zn	***MAD***	***2.8***		Zn	***MAD***	***2.3***		Zn	***MAD***	***2.0***

TABLE S8. "Angular Energies" (summed squared angular deviations from ideal) of clusters.

Cd_4 = 378.0

2	1	3	46.2	4	6	7	18.5	2	10	9	33.6	8	13	12	8.4
2	1	4	0.5	4	6	8	11.6	2	10	11	10.9	8	13	14	0.4
2	1	5	0.2	4	6	9	13.7	2	10	12	34.8	8	13	15	4.8
3	1	4	16.8	7	6	8	10.2	9	10	11	4.8	12	13	14	1.4
3	1	5	130.0	7	6	9	2.6	9	10	12	2.6	12	13	15	2.6
4	1	5	1.4	8	6	9	0.8	11	10	12	0.0	14	13	15	21.2
	Cd	***SSD***	***195.1***		Cd	***SSD***	***57.4***		Cd	***SSD***	***86.8***		Cd	***SSD***	***38.8***

Cd_3Zn Isomer 1 = 461.0

2	1	3	10.9	4	6	7	8.4	2	10	9	31.4	8	13	12	43.6
2	1	4	0.4	4	6	8	54.8	2	10	11	32.5	8	13	14	0.6
2	1	5	0.5	4	6	9	47.6	2	10	12	28.1	8	13	15	2.3
3	1	4	29.2	7	6	8	3.6	9	10	11	75.7	12	13	14	21.2
3	1	5	0.3	7	6	9	5.3	9	10	12	1.0	12	13	15	29.2
4	1	5	7.8	8	6	9	5.3	11	10	12	2.3	14	13	15	19.4
	Zn	***SSD***	***49.0***		Cd	***SSD***	***125.0***		Cd	***SSD***	***170.9***		Cd	***SSD***	***116.1***

Cd_3Zn Isomer 2 = 358.5

2	1	3	47.6	4	6	7	5.3	2	10	9	1.7	8	13	12	4.8
2	1	4	10.9	4	6	8	30.3	2	10	11	0.8	8	13	14	27.0
2	1	5	0.0	4	6	9	15.2	2	10	12	2.0	8	13	15	9.6
3	1	4	24.0	7	6	8	15.2	9	10	11	3.6	12	13	14	6.3
3	1	5	118.8	7	6	9	3.6	9	10	12	0.1	12	13	15	0.2
4	1	5	6.8	8	6	9	4.8	11	10	12	10.9	14	13	15	9.0
	Cd	***SSD***	***208.1***		Cd	***SSD***	***74.4***		Cd	***SSD***	***19.1***		Zn	***SSD***	***56.9***

Cd_3Zn Isomer 3 = 419.9

2	1	3	16.8	4	6	7	4.8	2	10	9	2.6	8	13	12	114.5
2	1	4	3.6	4	6	8	41.0	2	10	11	4.4	8	13	14	82.8
2	1	5	1.0	4	6	9	22.1	2	10	12	1.0	8	13	15	23.0
3	1	4	9.0	7	6	8	31.4	9	10	11	7.3	12	13	14	3.2
3	1	5	21.2	7	6	9	0.2	9	10	12	4.4	12	13	15	0.8
4	1	5	0.4	8	6	9	4.4	11	10	12	12.3	14	13	15	7.8
	Cd	***SSD***	***51.9***		Zn	***SSD***	***103.8***		Cd	***SSD***	***31.9***		Cd	***SSD***	***232.2***

Cd_3Zn Isomer 4 = 223.0

2	1	3	2.9	4	6	7	5.8	2	10	9	2.6	8	13	12	17.6
2	1	4	19.4	4	6	8	16.0	2	10	11	1.0	8	13	14	0.0
2	1	5	5.8	4	6	9	8.4	2	10	12	1.7	8	13	15	0.3
3	1	4	7.8	7	6	8	0.1	9	10	11	9.0	12	13	14	17.6
3	1	5	13.0	7	6	9	0.6	9	10	12	2.0	12	13	15	37.2
4	1	5	1.2	8	6	9	17.6	11	10	12	0.6	14	13	15	34.8
	Cd	***SSD***	***50.0***		Cd	***SSD***	***48.5***		Zn	***SSD***	***16.9***		Cd	***SSD***	***107.6***

Zn_4 = 311.0

2	1	3	13.7	4	6	7	0.4	2	10	9	20.3	8	13	12	29.2
2	1	4	1.0	4	6	8	50.4	2	10	11	13.7	8	13	14	14.4
2	1	5	0.8	4	6	9	34.8	2	10	12	6.3	8	13	15	0.8
3	1	4	23.0	7	6	8	13.7	9	10	11	46.2	12	13	14	3.6
3	1	5	0.5	7	6	9	3.6	9	10	12	2.6	12	13	15	9.6
4	1	5	12.3	8	6	9	1.7	11	10	12	0.1	14	13	15	8.4
		SSD	***51.3***			***SSD***	***104.6***			***SSD***	***89.1***			***SSD***	***66.0***

Cd_2Zn_2 Isomer 1 = 429.7

2	1	3	9.6	4	6	7	3.2	2	10	9	43.6	8	13	12	27.0
2	1	4	0.3	4	6	8	56.3	2	10	11	36.0	8	13	14	8.4
2	1	5	0.4	4	6	9	53.3	2	10	12	34.8	8	13	15	0.4
3	1	4	24.0	7	6	8	12.3	9	10	11	74.0	12	13	14	4.0
3	1	5	0.0	7	6	9	7.3	9	10	12	3.2	12	13	15	8.4
4	1	5	7.3	8	6	9	5.8	11	10	12	0.0	14	13	15	10.2
	Zn	***SSD***	***41.5***		Cd	***SSD***	***138.1***		Cd	***SSD***	***191.6***		Zn	***SSD***	***58.5***

Cd_2Zn_2 Isomer 2 = 514.7

2	1	3	6.3	4	6	7	5.3	2	10	9	64.0	8	13	12	7.8
2	1	4	16.8	4	6	8	114.5	2	10	11	26.0	8	13	14	0.3
2	1	5	0.5	4	6	9	53.3	2	10	12	56.3	8	13	15	0.0
3	1	4	10.9	7	6	8	20.3	9	10	11	72.3	12	13	14	1.0
3	1	5	1.0	7	6	9	1.4	9	10	12	2.0	12	13	15	15.2
4	1	5	9.0	8	6	9	6.3	11	10	12	1.4	14	13	15	23.0
	Zn	***SSD***	***44.4***		Zn	***SSD***	***201.0***		Cd	***SSD***	***221.9***		Cd	***SSD***	***47.4***

Cd_2Zn_2 Isomer 3 = 253.9

2	1	3	13.7	4	6	7	0.4	2	10	9	16.0	8	13	12	22.1
2	1	4	0.0	4	6	8	26.0	2	10	11	18.5	8	13	14	2.9
2	1	5	1.7	4	6	9	46.2	2	10	12	10.2	8	13	15	0.8
3	1	4	12.3	7	6	8	2.9	9	10	11	33.6	12	13	14	7.8
3	1	5	0.2	7	6	9	7.8	9	10	12	0.1	12	13	15	13.0
4	1	5	0.3	8	6	9	0.0	11	10	12	1.4	14	13	15	16.0
	Zn	***SSD***	***28.1***		Cd	***SSD***	***83.4***		Zn	***SSD***	***79.9***		Cd	***SSD***	***62.6***

Cd_2Zn_2 Isomer 4 = 163.9

2	1	3	0.0	4	6	7	2.9	2	10	9	6.3	8	13	12	37.2
2	1	4	11.6	4	6	8	20.3	2	10	11	3.6	8	13	14	10.9
2	1	5	6.3	4	6	9	9.0	2	10	12	2.6	8	13	15	1.0
3	1	4	1.2	7	6	8	0.6	9	10	11	11.6	12	13	14	7.3
3	1	5	0.4	7	6	9	0.4	9	10	12	1.2	12	13	15	9.0
4	1	5	0.2	8	6	9	7.8	11	10	12	1.2	14	13	15	11.6
	Cd	***SSD***	***19.6***		Cd	***SSD***	***41.0***		Zn	***SSD***	***26.4***		Zn	***SSD***	***77.0***

Cd_2Zn_2 Isomer 5 = 377.4

2	1	3	18.5	4	6	7	7.8	2	10	9	42.3	8	13	12	51.8
2	1	4	3.2	4	6	8	29.2	2	10	11	0.5	8	13	14	27.0
2	1	5	2.0	4	6	9	23.0	2	10	12	3.6	8	13	15	9.6
3	1	4	15.2	7	6	8	34.8	9	10	11	1.4	12	13	14	8.4
3	1	5	54.8	7	6	9	2.3	9	10	12	18.5	12	13	15	0.4
4	1	5	0.0	8	6	9	16.8	11	10	12	2.3	14	13	15	4.0
	Cd	***SSD***	***93.7***		Zn	***SSD***	***113.9***		Cd	***SSD***	***68.5***		Zn	***SSD***	***101.3***

Cd_2Zn_2 Isomer 6 = 372.8

2	1	3	2.0	4	6	7	1.0	2	10	9	20.3	8	13	12	62.4
2	1	4	0.1	4	6	8	68.9	2	10	11	16.0	8	13	14	3.2
2	1	5	5.8	4	6	9	36.0	2	10	12	9.6	8	13	15	0.8
3	1	4	4.4	7	6	8	10.2	9	10	11	43.6	12	13	14	33.6
3	1	5	2.3	7	6	9	4.4	9	10	12	1.4	12	13	15	29.2
4	1	5	3.2	8	6	9	0.0	11	10	12	0.0	14	13	15	14.4
	Cd	***SSD***	***17.7***		Zn	***SSD***	***120.5***		Zn	***SSD***	***90.9***		Cd	***SSD***	***143.7***

$CdZn_3$ Isomer 1 = 371.7

2	1	3	13.0	4	6	7	4.8	2	10	9	16.0	8	13	12	29.2
2	1	4	2.0	4	6	8	65.6	2	10	11	18.5	8	13	14	7.8
2	1	5	1.0	4	6	9	57.8	2	10	12	15.2	8	13	15	0.2
3	1	4	15.2	7	6	8	14.4	9	10	11	44.9	12	13	14	15.2
3	1	5	0.0	7	6	9	10.9	9	10	12	5.8	12	13	15	16.0
4	1	5	6.3	8	6	9	5.3	11	10	12	0.0	14	13	15	6.8
	Zn	***SSD***	***37.4***		Cd	***SSD***	***158.8***		Zn	***SSD***	***100.4***		Zn	***SSD***	***75.1***

$CdZn_3$ Isomer 2 = 191.3

2	1	3	1.4	4	6	7	11.6	2	10	9	0.0	8	13	12	33.6
2	1	4	17.6	4	6	8	22.1	2	10	11	1.4	8	13	14	11.6
2	1	5	6.3	4	6	9	17.6	2	10	12	1.2	8	13	15	0.6
3	1	4	4.0	7	6	8	16.8	9	10	11	8.4	12	13	14	10.9
3	1	5	2.9	7	6	9	0.2	9	10	12	1.2	12	13	15	12.3
4	1	5	0.2	8	6	9	0.0	11	10	12	0.4	14	13	15	9.0
	Cd	***SSD***	***32.4***		Zn	***SSD***	***68.3***		Zn	***SSD***	***12.7***		Zn	***SSD***	***78.0***

$CdZn_3$ Isomer 3 = 300.7

2	1	3	8.4	4	6	7	1.7	2	10	9	29.2	8	13	12	56.3
2	1	4	2.6	4	6	8	37.2	2	10	11	0.1	8	13	14	24.0
2	1	5	0.0	4	6	9	13.7	2	10	12	0.5	8	13	15	9.6
3	1	4	27.0	7	6	8	29.2	9	10	11	1.0	12	13	14	11.6
3	1	5	17.6	7	6	9	1.0	9	10	12	10.2	12	13	15	0.4
4	1	5	4.8	8	6	9	10.2	11	10	12	0.0	14	13	15	4.4
	Zn	***SSD***	***60.5***		Zn	***SSD***	***93.0***		Cd	***SSD***	***41.0***		Zn	***SSD***	***106.2***

$CdZn_3$ Isomer 4 = 220.8

2	1	3	6.3	4	6	7	8.4	2	10	9	39.7	8	13	12	16.0
2	1	4	1.2	4	6	8	16.8	2	10	11	0.3	8	13	14	1.2
2	1	5	1.4	4	6	9	14.4	2	10	12	16.8	8	13	15	2.6
3	1	4	25.0	7	6	8	10.9	9	10	11	4.0	12	13	14	3.2
3	1	5	18.5	7	6	9	0.6	9	10	12	4.4	12	13	15	3.6
4	1	5	6.8	8	6	9	1.2	11	10	12	1.4	14	13	15	16.0
	Zn	***SSD***	***59.1***		Zn	***SSD***	***52.4***		Zn	***SSD***	***66.6***		Cd	***SSD***	***42.6***

Cd_3 = 214.2

2	1	3	9.0	2	6	7	5.8	3	10	7	36.0
2	1	4	21.2	2	6	8	12.3	3	10	11	8.4
2	1	5	3.2	2	6	9	5.8	3	10	12	11.6
3	1	4	14.4	7	6	8	25.0	7	10	11	16.0
3	1	5	0.0	7	6	9	0.1	7	10	12	0.0
4	1	5	12.3	8	6	9	13.0	11	10	12	20.3
	Cd	***SSD***	***60.1***		Cd	***SSD***	***61.8***		Cd	***SSD***	***92.2***

Cd_2Zn Isomer 1 = 537.4

2	1	3	125.4	2	6	7	0.8	3	10	7	42.3
2	1	4	0.0	2	6	8	16.0	3	10	11	2.9
2	1	5	4.0	2	6	9	6.8	3	10	12	0.1
3	1	4	16.8	7	6	8	70.6	7	10	11	0.0
3	1	5	196.0	7	6	9	41.0	7	10	12	6.8
4	1	5	3.2	8	6	9	2.6	11	10	12	2.3
	Cd	***SSD***	***345.5***		Cd	***SSD***	***137.7***		Zn	***SSD***	***54.2***

Cd_2Zn Isomer 2 = 160.8

2	1	3	17.6	2	6	7	8.4	3	10	7	0.4
2	1	4	10.9	2	6	8	10.2	3	10	11	4.8
2	1	5	39.7	2	6	9	2.3	3	10	12	9.0
3	1	4	1.0	7	6	8	9.6	7	10	11	10.2
3	1	5	0.2	7	6	9	13.7	7	10	12	11.6
4	1	5	4.4	8	6	9	5.8	11	10	12	1.0
	Cd	***SSD***	***73.8***		Zn	***SSD***	***50.0***		Cd	***SSD***	***37.0***

Cd_2Zn Isomer 3 = 111.0

2	1	3	0.2	2	6	7	19.4	3	10	7	3.6
2	1	4	15.2	2	6	8	0.0	3	10	11	4.0
2	1	5	4.8	2	6	9	1.0	3	10	12	4.8
3	1	4	16.8	7	6	8	2.0	7	10	11	0.6
3	1	5	4.4	7	6	9	8.4	7	10	12	9.0
4	1	5	13.7	8	6	9	0.5	11	10	12	2.6
	Zn	***SSD***	***55.1***		Cd	***SSD***	***31.2***		Cd	***SSD***	***24.7***

$CdZn_2$ Isomer 1 = 225.5

2	1	3	24.0	2	6	7	24.0	3	10	7	0.0
2	1	4	9.6	2	6	8	25.0	3	10	11	5.3
2	1	5	4.8	2	6	9	8.4	3	10	12	7.8
3	1	4	0.3	7	6	8	16.0	7	10	11	23.0
3	1	5	5.3	7	6	9	19.4	7	10	12	10.2
4	1	5	9.6	8	6	9	32.5	11	10	12	0.2
	Zn	***SSD***	***53.6***		Zn	***SSD***	***125.3***		Cd	***SSD***	***46.6***

$CdZn_2$ Isomer 2 = 243.2

2	1	3	46.2	2	6	7	10.9	3	10	7	6.3
2	1	4	0.3	2	6	8	0.8	3	10	11	3.6
2	1	5	2.9	2	6	9	11.6	3	10	12	1.4
3	1	4	44.9	7	6	8	1.7	7	10	11	0.0
3	1	5	110.3	7	6	9	0.1	7	10	12	0.0
4	1	5	0.6	8	6	9	0.0	11	10	12	1.7
	Zn	***SSD***	***205.2***		Cd	***SSD***	***25.0***		Zn	***SSD***	***13.0***

$CdZn_2$ Isomer 3 = 190.4

2	1	3	26.0	2	6	7	7.8	3	10	7	4.4
2	1	4	32.5	2	6	8	4.4	3	10	11	0.0
2	1	5	2.6	2	6	9	2.9	3	10	12	1.4
3	1	4	2.0	7	6	8	23.0	7	10	11	5.8
3	1	5	4.8	7	6	9	36.0	7	10	12	28.1
4	1	5	0.3	8	6	9	4.0	11	10	12	4.4
	Cd	***SSD***	***68.1***		Zn	***SSD***	***78.2***		Zn	***SSD***	***44.1***

Zn_3 = 148.1

2	1	3	3.2	2	6	7	1.2	3	10	7	3.6
2	1	4	31.4	2	6	8	3.2	3	10	11	3.2
2	1	5	38.4	2	6	9	2.6	3	10	12	1.2
3	1	4	1.2	7	6	8	21.2	7	10	11	2.3
3	1	5	1.2	7	6	9	13.0	7	10	12	16.8
4	1	5	1.2	8	6	9	1.2	11	10	12	2.0
	Zn	***SSD***	***76.7***		Zn	***SSD***	***42.3***		Zn	***SSD***	***29.1***

TABLE S9. Computed electronic energy, Zero point energy + 3RT, and thermodynamic state functions (thermal energy, enthalpy, entropy, and Gibbs' free energy) at 298 K (TPSSh, def-TZVP). Most stable states are in bold.

Cluster	*Isomer*	E_{el} *(a.u.)*	*ZPE+3RT (kJ/mol)*	*E (kJ/mol)*	*H (kJ/mol)*	*TS (kJ/mol)*	*G (kJ/mol)*
Cd_4	1	**-5491.037747**	**1241.78**	**-14415149.7**	**-14415147.2**	**434.0**	**-14415581.2**
Cd_3Zn	1	-7102.737804	1239.06	-18646574.7	-18646572.2	422.3	-18646994.4
	2	-7102.753852	1244.87	-18646611.0	-18646608.5	430.7	-18647039.2
	3	**-7102.753956**	**1242.43**	**-18646613.7**	**-18646611.2**	**428.2**	**-18647039.4**
	4	-7102.752625	1242.24	-18646610.4	-18646607.9	428.8	-18647036.7
Cd_2Zn_2	1	-8714.438304	1239.26	-22877997.8	-22877995.3	415.3	-22878410.7
	2	-8714.438091	1244.68	-22877991.8	-22877989.3	431.6	-22878421.0
	3	-8714.438632	1244.61	-22877993.3	-22877990.8	428.9	-22878419.8
	4	-8714.448889	1242.55	-22878022.3	-22878019.8	417.9	-22878437.7
	5	**-8714.451631**	**1242.87**	**-22878029.2**	**-22878026.7**	**422.0**	**-22878448.7**
	6	-8714.448814	1239.67	-22878025.0	-22878022.5	419.1	-22878441.6
$CdZn_3$	1	-10326.14	1244.68	-27109418.3	-27109415.8	425.7	-27109841.5
	2	-10326.14	1242.67	-27109432.1	-27109429.6	410.8	-27109840.4
	3	-10326.14	1240.91	-27109428.7	-27109426.2	405.6	-27109831.8
	4	**-10326.14**	**1245.96**	**-27109427.1**	**-27109424.6**	**418.0**	**-27109842.7**
Zn_4	1	**-11937.84047**	**1245.15**	**-31340841.7**	**-31340839.2**	**419.9**	**-31341259.1**
Cd_3	1	**-4446.970947**	**1009.77**	**-11674246.7**	**-11674244.2**	**363.2**	**-11674607.5**
Cd_2Zn	1	**-6058.681992**	**1009.9**	**-15905697.7**	**-15905695.2**	**359.3**	**-15906054.5**
	2	-6058.68198	1007.51	-15905700.0	-15905697.5	347.5	-15906045.0
	3	-6058.673258	1012.81	-15905671.8	-15905669.3	367.3	-15906036.7
$CdZn_2$	1	-7670.372754	1013.29	-20137092.1	-20137089.6	351.8	-20137441.4
	2	-7670.372065	1012.78	-20137090.8	-20137088.3	363.7	-20137452.0
	3	**-7670.378699**	**1010.08**	**-20137110.9**	**-20137108.4**	**350.3**	**-20137458.7**
Zn_3	1	**-9282.073279**	**1008.05**	**-24368520.7**	**-24368518.2**	**331.8**	**-24368850.0**

TABLE S10. Computed volumes and areas of cluster cavities, from Cosmo (in Å^3 and Å^2).

Cluster A	*Formula*	*Isomer*	*Cavity volume*	*Cavity area*	*Positions*[a] $380^t - 381^b - 382^b - 379^t$
MT A calc.	Cd_4	1	5505.20	1887.79	Cd – Cd – Cd – Cd
MT A calc.	Cd_3Zn	1	5258.87	1820.99	Zn – Cd – Cd – Cd
MT A calc.		2	5400.44	1863.76	Cd – Cd – Cd – Zn
MT A calc.		3	5388.64	1863.81	Cd – Zn – Cd – Cd
MT A calc.		4	5263.08	1871.71	Cd – Cd – Zn – Cd
MT A calc.	Cd_2Zn_2	1	5235.46	1817.68	Zn – Cd – Cd – Zn
MT A calc.		2	5240.93	1814.62	Zn – Zn – Cd – Cd
MT A calc.		3	5191.44	1811.59	Zn – Cd – Zn – Cd
MT A calc.		4	5232.62	1852.57	Cd – Cd – Zn – Zn
MT A calc.		5	5326.44	1832.85	Cd – Zn – Cd – Zn
MT A calc.		6	5251.45	1831.70	Cd – Zn – Zn – Cd
MT A calc.	$CdZn_3$	1	5121.74	1767.31	Zn – Cd – Zn – Zn
MT A calc.		2	5119.94	1802.64	Cd – Zn – Zn – Zn
MT A calc.		3	5267.47	1815.32	Zn – Zn – Cd – Zn
MT A calc.		4	5184.61	1786.12	Zn – Zn – Zn – Cd
MT A calc.	Zn_4	1	5085.32	1763.76	Zn – Zn – Zn – Zn
Cluster B	*Formula*	*Isomer*			*Positions*[a] $378^t - 377^t - 376^t$
MT B calc.	Cd_3	1	4415.99	1600.30	Cd – Cd – Cd
MT B calc.	Cd_2Zn	1	4309.35	1569.12	Cd – Cd – Zn
MT B calc.		2	4355.04	1568.53	Cd – Zn – Cd
MT B calc.		3	4372.29	1600.59	Zn – Cd – Cd
MT B calc.	$CdZn_2$	1	4260.78	1544.57	Zn – Zn – Cd
MT B calc.		2	4289.01	1571.72	Zn – Cd – Zn
MT B calc.		3	4198.64	1528.77	Cd – Zn – Zn
MT B calc.	Zn_3	1	4168.65	1520.09	Zn – Zn – Zn
AVERAGE					

[a] The t and b refers to metal ions coordinating in "terminal" and "bridging" positions, respectively, in the A cluster, i.e. having two and one terminal sulfur atoms bound, respectively. In the B cluster, all metal ions bind two bridging and two terminal sulfur atoms and are designated "t".

TABLE S11. Deviation from ideal metal-sulfur bond lengths (Å).

Cluster A	Formula	Isomer	Cd-S^t_{av}	Zn-S^t_{av}	Cd-S^b_{av}	Zn-S^b_{av}	Positions[a] $380^t – 381^b – 382^b – 379^t$
Computed data, this work							
MT A calc.	Cd_4	1	-0.06	---	0.02	---	Cd – Cd – Cd – Cd
MT A calc.	Cd_3Zn	1	-0.06	-0.04	0.02	0.04	Zn – Cd – Cd – Cd
MT A calc.		2	-0.05	-0.05	0.02	0.05	Cd – Cd – Cd – Zn
MT A calc.		3	-0.05	-0.06	0.03	0.01	Cd – Zn – Cd – Cd
MT A calc.		4	-0.05	-0.03	0.03	0.03	Cd – Cd – Zn – Cd
MT A calc.	Cd_2Zn_2	1	-0.06	-0.04	0.01	0.04	Zn – Cd – Cd – Zn
MT A calc.		2	-0.05	-0.04	0.02	0.02	Zn – Zn – Cd – Cd
MT A calc.		3	-0.06	-0.04	0.02	0.02	Zn – Cd – Zn – Cd
MT A calc.		4	-0.05	-0.05	0.02	0.03	Cd – Cd – Zn – Zn
MT A calc.		5	-0.05	-0.05	0.02	0.02	Cd – Zn – Cd – Zn
MT A calc.		6	-0.05	-0.05	0.04	0.01	Cd – Zn – Zn – Cd
MT A calc.	$CdZn_3$	1	-0.06	-0.04	0.00	0.03	Zn – Cd – Zn – Zn
MT A calc.		2	-0.04	-0.04	0.03	0.02	Cd – Zn – Zn – Zn
MT A calc.		3	-0.06	-0.04	0.00	0.03	Zn – Zn – Cd – Zn
MT A calc.		4	-0.06	-0.04	0.05	0.02	Zn – Zn – Zn – Cd
MT A calc.	Zn_4	1	---	-0.04	---	0.02	Zn – Zn – Zn – Zn

Cluster B	Formula	Isomer	Cd-S^t_{av}	Zn-S^t_{av}	Cd-S^b_{av}	Zn-S^b_{av}	Positions[a] $378^t – 377^t – 376^t$
MT B calc.	Cd_3	1	-0.04	---	0.03	---	Cd – Cd – Cd
MT B calc.	Cd_2Zn	1	-0.04	-0.04	0.03	0.04	Cd – Cd – Zn
MT B calc.		2	-0.04	-0.03	0.03	0.03	Cd – Zn – Cd
MT B calc.		3	-0.04	-0.04	0.03	0.04	Zn – Cd – Cd
MT B calc.	$CdZn_2$	1	-0.04	-0.03	0.03	0.03	Zn – Zn – Cd
MT B calc.		2	-0.03	-0.04	0.02	0.04	Zn – Cd – Zn
MT B calc.		3	-0.04	-0.03	0.02	0.03	Cd – Zn – Zn
MT B calc.	Zn_3	1	---	-0.03	---	0.03	Zn – Zn – Zn
AVERAGE			-0.05	-0.04	0.02	0.03	
Experimental data, previous work							Notes
Human Cd_7-MT2	Cd_4		0.01	---	-0.01	---	1MHU.pdb A-cluster
Human Cd_7-MT2	Cd_3		0.00	---	0.02	---	2MHU.pdb B-cluster
Rat Cd_7-MT2	Cd_4+Cd_3		-0.06			---	
Rat Zn_7-MT2	Zn_4+Zn_3		---	-0.05			
Rat Cd_5Zn_2-MT	Cd_4		-0.10	---	-0.08	---	A cluster
Rat Cd_5Zn_2-MT	$CdZn_2$		-0.11	-0.03	-0.06	0.01	B cluster

[a] The t and b refers to metal sites being in “terminal” and “bridging” positions, i.e. having two or one terminal cysteines bound, respectively.
In the B cluster, all metal ions bind two bridging and two terminal sulfur atoms and are designated “t”.

TABLE S12. Computed atomic charges of isomers, derived from Mulliken population analysis.

Cluster A	Isomer	M380	S48[b]	S211[t]	S167[b]	S38[t]	M381	S126[t]	S363[b]	S79[b]	M382	S69[t]	S240[b]	M379	S332[t]	S353[t]
Cd_4	---	0.42	-0.30	-0.45	-0.30	-0.45	0.44	0.44	0.30	0.29	0.41	-0.44	-0.29	0.42	-0.44	-0.46
Cd_3Zn	1	0.45	-0.27	-0.46	-0.26	-0.46	0.44	-0.45	-0.30	-0.28	0.43	-0.45	-0.29	0.43	-0.44	-0.46
	2	0.42	-0.32	-0.45	-0.30	-0.45	0.44	-0.45	-0.25	-0.28	0.40	-0.45	-0.27	0.45	-0.40	-0.47
	3	0.41	-0.30	-0.46	-0.27	-0.46	0.45	-0.45	-0.25	-0.24	0.40	-0.45	-0.30	0.41	-0.43	-0.47
	4	0.40	-0.27	-0.45	-0.30	-0.47	0.43	-0.45	-0.30	-0.25	0.44	-0.45	-0.25	0.41	-0.44	-0.46
Cd_2Zn_2	1	0.45	-0.27	-0.46	-0.26	-0.46	0.42	-0.45	-0.27	-0.29	0.41	-0.45	-0.25	0.46	-0.42	-0.47
	2	0.44	-0.28	-0.46	-0.21	-0.47	0.44	-0.44	-0.27	-0.26	0.42	-0.44	-0.28	0.42	-0.45	-0.47
	3	0.45	-0.25	-0.46	-0.27	-0.46	0.41	-0.45	-0.30	-0.25	0.44	-0.45	-0.25	0.42	-0.45	-0.47
	4	0.40	-0.27	-0.45	-0.30	-0.47	0.41	-0.45	-0.27	-0.25	0.44	-0.45	-0.23	0.45	-0.42	-0.47
	5	0.41	-0.30	-0.46	-0.28	-0.47	0.45	-0.45	-0.22	-0.25	0.40	-0.45	-0.28	0.45	-0.42	-0.47
	6	0.39	-0.27	-0.46	-0.26	-0.47	0.44	-0.44	-0.27	-0.23	0.44	-0.44	-0.24	0.40	-0.45	-0.47
$CdZn_3$	1	0.45	-0.25	-0.46	-0.26	-0.46	0.40	-0.45	-0.27	-0.26	0.44	-0.44	-0.22	0.46	-0.43	-0.48
	2	0.38	-0.27	-0.45	-0.28	-0.47	0.44	-0.44	-0.26	-0.22	0.43	-0.46	-0.24	0.46	-0.43	-0.47
	3	0.45	-0.27	-0.47	-0.26	-0.44	0.44	-0.46	-0.22	-0.25	0.39	-0.45	-0.28	0.45	-0.42	-0.47
	4	0.45	-0.26	-0.47	-0.27	-0.44	0.44	-0.45	-0.27	-0.22	0.44	-0.43	-0.28	0.41	-0.45	-0.46
Zn_4	*---	0.45	-0.25	-0.46	-0.25	-0.47	0.43	-0.45	-0.26	-0.24	0.43	-0.45	-0.23	0.46	-0.44	-0.48
Avr.	*Total*	*0.43*	*-0.28*	*-0.46*	*-0.27*	*-0.46*	*0.43*	*-0.45*	*-0.27*	*-0.25*	*0.42*	*-0.45*	*-0.26*	*0.44*	*-0.43*	*-0.47*
	Cd t	*0.40*		*-0.45*		*-0.46*		*-0.45*				*-0.45*		*0.42*	*-0.44*	*-0.47*
	Zn t	*0.45*		*-0.46*		*-0.46*		*-0.45*				*-0.45*		*0.46*	*-0.42*	*-0.47*
	Cd b		*-0.29*		*-0.29*		*0.42*		*-0.28*	*-0.27*	*0.41*		*-0.28*			
	Zn b		*-0.26*		*-0.26*		*0.44*		*-0.25*	*-0.24*	*0.44*		*-0.24*			

Cluster B	Isomer	M378	S84[b]	S283[b]	S237[t]	S63[t]	M377	S168[b]	S314[t]	S144[t]	M376	S206[t]	S349[t]
Cd_3	---	0.44	-0.31	-0.30	-0.48	-0.45	0.43	-0.30	-0.47	-0.46	0.40	-0.46	-0.46
Cd_2Zn	1	0.41	-0.31	-0.25	-0.49	-0.44	0.42	-0.26	-0.46	-0.48	0.44	-0.48	-0.48
	2	0.41	-0.28	-0.32	-0.48	-0.47	0.48	-0.27	-0.45	-0.45	0.41	-0.48	-0.47
	3	0.46	-0.27	-0.29	-0.47	-0.47	0.40	-0.31	-0.47	-0.46	0.40	-0.46	-0.46
$CdZn_2$	1	0.47	-0.26	-0.29	-0.46	-0.45	0.46	-0.29	-0.48	-0.45	0.38	-0.49	-0.47
	2	0.45	-0.28	-0.25	-0.48	-0.47	0.39	-0.28	-0.47	-0.47	0.45	-0.47	-0.47
	3	0.40	-0.26	-0.28	-0.49	-0.48	0.47	-0.25	-0.45	-0.48	0.45	-0.48	-0.48
Zn_3	---	0.47	-0.26	-0.29	-0.49	-0.44	0.47	-0.26	-0.45	-0.48	0.45	-0.48	-0.49
Avr.	*Total*	*0.43*	*-0.28*	*-0.28*	*-0.48*	*-0.46*	*0.44*	*-0.28*	*-0.46*	*-0.46*	*0.42*	*-0.47*	*-0.47*
	Cd t	*0.43*			*-0.48*	*-0.45*	*0.46*		*-0.47*	*-0.45*	*0.42*	*-0.47*	*-0.47*
	Zn t	*0.44*			*-0.48*	*-0.47*	*0.42*		*-0.46*	*-0.47*	*0.42*	*-0.48*	*-0.47*
	cd b		*-0.29*	*-0.27*				*-0.29*					
	Zn b		*-0.27*	*-0.30*				*-0.28*					

[a] The t and b refers to metal sites being in "terminal" and "bridging" positions, i.e. having two or one terminal cysteines bound, respectively. In the B cluster, all metal ions bind two bridging and two terminal sulfur atoms and are designated "t".

TABLE S13. Bond orders (Computed overlap populations x 2), derived from Mulliken analysis.

Cd_4

	M380		M381		M382		M379
$S48^b$	0.57	$S167^b$	0.67	$S48^b$	0.66	$S363^b$	0.54
$S211^t$	0.90	$S126^t$	0.91	$S79^b$	0.65	$S240^b$	0.58
$S167^b$	0.61	$S363^b$	0.64	$S69^t$	0.88	$S332^t$	0.84
$S38^t$	0.83	$S79^b$	0.60	$S240^b$	0.66	$S353^t$	0.93

Cd_3Zn Isomer 1

	M380		M381		M382		M379
$S48^b$	0.81	$S167^b$	0.68	$S48^b$	0.62	$S363^b$	0.57
$S211^t$	0.98	$S126^t$	0.90	$S79^b$	0.59	$S240^b$	0.56
$S167^b$	0.77	$S363^b$	0.64	$S69^t$	0.90	$S332^t$	0.87
$S38^t$	0.98	$S79^b$	0.61	$S240^b$	0.67	$S353^t$	0.90

Cd_3Zn Isomer 2

	M380		M381		M382		M379
$S48^b$	0.55	$S167^b$	0.66	$S48^b$	0.64	$S363^b$	0.78
$S211^t$	0.89	$S126^t$	0.93	$S79^b$	0.62	$S240^b$	0.75
$S167^b$	0.62	$S363^b$	0.61	$S69^t$	0.91	$S332^t$	1.01
$S38^t$	0.82	$S79^b$	0.58	$S240^b$	0.67	$S353^t$	0.96

Cd_3Zn Isomer 3

	M380		M381		M382		M379
$S48^b$	0.58	$S167^b$	0.85	$S48^b$	0.66	$S363^b$	0.59
$S211^t$	0.88	$S126^t$	1.00	$S79^b$	0.63	$S240^b$	0.54
$S167^b$	0.63	$S363^b$	0.82	$S69^t$	0.90	$S332^t$	0.89
$S38^t$	0.79	$S79^b$	0.81	$S240^b$	0.67	$S353^t$	0.86

Cd_3Zn Isomer 4

	M380		M381		M382		M379
$S48^b$	0.58	$S167^b$	0.67	$S48^b$	0.83	$S363^b$	0.57
$S211^t$	0.88	$S126^t$	0.87	$S79^b$	0.83	$S240^b$	0.57
$S167^b$	0.61	$S363^b$	0.67	$S69^t$	0.99	$S332^t$	0.86
$S38^t$	0.81	$S79^b$	0.61	$S240^b$	0.87	$S353^t$	0.90

Cd_2Zn_2 Isomer 1

	M380		M381		M382		M379
$S48^b$	0.81	$S167^b$	0.68	$S48^b$	0.61	$S363^b$	0.77
$S211^t$	0.98	$S126^t$	0.90	$S79^b$	0.58	$S240^b$	0.76
$S167^b$	0.77	$S363^b$	0.64	$S69^t$	0.90	$S332^t$	1.00
$S38^t$	0.98	$S79^b$	0.61	$S240^b$	0.66	$S353^t$	0.97

Cd_2Zn_2 Isomer 2							
	M380		M381		M382		M379
$S48^b$	0.79	$S167^b$	0.84	$S48^b$	0.63	$S363^b$	0.58
$S211^t$	0.97	$S126^t$	0.97	$S79^b$	0.57	$S240^b$	0.54
$S167^b$	0.78	$S363^b$	0.80	$S69^t$	0.89	$S332^t$	0.85
$S38^t$	0.99	$S79^b$	0.84	$S240^b$	0.69	$S353^t$	0.90

Cd_2Zn_2 Isomer 3							
	M380		M381		M382		M379
$S48^b$	0.79	$S167^b$	0.69	$S48^b$	0.81	$S363^b$	0.56
$S211^t$	0.98	$S126^t$	0.87	$S79^b$	0.82	$S240^b$	0.59
$S167^b$	0.78	$S363^b$	0.65	$S69^t$	0.97	$S332^t$	0.85
$S38^t$	0.96	$S79^b$	0.61	$S240^b$	0.86	$S353^t$	0.89

Cd_2Zn_2 Isomer 4							
	M380		M381		M382		M379
$S48^b$	0.59	$S167^b$	0.66	$S48^b$	0.81	$S363^b$	0.77
$S211^t$	0.88	$S126^t$	0.88	$S79^b$	0.82	$S240^b$	0.75
$S167^b$	0.60	$S363^b$	0.67	$S69^t$	0.99	$S332^t$	1.01
$S38^t$	0.79	$S79^b$	0.61	$S240^b$	0.86	$S353^t$	0.98

Cd_2Zn_2 Isomer 5							
	M380		M381		M382		M379
$S48^b$	0.58	$S167^b$	0.83	$S48^b$	0.66	$S363^b$	0.78
$S211^t$	0.88	$S126^t$	1.00	$S79^b$	0.66	$S240^b$	0.77
$S167^b$	0.62	$S363^b$	0.81	$S69^t$	0.85	$S332^t$	1.00
$S38^t$	0.79	$S79^b$	0.83	$S240^b$	0.65	$S353^t$	0.96

Cd_2Zn_2 Isomer 6							
	M380		M381		M382		M379
$S48^b$	0.56	$S167^b$	0.84	$S48^b$	0.82	$S363^b$	0.57
$S211^t$	0.88	$S126^t$	0.98	$S79^b$	0.81	$S240^b$	0.59
$S167^b$	0.60	$S363^b$	0.82	$S69^t$	0.97	$S332^t$	0.86
$S38^t$	0.84	$S79^b$	0.84	$S240^b$	0.87	$S353^t$	0.87

$CdZn_3$ Isomer 1							
	M380		M381		M382		M379
$S48^b$	0.80	$S167^b$	0.69	$S48^b$	0.80	$S363^b$	0.78
$S211^t$	0.98	$S126^t$	0.88	$S79^b$	0.82	$S240^b$	0.76
$S167^b$	0.77	$S363^b$	0.63	$S69^t$	0.97	$S332^t$	1.00
$S38^t$	0.97	$S79^b$	0.61	$S240^b$	0.86	$S353^t$	0.97

$CdZn_3$ Isomer 2

	M380		M381		M382		M379
$S48^b$	0.60	$S167^b$	0.83	$S48^b$	0.82	$S363^b$	0.77
$S211^t$	0.86	$S126^t$	0.96	$S79^b$	0.83	$S240^b$	0.75
$S167^b$	0.61	$S363^b$	0.83	$S69^t$	0.97	$S332^t$	1.00
$S38^t$	0.79	$S79^b$	0.84	$S240^b$	0.87	$S353^t$	0.99

$CdZn_3$ Isomer 3

	M380		M381		M382		M379
$S48^b$	0.80	$S167^b$	0.84	$S48^b$	0.65	$S363^b$	0.78
$S211^t$	0.95	$S126^t$	1.00	$S79^b$	0.67	$S240^b$	0.78
$S167^b$	0.77	$S363^b$	0.81	$S69^t$	0.83	$S332^t$	1.00
$S38^t$	0.98	$S79^b$	0.83	$S240^b$	0.65	$S353^t$	0.96

$CdZn_3$ Isomer 4

	M380		M381		M382		M379
$S48^b$	0.80	$S167^b$	0.82	$S48^b$	0.84	$S363^b$	0.57
$S211^t$	0.95	$S126^t$	0.98	$S79^b$	0.85	$S240^b$	0.58
$S167^b$	0.78	$S363^b$	0.83	$S69^t$	0.95	$S332^t$	0.81
$S38^t$	0.98	$S79^b$	0.84	$S240^b$	0.82	$S353^t$	0.90

Zn_4

	M380		M381		M382		M379
$S48^b$	0.80	$S167^b$	0.85	$S48^b$	0.81	$S363^b$	0.77
$S211^t$	0.97	$S126^t$	0.98	$S79^b$	0.81	$S240^b$	0.78
$S167^b$	0.76	$S363^b$	0.82	$S69^t$	0.97	$S332^t$	0.99
$S38^t$	0.97	$S79^b$	0.85	$S240^b$	0.87	$S353^t$	0.97

Cd_3					
	M378		M377		M376
$S84^b$	0.62	$S84^b$	0.60	$S283^b$	0.62
$S283^b$	0.60	$S168^b$	0.64	$S168^b$	0.61
$S237^t$	0.83	$S314^t$	0.81	$S206^t$	0.86
$S63^t$	0.82	$S144^t$	0.87	$S349^t$	0.87

Cd_2Zn Isomer 1					
	M378		M377		M376
$S84^b$	0.59	$S84^b$	0.61	$S283^b$	0.78
$S283^b$	0.63	$S168^b$	0.64	$S168^b$	0.77
$S237^t$	0.83	$S314^t$	0.81	$S206^t$	0.99
$S63^t$	0.82	$S144^t$	0.83	$S349^t$	1.01

Cd_2Zn Isomer 2					
	M378		M377		M376
$S84^b$	0.63	$S84^b$	0.80	$S283^b$	0.57
$S283^b$	0.59	$S168^b$	0.81	$S168^b$	0.58
$S237^t$	0.86	$S314^t$	0.94	$S206^t$	0.84
$S63^t$	0.83	$S144^t$	0.94	$S349^t$	0.92

Cd_2Zn Isomer 3					
	M378		M377		M376
$S84^b$	0.80	$S84^b$	0.64	$S283^b$	0.61
$S283^b$	0.79	$S168^b$	0.65	$S168^b$	0.57
$S237^t$	0.94	$S314^t$	0.81	$S206^t$	0.89
$S63^t$	1.02	$S144^t$	0.80	$S349^t$	0.86

$CdZn_2$ Isomer 1					
	M378		M377		M376
$S84^b$	0.80	$S84^b$	0.82	$S283^b$	0.59
$S283^b$	0.84	$S168^b$	0.82	$S168^b$	0.56
$S237^t$	0.93	$S314^t$	0.89	$S206^t$	0.86
$S63^t$	0.94	$S144^t$	0.96	$S349^t$	0.90

$CdZn_2$ Isomer 2					
	M378		M377		M376
$S84^b$	0.80	$S84^b$	0.64	$S283^b$	0.78
$S283^b$	0.80	$S168^b$	0.66	$S168^b$	0.79
$S237^t$	0.91	$S314^t$	0.80	$S206^t$	0.99
$S63^t$	1.04	$S144^t$	0.78	$S349^t$	0.98

$CdZn_2$ Isomer 3					
	M378		M377		M376
$S84^b$	0.65	$S84^b$	0.82	$S283^b$	0.79
$S283^b$	0.61	$S168^b$	0.80	$S168^b$	0.82
$S237^t$	0.83	$S314^t$	0.95	$S206^t$	0.94
$S63^t$	0.82	$S144^t$	0.94	$S349^t$	1.01

Zn_3					
	M378		M377		M376
$S84^b$	0.82	$S84^b$	0.80	$S283^b$	0.79
$S283^b$	0.80	$S168^b$	0.82	$S168^b$	0.81
$S237^t$	0.91	$S314^t$	0.94	$S206^t$	0.95
$S63^t$	0.98	$S144^t$	0.93	$S349^t$	0.98

[a] The t and b refers to metal sites being in “terminal” and “bridging” positions, i.e. having two or one terminal cysteines bound, respectively. In the B cluster, all metal ions bind two bridging and two terminal sulfur atoms and are designated “t”.

Figure S1: Bond energies of metal-sulfur bonds in Cd_3 and Zn_3 clusters.