

complex 1 [Zn2(SO3)2(C2O4)0.5 (C6N2H13)].(H2O)2, 1

	Cart. Coordinates					Vector (M-O/F)			Unit Vector (M-O/F)			Distance	Charges	Z (Protons)	C_Grav	C_Charge	u_Debye						
	x	y	z	Occupancy		x	y	z	x	y	z						x	y	z				
S1	0.71353	-0.18826	0.85352	6	6.149202	-4.42524	6.865715	0.118325	1.384268	0.669904	0.077782	0.909962	0.440368	1.521237	-1.39346	16	8	0.333333	0.441666	1.30861	15.30923	7.408767	14.07973
O1	0.72726	-0.12937	0.9368	1	6.267527	-3.04097	7.535619	-0.12849	-0.9527	1.133239	-0.08423	-0.62448	0.742819	1.525592	-1.37716	8	8	0.333333	0.441238	-1.41437	-10.4866	12.47385	19.35245
O2	0.69862	-0.22879	0.9944	1	6.020707	-5.37794	7.998954	-0.12849	-0.9527	1.133239	-0.08423	-0.62448	0.742819	1.525592	-1.37716	8	8	0.333333	0.441238	-1.41437	-10.4866	12.47385	19.35245
O3	0.53771	-0.1902	0.69482	1	4.633985	-4.47084	5.589132	-1.51522	-0.0456	-1.27658	-0.98924	-0.02977	-0.83344	1.531701	-1.3546	8	8	0.333333	0.440644	-16.569	-0.49866	-13.9596	21.53971
																				-16.6748	4.323979	5.923067	17.63202

	Cart. Coordinates					Vector (M-O/F)			Unit Vector (M-O/F)			Distance	Charges	Z (Protons)	C_Grav	C_Charge	u_Debye						
	x	y	z	Occupancy		x	y	z	x	y	z						x	y	z				
S2	0.658446	0.159796	0.850667	4	5.674488	3.756165	6.842765									16	8	0.333333	0.441666	1.30861	15.30923	7.408767	14.07973
O4	0.47125	0.143101	0.752528	1	4.061233	3.363732	6.053335	-1.61326	-0.39243	-0.78943	-1.05495	-0.25662	-0.51623	1.529221	-1.36372	8	8	0.333333	0.441433	-17.7562	-4.31929	-8.68883	19.46152
O5	0.683937	0.200943	0.718929	1	5.894169	4.723366	5.783065	0.219681	0.967201	-1.0597	0.144947	0.638164	-0.6992	1.5156	-1.41486	8	8	0.333333	0.442776	2.453866	10.80375	-11.837	19.1681
O6	0.667743	0.195124	1.013741	1	5.754609	4.586585	8.154533	0.080122	0.83042	1.311767	0.05248	0.543931	0.859217	1.526702	-1.37303	8	8	0.333333	0.441678	0.884244	9.164744	14.47703	13.63374
																				-14.4181	15.6492	-6.04877	23.80675

	Cart. Coordinates					Vector (M-O/F)			Unit Vector (M-O/F)			Distance	Charges	Z (Protons)	C_Grav	C_Charge	u_Debye						
	x	y	z	Occupancy		x	y	z	x	y	z						x	y	z				
Zn1	0.344832	0.102198	0.873131	5	2.971762	2.402266	7.023466									30	8	0.210526	0.232116	-2.3517	2.417311	5.786434	5.78102
O1	0.272744	0.129365	1.063163	1	2.350508	3.040854	8.552083	-0.62125	0.638588	1.528617	-0.31431	0.323076	0.773364	1.976583	-0.47869	8	8	0.210526	0.232116	-2.3517	2.417311	5.786434	5.78102
O4	0.47125	0.143101	0.752528	1	4.061233	3.363732	6.053335	1.08947	0.961466	-0.97013	0.550499	0.48582	-0.4902	1.97906	-0.47549	8	8	0.210526	0.232049	4.1109	3.6279	-3.66059	7.370162
O7	0.576174	0.067759	1.073877	1	4.965468	1.592743	8.638267	1.993705	-0.80952	1.614801	0.929014	-0.37722	0.752455	2.146044	-0.30279	8	8	0.210526	0.228401	6.218075	-2.52478	5.036327	8.988888
O8	0.302754	0.016544	0.826517	1	2.609134	0.388883	6.648503	-0.36263	-2.01338	-0.37496	-0.17664	-0.98072	-0.18265	2.052957	-0.38941	8	8	0.210526	0.230235	-1.25001	-6.94031	-1.29253	6.638263
N1	0.109266	0.116369	0.638289	1	0.941654	2.73537	5.134397	-2.03011	0.333104	-1.88907	-0.93989	0.154219	-0.8746	2.159932	-0.30452	8	8	0.210526	0.228437	-6.34494	1.041089	-5.90414	9.012585
																				0.382321	-2.37879	-0.0345	2.395599

	Cart. Coordinates					Vector (M-O/F)			Unit Vector (M-O/F)			Distance	Charges	Z (Protons)	C_Grav	C_Charge	u_Debye						
	x	y	z	Occupancy		x	y	z	x	y	z						x	y	z				
Zn2	0.515575	0.242102	0.515184	4	4.443225	5.69085	4.14414									30	8	0.210526	0.233472	-7.42616	2.752576	-0.31015	7.969859
O2	0.30138	0.27121	0.5056	1	2.597293	6.375062	4.067046	-1.84593	0.684213	-0.07709	-0.95131	0.352612	-0.03973	1.940413	-0.52784	8	8	0.210526	0.233472	-7.42616	2.752576	-0.31015	7.969859
O3	0.462293	0.190205	0.305176	1	3.984041	4.470959	2.454836	-0.45918	-1.21989	-1.6893	-0.23197	-0.61626	-0.85339	1.979522	-0.4749	8	8	0.210526	0.232359	-1.75516	-4.66285	-6.45711	6.473004
O5	0.683937	0.200943	0.718929	1	5.894169	4.723366	5.783065	1.450944	-0.96748	1.638925	0.745984	-0.49742	0.842632	1.945007	-0.52133	8	8	0.210526	0.233335	5.801306	-3.86829	6.552911	10.59645
O6	0.667743	0.30488	0.5137	1	5.754609	7.166509	4.132203	1.311384	1.47566	-0.01194	0.663175	0.74625	-0.00604	1.977433	-0.47759	8	8	0.210526	0.232416	5.025927	5.65552	-0.04575	7.580138
																				1.645915	-0.12304	-0.2601	1.663027

complex 2 [C4N2H12]0.5[Zn2(SO3)2 (C2O4)0.5(H2O)2], 2

	Cart. Coordinates					Vector (M-O/F)			Unit Vector (M-O/F)			Distance	Charges	Z (Protons)	C_Grav	C_Charge	u_Debye						
	x	y	z	Occupancy		x	y	z	x	y	z						x	y	z				
S1	0.68336	0.068622	0	4	7.579146	0.761087	0									16	8	0.333333	0.44219	-1.19146	-16.7791	0	16.82136
O1	0.673741	-0.06684	0	1	7.472461	-0.74133	0	-0.10668	-1.50242	0	-0.07083	-0.99749	0	1.506203	-1.45125	8	8	0.333333	0.44219	-1.19146	-16.7791	0	16.82136
O2	0.608622	0.108651	0.137255	1	6.750227	1.205048	1.223628	-0.82892	0.443962	1.223628	-0.53714	0.287688	0.792915	1.543203	-1.31314	8	8	0.333333	0.438563	-8.89109	4.761987	13.12479	16.55258
O2	0.608622	0.108651	0.137255	1	6.750227	1.205048	1.223628	-0.82892	0.443962	1.223628	-0.53714	0.287688	0.792915	1.543203	-1.31314	8	8	0.333333	0.438563	-8.89109	4.761987	13.12479	16.55258
																				-18.9736	-7.25514	26.24957	33.1915

	Cart. Coordinates					Vector (M-O/F)			Unit Vector (M-O/F)			Distance	Charges	Z (Protons)	C_Grav	C_Charge	u_Debye						
	x	y	z	Occupancy		x	y	z	x	y	z						x	y	z				
Zn1	0.822446	-0.17755	0	6	9.121749	-1.96925	0									30	8	0.210526	0.231302	-5.96307	4.439588	0	7.434252
O1	0.673741	-0.06684	0	1	7.472461	-0.74133	0	-1.64929	1.227918	0	-0.80211	0.59718	0	2.056193	-0.38602	8	8	0.210526	0.231302	-5.96307	4.439588	0	7.434252
O1	0.673741	-0.06684	0	1	7.472461	-0.74133	0	-1.64929	1.227918	0	-0.80211	0.59718	0	2.056193	-0.38602	8	8	0.210526	0.231302	-5.96307	4.439588	0	7.434252
O3	0.928713	-0.07129	0.148371	1	10.30036	-0.79064	1.322727	1.178607	1.178607	1.322727	0.55389	0.55389	0.62162	2.127872	-0.31803	8	8	0.210526	0.229858	3.957667	3.957667	4.441611	7.145219
O3	0.928713	-0.07129	0.148371	1	10.30036	-0.79064	1.322727	1.178607	1.178607	1.322727	0.55389	0.55389	0.62162	2.127872	-0.31803	8	8	0.210526	0.229858	3.957667	3.957667	4.441611	7.145219
O1W	0.737047	-0.26295	0.178623	1	8.174588	-2.91641	1.592424	-0.94716	-0.94716	1.592424	-0.45517	-0.45517	0.765267	2.080875	-0.36111	8	8	0.210526	0.230774	-3.33509	-3.33509	5.607157	7.327064
O1W	0.737047	-0.26295	0.178623	1	8.174588	-2.91641	1.592424	-0.94716	-0.94716	1.592424	-0.45517	-0.45517	0.765267	2.080875	-0.36111	8	8	0.210526	0.230774	-3.33509	-3.33509	5.607157	7.327064
																				-10.681	10.12433	20.09754	24.90976

				Cart. Coordinates	Vector (M-O/F)			Unit Vector (M-O/F)			Distance	Charges	Z (Protons)	C_Grav	C_Charge	u_Debye						
				x	y	z	x	y	z	x	y	z				x	y	z				
Zn2		0.5	0	0.25	4	5.5455	0	2.22875					1.90574	30								
O2	0.608622	0.108651	0.137255	1	6.750227	1.205048	1.223628	1.204727	1.205048	-1.00512	0.608962	0.609125	-0.50807	1.978327	-0.47644	8	0.210526	0.231782	4.495123	4.496323	-3.75035	7.38161
O2	0.608622	0.108651	0.137255	1	6.750227	1.205048	1.223628	1.204727	1.205048	-1.00512	0.608962	0.609125	-0.50807	1.978327	-0.47644	8	0.210526	0.231782	4.495123	4.496323	-3.75035	7.38161
O2	0.608622	0.108651	0.137255	1	6.750227	1.205048	1.223628	1.204727	1.205048	-1.00512	0.608962	0.609125	-0.50807	1.978327	-0.47644	8	0.210526	0.231782	4.495123	4.496323	-3.75035	7.38161
O2	0.608622	0.108651	0.137255	1	6.750227	1.205048	1.223628	1.204727	1.205048	-1.00512	0.608962	0.609125	-0.50807	1.978327	-0.47644	8	0.210526	0.231782	4.495123	4.496323	-3.75035	7.38161
																	17.98049	17.98529	-15.0014	29.52644		

complex 3 [C4N2H12][Cd2(SO3)2(C2O4)](H2O).H2O 3

				Cart. Coordinates	Vector (M-O/F)			Unit Vector (M-O/F)			Distance	Charges	Z (Protons)	C_Grav	C_Charge	u_Debye						
				x	y	z	x	y	z	x	y	z				x	y	z				
S1	0.121568	0.377682	0.767288	6	0.756518	3.03645	12.83596						4.079845	16								
O5	0.052457	0.53222	0.82169	1	0.32644	4.278889	13.74605	-0.43008	1.242439	0.910091	-0.28134	0.812743	0.595337	1.528698	-1.36565	8	0.333333	0.439995	-4.68691	13.53988	9.918007	16.46397
O6	0.355502	0.266599	0.795358	1	2.212289	2.143376	13.30554	1.455771	-0.89307	0.469583	0.952521	-0.58434	0.307251	1.528336	-1.36698	8	0.333333	0.44003	15.87096	-9.73638	5.119439	16.80239
O7	-0.02285	0.261769	0.797958	1	-0.14217	2.104544	13.34904	-0.89869	-0.93191	0.513078	-0.58595	-0.60761	0.334531	1.533725	-1.34722	8	0.333333	0.43951	-9.74074	-10.1008	5.561176	16.62596
																	1.443308	-6.29728	20.59862	21.24786		

				Cart. Coordinates	Vector (M-O/F)			Unit Vector (M-O/F)			Distance	Charges	Z (Protons)	C_Grav	C_Charge	u_Debye						
				x	y	z	x	y	z	x	y	z				x	y	z				
S2	0.761234	0.96125	0.938041	4	4.737159	7.728162	15.69249						4.039581	16								
O8	0.624743	0.895489	0.879742	1	3.887776	7.199463	14.7172	-0.84938	-0.5287	-0.97528	-0.54997	-0.34233	-0.63149	1.544416	-1.30885	8	0.333333	0.437667	-9.04733	-5.63151	-10.3884	16.489
O9	0.764759	0.846604	1.014719	1	4.759095	6.806442	16.97523	0.021936	-0.92172	1.282746	0.014384	-0.60441	0.84115	1.52499	-1.3794	8	0.333333	0.439526	0.238608	-10.0259	13.95295	16.74187
O10	0.999215	0.892788	0.899816	1	6.218115	7.177748	15.05302	1.480956	-0.55041	-0.63947	0.966306	-0.35914	-0.41724	1.532596	-1.35133	8	0.333333	0.438788	15.97596	-5.93764	-6.8983	16.36845
																	7.167238	-21.5951	-3.33372	20.88051		

				Cart. Coordinates	Vector (M-O/F)			Unit Vector (M-O/F)			Distance	Charges	Z (Protons)	C_Grav	C_Charge	u_Debye						
				x	y	z	x	y	z	x	y	z				x	y	z				
Cd1	-0.10857	0.808439	0.771352	7	-0.67563	6.499041	12.90395						1.743739	48								
O1	0.267	0.8564	0.76361	1	1.661541	6.8846	12.77443	2.337172	0.385558	-0.12952	0.94211	0.155418	-0.05221	2.480784	-0.21037	8	0.142857	0.150741	4.817472	0.794728	-0.26696	5.109727
O2	-0.3928	0.7531	0.70157	1	-2.44439	6.054171	11.73656	-1.76876	-0.44487	-1.16738	-0.75717	-0.19044	-0.49973	2.336026	-0.3111	8	0.142857	0.152309	-4.37887	-1.10135	-2.89005	5.81248
O3	0.076237	0.736637	0.650506	1	0.474423	5.921825	10.88231	1.150054	-0.57722	-2.02163	0.50172	-0.25181	-0.88195	2.292225	-0.3502	8	0.142857	0.152916	3.032144	-1.52184	-5.33008	5.971133
O5	0.052457	0.532226	0.82169	1	0.32644	4.278565	13.74605	1.002071	-2.22048	0.842104	0.444441	-0.98483	0.373492	2.254676	-0.3876	8	0.142857	0.153496	2.796197	-6.19606	2.349823	6.351357
O8	-0.3753	0.8955	0.87974	1	-2.33549	7.198925	14.71717	-1.65986	0.699883	1.813223	-0.69655	0.2937	0.760903	2.382988	-0.27402	8	0.142857	0.151733	-3.85601	1.625895	4.212287	5.460685
O10	-0.0008	0.8928	0.89982	1	-0.00498	7.177219	15.05309	0.670653	0.678178	2.149141	0.270353	0.273387	0.866361	2.480654	-0.21045	8	0.142857	0.150742	1.38258	1.398094	4.430549	5.113736
O1W	-0.24775	1.093869	0.711886	1	-1.54172	8.793613	11.90913	-0.86609	2.294572	-0.99482	-0.368	0.974947	-0.42269	2.353536	-0.29672	8	0.142857	0.152086	-2.09291	5.544839	-2.40397	5.744858
																	3.793514	-5.00053	2.505564	5.818381		

				Cart. Coordinates	Vector (M-O/F)			Unit Vector (M-O/F)			Distance	Charges	Z (Protons)	C_Grav	C_Charge	u_Debye						
				x	y	z	x	y	z	x	y	z				x	y	z				
Cd2	0.252597	1.038925	0.863979	6	1.571911	8.351918	14.4535						2.114731	48								
O1	0.26697	0.856376	0.76361	1	1.661354	6.884407	12.77443	0.089443	-1.46751	-1.67907	0.039158	-0.64247	-0.73509	2.284167	-0.35791	8	0.142857	0.154082	0.26141	-4.289	-4.90732	6.615611
O6	0.3555	1.2666	0.79536	1	2.212277	10.1822	13.30558	0.640365	1.830279	-1.14793	0.274229	0.783797	-0.49159	2.335145	-0.31184	8	0.142857	0.153363	1.75019	5.002357	-3.13741	6.410782
O7	-0.0228	1.2618	0.79796	1	-0.14188	10.14361	13.34907	-1.7138	1.791692	-1.10443	-0.73971	0.773328	-0.47669	2.31686	-0.32764	8	0.142857	0.15361	-4.79539	5.013348	-3.09032	6.566037
O8	0.624743	0.895489	0.879742	1	3.887776	7.198836	14.7172	2.315865	-1.15308	0.263699	1.02423	-0.50997	0.116625	2.261078	-0.38095	8	0.142857	0.154441	6.988025	-3.47938	0.795701	6.844537
O9	0.2352	1.1534	0.98528	1	1.46365	9.272183	16.48275	-0.10826	0.920265	2.029244	-0.04773	0.405711	0.89462	2.268276	-0.37361	8	0.142857	0.154327	-0.32341	2.749069	6.06188	6.726518
O10	-0.0008	0.8928	0.89982	1	-0.00498	7.177219	15.05309	-1.57689	-1.1747	0.599584	-0.69187	-0.51541	0.263071	2.279175	-0.36277	8	0.142857	0.154158	-4.64022	-3.45672	1.764361	6.701216
																	-0.75939	1.539676	-2.51311	2.899167		