Structures from Powders: Polynuclear Hg(II) Complexes Containing the Flexible Bisimidazolylmethane Ligand.

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SUPPLEMENTARY MATERIAL

Figures S1-S6

Tables S1-S5

Figure S1 - TGA of compound 1

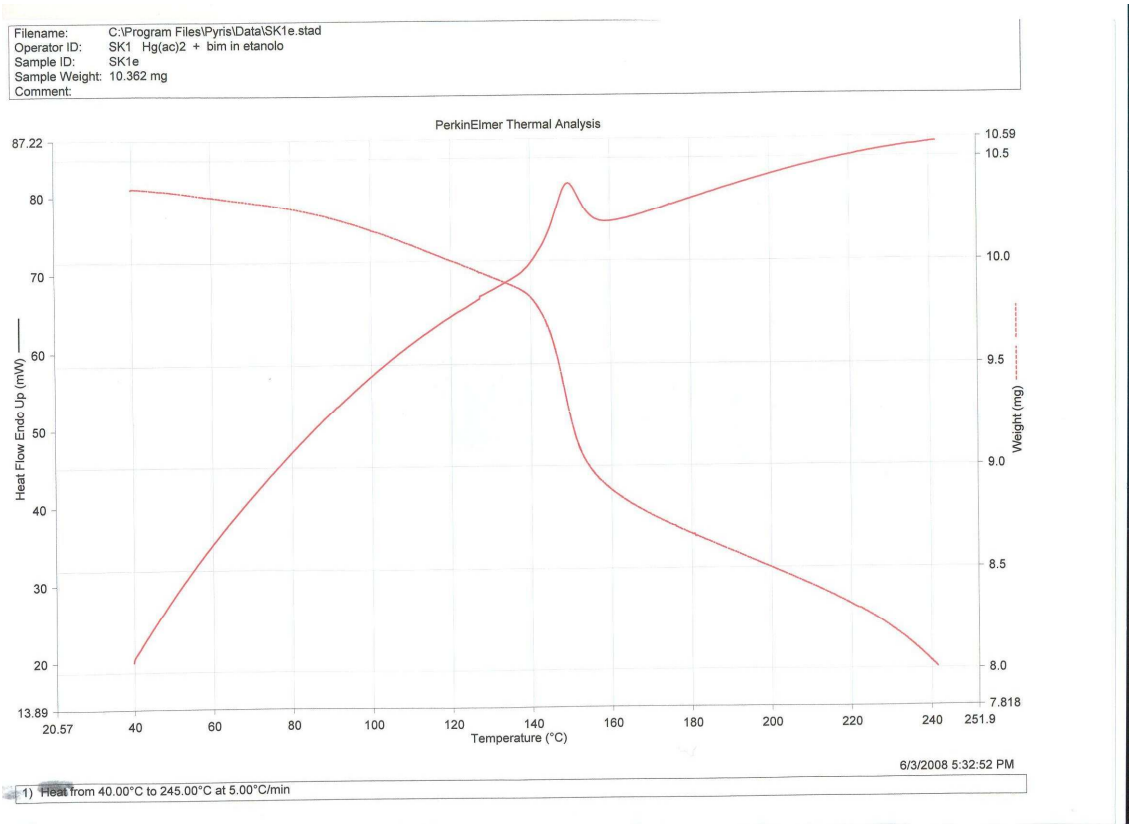


Figure S2 - TGA of compound 2

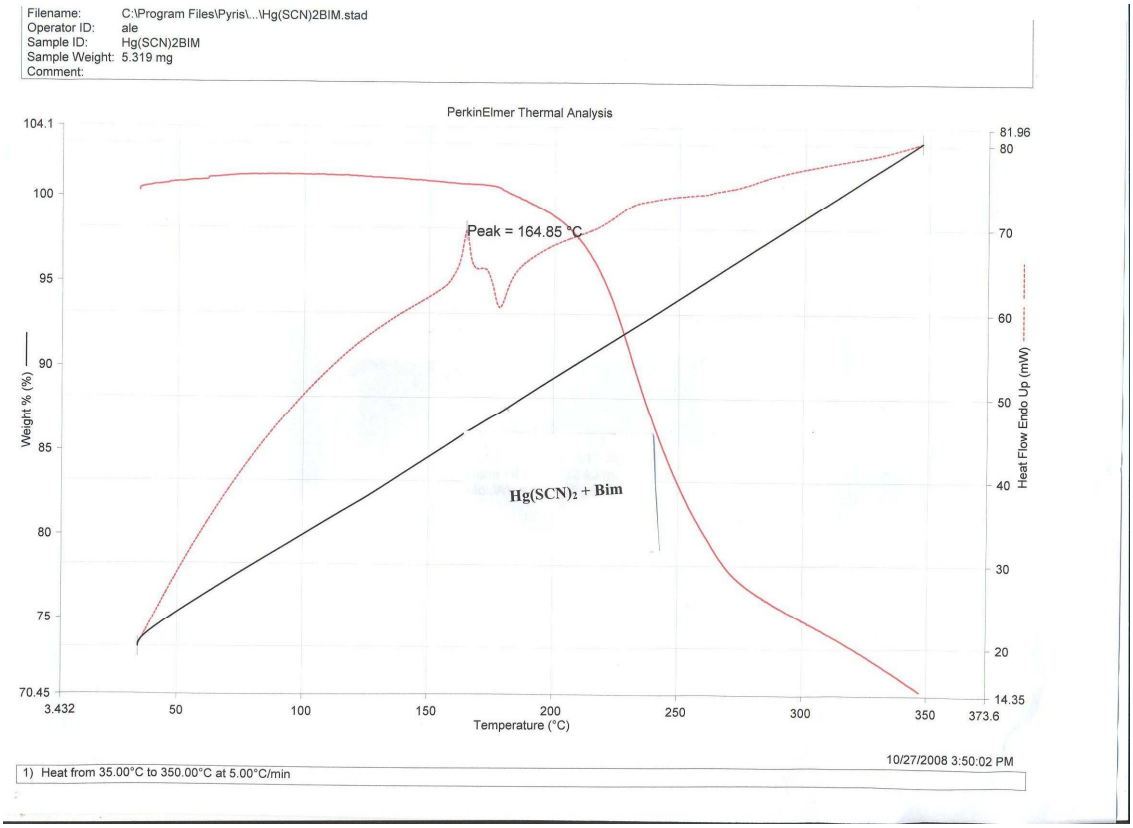


Figure S3 - TGA of compound 3

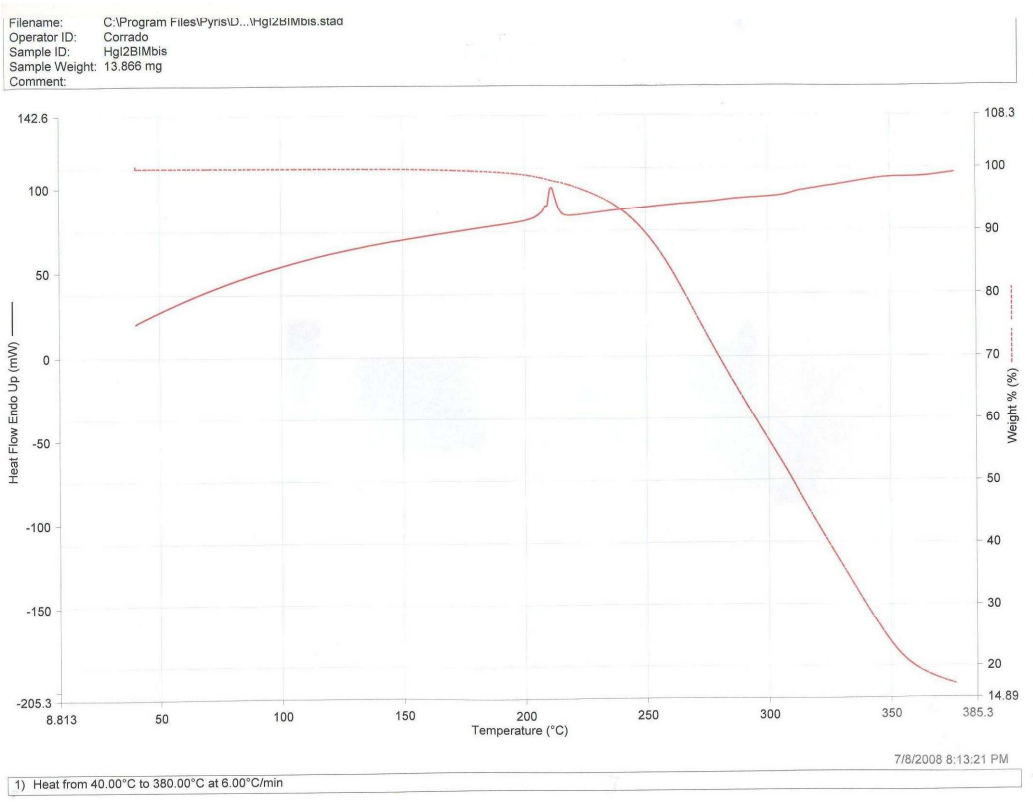


Figure S4 - TGA of compound 4

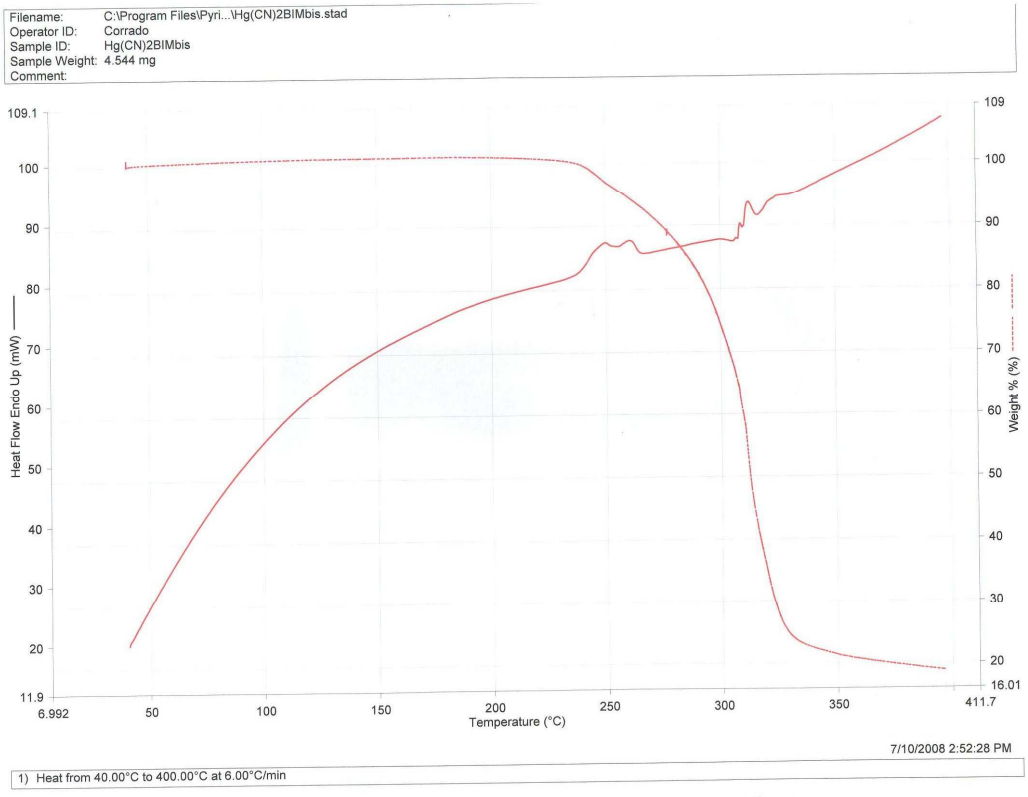


Figure S5 - TGA of compound 5

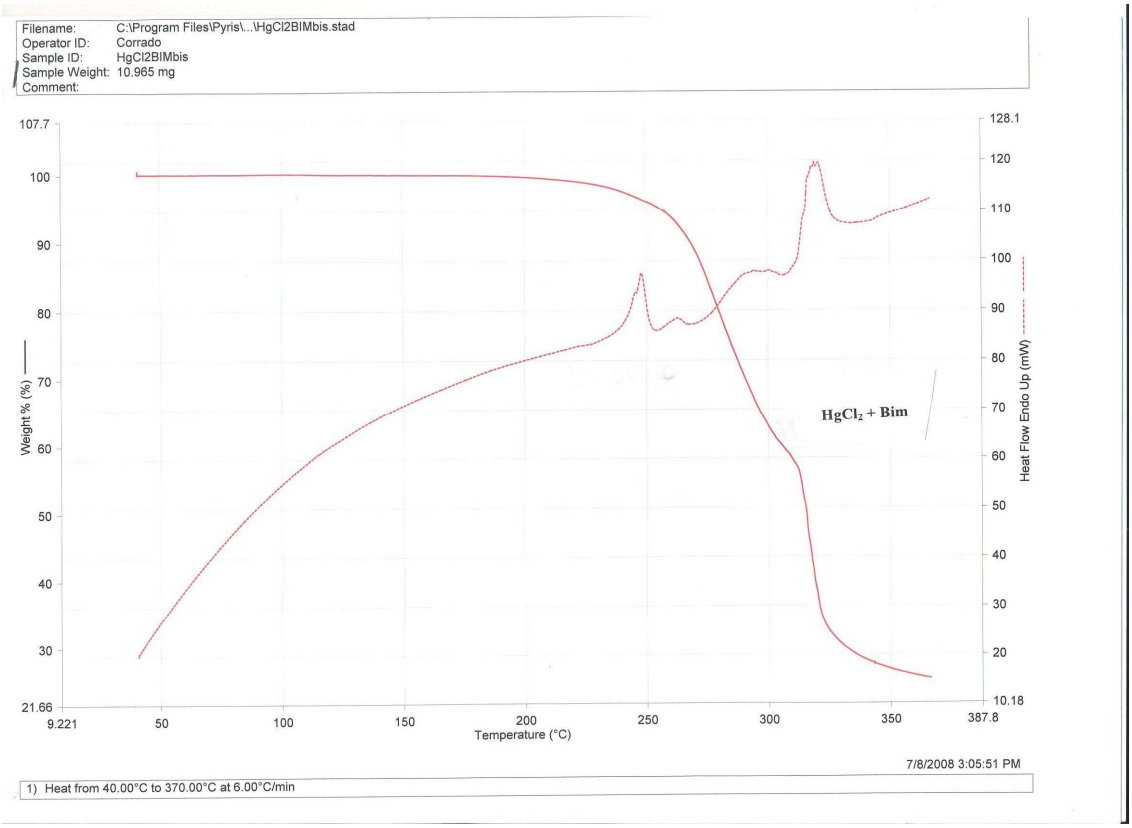
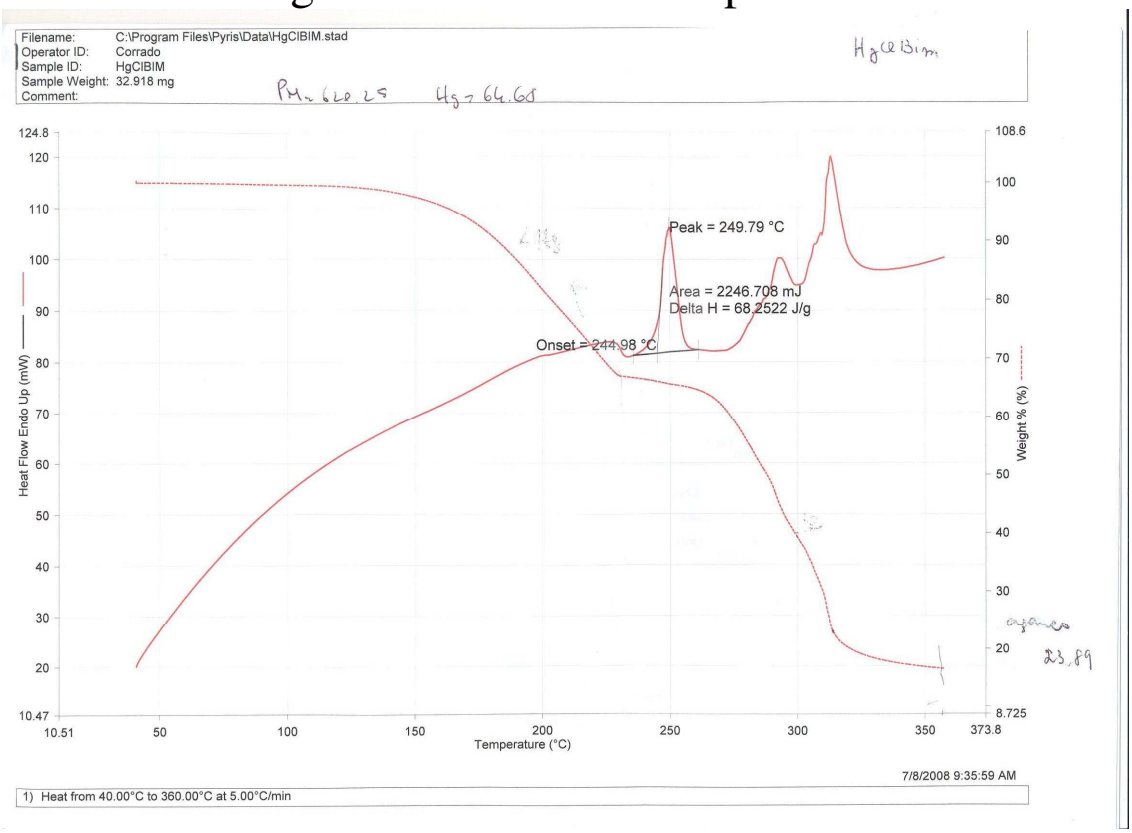


Figure S6 - TGA of compound 6



Thermodiffractometric analysis obtained by full-profile Rietveld-refinement for selected portions (typically 8<2θ<35°) of the whole diffraction pattern, sequentially collected in air on varying, stepwise the nominal temperature with a custom-made sample holder and temperature controller (supplied by Officina Elettrotecnica di Tenno, Italy). Axes are given in Angstrom (Å), angles in degree (°), volumes in Å^3 and metal-to-metal distance in Å.The Sample Height Displacement (SHD) suffered by misplacement of the average specimen surface, transparency effects and thermal expansion of the whole (metal-based) system, is expressed in mm. R_{wp} is the conventional weighted profile R factor.

Table S1. Thermodiffractometric data (ΔT = 100 °C) for $[BimHg(CH_3COO)_2]_2$, **1**.

T (°C)	a	b	c	α	β	γ	Volume	SHD	R_{wp}	Hg···Hg
25	9.440	14.992	10.219	90.000	96.395	90.000	1437.244	-0.07139	11.683	8.959
45	9.449	15.022	10.234	90.000	96.348	90.000	1443.736	-0.15608	8.278	8.954
65	9.456	15.052	10.248	90.000	96.286	90.000	1449.915	-0.18215	7.393	8.913
85	9.460	15.077	10.257	90.000	96.223	90.000	1454.318	-0.18597	7.135	8.907
105	9.464	15.101	10.268	90.000	96.151	90.000	1459.041	-0.19089	7.268	8.904
125	9.468	15.126	10.280	90.000	96.077	90.000	1463.93	-0.19837	6.974	8.904

Table S2. Thermodiffractometric data for $[BimHg(SCN)_2]_n$, **2**. ΔT = 135 °C.

T (°C)	a	b	c	α	β	γ	Volume	SHD	R_{wp}	Hg···Hg
30	14.219	11.002	9.154	90.000	110.299	90.000	1343.109	-0.064	0.0495	9.154
45	14.223	11.013	9.157	90.000	110.282	90.000	1345.389	-0.066	0.0476	9.157
65	14.229	11.030	9.162	90.000	110.252	90.000	1349.076	-0.070	0.0465	9.162
85	14.233	11.051	9.166	90.000	110.211	90.000	1352.906	-0.072	0.0458	9.166
105	14.235	11.074	9.169	90.000	110.147	90.000	1357.027	-0.076	0.0461	9.169
125	14.237	11.098	9.171	90.000	110.073	90.000	1361.122	-0.082	0.0466	9.171
145	14.239	11.122	9.173	90.000	109.978	90.000	1362.122	-0.081	0.0471	9.173
165	14.244	11.154	9.179	90.000	109.846	90.000	1371.658	-0.085	0.044	9.179

Table S3. Thermodiffractometric data for $[BimHg(CN)_2]_n$, **3**. ΔT = 215 °C.

T (℃)	a	b	c	α	β	γ	Volume	SHD	R_{wp}	Hg···Hg
30	14.272	11.936	14.851	90.000	65.777	90.000	2307.21	-0.129	4.771	9.30
45	14.281	11.944	14.856	90.000	65.793	90.000	2311.10	-0.126	4.782	9.31
65	14.296	11.957	14.866	90.000	65.808	90.000	2318.03	-0.134	4.887	9.32
85	14.309	11.968	14.874	90.000	65.825	90.000	2323.94	-0.135	4.718	9.33
105	14.321	11.978	14.880	90.000	65.843	90.000	2328.970	-0.130	4.584	9.34
125	14.332	11.988	14.886	90.000	65.861	90.000	2333.91	-0.125	4.529	9.34
145	14.345	11.999	14.894	90.000	65.880	90.000	2339.76	-0.128	4.531	9.35
165	14.366	12.020	14.908	90.000	65.900	90.000	2350.07	-0.164	4.594	9.36
185	14.372	12.025	14.910	90.000	65.919	90.000	2352.62	-0.149	4.381	9.37
205	14.386	12.037	14.920	90.000	65.931	90.000	2359.09	-0.167	3.878	9.38
225	14.397	12.048	14.927	90.000	65.948	90.000	2364.33	-0.176	3.6	9.39
245	14.391	12.037	14.915	90.000	65.960	90.000	2359.59	-0.163	4.024	9.38

Table S4. Thermodiffractometric data for $[BimHgI_2]_n$, **4**. ΔT = 175 °C.

T (℃)	a	b	c	α	β	γ	Volume	SHD	R_{wp}	Hg···Hg
30	9.117	9.427	8.406	90.000	118.523	90.000	634.72	-0.230	6.370	9.43
45	9.121	9.428	8.413	90.000	118.522	90.000	635.68	-0.222	5.624	9.43
65	9.126	9.427	8.421	90.000	118.521	90.000	636.51	-0.205	6.043	9.43
85	9.134	9.428	8.432	90.000	118.526	90.000	637.97	-0.212	5.689	9.43
105	9.144	9.433	8.444	90.000	118.531	90.000	639.857	-0.213	5.704	9.43
125	9.151	9.434	8.455	90.000	118.539	90.000	641.23	-0.224	5.891	9.43
145	9.161	9.438	8.468	90.000	118.551	90.000	643.09	-0.238	5.757	9.44
165	9.167	9.437	8.477	90.000	118.566	90.000	644.01	-0.267	5.495	9.44
185	9.179	9.441	8.492	90.000	118.596	90.000	646.18	-0.291	6.956	9.44
205	9.195	9.444	8.509	90.000	118.620	90.000	648.60	-0.218	15.96	9.44

Table S5. Thermodiffractometric data for $[BimHgCl_2]_n$, **5**. ΔT = 195 °C.

T (℃)	a	b	c	α	β	γ	Volume	SHD	R_{wp}	Hg···Hg
30	8.345	9.432	6.864	90.000	90.762	90.000	540.20	-0.221	5.302	9.432
45	8.354	9.433	6.867	90.000	90.778	90.000	541.09	-0.223	5.060	9.433
65	8.367	9.434	6.869	90.000	90.812	90.000	542.14	-0.220	5.079	9.434
85	8.381	9.436	6.873	90.000	90.837	90.000	543.44	-0.228	5.224	9.436
105	8.396	9.439	6.877	90.000	90.863	90.000	544.98	-0.243	5.085	9.439
125	8.408	9.440	6.880	90.000	90.896	90.000	545.98	-0.244	5.163	9.440
145	8.418	9.439	6.880	90.000	90.925	90.000	546.66	-0.232	5.237	9.439
165	8.432	9.442	6.884	90.000	90.958	90.000	548.05	-0.244	5.085	9.442
185	8.446	9.444	6.886	90.000	90.996	90.000	549.19	-0.246	5.049	9.444
205	8.456	9.442	6.887	90.000	91.033	90.000	549.81	-0.258	5.110	9.442
225	8.474	9.447	6.893	90.000	91.057	90.000	551.71	-0.310	5.123	9.447