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Supporting information for article:

Tailoring the dimensionality of metal complexes via ligand modifications

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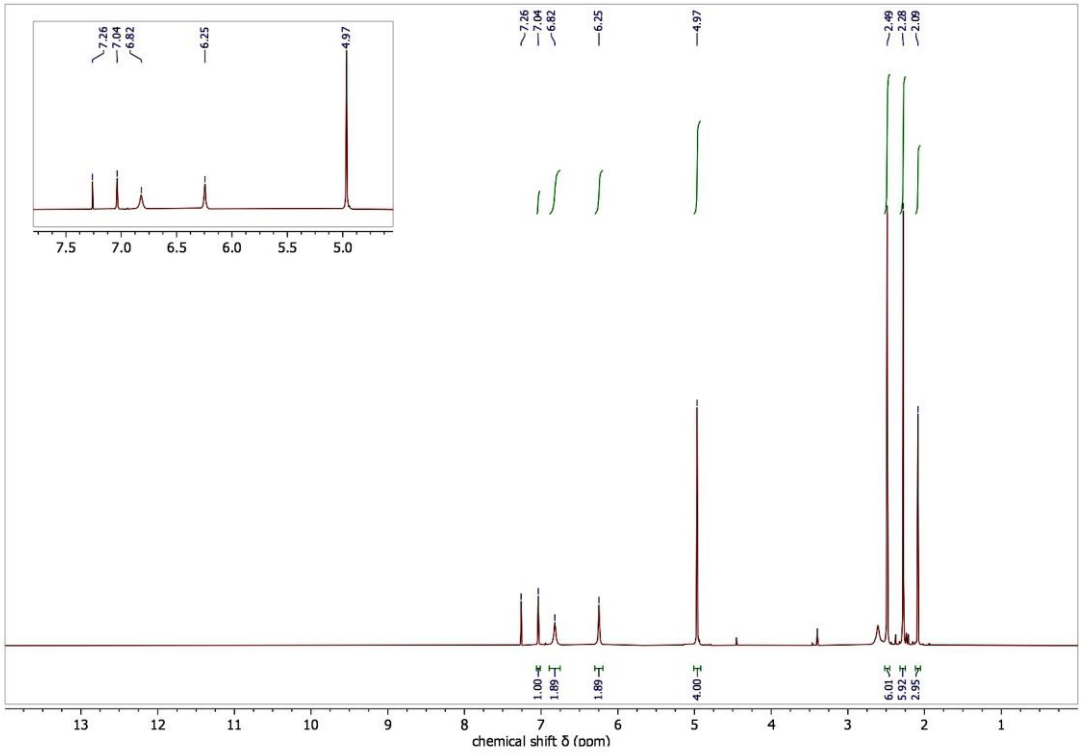
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chemical shift δ (ppm)

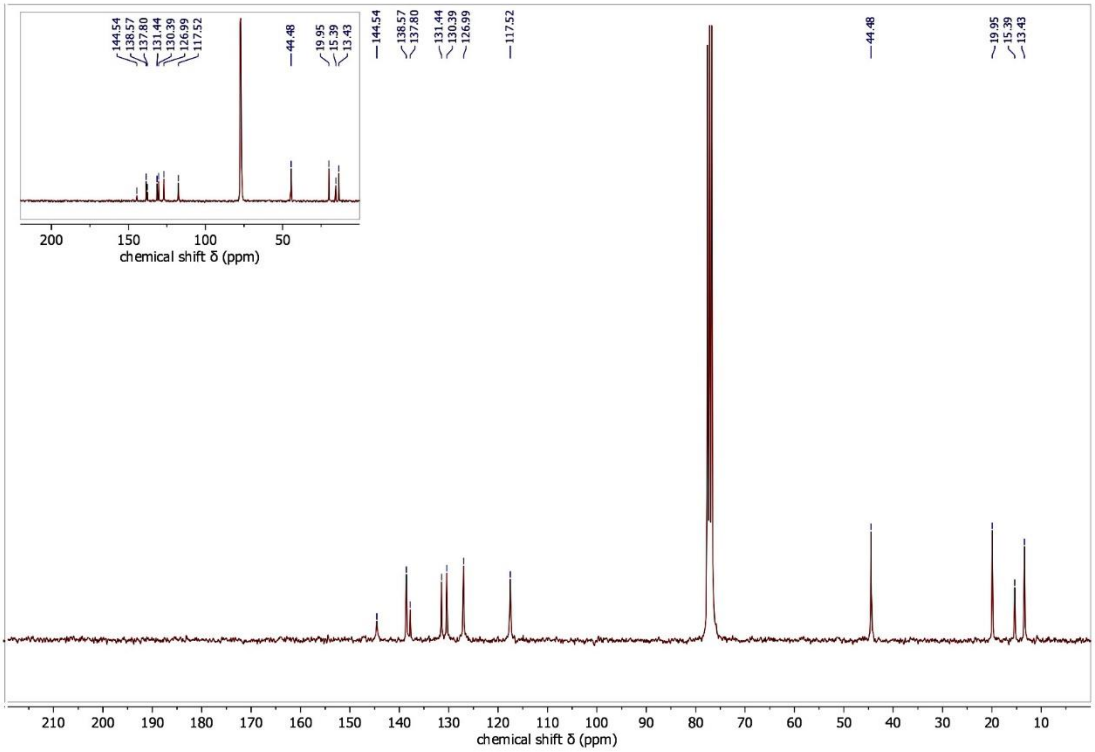

Figure S1 NMR spectra for **L4**.

Table S1 Intermolecular interactions in **1**-**4**.

Complexes	D-H---A	H---A (Å)	D---A (Å)	D-H---A (°)
1	C15-H15---N19^{i}	2.914	3.798(4)	156
	C5-H5---N19^{ii}	2.846	3.342(4)	114
	C6-H6A---N1^{iii}	2.752	3.492(3)	132
	C4-H4---O20^{ii}	2.845	3.334(3)	113
	C5-H5---O22ii	2.684	3.418(3)	134
	C13-H13A---O22i	2.793	3.661(4)	147
	C15-H15---O22i	2.423	3.274(4)	149
	C4-H4---O22iv	2.607	3.335(4)	134
	C6-H6A---O22iv	2.620	3.420(4)	138
	C12-H12---O22iv	2.661	3.442(3)	140
	C13-H13A---O21i	2.820	3.657(4)	143
	C6-H6B---O21v	2.438	3.323(4)	149
	C17-H17---O21^{vi}	2.849	3.365(4)	115
	C6-H6A---Cg1^{vii}	2.75	3.2571(14)	112
	C17-H17---Cg1^{viii}	2.98	3.4401(15)	111
	C13-H13B---Cg3^{ix}	2.86	3.6288(16)	135
2	C15-H15---N19^{i}	2.971	3.729(5)	138
	C10-H10---N19^{ii}	2.942	3.628 (5)	130
	C6-H6B---N1^{iii}	2.939	3.615(5)	126
	C6-H6B---N16^{iv}	2.789	3.602(6)	140
	C15-H15---O20^{i}	2.944	3.435(5)	113
	C17-H17---O20^{v}	2.601	3.147(5)	117
	C4-H4---O20^{iii}	2.795	3.563(5)	139

	C6-H6B---O20^{iii}	2.810	3.693(6)	149
	C6-H6A---O21^{vi}	2.625	3.562(5)	158
	C15-H15---O21^{i}	2.363	3.265(5)	159
	C4-H4---O21^{vii}	2.700	3.167(5)	111
	C5-H5---O21^{vii}	2.728	3.186(6)	110
	C10-H10---O21^{ii}	2.693	3.560(5)	152
	C4-H4---O22^{iii}	2.866	3.771(5)	159
	C2-H2---O22^{vi}	2.736	3.645(5)	160
	C12-H12---O22^{iii}	2.924	3.828(6)	159
	C11-H11---O22^{ii}	2.692	3.485(5)	141
	C2-H2---Cg2i	2.97	3.498(5)	116
	C6-H6B---Cg2^{iv}	2.95	3.561(5)	121
	C6-H6B---N3^{i}	2.887	3.366(5)	111
	C18-H18---N20^{ii}	2.707	3.432(6)	134
	C6-H6A---O21^{i}	2.537	3.510(5)	167
3	C16-H16---O21^{iii}	2.476	3.070(6)	121
	C18-H18---O21^{iv}	2.680	3.219(5)	117
	C12-H12---O23^{i}	2.619	3.501(5)	155
	C13-H13A---O23^{v}	2.758	3.527(6)	136
	C8-H8---O23^{vi}	2.669	3.527(7)	151
	C14-H14B---O23^{vi}	2.693	3.377(6)	127
	C19-H19---O23^{ii}	2.656	3.211(6)	118
	C16-H16---O23^{iii}	2.833	3.632(7)	143
	C2-H2---O22^{vi}	2.479	3.359(7)	154
	C8-H8---O22^{vi}	2.667	3.565(6)	158

	C18-H18---O22^{ii}	2.762	3.520(6)	137
	C5-H5---O22^{vii}	2.633	3.385(6)	136
	C6-H6B---Cg1^{i}	2.76	3.379(4)	121
	C13-H13B---Cg3^{viii}	2.94	3.752(6)	141
	C14-H14A---Cg3^{ix}	2.79	3.602(6)	139
4	O2-H2---N1^{i}	2.197	3.160	170
	O1-H1---N1^{ii}	2.650	3.574	168
	C7-H6---N2^{iii}	2.744	3.495	133
	O2-H2---O3^{iv}	1.876	2.792	156
	O1-H1---O3^{ii}	2.590	3.379	142
	C7-H7---O3^{v}	2.524	3.370	143
	C8-H8---O3^{i}	2.659	3.391	134
	C10-H10---O3^{v}	2.542	3.172	124
	O1-H1---O3^{ii}	2.07	2.992	168
	O2-H2---O4^{i}	2.752	3.656	155
	C2-H3---O4^{vi}	2.670	3.412	135
	C11-H1---O4^{vi}	2.588	3.451	146
	C13-H14---O4^{ii}	2.719	3.324	122
	C15-H18---O4^{vii}	2.851	3.533	127
	O2-H2---O5^{i}	2.669	3.511	145
	C6-H5---O5^{i}	2.565	3.489	165
	C8-H8---O5^{i}	2.597	3.546	176
	C14-H15---O5^{vi}	2.423	3.365	171
	C7-H6---Cg1^{v}	2.90	3.716	140
	C11-H11---Cg3^{vii}	2.59	3.545	162

C15-H16---Cg3^{viii}	2.95	3.817	147

(1) Cg1 is the centroid of imidazole ring N1-C5, Cg3 is the centroid of benzene ring C7-C12, **(2)** Cg2 is the centroid of imidazole ring N14-C18, **(3)** Cg1 is the centroid of imidazole ring N1-C5, Cg3 is the centroid of benzene ring C7-C12, **(4)** Cg1 is the centroid of imidazole ring N2-C10, Cg3 is the centroid of benzene ring C1-C6; Symmetry codes (**1**): (i) -x,-y,-z, (ii) 1-x,y-1/2,1/2-z, (iii) 1-x,-y-1,-z, (iv) x,y-1,z, (v) x,-y-1/2,z-1/2, (vi) -x,y-1/2,-z-1/2, (vii) 1-x,1-y,-z, (viii) x,y,z (ix) 2-x,-1/2+y,1/2-z; (**2**): (i) -x,y,3/2-z, (ii) 1/2+x,1/2-y,1/2+z, (iii) 1/2-x,1/2-y,1-z, (iv) 1/2-x,1/2+y,3/2-z, (v) x,-y,1/2+z, (vi) -x,1-y,1-z, (vii) 1/2+x,y-1/2,z; (**3**): (i) 1-x,3-y,-z, (ii) x,y,1+z, (iii) x-1,y,1+z, (iv) 1-x,2-y,1-z, (v) x-1,1+y,1+z, (vi) 1-x,2-y,-z, (vii) 2-x,2-y,-z, (viii) 1-x,3-y,1-z, (ix) -x,3-y,1-z; (**4**): (i) x,y,z, (ii) x,1+y,z, (iii) 2-x,-y,1-z, (iv) -x,y,1/2-z, (v) -x,-y,1-z, (vi) x,-y,1/2+z, (vii) 1/2-x,1/2+y,z, (viii) 1/2-x,-1/2+y,z.

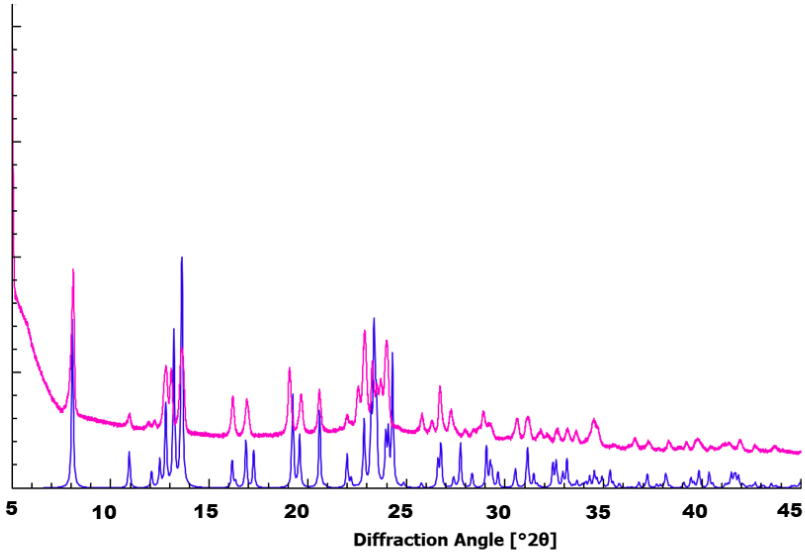

Figure S2 Result of PXRD analysis for **3** indicating dominancy of this particular phase in the bulk: blue – calculated for **3**, purple - experimental trace for bulk material **3**.

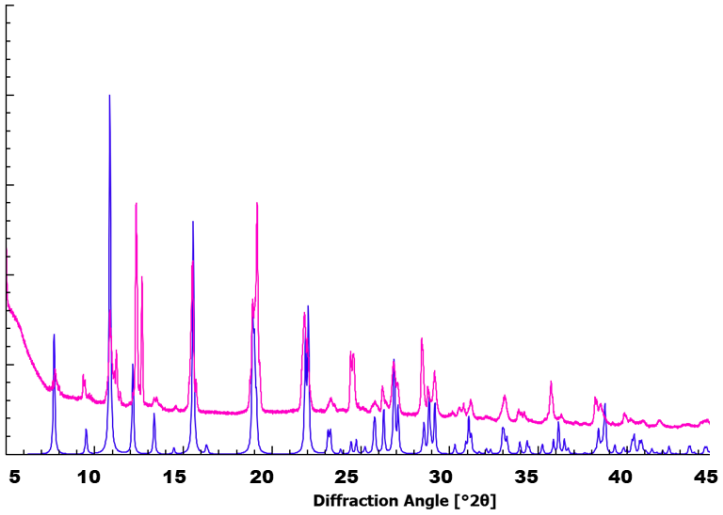

Figure S1 Result of PXRD analysis for **5**: blue – calculated for **5**, purple - experimental trace for bulk material **5**.

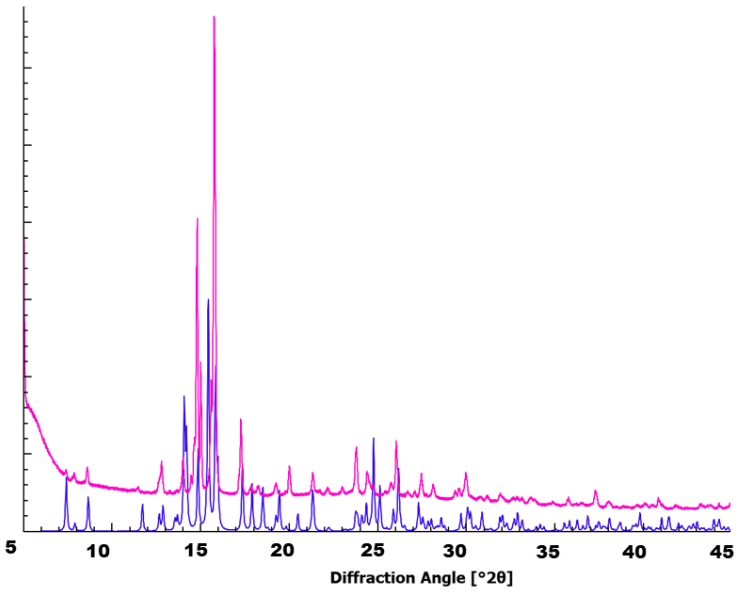

Figure S4 Result of PXRD analysis for **6** indicating dominancy of this particular phase in the bulk: blue – calculated for **6**, purple - experimental trace for bulk material **6**.

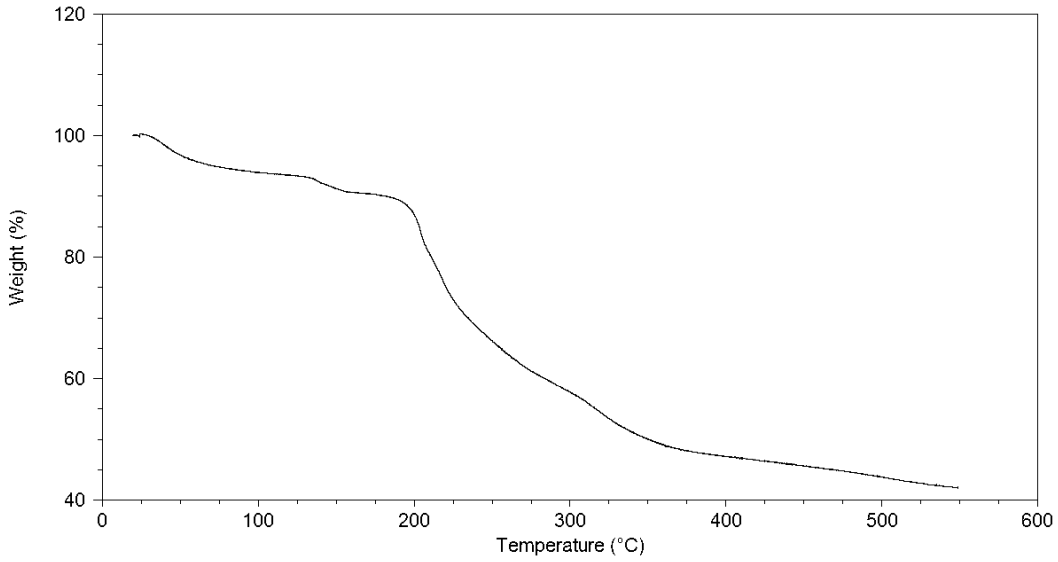

Figure S5 Thermogram of **5**.