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Supporting information for article:

Novel Ba^{2+} and Pb^{2+} metal–organic frameworks based on a semi-rigid tetracarboxylic acid: syntheses, structures, topologies and luminescence properties

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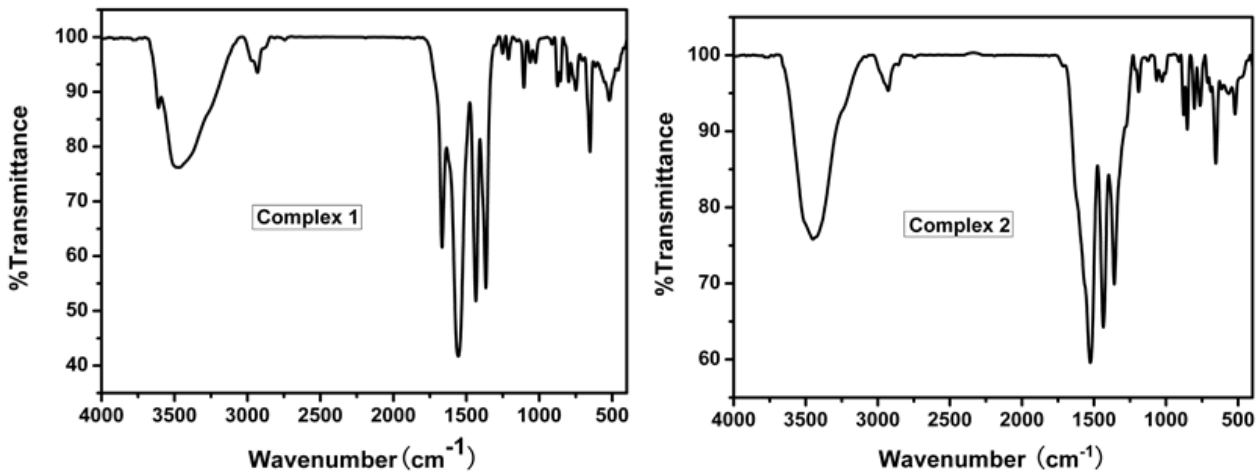
(1)Table S1 Selected bond lengths (Å) and angles (º) for 1 – 2.

Complex **1**[a]							
Ba1—O9	2.658 (4)	Ba1—O1	2.704(3)	Ba1—O4^{i}	2.744 (3)	Ba1—O8^{ii}	2.760 (3)
Ba1—O6^{iii}	2.765 (3)	Ba1—O1W	2.778 (3)	Ba1—O7^{ii}	2.920 (3)	Ba1—O5^{iii}	3.035 (3)
Ba2—O4W	2.713 (3)	Ba2—O7^{ii}	2.678 (3)	Ba2—O3W	2.694 (3)	Ba2—O2	2.699 (3)
Ba2—O2W^{v}	3.012 (4)	Ba2—O3^{iv}	2.720 (3)	Ba2—O1W	2.940 (3)	Ba2—O2W	2.956 (4)
O9—Ba1—O1	92.52 (16)	O1—Ba1—O4^{i}	90.64 (11)	O4^{i}—Ba1—O1W	79.95 (9)	O8^{ii}—Ba1—O1W	116.02 (9)
O9—Ba1—O4^{i}	85.22 (11)	O1—Ba1—O8^{ii}	85.56 (11)	O1W—Ba1—O7^{ii}	71.04 (8)	O6^{iii}—Ba1—O1W	108.48 (12)
O9—Ba1—O8^{ii}	78.35 (11)	O1—Ba1—O6^{iii}	155.32 (11)	O1W—Ba1—O5^{iii}	83.18 (10)	O6^{iii}—Ba1—O5^{iii}	43.98 (9)
O9—Ba1—O6^{iii}	80.98 (16)	O1—Ba1—O1W	83.56 (12)	O2—Ba2—O4W	81.47 (13)	O4W—Ba2—O3^{iv}	130.88 (10)
O9—Ba1—O1W	164.60 (12)	O1—Ba1—O7^{ii}	87.00 (11)	O2—Ba2—O3^{iv}	146.90 (12)	O4W—Ba2—O1W	155.23 (10)
O9—Ba1—O7^{ii}	123.77 (11)	O1—Ba1—O5^{iii}	160.48 (10)	O2—Ba2—O1W	78.68 (13)	O4W—Ba2—O2W	60.91 (12)
O9—Ba1—O5^{iii}	96.50 (14)	O3W—Ba2—O2	81.13 (11)	O2—Ba2—O2W	130.42 (11)	O4W—Ba2—O2Wv	70.29 (11)
O7^{ii}—Ba2—O3W	135.93 (10)	O3W—Ba2—O4W	124.11 (12)	O2—Ba2—O2W^{v}	129.88 (13)	O3^{iv}—Ba2—O1W	68.31 (9)
O7^{ii}—Ba2—O2	75.30 (11)	O3W—Ba2—O3^{iv}	83.94 (10)	O1W—Ba2—O2W	124.31 (11)	O3^{iv}—Ba2—O2W	73.91 (10)
O7^{ii}—Ba2—O4W	88.68 (11)	O3W—Ba2—O1W	67.06 (10)	O1W—Ba2—O2W^{v}	134.36 (10)	O3W—Ba2—O2W^{v}	81.79 (10)
O7^{ii}—Ba2—O1W	72.08 (9)	O3W—Ba2—O2W	146.09 (10)	O2W—Ba2—O2W^{v}	68.36 (12)	O7ii—Ba2—O2W	72.94 (9)

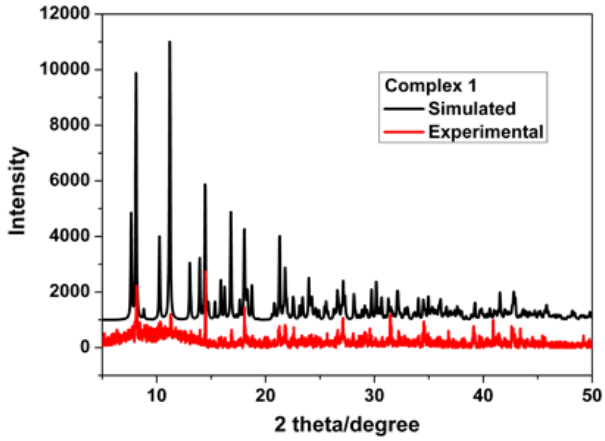
Complex **2**[b]							
Pb1—O1	2.597 (9)	Pb1—O1W	2.662 (10)	Pb1—O2	2.510 (8)	Pb1—O5^{vi}	2.397 (0)
Pb1—O5^{vii}	2.498 (10)	Pb1—O4^{vii}	2.769(5)	Pb2—O7	2.640 (11)	Pb2—O8	2.313 (9)
Pb2—O2W	2.67 (2)	Pb2—O4^{i}	2.635 (9)	Pb2—O3^{i}	2.469 (10)	Pb2—O3^{viii}	2.449 (12)
O5^{vii}—Pb1—O1	127.0 (3)	O5^{vi}—Pb1—O2	80.6 (3)	O5^{vii}—Pb1—O2	76.3 (3)	O5^{vi}—Pb1—O1	99.4 (3)
O2—Pb1—O1W	150.6 (4)	O2—Pb1—O1	50.8 (3)	O5^{vi}—Pb1—O1W	77.8 (3)	O5^{vii}—Pb1—O1W	77.7 (3)
O3^{viii}—Pb2—O3^{i}	77.2 (4)	O1—Pb1—O1W	153.0 (3)	O8—Pb2—O3^{viii}	91.5 (4)	O8—Pb2—O3^{i}	82.4 (3)
O8—Pb2—O4^{i}	83.7 (3)	O8—Pb2—O7	49.9 (4)	O3^{viii}—Pb2—O7	135.0 (4)	O3^{i}—Pb2—O7	112.8 (3)
O8—Pb2—O2W	122.9 (5)	O3^{viii}—Pb2—O2W	140.7 (5)	O^{3i}—Pb2—O4i	47.8 (4)	O7—Pb2—O4^{i}	78.6 (4)
O4^{i}—Pb2—O2W	81.2 (5)			O^{3i}—Pb2—O2W	122.0 (5)	O7—Pb2—O2W	73.1 (5)

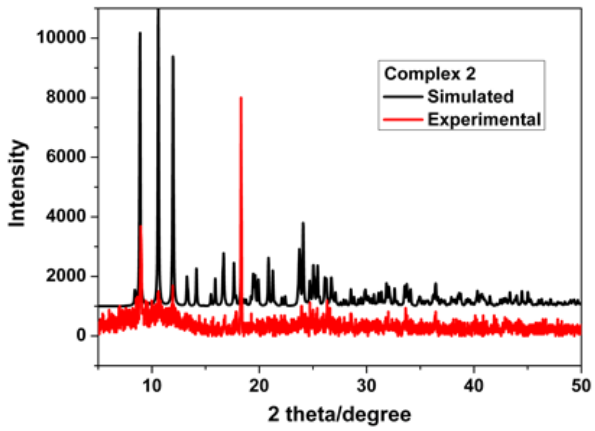
[a] Symmetry codes: (i) −x+1/2, y+1/2, −z+1/2; (ii) −x+1/2, y−1/2, −z+1/2; (iii) x+1, y, z; (iv) x+1/2, −y+1/2, z−1/2; (v) −x+1, −y, −z; (vi) x−1, y, z; (vii) x−1/2, −y+1/2, z+1/2. [b] Symmetry codes: (i) x−1/2, −y+3/2, z+1/2; (ii) −x+3/2, y+1/2, −z+1/2; (iii) x+1/2, −y+3/2, z−1/2; (iv) −x+3/2, y−1/2, −z−1/2; (v) x+1/2, −y+3/2, z+1/2; (vi) −x+3/2, y+1/2, −z−1/2; (vii) x−1/2, −y+3/2, z−1/2; (viii) −x+3/2, y−1/2, −z+1/2.

(2) Fig. S1: IR spectra of complexes 1-2.



(3) Fig. S2: The powder XRD pattern and the simulated one from the single-crystal diffraction data for complexes 1-2.


Complex 1
Simulated
Experimental
Intensity
2 theta/degree
0
2000
4000
6000
8000
10000
12000
10
20
30
40
50


Complex 2
Simulated
Experimental
Intensity
2 theta/degree
0
2000
4000
6000
8000
10000
10
20
30
40
50