

Supplementary Material (ESI) for Dalton Transactions
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Isopolymolybdate-based inorganic–organic hybrid compounds constructed by multidentate N-donor ligands: syntheses, structures and properties

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Table S1 Selected bond lengths and angles for compounds 1–5.

Compound 1			
Mo1-O3	1.717(2)	Mo1-N3	2.302(2)
Mo1-O1	1.7379(19)	Mo1-N2	2.323(2)
Mo1-O2	1.743(2)	Mo1-N1	2.3930(18)
O3-Mo1-O1	106.63(10)	O2-Mo1-N2	85.35(9)
O3-Mo1-O2	106.57(10)	N3-Mo1-N2	73.06(7)
O1-Mo1-O2	106.70(11)	O3-Mo1-N1	155.44(9)
O3-Mo1-N3	87.60(9)	O1-Mo1-N1	87.44(8)
O1-Mo1-N3	89.08(9)	O2-Mo1-N1	87.75(8)
O2-Mo1-N3	154.12(8)	N3-Mo1-N1	72.28(7)
O3-Mo1-N2	89.23(9)	N2-Mo1-N1	71.79(7)
O1-Mo1-N2	155.77(8)		

Compound 2			
Cu1-O1W	1.955(4)	Cu1-N3	2.071(5)
Cu1-N1	1.995(5)	Cu1-N4	2.070(6)
Cu1-N2	2.057(5)		
O1W-Cu1-N1	178.0(2)	N2-Cu1-N4	116.9(2)
O1W-Cu1-N2	97.4(2)	O1W-Cu1-N3	97.1(2)
N1-Cu1-N2	81.9(2)	N1-Cu1-N3	81.5(2)
O1W-Cu1-N4	100.4(2)	N2-Cu1-N3	113.0(2)
N1-Cu1-N4	81.6(2)	N4-Cu1-N3	123.9(2)

Compound 3			
Co1-O1	2.037(5)	Co1-N3	2.120(7)
Co1-N2	2.096(7)	Co1-N1	2.198(7)
Co1-N4	2.115(7)	Co1-O9#2	2.217(5)
O1-Co1-N2	99.4(2)	N4-Co1-N1	76.7(3)
O1-Co1-N4	106.4(2)	N3-Co1-N1	78.7(3)
N2-Co1-N4	149.8(3)	O1-Co1-O9#2	82.7(2)
O1-Co1-N3	92.9(2)	N2-Co1-O9#2	86.0(2)

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N2-Co1-N3	84.5(3)	N4-Co1-O9#2	82.0(2)
N4-Co1-N3	109.2(3)	N3-Co1-O9#2	168.8(2)
O1-Co1-N1	171.7(2)	N1-Co1-O9#2	105.5(2)
N2-Co1-N1	80.1(3)		

2 -1-x, -y, -z

Compound 4

Co1-O1	1.978(2)	Co1-N2	2.106(3)
Co1-O12#1	2.252(2)	Co1-N1	2.149(3)
Co1-N4	2.140(3)	Co1-N3	2.151(3)
O1-Co1-O12#1	87.21(9)	N2-Co1-O12#1	171.16(11)
O1-Co1-N4	101.43(11)	N2-Co1-N4	105.24(12)
O1-Co1-N2	88.46(11)	N2-Co1-N1	80.94(12)
O1-Co1-N1	168.67(11)	N2-Co1-N3	81.30(12)
O1-Co1-N3	103.13(12)	N1-Co1-O12#1	103.83(10)
N4-Co1-O12#1	83.18(10)	N1-Co1-N3	79.30(12)
N4-Co1-N1	77.76(12)	N3-Co1-O12#1	92.19(10)
N4-Co1-N3	154.74(12)		

#1 2-x, -y, 1-z

Compound 5

Cu1-N4	2.004(4)	Cu1-N5	1.967(4)
Cu1-N1	2.089(4)	Cu2-O1	2.325(3)
Cu1-N2	2.045(4)	Cu2-N8	2.091(4)
Cu1-N3	2.119(4)	Cu2-N9	1.990(3)
N5-Cu1-N1	100.55(16)	N5-Cu1-N4	178.22(15)
N5-Cu1-N2	97.66(18)	O1-Cu2-O1#2	180.00(16)
N5-Cu1-N3	98.19(16)	N8-Cu2-O1	89.20(13)
N4-Cu1-N1	81.23(15)	N8-Cu2-N8#2	180
N4-Cu1-N2	81.55(17)	N9-Cu2-O1	88.01(13)
N4-Cu1-N3	80.82(15)	N9-Cu2-N8#2	88.48(14)
N1-Cu1-N3	118.73(16)	N9-Cu2-N8	91.52(14)
N2-Cu1-N1	116.59(17)	N9#2-Cu2-N8	88.48(14)
N2-Cu1-N3	117.79(16)	N9#2-Cu2-N9	180

#2 2-x, 1-y, -z

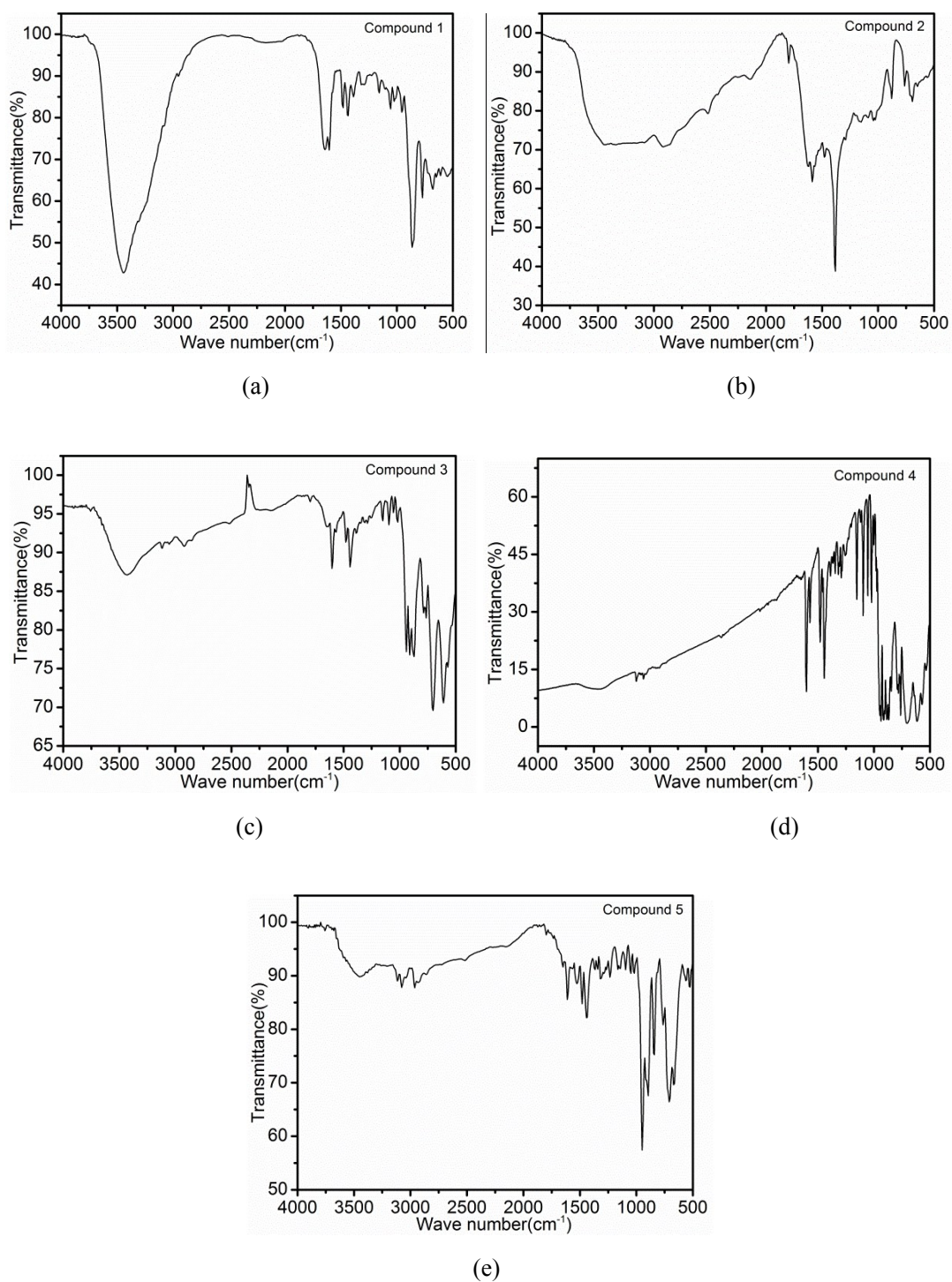


Fig. S1 The IR spectra of compounds 1–5.

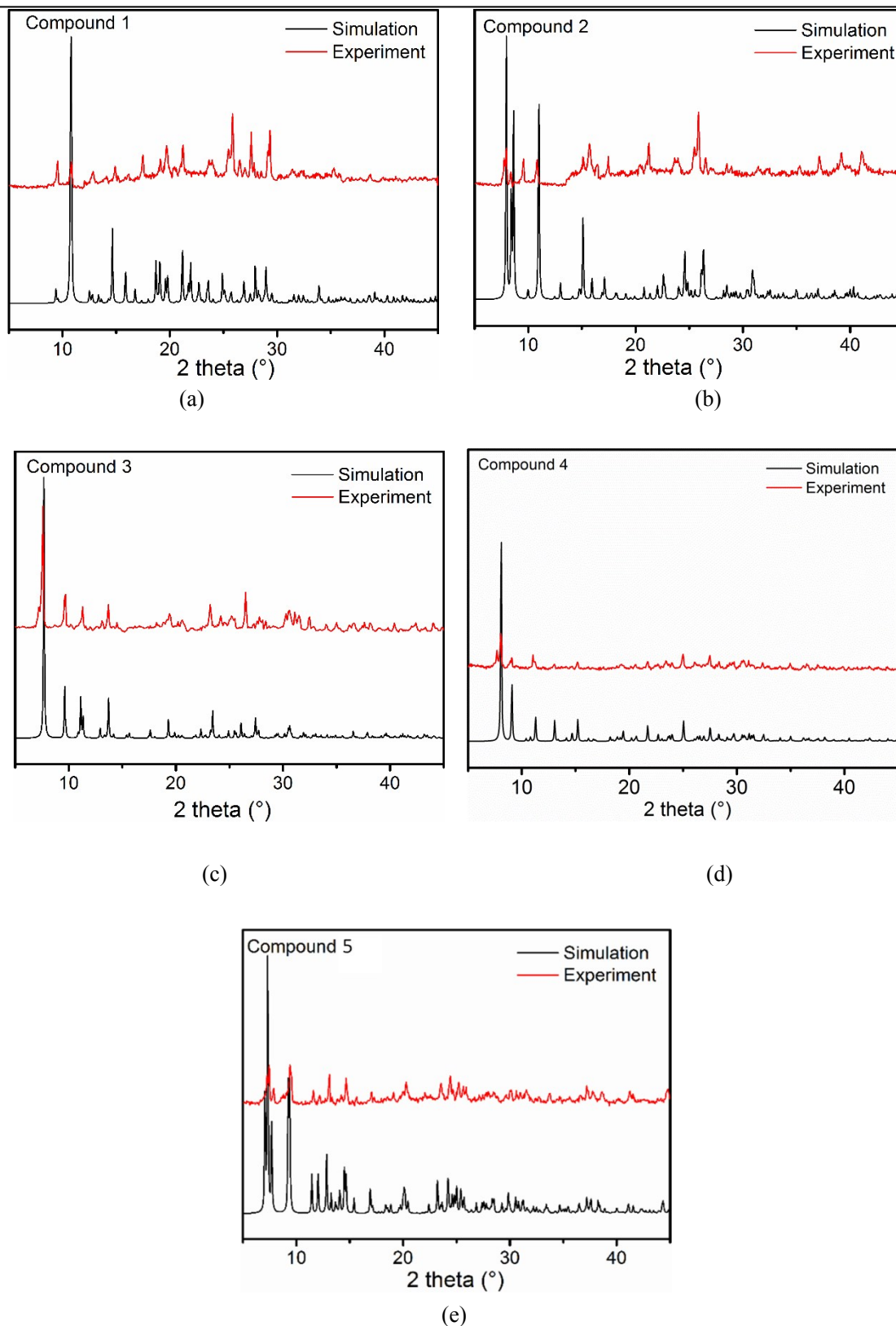


Fig. S2 The powder X-ray diffraction of compounds 1–5.

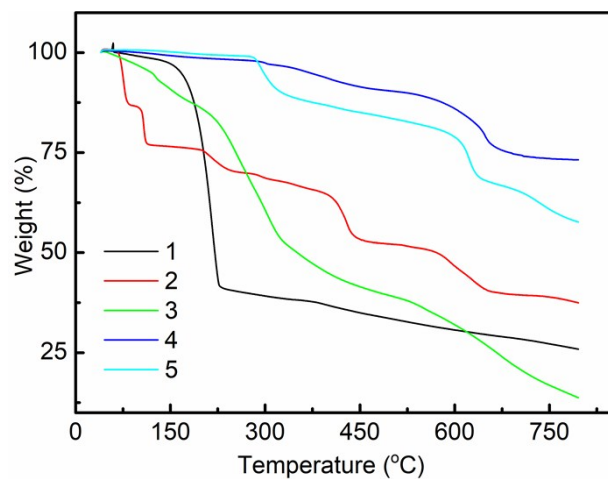

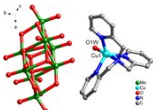
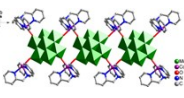
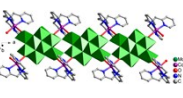
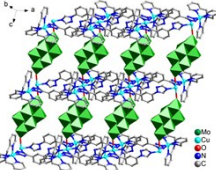


Fig. S3 The TG curves of compounds 1–5.

Table S2 Relationship between structure and property of compounds 1–5.

Compound	1	2	3	4	5
Crystal Structure					
Thermal Stability	✗	✗	✗	✓	✓
Electrocatalytic	✗	✗	✗	✗	✓
Photocatalytic	✗	✗	✗	✓	✓