Supporting Information

Characterization of a new porous Pt-containing metal-organic framework containing potentially catalytically active sites: Local electronic structure at the metal centers.

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The structure of Pt/Gd-MOF was determined by single crystal X-ray diffraction using a Siemens Bruker Smart CCD diffractometer. A total of 915 frames were collected ($\Delta\omega$ = 0.6°, 45 s per frame), covering one hemisphere of the reciprocal space. Data reduction and empirical absorption correction were carried out using the programs SAINT+[1] and SADABS,[2] respectively. The structure was solved by direct methods and refined using the SHELXTL[3] program package. A detailed description on both data acquisition and data analysis has been reported elsewhere.[4] Table S1 reports a selection of atomic distances and angles.

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Table S1. Selection of bond distances (Å) and angles (°), with corresponding e.s.d., from structure determination of the Pt/Gd-MOF (single crystal data).[4]

Pt(1)-N(2)	2.036(19)	Gd(1)-O(11)	2.349(16)
Pt(1)-N(1)	2.03(2)	Gd(1)-OW5	2.378(18)
Pt(1)-Cl(2)	2.304(7)	Gd(1)-OW6	2.479(17)
Pt(1)-Cl(1)	2.305(6)	Gd(1)-O(2)	2.490(18)
Pt(2)-N(3)	2.022(19)	Gd(1)-OW4	2.505(17)
Pt(2)-N(4)	2.03(2)	Gd(1)-O(1)	2.500(18)
Pt(2)-Cl(3)	2.309(6)	Gd(2)-O(6)	2.302(17)
Pt(2)-Cl(4)	2.313(6)	Gd(2)-O(4)	2.343(17)
Pt(3)-N(6)	2.034(17)	Gd(2)-O(9)	2.348(16)
Pt(3)-N(5)	2.07(2)	Gd(2)-OW1	2.348(16)
Pt(3)-Cl(6)	2.303(6)	Gd(2)-OW3	2.387(16)
Pt(3)-Cl(5)	2.315(7)	Gd(2)-OW2	2.459(16)
Gd(1)-O(5)	2.261(19)	Gd(2)-O(8)	2.516(17)
Gd(1)-O(3)	2.340(18)	Gd(2)-O(7)	2.527(17)
Pt(1)-Pt(2)	3.386(2)	Pt(2)-Pt(3)	3.291(2)
Pt(1)-C(3)	2.88(2)	Pt(1)-C(1)	2.99(2)
Pt(1)-C(12)	2.90(4)	Pt(1)-C(10)	3.01(3)
Pt(2)-C(21)	2.90(2)	Pt(2)-C(14)	3.00(2)
Pt(2)-C(19)	2.92(3)	Pt(2)-C(15)	3.06(2)
Pt(3)-C(26)	2.88(3)	Pt(3)-C(32)	3.04(2)
Pt(3)-C(30)	2.90(2)	Pt(3)-C(25)	3.07(3)
N(1)-Pt(1)-N(2)	81.9(8)	N(3)-Pt(2)-Cl(4)	176.4(6)
N(1)-Pt(1)-Cl(2)	176.3(6)	N(4)-Pt(2)-Cl(4)	96.0(7)
N(2)-Pt(1)-Cl(2)	94.5(6)	Cl(3)-Pt(2)-Cl(4)	88.0(2)
N(1)-Pt(1)-Cl(1)	94.9(6)	N(6)-Pt(3)-N(5)	81.2(8)
N(2)-Pt(1)-Cl(1)	176.2(6)	N(6)-Pt(3)-Cl(6)	176.7(5)
Cl(2)-Pt(1)-Cl(1)	88.7(2)	N(5)-Pt(3)-Cl(6)	96.0(6)
N(3)-Pt(2)-N(4)	80.5(8)	N(6)-Pt(3)-Cl(5)	95.1(5)
N(3)-Pt(2)-Cl(3)	95.6(6)	N(5)-Pt(3)-Cl(5)	176.2(6)
N(4)-Pt(2)-Cl(3)	176.0(7)	Cl(6)-Pt(3)-Cl(5)	87.7(2)

The XRPD pattern of the dehydrated material has been indexed and then refined by using the whole profile in a Pawley refinement. The result of this refinement is shown in Figure S1.

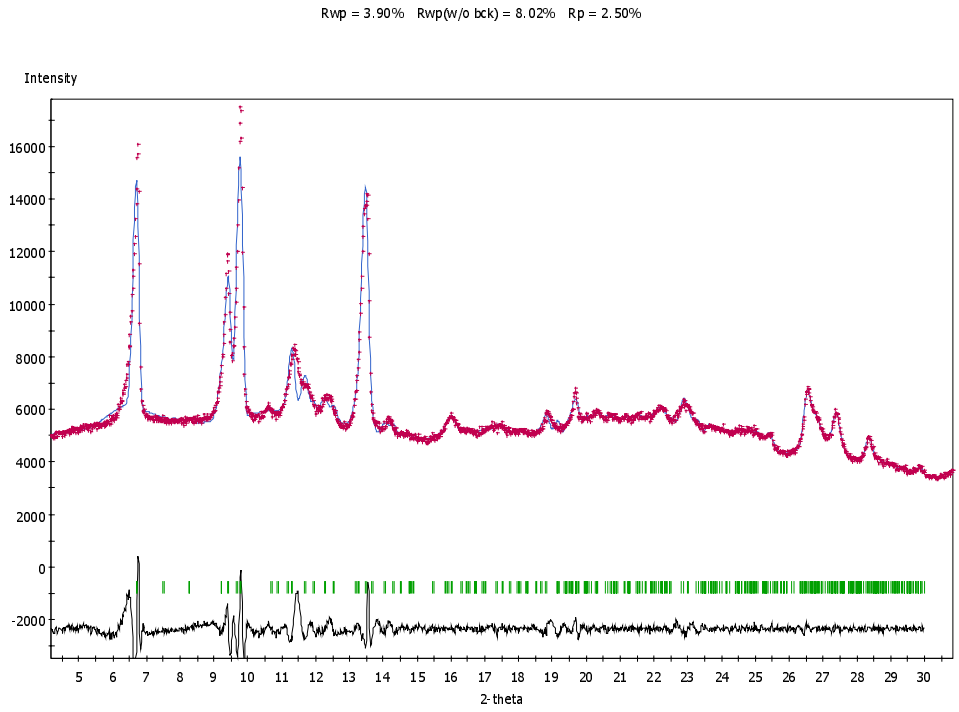

Figure S1. Pawley refinement of the dehydrated Pt-Gd MOF: experimental (red scattered points), theoretical (blue curve) and residual (black curve). Green bars represents the expected reflections after indexing.

References

(1) Bruker AXS, SAINT+ version 6.22, Bruker AXS, Madison, WI, USA, 2001.

(2) Sheldrick, G. M. SADABS, Empirical Absorption Corrections Program, University of Göttingen, Germany, 1997.

(3) Sheldrick, G. M. Shelxl-97, A program for crystal structure refinement, University of Göttingen, Germany, 1997.

(4) Szeto, K. C.; Kongshaug, K. O.; Jakobsen, S.; Tilset, M.; Lillerud, K. P. *Dalton Trans.* **2006**, submitted.