Influence of the Lanthanide (III) ion in $\{[Cu_3Ln_2(oda)_6(H_2O)_6]\bullet nH_2O\}_n$ (Ln^{III}: La,Gd,Yb) Catalysts on the Heterogeneous Oxidation of Olefins.

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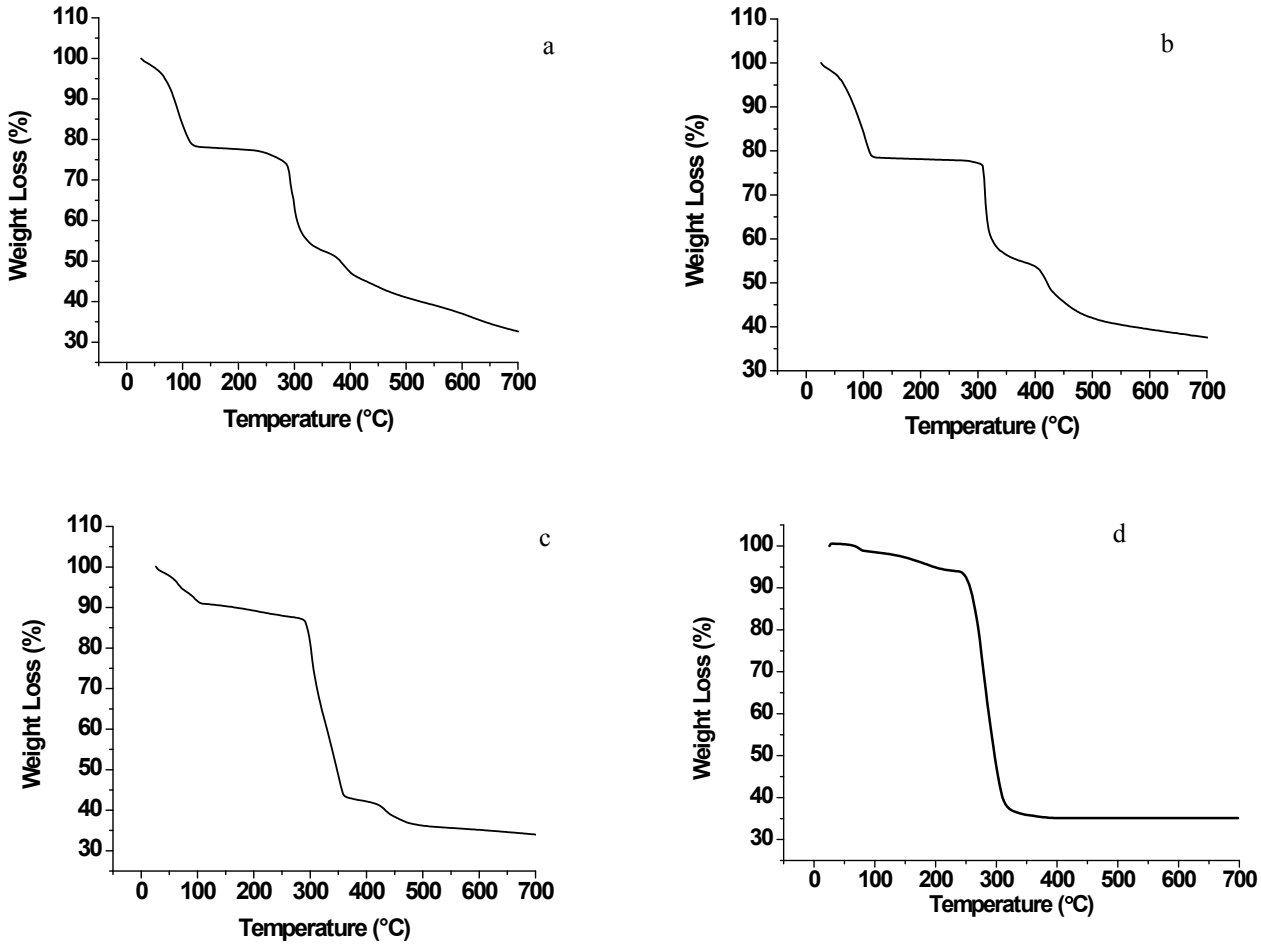


Fig S1. Thermograms for (a) $\{[Cu_3La_2(oda)_6(H_2O)_6]\bullet 12H_2O\}_n$ **(1);** (b) $\{[Cu_3Gd_2(oda)_6(H_2O)_6]\bullet 12H_2O\}_n$ **(2)**;(c) $\{[Cu_3Yb_2(oda)_6(H_2O)_6]\}_n$ **(3);** (d) $\{[Cu(oda)_2] \bullet 0.5H_2O\}_n$ **(4)**.

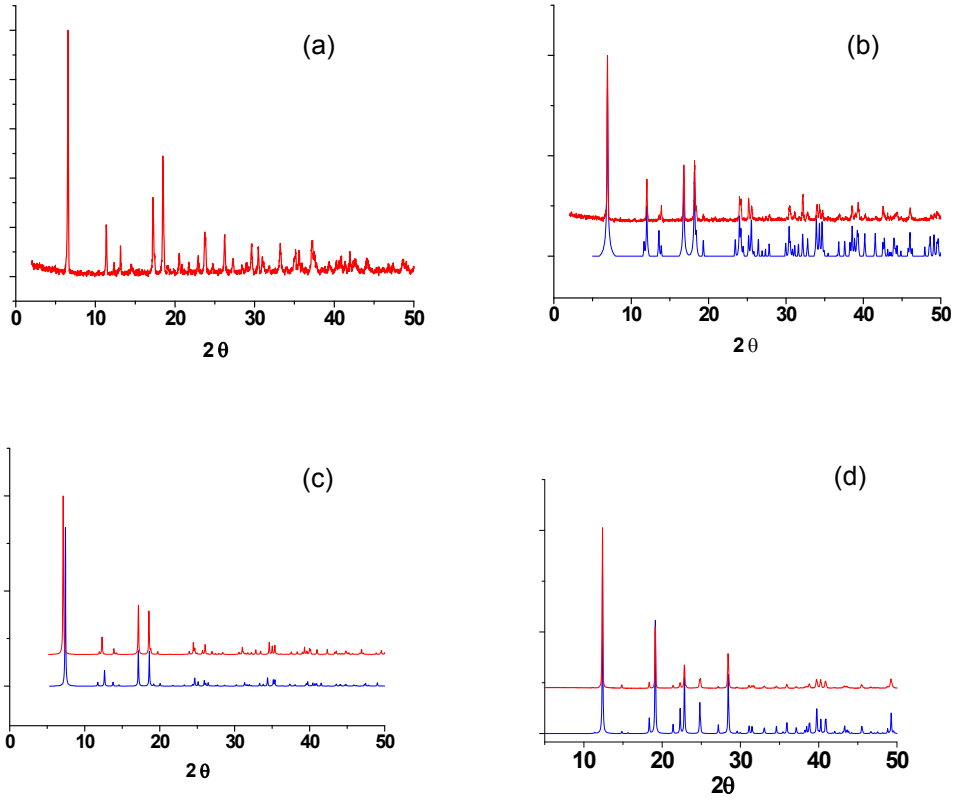


Fig S2. Powder diffractograms corresponding to (a) $\{[Cu_3La_2(oda)_6(H_2O)_6]\bullet 12H_2O\}_n$; (b) $\{[Cu_3Gd_2(oda)_6(H_2O)_6]\bullet 12H_2O\}_n$; (c) $\{[Cu_3Yb_2(oda)_6(H_2O)_6]\}_n$; (d) $\{[Cu(oda)_2]\bullet 0.5H_2O\}_n$. (Blue: simulated; Red: experimental).

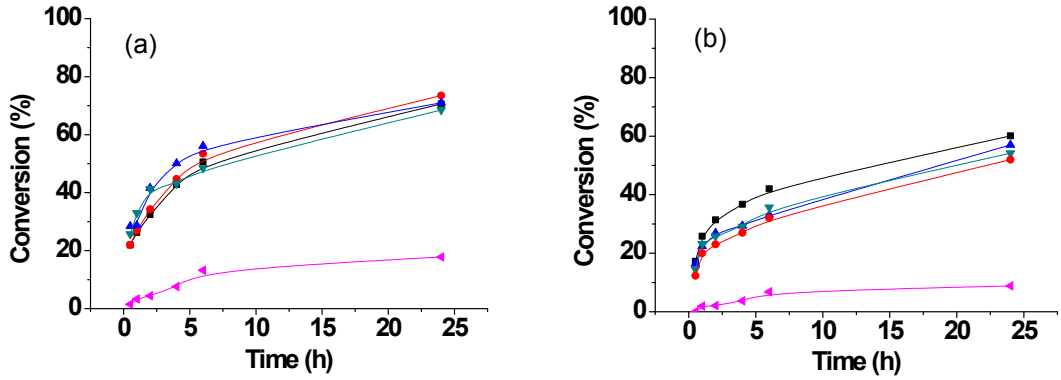


Fig S3. Oxidation of (a) styrene or (b) cyclohexene, catalyzed by CuGdMOF, using different S/O/C ratios. 400/400/1 (●); 800/800/1 (▲); 1200/1200/1 (▼); 2400/2400/1 (■); blank (◄).

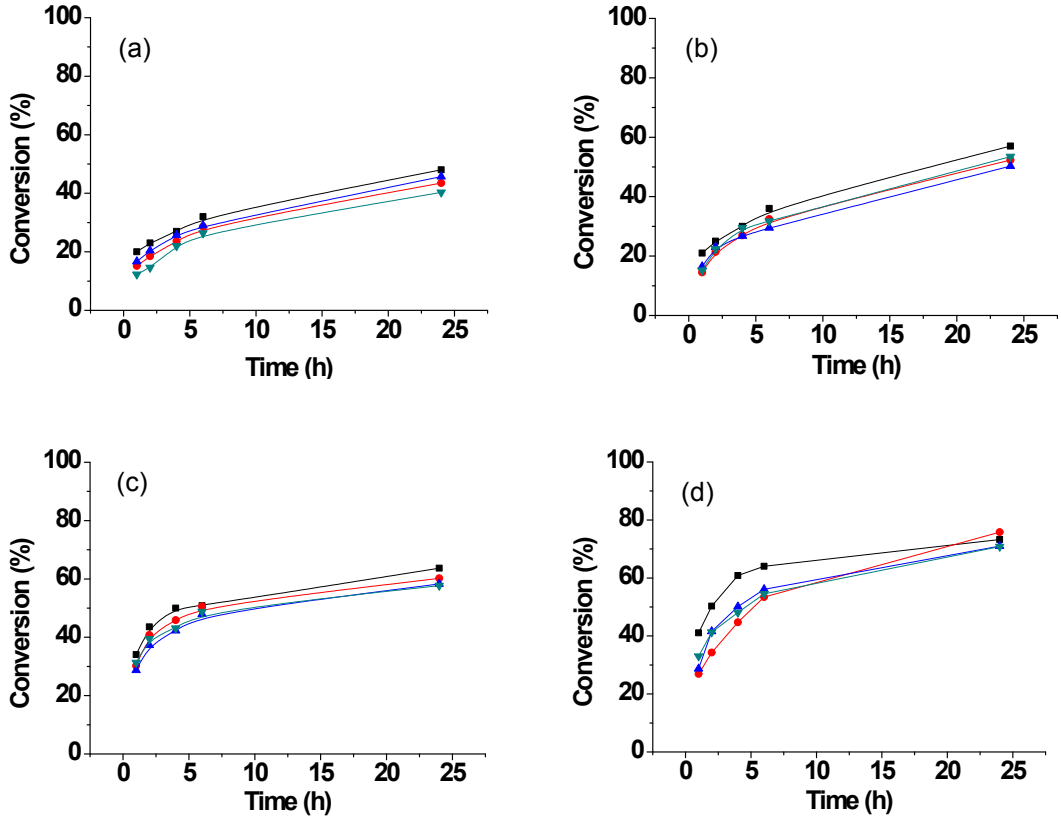


Fig S4. Reusability of catalysts for the oxidation reactions. (■): Run 1; (●): Run 2; (▲): Run 3; (▼): Run 4. Oxidation of cyclohexene: (a) $\{[Cu_3La_2(oda)_6(H_2O)_6]\bullet 12H_2O\}_n$; (b) $\{[Cu_3Yb_2(oda)_6(H_2O)_6]\}_n$; Oxidation of styrene: (c) $\{[Cu_3La_2(oda)_6(H_2O)_6]\bullet 12H_2O\}_n$; (d) $\{[Cu_3Yb_2(oda)_6(H_2O)_6]\}_n$

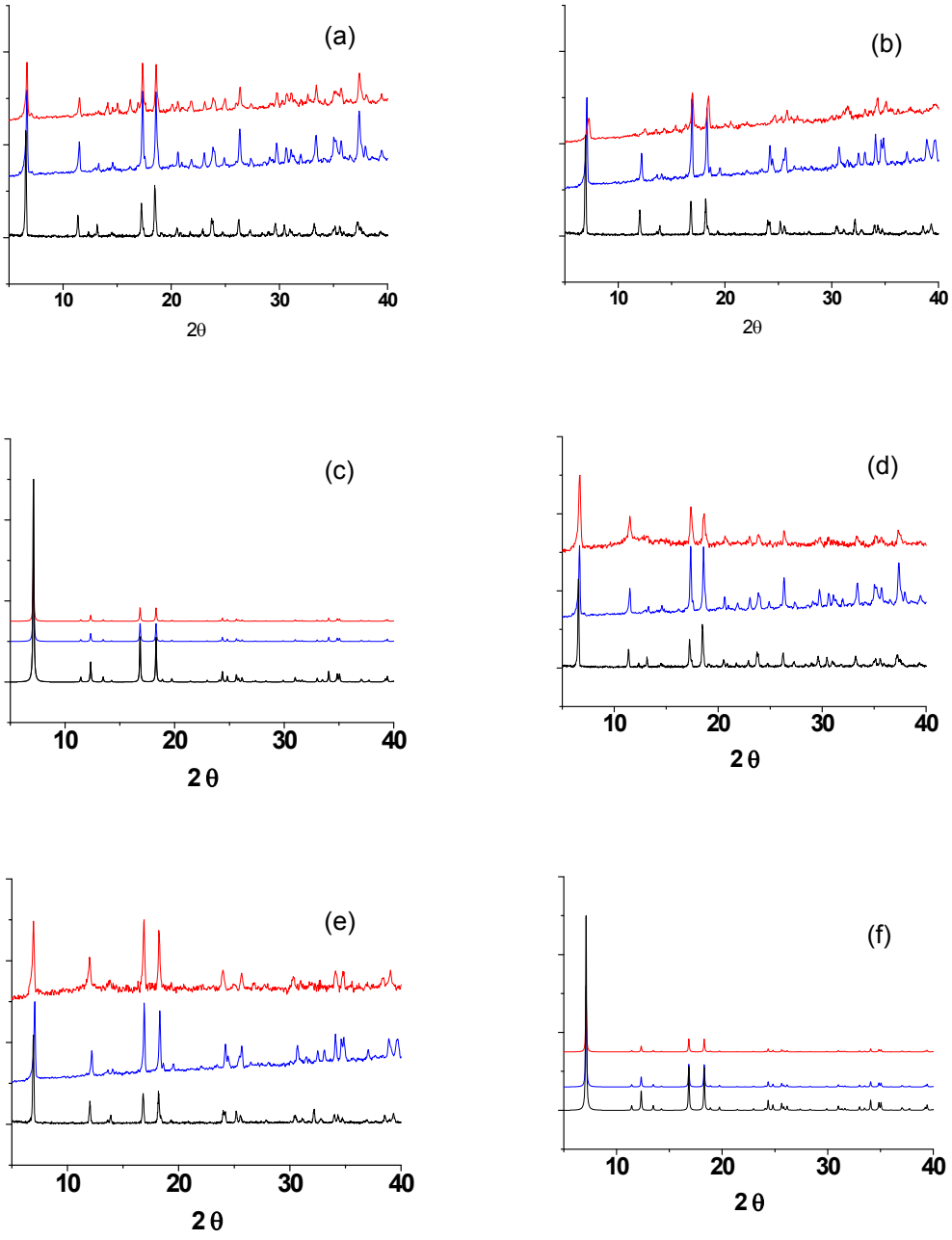


Fig S5. Powder diffractograms corresponding to reusability of the catalysts in oxidations reactions. Oxidation of cyclohexene: (a) $\{[Cu_3La_2(oda)_6(H_2O)_6]\bullet 12H_2O\}_n$; (b) $\{[Cu_3Gd_2(oda)_6(H_2O)_6]\bullet 12H_2O\}_n$; (c) $\{[Cu_3Yb_2(oda)_6(H_2O)_6]\}_n$; Oxidation of styrene: (d) $\{[Cu_3La_2(oda)_6(H_2O)_6]\bullet 12H_2O\}_n$; (e) $\{[Cu_3Gd_2(oda)_6(H_2O)_6]\bullet 12H_2O\}_n$ (f) $\{[Cu_3Yb_2(oda)_6(H_2O)_6]\}_n$. (Black: fresh catalyst; Blue: after run 1; Red: after run 4).

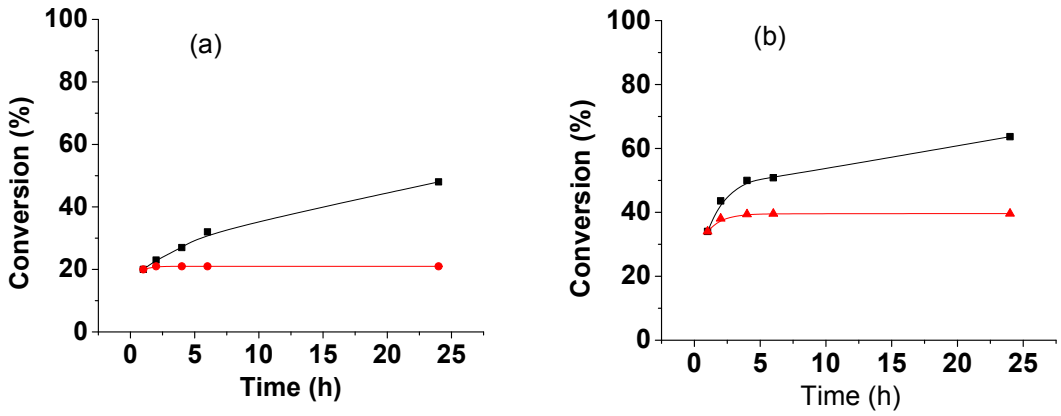


Figure S6. Hot test filtration using CuLaMOF as catalyst for the cyclohexene oxidation (a) and styrene oxidation (b). with catalyst (■); filtered after 1 hour (●).

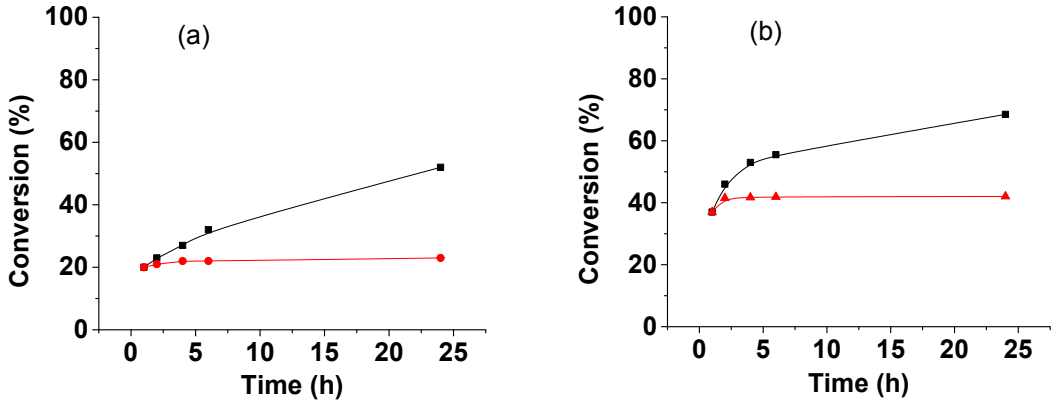


Figure S7. Hot test filtration using CuGdMOF as catalyst for the cyclohexene oxidation (a) and styrene oxidation (b). with catalyst (■); filtered after 1 hour (●).

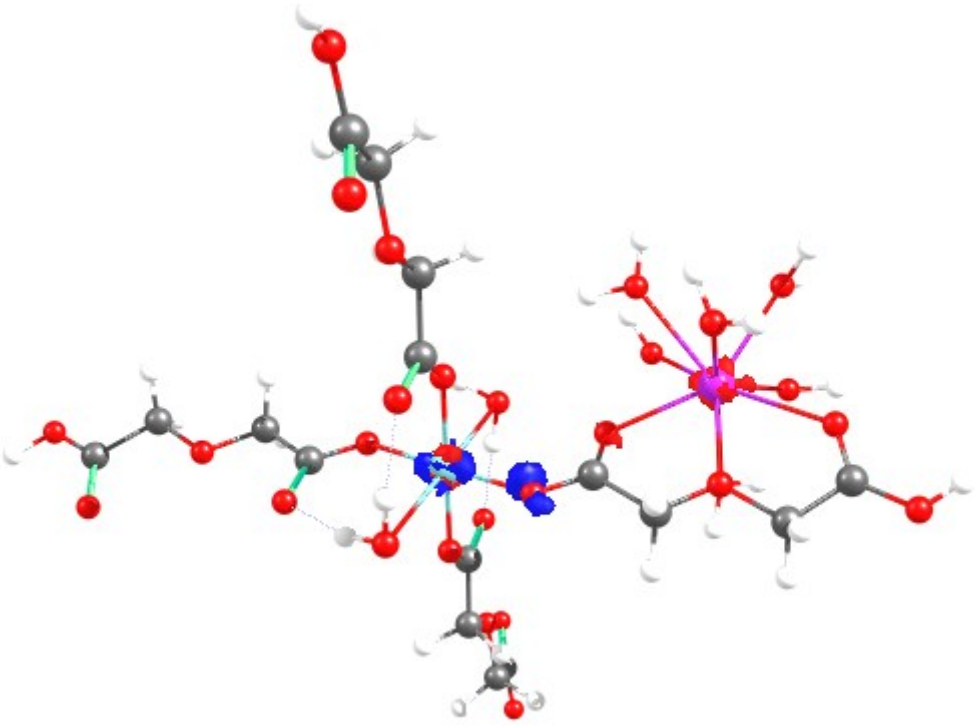
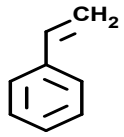


Figure S8. Difference in electronic density (CuLaMOF geometry) between CuLaMOF and CuGdMOF. Positive (red) values indicate an enhancement of electron density in CuGdMOF with respect to CuLaMOF. Blue regions represent a depletion of electon density. Presented results correspond to TPSSh functional, def2-QZVPP basis set and COSMO solvation model for water. Plot isovalue is $2 \cdot 10^{-5}$.

Table S1. Percentage of weight loss associated with $\{[Cu_3Ln_2(oda)_6(H_2O)_6]\bullet nH_2O\}_n$.

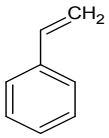
MOF	Species	% Calc	%Exp
(**1**) $\{[Cu_3La_2(oda)_6(H_2O)_6]\bullet 12H_2O\}_n$ P.M. = 1584.3 g/mole	H_20 (crystalization)	13.6	21
	H_20 (coordination)	6.8	
	oda	50.7	48
(**2**) $\{[Cu_3Gd_2(oda)_6(H_2O)_6]\bullet 12H_2O\}_n$ P.M. = 1621.1 g/mole	H_20 (crystalization)	13.3	21
	H_20 (coordination)	6.7	
	oda	49.6	44
(**3**) $\{[Cu_3Yb_2(oda)_6(H_2O)_6]\}_n$ P.M. = 1440.6 g/mole	H_20 (crystalization)	7.5	9
	H_20 (coordination)	0	
	Oda	55.8	55.2
(**4**) $\{[Cu(oda)_2] \bullet 0.5H_2O\}_n$ P.M. = 204.6 g/mole	H_20 (crystalization)	4.4	3.2
	H_20 (coordination)	0	
	Oda	64.6	61.7

Table S2. TOF and TON values obtained at 1 and 24 h, with different S/O/C ratios, for the oxidation of styrene and cyclohexene using CuGdMOF as catalyst.

Substrate	**S/O/C**	**400:400:1**	**800:800:1**	**1200:1200:1**	**2400:2400:1**
		1h / 24h	**1h / 24h**	**1h / 24h**	**1h / 24h**
	**TOF (h^{-1})**	105 / 11.8	215 / 24.5	344 / 35.5	792 / 68.5
	TON	105 / 283	215 / 588	344 / 852	792/ 1644
	**TOF (h^{-1})**	103 / 10.0	179 / 19.0	278 / 27.1	480 / 52.0
	TON	103 / 240	179 / 456	278 / 650	480/ 1248

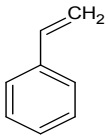
Reaction conditions: Solvent: 1,2-dichloroethane; Oxidant: *tert*-butylhydroperoxide in aqueous medium; Temperature: 75 °C. TON calculated as moles of products per mole of catalyst; TOF calculated as moles of products per mole of catalyst per hour.

Table S3. Conversion and yields at 24 h of the different products for the oxidation of styrene and cyclohexene, using different solvents and CuGdMOF as the catalyst.

	Solvent	Conversion (%)	(A) (%)	(B) (%)	(C) (%)	(D) (%)
	**DCE/water**	69	25	48	27	0
	n-decane	73	34	42	19	5
	**DCE/water**	52	58	30	4	8
	n-decane	60	54	28	6	12

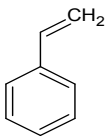
Reaction conditions: S/O/C ratios: 2400/2400/1; Oxidant: *tert*-butylhydroperoxide in aqueous medium; Temperature: 75 °C.

Table S4. Conversion and yields at 24 h of the different products for the oxidation of styrene and cyclohexene, using different solvents and CuYbMOF as the catalyst.

	Solvent	Conversion (%)	(1) (%)	(2) (%)	(3) (%)	(4) (%)
	**DCE/water**	73	23	43	34	0
	n-decane	86	24	39	17	20
	**DCE/water**	57	58	30	5	7
	n-decane	66	54	31	4	11

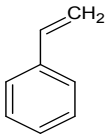
Reaction conditions: S/O/C ratios: 2400/2400/1; Oxidant: *tert*-butylhydroperoxide in aqueous medium; Temperature: 75 °C.

Table S5. Conversion and yields at 24 h of the different products for the oxidation of styrene and cyclohexene in DCE/water, using different temperatures and CuLaMOF as catalyst.

Substrate	Temperature	Conversion (%)	(1) (%)	(2) (%)	(3) (%)	(4) (%)
	**75ºC**	64	27	44	29	0
	60ºC	36	26	49	18	7
	25ºC	22	72	11	11	6
	**75ºC**	48	58	29	4	9
	60ºC	30	56	28	4	12
	25ºC	18	54	44	2	0

Reaction conditions: S/O/C ratios: 2400/2400/1; Solvent: 1,2-dichloroethane; Oxidant: *tert*-butylhydroperoxide in aqueous medium.

Table S6. Conversion and yields at 24 h of the different products for the oxidation of styrene and cyclohexene in DCE/water, using different temperatures and CuGdMOF as catalyst.

Substrate	Temperature	Conversion (%)	(1) (%)	(2) (%)	(3) (%)	(4) (%)
	**75ºC**	69	25	48	27	0
	60ºC	49	27	52	18	3
	25ºC	30	68	12	12	8
	**75ºC**	52	58	30	4	8
	60ºC	37	56	29	4	11
	25ºC	15	54	41	2	3

Reaction conditions: S/O/C ratios: 2400/2400/1; Solvent: 1,2-dichloroethane; Oxidant: *tert*-butylhydroperoxide in aqueous medium.

Table S7. Total energies (eV) for *large* and *small-Cu^{II}* models, calculated using FHI-AIMS

Model	CuLaMOF	CuGdMOF
Large	-1097923.040467470	1411495.847828116
Small-Cu^{II}	-107290.413614348	-107290.427761725
In CuLaMOF-geometry	-	-1411495.734553497
In CuGdMOF-geometry	-1097921.227966883	-

Table S8. Energy of the Cu^{II} d_{x2-y2} orbital (eV) for *large* and *small-Cu^{II}* models, calculated using FHI-AIMS

Model	CuLaMOF	CuGdMOF
Large	-23.52155	-23.61944
Small-Cu^{II}	2.29825	2.28911
In CuLaMOF-geometry	-	-23.79782
In CuGdMOF-geometry	-23.60277	-

All presented energies correspond to spin unrestricted PBE calculations employing the 'tight' basis set

Table S9. Electron affinities (eV) of *small-Cu^{II}Ln^{III}* models using different density functionals, basis sets in gas phase and in water solvent.

DFT functional	basis set	water					gas				
		Gd, geoGd	Gd, geoLa	La, geoLa	La, geoGd	Gd-La	Gd, geoGd	Gd, geoLa	La, geoLa	La, geoGd	Gd-La
B3LYP	def2-TZVP	-1.59	-1.64	-1.56	-1.50	-0.03	-4.81	-5.07	-3.87	-3.80	-0.95
	def2-QZVPP	-1.59	-1.64	-1.56	-1.50	-0.03	-4.81	-5.07	-3.87	-3.80	-0.95
PBE	def2-TZVP	-2.61	-2.73	-2.16	-2.14	-0.45	-4.75	-4.74	-4.54	-4.53	-0.22
	def2-QZVPP	-2.61	-2.73	-2.16	-2.14	-0.45	-4.75	-4.74	-4.54	-4.51	-0.22
TPSSh	def2-TZVP	-1.88	-1.96	-1.65	-1.61	-0.22	-4.63	-4.81	-4.14	-3.89	-0.50
	def2-QZVPP	-1.88	-1.96	-1.66	-1.61	-0.22	-4.63	-4.81	-4.14	-3.89	-0.50

Cartesian coordinates for all models

CuLaMOF, *large* model
La 7.60036000 4.38719200 10.93822500
La 0.00000000 8.77438500 10.93822500
La 7.59884000 4.38719200 3.64607500
La -0.00076000 8.77570100 3.64607500
Cu 3.79980000 6.58144700 7.29215000
H 7.09853566 0.46312291 0.74344670
C 4.65095500 4.69810000 9.33643100
C 2.94864500 8.46479300 9.33643100
C 1.20544900 11.48409800 2.04428100
C 1.20544900 11.48409800 12.54001900
C 2.94864500 8.46479300 5.24786900
C 4.65095500 4.69810000 5.24786900
C 6.39415100 1.67879500 12.54001900
C 6.39415100 1.67879500 2.04428100
C 3.34093600 9.62075900 4.36858100
C 4.25866400 3.54213500 4.36858100
C 5.19691000 1.91704400 11.66073100
C 5.19691000 1.91704400 2.92356900
C 4.25866400 3.54213500 10.21571900
C 3.34093600 9.62075900 10.21571900
C 2.40269000 11.24585000 2.92356900
C 2.40269000 11.24585000 11.66073100

O -1.46687500 7.59604200 5.24043100
O -1.46687500 7.59604200 9.34386900
O -1.75467200 8.09452100 2.05171900
O -1.75467200 8.09452100 12.53258100
O -0.00035000 6.21854600 3.64607500
O -2.21435600 10.05331800 10.93822500
O 0.00035000 6.21854600 10.93822500
O -2.21400700 10.05392300 3.64607500
O 1.25203400 6.25829800 7.29215000
O 1.46687500 7.59604200 2.05171900
O 1.46687500 7.59604200 12.53258100
O -0.28779700 10.63522300 5.24043100
O -0.28779700 10.63522300 9.34386900
O 1.75467200 8.09452100 5.24043100
O 1.75467200 8.09452100 9.34386900
O 0.28779700 10.63522300 2.05171900
O 0.28779700 10.63522300 12.53258100
O 6.35030200 0.63616300 1.36465300
O 6.35030200 0.63616300 13.21964700
O 3.72608400 5.18144100 5.92749700
O 3.72608400 5.18144100 8.65680300
O 5.38559300 3.10897000 10.93822500
O 5.38524400 3.10957600 3.64607500
O 2.21435600 10.05331800 3.64607500
O 2.21435600 10.05331800 10.93822500
O 3.87351600 7.98145200 5.92749700
O 3.87351600 7.98145200 8.65680300
O 1.24929800 12.52673100 1.36465300
O 1.24929800 12.52673100 13.21964700
O 7.31180300 2.52767000 2.05171900
O 7.31180300 2.52767000 12.53258100
O 5.84492800 5.06837200 5.24043100
O 5.84492800 5.06837200 9.34386900
O 7.88739700 2.52767000 5.24043100
O 7.88739700 2.52767000 9.34386900
O 6.13272500 5.56685100 2.05171900
O 6.13272500 5.56685100 12.53258100
O 6.34756600 6.90459600 7.29215000
O 9.81360700 3.10897000 3.64607500
O 7.59925000 6.94434800 3.64607500
O 7.59925000 6.94434800 10.93822500
O 9.81395600 3.10957600 10.93822500
O 9.35427200 5.06837200 2.05171900
O 9.35427200 5.06837200 12.53258100
O 9.06647500 5.56685100 5.24043100
O 9.06647500 5.56685100 9.34386900
H 1.32966303 6.83496151 6.50310634
H 1.26577043 6.90095785 8.03247736
H 3.74557123 10.43303516 4.99738737
H 4.15271669 9.31780053 3.68538614
H 3.44431078 3.83939777 3.68558163
H 3.85427353 2.73192458 5.00000060
H 5.04771815 1.04797437 10.99461045
H 4.29871133 1.96371202 12.30344670
H 4.29763126 1.96251917 2.28209073

H 5.04628949 1.04991440 3.59176016
H 3.85057493 2.72819987 9.59132195
H 3.44988564 3.84461123 10.90299472
H 4.15050669 9.31483095 10.90019379
H 3.74748430 10.43305074 9.58813667
H 2.55417907 12.11370152 3.59075228
H 3.30099281 11.19900141 2.28090319
H 3.30063443 11.19801063 12.30360323
H 2.55173501 12.11434204 10.99393346
H 7.10127432 0.46437467 13.83748324
H 0.50178644 12.69922773 0.74233982
H 0.50006832 12.69943851 13.83976488
H 6.31258268 7.79467340 6.90159062
H 6.24566037 6.30007680 6.52178189
H 10.72396540 3.46274619 3.60537939
H 9.90697453 2.23014118 3.22424939
H 8.81987170 2.23758564 5.26817298
H 7.36187644 1.76401695 5.53268100
H 9.79202625 4.41777805 1.46668716
H 9.61238812 5.92408326 1.65454597
H 6.57851851 6.05503194 1.33026935
H 5.45035123 5.06182825 1.57082865
H 8.38152575 7.47962181 3.87066017
H 7.00331276 7.55277055 3.17864954
H 10.03827610 5.61683863 5.30842637
H 8.72295504 6.03152877 6.02651634
H 8.16256764 7.60443286 11.38678086
H 7.01298454 7.44049335 10.33879853
H 9.96095001 5.34544244 9.02854978
H 9.06739243 6.53143488 9.46601886
H 8.67780815 2.00078079 9.57196216
H 7.27017213 1.91671051 8.90933263
H 10.69645403 3.06105367 10.52026174
H 9.92877421 2.56915221 11.74766150
H 10.31513756 4.94967716 12.41579669
H 9.28271021 5.37918312 13.45814126
H 6.33822493 6.48601372 12.77342692
H 5.77524728 5.16477438 13.34790895
H 0.49251690 5.62598289 10.34163734
H -0.60907128 5.63767125 11.43531256
H -1.64851461 6.65067233 9.48393042
H -2.23855690 7.93174228 8.85386412
H 0.29966360 11.28029999 8.91696003
H -1.10820562 11.11851869 9.56735006
H -2.31729846 10.63681360 11.71925828
H -3.11775656 10.03187274 10.56435798
H -1.67441556 7.77409607 13.45451831
H -2.71467699 8.23567241 12.43463534
H 1.80835801 7.96796708 13.36891220
H 1.30727822 6.65476792 12.71582700
H 0.23573123 11.41136892 5.50222698
H -1.22116223 10.92213760 5.27036672
H -1.13254337 6.86534617 5.79244498
H -2.43420734 7.59900369 5.36278220
H 0.76341529 5.61878455 3.67570264

H -0.77739573 5.62887793 3.64857248
H -1.99502234 7.25371010 1.61313795
H -2.18056356 8.76102911 1.47600301
H 1.95066766 8.08598707 1.35893559
H 1.04823356 6.86402140 1.56048128
H -2.31271270 10.93896440 3.23863802
H -3.11860707 9.68805802 3.58338002

CuLaMOF, *small-Cu^{II}* model

Cu	3.799800000	6.581447000	7.292150000
H	7.098535660	0.463122910	0.743446700
C	4.650955000	4.698100000	9.336431000
C	2.948645000	8.464793000	9.336431000
C	1.205449000	11.484098000	2.044281000
C	1.205449000	11.484098000	12.540019000
C	2.948645000	8.464793000	5.247869000
C	4.650955000	4.698100000	5.247869000
C	6.394151000	1.678795000	12.540019000
C	6.394151000	1.678795000	2.044281000
C	3.340936000	9.620759000	4.368581000
C	4.258664000	3.542135000	4.368581000
C	5.196910000	1.917044000	11.660731000
C	5.196910000	1.917044000	2.923569000
C	4.258664000	3.542135000	10.215719000
C	3.340936000	9.620759000	10.215719000
C	2.402690000	11.245850000	2.923569000
C	2.402690000	11.245850000	11.660731000
O	1.252034000	6.258298000	7.292150000
O	1.754672000	8.094521000	5.240431000
O	1.754672000	8.094521000	9.343869000
O	0.287797000	10.635223000	2.051719000
O	0.287797000	10.635223000	12.532581000
O	6.350302000	0.636163000	1.364653000
O	6.350302000	0.636163000	13.219647000
O	3.726084000	5.181441000	5.927497000
O	3.726084000	5.181441000	8.656803000
O	5.385593000	3.108970000	10.938225000
O	5.385244000	3.109576000	3.646075000
O	2.214356000	10.053318000	3.646075000
O	2.214356000	10.053318000	10.938225000
O	3.873516000	7.981452000	5.927497000
O	3.873516000	7.981452000	8.656803000
O	1.249298000	12.526731000	1.364653000
O	1.249298000	12.526731000	13.219647000
O	7.311803000	2.527670000	2.051719000
O	7.311803000	2.527670000	12.532581000
O	5.844928000	5.068372000	5.240431000
O	5.844928000	5.068372000	9.343869000
O	6.347566000	6.904596000	7.292150000
H	1.329663030	6.834961510	6.503106340
H	1.265770430	6.900957850	8.032477360
H	3.745571230	10.433035160	4.997387370
H	4.152716690	9.317800530	3.685386140
H	3.444310780	3.839397770	3.685581630

H	3.854273530	2.731924580	5.000000600
H	5.047718150	1.047974370	10.994610450
H	4.298711330	1.963712020	12.303446700
H	4.297631260	1.962519170	2.282090730
H	5.046289490	1.049914400	3.591760160
H	3.850574930	2.728199870	9.591321950
H	3.449885640	3.844611230	10.902994720
H	4.150506690	9.314830950	10.900193790
H	3.747484300	10.433050740	9.588136670
H	2.554179070	12.113701520	3.590752280
H	3.300992810	11.199001410	2.280903190
H	3.300634430	11.198010630	12.303603230
H	2.551735010	12.114342040	10.993933460
H	7.101274320	0.464374670	13.837483240
H	0.501786440	12.699227730	0.742339820
H	0.500068320	12.699438510	13.839764880
H	6.312582680	7.794673400	6.901590620
H	6.245660370	6.300076800	6.521781890

CuLaMOF, *small-*$Cu^{II}Ln^{III}$ model

La	7.600360000	4.387192000	10.938225000
Cu	3.799800000	6.581447000	7.292150000
H	7.104638860	0.470906520	0.742433040
C	4.650955000	4.698100000	9.336431000
C	2.948645000	8.464793000	9.336431000
C	1.205449000	11.484098000	2.044281000
C	1.205449000	11.484098000	12.540019000
C	2.948645000	8.464793000	5.247869000
C	4.650955000	4.698100000	5.247869000
C	6.394151000	1.678795000	12.540019000
C	6.394151000	1.678795000	2.044281000
C	3.340936000	9.620759000	4.368581000
C	4.258664000	3.542135000	4.368581000
C	5.196910000	1.917044000	11.660731000
C	5.196910000	1.917044000	2.923569000
C	4.258664000	3.542135000	10.215719000
C	3.340936000	9.620759000	10.215719000
C	2.402690000	11.245850000	2.923569000
C	2.402690000	11.245850000	11.660731000
O	1.252034000	6.258298000	7.292150000
O	1.754672000	8.094521000	5.240431000
O	1.754672000	8.094521000	9.343869000
O	0.287797000	10.635223000	2.051719000
O	0.287797000	10.635223000	12.532581000
O	6.350302000	0.636163000	1.364653000
O	6.350302000	0.636163000	13.219647000
O	3.726084000	5.181441000	5.927497000
O	3.726084000	5.181441000	8.656803000
O	5.385593000	3.108970000	10.938225000
O	5.385244000	3.109576000	3.646075000
O	2.214356000	10.053318000	3.646075000
O	2.214356000	10.053318000	10.938225000
O	3.873516000	7.981452000	5.927497000
O	3.873516000	7.981452000	8.656803000
O	1.249298000	12.526731000	1.364653000

O	1.249298000	12.526731000	13.219647000
O	7.311803000	2.527670000	2.051719000
O	7.311803000	2.527670000	12.532581000
O	5.844928000	5.068372000	5.240431000
O	5.844928000	5.068372000	9.343869000
O	7.887397000	2.527670000	9.343869000
O	6.132725000	5.566851000	12.532581000
O	6.347566000	6.904596000	7.292150000
O	7.599250000	6.944348000	10.938225000
O	9.813956000	3.109576000	10.938225000
O	9.354272000	5.068372000	12.532581000
O	9.066475000	5.566851000	9.343869000
H	1.331134360	6.835999870	6.502166600
H	1.264930740	6.903310350	8.032735340
H	3.745303880	10.432913300	4.998594870
H	4.152730070	9.316833780	3.684822340
H	3.443885800	3.839539120	3.685100530
H	3.854509490	2.732276690	5.001491360
H	5.047894030	1.046956040	10.995546730
H	4.300012690	1.963877820	12.305667590
H	4.298981670	1.962206260	2.279852860
H	5.046555120	1.049013530	3.590957570
H	3.850365410	2.728375390	9.590328780
H	3.450306740	3.845932940	10.903921120
H	4.149956140	9.313285790	10.901187120
H	3.747776980	10.432939420	9.587326240
H	2.554234140	12.114644700	3.589815130
H	3.299583210	11.198960200	2.278552760
H	3.299261930	11.197800690	12.305902980
H	2.551498440	12.115352100	10.994896750
H	7.107261920	0.471988100	13.838561370
H	0.495864300	12.691357400	0.741045530
H	0.494199550	12.691415550	13.841128610
H	6.312417950	7.787917380	6.879908270
H	6.246938020	6.285974220	6.531344180
H	8.153459090	7.614680840	11.388769770
H	7.014861470	7.434858990	10.326928970
H	9.970207420	5.342209170	9.050392860
H	9.076734480	6.532602690	9.482195140
H	8.663728890	1.976184840	9.575440810
H	7.255554790	1.929535540	8.906980480
H	10.692615250	3.036116450	10.510026470
H	9.935660680	2.580952590	11.758836920
H	10.318837120	4.955995640	12.413265730
H	9.286577000	5.368652900	13.464958410
H	6.340807700	6.486981410	12.778883780
H	5.775489090	5.162818420	13.350312680

CuGdMOF, *large* model
Gd 7.35933600 4.24806500 11.37697500
Gd 0.00000000 8.49613000 11.37697500
Gd 7.35786400 4.24806500 3.79232500
Gd -0.00073600 8.49740400 3.79232500
Cu 3.67930000 6.37273500 7.58465000
H 6.87523327 0.48908057 0.74947623

C 4.52186000 4.52770000 9.69272800
C 2.83674000 8.21776900 9.69272800
C 1.17656700 11.09327400 2.10807800
C 1.17656700 11.09327400 13.06122200
C 2.83674000 8.21776900 5.47657200
C 4.52186000 4.52770000 5.47657200
C 6.18203300 1.65219500 13.06122200
C 6.18203300 1.65219500 2.10807800
C 3.23807800 9.37174300 4.60130400
C 4.12052200 3.37372600 4.60130400
C 4.98199300 1.88161400 12.18595400
C 4.98199300 1.88161400 2.98334600
C 4.12052200 3.37372600 10.56799600
C 3.23807800 9.37174300 10.56799600
C 2.37660700 10.86385500 2.98334600
C 2.37660700 10.86385500 12.18595400
O 8.77747100 5.33961200 9.76020100
O 5.70422500 4.93170600 9.76020100
O 7.59410500 2.47415000 9.76020100
O 1.65437500 7.81376300 9.76020100
O -0.23550500 10.27131900 9.76020100
O 5.93972900 5.33961200 2.17555100
O 9.01297500 4.93170600 2.17555100
O 0.23550500 10.27131900 2.17555100
O 1.41887100 7.40585700 2.17555100
O -1.65437500 7.81376300 2.17555100
O 8.77747100 5.33961200 5.40909900
O 0.23550500 10.27131900 12.99374900
O -1.41887100 7.40585700 5.40909900
O 1.65437500 7.81376300 5.40909900
O -0.23550500 10.27131900 5.40909900
O 5.70422500 4.93170600 5.40909900
O 7.59410500 2.47415000 5.40909900
O 1.41887100 7.40585700 12.99374900
O -1.65437500 7.81376300 12.99374900
O 7.12309500 2.47415000 12.99374900
O 5.93972900 5.33961200 12.99374900
O 9.01297500 4.93170600 12.99374900
O -1.41887100 7.40585700 9.76020100
O 7.12309500 2.47415000 2.17555100
O 3.62411100 4.97404700 8.94958400
O 3.73449000 7.77142200 8.94958400
O 1.23889400 12.09392100 1.36493400
O 1.23889400 12.09392100 13.80436600
O 3.73449000 7.77142200 6.21971600
O 3.62411100 4.97404700 6.21971600
O 6.11970600 0.65154800 13.80436600
O 6.11970600 0.65154800 1.36493400
O -0.00005900 6.01369500 3.79232500
O 2.15061700 9.73857100 3.79232500
O -2.15055800 9.73867300 3.79232500
O 5.20798300 3.00689800 3.79232500
O 9.50915800 3.00679600 3.79232500
O 0.00005900 6.01369500 11.37697500
O -2.15061700 9.73857100 11.37697500

O 5.20804200 3.00679600 11.37697500
O 7.35854100 6.73177400 11.37697500
O 9.50921700 3.00689800 11.37697500
O 2.15061700 9.73857100 11.37697500
O 7.35854100 6.73177400 3.79232500
O 6.17622000 6.63325200 7.58465000
O 1.18238000 6.11221700 7.58465000
H 6.20108230 6.03458625 6.81016903
H 6.23397317 6.02719096 8.34997699
H 1.14036943 5.19465866 7.90225681
H 1.16658012 6.66649018 8.39641693
H 3.57029681 10.21612641 5.23096633
H 4.10432033 9.09029071 3.97780199
H 3.25170379 3.65691946 3.98296734
H 3.79263586 2.53000892 5.23396839
H 4.78497827 0.97400475 11.58659441
H 4.09684834 2.01517960 12.83484584
H 4.09608772 2.01390754 2.33480493
H 4.78204960 0.97430028 3.58241900
H 3.78952782 2.53014290 9.93626101
H 3.25389741 3.65615782 11.19064482
H 4.10886074 9.09111906 11.18471186
H 3.56613430 10.21366569 9.93304786
H 2.57537445 11.77161973 3.58201803
H 3.26152504 10.73040757 2.33406406
H 3.26444689 10.73393593 12.83230908
H 2.57313119 11.77090250 11.58550850
H 6.87745725 0.48928372 14.41731377
H 0.48027127 12.25213304 0.75275418
H 0.48104729 12.25975370 14.41609203
H 1.87285359 7.94559392 13.66882942
H 1.00449039 6.69497725 13.51663265
H 0.80959886 5.54914812 11.10848461
H -0.57052344 5.33014552 11.77695145
H -2.06389272 6.99664969 13.33985205
H -1.91226256 8.48253364 13.66021939
H -1.56792266 6.44660481 9.79826043
H -2.23397716 7.78433430 9.38319225
H 0.38829988 10.93420798 9.42177380
H -1.11974274 10.67846580 9.70162159
H -2.26695907 10.63593407 11.74929119
H -3.01621797 9.31656354 11.54143427
H 10.40849777 3.13711726 11.01777351
H 9.63623560 2.33950517 12.08307079
H 9.93877440 4.62769337 13.00138438
H 8.90196809 5.33234271 13.87889098
H 8.39801804 1.94793549 9.93786612
H 6.94816108 1.86278590 9.37047325
H 9.26054348 4.88503280 9.04847950
H 9.32307819 6.11775014 9.97437026
H 8.00229991 7.29701614 11.84642899
H 7.06317138 7.25415261 10.61034970
H 6.06947535 6.29504875 13.11710494
H 5.70481302 4.98211739 13.87107898
H 8.50120790 2.11872286 5.46410049

H 7.00562374 1.72894399 5.61535347
H 10.35899990 3.43472176 3.56952938
H 9.61748496 2.10431817 3.42996054
H 9.24031538 4.28704385 1.47492214
H 9.40556144 5.76111555 1.83932155
H 9.68463540 5.07957512 5.65144098
H 8.74284140 6.30489053 5.51600578
H 7.97342918 7.40863227 3.45102325
H 6.64840823 7.22905686 4.23442838
H 6.27939183 6.16930712 1.79655630
H 5.57791161 4.85726195 1.40784556
H 1.64159187 7.74613147 1.28887113
H 1.21292640 6.46086877 2.06364896
H 0.40086821 10.95217895 5.68191575
H -1.08352564 10.73384993 5.26770719
H -1.56115608 7.30752624 1.34467039
H -2.53923734 8.21362759 2.09693131
H -2.27855765 10.41852167 3.09905443
H -3.03929406 9.63357789 4.18401725
H 0.41635361 5.56518643 4.54756154
H -0.78561791 5.48278706 3.56468923
H -0.99558937 7.00699501 6.19085072
H -2.33842169 7.08660322 5.39187833

CuGdMOF, *small-Cu*^{II} model

Cu	3.679300000	6.372735000	7.584650000
H	6.875233270	0.489080570	0.749476230
C	4.521860000	4.527700000	9.692728000
C	2.836740000	8.217769000	9.692728000
C	1.176567000	11.093274000	2.108078000
C	1.176567000	11.093274000	13.061222000
C	2.836740000	8.217769000	5.476572000
C	4.521860000	4.527700000	5.476572000
C	6.182033000	1.652195000	13.061222000
C	6.182033000	1.652195000	2.108078000
C	3.238078000	9.371743000	4.601304000
C	4.120522000	3.373726000	4.601304000
C	4.981993000	1.881614000	12.185954000
C	4.981993000	1.881614000	2.983346000
C	4.120522000	3.373726000	10.567996000
C	3.238078000	9.371743000	10.567996000
C	2.376607000	10.863855000	2.983346000
C	2.376607000	10.863855000	12.185954000
O	5.704225000	4.931706000	9.760201000
O	1.654375000	7.813763000	9.760201000
O	0.235505000	10.271319000	2.175551000
O	0.235505000	10.271319000	12.993749000
O	1.654375000	7.813763000	5.409099000
O	5.704225000	4.931706000	5.409099000
O	7.123095000	2.474150000	12.993749000
O	7.123095000	2.474150000	2.175551000
O	3.624111000	4.974047000	8.949584000
O	3.734490000	7.771422000	8.949584000
O	1.238894000	12.093921000	1.364934000

O	1.238894000	12.093921000	13.804366000
O	3.734490000	7.771422000	6.219716000
O	3.624111000	4.974047000	6.219716000
O	6.119706000	0.651548000	13.804366000
O	6.119706000	0.651548000	1.364934000
O	2.150617000	9.738571000	3.792325000
O	5.207983000	3.006898000	3.792325000
O	5.208042000	3.006796000	11.376975000
O	2.150617000	9.738571000	11.376975000
O	6.176220000	6.633252000	7.584650000
O	1.182380000	6.112217000	7.584650000
H	6.201082300	6.034586250	6.810169030
H	6.233973170	6.027190960	8.349976990
H	1.140369430	5.194658660	7.902256810
H	1.166580120	6.666490180	8.396416930
H	3.570296810	10.216126410	5.230966330
H	4.104320330	9.090290710	3.977801990
H	3.251703790	3.656919460	3.982967340
H	3.792635860	2.530008920	5.233968390
H	4.784978270	0.974004750	11.586594410
H	4.096848340	2.015179600	12.834845840
H	4.096087720	2.013907540	2.334804930
H	4.782049600	0.974300280	3.582419000
H	3.789527820	2.530142900	9.936261010
H	3.253897410	3.656157820	11.190644820
H	4.108860740	9.091119060	11.184711860
H	3.566134300	10.213665690	9.933047860
H	2.575374450	11.771619730	3.582018030
H	3.261525040	10.730407570	2.334064060
H	3.264446890	10.733935930	12.832309080
H	2.573131190	11.770902500	11.585508500
H	6.877457250	0.489283720	14.417313770
H	0.480271270	12.252133040	0.752754180
H	0.481047290	12.259753700	14.416092030

CuGdMOF, *small-Cu^{II}Ln^{III}* model

Gd	7.359336000	4.248065000	11.376975000
Cu	3.679300000	6.372735000	7.584650000
H	6.881514320	0.495773860	0.748906860
C	4.521860000	4.527700000	9.692728000
C	2.836740000	8.217769000	9.692728000
C	1.176567000	11.093274000	2.108078000
C	1.176567000	11.093274000	13.061222000
C	2.836740000	8.217769000	5.476572000
C	4.521860000	4.527700000	5.476572000
C	6.182033000	1.652195000	13.061222000
C	6.182033000	1.652195000	2.108078000
C	3.238078000	9.371743000	4.601304000
C	4.120522000	3.373726000	4.601304000
C	4.981993000	1.881614000	12.185954000
C	4.981993000	1.881614000	2.983346000
C	4.120522000	3.373726000	10.567996000
C	3.238078000	9.371743000	10.567996000
C	2.376607000	10.863855000	2.983346000
C	2.376607000	10.863855000	12.185954000

O	8.777471000	5.339612000	9.760201000
O	5.704225000	4.931706000	9.760201000
O	7.594105000	2.474150000	9.760201000
O	1.654375000	7.813763000	9.760201000
O	0.235505000	10.271319000	2.175551000
O	0.235505000	10.271319000	12.993749000
O	1.654375000	7.813763000	5.409099000
O	5.704225000	4.931706000	5.409099000
O	7.123095000	2.474150000	12.993749000
O	5.939729000	5.339612000	12.993749000
O	9.012975000	4.931706000	12.993749000
O	7.123095000	2.474150000	2.175551000
O	3.624111000	4.974047000	8.949584000
O	3.734490000	7.771422000	8.949584000
O	1.238894000	12.093921000	1.364934000
O	1.238894000	12.093921000	13.804366000
O	3.734490000	7.771422000	6.219716000
O	3.624111000	4.974047000	6.219716000
O	6.119706000	0.651548000	13.804366000
O	6.119706000	0.651548000	1.364934000
O	2.150617000	9.738571000	3.792325000
O	5.207983000	3.006898000	3.792325000
O	5.208042000	3.006796000	11.376975000
O	7.358541000	6.731774000	11.376975000
O	9.509217000	3.006898000	11.376975000
O	2.150617000	9.738571000	11.376975000
O	6.176220000	6.633252000	7.584650000
O	1.182380000	6.112217000	7.584650000
H	6.200605850	6.030993100	6.810766890
H	6.231621440	6.026591640	8.352047100
H	1.134660160	5.202023580	7.930157260
H	1.161911680	6.686148470	8.384658640
H	3.570493330	10.215958150	5.231883070
H	4.103520450	9.088721100	3.976349750
H	3.252021050	3.658677780	3.982228860
H	3.792557470	2.530084000	5.234771720
H	4.786124740	0.972875590	11.587637880
H	4.098254630	2.015633580	12.836944920
H	4.097364440	2.014191230	2.332819390
H	4.782770740	0.973197210	3.581274540
H	3.789263960	2.530222080	9.935471840
H	3.254625730	3.657569090	11.192075520
H	4.109279650	9.090385500	11.184916580
H	3.565815760	10.213431410	9.931775230
H	2.574621450	11.772745480	3.580907840
H	3.260233120	10.729942030	2.332034950
H	3.263661260	10.734592200	12.833685890
H	2.571453580	11.771997840	11.586193540
H	6.883744330	0.496106090	14.417892510
H	0.474113510	12.245235140	0.752068730
H	0.474478140	12.253323640	14.416235880
H	10.407819480	3.125547600	11.004439470
H	9.644440010	2.338450850	12.085925970
H	9.939033120	4.617591940	13.004731120
H	8.905960930	5.328059210	13.884827970

H	8.389716740	1.929329620	9.938300000
H	6.938299250	1.871613220	9.366046200
H	9.232480530	4.883242480	9.027652180
H	9.358715310	6.094923060	9.978671730
H	8.008758260	7.298185660	11.842748400
H	7.081081750	7.249562030	10.596405740
H	6.066639290	6.298916590	13.116215420
H	5.707181370	4.984368630	13.876086140