Supporting Information for:

Efficient MOF-based degradation of organophosphorous compounds in non-aqueous environments

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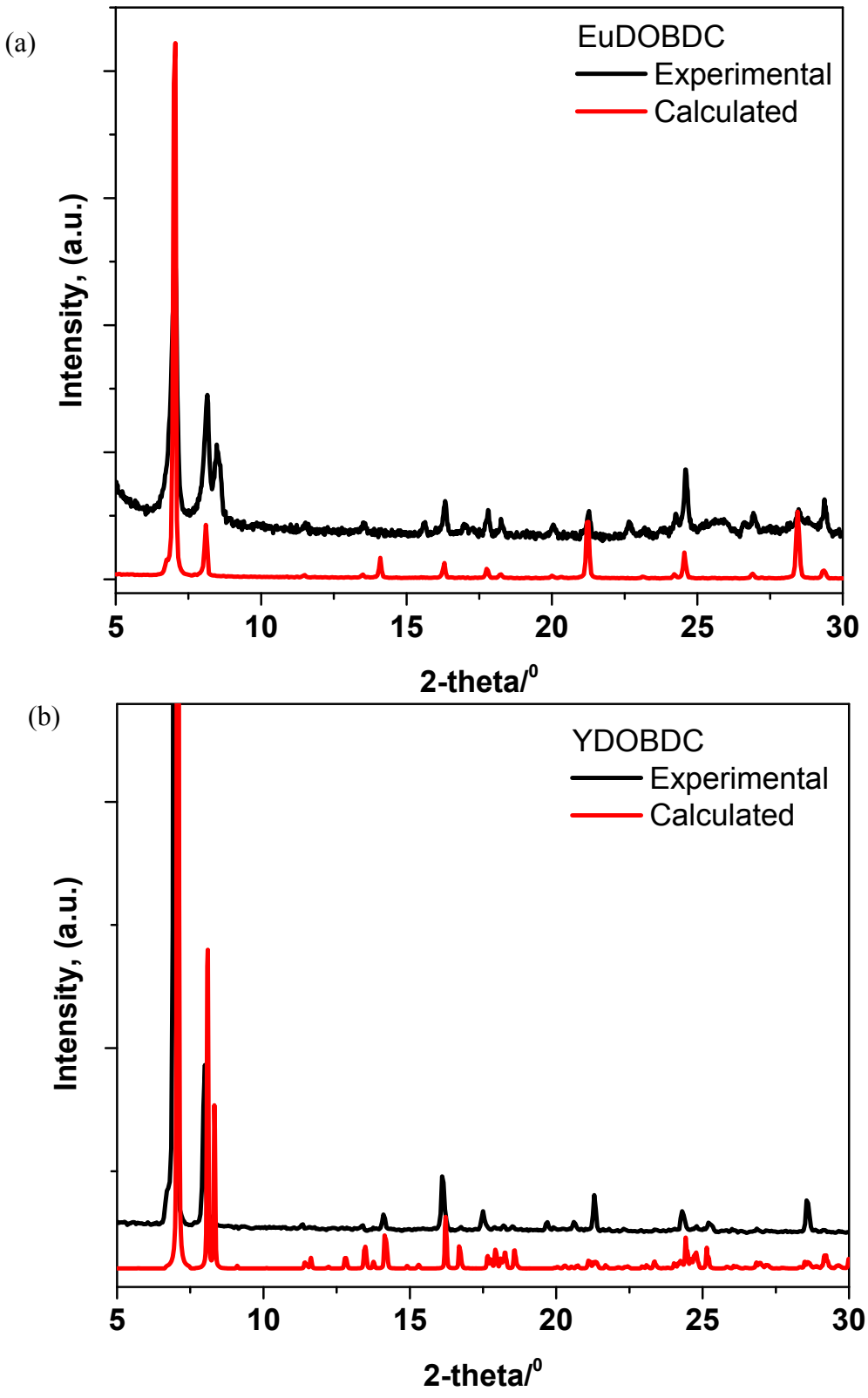
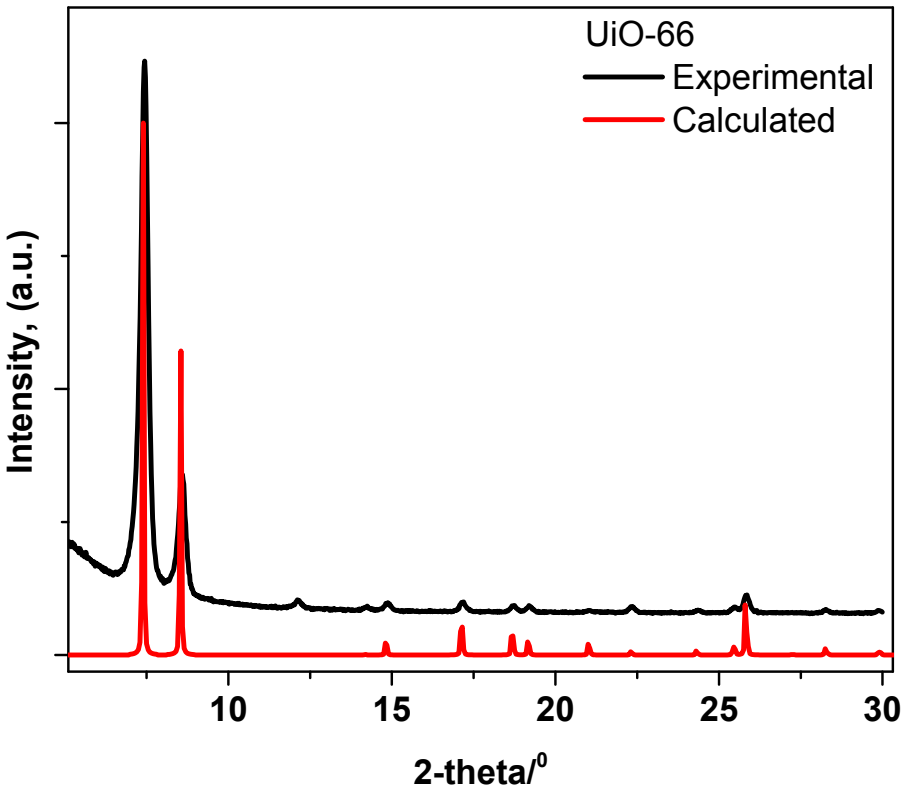
Fig. S1 Experimental (black trace) vs. calculated (red trace) powder X-ray diffraction patters for (a) EuDOBDC, (b) YDOBDC, (c) UiO-66 and (d) UiO-66-DOBDC materials.



(c)


UiO-66
Experimental
Calculated
Intensity, (a.u.)
10
15
20
25
30
2-theta/0

(d)

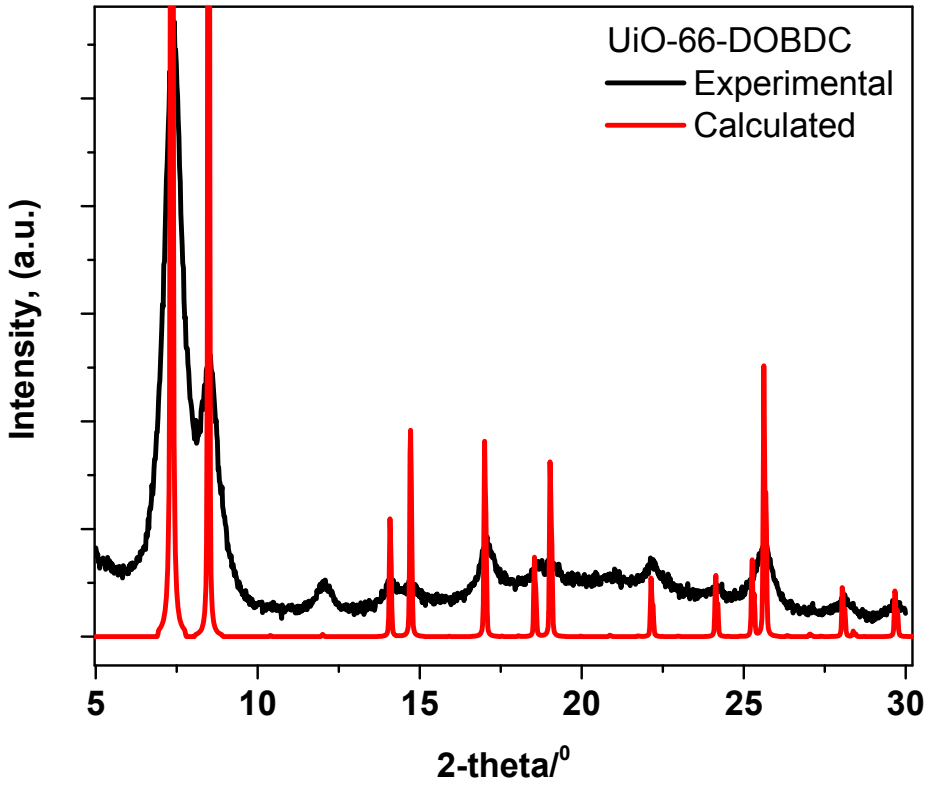

UiO-66-DOBDC
Experimental
Calculated
Intensity, (a.u.)
5
10
15
20
25
30
2-theta/0

Fig.S2 Nitrogen sorption isotherm measured at 77K on the UiO-66-DOBDC sample.

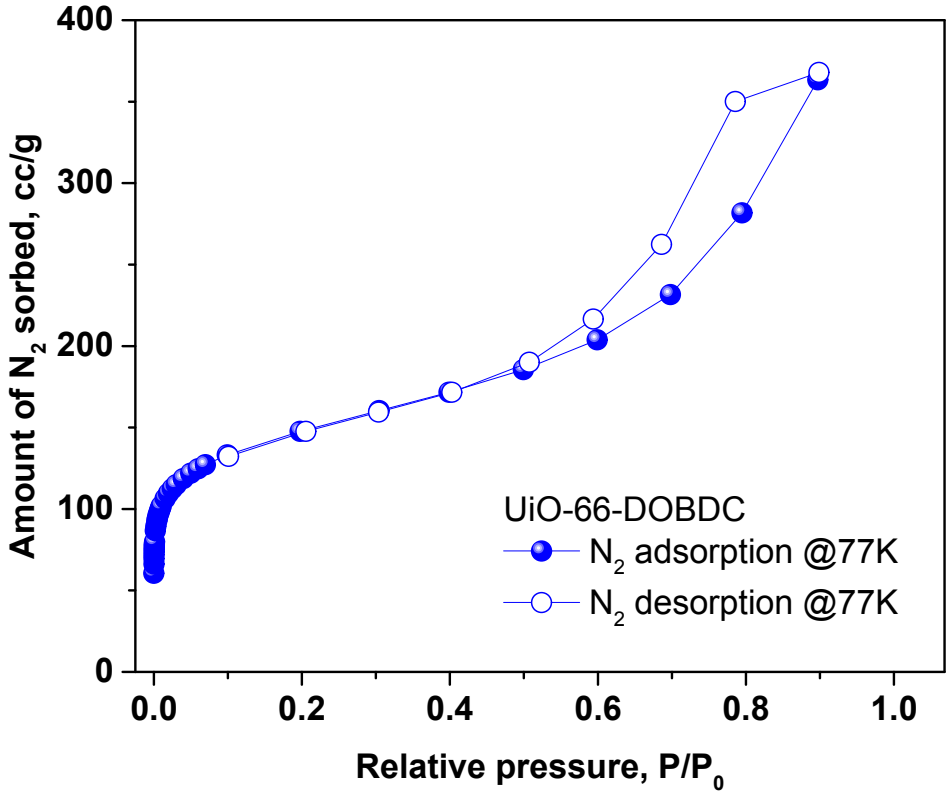


Table S1. Optimized cell parameters for UiO-66, UiO-66-DOBDC, Y-DOBDC, and Eu-DOBDC with corresponding experimental values. [a]*Chem. Mater.*, **2011**, 23, 1700-1718. [b]*ACS Appl. Mater. Interfaces*, **2017**, 9, 22268-22277.

System	a (Å)	b	c	α (°)	β	γ
UiO-66 (sim)	14.679	14.679	14.679	60.000	60.000	59.948
UiO-66 (exp[a])	14.668	14.668	14.668	60.000	60.000	60.000
UiO-66-DOBDC	14.698	14.698	14.698	60.000	60.000	59.864
YDOBDC	15.464	15.529	21.096	89.952	89.987	89.990
EuDOBDC (sim)	15.575	15.631	21.330	89.988	89.959	90.002
EuDOBDC (exp[b])	15.560	15.560	21.330	90.000	90.000	90.000

Fig.S3 Snapshots from DFT vibrational analysis highlighting the effect of the ligand (UiO-66-DOBDC, (a) and (b)) and that of the metal (YDOBDC, EuDOBDC and UiO-66-DOBDC, (c) and (d)) for select IR modes.

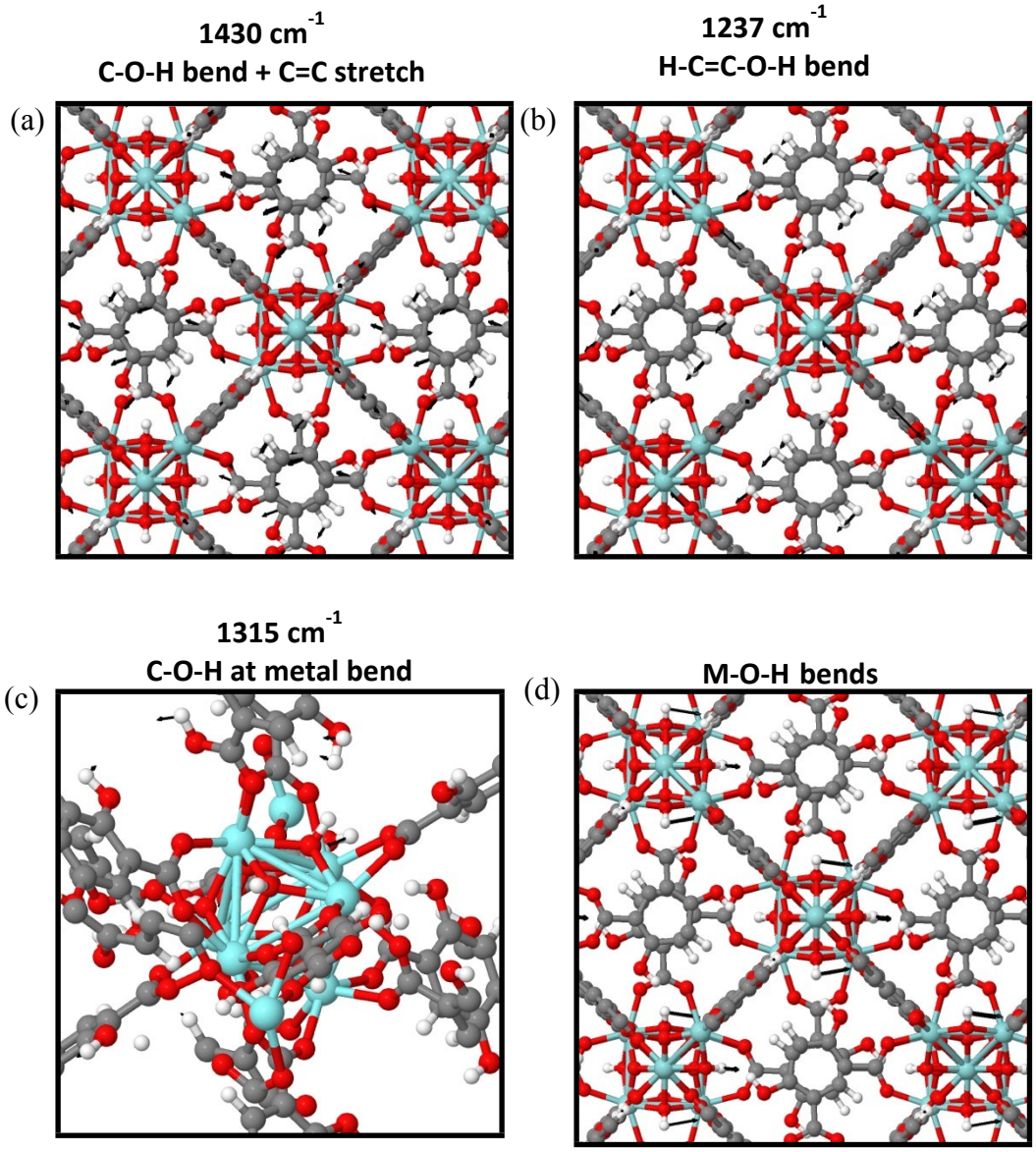


Table S2. Selected modes and frequencies (cm^{-1}) from simulated vibrational spectrum for UiO-66, UiO-66-DOBDC, YDOBDC, and EuDOBDC.

UiO-66	UiO-66-DOBDC	YDOBDC	EuDOBDC	Description
		1706	1705	C=O stretch + $C_{carboxyate}$-O-H bend
		1590	1589	C=O stretch in carboxlyate + C=C stretch + C-O-H bend
1565	1575			C=O stretch in carboxylate
1484				C-C stretch at carboxylate + H-C=C-H rocking
	1430	1440	1441	C=C stretch + H-C=C-O-H rocking/scissoring
1417				C-C stretch at carboxylate
1400				C=C stretch + H-C=C-H rocking/scissoring
1380				C-C stretch + H-C=C-H rocking/scissoring
	1370	1367	1365	C-C stretch at carboxylate + C=C stretch + H-C=C-O-H rocking/scissoring
1366				C-C stretch at carboxylate + H-C=C-H rocking/scissoring
		1315	315	C-C stretch at carboxylate + C-O-H bend at monodentate linker
1255				H-C=C-H rocking
	1239	1231	120	H-C=C-O-H rocking
	1155	1136	1135	H-C=C-O-H scissoring

Fig. S4 Representative ^{31}P NMR plot for DECP degradation in MeOH.

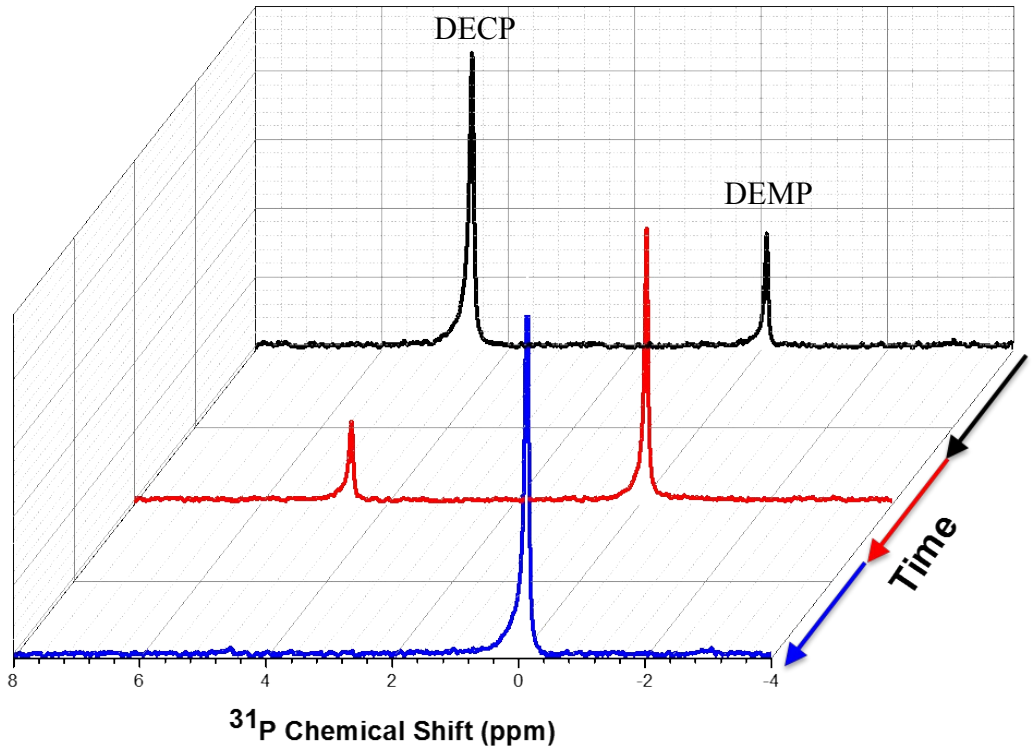


Fig. S5 Sum of product and reactant ^{31}P NMR peak integrals for DECP degradation in (a) MeOH blank and (b) UiO-66.

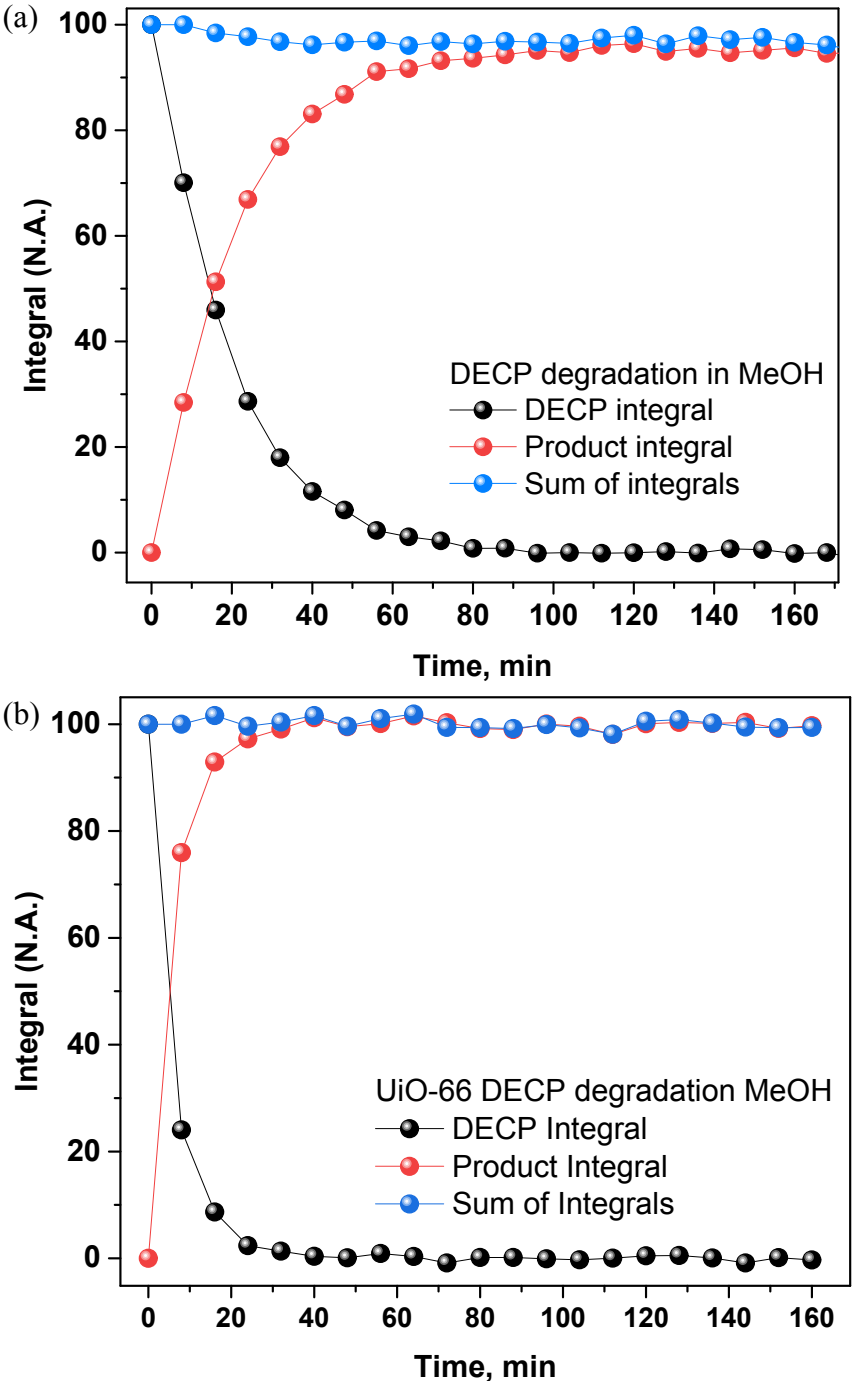


Fig. S6 UiO-66 supported degradation of DECP in MeOH as function of temperature and amount of catalyst as determined from ^{31}P NMR.

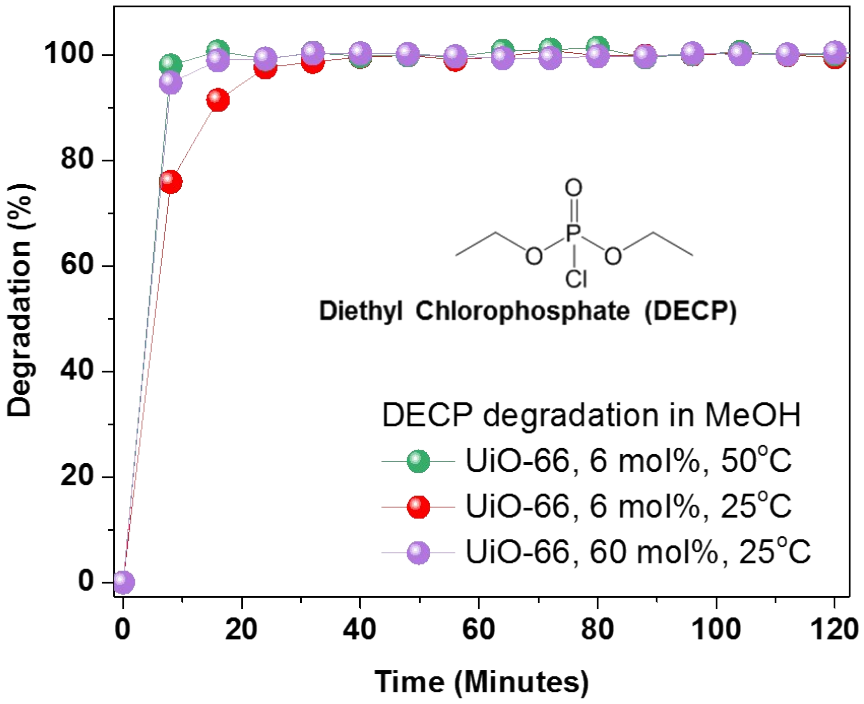


Table S3. Representative half-lives of UiO-66 supported degradation of DECP in MeOH as function of temperature and amount of catalyst.

Sample	$t_{1/2}$, min
UiO-66, 6 mol%, 50°C	1.41
UiO-66, 60 mol%, 25°C	3.35
UiO-66, 6 mol%, 25°C	7.58