Electronic Supplementary Information for

Kinetics and Adsorption Calculations: Insights into the MgO-Catalyzed Detoxification of Simulants of Organophosphorus Biocides

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Summary

1. Synthesis of the phosphate triesters

The phosphate triester chlorpyrifos methyl *O*-analog (CPO) was purchased (Sigma Aldrich) and used as received. The other substrates were synthesized as described previously;[1-5] the procedures and characterization data are detailed below (for ^{1}H NMR data, chemical shifts are referred to internal tetramethylsilane, while external H_3PO_4 85% was used as standard for $^{31}P\{^{1}H\}$ NMR).

Methyl paraoxon (dimethyl 4-nitrophenyl phosphate). Triethylamine (5.5 mmol) was added to a solution of 4-nitrophenol (5.0 mmol) in dry $CHCl_3$ (25 mL) in a round bottomed vessel under magnetic stirring and argon atmosphere. The system was cooled to 0° and a solution of dimethyl chlorophosphate (5.0 mmol) was added dropwise. The system was kept at 0ºC for 10 minutes and then at room temperature for 3 hours. Triethylammonium chloride was removed by filtration. The filtrate was extracted with $NaHCO_3$ saturated solution (2 x 25 mL) and once with 25 mL of brine. The organic phase was dried over $MgSO_4$ and the solvent was removed under reduced pressure to give a yellowish oil (60%); $^{31}P\{^{1}H\}$ NMR (81 MHz, $CDCl_3$): δ = –4.56 ppm. ESI-MS positive ion mode (*m*/*z*): calcd for $C_8H_{11}NO_6P^+$: 248.0; found 248.2 (100) $[M]^+$.

Dimethyl 2,4-dinitrophenyl phosphate (DMDNPP). Triethylamine (5.5 mmol) was added to a solution of 2,4-dinitrophenol (5.0 mmol) in dry $CHCl_3$ (25 mL) in a round bottomed vessel under magnetic stirring and argon atmosphere. The system was cooled to 0° and a solution of dimethyl chlorophosphate (5.0 mmol) was added dropwise. The system was kept at 0ºC for 10 minutes and then at room temperature for 3 hours. Triethylammonium chloride was removed by filtration. The filtrate was extracted with $NaHCO_3$ saturated solution (2 x 25 mL) and once with 25 mL of brine. The organic phase was dried over $MgSO_4$ and the solvent was removed under reduced pressure, yielding the product in 54%; $^{31}P\{^{1}H\}$ NMR (81 MHz, $CDCl_3$): δ = –3.83 ppm.

Diethyl 2,4-dinitrophenyl phosphate (DEDNPP). The triester was prepared according to the procedure described by Ba-Saif and Williams[3] as follows: Triethylamine (22.0 mmol) was added to a solution of 2,4-dinitrophenol (20.0 mmol) in dry benzene (75 mL) in a round bottomed vessel under magnetic stirring and argon atmosphere. The system was cooled to 0° and a solution of diethyl chlorophosphate (20.0 mmol) in 25.0

mL of dry benzene was added dropwise. The temperature was raised slowly and the system was refluxed for 14 hours at 70-80ºC. Triethylammonium chloride was removed by filtration. The filtrate was extracted five times with 100 mL of water. The organic phase was dried over $MgSO_4$ and the solvent was removed under reduced pressure to give a yellow oil (54%). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 1.40 (t, *J* = 6.96 Hz, 6H), 4.31 (m, *J* = 6.96 Hz, 4H), 7.86 (dd, *J* = 9.16 and 1.10 Hz, 1H), 8.46 (dd, *J* = 9.16 and 2.93 Hz, 1H), 8.81 (dd, *J* = 2.93 and 1.10 Hz, 1H). ^{31}P{^{1}H} NMR (81 MHz, $CDCl_3$): δ = –7.64 ppm.

***tris*-2-Pyridyl phosphate (T2PyP)**. Triethylamine (22.3 mmol) was added to a solution of 2-hydroxypyridine (21.8 mmol) in dry chloroform (15 mL) in a round bottomed vessel under magnetic stirring and argon atmosphere. The mixture was cooled to 0° and a solution of $POCl_3$ (5.5 mmol, 0.5 mL) in chloroform (1.5 mL) was added dropwise. The system was kept at 0ºC for 10 minutes and at room temperature for 2 hours. Triethylammonium chloride was removed by filtration. The filtrate was extracted with $NaHCO_3$ saturated solution (3 x 10 mL) and then with brine (2 x 10 mL). The organic phase was dried over $MgSO_4$ and the solvent was removed under reduced pressure to give a light brown oil, which crystallized after four days in a freezer, yielding 1.8 g of pale crystals (90%). m.p. 55-56ºC (uncorrected). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.17 (dd, *J* = 5.0 and 7.5 Hz, 1H), 7.23 (d, *J* = 7.5 Hz, 1H), 7.77 (t, *J* = 7.5 Hz, 1H), 8.28 (d, *J* = 5.0 Hz, 1H). ^{31}P{^{1}H} NMR (81 MHz, $CDCl_3$): δ = –20.69 ppm. ESI-MS positive ion mode (*m*/*z*): calcd for $C_{15}H_{13}N_3O_4P^+$: 330.06; found 330.05 (100) $[M]^+$.

***tris*-4-Nitrophenyl phosphate (T4NPP)**. Triethylamine (3 equiv.) was added to a solution of 3 equivalents of 4-nitrophenol in dry acetonitrile (1.23 mmols of 4-nitrophenol/mL of solvent) in a round bottomed vessel under magnetic stirring and argon atmosphere. The system was then cooled to 0ºC and a solution of 1 equivalent of $POCl_3$ in acetonitrile (0.82 mmol/mL) was added dropwise. Stirring was continued for a further 10 minutes at 0ºC and then at room temperature for 1 hour. The triester was then precipitated with the addition of ice-cold water, and purification was performed by recrystallization in acetone/water to achieve the pure compound. m.p. 156-158ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.44 (dd, *J* = 9.3 and 1.1 Hz), 8.31 (dd, *J* = 9.2 and 0.6 Hz).

2. Characterization of MgO

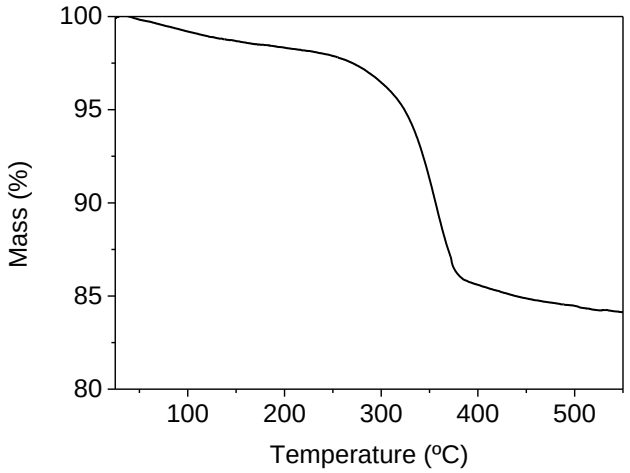

Figure S1. Thermogravimetric analysis of commercial MgO.

Table S1. Semi-quantitative EDXRF analysis of commercial MgO.

Composition expressed as *n* = 2	**1 A (%)**	**1 B (%)**	**Mass fraction, dried sample Mean value ± Std. error (%)**
MgO	78.1	78.0	78.1
CaO	1.0	1.0	1.0
SO_3	0.4	0.3	0.4
SiO_2	0.2	0.3	0.3
Cl	0.1	0.1	0.1
Fe_2O_3	0.1	0.1	0.1
Mineral Part	--	--	79.9
LOI (*n* = 3) 750 ºC	--	--	20.2 ± 0.1
Total			100.1 ± 0.1

n = number of individual determinations.
LOI = Fire assay (mainly H_2O + CO_2).

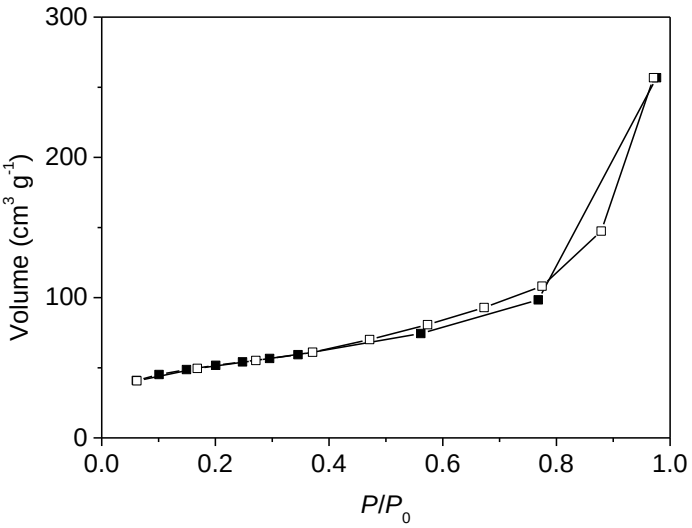

Figure S2. Nitrogen adsorption/desorption isotherms for commercial MgO.

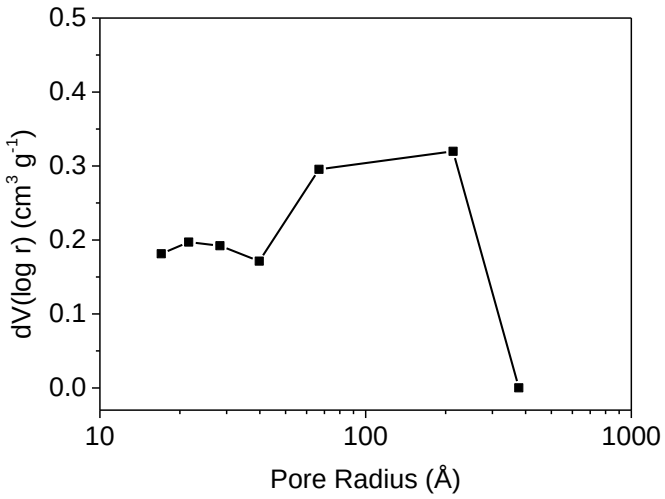

Figure S3. Pore radius distribution of commercial MgO, calculated by the BJH method using the desorption curve.

3. Kinetic data

Table S2. Optimization of the reaction variables (stirring rate and temperature) in the propanolysis of methyl paraoxon catalyzed by MgO.

Substrate/catalyst (mol g^{-1})	Stirring rate (rpm)	Temperature (ºC)	k_1 (s^{-1})
4.61×10^{-6}	100	30	3.84×10^{-4}
4.61×10^{-6}	640	30	4.38×10^{-4}
4.61×10^{-6}	640	80	2.65×10^{-3}

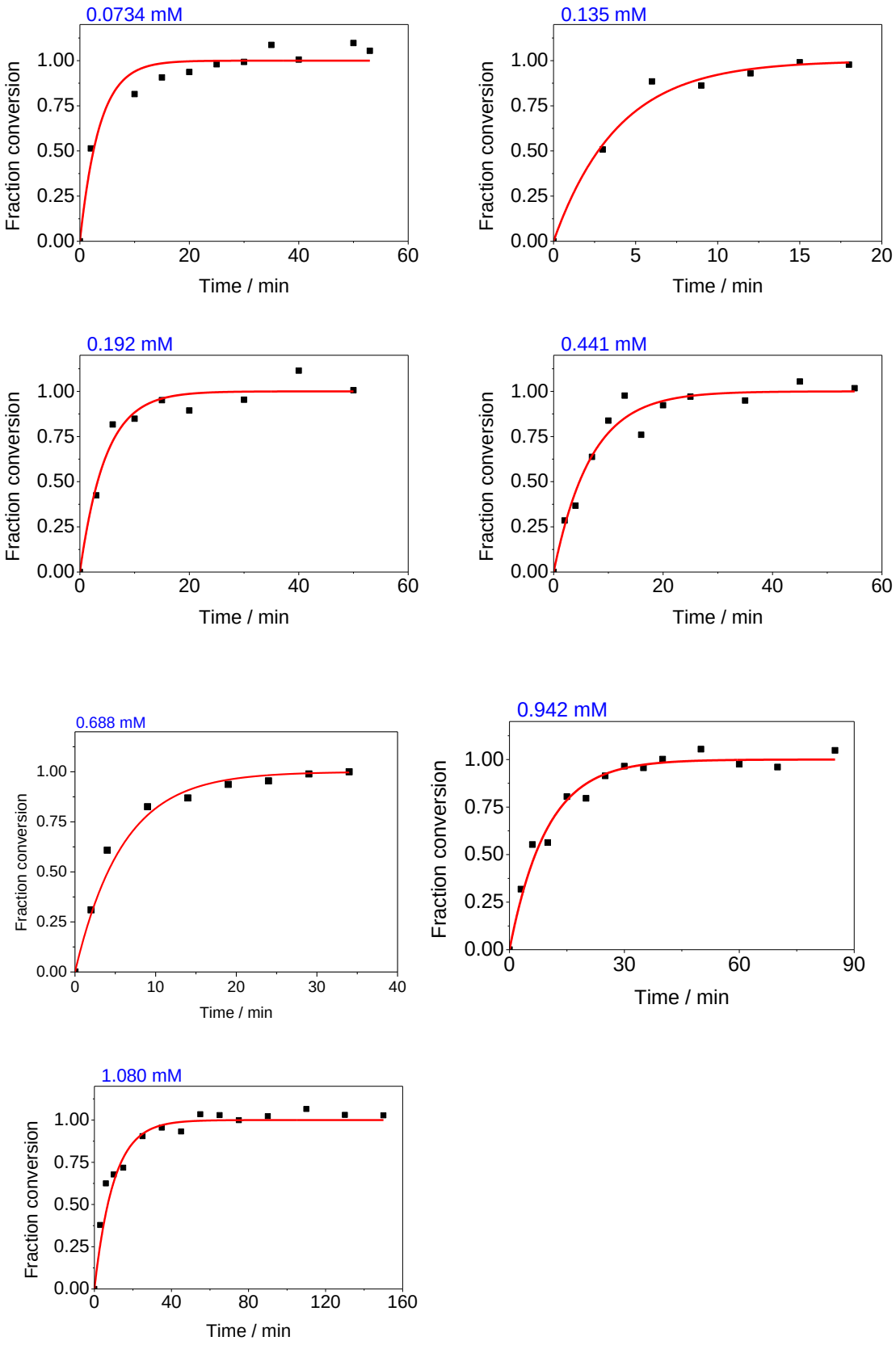

Figure S4. Kinetic profiles of the MgO-catalyzed propanolysis of methyl paraoxon employing 300 mg of catalyst and different concentrations of the substrate, as indicated in the figure, at 80ºC. The ratio of mols of substrate per gram of catalyst are in the range 5 x 10^{-6} to 7.2 x 10^{-5}. The solid lines represent fitting to a first order exponential (eq. 1 in the main text).

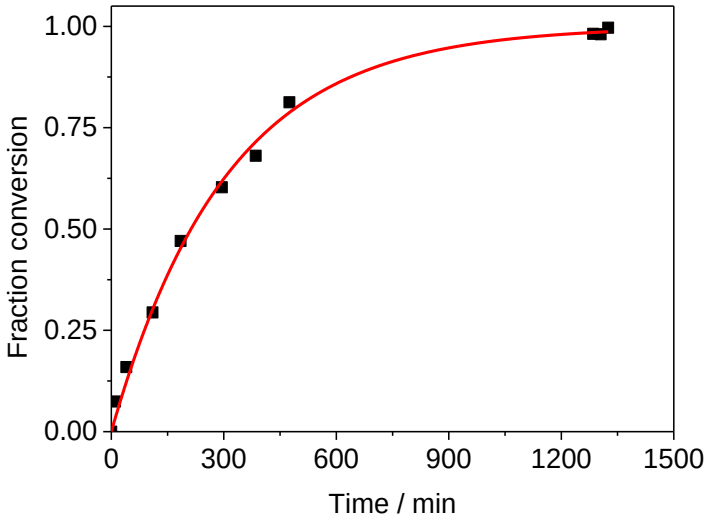

Figure S5. Kinetic profile of the MgO-catalyzed propanolysis of methyl paraoxon employing 30 mg of catalyst and 0.647 mM of the substrate, at 80ºC. The solid line represents fitting to a first order exponential (eq. 1 in the main text).

4. Catalyst recycling

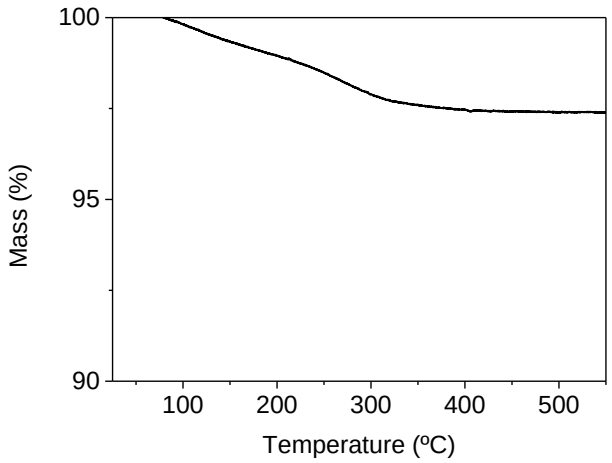

Table S6. Thermogravimetric analysis of commercial MgO subjected to one reactivation procedure.

Table S3. Semi-quantitative EDXRF analysis of commercial MgO reactivated after the second use.

Composition expressed as *n* = 2	**1 A (%)**	**1 B (%)**	**Mass fraction; dried sample Mean value ± Std. error (%)**
MgO	78.3	78.3	78.3
Na_2O	0.6	0.4	0.5 ± 0.1
SiO_2	0.4	0.4	0.4
Fe_2O_3	0.1	0.1	0.1
Al_2O_3	--	0.1	0.1
CaO	0.1	0.2	0.15
Cl	0.1	0.1	0.1
K_2O	0.1	0.1	0.1
SO_3	0.1	0.1	0.1
Mineral Part	--	--	79.9
LOI (*n* = 3) 750 ºC	--	--	20.2 ± 0.1
Total			100.1 ± 0.2

n = number of individual determinations.
LOI = Fire assay (mainly $H_2O + CO_2$).

5. Kinetic treatment of the data for the MgO-catalyzed propanolysis of the triaryl phosphate esters

For the propanolyis of the triaryl phosphates catalyzed by MgO, up to three consecutive irreversible first order reactions were observed, and thus the profiles of absorbance against time can be described by the general eq. S1 below,

$[ArOH]_t = [ArOH]_i + [ArOH]_{ii} + [ArOH]_{iii}$ (S1)

were $[ArOH]_t$ denotes the total concentration of the aromatic leaving group, and $[ArOH]_i$, $[ArOH]_{ii}$ and $[ArOH]_{iii}$ stand for the concentration of the aromatic leaving group from the first, second and third step, respectively, given by eqs. S2–S4.

$$[\mathrm{ArOH}]_i = [\mathrm{A}]_0\left(1 - e^{-k_1 t}\right) \quad \text{(S2)}$$

$$[\mathrm{ArOH}]_{ii} = [\mathrm{A}]_0\left[1 + \frac{\left(k_2 e^{-k_1 t} - k_1 e^{-k_2 t}\right)}{\left(k_1 - k_2\right)}\right] \quad \text{(S3)}$$

$$[\mathrm{ArOH}]_{iii} = [\mathrm{A}]_0\left[1 - \frac{k_2 k_3 e^{-k_1 t}}{\left(k_2 - k_1\right)\left(k_3 - k_1\right)} - \frac{k_1 k_3 e^{-k_2 t}}{\left(k_1 - k_2\right)\left(k_3 - k_2\right)} - \frac{k_1 k_2 e^{-k_3 t}}{\left(k_1 - k_3\right)\left(k_2 - k_3\right)}\right] \quad \text{(S4)}$$

where $[A]_0$ is the initial concentration of the substrate, and k_1, k_2 and k_3 represent the observed first order rate constants of the first, second and third steps, respectively.

For the scenario with two consecutive irreversible first order reactions, eq. S1 reduces to eq. S5.

$[ArOH]_t = [ArOH]_i + [ArOH]_{ii}$ eq. S5

For the T4NPP substrate, it was observed the substitution of the three aryloxide substituents, and the kinetic data was fitted to eq. S1, while eq. S5 was used to fit the kinetic data of the T2PyP substrate, since two substitution reactions were observed up to ~175 min.

6. Experiments of LC-ESI-MS

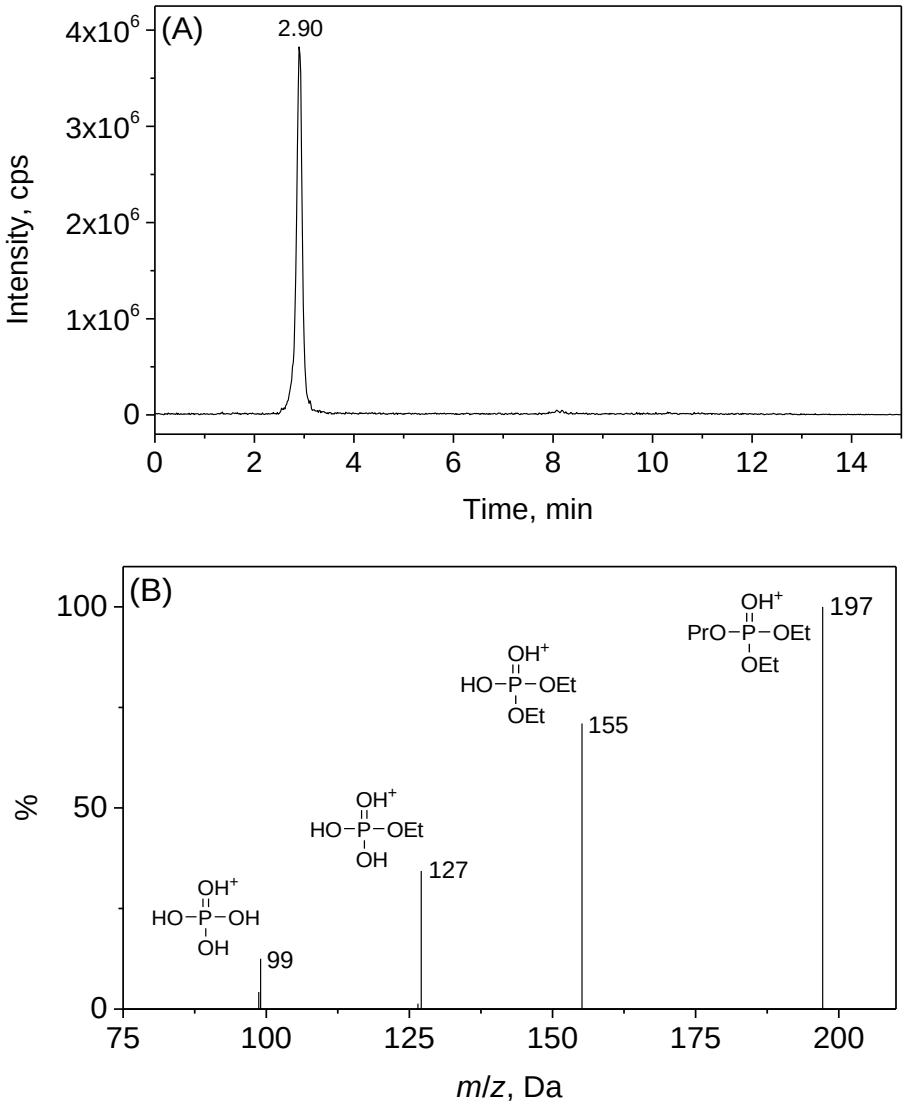

Figure S7. **(A)** Total ion current chromatogram of product ion of *m*/*z* 197, from an aliquot of the reaction products of the MgO-catalyzed propanolysis of DEDNPP obtained by LC/MS with ESI(+)-MS detection. **(B)** ESI(+)-MS/MS of the peak eluted at 2.90 min.

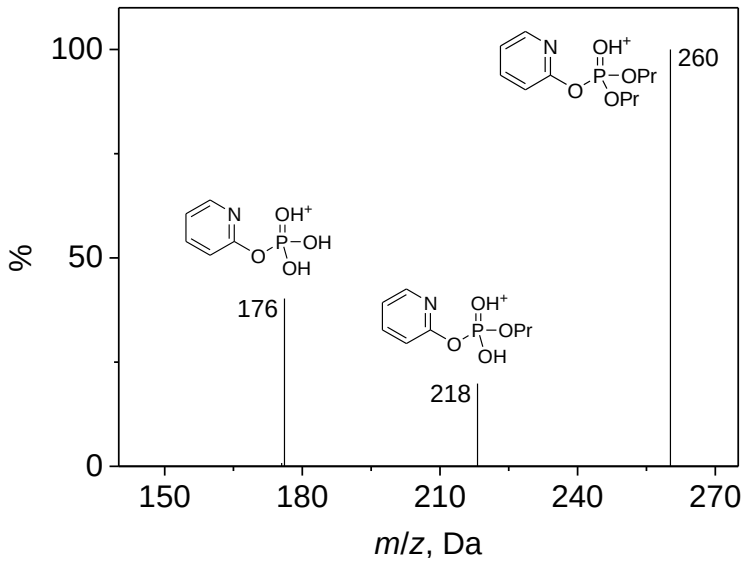

Figure S8. ESI(+)-MS/MS of the product ion of *m*/*z* 260 eluted at 3.45 min, obtained from a LC-ESI-MS analysis of the MgO-catalyzed propanolysis of the T2PyP substrate.

7. Characterization of commercial γ-Al_2O_3 and kinetic data of methyl paraoxon propanolysis catalyzed by γ-Al_2O_3

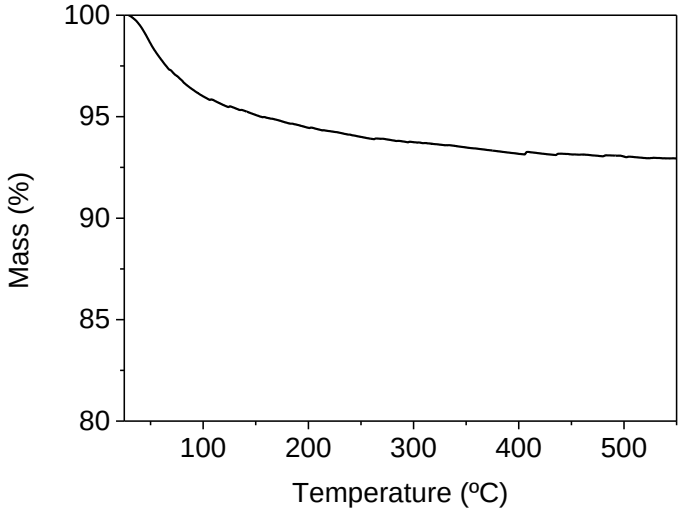

Figure S9. Thermogravimetric analysis of commercial γ-Al_2O_3.

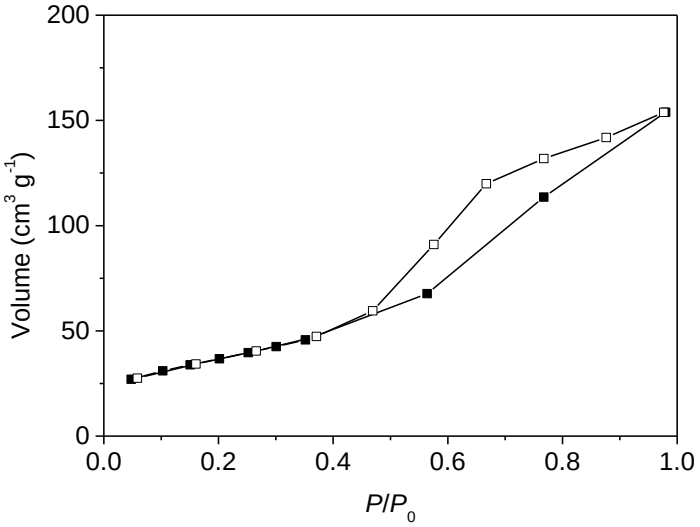

Table S10. Nitrogen adsorption/desorption isotherms for commercial γ-Al_2O_3.

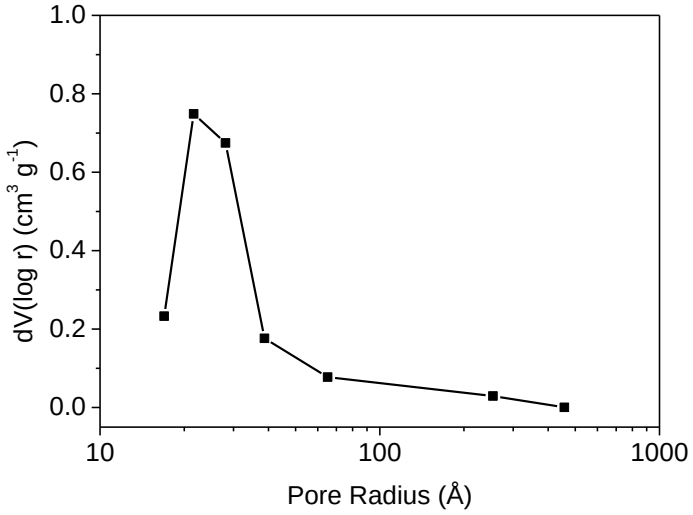

Figure S11. Pore radius distribution of commercial γ-Al_2O_3, calculated by the BJH method using the desorption curve.

Table S4. Summary of textural properties of commercial γ-Al_2O_3 obtained by nitrogen adsorption/desorption measurements.

S_{BET} (m^2 g^{-1})[a]	132.5
V_{BJH} (cm^3 g^{-1})[b]	0.238
RP (Å)[c]	35.9

[a] Specific surface area. [b] Pore volume. [c] Mean pore radius.

Table S5. Base site density of commercial γ-Al_2O_3 (μmol CO_2/g catalyst).

Total	218.60
Weak	61.30
Medium	81.40
Strong	75.90

Table S6. Optimization of the reaction variables (stirring rate and temperature) in the propanolysis of methyl paraoxon catalyzed by γ-Al_2O_3.

Substrate/catalyst (mol g^{-1})	Stirring rate (rpm)	Temperature (ºC)	k_1 (s^{-1})
4.6×10^{-6}	100	30	3.33×10^{-5}
4.6×10^{-6}	640	30	3.25×10^{-5}
4.6×10^{-6}	640	80	1.05×10^{-4}
4.6×10^{-5}	640	80	1.20×10^{-4}
4.6×10^{-4}	640	80	3.50×10^{-5}

8. Data from DFT calculations

In all cases, calculations employed the methodology described in the main text.

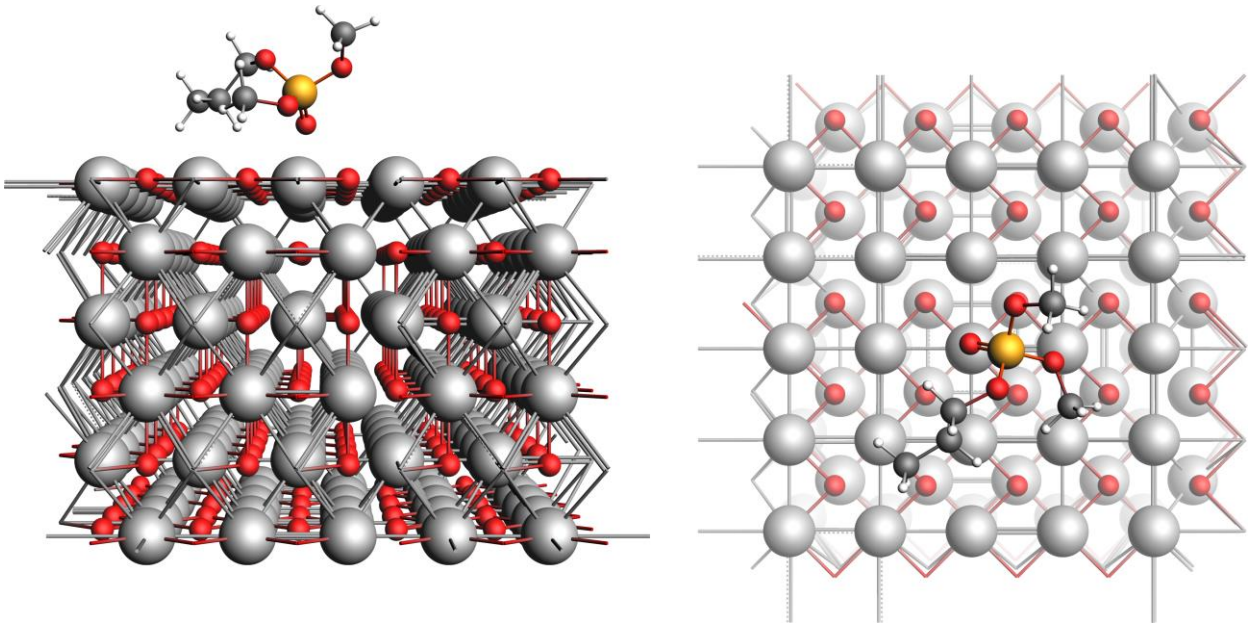

Figure S12. Structure of the adsorbed phosphate product, whose calculated binding energy was -36.901 kcal/mol.

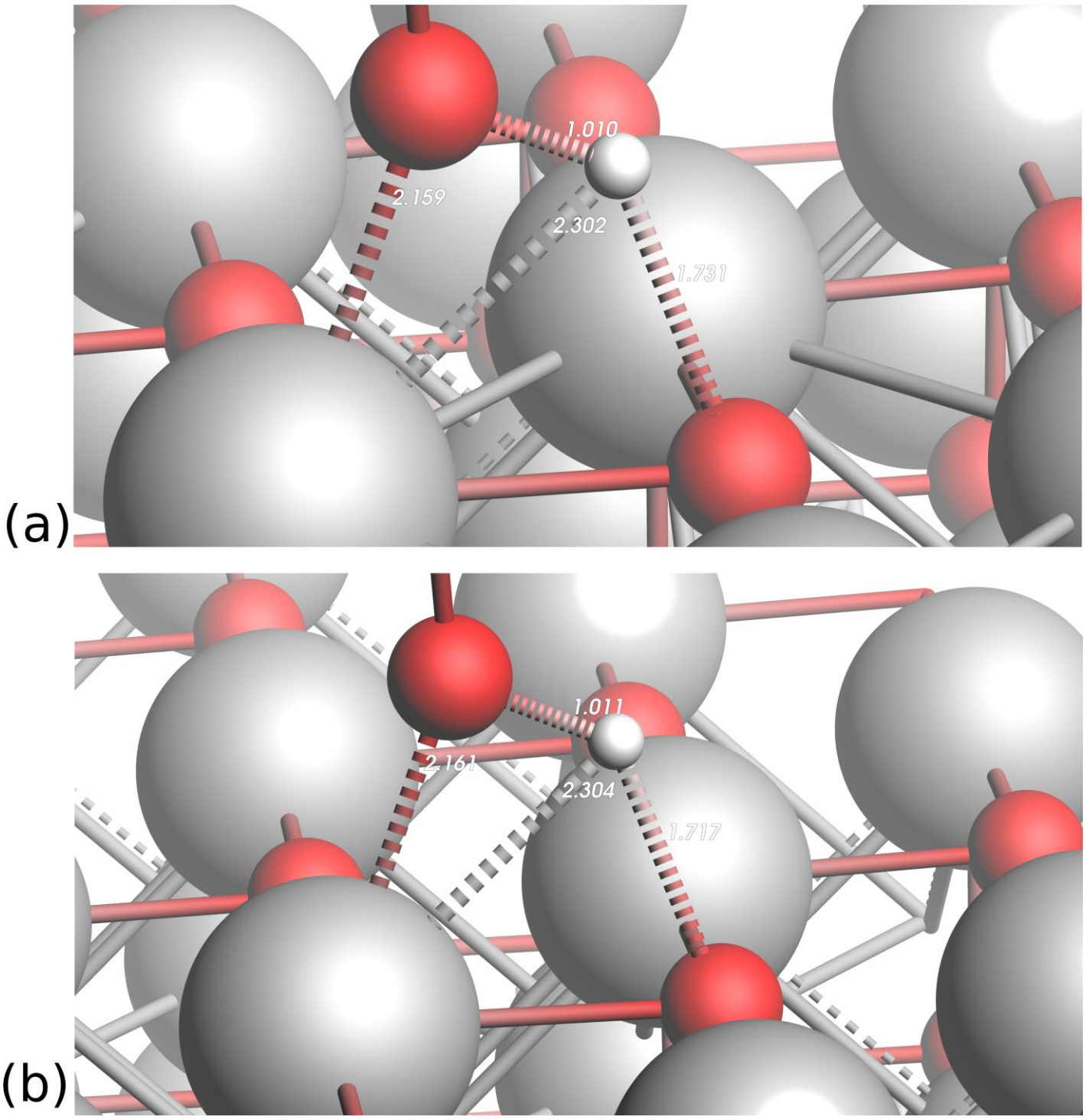

Figure S13. Selected geometry parameters (Å) of (a) adsorbed 1-propanol and (b) 1-propoxide.

Atomic coordinates (Å) for the slab unit cell (of size 14.884 x 14.884 Å² in all cases) of all studied structures are shown below, together with their respective final electronic energies (formation energies w.r.t. spherically-symmetric spin-restricted atoms, in hartree, Eh). Unit cell vectors are always v_1 = (14.883665032, 0.0, 0.0) and v_2 = (0.0, 14.883665032, 0.0).

```
26
phosphate (-5.72121647 Eh)
H       0.148876221     1.284903540    -1.612049145
H      -1.694526607     2.952936058    -1.244981459
H       3.037852793    -4.036014547    -1.069824642
H       2.255588123    -3.043761743    -2.359183202
H       3.167472359     0.952047191     1.930496494
H       3.032811284    -0.836932761     1.746264808
H       1.541215200     0.174762198     1.901893435
H       1.274015910    -3.667252029    -0.972381579
H      -3.448424004     0.404141711     1.746155861
H      -1.588291676    -1.270425398     1.405504446
P       1.871574831    -0.731016890    -0.893616809
O       1.824861138    -0.332663708    -2.320457346
O       2.609901332    -2.106595733    -0.495235848
O       2.564886583     0.355758712     0.063556929
O      -4.586103802     2.487103726     1.354972829
O      -3.698826208     3.790033427    -0.206534071
O       0.385135047    -1.038841693    -0.195971603
C       2.569209203     0.132350590     1.511755553
C       2.259954552    -3.292280473    -1.287692033
C      -2.651990667     1.766840000     0.277143785
C      -2.650533237     0.581877275     1.026904548
C      -1.622128449    -0.339995690     0.837139959
C      -0.605553774    -0.072821557    -0.099032503
C      -0.622970921     1.106290789    -0.864569037
C      -1.652919105     2.029814021    -0.668813691
N      -3.721086127     2.749742981     0.488554321

12
propanol (-2.26222347 Eh)
C      -0.600834458    -0.581452734     1.338526216
C      -0.461798685    -0.434510391    -0.184200866
C       0.612570765     0.582579630    -0.564231269
O       0.675817479     0.658030592    -2.009248506
H       1.363952179     1.320816339    -2.228484354
H       0.347459705    -0.915731289     1.795449945
H      -1.377240862    -1.322043342     1.591389608
H      -0.881938964     0.377814452     1.808134235
H      -1.421196288    -0.115437165    -0.629746980
H      -0.203854099    -1.405930403    -0.642979046
H       1.588864254     0.265151925    -0.144701274
H       0.358198973     1.570712387    -0.129907710

23
phosphate product (-4.53374214 Eh)
H      -3.422432970     0.166066821    -1.716071293
H       2.227594195    -1.896861043    -1.208533162
H       1.366016124    -2.190213632     0.351700375
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H       2.933118786     1.632342630     1.889845110
H       3.165965048    -2.283992949     0.284717336
H       1.186512717     1.949355149     2.221462927
H       2.272383854     3.302224863     1.725357495
H      -1.365523250     1.260292256    -0.515267908
H      -1.958747489     0.592629152     1.042476511
H      -1.747085029    -1.732545131     0.080314888
H      -1.202878834    -1.020441465    -1.463307930
H      -3.976845287    -0.516503845    -0.160827277
H      -3.670192027    -1.591508174    -1.550783442
O       1.756720401     2.048177312     0.189044623
O       2.423398143    -0.367103450     0.232361164
O       0.939365599     0.585274396    -1.773807022
O       0.013398144     0.172988598     0.664168672
C       2.054379114     2.231780888     1.604742357
C      -1.348092608     0.381641318     0.149374478
C       2.275418855    -1.778592518    -0.114644554
C      -1.850350264    -0.857398247    -0.586185066
C      -3.313492191    -0.689432061    -1.026955980
P       1.241368967     0.601819130    -0.319182302

300
surface (-65.93125593 Eh)
O      -0.496122168     2.480610839    -5.253722476
O      -0.496122168     5.457343845    -5.253722476
O       2.480610839    -6.449588181    -5.253722476
O       2.480610839    -3.472855174    -5.253722476
O       2.480610839    -0.496122168    -5.253722476
O       2.480610839     2.480610839    -5.253722476
O       2.480610839     5.457343845    -5.253722476
O       5.457343845    -6.449588181    -5.253722476
O       5.457343845    -3.472855174    -5.253722476
O       5.457343845    -0.496122168    -5.253722476
O       5.457343845     2.480610839    -5.253722476
O       5.457343845     5.457343845    -5.253722476
O      -6.449588181    -6.449588181    -5.253722476
O      -6.449588181    -3.472855174    -5.253722476
O      -6.449588181    -0.496122168    -5.253722476
O      -6.449588181     2.480610839    -5.253722476
O      -6.449588181     5.457343845    -5.253722476
O      -3.472855174    -6.449588181    -5.253722476
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O      -3.472855174     2.480610839    -5.253722476
O      -3.472855174     5.457343845    -5.253722476
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O      -0.496122168    -3.472855174    -5.253722476
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O      -6.449588181    -3.472855174    -1.043986287
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O      -6.449588181     2.480610839    -1.043986287
O      -6.449588181     5.457343845    -1.043986287
O      -3.472855174    -6.449588181    -1.043986287
O      -3.472855174    -3.472855174    -1.043986287
O      -3.472855174    -0.496122168    -1.043986287
O      -3.472855174     2.480610839    -1.043986287
O      -3.472855174     5.457343845    -1.043986287
O      -0.496122168    -6.449588181    -1.043986287
O      -0.496122168    -3.472855174    -1.043986287
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O	-0.496122168	2.480610839	-1.043986287
O	-0.496122168	5.457343845	-1.043986287
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O	2.480610839	-3.472855174	-1.043986287
O	2.480610839	-0.496122168	-1.043986287
O	2.480610839	2.480610839	-1.043986287
O	2.480610839	5.457343845	-1.043986287
O	5.457343845	-6.449588181	-1.043986287
O	5.457343845	-3.472855174	-1.043986287
O	5.457343845	-0.496122168	-1.043986287
O	5.457343845	2.480610839	-1.043986287
O	5.457343845	5.457343845	-1.043986287
O	-4.961221677	-4.961221677	-3.148854381
O	-4.961221677	-1.984488671	-3.148854381
O	-4.961221677	0.992244335	-3.148854381
O	-4.961221677	3.968977342	-3.148854381
O	-4.961221677	6.945710348	-3.148854381
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O	-1.984488671	-1.984488671	-3.148854381
O	-1.984488671	0.992244335	-3.148854381
O	-1.984488671	3.968977342	-3.148854381
O	-1.984488671	6.945710348	-3.148854381
O	0.992244335	-4.961221677	-3.148854381
O	0.992244335	-1.984488671	-3.148854381
O	0.992244335	0.992244335	-3.148854381
O	0.992244335	3.968977342	-3.148854381
O	0.992244335	6.945710348	-3.148854381
O	3.968977342	-4.961221677	-3.148854381
O	3.968977342	-1.984488671	-3.148854381
O	3.968977342	0.992244335	-3.148854381
O	3.968977342	3.968977342	-3.148854381
O	3.968977342	6.945710348	-3.148854381
O	6.945710348	-4.961221677	-3.148854381
O	6.945710348	-1.984488671	-3.148854381
O	6.945710348	0.992244335	-3.148854381
O	6.945710348	3.968977342	-3.148854381
O	6.945710348	6.945710348	-3.148854381
Mg	-6.449588181	-6.449588181	5.228307570
Mg	-6.449588181	-3.472855174	5.228307570
Mg	-6.449588181	-0.496122168	5.228307570
Mg	-6.449588181	2.480610839	5.228307570
Mg	-6.449588181	5.457343845	5.228307570
Mg	-3.472855174	-6.449588181	5.228307570
Mg	-3.472855174	-3.472855174	5.228307570
Mg	-3.472855174	-0.496122168	5.228307570
Mg	-3.472855174	2.480610839	5.228307570
Mg	-3.472855174	5.457343845	5.228307570
Mg	-0.496122168	-6.449588181	5.228307570
Mg	-0.496122168	-3.472855174	5.228307570
Mg	-0.496122168	-0.496122168	5.228307570
Mg	-0.496122168	2.480610839	5.228307570
Mg	-0.496122168	5.457343845	5.228307570
Mg	2.480610839	-6.449588181	5.228307570
Mg	2.480610839	-3.472855174	5.228307570
Mg	2.480610839	-0.496122168	5.228307570
Mg	2.480610839	2.480610839	5.228307570
Mg	2.480610839	5.457343845	5.228307570
Mg	5.457343845	-6.449588181	5.228307570
Mg	5.457343845	-3.472855174	5.228307570

Mg	5.457343845	-0.496122168	5.228307570
Mg	5.457343845	2.480610839	5.228307570
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Mg	-1.984488671	3.968977342	3.145335360
Mg	-1.984488671	6.945710348	3.145335360
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Mg	0.992244335	-1.984488671	3.145335360
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Mg	3.968977342	-4.961221677	3.145335360
Mg	3.968977342	-1.984488671	3.145335360
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Mg	3.968977342	3.968977342	3.145335360
Mg	3.968977342	6.945710348	3.145335360
Mg	6.945710348	-4.961221677	3.145335360
Mg	6.945710348	-1.984488671	3.145335360
Mg	6.945710348	0.992244335	3.145335360
Mg	6.945710348	3.968977342	3.145335360
Mg	6.945710348	6.945710348	3.145335360
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Mg	-6.449588181	-3.472855174	1.046730089
Mg	-6.449588181	-0.496122168	1.046730089
Mg	-6.449588181	2.480610839	1.046730089
Mg	-6.449588181	5.457343845	1.046730089
Mg	-3.472855174	-6.449588181	1.046730089
Mg	-3.472855174	-3.472855174	1.046730089
Mg	-3.472855174	-0.496122168	1.046730089
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Mg	-3.472855174	5.457343845	1.046730089
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Mg	-0.496122168	-3.472855174	1.046730089
Mg	-0.496122168	-0.496122168	1.046730089
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Mg	-0.496122168	5.457343845	1.046730089
Mg	2.480610839	-6.449588181	1.046730089
Mg	2.480610839	-3.472855174	1.046730089
Mg	2.480610839	-0.496122168	1.046730089
Mg	2.480610839	2.480610839	1.046730089
Mg	2.480610839	5.457343845	1.046730089
Mg	5.457343845	-6.449588181	1.046730089
Mg	5.457343845	-3.472855174	1.046730089
Mg	5.457343845	-0.496122168	1.046730089
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O	-4.961221677	-4.961221677	5.284178922

O	-4.961221677	-1.984488671	5.284178922
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O	0.992244335	-4.961221677	5.284178922
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O	0.992244335	3.968977342	5.284178922
O	3.968977342	6.945710348	5.284178922
O	3.968977342	-4.961221677	5.284178922
O	3.968977342	-1.984488671	5.284178922
O	3.968977342	0.992244335	5.284178922
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O	-3.472855174	-0.496122168	3.139822455
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O	-0.496122168	2.480610839	3.139822455
O	-0.496122168	5.457343845	3.139822455
O	2.480610839	-6.449588181	3.139822455
O	2.480610839	-3.472855174	3.139822455
O	2.480610839	-0.496122168	3.139822455
O	2.480610839	2.480610839	3.139822455
O	2.480610839	5.457343845	3.139822455
O	5.457343845	-6.449588181	3.139822455
O	5.457343845	-3.472855174	3.139822455
O	5.457343845	-0.496122168	3.139822455
O	5.457343845	2.480610839	3.139822455
O	5.457343845	5.457343845	3.139822455
O	-4.961221677	-4.961221677	1.048751890
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O	-4.961221677	0.992244335	1.048751890
O	-4.961221677	3.968977342	1.048751890
O	-4.961221677	6.945710348	1.048751890
O	-1.984488671	-4.961221677	1.048751890
O	-1.984488671	-1.984488671	1.048751890
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O	0.992244335	0.992244335	1.048751890
O	0.992244335	3.968977342	1.048751890
O	0.992244335	6.945710348	1.048751890
O	3.968977342	-4.961221677	1.048751890
O	3.968977342	-1.984488671	1.048751890

O	3.968977342	0.992244335	1.048751890
O	3.968977342	3.968977342	1.048751890
O	3.968977342	6.945710348	1.048751890
O	6.945710348	-4.961221677	1.048751890
O	6.945710348	-1.984488671	1.048751890
O	6.945710348	0.992244335	1.048751890
O	6.945710348	3.968977342	1.048751890
O	6.945710348	6.945710348	1.048751890
Mg	-4.961221677	-4.961221677	-1.043986287
Mg	-4.961221677	-1.984488671	-1.043986287
Mg	-4.961221677	0.992244335	-1.043986287
Mg	-4.961221677	3.968977342	-1.043986287
Mg	-4.961221677	6.945710348	-1.043986287
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Mg	-1.984488671	-1.984488671	-1.043986287
Mg	-1.984488671	0.992244335	-1.043986287
Mg	-1.984488671	3.968977342	-1.043986287
Mg	-1.984488671	6.945710348	-1.043986287
Mg	0.992244335	-4.961221677	-1.043986287
Mg	0.992244335	-1.984488671	-1.043986287
Mg	0.992244335	0.992244335	-1.043986287
Mg	0.992244335	3.968977342	-1.043986287
Mg	0.992244335	6.945710348	-1.043986287
Mg	3.968977342	-4.961221677	-1.043986287
Mg	3.968977342	-1.984488671	-1.043986287
Mg	3.968977342	0.992244335	-1.043986287
Mg	3.968977342	3.968977342	-1.043986287
Mg	3.968977342	6.945710348	-1.043986287
Mg	6.945710348	-4.961221677	-1.043986287
Mg	6.945710348	-1.984488671	-1.043986287
Mg	6.945710348	0.992244335	-1.043986287
Mg	6.945710348	3.968977342	-1.043986287
Mg	6.945710348	6.945710348	-1.043986287
Mg	-6.449588181	-6.449588181	-3.148854381
Mg	-6.449588181	-3.472855174	-3.148854381
Mg	-6.449588181	-0.496122168	-3.148854381
Mg	-6.449588181	2.480610839	-3.148854381
Mg	-6.449588181	5.457343845	-3.148854381
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Mg	-3.472855174	-3.472855174	-3.148854381
Mg	-3.472855174	-0.496122168	-3.148854381
Mg	-3.472855174	2.480610839	-3.148854381
Mg	-3.472855174	5.457343845	-3.148854381
Mg	-0.496122168	-6.449588181	-3.148854381
Mg	-0.496122168	-3.472855174	-3.148854381
Mg	-0.496122168	-0.496122168	-3.148854381
Mg	-0.496122168	2.480610839	-3.148854381
Mg	-0.496122168	5.457343845	-3.148854381
Mg	2.480610839	-6.449588181	-3.148854381
Mg	2.480610839	-3.472855174	-3.148854381
Mg	2.480610839	-0.496122168	-3.148854381
Mg	2.480610839	2.480610839	-3.148854381
Mg	2.480610839	5.457343845	-3.148854381
Mg	5.457343845	-6.449588181	-3.148854381
Mg	5.457343845	-3.472855174	-3.148854381
Mg	5.457343845	-0.496122168	-3.148854381
Mg	5.457343845	2.480610839	-3.148854381
Mg	5.457343845	5.457343845	-3.148854381
Mg	-4.961221677	-4.961221677	-5.253722476
Mg	-4.961221677	-1.984488671	-5.253722476

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Mg     -4.961221677     0.992244335    -5.253722476
Mg     -4.961221677     3.968977342    -5.253722476
Mg     -4.961221677     6.945710348    -5.253722476
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Mg     -1.984488671    -1.984488671    -5.253722476
Mg     -1.984488671     0.992244335    -5.253722476
Mg     -1.984488671     3.968977342    -5.253722476
Mg     -1.984488671     6.945710348    -5.253722476
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Mg      0.992244335     0.992244335    -5.253722476
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Mg      0.992244335     6.945710348    -5.253722476
Mg      3.968977342    -4.961221677    -5.253722476
Mg      3.968977342    -1.984488671    -5.253722476
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Mg      3.968977342     3.968977342    -5.253722476
Mg      3.968977342     6.945710348    -5.253722476
Mg      6.945710348    -4.961221677    -5.253722476
Mg      6.945710348    -1.984488671    -5.253722476
Mg      6.945710348     0.992244335    -5.253722476
Mg      6.945710348     3.968977342    -5.253722476
Mg      6.945710348     6.945710348    -5.253722476

326
phosphate over MgO surface (-71.74465769 Eh)
O       0.107726769     2.487029447    -5.942516709
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O       3.084459776    -6.443169572    -5.942516709
O       3.084459776    -3.466436565    -5.942516709
O       3.084459776    -0.489703559    -5.942516709
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O       3.084459776     5.463762454    -5.942516709
O       6.061192782    -6.443169572    -5.942516709
O       6.061192782    -3.466436565    -5.942516709
O       6.061192782    -0.489703559    -5.942516709
O       6.061192782     2.487029447    -5.942516709
O       6.061192782     5.463762454    -5.942516709
O      -7.338396797     6.953558991     4.591161420
O      -7.333682738    -4.953008314     4.597406812
O      -7.330997558    -1.976084065     4.599850017
O      -7.324894904     0.998297898     4.609291493
O      -7.331923727     3.969832004     4.598487053
O      -4.362954554     6.957988696     4.566783502
O      -4.355271514    -4.952277561     4.601153947
O      -4.361853871    -1.974908629     4.595709379
O      -4.355260308     0.995541539     4.570256494
O      -4.353917993     3.972537773     4.578356388
O      -1.375380817     6.956561754     4.593931614
O      -1.378143330    -4.955838581     4.615910963
O      -1.388213661    -1.990724467     4.581581282
O      -1.388938661     1.008127786     4.575804168
O      -1.376370691     3.978117182     4.606826427
O       1.597200624     6.952277902     4.597230350
O       1.592221220    -4.956773748     4.600668331
O       1.609048192    -1.996490851     4.585940942
O       1.606870295     1.010238442     4.586752495
O       1.593434577     3.978219128     4.600986658
O       4.571323918     6.951576187     4.595716787
O       4.571823225    -4.955497545     4.597291050
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O	4.576862057	-1.978737061	4.598778677
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312
1-propanol over MgO surface (-68.22279727 Eh)
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O	3.758991961	-5.078538866	0.687820248
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C	-1.398820797	-1.226913984	8.813880927
C	-0.322087514	-0.206655286	8.442113813
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H       0.657587237    -0.524235708     8.850697680
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312
propoxide over MgO surface (-68.22251203 Eh)
O       0.007816607     2.982738529    -5.612763998
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O       5.961282620    -5.947460491    -5.612763998
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O      -7.432971361    -1.480211571     4.924907475
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O      -7.430528045     4.473690744     4.925240253
O      -4.455395363    -7.433788864     4.923878247
O      -4.456719234    -4.458398742     4.924778353
O      -4.459916320    -1.480352052     4.926335926
O      -4.460326162     1.496026564     4.925618532
O      -4.455222551     4.473042044     4.923868545
O      -1.478528800    -7.434651074     4.924903000
O      -1.478749298    -4.461542206     4.926760397
O      -1.495807506    -1.497387989     4.926787026
O      -1.496128749     1.507784094     4.892050742
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O       1.498384187    -7.432756918     4.925157646
O       1.497674247    -4.461533429     4.926173490
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O       1.497575213     4.477285770     4.928931885
O       4.475584499    -7.432476677     4.925076764
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O       4.479064685    -1.481713458     4.924204455
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O       4.479167263     4.477251498     4.924959569
O      -5.944532986    -5.946325117     2.778926174
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323
phosphate product over MgO surface (-70.52380287 Eh)
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