Supporting Information

MAPO-18 catalysts for the Methanol to Olefins (MTO) process: Influence of catalyst acidity in high-pressure syngas (CO and H₂) environment

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Supporting Figure 1. Dual-cycle hydrocarbon pool mechanism for the MTO reaction, from Olsbye et al.\textsuperscript{1}, with permission from John Wiley and Sons.
S2: Supporting catalyst characterization

Supporting Figure 2. SEM images of calcined MAPO-18s (0.05): (a) SiAPO-18, (b) MgAPO-18, (c) CoAPO-18 and (d) ZnAPO-18.

Supporting Table 1. Atomic percent (%) obtained using SEM-EDS for the MAPO-18s. Consistent elemental composition was obtained from different locations, hence suggesting the homogeneity of the catalysts.

|        | Al   | P    | O    | M    |
|--------|------|------|------|------|
| SAPO-18|      |      |      |      |
|        | 12.55| 12.99| 67.60| 1.49 |
|        | 13.27| 12.48| 67.61| 1.59 |
|        | 12.42| 13.13| 67.84| 1.61 |
|        | 13.88| 11.49| 67.36| 1.62 |
|        | 12.42| 12.75| 68.00| 1.50 |
| MgAPO-18|     |      |      |      |
|        | 12.45| 14.36| 67.79| 1.37 |
|        | 11.90| 14.48| 67.57| 1.37 |
|        | 12.22| 14.02| 67.31| 1.35 |
|        | 12.38| 13.99| 67.61| 1.48 |
|        | 12.56| 13.89| 67.50| 1.49 |
|        | 12.44| 13.88| 67.53| 1.45 |
| CoAPO-18|     |      |      |      |
|        | 11.42| 12.01| 70.10| 1.86 |
|        | 11.59| 12.08| 70.11| 1.85 |
|        | 11.92| 11.55| 70.00| 1.89 |
|        | 11.79| 11.59| 70.17| 1.89 |
|        | 11.09| 12.26| 70.14| 1.97 |
| ZnAPO-18|   |      |      |      |
|        | 13.00| 13.94| 67.18| 1.82 |
|        | 12.53| 14.04| 67.18| 1.94 |
|        | 12.42| 14.44| 67.50| 1.64 |
|        | 12.60| 14.06| 67.20| 1.80 |
Supporting Figure 3. PXRD patterns of as-synthesized (uncalcined) and calcined MAPO-18 catalysts. (a) PXRD patterns of SAPO-18 samples as-synthesised (left panel) and calcined (right panel), at displayed Si/T atom ratios. Phase deconvolution is only reported for the Si/T: 0.05 samples, as the other samples within the series display nearly identical patterns. Measured pattern: blue dots, calculated pattern: red line, deconvoluted phases: green lines, difference (experimental - calculated pattern): grey lines. (b) PXRD patterns of Mg-AlPO-18 samples as-synthesised (left panel) and calcined (right panel), at displayed Mg/T atom ratios. Phase deconvolution is only reported for the Mg/T: 0.05 sample, as the other samples within the series contain the same phases. Measured pattern: red dots, calculated pattern: black line, deconvoluted phases: green lines, difference (experimental - calculated pattern): grey lines. (c) PXRD patterns of Co-AlPO-18 (left panel) and Zn-AlPO-18 (right panel) samples, at 0.05 M/T-atom ratios. Measured pattern: yellow (Co-AlPO-18) and grey (Zn-AlPO-18) dots, calculated pattern: black line, deconvoluted phases: green lines, difference (experimental - calculated pattern): grey lines.

The SAPO-18 samples display a pure AEI structure, with minor presence of CHA intergrowth which is regularly observed for CHA and AEI materials. The Mg-AlPO-18 samples display a mixture of CHA and AEI phases as synthesized, with a minor presence of CHA still visible after calcination. The Co- and Zn-AlPO-18 samples display a mixture of CHA and AEI phases as synthesized, with a minor presence of CHA still visible in the Co-AlPO-18 sample after calcination.
The Zn-AlPO-18 decomposes upon calcination to tridymite and low-cristobalite AlPO₄. No separate ZnO phases are detected.

The evaluation of the samples’ structure is complex due to several factors. (1) The significant phase change of the AEI materials upon calcination, (2) the small domain size and high disorder in all samples (which is intentional to improve their performance as catalysts) and (3) the absence of accurate structure models. The lack of accurate structure models, and the low signal to noise ratio of the data, prevents the effective refinement of known AEI/CHA stacking faults, and the quantification of the AEI/CHA ratio in the samples where large CHA crystallites are present.

SAPO-34 is regularly obtained as cuboid crystals, whereas SAPO-18 synthesized with the DIPEA SDA tends to give elongated crystallites with diagonal facets (Figure S3). The M-AlPO-18 (M=Si, Zn) materials obtained in this study occur as disordered agglomerates of nanosized (10-200 nm) crystals with elongated shape, whereas the M-AlPO-18 (M=Mg,Co) materials occur as cuboid or prism-like particles (0.1 – 1 micron) with uneven surfaces.

Analysis of the PXRD patterns of SAPO-18 by Rietveld refinement against published structures shows a close agreement to the calculated pattern and high phase purity. For the non-calcined sample, peak broadening of certain peaks point to the presence of stacking faults.

Inspection of the PXRD patterns of Co/Mg-AlPO-18 before and after calcination reveals that the material consists of two distinct phases, AEI and CHA. The peak profiles of non-overlapping peaks from the two phases are significantly different, where the CHA peaks are sharper indicating larger diffracting domains. This was confirmed qualitatively by a combined Rietveld/Pawley fit, giving a domain size ratio of CHA/AEI of ≈2:1. Thus, the presented evidence points towards large cuboid CHA crystals, with AEI surface growth, closely resembling previously reported SAPO-18 surface crystallites on cuboid SAPO-34 crystals.

In both the Mg-AlPO-18 and Co-AlPO-18 samples, the CHA phase is no longer clearly observed in the PXRD patterns after calcination, indicating a lower thermal stability of this CHA phase than pure AlPO-18. The experiments have been reproduced several times, with varying degree of CHA content before calcination, with no discernable effect on the catalytic performance. Thus, we expect that the active phase in the materials reported herein is AEI in all cases.
Supporting Figure 4. N₂ physisorption analysis of calcined MAPO-18s (0.05). (a) SAPO-18, (b) MgAPO-18, (c) CoAPO-18 and (d) ZnAPO-18. All MAPO-18 (except ZnAPO-18) showed a similar Type I isotherm. The ZnAPO-18 isotherm also confirmed the presence of a largely dense phase in the calcined material.

Supporting Figure 5. Propylamine-TPD analysis of calcined MAPO-18s (0.05). (a) SAPO-18, (b) MgAPO-18, (c) CoAPO-18 and (d) ZnAPO-18. Product desorption temperature is expected to be inversely proportional to the acidic strength of BAS, since its main contributor is propyl amine cracking temperature, but product diffusion rates may also influence the observed desorption temperature.
Supporting Figure 6. IR spectra of MAPOs-18: (a) SAPO-18, (b) MgAPO-18, (c) CoAPO-18, (d) ZnAPO-18 in presence of adsorbed CO at 77K at decreasing coverages. Left panels: OH stretching region (from 3800 to 2600 cm$^{-1}$) of activated samples (dark lines) and in presence of the highest CO coverage (light lines). Right panels: CO stretching region (from 2250 to 2050 cm$^{-1}$) of spectra recorded in presence of decreasing CO equilibrium pressure (from lighter to darker lines).

Left panel illustrates the effect of CO interaction towards the variety of OH groups. Upon interaction with CO in all the samples, most of the P-OH are eroded, with the parallel growth of a band at 3510 cm$^{-1}$, confirming the low acidic character of these species. More complex is the evolution of BAS. In particular, BAS signals are downward shifted to 3350 cm$^{-1}$ for SAPO-18, and to 3280 cm$^{-1}$ for MgAPO-18 respectively, following the trend observed for the $\nu$(OH) (see main text). In case of CoAPO-18 the BAS species interacting with CO generate a very broad band extending from 3300 to 3000 cm$^{-1}$.

Right panels show the corresponding CO stretching range. All the samples are characterized by a strong component due to physisorbed CO at 2140 cm$^{-1}$ and a contribution around 2160 cm$^{-1}$, associated to CO interacting with the low acidic P-OH. Moreover, the interaction of CO with BAS is observed at 2170 cm$^{-1}$ and at 2178 cm$^{-1}$ in case SAPO and MgAPO-18 respectively. In MgAPO-18, a minor contribution is also observed at 2205 cm$^{-1}$, corresponding to the interaction of CO with extraframework Mg$^{2+}$ cation. As regards the CoAPO-18, a very strong band is centred at 2180 cm$^{-1}$. The literature assigns this band to a convolution of different contributions, nominally the interaction of CO with Co$^{2+}$ Lewis acid centres with different coordination within the framework (tetracoordinated Co$^{2+}$ at 2180 cm$^{-1}$ and defective tricoordinated Co$^{2+}$ at 2185 cm$^{-1}$) and a component assigned to tetracoordinated Co$^{3+}$ at 2178 cm$^{-1}$, due to the oxidation process caused by
exposure of the sample to atmospheric moisture. From our experimental data (the evolution of the IR spectra in the OH region) we suggest that the component at 2180 cm\(^{-1}\) contains also the contribution of CO interacting with BAS, as this signal decreases together with the band extending from 3300 to 3000 cm\(^{-1}\), while the BAS band is being restored. Finally, at low pressures of CO a small band is visible at 2210 cm\(^{-1}\), generated by the interaction of the probe with a minor fraction of extraframework Co\(^{2+}\) cations. ZnAPO shows, apart the signal of CO liquid like and CO interacting with P-OH, a component at very high frequency (2210 cm\(^{-1}\)) suggesting the presence of highly unsaturated Zn\(^{2+}\) sites.

Supporting Table 2. Textural and acidic properties of the SAPO-18 and MgAPO-18 catalysts with varied M/T atomic ratios. SAPO-18 and MgAPO-18 were catalysts discussed in the manuscript as part of the series of MAPO-18 (M = Si, Mg, Co and Zn). SAPO-18_a to d and MgAPO-18_a to c were prepared by varying M/T ratios in the synthesis gel recipes.

|                  | Crystal size (µm)\(^{a}\) | \(S_{\text{BET}}\) (m\(^2\)/g)\(^{b}\) | Elemental Composition\(^{c}\) | Density of M (mmol/g\(_{\text{cat}}\)) \(\text{P/Al}\) | M/Al | M/T Atoms | Brønsted Acidity (mmol/g\(_{\text{cat}}\)) \(\text{P/Al}\) | M/Al | M/T Atoms |
|------------------|--------------------------|-------------------------------------|-------------------------------|---------------------------------|-------|------------|---------------------------------|-------|------------|
| SAPO-18          | ~ 0.5                    | 749                                 | 1.0                           | 0.12                            | 0.06  | 0.61       | 0.29                            |
| SAPO-18\(_a\)    | ~ 0.5                    | 729                                 | 1.0                           | 0.06                            | 0.03  | 0.51       | 0.33                            |
| SAPO-18\(_b\)    | ~ 0.5                    | 772                                 | 1.0                           | 0.09                            | 0.04  | 0.71       | 0.41                            |
| SAPO-18\(_c\)    | ~ 0.5                    | 685                                 | 0.9                           | 0.12                            | 0.06  | 0.94       | 0.45                            |
| SAPO-18\(_d\)    | ~ 0.5                    | 749                                 | 0.9                           | 0.12                            | 0.06  | 1.01       | 0.25                            |
| MgAPO-18         | ~ 0.5                    | 730                                 | 1.1                           | 0.12                            | 0.05  | 0.55       | 0.17                            |
| MgAPO-18\(_a\)   | ~ 0.5                    | 748                                 | 1.0                           | 0.06                            | 0.03  | 0.49       | 0.23                            |
| MgAPO-18\(_b\)   | ~ 0.5                    | 755                                 | 1.0                           | 0.08                            | 0.04  | 0.65       | 0.30                            |
| MgAPO-18\(_c\)   | ~ 0.5                    | 741                                 | 1.0                           | 0.11                            | 0.05  | 0.81       | 0.39                            |

Properties determined using \(^{a}\) SEM, \(^{b}\) N\(_2\)-physorption using BET method, \(^{c}\) SEM-EDS, \(^{d}\) propylamine-TPD.
Supporting Figure 7. SEM images of calcined SAPO-18s. (a) SAPO-18_a, (b) SAPO-18_b, (c) SAPO-18_c, and (d) SAPO-18_d all showed characteristic small rods.

Supporting Figure 8. N\textsubscript{2} adsorption desorption isotherms of calcined SAPO-18s. (a) SAPO-18_a, (b) SAPO-18_b, (c) SAPO-18_c and (d) SAPO-18_d. All showed a similar Type I isotherm behavior.
Supporting Figure 9. SEM images of calcined MgAPO-18s. (a) MgAPO-18_a, (b) MgAPO-18_b and (c) MgAPO-18_c all appeared cubic with irregular and rough surfaces. This was different to the SiAPO-18 materials and may be as a consequence of the use of magnesium in the synthesis. This suggests that the crystallization process consisted of agglomerates of smaller crystals. The size and morphology of the crystallites was consistent between samples of varying Mg-content.

![SEM images of calcined MgAPO-18s](image)

Supporting Figure 10. N$_2$ adsorption desorption isotherms of calcined MgAPO-18s. (a) MgAPO-18_a, (b) MgAPO-18_b and (c) MgAPO-18_c. All showed a similar Type I isotherm behavior with capillary condensation seen at high relative pressure.

![N$_2$ adsorption desorption isotherms](image)
Supporting Figure 11. OH stretching region of IR spectra of activated SAPO-18s and MgAPOs. (a) SAPO-18_a, (b) SAPO-18_b, (c) SAPO-18_c, (d) MgAPO-18_a, (e) MgAPO-18_b and (f) MgAPO-18_c. The spectra are normalized to the pellets’ thickness.

The IR spectra of all samples are characterized by the components already described in the main text. Notably, the variation of BAS bands intensities, moving from the bottom to the top of the series is not proportional to the increment of the heteroatom contents but it follows the trend evaluated by propylamine-TPD (Table S2). The decreased amount of BAS observed for the sample with the higher amount of Si, indicates that in this sample Si is present aggregated in islands as widely reported in the literature.\(^7,8\) In case of MgAPO-18_a (Figure S12 below); MgAPO-18_b and MgAPO-18_c samples, CO adsorption at low temperature did not evidence the presence of any Mg\(^{2+}\) counterion: lack of the band at 2205 cm\(^{-1}\).

Supporting Figure 12. IR spectra of MgAPO-18_a in presence of adsorbed CO at 77K at decreasing coverages. Left panels: OH stretching region (from 3800 to 3000 cm\(^{-1}\)) of activated samples (dark lines) and in presence of the highest CO coverage (light lines). Right panels: CO stretching region (from 2250 to 2050 cm\(^{-1}\)) of spectra recorded in presence of decreasing CO equilibrium pressure (from lighter to darker lines).
S3: Supporting catalyst performance

Supporting Figure 13. Catalytic performance of commercial SAPO-34 (from ACS Materials) at MTO reaction conditions. Reaction conditions: 350 °C, 1 bar, 0.13 bar MeOH (WHSV = 0.25 g<sub>MeOH</sub> g<sub>cat</sub>⁻¹ h⁻¹), 0.87 bar He. (a) Activity in terms % sum of MeOH and DME conversion over MeOH conversion capacity. The MAPO-18s were tested at identical conditions except with a higher WHSV (MeOH) = 4 g<sub>MeOH</sub> g<sub>cat</sub>⁻¹ h⁻¹. (b) Selectivity vs. conversion of SAPO-34. Conversion variation was due to catalyst deactivation during runtime.
Supporting Figure 14. Selectivity vs. conversion of MAPO-18s at MTO reaction conditions (a to h) and reproducibility runs of MgAPO-18 (i to o) with error bars at 95 % confidence interval. Reaction conditions: 350 °C, 1 bar, 0.13 bar MeOH (WHSV = 4 gMeOH gcat⁻¹ h⁻¹), 0.87 bar He. Conversion variation was due to catalyst deactivation during runtime.
Supporting Figure 15. Paraffin selectivity vs. conversion of MAPO-18s in various reaction feeds. Reaction conditions: 350 °C, 20 bar, 1 bar MeOH (WHSV = 2.5 gMeOH gcat⁻¹ h⁻¹), 0.6 bar Ar internal standard, 18.4 bar N₂ or H₂ or H₂/X = 3 (in which X = N₂, CO₂ or CO), GHSV ≈ 16 000 mL total flow mLcat⁻¹ h⁻¹. Conversion variation was due to catalyst deactivation during runtime.
Supporting Figure 15 (II). Olefin selectivity vs. conversion of MAPO-18s in various reaction feeds. Reaction conditions: 350 °C, 20 bar, 1 bar MeOH (WHSV = 2.5 gMeOH g\texttext{cat}^{-1} h^{-1}), 0.6 bar Ar internal standard, 18.4 bar N\texttext{2} or H\texttext{2} or H\texttext{2}/X = 3 (in which X = N\texttext{2}, CO\texttext{2} or CO), GHSV ≈ 16 000 mL\texttext{total flow} mL\texttext{cat}^{-1} h^{-1}. Conversion variation was due to catalyst deactivation during runtime.
Supporting Figure 16. Reproducibility runs of CoAPO-18 with error bars at 95% confidence interval. Reaction conditions: 350 °C, 20 bar, 1 bar MeOH (WHSV = 2.5 g\textsubscript{MeOH} g\textsubscript{cat}\textsuperscript{-1} h\textsuperscript{-1}), 0.6 bar Ar internal standard, 18.4 bar H\textsubscript{2}/CO = 3, GHSV ≈ 16 000 mL\textsubscript{total flow} mL\textsubscript{cat}\textsuperscript{-1} h\textsuperscript{-1}.

Supporting Figure 17. Catalytic performance of commercial SAPO-34 (from ACS Materials) at high pressure MTO reaction conditions. Reaction conditions: 350 °C, 20 bar, 1 bar MeOH (WHSV = 2.0 g\textsubscript{MeOH} g\textsubscript{cat}\textsuperscript{-1} h\textsuperscript{-1}), 0.6 bar Ar internal standard, 18.4 bar N\textsubscript{2}, GHSV ≈ 14 000 mL\textsubscript{total flow} mL\textsubscript{cat}\textsuperscript{-1} h\textsuperscript{-1}. (a) Activity in terms % sum of MeOH and DME conversion over MeOH conversion capacity. The MAPO-18s were tested at identical conditions except with a higher WHSV (MeOH) = 2.5 g\textsubscript{MeOH} g\textsubscript{cat}\textsuperscript{-1} h\textsuperscript{-1}. (b) Selectivity vs. conversion of SAPO-34. Conversion variation was due to catalyst deactivation during runtime.
**Supporting Table 3.** Catalytic performance of MAPO-18s in various reaction feeds. Reaction conditions: 350 °C, 20 bar, 1 bar MeOH (WHSV = 2.5 g\textsubscript{MeOH} g\textsuperscript{-1} cat h\textsuperscript{-1}), 0.6 bar Ar internal standard, 18.4 bar N\textsubscript{2} or H\textsubscript{2} or H\textsubscript{2}/X = 3 (in which X = N\textsubscript{2}, CO\textsubscript{2} or CO), GHSV ≈ 16 000 mL\textsubscript{total} flow mL\textsubscript{cat} h\textsuperscript{-1}.

| Catalyst | Reaction Conditions | Olefin-to-paraffin ratio | Ethylene/Propylene ratio | DME/MeOH ratio |
|----------|---------------------|--------------------------|--------------------------|----------------|
|          |                     | C2 =/- | C3 =/- | C4 =/- |                  |                   |
| N\textsubscript{2} |                      | 39.2 | 53.6 | 27.2 | 0.38 | 5.4 |
| H\textsubscript{2} |                      | 0.0 | 0.2 | 0.6 | 0.00 | 4.5 |
| H\textsubscript{2}/N\textsubscript{2} = 3 |                   | 0.3 | 1.0 | 0.9 | 0.09 | 5.0 |
| H\textsubscript{2}/CO\textsubscript{2} = 3 |                   | 0.4 | 1.8 | 1.9 | 0.12 | 5.0 |
| H\textsubscript{2}/CO = 3 |                   | 5.2 | 13.6 | 8.1 | 0.27 | 4.8 |
| MgAPO-18 | H\textsubscript{2}/N\textsubscript{2} = 3 | 0.5 | 1.0 | 1.8 | 0.04 | 21.6 |
|          | H\textsubscript{2}/CO\textsubscript{2} = 3 | 0.1 | 1.0 | 2.2 | 0.03 | 21.3 |
|          | H\textsubscript{2}/CO = 3 | 16.4 | 19.4 | 38.0 | 0.20 | 19.0 |
| CoAPO-18 | H\textsubscript{2}/N\textsubscript{2} = 3 | 0.3 | 1.7 | 2.7 | 0.09 | 21.6 |
|          | H\textsubscript{2}/CO\textsubscript{2} = 3 | 0.1 | 1.2 | 2.3 | 0.05 | 18.5 |
|          | H\textsubscript{2}/CO = 3 | 22.8 | 19.9 | 30.6 | 0.28 | 23.9 |
| ZnAPO-18 | H\textsubscript{2}/N\textsubscript{2} = 3 | 0.5 | 0.9 | 1.0 | 0.20 | 0.7 |
|          | H\textsubscript{2}/CO\textsubscript{2} = 3 | 0.4 | 1.5 | 2.0 | 0.15 | 0.8 |
|          | H\textsubscript{2}/CO = 3 | 60.8 | 105.8 | 93.6 | 0.30 | 0.8 |
Supporting Figure 18. Catalytic performance of SAPO-18 in MeOH carbonylation reaction. Reaction conditions: 350 °C, 20 bar, 1 bar MeOH (WHSV = 2.5 g_{MeOH} g_{cat}^{-1} h^{-1}), 0.6 bar Ar internal standard, 18.4 bar N₂ or CO, GHSV ≈ 16 000 mL_total flow mL_{cat}^{-1} h^{-1}.
Supporting Figure 19. Catalytic performance of MgAPO-18 in MeOH carbonylation reaction. Reaction conditions: 350 °C, 20 bar, 1 bar MeOH (WHSV = 2.5 g\textsubscript{MeOH} g\textsubscript{cat}\textsuperscript{-1} h\textsuperscript{-1}), 0.6 bar Ar internal standard, 18.4 bar N\textsubscript{2} or CO, GHSV ≈ 16 000 mL\textsubscript{total flow} mL\textsubscript{cat}\textsuperscript{-1} h\textsuperscript{-1}.
Supporting Figure 20. Catalytic performance of CoAPO-18 in MeOH carbonylation reaction. Reaction conditions: 350 °C, 20 bar, 1 bar MeOH (WHSV = 2.5 gMeOH g\text{cat}$^{-1}$ h$^{-1}$), 0.6 bar Ar internal standard, 18.4 bar N$_2$ or H$_2$ or CO, GHSV $\approx$ 16 000 mL$_{\text{total flow}}$ mL$_{\text{cat}}^{-1}$ h$^{-1}$.
Supporting Figure 21. Effect of CO on the catalytic performance of SAPO-18s. Reaction conditions: 350 °C, 20 bar, 0.5 bar MeOH (WHSV = 2.5 gMeOH gcat⁻¹ h⁻¹), 0.7 bar Ar internal standard, 18.8 bar H₂/COx = 3, GHSV ≈ 16 000 mLtotal flow mLcat⁻¹ h⁻¹. (a and b) Activity in terms % sum of MeOH and DME conversion over time-on-stream, and (c and d) Product selectivity at TOS = 10 h.
Supporting Figure 2. Effect of MAPO-18 M/T ratio on the catalytic performance of MAPO-18s. Reaction conditions: 350 °C, 20 bar, 1 bar MeOH (WHSV = 2.5 gMeOH g\text{cat}^{-1} h^{-1}), 0.6 bar Ar internal standard, 18.4 bar H\text{2}/CO = 3, GHSV ≈ 16 000 mL\text{total flow} mL\text{cat}^{-1} h^{-1}. a – b | Activity in terms % sum of MeOH and DME conversion over time-on-stream for (a) SAPO-18, (b) MgAPO-18. c – d | Product selectivity at TOS = 10 h for (c) SAPO-18, (d) MgAPO-18.
S4: Supporting DFT calculations

Optimized SAPO-18 lattice with ethene molecule

Final Coordinates Ethene in SAPO-18 (Angstroms)

Lattice:

translation vector [a0] 1 25.910790790 0.000000000 0.000000000
translation vector [a0] 2 0.000000000 24.059048160 0.000000000
translation vector [a0] 3 -0.006124912 0.000000000 35.093158470

Final Coordinates (Angstroms)

| ATOM | X     | Y     | Z     |
|------|-------|-------|-------|
| 1    | 1.463004 | 0.626289 | 3.034494 |
| 2    | 1.500503 | 10.018531 | 17.569548 |
| 3    | 10.540843 | 11.659187 | 0.886299 |
| 4    | 3.102360 | 11.569994 | 1.046574 |
| 5    | 12.177948 | 10.007021 | 17.422238 |
| 6    | 12.147021 | 0.486896 | 3.001458 |
| 7    | 11.151262 | 12.205783 | 2.427644 |
| 8    | 11.901423 | 11.070626 | -0.065851 |
| 9    | -0.136920 | 9.415814 | 17.641097 |
| 10   | 1.906715 | 10.725085 | 0.555199 |
| 11   | 2.675555 | 12.371926 | 2.277719 |
| 12   | 13.566884 | 0.128937 | 2.510969 |
| 13   | 11.804948 | 1.916828 | 2.550784 |
| 14   | 9.330346 | 10.440339 | 1.122897 |
| 15   | 1.545871 | 0.443031 | 4.758351 |
| 16   | 2.609140 | 8.741993 | 17.170499 |
| 17   | 12.102169 | 10.675570 | 16.037289 |
| 18   | 9.877172 | 0.280245 | 18.543214 |
| 19   | 8.317358 | 6.832600 | 3.020084 |
| 20   | 8.450832 | 3.677573 | 17.334300 |
|   |   |   |   |   |
|---|---|---|---|---|
| 21 | Al | 3.714182 | 5.305472 | 0.818205 |
| 22 | P  | 9.958861 | 5.266278 | 0.918873 |
| 23 | Si | 5.338827 | 3.552416 | 17.440827 |
| 24 | P  | 5.271536 | 6.765604 | 2.986099 |
| 25 | O  | 4.276218 | 5.752733 | 2.420046 |
| 26 | O  | 5.037739 | 4.795277 | -0.177794 |
| 27 | O  | 6.851318 | 3.075510 | 17.370974 |
| 28 | O  | 8.736239 | 4.754184 | 0.134144 |
| 29 | O  | 9.485884 | 5.764329 | 2.291135 |
| 30 | O  | 6.692642 | 6.419704 | 2.489684 |
| 31 | O  | 4.917114 | 8.192728 | 2.534038 |
| 32 | O  | 2.450913 | 4.115642 | 1.003109 |
| 33 | O  | 8.376161 | 6.719435 | 4.751499 |
| 34 | O  | 9.642622 | 2.418891 | 17.278550 |
| 35 | O  | 5.043066 | 4.312238 | 15.878208 |
| 36 | O  | 3.063157 | 6.754313 | 18.602005 |
| 37 | Al | 12.181819 | 0.603652 | 6.236590 |
| 38 | Al | 12.148924 | 10.012373 | 10.270571 |
| 39 | Al | 3.104334 | 11.663916 | 8.379202 |
| 40 | P  | 10.513226 | 11.600235 | 8.244081 |
| 41 | P  | 1.471561 | 10.008179 | 10.422513 |
| 42 | P  | 1.482418 | 0.483894 | 6.277779 |
| 43 | O  | 2.495008 | 12.212392 | 6.839846 |
| 44 | O  | 1.751960 | 11.044019 | 9.314504 |
| 45 | O  | 13.790993 | 9.407590 | 10.197686 |
| 46 | O  | 11.727093 | 10.799821 | 8.760355 |
| 47 | O  | 10.938907 | 12.401192 | 7.014403 |
| 48 | O  | 0.069978 | 0.103947 | 6.779890 |
| 49 | O  | 1.813512 | 1.910850 | 6.750608 |
| 50 | O  | 4.340273 | 10.476662 | 8.149109 |
|   |   |   |   |   |
|---|---|---|---|---|
| 51 | O | 12.059028 | 0.430265 | 4.523007 |
| 52 | O | 11.076683 | 8.684854 | 10.588761 |
| 53 | O | 1.531792  | 10.707732 | 11.790656 |
| 54 | O | 3.756528  | 0.278789  | 9.305959  |
| 55 | Al| 5.283448  | 6.887519  | 6.224279  |
| 56 | Al| 5.239198  | 3.690797  | 10.414966 |
| 57 | Al| 9.903816  | 5.264129  | 8.393070  |
| 58 | P | 3.691833  | 5.252205  | 8.335985  |
| 59 | P | 8.348524  | 3.615790  | 10.528185 |
| 60 | P | 8.323544  | 6.761196  | 6.272489  |
| 61 | O | 9.272925  | 5.689990  | 6.824794  |
| 62 | O | 8.595655  | 4.631992  | 9.393691  |
| 63 | O | 6.892861  | 3.133955  | 10.462124 |
| 64 | O | 4.948160  | 4.580169  | 8.936230  |
| 65 | O | 4.082685  | 5.893787  | 7.004753  |
| 66 | O | 6.897276  | 6.464138  | 6.787097  |
| 67 | O | 8.747370  | 8.157958  | 6.758142  |
| 68 | O | 11.186938 | 4.114777  | 8.234356  |
| 69 | O | 5.206199  | 6.704990  | 4.510708  |
| 70 | O | 4.132719  | 2.364010  | 10.602117 |
| 71 | O | 8.605901  | 4.308117  | 11.885959 |
| 72 | O | 10.500784 | 6.707272  | 9.191643  |
| 73 | Al| 12.143870 | 12.334579 | 15.458433 |
| 74 | Al| 12.126942 | 2.865054  | 1.106701  |
| 75 | Al| 3.038973  | 1.249774  | 17.709266 |
| 76 | P | 10.590762 | 1.274430  | 17.601906 |
| 77 | P | 1.488592  | 2.951478  | 1.198487  |
| 78 | P | 1.487113  | 12.523480 | 15.540299 |
| 79 | O | 2.424670  | 0.857715  | 16.112001 |
| 80 | O | 1.709687  | 1.855841  | 18.704576 |

26
|   |   |   |   |
|---|---|---|---|
| 81 | O | 13.761212 | 3.473048 | 1.071748 |
| 82 | O | 11.869766 | 1.802800 | 18.288986 |
| 83 | O | 10.975253 | 0.582598 | 16.290707 |
| 84 | O | 0.034751 | 13.022259 | 15.650367 |
| 85 | O | 1.638285 | 11.203903 | 16.301186 |
| 86 | O | 4.315260 | 2.355832 | 17.532397 |
| 87 | O | 11.764844 | 12.263657 | 13.763538 |
| 88 | O | 10.979427 | 4.156284 | 1.127072 |
| 89 | O | 1.697509 | 2.319555 | 2.592810 |
| 90 | O | 3.574403 | 12.491972 | -0.089018 |
| 91 | Al | 5.352847 | 6.076051 | 15.540971 |
| 92 | Al | 5.257399 | 9.274451 | 1.196479 |
| 93 | Al | 9.928782 | 7.676993 | 17.702333 |
| 94 | P | 3.680172 | 7.745464 | 17.604960 |
| 95 | P | 8.362932 | 9.263233 | 1.215380 |
| 96 | P | 8.388595 | 6.099819 | 15.528626 |
| 97 | O | 9.393483 | 7.071697 | 16.153259 |
| 98 | O | 8.548755 | 8.315479 | 18.580860 |
| 99 | O | 6.926460 | 9.791063 | 1.194487 |
| 100 | O | 4.884055 | 8.468552 | 18.244926 |
| 101 | O | 4.158260 | 7.031126 | 16.327767 |
| 102 | O | 6.976484 | 6.437454 | 16.075499 |
| 103 | O | 8.728497 | 4.643060 | 15.867546 |
| 104 | O | 11.158299 | 8.879921 | 17.514008 |
| 105 | O | 5.266752 | 6.099671 | 13.806218 |
| 106 | O | 4.267721 | 10.674009 | 1.455926 |
| 107 | O | 8.636940 | 8.494490 | 2.521820 |
| 108 | O | 10.626955 | 6.404240 | 0.124795 |
| 109 | Al | 1.490278 | 12.359546 | 12.389132 |
| 110 | Al | 1.514954 | 2.880846 | 8.180425 |
|   |   |   |   |
|---|---|---|---|
| 111 | Al | 10.548394 | 1.249883 | 10.168557 |
| 112 | P  | 3.101561  | 1.287713 | 10.267366 |
| 113 | P  | 12.144568 | 2.937667 | 8.087893  |
| 114 | P  | 12.140175 | 12.505661| 12.305156 |
| 115 | O  | 11.190259 | 0.833309 | 11.733514 |
| 116 | O  | 11.852975 | 1.876195 | 9.170018  |
| 117 | O  | -0.132428 | 3.446782 | 8.268082  |
| 118 | O  | 1.848925  | 1.897567 | 9.605298  |
| 119 | O  | 2.685701  | 0.612255 | 11.579468 |
| 120 | O  | 13.588542 | 13.018966| 12.168178 |
| 121 | O  | 11.990009 | 11.180311| 11.550876 |
| 122 | O  | 9.267637  | 2.408512 | 10.378033 |
| 123 | O  | 1.882843  | 12.284249| 14.079825 |
| 124 | O  | 2.602525  | 4.220903 | 8.081086  |
| 125 | O  | 11.975287 | 2.297822 | 6.698467  |
| 126 | O  | 9.985003  | 12.531402| 9.354860  |
| 127 | Al | 8.344324  | 6.010093 | 12.300013 |
| 128 | Al | 8.392782  | 9.262550 | 8.076393  |
| 129 | Al | 3.745514  | 7.694573 | 10.183145 |
| 130 | P  | 9.956333  | 7.720237 | 10.214379 |
| 131 | P  | 5.284311  | 9.284938 | 8.031741  |
| 132 | P  | 5.300729  | 6.123984 | 12.277323 |
| 133 | O  | 4.341185  | 7.199848 | 11.758583 |
| 134 | O  | 5.074627  | 8.311913 | 9.213373  |
| 135 | O  | 6.729143  | 9.786361 | 8.067756  |
| 136 | O  | 8.753659  | 8.476054 | 9.609844  |
| 137 | O  | 9.509307  | 7.008535 | 11.493153 |
| 138 | O  | 6.719685  | 6.428117 | 11.755973 |
| 139 | O  | 4.875071  | 4.727487 | 11.790594 |
| 140 | O  | 2.512117  | 8.892529 | 10.385756 |
Optimized MgAPO-18 lattice with ethene molecule

Final Coordinates Ethene in MgALPO-18 (Angstroms)

Lattice:

| Translation Vector [a0] | 1 | 25.910790790 | 0.000000000 | 0.000000000 |
|--------------------------|---|---------------|--------------|--------------|
| Translation Vector [a0]  | 2 | 0.000000000 | 24.059048160 | 0.000000000 |
| Translation Vector [a0]  | 3 | -0.006124912 | 0.000000000 | 35.093158470 |

ATOM                    X    Y    Z
---------------------------------------
1  Al                     1.409561 0.370744 3.081720
2  Al                     1.571263 9.835621 17.432512
3  Al                      10.602115 11.580913 0.820240
4  P                       3.047490 11.398618 1.040635
5  P                      12.110325 9.894053 17.378241
6  P                      12.106387 0.402157 3.063203
7  O                      11.042890 12.290986 2.351125
8  O                       11.934036 10.637556 0.145806
9  O                      -0.124302 9.537146 17.210321
10 O                       1.886659 10.593203 0.416259
|    | Atom | X      | Y      | Z      |
|----|------|--------|--------|--------|
|   11| O    | 2.558011|12.035690|2.343189|
|   12| O    | 13.495671|-0.021705|2.537733|
|   13| O    | 11.899205| 1.906349|2.820520|
|   14| O    | 9.234692 |10.527791|1.028244|
|   15| O    | 1.469556 | 0.197414|4.803339|
|   16| O    | 2.396998 | 8.318256|17.291345|
|   17| O    | 11.624599|10.774876|16.212428|
|   18| O    | 10.166694| 0.086887|18.234751|
|   19| Al   | 8.540739 | 6.975419|3.061319|
|   20| Mg   | 8.349916 | 3.387782|17.818615|
|   21| Al   | 3.853354 | 5.072668|0.977526|
|   22| P    | 10.032259| 5.242949|1.041808|
|   23| P    | 5.254364 | 3.353624|17.370342|
|   24| P    | 5.482809 | 6.664297|3.026322|
|   25| O    | 4.588807 | 5.540399|2.490639|
|   26| O    | 5.080699 | 4.456058|-0.115016|
|   27| O    | 6.615238 | 2.720652|17.479971|
|   28| O    | 8.698592 | 4.655640|0.629089|
|   29| O    | 9.848874 | 6.146995|2.280580|
|   30| O    | 6.946124 | 6.325001|2.700477|
|   31| O    | 5.098892 | 8.009327|2.391664|
|   32| O    | 2.589219 | 3.928143|1.288496|
|   33| O    | 8.800789 | 6.840310|4.769394|
|   34| O    | 9.936517 | 2.444383|17.388960|
|   35| O    | 5.076586 | 4.046464|15.985340|
|   36| O    | 3.189057 | 6.500159|18.773535|
|   37| Al   | 12.131862| 0.520011|6.253348|
|   38| Al   | 12.142466| 9.994230|10.384447|
|   39| Al   | 3.042316 |11.442887|8.398375|
|   40| P    | 10.546685|11.593964|8.372726|
| 101 | O  | 4.050334 | 6.714043 | 16.403332 |
| 102 | O  | 6.858789 | 6.289015 | 16.017048 |
| 103 | O  | 8.660513 | 4.556211 | 16.088473 |
| 104 | O  | 11.291136 | 8.605688 | 17.344586 |
| 105 | O  | 5.029913 | 6.017321 | 13.872352 |
| 106 | O  | 4.223262 | 10.488730 | 1.381209 |
| 107 | O  | 8.520793 | 8.664738 | 2.547169 |
| 108 | O  | 10.633122 | 6.095227 | -0.112346 |
| 109 | Al | 1.640403 | 12.208851 | 12.445320 |
| 110 | Al | 1.639796 | 2.730194 | 8.104816 |
| 111 | Al | 10.714892 | 1.316721 | 10.196294 |
| 112 | P  | 3.139677 | 1.148385 | 10.206835 |
| 113 | P  | 12.236001 | 2.934880 | 7.976558 |
| 114 | P  | 12.233210 | 12.504464 | 12.390785 |
| 115 | O  | 11.469048 | 0.909629 | 11.706004 |
| 116 | O  | 11.956147 | 1.962454 | 9.141394 |
| 117 | O  | 0.005285 | 3.328707 | 8.021153 |
| 118 | O  | 1.901560 | 1.857692 | 9.616314 |
| 119 | O  | 2.733681 | 0.449077 | 11.502395 |
| 120 | O  | 13.729153 | 12.868904 | 12.405688 |
| 121 | O  | 12.028631 | 11.173557 | 11.658649 |
| 122 | O  | 9.427983 | 2.447098 | 10.481220 |
| 123 | O  | 2.267381 | 12.208006 | 14.067873 |
| 124 | O  | 2.778197 | 4.032729 | 8.016391 |
| 125 | O  | 11.898882 | 2.232710 | 6.645563 |
| 126 | O  | 10.094574 | 12.596474 | 9.449852 |
| 127 | Al | 8.218045 | 6.036781 | 12.299754 |
| 128 | Al | 8.361206 | 9.268644 | 8.175778 |
| 129 | Al | 3.660603 | 7.465191 | 10.172560 |
| 130 | P  | 9.945256 | 7.657370 | 10.359877 |
|   |   |   |   |
|---|---|---|---|
| 131 | P | 5.309220 | 9.133630 | 8.230492 |
| 132 | P | 5.211310 | 5.880996 | 12.365559 |
| 133 | O | 4.095012 | 6.649957 | 11.653873 |
| 134 | O | 5.075943 | 8.226182 | 9.457758 |
| 135 | O | 6.700283 | 9.763242 | 8.357361 |
| 136 | O | 8.787966 | 8.188506 | 9.494100 |
| 137 | O | 9.364303 | 7.189460 | 11.702470 |
| 138 | O | 6.570953 | 6.485920 | 11.933757 |
| 139 | O | 5.185890 | 4.386573 | 11.996019 |
| 140 | O | 2.424966 | 8.641102 | 10.491012 |
| 141 | O | 8.432269 | 5.918948 | 14.038241 |
| 142 | O | 9.372248 | 10.663101 | 8.096309 |
| 143 | O | 5.193434 | 8.319074 | 6.934174 |
| 144 | O | 3.075587 | 6.306673 | 8.988605 |
| 145 | H | 22.863202 | 16.729328 | 15.421027 |
| 146 | C | 10.306364 | 15.646491 | 13.921076 |
| 147 | C | 9.148590 | 15.020300 | 14.096264 |
| 148 | H | 11.181195 | 15.386351 | 14.505559 |
| 149 | H | 10.426272 | 16.412754 | 13.162954 |
| 150 | H | 9.039036 | 14.230759 | 14.832082 |
| 151 | H | 8.268846 | 15.264179 | 13.507129 |
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