Supplementary material for Bordat *et al.*

'Structure and dynamics of $AlPO_4$-5 and other aluminophosphates'

BKS_model_P1min.out: unit cell and fractional coordinates of the analytically minimised structure of $AlPO_4$-5 in the BKS model.

zeroed_structure.xyz: XYZ file for the atomic cartesian coordinates in the minimum (BKS model) obtained by coupling an MD simulation to a heat bath at 0K.

averaged_structure_300K.xyz: XYZ file with the thermally averaged atomic coordinates, averaged over a particular period (about 10ps) during which the simulation with the BKS model remained in one of the three settings obtained by energy minimisation (the same setting as in zeroed_structure.xyz)

smallcluster.xyz and *bigcluster.xyz:* sample AlO_4 tetrahedron and $Al_4P_4O_{16}$ cluster, i.e. Al with zero and four phosphorous atoms in the second coordination shell, cut out of the $AlPO_4$-5 crystal optimised with the BKS force-field and saturated with hydrogens (which were optimised in *ab initio* calculations before GIAO calculation of the ^{27}Al chemical shifts).