Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supplementary information

The curious effects of integrating bimetallic active centres within nanoporous architectures for acid-catalysed transformations

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Structural characterisation data

Table S1: Full ICP data

System	Al/wt%	P/wt%	Zn/wt%	Mg/wt%	Si/wt%
AlPO-5	18.1	16.7	-	-	-
MgAlPO-5	15.9	20.6	-	0.85	-
ZnAlPO-5	16.4	21.2	2.11	-	-
SiAlPO-5	19.8	14.7	-	-	1.69
MgZnAlPO-5	17.0	22.9	1.86	0.72	-
MgSiAlPO-5	18.0	14.6	-	0.89	1.70
ZnSiAlPO-5	18.7	15.9	1.33	-	1.66

Table S2: XRD parameters, particle size and surface area summary

System	Optimized XRD parameters for P6cc		Particle size/nm	BET SSA/m^2 g^{-1}
	a/Å	c/Å		
AlPO-5	13.69	8.43	56.5	295.1
ZnAlPO-5	13.68	8.34	55.5	165.4
MgAlPO-5	13.71	8.40	55.5	193.3
SiAlPO-5	13.70	8.39	54.8	181.9
MgZnAlPO-5	13.80	8.41	66.3	283.3
MgSiAlPO-5	13.71	8.39	52.6	168.1
ZnSiAlPO-5	13.76	8.40	64.2	236.2

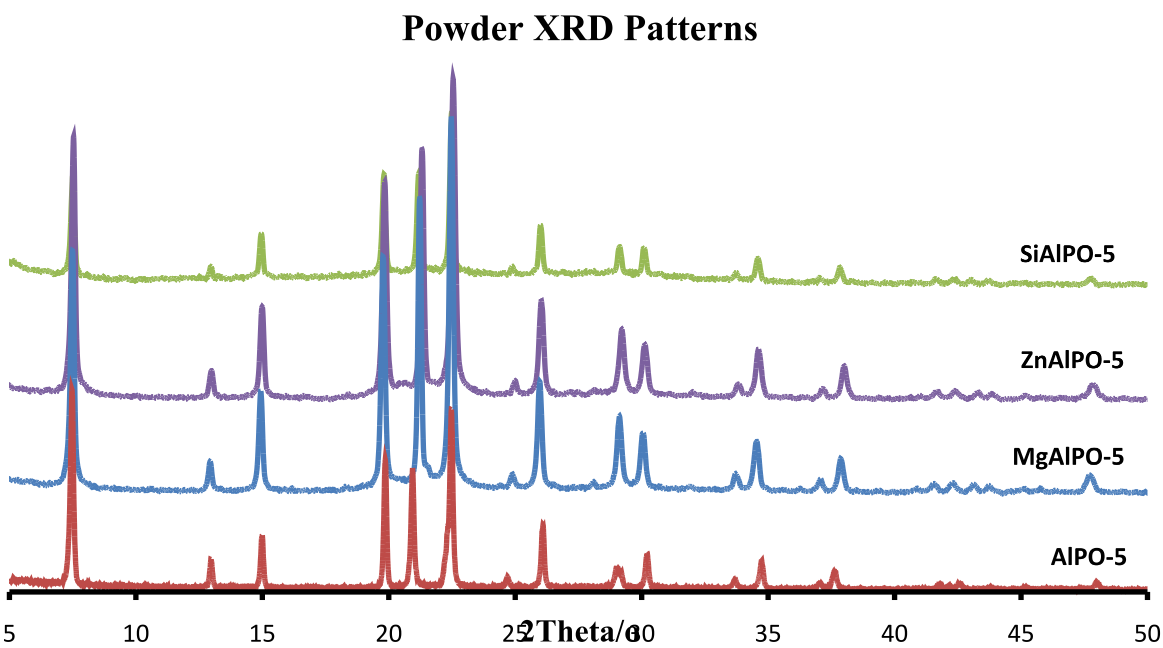

Figure S1: Powder X-ray diffraction pattern of monometallic AlPO-5 systems

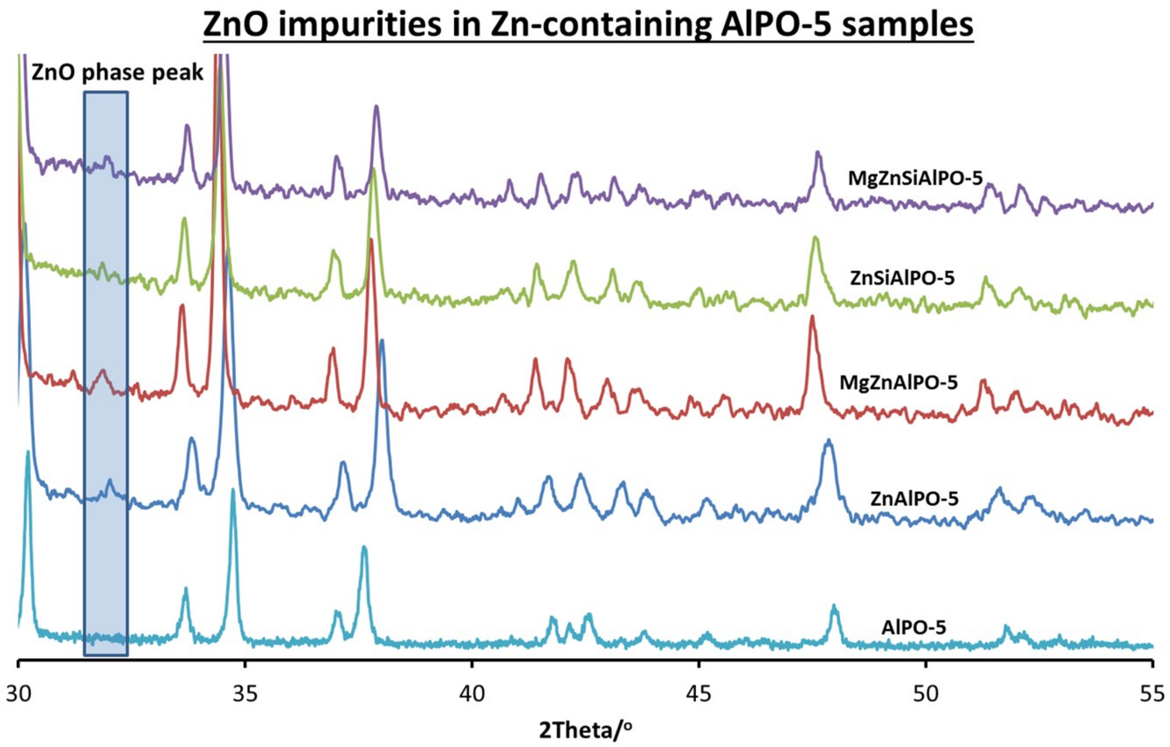

Figure S2: Zoomed XRD pattern of Zn-containing species revealing trace quantities of ZnO hexagonal phase.

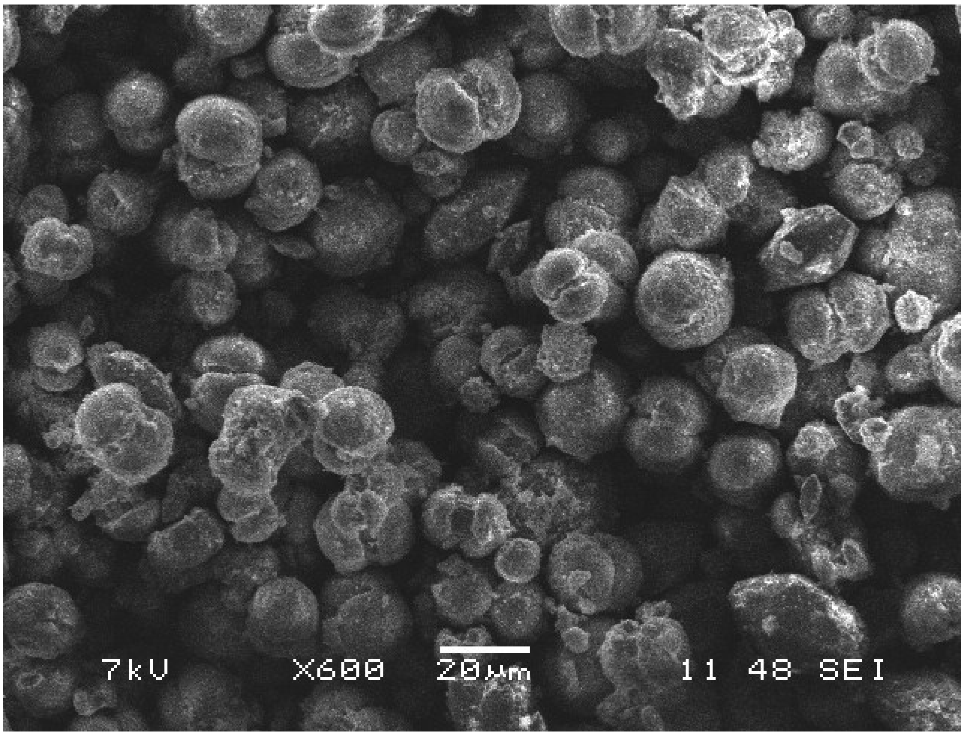

Figure S3: SEM image of monometallic MgAlPO-5

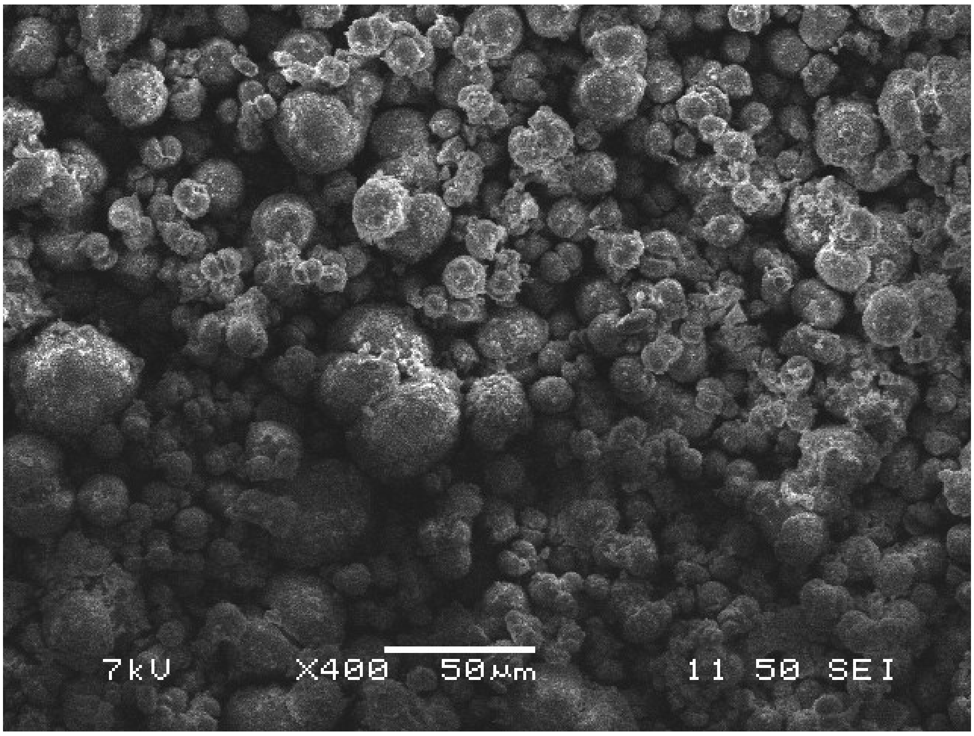

Figure S4: SEM image of monometallic ZnAlPO-5

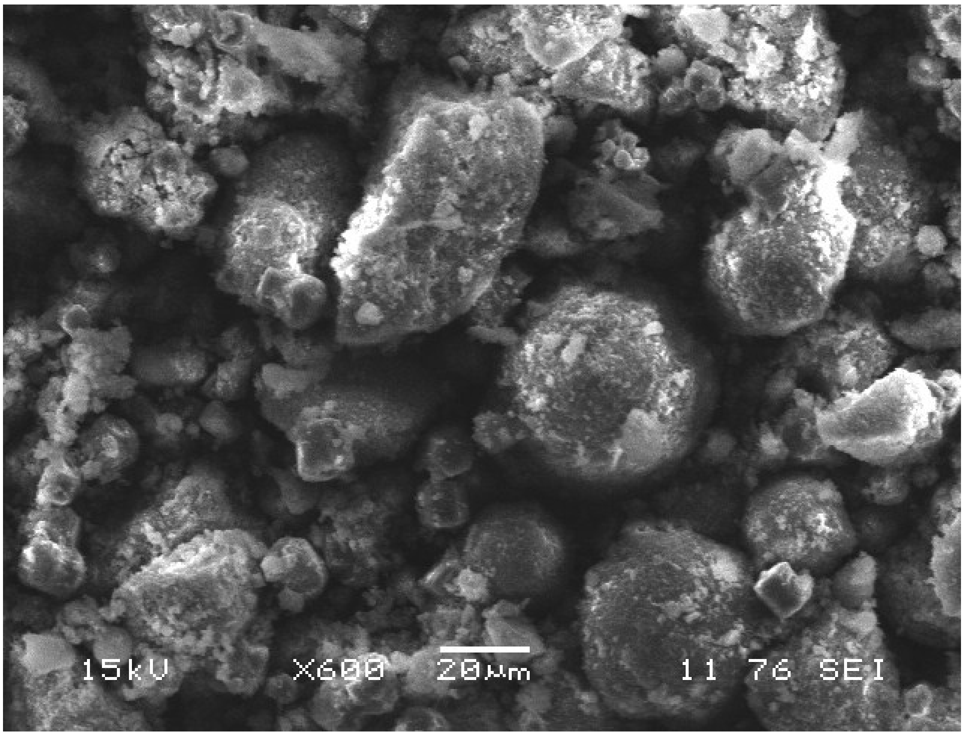

Figure S5: SEM image of monometallic SiAlPO-5

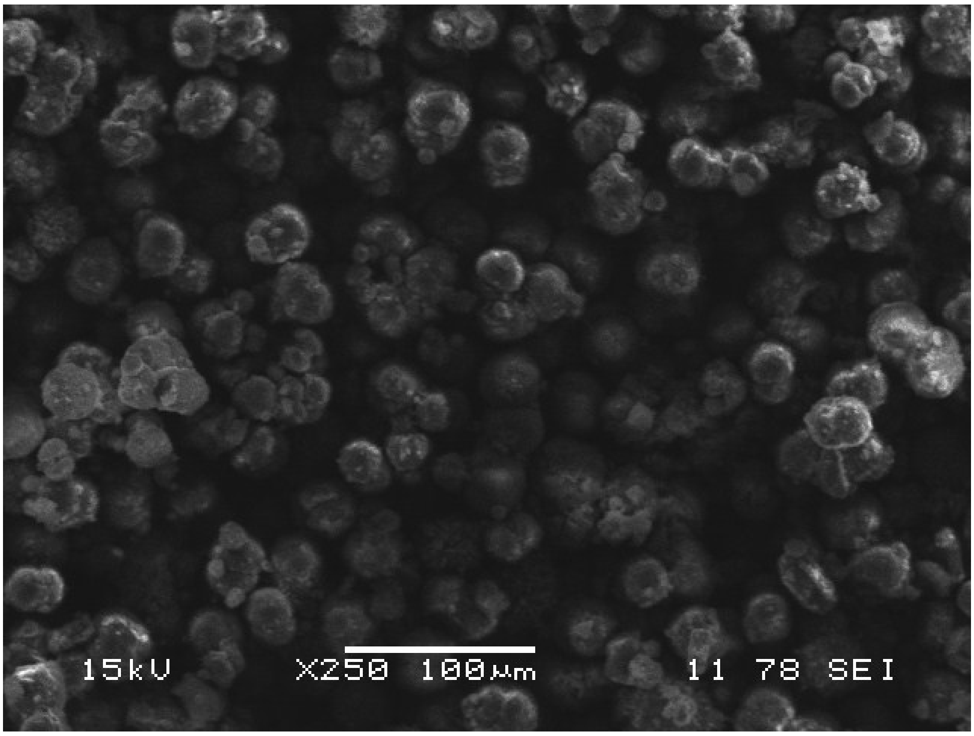

Figure S6: SEM image of bimetallic MgZnAlPO-5

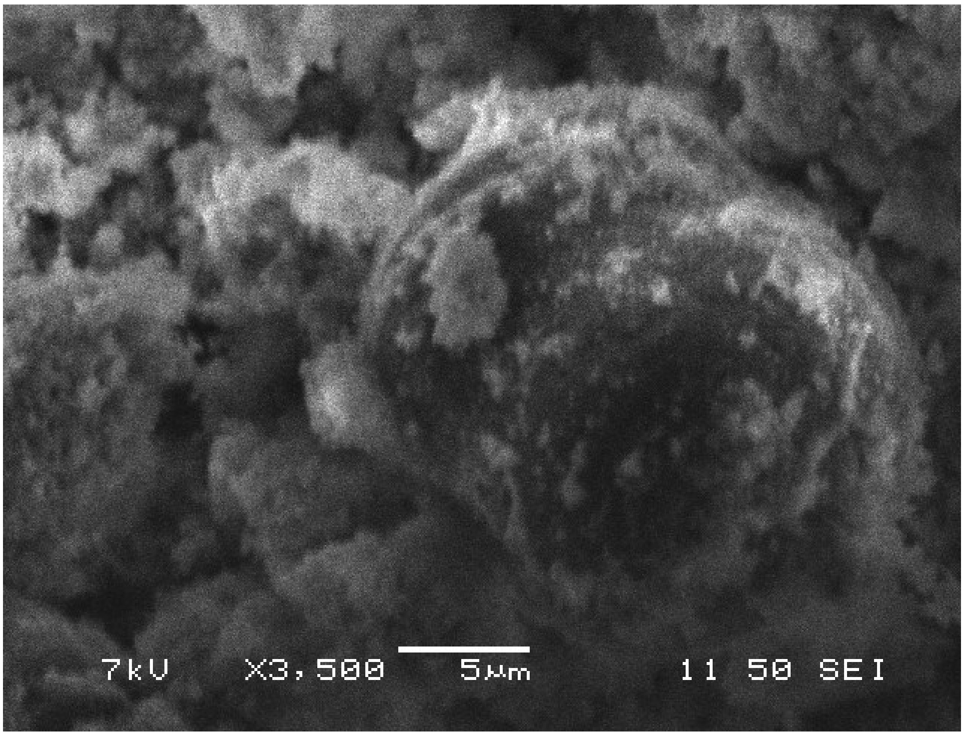

Figure S7: SEM image of bimetallic MgSiAlPO-5

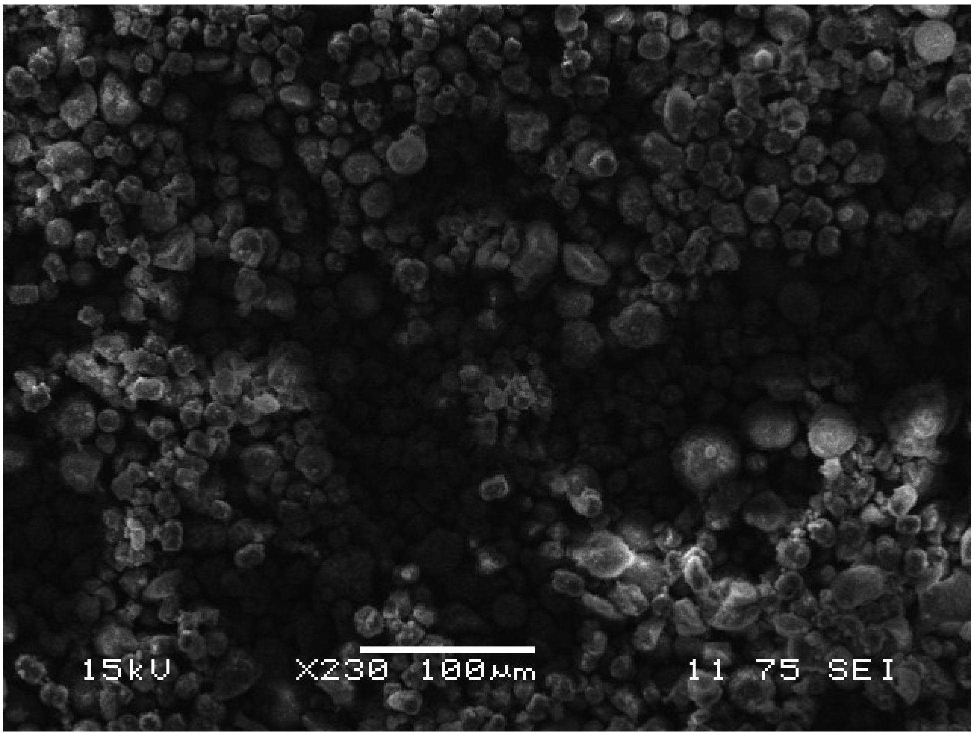

Figure S8: SEM image of bimetallic ZnSiAlPO-5

Full catalysis data

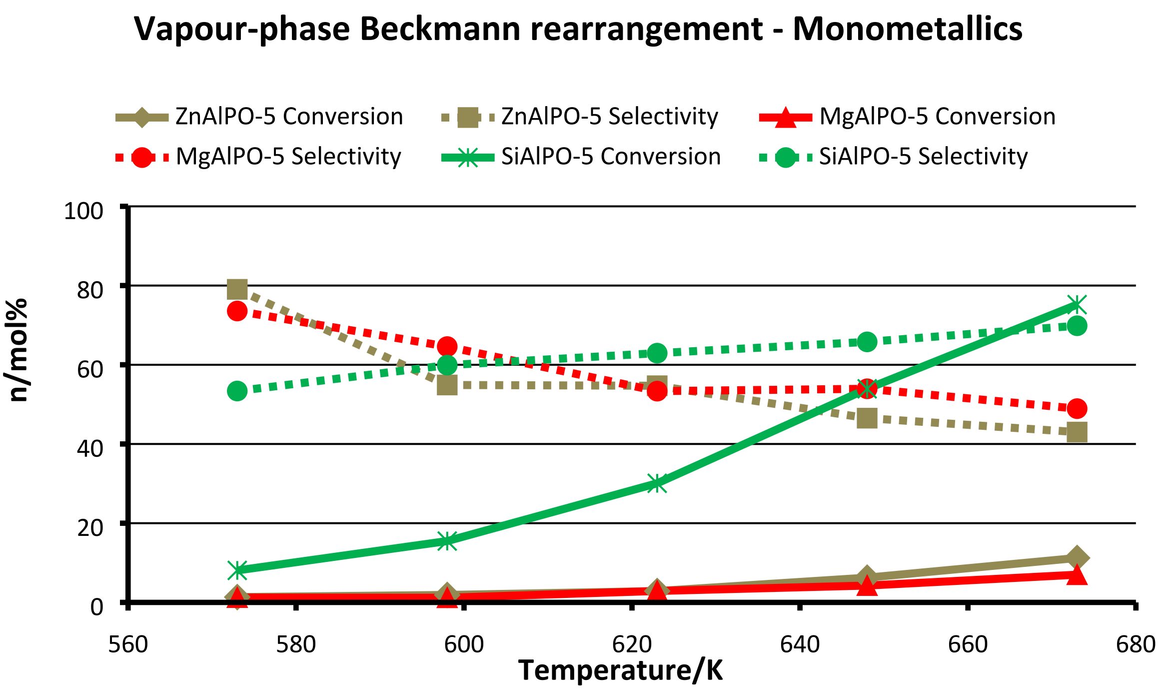

Figure S9: Full catalytic data for the vapour-phase Beckmann rearrangement of cyclohexanone oxime using monometallic AlPO-5 systems. Reaction conditions: WHSV 3.3 hr^{-1}, Helium carrier gas flow 20 ml/min, 0.3 g of catalyst, liquid feed 300g/l of cyclohexanone oxime in methanol, temperature as shown.

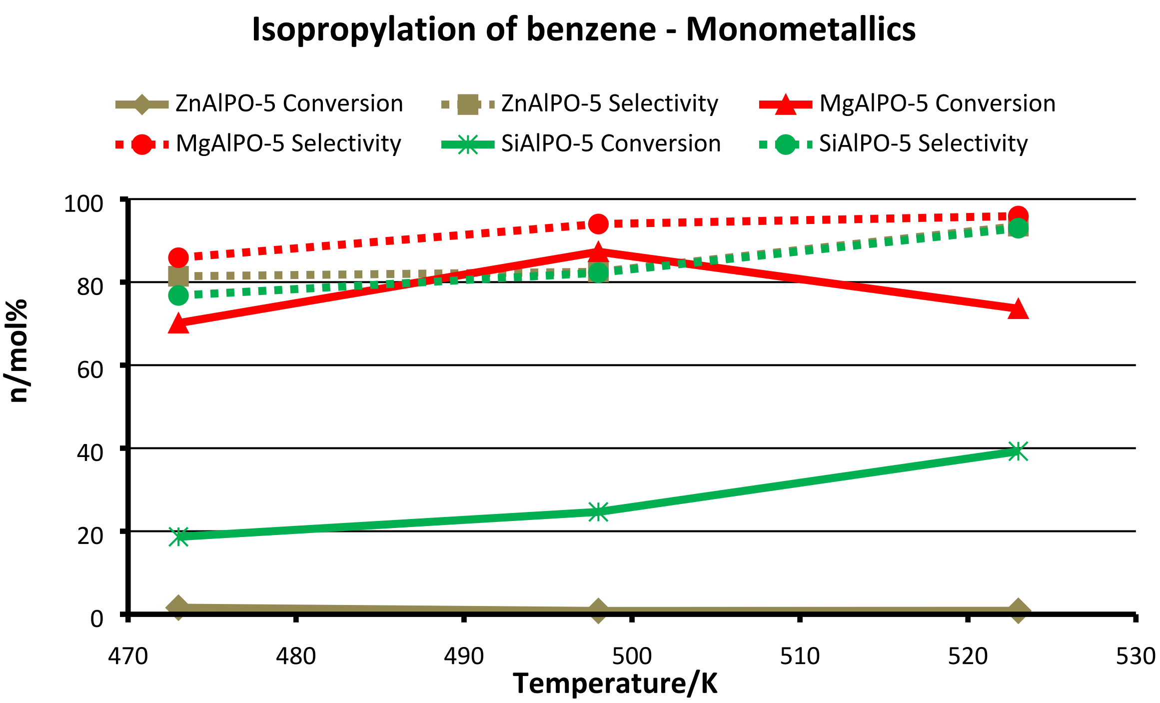

Figure S10: Full catalytic data for the isopropylation of benzene using monometallic AlPO-5 systems. Reaction conditions: WHSV of 3.5 hr^{-1}, Helium carrier gas of 10 ml/min, feed 6:1 mole ratio of benzene:isopropanol, temperature as shown.

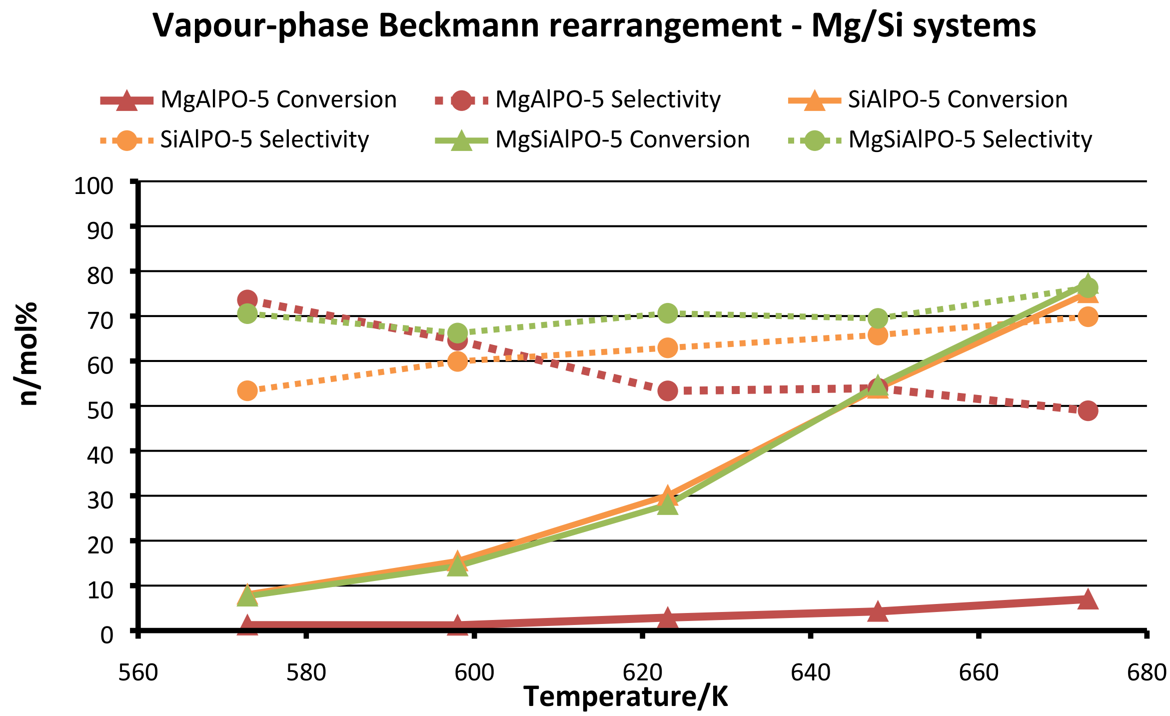

Figure S11: Full catalytic data for the vapour-phase Beckmann rearrangement of cyclohexanone oxime using Mg and Si-containing AlPO-5 systems. Reaction conditions: WHSV 3.3 hr^{-1}, Helium carrier gas flow 20 ml/min, 0.3 g of catalyst, liquid feed 300g/l of cyclohexanone oxime in methanol, temperature as shown

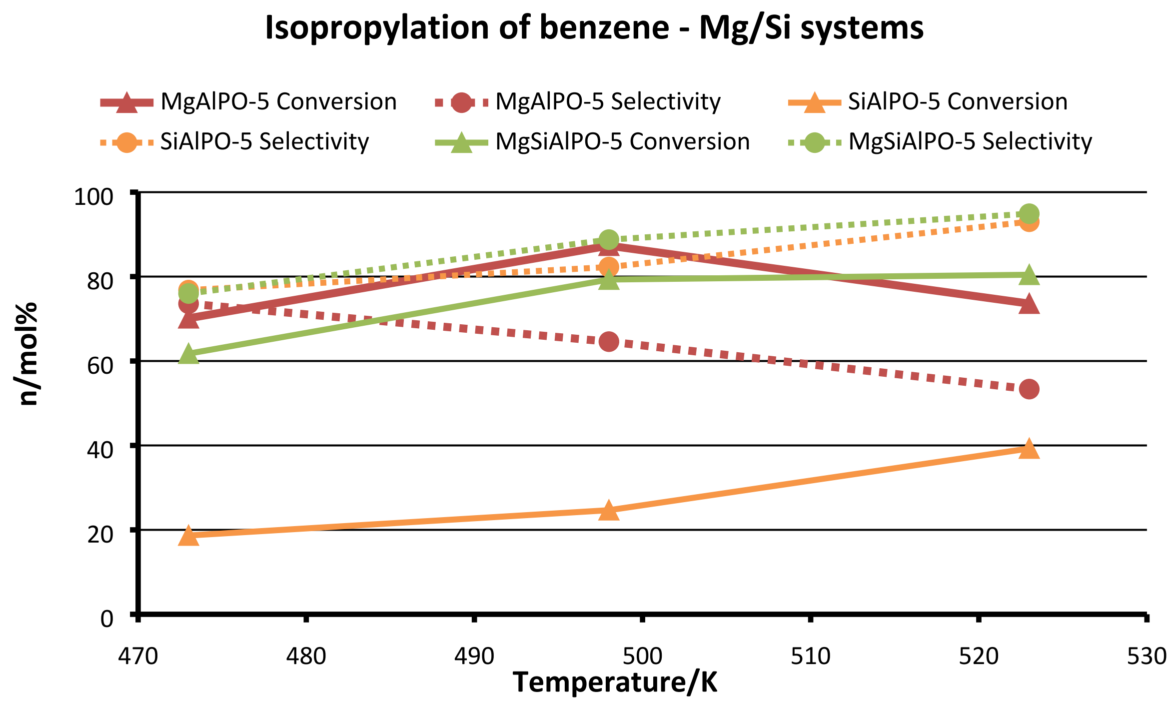

Figure S12: Full catalytic data for the isopropylation of benzene using Mg and Si-containing AlPO-5 systems. Reaction conditions: WHSV of 3.5 hr^{-1}, Helium carrier gas of 10 ml/min, feed 6:1 mole ratio of benzene:isopropanol, temperature as shown.

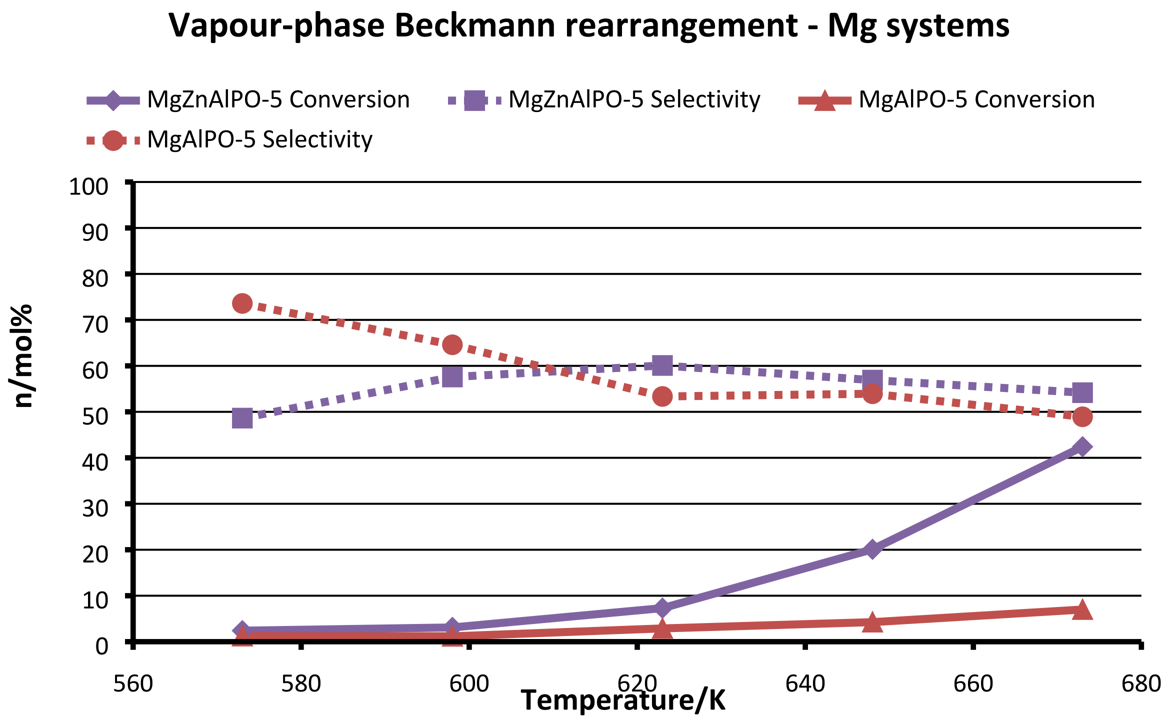

Figure S13: Full catalytic data for the vapour-phase Beckmann rearrangement of cyclohexanone oxime using Mg-containing AlPO-5 systems. Reaction conditions: WHSV 3.3 hr^{-1}, Helium carrier gas flow 20 ml/min, 0.3 g of catalyst, liquid feed 300g/l of cyclohexanone oxime in methanol, temperature as shown.

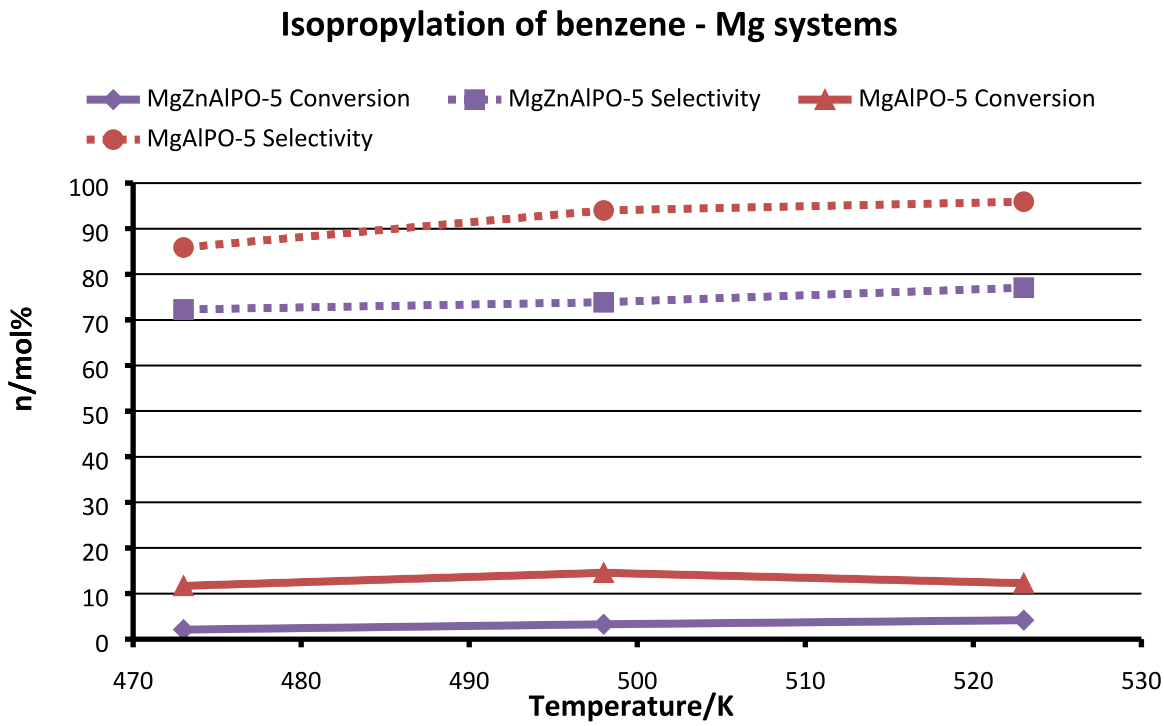

Figure S14: Full catalytic data for the isopropylation of benzene using Mg-containing AlPO-5 systems. Reaction conditions: WHSV of 3.5 hr^{-1}, Helium carrier gas of 10 ml/min, feed 6:1 mole ratio of benzene:isopropanol, temperature as shown.

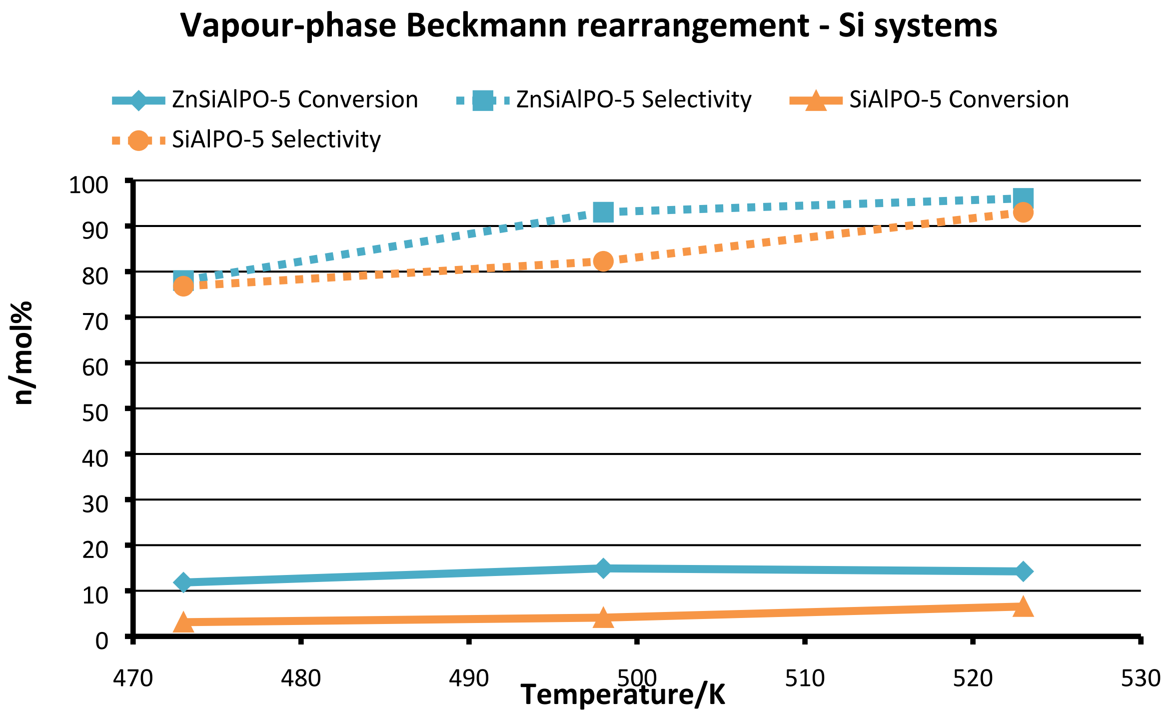

Figure S15: Full catalytic data for the vapour-phase Beckmann rearrangement of cyclohexanone oxime using Si-containing AlPO-5 systems. Reaction conditions: WHSV 3.3 hr^{-1}, Helium carrier gas flow 20 ml/min, 0.3 g of catalyst, liquid feed 300g/l of cyclohexanone oxime in methanol, temperature as shown.

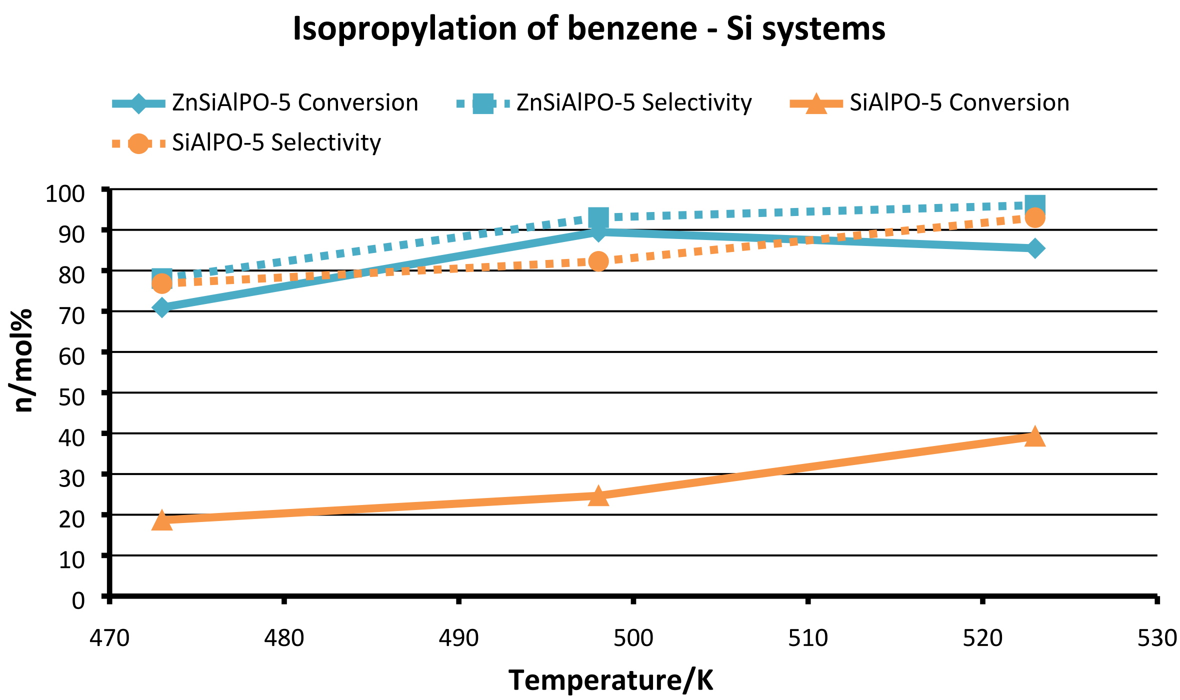

Figure S16: Full catalytic data for the isopropylation of benzene using Si-containing AlPO-5 systems. Reaction conditions: WHSV of 3.5 hr^{-1}, Helium carrier gas of 10 ml/min, feed 6:1 mole ratio of benzene:isopropanol, temperature as shown.

Mechanistic pathways

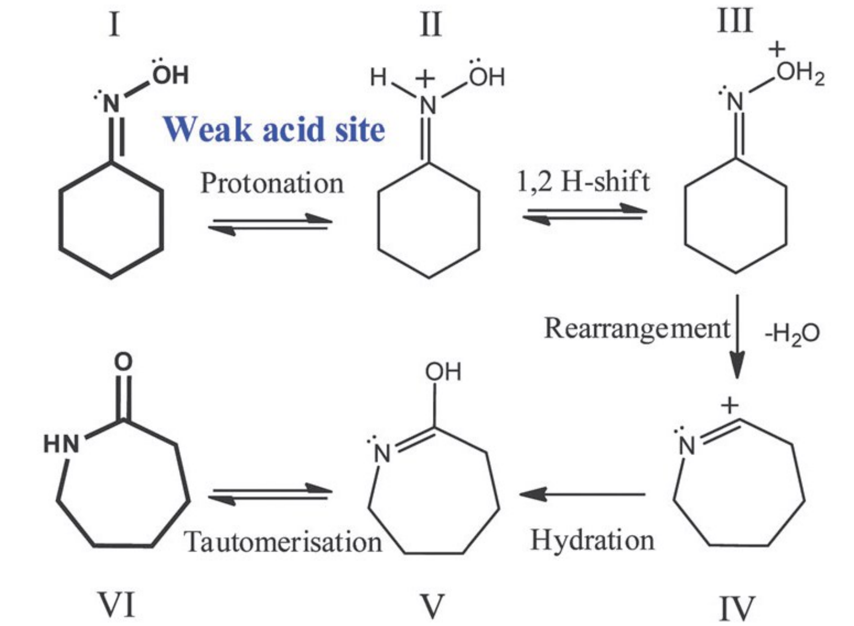

Figure S17: Mechanistic pathway of the Beckmann rearrangement of cyclohexanone oxime.

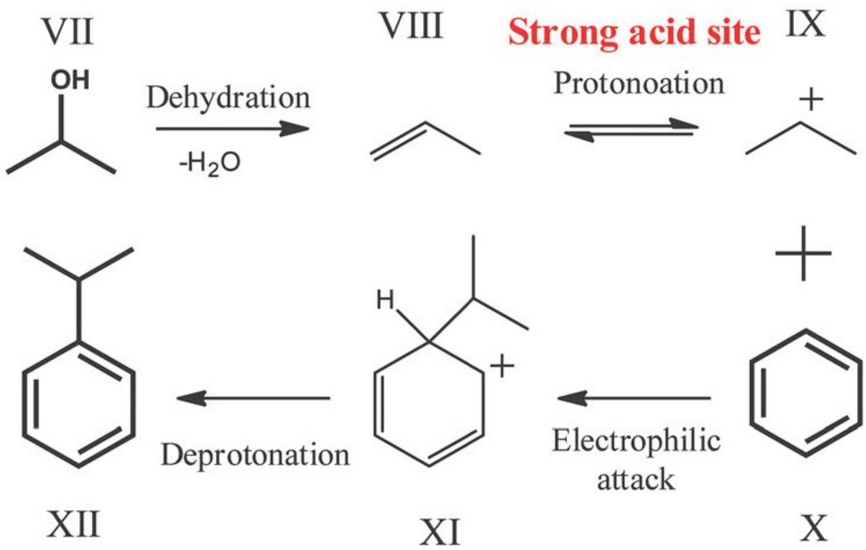

Figure S18: Mechanistic pathway of the isopropylation of benzene to cumene.