CHARACTERISATION OF INORGANIC MATERIALS USING SOLID-STATE NMR SPECTROSCOPY

Appendix B

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Appendix B

B.1 Unit cell parameters for as-prepared AlPOs pre- and post-DFT optimisation

Table B.1: Unit cell parameters for as-prepared AlPOs pre- and post-DFT optimisation.

	a / Å	*b* / Å	*c* / Å	Volume / Å^3	α	β	γ
AlPO-14(isopropylammonium hydroxide)							
[A]	9.6599	9.6639	10.6181	918.2050	74.719	74.140	88.983
[D]	9.6752	9.7569	10.7708	942.6373	74.830	74.190	88.979
[E]	9.5443	9.5706	10.5811	898.2592	75.373	74.101	88.748
[F]	9.5794	9.6261	10.5845	906.3303	75.127	74.182	88.812
AlPO-15(ammonium hydroxide)							
[A]	9.5560	9.5630	9.6150	854.0928	90.000	103.580	90.000
[D]	9.6275	9.6603	9.7241	877.8126	90.000	103.924	90.000
[E]	9.5534	9.5284	9.5876	848.8842	90.000	103.430	90.000
[F]	9.5647	9.5260	9.6395	852.7067	90.000	103.862	90.000

Table B.1: *Continued...*

	a / Å	*b* / Å	*c* / Å	Volume / Å^3	α	β	γ
JDF-2(methylammonium hydroxide)							
[A]	10.2810	13.8440	17.0640	2428.7219	90.000	90.000	90.000
[D]	10.3196	14.1501	17.0678	2492.2908	90.000	90.000	90.000
[E]	10.1856	14.0395	16.8507	2409.6665	90.000	90.000	90.000
[F]	10.1900	14.0233	16.8528	2408.2151	90.000	90.000	90.000
AlPO-34(morpholinium fluoride)							
[A]	9.3330	9.1830	9.1620	764.6919	88.450	102.570	93.760
[D]	9.4072	9.2988	9.1905	779.2521	88.973	103.551	94.409
[E]	9.3216	9.2190	9.0813	751.9572	89.853	104.619	95.129
[F]	9.3425	9.2153	9.0838	755.4825	89.108	104.287	94.545
SIZ-4(dimethylimidazolium fluoride)							
[A]	9.074	9.230	9.309	757.1282	76.446	87.343	89.388
[D]	9.1846	9.3401	9.4075	784.9020	76.828	87.291	89.396
[E]	9.0639	9.2301	9.3034	752.1646	75.419	86.981	89.911
[F]	9.0611	9.2360	9.3273	753.7809	75.252	87.150	89.989

B.2 Simulated powder X-ray diffraction patterns for as-prepared AlPOs

B.2.1 AlPO-14(isopropylammonium hydroxide)

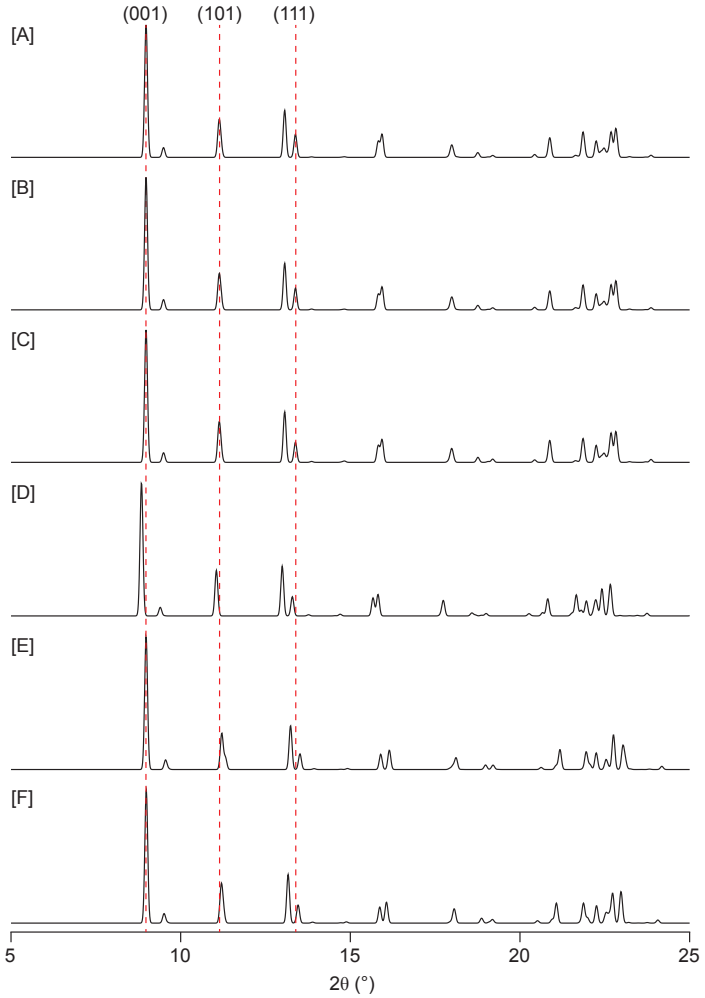

Figure B.1: Simulated powder X-ray diffraction patterns, using Cu $K_{\alpha 1}$ radiation for AlPO-14(isopropylammonium hydroxide) structures [A]-[F]. The red dotted lines are included as a guide to the changes in the positions of selected diffraction peaks. See Table 4.7 for a description of the optimisation strategy.

B.2.2 AlPO-15(ammonium hydroxide)

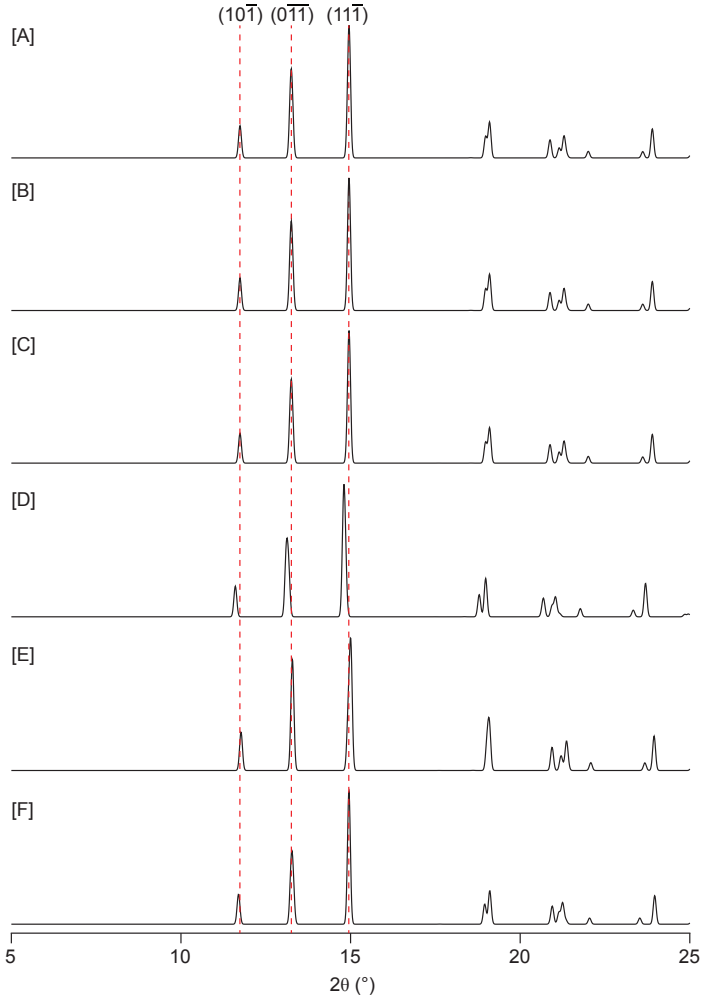

Figure B.2: Simulated powder X-ray diffraction patterns, using Cu $K_{\alpha 1}$ radiation for AlPO-15(ammonium hydroxide) structures [A]-[F]. The red dotted lines are included as a guide to the changes in the positions of selected diffraction peaks. See Table 4.7 for a description of the optimisation strategy.

B.2.3 AlPO-34(morpholinium fluoride)

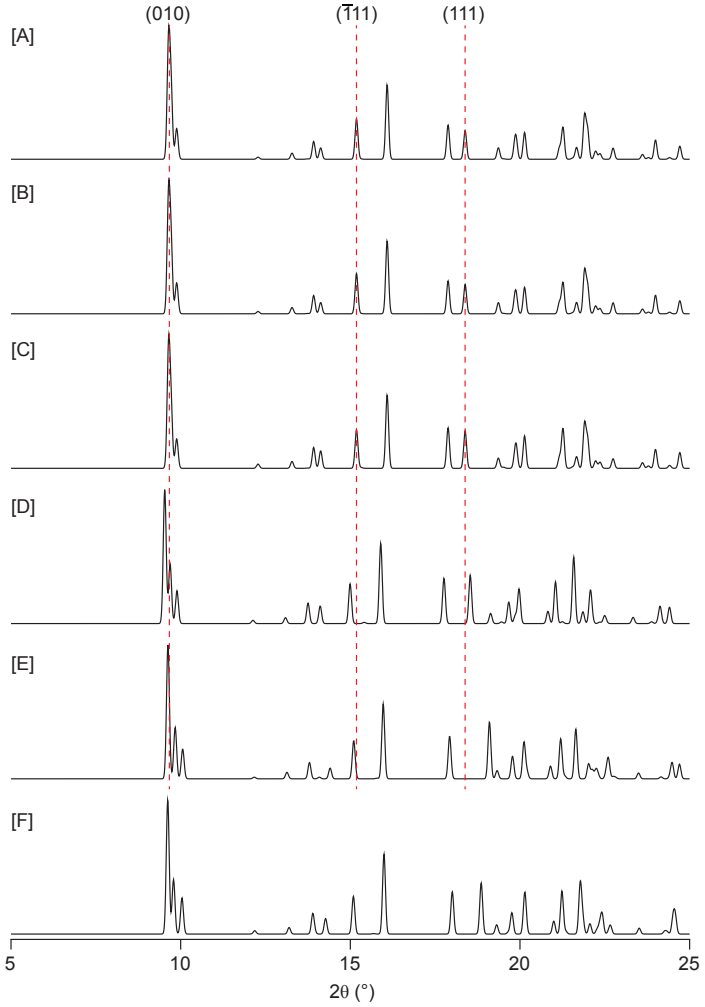

Figure B.3: Simulated powder X-ray diffraction patterns, using Cu $K_{\alpha 1}$ radiation for AlPO-34(morpholinium fluoride) structures [A]-[F]. The red dotted lines are included as a guide to the changes in the positions of selected diffraction peaks. See Table 4.7 for a description of the optimisation strategy.

B.2.4 SIZ-4(dimethylimidazolium fluoride)

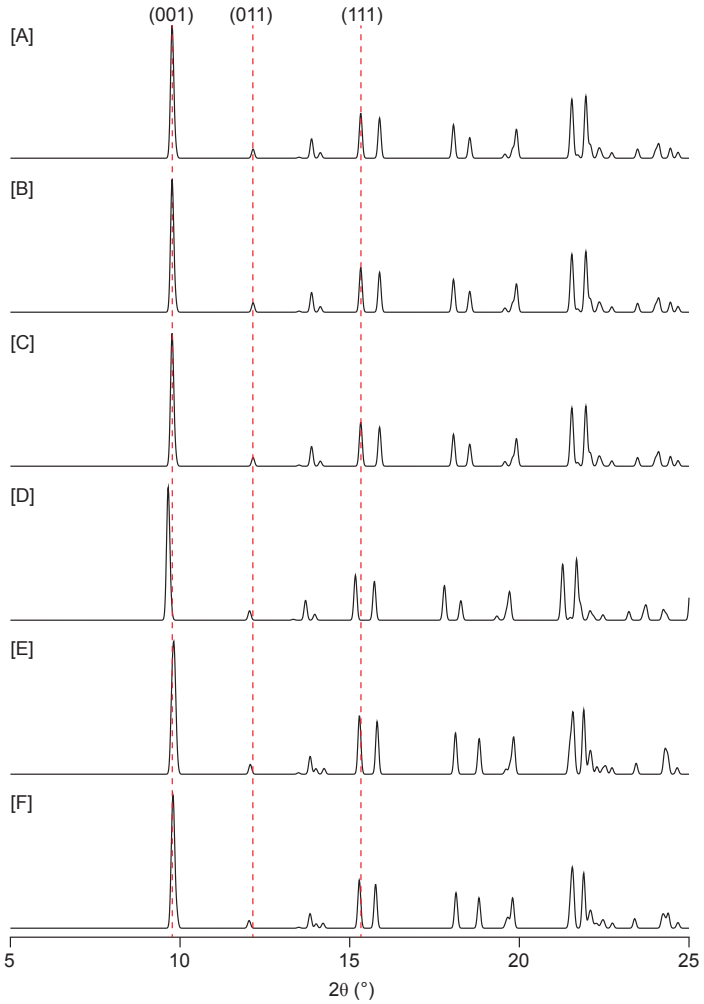

Figure B.4: Simulated powder X-ray diffraction patterns, using Cu $K_{\alpha 1}$ radiation for SIZ-4(dimethylimidazolium fluoride) structures [A]-[F]. The red dotted lines are included as a guide to the changes in the positions of selected diffraction peaks. See Table 4.7 for a description of the optimisation strategy.

B.3 Unit cell parameters for calcined AlPOs pre- and post-DFT optimisation

Table B.2: Unit cell parameters for calcined AlPOs pre- and post-DFT optimisation.

	a / Å	*b* / Å	*c* / Å	volume / Å^3	α	β	γ
AlPO-14							
[A]	9.7041	9.7361	10.2018	919.8089	77.811	77.504	87.691
[D]	9.7840	9.8389	10.3104	946.3046	77.619	77.462	87.602
[E]	9.7454	9.8071	10.2641	935.9734	77.736	77.533	87.731
[F]	9.7448	9.8012	10.2548	934.3540	77.727	77.498	87.616
AlPO-53(B)							
[A]	18.0240	13.9170	9.6550	2421.8603	90.000	90.000	90.000
[D]	18.1952	14.0757	9.7654	2501.0043	90.000	90.000	90.000
[E]	18.1535	13.9661	9.7138	2462.7563	90.000	90.000	90.000
[F]	18.1179	13.9754	9.7033	2456.9258	90.000	90.000	90.000
AlPO-34							
[A]	13.7157	13.7157	14.9273	2431.9174	90.000	90.000	120.000
[D]	13.8103	13.8103	15.0442	2484.8621	90.000	90.000	120.000
[E]	13.7919	13.7919	15.0252	2475.1516	90.000	90.000	120.000
[F]	13.7806	13.7806	15.0093	2468.4509	90.000	90.000	120.000

Table B.2: *Continued...*

	a / Å	*b* / Å	*c* / Å	volume / Å^3	α	β	γ
AlPO-17							
[A]	13.0898	13.0898	15.3302	2274.8031	90.000	90.000	120.000
[D]	13.2166	13.2166	15.5134	2346.8130	90.000	90.000	120.000
[E]	13.2048	13.2048	15.4548	2333.7620	90.000	90.000	120.000
[F]	13.1944	13.1944	15.4346	2327.0344	90.000	90.000	120.000
AlPO-18							
[A]	13.7114	12.7314	18.5703	3241.7303	90.000	90.010	90.000
[D]	13.8254	12.8333	18.7095	3319.5244	90.000	89.939	90.000
[E]	13.8098	12.7966	18.6730	3299.8570	90.000	89.913	90.000
[F]	13.7995	12.7791	18.6555	3289.8045	90.000	89.764	90.000

B.4 Simulated powder X-ray diffraction patterns for calcined AlPOs

B.4.1 Calcined AlPO-14

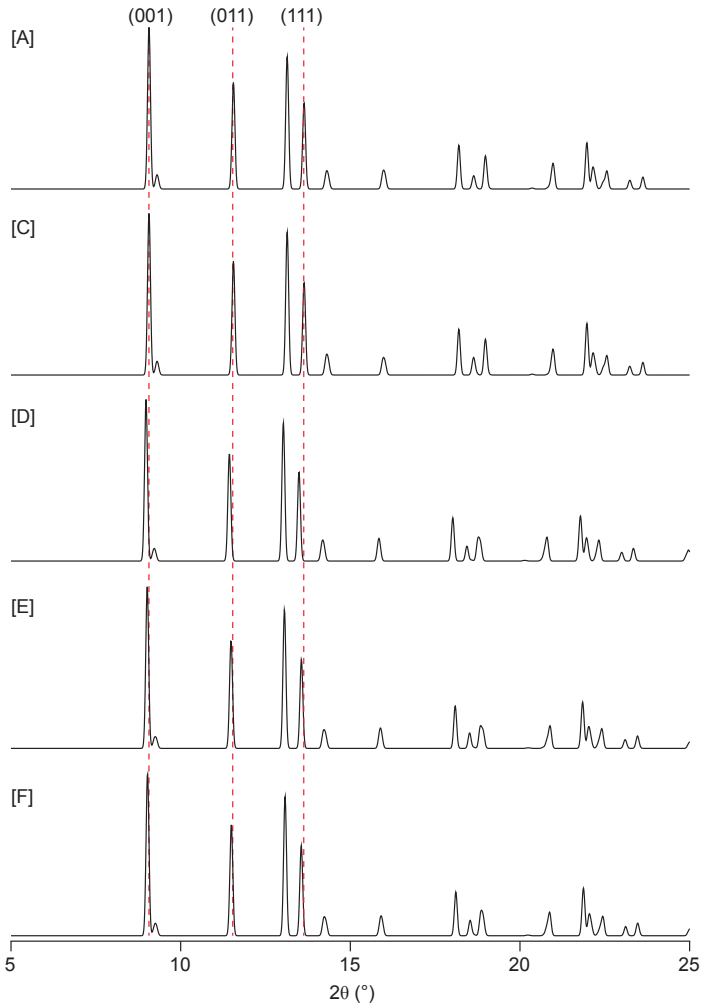

Figure B.5: Simulated powder X-ray diffraction patterns, using Cu $K_{\alpha 1}$ radiation for calcined AlPO-14 structures [A]-[F]. The red dotted lines are included as a guide to the changes in the positions of selected diffraction peaks. See Table 4.7 for a description of the optimisation strategy.

B.4.2 Calcined AlPO-53(B)

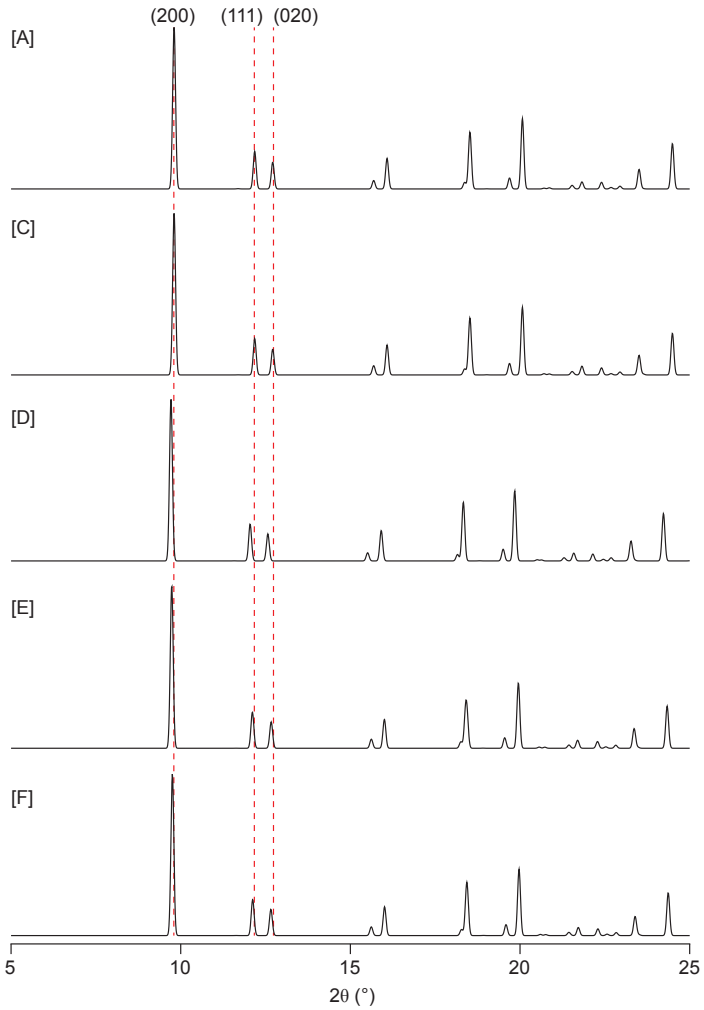

Figure B.6: Simulated powder X-ray diffraction patterns, using Cu $K_{\alpha 1}$ radiation for calcined AlPO-53(B) structures [A]-[F]. The red dotted lines are included as a guide to the changes in the positions of selected diffraction peaks. See Table 4.7 for a description of the optimisation strategy.

B.4.3 Calcined AlPO-17

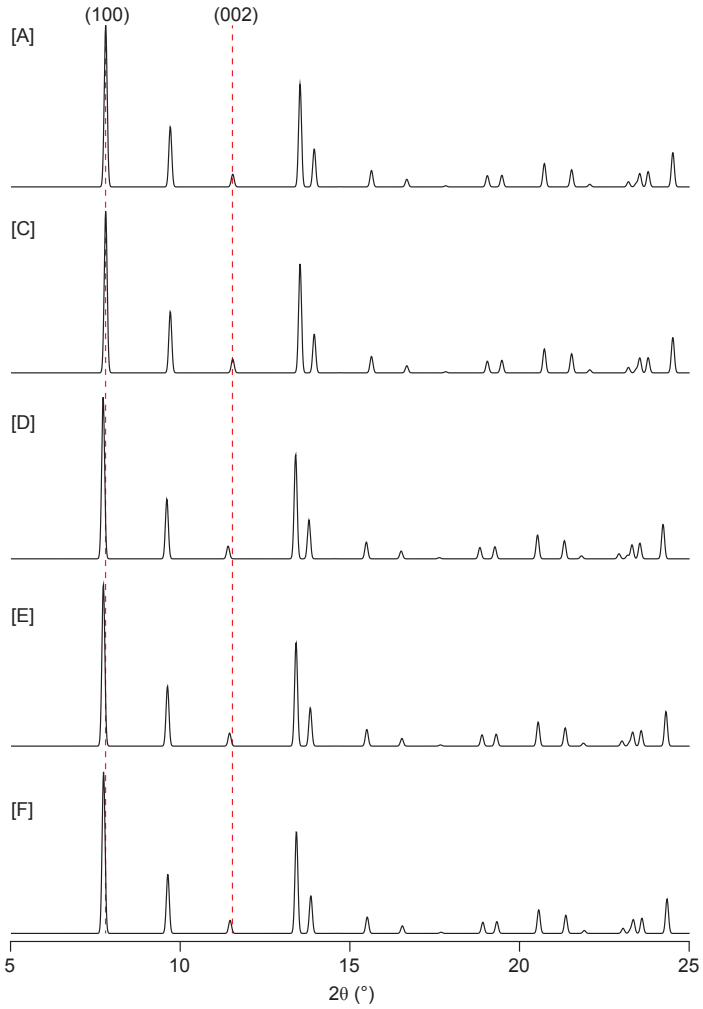

Figure B.7: Simulated powder X-ray diffraction patterns, using Cu $K_{\alpha 1}$ radiation for calcined AlPO-17 structures [A]-[F]. The red dotted lines are included as a guide to the changes in the positions of selected diffraction peaks. See Table 4.7 for a description of the optimisation strategy.

B.4.4 Calcined AlPO-18

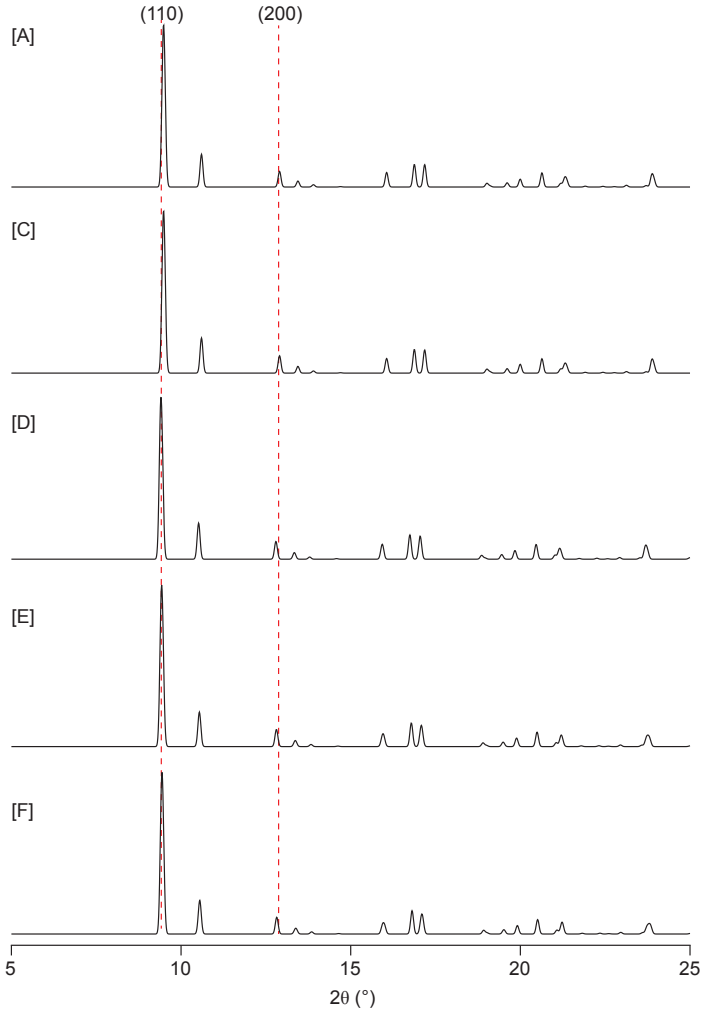

Figure B.8: Simulated powder X-ray diffraction patterns, using Cu $K_{\alpha 1}$ radiation for calcined AlPO-18 structures [A]-[F]. The red dotted lines are included as a guide to the changes in the positions of selected diffraction peaks. See Table 4.7 for a description of the optimisation strategy.