Supplementary Material

Calcined-dehydrated AlPO-14

i. Atomic positions (x, y, z fractional co-ordinates) of all atoms in the unit cell before any optimization (Broach)

Unit cell	*a*	9.70413 Å	*b*	9.73611 Å	*c*	10.2018 Å
	α	77.811°	β	77.504°	γ	87.691°

Atom type	x	y	z
O	0.0766	0.4368	0.8348
O	0.9234	0.5632	0.1652
O	0.3024	0.3126	0.8628
O	0.6976	0.6874	0.1372
O	0.7757	0.2329	0.9823
O	0.2243	0.7671	0.0177
O	0.4396	0.0642	0.8307
O	0.5604	0.9358	0.1693
O	0.4431	0.8367	0.7641
O	0.5569	0.1633	0.2359
O	0.2989	0.5607	0.8480
O	0.7011	0.4393	0.1520
O	0.0245	0.3297	0.3318
O	0.9755	0.6703	0.6682
O	0.8582	0.1495	0.4864
O	0.1418	0.8505	0.5136
O	0.9407	0.9216	0.6755
O	0.0593	0.0784	0.3245
O	0.1609	0.4094	0.0595
O	0.8391	0.5906	0.9405
O	0.8659	0.1898	0.2366
O	0.1341	0.8102	0.7634
O	0.6009	0.2911	0.8439
O	0.3991	0.7089	0.1561
O	0.8048	0.1556	0.7691
O	0.1952	0.8444	0.2309
O	0.3519	0.0299	0.3184
O	0.6481	0.9701	0.6816
O	0.4183	0.1391	0.0786
O	0.5817	0.8609	0.9214
O	0.8210	0.4141	0.7623
O	0.1790	0.5859	0.2377
Al	0.2730	0.7425	0.8445
Al	0.7270	0.2575	0.1555

Al	0.4322	0.2004	0.908
Al	0.5678	0.7996	0.092
Al	0.8141	0.0506	0.6558
Al	0.1859	0.9494	0.3442
Al	0.0699	0.4732	0.2015
Al	0.9301	0.5268	0.7985
P	0.5246	0.9351	0.7996
P	0.4754	0.0649	0.2004
P	0.2010	0.4282	0.9010
P	0.7990	0.5718	0.0990
P	0.9511	0.1884	0.3437
P	0.0489	0.8116	0.6563
P	0.7520	0.2740	0.8400
P	0.2480	0.7260	0.1600

ii. New atomic positions (x, y, z fractional co-ordinates) of all atoms in the unit cell after optimization with CASTEP with a fixed unit cell size (Optfix)

Unit cell	*a*	9.70413 Å	*b*	9.73611 Å	*c*	10.2018 Å
	α	77.811°	β	77.504°	γ	87.691°

Atom type	x	y	z
O	0.076732	0.435454	0.836396
O	0.923268	0.564546	0.163604
O	0.291526	0.300515	0.866759
O	0.708474	0.699485	0.133241
O	0.772641	0.242078	0.984688
O	0.227359	0.757922	0.015312
O	0.436560	0.054421	0.825396
O	0.563440	0.945579	0.174604
O	0.432223	0.822600	0.761646
O	0.567777	0.177400	0.238354
O	0.296276	0.560223	0.841916
O	0.703724	0.439777	0.158084
O	0.023849	0.326936	0.333980
O	0.976151	0.673064	0.666020
O	0.846427	0.154206	0.484720
O	0.153573	0.845794	0.515280
O	0.943148	0.928550	0.667979
O	0.056852	0.071450	0.332021
O	0.159423	0.408678	0.057143
O	0.840577	0.591322	0.942857
O	0.866703	0.199718	0.231678
O	0.133297	0.800282	0.768322
O	0.589267	0.292627	0.840321
O	0.410733	0.707373	0.159679
O	0.805782	0.153942	0.769639
O	0.194218	0.846058	0.230361

O	0.352217	0.029209	0.328710
O	0.647783	0.970791	0.671290
O	0.411579	0.140122	0.080592
O	0.588421	0.859878	0.919408
O	0.821544	0.412563	0.757049
O	0.178456	0.587437	0.242951
Al	0.272921	0.738169	0.844974
Al	0.727079	0.261831	0.155026
Al	0.432242	0.197184	0.903637
Al	0.567758	0.802816	0.096363
Al	0.811635	0.050998	0.648712
Al	0.188365	0.949002	0.351288
Al	0.071746	0.471621	0.200681
Al	0.928254	0.528379	0.799319
P	0.526239	0.927003	0.794744
P	0.473761	0.072997	0.205256
P	0.205384	0.427106	0.901031
P	0.794616	0.572894	0.098969
P	0.948705	0.187741	0.345844
P	0.051295	0.812259	0.654156
P	0.747266	0.275147	0.837896
P	0.252734	0.724853	0.162104

iii. New atomic positions (x, y, z fractional co-ordinates) of all atoms in the unit cell after optimization with CASTEP with a variable unit cell (Opt)

Unit cell	a	9.786066 Å	b	9.840522 Å	c	10.311201 Å
	α	77.586741°	β	77.461648°	γ	87.592192°

Atom type	x	y	z
O	0.081321	0.437902	0.836391
O	0.918679	0.562098	0.163609
O	0.298621	0.309475	0.868113
O	0.701379	0.690525	0.131887
O	0.775912	0.235817	0.985977
O	0.224088	0.764183	0.014023
O	0.439870	0.060187	0.826437
O	0.560130	0.939813	0.173563
O	0.430559	0.830684	0.764828
O	0.569441	0.169316	0.235172
O	0.294125	0.566754	0.846382
O	0.705875	0.433246	0.153618
O	0.020504	0.326911	0.329590
O	0.979496	0.673089	0.670410
O	0.855842	0.149293	0.486950
O	0.144158	0.850707	0.513050
O	0.939074	0.924629	0.675335
O	0.060926	0.075371	0.324665

O	0.158349	0.410408	0.056597
O	0.841651	0.589592	0.943403
O	0.861346	0.194894	0.238131
O	0.138654	0.805106	0.761869
O	0.594129	0.292746	0.843329
O	0.405871	0.707254	0.156671
O	0.808675	0.157291	0.767983
O	0.191325	0.842709	0.232017
O	0.351241	0.025679	0.323419
O	0.648759	0.974321	0.676581
O	0.414655	0.138585	0.078472
O	0.585345	0.861415	0.921528
O	0.825447	0.411197	0.763592
O	0.174553	0.588803	0.236408
Al	0.272596	0.744415	0.845030
Al	0.727404	0.255585	0.154970
Al	0.435839	0.201536	0.903873
Al	0.564161	0.798464	0.096127
Al	0.813563	0.051364	0.651791
Al	0.186437	0.948636	0.348209
Al	0.068339	0.471697	0.198232
Al	0.931661	0.528303	0.801768
P	0.526145	0.931907	0.797546
P	0.473855	0.068093	0.202454
P	0.207808	0.432023	0.902020
P	0.792192	0.567977	0.097980
P	0.949712	0.186181	0.345272
P	0.050288	0.813819	0.654728
P	0.751057	0.274167	0.840296
P	0.248943	0.725833	0.159704

***ipa*-AlPO-14**

i. Atomic positions (x, y, z fractional co-ordinates) of all atoms in the unit cell after initial optimization with CASTEP of only ^{1}H positions with a fixed unit cell size (Broach)

Unit cell	*a*	9.6599 Å	*b*	9.6639 Å	*c*	10.6181 Å
	α	77.7194°	β	74.14°	γ	88.983°

Atom type	x	y	z
H	0.272920	0.033824	0.038837
H	0.727080	0.966176	0.961163
H	0.469899	0.293936	0.228914
H	0.530101	0.706064	0.771086
H	0.292931	0.276106	0.289566

H	0.707069	0.723894	0.710434
H	0.373313	0.439252	0.238217
H	0.626687	0.560748	0.761783
H	0.490015	0.411597	0.396092
H	0.509985	0.588403	0.603908
H	0.251279	0.502101	0.443859
H	0.748721	0.497899	0.556141
H	0.178298	0.332599	0.535598
H	0.821702	0.667401	0.464402
H	0.301614	0.420151	0.589004
H	0.698386	0.579849	0.410996
H	0.532917	0.158373	0.427911
H	0.467083	0.841627	0.572089
H	0.478496	0.224108	0.577184
H	0.521504	0.775892	0.422816
H	0.356324	0.12126	0.535870
H	0.643676	0.87874	0.464130
H	0.813401	0.835708	0.111364
H	0.186599	0.164292	0.888636
H	0.955212	0.862235	-0.005602
H	0.044788	0.137765	1.005602
C	0.396000	0.336000	0.423000
C	0.604000	0.664000	0.577000
C	0.278000	0.400000	0.499000
C	0.722000	0.600000	0.501000
C	0.443000	0.204000	0.493000
C	0.557000	0.796000	0.507000
N	0.382000	0.336000	0.288000
N	0.618000	0.664000	0.712000
O	0.559000	0.832000	0.164000
O	0.441000	0.168000	0.836000
O	0.617000	0.603000	0.123000
O	0.383000	0.397000	0.877000
O	0.840000	0.195000	0.992000
O	0.160000	0.805000	0.008000
O	0.093000	0.452000	0.847000
O	0.907000	0.548000	0.153000
O	0.912000	0.381000	0.748000
O	0.088000	0.619000	0.252000
O	0.368000	0.655000	0.165000
O	0.632000	0.345000	0.835000
O	0.364000	0.002000	0.289000
O	0.636000	0.998000	0.711000
O	0.168000	0.898000	0.502000
O	0.832000	0.102000	0.498000
O	0.350000	0.965000	0.052000
O	0.650000	0.035000	0.948000
O	0.552000	0.790000	0.939000
O	0.448000	0.210000	0.061000
O	0.149000	0.864000	0.278000
O	0.851000	0.136000	0.722000
O	0.723000	0.334000	0.149000

O	0.277000	0.666000	0.851000
O	0.883000	0.144000	0.217000
O	0.117000	0.856000	0.783000
O	0.025000	0.638000	0.684000
O	0.975000	0.362000	0.316000
O	0.848000	0.554000	0.904000
O	0.152000	0.446000	0.096000
O	0.639000	0.073000	0.200000
O	0.361000	0.927000	0.800000
O	0.121000	0.102000	0.325000
O	0.879000	0.898000	0.675000
O	0.85000	0.855000	0.014000
O	0.150000	0.145000	0.986000
Al	0.222000	0.769000	0.157000
Al	0.778000	0.231000	0.843000
Al	0.775000	0.516000	0.079000
Al	0.225000	0.484000	0.921000
Al	0.046000	0.823000	0.659000
Al	0.954000	0.177000	0.341000
Al	0.502000	0.021000	0.127000
Al	0.498000	0.979000	0.873000
P	0.962000	0.502000	0.797000
P	0.038000	0.498000	0.203000
P	0.519000	0.726000	0.093000
P	0.481000	0.274000	0.907000
P	0.201000	0.964000	0.348000
P	0.799000	0.036000	0.652000
P	0.768000	0.183000	0.142000
P	0.232000	0.817000	0.858000

ii. New atomic positions (x, y, z fractional co-ordinates) of all atoms in the unit cell after optimization with CASTEP with a fixed unit cell size (Optfix)

Unit cell	*a*	9.6599 Å	*b*	9.6639 Å	*c*	10.6181 Å
	α	77.7194°	β	74.14°	γ	88.983°

Atom type	x	y	z
H	0.285736	0.027463	0.038189
H	0.714264	0.972537	0.961811
H	0.463541	0.314079	0.222614
H	0.536459	0.685921	0.777386
H	0.289924	0.277783	0.301784
H	0.710076	0.722217	0.698216
H	0.353115	0.448644	0.239583
H	0.646885	0.551356	0.760417
H	0.495672	0.430562	0.392275
H	0.504328	0.569438	0.607725

H	0.243531	0.516811	0.454891
H	0.756470	0.483189	0.545109
H	0.176746	0.339916	0.531856
H	0.823254	0.660084	0.468144
H	0.291057	0.423979	0.599668
H	0.708943	0.576021	0.400332
H	0.531356	0.166716	0.423777
H	0.468644	0.833284	0.576223
H	0.469732	0.219311	0.579555
H	0.530268	0.780689	0.420445
H	0.348625	0.134365	0.519163
H	0.651375	0.865635	0.480837
H	0.792675	0.841445	0.114768
H	0.207325	0.158555	0.885232
H	0.944050	0.850303	0.010250
H	0.055950	0.149696	0.989750
C	0.402762	0.355223	0.420330
C	0.597238	0.644777	0.579670
C	0.271144	0.413047	0.505399
C	0.728856	0.586954	0.494601
C	0.440780	0.210721	0.488496
C	0.559220	0.789279	0.511504
N	0.375430	0.348505	0.288032
N	0.624570	0.651495	0.711968
O	0.552019	0.834611	0.165000
O	0.447981	0.165389	0.835000
O	0.612749	0.596529	0.112326
O	0.387251	0.403471	0.887674
O	0.852160	0.191266	0.991883
O	0.147840	0.808734	0.008117
O	0.108577	0.447924	0.834633
O	0.891423	0.552076	0.165367
O	0.913167	0.379426	0.747573
O	0.086832	0.620574	0.252427
O	0.362882	0.666864	0.151918
O	0.637118	0.333136	0.848082
O	0.360329	0.010190	0.295209
O	0.639671	0.989809	0.704791
O	0.172420	0.889315	0.499794
O	0.827580	0.110685	0.500206
O	0.359542	0.956551	0.051164
O	0.640458	0.043449	0.948836
O	0.546972	0.787464	0.938453
O	0.453028	0.212536	0.061547
O	0.143823	0.876993	0.276517
O	0.856177	0.123007	0.723483
O	0.714987	0.336714	0.149891
O	0.285013	0.663286	0.850109
O	0.883973	0.153643	0.219907
O	0.116027	0.846357	0.780093
O	0.014933	0.630669	0.674818
O	0.985068	0.369331	0.325183

O	0.861326	0.544120	0.907610
O	0.138675	0.455880	0.092390
O	0.646103	0.080404	0.196470
O	0.353897	0.919596	0.803530
O	0.117654	0.109115	0.348099
O	0.882347	0.890885	0.651901
O	0.840217	0.850451	0.019535
O	0.159783	0.149550	0.980465
Al	0.209633	0.773614	0.156563
Al	0.790367	0.226386	0.843437
Al	0.774161	0.514186	0.077945
Al	0.225839	0.485814	0.922055
Al	0.048300	0.814575	0.651545
Al	0.951701	0.185425	0.348455
Al	0.499346	0.024668	0.133219
Al	0.500654	0.975332	0.866781
P	0.974151	0.499085	0.790957
P	0.025849	0.500915	0.209043
P	0.521371	0.725950	0.089146
P	0.478629	0.274050	0.910854
P	0.201030	0.970116	0.353050
P	0.798970	0.029884	0.646950
P	0.771770	0.187706	0.140668
P	0.228230	0.812294	0.859332

iii. New atomic positions (x, y, z fractional co-ordinates) of all atoms in the unit cell after optimization with CASTEP with a variable unit cell (Opt)

Unit cell	*a*	9.687163 Å	*b*	9.740585 Å	*c*	10.719979 Å
	α	75.223602°	β	74.286875°	γ	89.023471°

Atom type	x	y	z
H	0.286543	0.025772	0.037092
H	0.713475	0.974208	0.962909
H	0.465344	0.313306	0.225027
H	0.534661	0.686694	0.774970
H	0.291159	0.275170	0.302331
H	0.708849	0.724834	0.697669
H	0.355184	0.447452	0.236915
H	0.644822	0.552553	0.763081
H	0.496219	0.427439	0.389027
H	0.503789	0.572566	0.610970
H	0.245877	0.512011	0.448849
H	0.754126	0.487994	0.551147
H	0.177873	0.334169	0.532524
H	0.822136	0.665837	0.467472
H	0.294467	0.418464	0.594996

H	0.705531	0.581537	0.404989
H	0.531217	0.163905	0.427474
H	0.468793	0.836095	0.572522
H	0.470943	0.213973	0.580686
H	0.529055	0.786025	0.419297
H	0.349120	0.128391	0.524595
H	0.650887	0.871615	0.475401
H	0.798373	0.839599	0.113919
H	0.201615	0.160402	0.886095
H	0.946156	0.852811	0.005307
H	0.053818	0.147194	0.994689
C	0.403271	0.351173	0.419401
C	0.596739	0.648834	0.580589
C	0.272853	0.407774	0.502505
C	0.727157	0.592229	0.497475
C	0.441127	0.206044	0.491001
C	0.558876	0.793963	0.508978
N	0.376530	0.346228	0.287719
N	0.623475	0.653777	0.712278
O	0.553467	0.832224	0.166774
O	0.446532	0.167764	0.833262
O	0.614800	0.596446	0.117708
O	0.385188	0.403550	0.882348
O	0.848508	0.194168	0.992763
O	0.151469	0.805801	0.007283
O	0.102547	0.450445	0.842799
O	0.897436	0.549561	0.157223
O	0.912872	0.383938	0.749467
O	0.087145	0.616050	0.250538
O	0.364454	0.664683	0.157375
O	0.635528	0.335294	0.842677
O	0.359722	0.004824	0.292682
O	0.640288	0.995172	0.707310
O	0.169428	0.889055	0.499536
O	0.830594	0.110982	0.500393
O	0.358817	0.953672	0.051699
O	0.641178	0.046300	0.948352
O	0.548232	0.790574	0.942214
O	0.451771	0.209402	0.057838
O	0.144893	0.869111	0.278367
O	0.855124	0.130872	0.721609
O	0.712643	0.333972	0.150126
O	0.287340	0.666022	0.849907
O	0.880114	0.149566	0.220994
O	0.119881	0.850445	0.778999
O	0.014743	0.636268	0.676927
O	0.985270	0.363744	0.323047
O	0.854682	0.543440	0.906733
O	0.145307	0.456552	0.093301
O	0.642911	0.077557	0.196949
O	0.357080	0.922419	0.803071
O	0.118098	0.104472	0.337196

O	0.881929	0.895564	0.662755
O	0.842161	0.854826	0.017831
O	0.157819	0.145163	0.982201
Al	0.212008	0.772107	0.157257
Al	0.787993	0.227902	0.842707
Al	0.773506	0.513068	0.077922
Al	0.226487	0.486940	0.922050
Al	0.047858	0.818963	0.655033
Al	0.952130	0.181043	0.344952
Al	0.499223	0.022092	0.132897
Al	0.500773	0.977924	0.867072
P	0.970770	0.501415	0.793979
P	0.029230	0.498591	0.206000
P	0.522824	0.725407	0.093373
P	0.477170	0.274600	0.906643
P	0.200171	0.965541	0.349735
P	0.799835	0.034479	0.650238
P	0.768697	0.186151	0.140876
P	0.231292	0.813839	0.859110

Figure S1

Experimental (flat plate) X-ray powder diffraction pattern and simulated patterns (Cu-Kα_1 radiation) for the experimental (Broach) and optimized (Optfix) structures of calcined-dehydrated AlPO-14.

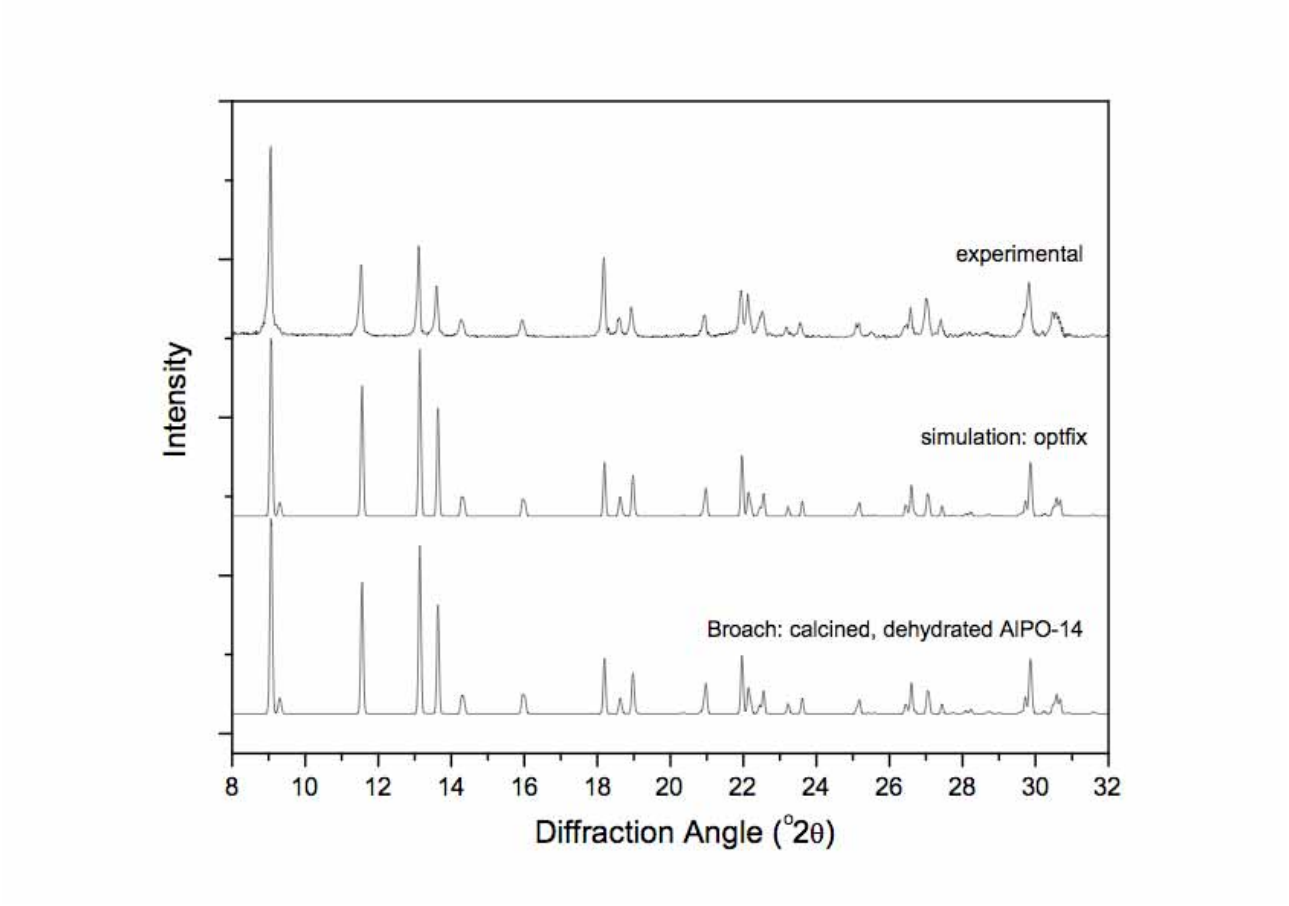

Figure S2

Experimental (flat plate) X-ray powder diffraction pattern and simulated patterns (Cu-Kα_1 radiation) for the experimental (Broach) and optimized (Optfix) structures of *ipa*-AlPO-14.