Can Laue microdiffraction be used to solve and refine complex inorganic structures?

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Supplementary information

Table 1 Simulation results for sanidine and the DET-90 configuration

Dataset	HarmAll	HarmAll	HarmAll	Harm012	Harm012	Harm012	Harm0	Harm0	Harm0
No. pattern	1	4	8	1	4	8	1	4	8
Resolution range (Å)	0.34-2.12	0.34-2.61	0.34-2.61	0.34-1.66	0.34-2.42	0.34-2.58	0.34-1.17	0.34-1.17	0.34-1.17
Total reflections	569	2306	4577	531	2163	4316	423	1709	3409
Unique reflections	567	1730	2673	529	1631	2530	421	1316	2062
Completeness (%)	6	17	26	6	16	25	5	13	21
Resolution range (Å)	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5
Unique reflections	192	540	725	177	495	666	117	349	467
Completeness (%)	11	32	43	11	29	40	7	21	28
XS[a]	-	RE=0.453 G3	RE=0.467 G1	-	RE=0.445 G1	RE=0.48 G3	-	-	-
XD[a]	R=0.441 G3	R=0.280 G1	R=0.298 G1	R=0.430 G3	R=0.260 G1	R=0.288 G1	R=0.414 G3	R=0.241 G1	R=0.292 G1

[a] Structure solution results from direct (XS) and dual-space (XD) methods are indicated by the RE and R factors, respectively.
G1: Group1 (full structure); G2: Group2 (partial structure); G3: Group3 (no solution); -: insufficient data for XS

Table 2 Simulation results for sanidine and the DET-60 configuration

Dataset	HarmAll	HarmAll	HarmAll	Harm012	Harm012	Harm012	Harm0	Harm0	Harm0
No. pattern	1	4	8	1	4	8	1	4	8
Resolution range (Å)	0.44-3.54	0.43-3.54	0.42-3.54	0.44-2.79	0.43-2.79	0.42-3.54	0.44-2.39	0.43-2.39	0.42-2.39
Total reflections	273	1105	2208	256	1034	2072	197	802	1612
Unique reflections	239	876	1599	222	812	1509	174	644	1225
Completeness (%)	5	18	32	5	17	30	4	13	24
Resolution range (Å)	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5
Unique reflections	93	299	490	82	268	447	56	186	324
Completeness (%)	12	40	65	11	36	59	7	25	43
XS[a]	RE=0.468 G3	RE=0.413 G1	RE=0.363 G1	RE=0.450 G3	RE=0.42 G1	RE=0.526 G3	RE=0.482 G3	RE=0.469 G3	RE=0.512 G3
XD[a]	R=0.351 G2	R=0.27 G1	R=0.307 G1	R=0.342 G3	R=0.272 G1	R=0.281 G1	R=0.352 G3	R=0.259 G1	R=0.265 G1

[a] Structure solution results from direct (XS) and dual-space (XD) methods are indicated by the RE and R factors, respectively.
G1: Group1 (full structure); G2: Group2 (partial structure); G3: Group3 (no solution); -: insufficient data for XS

Table 3 Simulation results for sanidine and the DET-46 configuration

Dataset	HarmAll	HarmAll	HarmAll	Harm012	Harm012	Harm012	Harm0	Harm0	Harm0
No. pattern	1	4	8	1	4	8	1	4	8
Resolution range (Å)	0.49-3.95	0.49-6.46	0.49-6.50	0.49-2.89	0.49-6.46	0.49-6.50	0.49-2.89	0.49-2.89	0.49-6.50
Total reflections	188	761	1483	178	716	1391	139	549	1084
Unique reflections	174	628	1065	167	589	1004	131	471	819
Completeness (%)	5	19	32	5	18	30	4	15	24
Resolution range (Å)	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0
Unique reflections	75	244	376	72	225	345	51	166	259
Completeness (%)	14	46	71	14	42	65	10	31	49
XS[a]	RE=0.445 G3	RE=0.441 G1	RE=0.341 G1	RE=0.376 G3	RE=0.424 G1	RE=0.37 G1	-	RE=0.512 G3	RE=0.494 G3
XD[a]	R=0.396 G3	R=0.272 G1	R=0.311 G1	R=0.381 G3	R=0.279 G1	R=0.316 G1	R=0.368 G3	R=0.324 G2	R=0.356 G2

[a] Structure solution results from direct (XS) and dual-space (XD) methods are indicated by the RE and R factors, respectively.
G1: Group1 (full structure); G2: Group2 (partial structure); G3: Group3 (no solution); -: insufficient data for XS

Table 4 Simulation results for KTP and the DET-90 configuration

Dataset	HarmAll	HarmAll	HarmAll	Harm012	Harm012	Harm012	Harm0	Harm0	Harm0
No. pattern	1	4	8	1	4	8	1	4	8
Resolution range (Å)	0.33-2.86	0.33-2.86	0.33-2.86	0.33-1.88	0.33-2.40	0.33-2.40	0.33-1.14	0.33-1.24	0.33-1.26
Total reflections	1421	5342	10882	1351	5090	10298	1060	4021	8161
Unique reflections	942	3339	5225	884	3173	4972	685	2556	4082
Completeness (%)	6	14	21	6	13	20	4	11	17
Resolution range (Å)	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5
Unique reflections	479	984	1330	440	912	1228	277	622	884
Completeness (%)	12	25	34	11	23	31	7	16	22
XS[a]	-	RE=0.492 G3	RE=0.487 G3	-	RE=0.47 G3	RE=0.49 G3	-	-	-
XD[a]	R=0.275 G2	R=0.232 G2	R=0.21 G1	R=0.264 G2	R=0.233 G2	R=0.192 G1	R=0.315 G3	R=0.267 G2	R=0.204 G2

[a] Structure solution results from direct (XS) and dual-space (XD) methods are indicated by the RE and R factors, respectively.
G1: Group1 (full structure); G2: Group2 (partial structure); G3: Group3 (no solution); -: insufficient data for XS

Table 5 Simulation results for KTP and the DET-60 configuration

Dataset	HarmAll	HarmAll	HarmAll	Harm012	Harm012	Harm012	Harm0	Harm0	Harm0
No. pattern	1	4	8	1	4	8	1	4	8
Resolution range (Å)	0.42-4.53	0.42-5.29	0.42-5.29	0.42-4.53	0.42-5.29	0.42-5.29	0.42-2.21	0.42-2.21	0.42-2.40
Total reflections	681	2584	5208	617	2441	4917	519	1967	3883
Unique reflections	449	2028	3547	411	1911	3376	340	1597	2818
Completeness (%)	6	16	29	5	15	27	4	13	23
Resolution range (Å)	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5
Unique reflections	238	616	988	206	563	923	151	417	697
Completeness (%)	14	36	58	12	33	54	9	25	41
XS[a]	RE=0.396 G3	RE=0.411 G2	RE=0.397 G1	RE=0.394 G3	RE=0.404 G3	RE=0.385 G1	-	RE=0.429 G3	RE=0.381 G1
XD[a]	R=0.236 G2	R=0.179 G2	R=0.182 G1	R=0.274 G2	R=0.172 G2	R=0.148 G1	R=0.331 G3	R=0.23 G3	R=0.19 G2

[a] Structure solution results from direct (XS) and dual-space (XD) methods are indicated by the RE and R factors, respectively.
G1: Group1 (full structure); G2: Group2 (partial structure); G3: Group3 (no solution); -: insufficient data for XS

Table 6 Simulation results for KTP and the DET-46 configuration

Dataset	HarmAll	HarmAll	HarmAll	Harm012	Harm012	Harm012	Harm0	Harm0	Harm0
No. pattern	1	4	8	1	4	8	1	4	8
Resolution range (Å)	0.48-5.04	0.48-5.73	0.48-5.73	0.48-5.04	0.48-5.73	0.48-5.73	0.48-3.89	0.48-5.73	0.48-5.73
Total reflections	435	1704	3455	423	1648	3321	329	1293	2598
Unique reflections	316	1283	2027	306	1246	1969	241	997	1608
Completeness (%)	5	16	25	5	15	24	4	12	20
Resolution range (Å)	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0
Unique reflections	170	454	510	162	435	486	103	302	367
Completeness (%)	14	38	55	13	36	53	9	25	39
XS[a]	RE=0.369 G3	RE=0.37 G1	RE=0.318 G1	RE=0.416 G3	RE=0.363 G1	RE=0.327 G1	RE=0.399 G3	RE=0.408 G3	RE=0.418 G2
XD[a]	R=0.256 G2	R=0.187 G1	R=0.154 G1	R=0.307 G3	R=0.211 G2	R=0.172 G1	R=0.330 G3	R=0.25 G2	R=0.21 G1

[a] Structure solution results from direct (XS) and dual-space (XD) methods are indicated by the RE and R factors, respectively.
G1: Group1 (full structure); G2: Group2 (partial structure); G3: Group3 (no solution); -: insufficient data for XS

Table 7 Simulation results for ZSM-5 and the DET-90 configuration

Dataset	HarmAll	HarmAll	HarmAll	Harm012	Harm012	Harm012	Harm0	Harm0	Harm0
No. pattern	1	4	8	1	4	8	1	4	8
Resolution range (Å)	0.33-2.75	0.33-2.75	0.33-2.91	0.33-2.32	0.33-2.41	0.33-2.57	0.33-1.26	0.33-1.27	0.33-1.27
Total reflections	8137	32306	64980	7739	30695	61625	6091	24207	48605
Unique reflections	6076	13161	27469	5747	12582	26075	4597	10406	21127
Completeness (%)	8	17	36	8	17	34	6	14	28
Resolution range (Å)	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5
Unique reflections	1695	3296	7828	1551	3088	7250	1007	2330	5127
Completeness (%)	14	27	63	13	25	59	8	19	42
XS[a]	RE=0.600 G3	RE=0.475 G3	RE=0.466 G3	RE=0.594 G3	RE=0.559 G3	RE=0.468 G2	-	-	RE=0.478 G2
XD[a]	R=0.339 G2	R=0.204 G1	R=0.173 G1	R=0.243 G1	R=0.223 G1	R=0.178 G1	R=0.265 G1	R=0.221 G1	R=0.187 G1

[a] Structure solution results from direct (XS) and dual-space (XD) methods are indicated by the RE and R factors, respectively.
G1: Group1 (full structure); G2: Group2 (partial structure); G3: Group3 (no solution); -: insufficient data for XS

Table 8 Simulation results for ZSM-5 and the DET-60 configuration

Dataset	HarmAll	HarmAll	HarmAll	Harm012	Harm012	Harm012	Harm0	Harm0	Harm0
No. pattern	1	4	8	1	4	8	1	4	8
Resolution range (Å)	0.43-4.54	0.42-5.53	0.42-6.05	0.43-3.75	0.42-5.53	0.42-5.53	0.43-2.43	0.42-2.78	0.42-2.78
Total reflections	3883	15471	31156	3683	14617	29493	2921	11587	23253
Unique reflections	3217	7396	14026	3054	7086	13416	2450	5970	11107
Completeness (%)	9	20	37	9	19	36	7	16	30
Resolution range (Å)	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5
Unique reflections	858	2024	4052	779	1911	3813	486	1540	2904
Completeness (%)	22	37	75	20	35	70	13	28	54
XS[a]	RE=0.475 G3	RE=0.343 G2	RE=0.352 G2	RE=0.481 G3	RE=0.353 G2	RE=0.339 G2	RE=0.449 G3	RE=0.42 G3	RE=0.286 G2
XD[a]	R=0.278 G1	R=0.217 G1	R=0.187 G1	R=0.289 G1	R=0.228 G1	R=0.188 G1	R=0.382 G2	R=0.291 G1	R=0.194 G1

[a] Structure solution results from direct (XS) and dual-space (XD) methods are indicated by the RE and R factors, respectively.
G1: Group1 (full structure); G2: Group2 (partial structure); G3: Group3 (no solution); -: insufficient data for XS

Table 9 Simulation results for ZSM-5 and the DET-46 configuration

Dataset	HarmAll	HarmAll	HarmAll	Harm012	Harm012	Harm012	Harm0	Harm0	Harm0
No. pattern	1	4	8	1	4	8	1	4	8
Resolution range (Å)	0.48-6.35	0.48-7.44	0.48-8.02	0.48-6.35	0.48-6.35	0.48-6.35	0.48-4.56	0.48-4.60	0.48-4.69
Total reflections	2700	10923	21626	2540	10277	20432	2002	8097	16109
Unique reflections	2336	6880	10666	2212	6542	10174	1788	5451	8494
Completeness (%)	9	26	41	9	25	39	7	21	32
Resolution range (Å)	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0
Unique reflections	896	2106	3104	835	1963	2908	602	1504	2257
Completeness (%)	23	55	81	22	51	76	16	39	59
XS[a]	RE=0.43 G3	RE=0.347 G2	RE=0.31 G2	RE=0.389 G3	RE=0.355 G2	RE=0.307 G2	RE=0.447 G3	RE=0.359 G2	RE=0.405 G2
XD[a]	R=0.411 G3	R=0.193 G1	R=0.192 G1	R=0.416 G3	R=0.196 G1	R=0.207 G1	R=0.435 G3	R=0.251 G1	R=0.219 G1

[a] Structure solution results from direct (XS) and dual-space (XD) methods are indicated by the RE and R factors, respectively.
G1: Group1 (full structure); G2: Group2 (partial structure); G3: Group3 (no solution); -: insufficient data for XS

Table 10 Simulation results for AlPO-17 and the DET-90 configuration

Dataset	HarmAll	HarmAll	HarmAll	Harm012	Harm012	Harm012	Harm0	Harm0	Harm0
No. pattern	1	4	8	1	4	8	1	4	8
Resolution range (Å)	0.34-2.67	0.34-2.67	0.34-2.67	0.34-2.16	0.34-2.23	0.34-2.47	0.34-1.22	0.34-1.25	0.34-1.25
Total reflections	3583	14208	28392	3355	13393	26700	2621	10441	20845
Unique reflections	3394	8127	11118	3194	7717	10593	2537	6184	8652
Completeness (%)	16	38	52	15	37	50	12	30	42
Resolution range (Å)	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5	0.6-1.5
Unique reflections	1068	2452	3029	979	2274	2822	647	1566	2076
Completeness (%)	31	70	87	28	65	81	19	45	60
XS[a]	RE=0.578 G3	RE=0.465 G3	RE=0.438 G3	RE=0.584 G3	RE=0.573 G3	RE=0.581 G3	-	-	RE=0.598 G3
XD[a]	R=0.193 G2	R=0.108 G1	R=0.114 G1	R=0.203 G2	R=0.101 G1	R=0.111 G1	R=0.287 G2	R=0.155 G2	R=0.151 G2

[a] Structure solution results from direct (XS) and dual-space (XD) methods are indicated by the RE and R factors, respectively.
G1: Group1 (full structure); G2: Group2 (partial structure); G3: Group3 (no solution); -: insufficient data for XS

Table 11 Simulation results for AlPO-17 and the DET-60 configuration

Dataset	HarmAll	HarmAll	HarmAll	Harm012	Harm012	Harm012	Harm0	Harm0	Harm0
No. pattern	1	4	8	1	4	8	1	4	8
Resolution range (Å)	0.43-4.53	0.42-5.34	0.42-5.73	0.43-4.52	0.42-4.52	0.42-4.52	0.43-2.16	0.42-2.44	0.42-2.65
Total reflections	1703	6727	13447	1598	6299	12642	1247	4954	9917
Unique reflections	1314	3910	5606	1236	3719	5357	974	3051	4515
Completeness (%)	13	37	54	12	36	51	10	29	43
Resolution range (Å)	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5	0.8-2.5
Unique reflections	461	1213	1424	422	1137	1340	283	848	1073
Completeness (%)	30	79	92	27	74	87	18	55	70
XS[a]	RE=0.475 G3	RE=0.394 G3	RE=0.366 G1	RE=0.476 G3	RE=0.438 G3	RE=0.409 G1	RE=0.453 G3	RE=0.477 G3	RE=0.417 G1
XD[a]	R=0.236 G2	R=0.174 G2	R=0.118 G1	R=0.30 G2	R=0.17 G2	R=0.139 G1	R=0.377 G3	R=0.184 G2	R=0.130 G1

[a] Structure solution results from direct (XS) and dual-space (XD) methods are indicated by the RE and R factors, respectively.
G1: Group1 (full structure); G2: Group2 (partial structure); G3: Group3 (no solution); -: insufficient data for XS

Table 12 Simulation results for AlPO-17 and the DET-46 configuration

Dataset	HarmAll	HarmAll	HarmAll	Harm012	Harm012	Harm012	Harm0	Harm0	Harm0
No. pattern	1	4	8	1	4	8	1	4	8
Resolution range (Å)	0.49-6.62	0.48-7.38	0.48-7.38	0.49-6.04	0.48-7.38	0.48-7.38	0.49-6.04	0.48-6.04	0.48-6.04
Total reflections	1163	4656	9321	1100	4420	8840	852	3439	6864
Unique reflections	983	2745	3844	930	2636	3695	748	2160	3115
Completeness (%)	14	38	53	13	36	51	11	30	43
Resolution range (Å)	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0	0.9-3.0
Unique reflections	346	794	962	320	747	905	235	562	759
Completeness (%)	32	73	89	29	69	83	22	52	70
XS[a]	RE=0.366 G3	RE=0.37 G1	RE=0.364 G1	RE=0.469 G3	RE=0.366 G1	RE=0.382 G1	RE=0.513 G3	RE=0.544 G3	RE=0.493 G2
XD[a]	R=0.245 G2	R=0.166 G2	R=0.099 G1	R=272 G2	R=0.17 G2	R=0.103 G1	R=0.382 G3	R=0.186 G2	R=0.129 G1

[a] Structure solution results from direct (XS) and dual-space (XD) methods are indicated by the RE and R factors, respectively.
G1: Group1 (full structure); G2: Group2 (partial structure); G3: Group3 (no solution); -: insufficient data for XS

Table 13 Refinement results for sanidine. Dataset was obtained after combining 3 DET-90 and 3 DET-60 patterns, and by extraction only reflections with no harmonic.

Atoms	X	Y	Z	Occ.	Ueq
K1	0.2145(2)	0.5	0.3612(5)	0.45	0.029(1)
Na1	0.2145(2)	0.5	0.3612(5)	0.05	0.029(1)
Si1	0.9908(2)	0.18501(9)	0.2766(4)	0.66	0.0119(6)
Al1	0.9908(2)	0.18501(9)	0.2766(4)	0.34	0.0119(6)
Si2	0.2097(2)	0.38202(8)	0.8446(3)	0.88	0.0124(6)
Al2	0.2097(2)	0.38202(8)	0.8446(3)	0.12	0.0124(6)
O1	0.1396(7)	0.5	0.789(1)	0.50	0.024(3)
O2	0.3190(6)	0.3739(3)	0.096(1)	1.00	0.021(2)
O3	0.0	0.1453(5)	0.5	0.50	0.023(3)
O4	0.0357(5)	0.3114(3)	0.760(1)	1.00	0.022(2)
O5	0.1712(6)	0.1477(3)	0.271(1)	1.00	0.028(2)

Table 14 Refinement results for sanidine. Dataset was obtained after combining 3 DET-90 and 3 DET-60 patterns, and by extraction reflections with no harmonic, 1 harmonics and 2 harmonics.

Atoms	X	Y	Z	Occ.	Ueq
K1	0.2143(2)	0.5	0.3610(6)	0.45	0.027(1)
Na1	0.2143(2)	0.5	0.3610(6)	0.05	0.027(1)
Si1	0.9908(2)	0.18506(9)	0.2766(4)	0.66	0.0106(7)
Al1	0.9908(2)	0.18506(9)	0.2766(4)	0.34	0.0106(7)
Si2	0.2098(2)	0.38207(9)	0.8448(4)	0.88	0.0116(7)
Al2	0.2098(2)	0.38207(9)	0.8448(4)	0.12	0.0116(7)
O1	0.1396(8)	0.5	0.790(1)	0.50	0.023(3)
O2	0.3194(6)	0.3737(3)	0.096(1)	1.00	0.018(2)
O3	0.0	0.1453(5)	0.5	0.50	0.021(4)
O4	0.0358(5)	0.3113(3)	0.760(1)	1.00	0.020(2)
O5	0.1714(6)	0.1477(4)	0.270(1)	1.00	0.029(3)

Table 15 Refinement results for KTP. Dataset was obtained after combining 3 DET-90 and 3 DET-46 patterns, and by extraction only reflections with no harmonic.

Atoms	X	Y	Z	Occ.	Ueq
K1	0.3779(2)	0.7807(3)	0.6890(3)	1.00	0.0194(5)
K2	0.1055(2)	0.7001(3)	0.9337(3)	1.00	0.0194(5)
Ti1	0.3728(1)	0.4997(1)	0.9992(2)	1.00	0.0055(2)
Ti2	0.24687(9)	0.2693(2)	0.7476(2)	1.00	0.0055(2)
P1	0.4979(2)	0.3360(2)	0.7401(3)	1.00	0.0060(3)
P2	0.1809(2)	0.5017(2)	0.4880(3)	1.00	0.0060(3)
O1	0.4861(6)	0.4896(7)	0.8509(7)	1.00	0.0070(6)
O2	0.5098(6)	0.4648(9)	0.6182(8)	1.00	0.0096(7)
O3	0.3990(6)	0.1995(7)	0.7211(7)	1.00	0.0079(7)
O4	0.5941(6)	0.1923(8)	0.7608(8)	1.00	0.0093(8)
O5	0.1128(6)	0.3105(7)	0.4578(6)	1.00	0.0067(6)
O6	0.1109(6)	0.6925(7)	0.5142(7)	1.00	0.0071(6)
O7	0.2516(5)	0.5383(9)	0.3713(8)	1.00	0.0080(7)
O8	0.2539(5)	0.4586(8)	0.6018(7)	1.00	0.0063(7)
O9	0.2247(6)	0.9684(9)	0.3560(7)	1.00	0.0089(7)
O10	0.2246(5)	0.0426(7)	0.6106(6)	1.00	0.0062(6)

Table 16 Refinement results for ZSM-5. Dataset was obtained after combining 6 DET-90 and 6 DET-60 patterns, and by extraction only reflections with no harmonic.

Atoms	X	Y	Z	Occ.	Ueq
Si1	0.4227(1)	0.0575(1)	-0.3341(1)	1.0	0.0197(4)
Si2	0.3088(2)	0.0293(1)	-0.1872(2)	1.0	0.0214(5)
Si3	0.2790(1)	0.0614(1)	0.0330(2)	1.0	0.0204(5)
Si4	0.1222(1)	0.0627(1)	0.0300(2)	1.0	0.0217(5)
Si5	0.0721(1)	0.0275(1)	-0.1832(2)	1.0	0.0189(5)
Si6	0.1873(1)	0.0591(1)	-0.3262(1)	1.0	0.0204(5)
Si7	0.4239(1)	-0.1723(1)	-0.3248(2)	1.0	0.0195(5)
Si8	0.3093(1)	-0.1289(1)	-0.1839(1)	1.0	0.0204(5)
Si9	0.2751(1)	-0.1727(1)	0.0320(2)	1.0	0.0215(5)
Si10	0.1219(1)	-0.1734(1)	0.0302(2)	1.0	0.0210(5)
Si11	0.0709(1)	-0.1301(1)	-0.1810(2)	1.0	0.0198(5)
Si12	0.1884(1)	-0.17325(9)	-0.3178(2)	1.0	0.0194(5)
O1	0.3742(4)	0.0550(8)	-0.2395(6)	1.0	0.050(2)
O2	0.3071(4)	0.0590(4)	-0.0760(4)	1.0	0.034(1)
O3	0.1994(4)	0.0605(8)	0.0329(9)	1.0	0.071(3)
O4	0.0974(4)	0.0600(4)	-0.0838(4)	1.0	0.039(2)
O5	0.1170(4)	0.0553(5)	-0.2743(5)	1.0	0.038(2)
O6	0.2457(4)	0.0545(8)	-0.2470(4)	1.0	0.042(2)
O7	0.3768(4)	-0.1566(6)	-0.2344(6)	1.0	0.041(2)
O8	0.3096(5)	-0.1532(5)	-0.0722(5)	1.0	0.042(2)
O9	0.1972(5)	-0.1538(4)	0.0320(7)	1.0	0.045(2)
O10	0.0894(5)	-0.1628(5)	-0.0759(6)	1.0	0.047(2)
O11	0.1177(4)	-0.1580(5)	-0.2665(5)	1.0	0.036(2)
O12	0.2461(4)	-0.1563(9)	-0.2412(6)	1.0	0.051(4)
O13	0.3088(6)	-0.0499(3)	-0.1872(5)	1.0	0.050(2)
O14	0.0764(5)	-0.0505(3)	-0.1769(6)	1.0	0.045(2)
O15	0.4171(4)	0.1274(3)	-0.3891(6)	1.0	0.042(2)
O16	0.4061(6)	-0.0010(4)	-0.4110(6)	1.0	0.048(2)

O17	0.4024(6)	-0.1312(4)	-0.4217(6)	1.0	0.048(2)
O18	0.1902(5)	0.1292(3)	-0.3830(5)	1.0	0.038(2)
O19	0.1938(6)	0.0007(3)	-0.4063(6)	1.0	0.043(2)
O20	0.1980(5)	-0.1292(3)	-0.4196(5)	1.0	0.035(2)
O21	-0.0038(3)	0.0504(5)	-0.2066(5)	1.0	0.036(2)
O22	-0.0017(4)	-0.1522(6)	-0.2105(5)	1.0	0.038(2)
O23	0.4225(7)	0.75	-0.3476(8)	0.5	0.037(2)
O24	0.1885(7)	0.75	-0.3486(7)	0.5	0.037(2)
O25	0.2861(8)	0.75	0.0550(8)	0.5	0.048(4)
O26	0.1109(6)	0.75	0.0594(8)	0.5	0.037(3)

Table 17 Refinement results for ZSM-5. Dataset was obtained after combining 6 DET-90 and 6 DET-60 patterns, and by extraction reflections with no harmonic, 1 harmonics and 2 harmonics.

Atoms	X	Y	Z	Occ.	Ueq
Si1	0.4227(1)	0.05762(8)	-0.3339(1)	1.0	0.0198(4)
Si2	0.3088(1)	0.02915(8)	-0.1869(1)	1.0	0.0217(4)
Si3	0.2788(1)	0.06146(8)	0.0328(1)	1.0	0.0195(4)
Si4	0.1223(1)	0.06267(8)	0.0298(1)	1.0	0.0211(4)
Si5	0.0720(1)	0.02754(8)	-0.1831(1)	1.0	0.0184(4)
Si6	0.1872(1)	0.05934(8)	-0.3263(1)	1.0	0.0196(4)
Si7	0.4238(1)	-0.17223(8)	-0.3249(1)	1.0	0.0195(4)
Si8	0.3094(1)	-0.12906(8)	-0.1839(1)	1.0	0.0204(4)
Si9	0.2749(1)	-0.17278(8)	0.0316(1)	1.0	0.0213(4)
Si10	0.1209(1)	-0.17357(8)	0.0300(1)	1.0	0.0203(4)
Si11	0.0708(1)	-0.13027(8)	-0.1810(1)	1.0	0.0198(4)
Si12	0.1883(1)	-0.17306(7)	-0.3177(1)	1.0	0.0190(4)
O1	0.3741(3)	0.0555(4)	-0.2412(4)	1.0	0.043(1)
O2	0.3071(3)	0.0588(3)	-0.0762(3)	1.0	0.033(1)
O3	0.2002(3)	0.0589(4)	0.0321(5)	1.0	0.054(2)
O4	0.0958(4)	0.0610(3)	-0.0815(4)	1.0	0.039(1)

O5	0.1173(3)	0.0552(3)	-0.2722(4)	1.0	0.037(1)
O6	0.2459(3)	0.0545(5)	-0.2469(4)	1.0	0.040(1)
O7	0.3761(3)	-0.1562(4)	-0.2349(4)	1.0	0.040(1)
O8	0.3097(3)	-0.1538(3)	-0.0718(4)	1.0	0.038(1)
O9	0.1970(4)	-0.1548(3)	0.0294(5)	1.0	0.044(1)
O10	0.0901(4)	-0.1620(4)	-0.0752(4)	1.0	0.046(2)
O11	0.1183(3)	-0.1578(4)	-0.2670(4)	1.0	0.038(1)
O12	0.2458(3)	-0.1567(5)	-0.2415(5)	1.0	0.052(2)
O13	0.3095(5)	-0.0498(2)	-0.1862(5)	1.0	0.059(2)
O14	0.0767(4)	-0.0505(2)	-0.1761(5)	1.0	0.048(2)
O15	0.4169(3)	0.1274(2)	-0.3897(5)	1.0	0.039(1)
O16	0.4070(4)	-0.0014(3)	-0.4091(5)	1.0	0.046(2)
O17	0.4027(4)	-0.1313(3)	-0.4226(4)	1.0	0.043(2)
O18	0.1902(4)	0.1290(2)	-0.3839(4)	1.0	0.035(1)
O19	0.1933(4)	0.0003(2)	-0.4057(4)	1.0	0.040(1)
O20	0.1976(4)	-0.1298(2)	-0.4175(4)	1.0	0.033(1)
O21	-0.0034(3)	0.0507(3)	-0.2072(4)	1.0	0.036(1)
O22	-0.0023(3)	-0.1519(4)	-0.2099(4)	1.0	0.037(1)
O23	0.4221(5)	0.75	-0.3493(6)	0.5	0.040(2)
O24	0.1894(5)	0.75	-0.3472(6)	0.5	0.036(2)
O25	0.2874(6)	0.75	0.0570(7)	0.5	0.049(3)
O26	0.1082(5)	0.75	0.0608(6)	0.5	0.040(2)