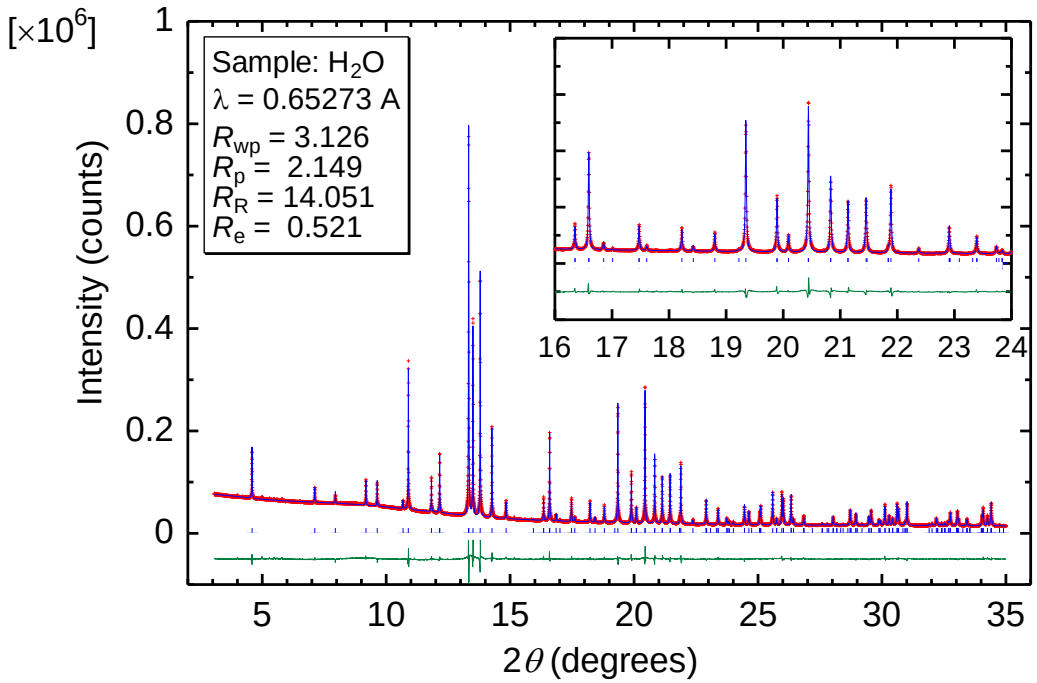
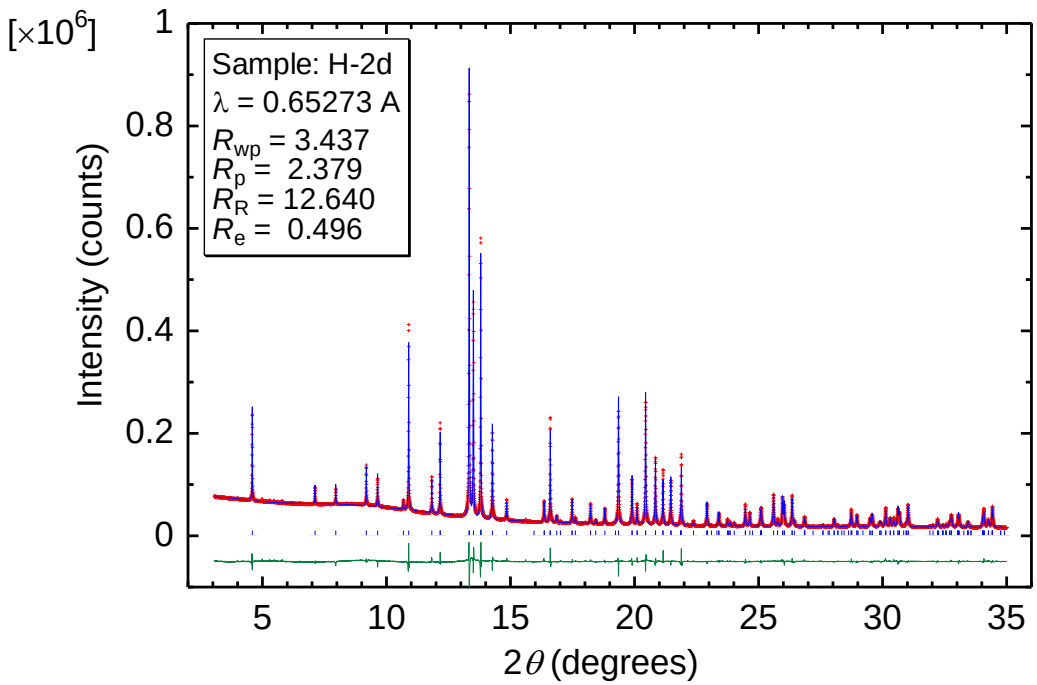
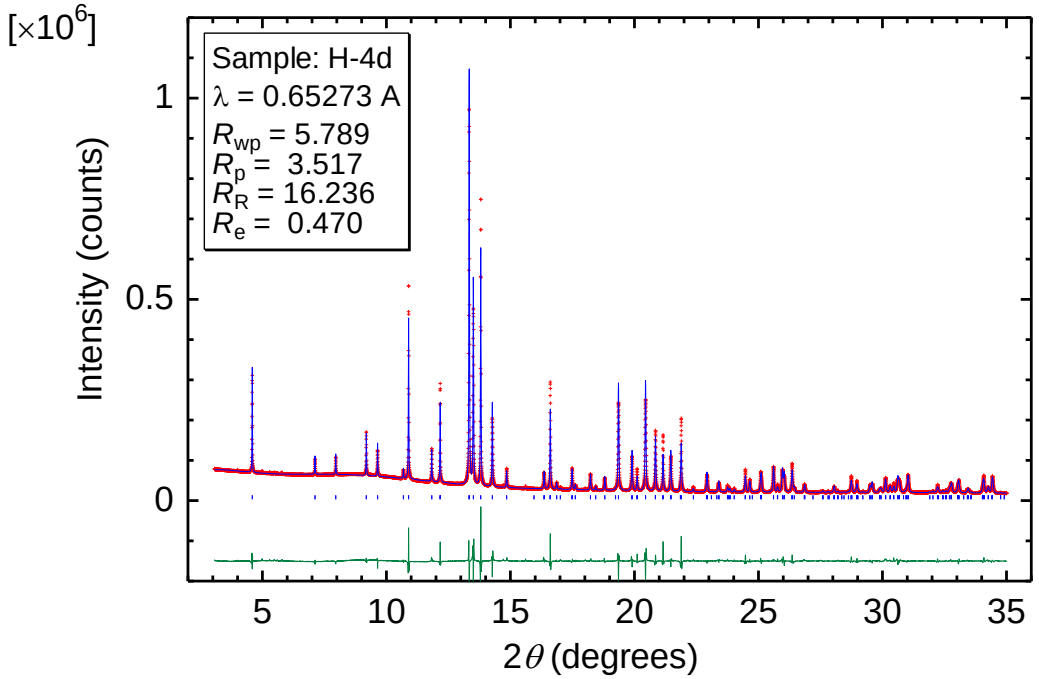
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.



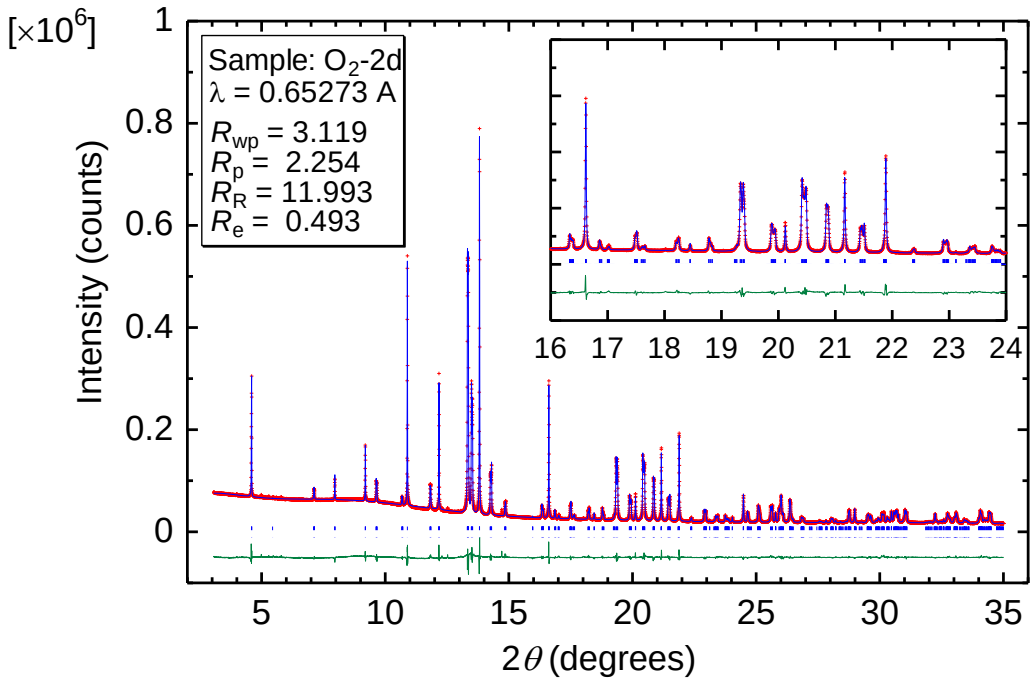
Sample	H_2O-6d		Space group		*P*63/*m* (176)	
Lattice constant	*a*	*b*	*c*	*α*	*β*	*γ*
	9.3877(1)	= *a*	6.8555(1)	90	90	120
Atom	Site	*g*	*x*	*y*	*z*	*B*
Ca1	4f	1.0	1/3	2/3	0.0018(2)	0.62(3)
Ca2	6h	1.0	0.2465(2)	0.2541(2)	1/4	0.43(3)
P	6h	1.0	0.3981(2)	0.0300(2)	1/4	0.53(3)
O1	6h	1.0	0.1567(4)	0.4829(4)	1/4	0.57(7)
O2	6h	1.0	0.5874(4)	0.1216(4)	1/4	1.05(7)
O3	12i	1.0	0.3404(2)	0.0845(2)	0.0703(4)	1.05(5)
O4	4e	0.537(4)	0	0	0.1948(8)	1.3(2)



Sample	H-2d		Space group		*P*63/*m* (176)	
Lattice constant	*a*	*b*	*c*	*α*	*β*	*γ*
	9.38410	9.38410	6.85680	90	90	120
Atom	Site	*g*	*x*	*y*	*z*	*B*
Ca1	4f	1.0	1/3	2/3	0.0022(2)	0.47(3)
Ca2	6h	1.0	0.2458(2)	0.2537(2)	1/4	0.61(3)
P	6h	1.0	0.3979(2)	0.0298(2)	1/4	0.56(3)
O1	6h	1.0	0.1574(4)	0.4843(4)	1/4	0.53(7)
O2	6h	1.0	0.5866(4)	0.1221(4)	1/4	0.99(8)
O3	12i	1.0	0.3395(2)	0.0843(2)	0.0704(4)	1.50(5)
O4	4e	0.4219	0	0	0.199(2)	1.7(3)



Sample	H-4d		Space group		*P*63/*m* (176)	
Lattice constant	*a*	*b*	*c*	*α*	*β*	*γ*
	9.3657(1)	= *a*	6.8456(1)	90	90	120
Atom	Site	*g*	*x*	*y*	*z*	*B*
Ca1	4f	1.0	1/3	2/3	0.0024(4)	0.44(4)
Ca2	6h	1.0	0.2454(2)	0.2533(4)	1/4	0.59(3)
P	6h	1.0	0.3977(4)	0.0299(4)	1/4	0.51(1)
O1	6h	1.0	0.1594(5)	0.4852(4)	1/4	0.58(10)
O2	6h	1.0	0.5859(5)	0.1218(5)	1/4	0.94(10)
O3	12i	1.0	0.3401(4)	0.0845(4)	0.0705(4)	1.44(8)
O4	4e	0.401(5)	0	0	0.200(2)	1.9 (4)



Sample	O2-2d		Space group		*P*-1 (2)	
Lattice constant	*a*	*b*	*c*	*α*	*β*	*γ*
	6.8780(1)	9.4040(1)	9.4050(1)	60.011(1)	89.845(1)	89.764(1)
Atom	Site	*g*	*x*	*y*	*z*	*B*
Ca1a	2i	1.0	0.5013(7)	0.3396(7)	0.3316(5)	0.47(3)
Ca1b	2i	1.0	0.0024(7)	0.6742(7)	0.6638(5)	= Ca1a
Ca2a	2i	1.0	0.2532(7)	0.7561(7)	0.2513(7)	0.82(2)
Ca2b	2i	1.0	0.7498(7)	0.0095(7)	0.2436(7)	= Ca2a
Ca2c	2i	1.0	0.2462(5)	0.2556(7)	0.9907(5)	= Ca2a
Pa	2i	1.0	0.2484(7)	0.6025(8)	0.0301(7)	0.53(3)
Pb	2i	1.0	0.2411(7)	0.3644(7)	0.6048(7)	= Pa
Pc	2i	1.0	0.2485(7)	0.0261(8)	0.3718(7)	= Pa
O1a	2i	1.0	0.7431(14)	0.3254(14)	0.1586(14)	0.66(7)
O1b	2i	1.0	0.2396(13)	0.4891(15)	0.6698(13)	= O1a
O1c	2i	1.0	0.7372(14)	0.1566(16)	0.5170(14)	= O1a
O2a	2i	1.0	0.2468(17)	0.4132(14)	0.1263(15)	1.19(8)
O2b	2i	1.0	0.2504(14)	0.4653(15)	0.4194(13)	= O2a
O2c	2i	1.0	0.2750(15)	0.1218(14)	0.4666(13)	= O2a
O3a	2i	1.0	0.4266(14)	0.6513(13)	0.0974(14)	1.35(6)
O3b	2i	1.0	0.4159(14)	0.2526(14)	0.6836(13)	= O3a
O3c	2i	1.0	0.4147(13)	0.0712(11)	0.2307(13)	= O3a
O3d	2i	1.0	0.0727(13)	0.6551(13)	0.0842(13)	= O3a
O3e	2i	1.0	0.0520(15)	0.2677(14)	0.6400(13)	= O3a
O3f	2i	1.0	0.0623(13)	0.0922(13)	0.2656(13)	= O3a
O4a	2i	0.38(4)	0.177(5)	0.002(4)	0.010(7)	1.9(4)
O4b	2i	0.44(4)	0.274(4)	0.007(4)	0.985(6)	= O4a