Electronic Supplementary Information to:

A new structural model for disorder in vaterite from first-principles calculations.

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Fractional coordinates of the minimum energy vaterite structures as obtained with the PBEsol functional.

Table 1 *P6₅* (space group number, SGN=170, hexagonal; *a*=7.1120 Å, *c*= 25.4089 Å)

	x/a	*y/b*	*z/c*
Ca	0.95661	0.97935	0.08650
Ca	0.67921	0.31096	0.08050
Ca	0.30019	0.62994	0.08153
C	0.04111	0.35589	0.99496
C	0.65885	0.61228	0.00485
C	0.01935	0.31215	0.66700
O	0.03599	0.14063	0.67262
O	0.00532	0.36944	0.61897
O	0.58087	0.59863	0.37438
O	0.95631	0.25748	0.95143
O	0.64138	0.66134	0.05336
O	0.21600	0.54229	0.99401
O	0.67527	0.44184	0.99694
O	0.95776	0.27600	0.04054
O	0.66170	0.72781	0.96587

Table 2 *P3₂21* (SGN=154, hexagonal; *a*=7.1239 Å, *c*= 25.3203 Å). This is the least-energy structure.

	x/a	*y/b*	*z/c*
Ca	0.98731	0.00884	0.25020
Ca	0.66938	0.29692	0.25375
Ca	0.30357	0.63281	0.24648
C	0.03394	0.36633	0.16169
C	0.94957	0.62773	0.66089
C	0	0.30149	5/6
C	0	0.69852	1/3
O	0	0.11971	5/6
O	0	0.87944	1/3
O	0.98084	0.37860	0.78859
O	0.99342	0.60886	0.28838
O	0.92793	0.26758	0.12000
O	0.99651	0.67669	0.61111
O	0.21701	0.54412	0.15803
O	0.77434	0.44983	0.67169
O	0.96475	0.29501	0.20912
O	0.07260	0.75107	0.69768

Table 3 *Ama2* (SGN=40, orthorhombic; *a*=8.4905 Å, *b*=6.3905 Å, *c*=4.5026 Å)

	x/a	*y/b*	*z/c*
Ca	1/2	0	0.50868
C	1/4	0.14432	0.94400
O	0.38423	0.16589	0.07718
O	1/4	0.10559	0.66336

Table 4 *P2₁2₁2₁* (SGN=19, orthorhombic; *a*=4.3668 Å, *b*=6.5831 Å, *c*=8.4282 Å)

	x/a	*y/b*	*z/c*
Ca	0.28955	0.98906	0.51457
C	0.22679	0.63243	0.24756
O	0.98002	0.53149	0.22359
O	0.31307	0.66026	0.39468
O	0.11592	0.29549	0.63138

Table 5 *P112₁* (SGN=4, monoclinic; *a*=7.1115 Å, *b*=7.1013 Å, *c*=25.3601 Å, γ=60.34 degrees)

	x/a	*y/b*	*z/c*
Ca	0.03048	0.01021	0.91600
Ca	0.00358	0.98939	0.25061
Ca	0.99067	0.01696	0.58150
Ca	0.33271	0.32070	0.91682
Ca	0.32519	0.38051	0.25303
Ca	0.39467	0.31746	0.58319
Ca	0.68393	0.63524	0.91794
Ca	0.69467	0.66844	0.24748
Ca	0.66489	0.70193	0.58607
C	0.95198	0.36682	0.00457
C	0.36547	0.68393	0.33905
C	0.67493	0.96202	0.67233
C	0.32695	0.62360	0.99400
C	0.03511	0.33458	0.66160
C	0.62352	0.04956	0.32845
C	0.99717	0.30398	0.33296
C	0.30178	0.70083	0.66675
C	0.70123	0.98724	0.00011
O	0.97450	0.13478	0.33495
O	0.12301	0.88341	0.66567
O	0.87469	0.00122	0.99548
O	0.00660	0.39463	0.37614
O	0.37561	0.60859	0.71201
O	0.63519	0.98449	0.04806
O	0.39984	0.61847	0.62261
O	0.00969	0.37557	0.28661
O	0.60165	0.97605	0.95887
O	0.04295	0.28012	0.04866
O	0.30733	0.69575	0.38839
O	0.66430	0.06888	0.71410
O	0.32925	0.67596	0.94472
O	0.92940	0.34740	0.61942
O	0.68221	0.98879	0.27995
O	0.75922	0.53118	0.00465
O	0.55185	0.66447	0.32964
O	0.67795	0.77942	0.67528
O	0.34209	0.43874	0.00360
O	0.21855	0.33007	0.65885
O	0.45646	0.23766	0.33591
O	0.04517	0.29634	0.95934
O	0.24189	0.68994	0.30154
O	0.68180	0.03097	0.62518
O	0.31045	0.75161	0.03156
O	0.96635	0.32567	0.70849
O	0.72603	0.92955	0.36789

Notes and references

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