

Supplementary Information for “Simulating preferential sorption of tartrate on prismatic calcite surfaces”

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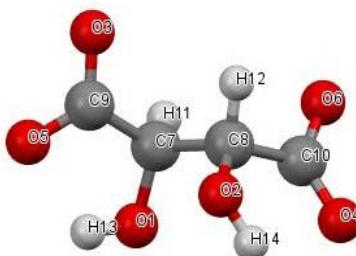


Fig. S1. Tartrate molecule structure and atom names.

Table S1. Atom names, atom types and RESP charges of tartrate.

Atom	GAFF atom type	RESP Charge
O1	oh	-0.7468
O2	oh	-0.7804
O3	o	-0.8449
O4	o	-0.8591
O5	o	-0.8202
O6	o	-0.8166
C7	c3	0.2351
C8	c3	0.3247
C9	c	0.8092
C10	c	0.8127
H11	h1	-0.0468
H12	h1	-0.0771
H13	ho	0.3975
H14	ho	0.4125