

!BIOSYM archive 3

PBC=ON

Optimized structure of hydronium alunite at the AM05/TZ2P level from Gale et al

!DATE Wed Feb 24 11:08:07 2010

PBC 7.0569 7.0351 16.9607 90.0161 90.0253 119.5894 (P1)

S	3.612518012	2.022695788	10.833376724	CORE 1	?	S	6.000
O	3.597133746	2.016402086	12.322407628	CORE 1	?	O	-2.000
O	4.965229115	1.248840894	8.041306568	CORE 1	?	O	-2.000
H	5.722033387	0.807284282	7.579458649	CORE 1	?	H	1.000
O	3.649196516	3.601510207	8.123612463	CORE 1	?	O	-2.000
H	3.639592216	4.336096365	7.464569306	CORE 1	?	H	1.000
O	2.328356718	1.278997602	7.894844977	CORE 1	?	O	-2.000
H	1.513849939	0.840027613	7.532618342	CORE 1	?	H	1.000
Al	-1.666084953	3.016057441	8.498787436	CORE 1	?	Al	3.000
O	-1.139159087	3.385397373	6.679904729	CORE 1	?	O	-2.000
Al	3.652651387	-0.004149792	8.481046841	CORE 1	?	Al	3.000
O	0.104841733	5.485848044	6.645282600	CORE 1	?	O	-2.000
Al	1.864254548	3.085074655	8.506256268	CORE 1	?	Al	3.000
O	1.327725869	3.363433468	6.647670502	CORE 1	?	O	-2.000
O	2.391707014	2.730143297	10.329873057	CORE 1	?	O	-2.000
O	3.602784593	0.610566940	10.324040937	CORE 1	?	O	-2.000
O	4.858082200	2.715038555	10.357835043	CORE 1	?	O	-2.000
S	0.092331871	4.062108153	6.159245272	CORE 1	?	S	6.000
O	0.072319280	4.039346513	4.672639925	CORE 1	?	O	-2.000
O	1.466587635	4.856255531	8.901614353	CORE 1	?	O	-2.000
H	2.165392870	5.249101357	9.478356024	CORE 1	?	H	1.000
O	0.110050030	2.505513602	8.917764200	CORE 1	?	O	-2.000
H	0.099647312	1.670093375	9.449521239	CORE 1	?	H	1.000
O	-1.165248662	4.828363146	9.104991271	CORE 1	?	O	-2.000
H	-1.987484996	5.277437467	9.432940928	CORE 1	?	H	1.000
S	3.582352044	6.093712525	5.186649244	CORE 2	?	S	6.000
O	-3.448111410	6.107460595	6.667147708	CORE 2	?	O	-2.000
O	-2.105567507	5.286902051	2.405117984	CORE 2	?	O	-2.000
H	-1.359108543	4.851930356	1.921049629	CORE 2	?	H	1.000
O	0.035339552	1.439389489	2.225174364	CORE 2	?	O	-2.000
H	0.016594268	2.374306388	1.894191448	CORE 2	?	H	1.000
O	2.246686923	5.270303200	2.452695066	CORE 2	?	O	-2.000
H	1.602593753	4.907457573	1.797112918	CORE 2	?	H	1.000
Al	1.810964605	0.930599620	2.845227152	CORE 2	?	Al	3.000
O	2.324908219	1.290693895	1.003472886	CORE 2	?	O	-2.000
Al	3.613148721	4.043222064	2.851610157	CORE 2	?	Al	3.000
O	3.549932574	3.408006624	1.022924142	CORE 2	?	O	-2.000
Al	5.293618573	0.946049381	2.812920842	CORE 2	?	Al	3.000
O	4.772797172	1.270838117	0.978500231	CORE 2	?	O	-2.000
O	5.812917242	0.692633711	4.693372734	CORE 2	?	O	-2.000
O	3.586700090	4.684710451	4.689155615	CORE 2	?	O	-2.000
O	1.197803560	0.705907016	4.657314539	CORE 2	?	O	-2.000
S	3.549502779	2.003385364	0.502541654	CORE 2	?	S	6.000
O	3.536405713	2.015933116	15.976801691	CORE 2	?	O	-2.000
O	4.940332331	2.751583499	3.253015255	CORE 2	?	O	-2.000
H	-1.431716092	3.143729932	3.849417478	CORE 2	?	H	1.000
O	3.551917658	0.425896967	3.287093623	CORE 2	?	O	-2.000
H	0.090532386	5.670844932	3.756896808	CORE 2	?	H	1.000

O	2.282116151	2.717022740	3.439723158	CORE 2	?	O	-2.000
H	1.502166312	3.205595053	3.821453457	CORE 2	?	H	1.000
Al	-1.729230459	5.125511520	14.110040510	CORE 3	?	Al	3.000
O	-1.217005219	4.858451601	15.990467808	CORE 3	?	O	-2.000
Al	0.065778228	2.098064634	14.158379807	CORE 3	?	Al	3.000
O	0.018728168	2.725942524	15.984523238	CORE 3	?	O	-2.000
Al	1.837438459	5.109484029	14.120672519	CORE 3	?	Al	3.000
O	1.226233846	4.856060216	15.945383955	CORE 3	?	O	-2.000
S	0.003670565	0.080438514	11.788541860	CORE 3	?	S	6.000
O	0.006477521	0.075147688	10.308588345	CORE 3	?	O	-2.000
O	1.382165293	0.807895207	14.562041532	CORE 3	?	O	-2.000
H	2.112547808	1.223576706	15.088495625	CORE 3	?	H	1.000
O	3.582725088	4.596084320	14.563170099	CORE 3	?	O	-2.000
H	3.579905853	3.763326971	15.095465133	CORE 3	?	H	1.000
O	5.794710735	0.781671769	14.733120281	CORE 3	?	O	-2.000
H	5.006756137	1.250801195	15.121623005	CORE 3	?	H	1.000
S	0.028206574	4.141188443	16.480823001	CORE 3	?	S	6.000
O	0.053209684	4.144539417	1.000067509	CORE 3	?	O	-2.000
O	1.401343121	3.335343478	13.698074298	CORE 3	?	O	-2.000
H	2.119054033	2.905659515	13.169620024	CORE 3	?	H	1.000
O	0.061591174	5.603094280	13.538917422	CORE 3	?	O	-2.000
H	3.525238989	0.401958982	13.143085794	CORE 3	?	H	1.000
O	-1.301223381	3.325753727	13.710770769	CORE 3	?	O	-2.000
H	5.018686693	2.904601488	13.199546064	CORE 3	?	H	1.000
O	2.360334739	5.519539849	12.309412478	CORE 3	?	O	-2.000
O	0.014990801	1.511998528	12.287650661	CORE 3	?	O	-2.000
O	-2.251042257	5.482412375	12.286762427	CORE 3	?	O	-2.000
H	-0.116176667	3.194019637	11.520132883	CORE 4	?	H	1.000
H	-0.484817984	4.452538219	10.445669121	CORE 4	?	H	1.000
H	-0.003169703	4.733164174	12.122185746	CORE 4	?	H	1.000
O	0.059210840	4.144102790	11.286606213	CORE 4	?	O	-2.000
H	4.286058511	1.405247479	5.444915529	CORE 5	?	H	1.000
H	3.015210414	1.701355746	6.497477717	CORE 5	?	H	1.000
H	2.984294916	2.238957705	4.822123242	CORE 5	?	H	1.000
O	3.539592718	2.024914014	5.667402792	CORE 5	?	O	-2.000
H	-0.492792702	0.383390696	16.123677464	CORE 6	?	H	1.000
H	0.877075359	-0.342243565	16.738099117	CORE 6	?	H	1.000
H	0.010204525	0.641846713	17.793530215	CORE 6	?	H	1.000
O	-0.023006379	0.018748893	16.966238717	CORE 6	?	O	-2.000

end  
end