Deposited Table 7 Anisotropic displacement parameters for sartorite

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pb1	0.0477(5)	0.0568(5)	0.0562(6)	-0.0040(4)	0.0081(4)	-0.0069(4)
Pb2	0.0549(5)	0.0565(5)	0.0731(7)	0.0047(5)	0.0243(5)	0.0134(4)
Pb3	0.0440(5)	0.0579(5)	0.0511(6)	-0.0009(4)	0.0068(4)	0.0050(4)
Pb4	0.0473(5)	0.0461(5)	0.0815(7)	0.0013(5)	0.0233(5)	-0.0002(4)
Pb5	0.0390(4)	0.0641(5)	0.0571(6)	-0.0053(4)	0.0107(4)	-0.0012(4)
Pb6	0.0395(4)	0.0475(5)	0.0587(6)	-0.0047(4)	0.0083(4)	0.0047(3)
Pb7	0.0420(5)	0.0603(5)	0.0830(8)	-0.0065(5)	0.0158(5)	-0.0081(4)
Pb8	0.0446(5)	0.0538(5)	0.0684(7)	-0.0078(5)	0.0139(4)	-0.0090(4)
Pb9	0.0515(5)	0.0526(5)	0.0606(6)	0.0094(4)	0.0224(4)	0.0141(4)
As1	0.0350(10)	0.0437(11)	0.0434(13)	0.0062(10)	0.0064(9)	0.0000(8)
As2	0.0373(10)	0.0384(10)	0.0403(13)	-0.0036(9)	0.0101(9)	0.0025(8)
As3	0.0441(11)	0.0476(11)	0.0403(13)	-0.0078(10)	0.0095(9)	-0.0098(9)
As4	0.0367(10)	0.0423(11)	0.0422(13)	-0.0037(10)	0.0009(9)	0.0015(8)
As6	0.0537(13)	0.0401(11)	0.0448(13)	0.0017(10)	0.0158(10)	0.0008(9)
As7	0.0391(11)	0.0606(13)	0.0448(14)	0.0008(11)	0.0090(10)	0.0003(10)
As8	0.0377(10)	0.0392(10)	0.0487(13)	-0.0005(9)	0.0074(9)	0.0031(8)
As9a	0.076(7)	0.045(3)	0.059(3)	-0.002(3)	0.032(4)	0.001(5)
As9b	0.011(5)	0.016(5)	0.036(4)	-0.005(3)	-0.002(3)	-0.012(3)
As10	0.0381(11)	0.0453(11)	0.0423(13)	0.0047(10)	0.0070(9)	0.0012(9)
As11	0.0374(10)	0.0409(10)	0.0347(12)	0.0009(9)	0.0068(9)	0.0055(8)
As12	0.118(2)	0.0452(13)	0.0497(16)	-0.0138(12)	0.0392(15)	-0.0336(13)
M13a	0.042(3)	0.027(3)	0.045(3)	-0.005(2)	0.012(2)	-0.007(2)
M13b	0.046(2)	0.037(2)	0.078(3)	0.015(2)	0.028(2)	0.0021(18)
As14	0.0308(10)	0.0448(11)	0.0404(13)	0.0032(9)	0.0044(9)	0.0008(8)
As15	0.0349(10)	0.0440(11)	0.0488(14)	0.0082(10)	-0.0008(9)	-0.0001(9)
As16	0.0631(13)	0.0360(11)	0.0404(13)	-0.0027(9)	-0.0029(10)	0.0023(10)
As17	0.0559(13)	0.0583(14)	0.0452(14)	-0.0035(11)	0.0028(11)	0.0082(11)
As18	0.0326(10)	0.0374(10)	0.0388(12)	-0.0060(9)	0.0045(9)	-0.0002(8)
S1	0.035(2)	0.037(2)	0.037(3)	-0.004(2)	0.002(2)	-0.0041(19)
S2	0.059(3)	0.037(3)	0.055(4)	0.003(2)	0.003(3)	-0.005(2)
S3	0.034(2)	0.049(3)	0.040(3)	0.007(2)	0.007(2)	0.000(2)
S4	0.035(2)	0.033(2)	0.042(3)	0.001(2)	0.009(2)	-0.0021(19)
S5	0.037(3)	0.038(3)	0.057(4)	-0.011(3)	0.007(2)	-0.002(2)
S6	0.048(3)	0.045(3)	0.033(3)	0.000(2)	0.012(2)	-0.002(2)
S7	0.034(3)	0.044(3)	0.071(4)	0.006(3)	0.012(3)	-0.003(2)
S8	0.039(3)	0.045(3)	0.047(3)	-0.001(2)	0.006(2)	0.001(2)
S9	0.038(3)	0.037(3)	0.039(3)	-0.001(2)	0.009(2)	0.0022(19)
S10	0.055(3)	0.036(3)	0.056(4)	0.001(2)	0.017(3)	-0.002(2)
S11	0.074(4)	0.048(3)	0.063(4)	-0.011(3)	-0.004(3)	-0.006(3)
S12	0.043(3)	0.028(2)	0.050(3)	0.003(2)	0.009(2)	-0.003(2)
S13	0.037(3)	0.040(3)	0.059(4)	-0.008(3)	0.006(2)	0.004(2)
S14	0.042(3)	0.048(3)	0.040(3)	-0.002(2)	0.009(2)	-0.007(2)
S15	0.055(3)	0.042(3)	0.065(4)	0.008(3)	0.026(3)	0.009(2)
S16	0.049(3)	0.053(3)	0.050(4)	0.000(3)	0.013(3)	-0.012(2)
S17	0.047(3)	0.042(3)	0.059(4)	0.003(3)	0.022(3)	0.006(2)
S18	0.043(3)	0.048(3)	0.041(3)	0.002(2)	0.006(2)	0.001(2)
S19	0.038(3)	0.039(3)	0.046(3)	-0.001(2)	0.009(2)	-0.004(2)
S20	0.039(3)	0.043(3)	0.050(3)	0.001(2)	0.006(2)	0.004(2)
S21	0.037(3)	0.041(3)	0.044(3)	0.001(2)	0.004(2)	-0.005(2)
S22	0.043(3)	0.037(2)	0.052(3)	0.003(2)	0.011(2)	-0.002(2)
S23	0.039(3)	0.041(3)	0.048(3)	-0.004(2)	0.010(2)	-0.001(2)
S24	0.032(2)	0.038(3)	0.052(3)	0.002(2)	0.011(2)	0.0004(19)
S25	0.037(3)	0.039(3)	0.037(3)	-0.001(2)	0.004(2)	-0.003(2)
S26	0.030(2)	0.046(3)	0.053(3)	0.012(2)	0.009(2)	0.005(2)
S27	0.040(3)	0.037(2)	0.037(3)	-0.006(2)	0.001(2)	0.002(2)
S28	0.034(2)	0.039(2)	0.046(3)	-0.004(2)	0.006(2)	-0.002(2)
S29	0.044(3)	0.040(3)	0.047(3)	0.006(2)	0.004(2)	0.007(2)
S30	0.035(3)	0.052(3)	0.043(3)	0.007(3)	0.006(2)	0.002(2)
S31	0.042(3)	0.039(3)	0.039(3)	0.002(2)	0.008(2)	0.000(2)
S32	0.035(3)	0.038(3)	0.046(3)	-0.004(2)	0.008(2)	0.002(2)
S33	0.036(2)	0.042(3)	0.031(3)	0.001(2)	0.006(2)	-0.004(2)
S34	0.035(3)	0.048(3)	0.116(6)	0.022(3)	0.003(3)	0.001(2)
S35	0.036(2)	0.037(2)	0.036(3)	0.002(2)	0.009(2)	0.004(2)

Deposited Table 8 Bond distances and angles (full Table)

Pb1	S32	S1	S5	S4	S28	S31	S30	S6	S2
S32	3.172(5)	84.3(1)	136.3(1)	66.4(1)	81.6(1)	67.8(1)	128.6(1)	136.8(1)	71.0(1)
S1	4.258(7)	3.175(5)	85.6(1)	69.1(1)	135.6(1)	144.2(1)	65.3(1)	132.4(1)	78.2(1)
S5	5.895(7)	4.319(7)	3.180(5)	70.2(1)	76.5(1)	130.0(1)	83.8(1)	77.3(1)	146.8(1)
S4	3.479(8)	3.604(8)	3.659(7)	3.182(6)	66.6(1)	115.4(1)	128.6(1)	139.5(1)	127.9(1)
S28	4.177(7)	5.923(7)	3.964(7)	3.517(6)	3.222(6)	63.8(1)	148.6(1)	82.9(1)	134.2(1)
S31	3.616(7)	6.174(7)	5.885(7)	5.488(8)	3.452(8)	3.312(5)	115.4(1)	69.2(1)	72.0(1)
S30	5.851(8)	3.505(7)	4.342(9)	5.859(9)	6.300(8)	5.606(8)	3.321(6)	68.9(1)	63.2(1)
S6	6.051(7)	5.958(7)	4.071(8)	6.113(8)	4.344(8)	3.776(7)	3.767(7)	3.335(5)	92.5(1)
S2	3.793(9)	4.123(8)	6.264(8)	5.872(9)	6.059(9)	3.918(8)	3.498(7)	4.833(8)	3.355(6)

Pb2	S5	S8	S6	S9	S24	S10	S26	S27	S28
S5	2.995(5)	71.2(1)	84.4(1)	85.7(1)	135.5(1)	148.4(1)	84.3(1)	127.8(1)	76.2(1)
S8	3.521(8)	3.054(6)	148.4(1)	66.6(1)	65.3(1)	129.4(1)	126.8(1)	114.9(1)	71.0(1)
S6	4.071(8)	5.888(9)	3.065(6)	132.6(1)	130.9(1)	81.6(1)	67.9(1)	65.1(1)	84.1(1)
S9	4.164(7)	3.392(7)	5.668(8)	3.124(5)	85.6(1)	83.3(1)	65.1(1)	146.0(1)	137.3(1)
S24	5.721(7)	3.370(7)	5.686(9)	4.289(7)	3.185(6)	73.0(1)	129.8(1)	67.0(1)	81.2(1)
S10	5.979(7)	5.671(8)	4.106(8)	4.214(7)	3.810(8)	3.218(5)	64.2(1)	70.1(1)	129.8(1)
S26	4.239(7)	5.692(9)	3.567(7)	3.464(9)	5.882(8)	3.469(7)	3.311(6)	117.4(1)	147.4(1)
S27	5.722(7)	5.422(8)	3.474(8)	6.214(7)	3.621(8)	3.789(7)	5.712(7)	3.373(5)	60.2(1)
S28	3.964(7)	3.764(7)	4.344(8)	6.084(7)	4.294(7)	6.000(7)	6.447(7)	3.402(7)	3.407(5)

Pb3	S13	S14	S10	S9	S12	S22	S20	S24	S23
S13	3.025(5)	84.6(1)	151.4(1)	86.2(1)	69.6(1)	84.4(1)	75.8(1)	133.1(1)	128.8(1)
S14	4.092(8)	3.055(5)	83.0(1)	137.8(1)	144.0(1)	68.8(1)	84.7(1)	130.4(1)	66.7(1)
S10	5.918(8)	4.067(8)	3.083(6)	85.8(1)	130.9(1)	67.1(1)	128.3(1)	73.1(1)	68.4(1)
S9	4.194(8)	5.751(7)	4.214(7)	3.110(5)	67.1(1)	69.3(1)	132.3(1)	83.8(1)	143.1(1)
S12	3.533(7)	5.910(8)	5.679(9)	3.467(8)	3.160(6)	130.0(1)	65.2(1)	64.3(1)	110.2(1)
S22	4.173(9)	3.529(7)	3.465(7)	3.581(7)	5.752(9)	3.187(6)	148.3(1)	132.8(1)	119.3(1)
S20	3.874(7)	4.268(8)	5.721(9)	5.838(8)	3.466(7)	6.215(8)	3.273(6)	77.7(1)	60.7(1)
S24	5.813(7)	5.778(7)	3.810(8)	4.289(7)	3.444(8)	5.952(7)	4.130(7)	3.310(5)	64.2(1)
S23	5.719(7)	3.511(7)	3.600(8)	6.095(7)	5.313(7)	5.611(7)	3.328(8)	3.518(7)	3.316(5)

Pb4	S16	S13	S14	S18	S17	S16	S19	S20
S16	3.083(6)	82.6(1)	139.8(1)	68.6(1)	87.7(1)	80.2(2)	144.2(1)	128.1(1)
S13	4.075(8)	3.089(5)	82.4(1)	84.0(1)	150.1(1)	130.3(1)	129.5(1)	73.6(1)
S14	5.828(9)	4.092(8)	3.123(6)	72.9(1)	87.0(1)	136.0(1)	69.3(1)	82.1(1)
S18	3.498(9)	4.161(7)	3.714(7)	3.126(5)	66.1(1)	130.1(1)	123.0(1)	148.4(1)
S17	4.351(8)	6.070(7)	4.349(8)	3.446(7)	3.194(5)	75.1(1)	70.8(1)	132.5(1)
S16	4.055(8)	5.719(8)	5.875(9)	5.747(8)	3.903(8)	3.213(6)	67.0(1)	81.4(1)
S19	6.047(8)	5.753(7)	3.636(8)	5.622(7)	3.748(7)	3.577(9)	3.271(5)	62.1(1)
S20	5.803(7)	3.874(7)	4.268(8)	6.250(7)	6.008(7)	4.293(8)	3.424(7)	3.368(5)

Pb5	S20	S16	S15	S19	S17	S21	S16	S13
S20	2.948(5)	93.0(2)	80.2(1)	69.3(1)	150.2(1)	90.9(1)	135.3(1)	82.7(1)
S16	4.293(8)	2.969(6)	81.0(2)	72.6(1)	91.8(2)	153.5(2)	79.5(2)	134.2(1)
S15	3.818(9)	3.861(8)	2.976(6)	137.9(1)	71.6(1)	73.9(1)	139.9(1)	141.7(1)
S19	3.424(7)	3.577(9)	5.644(9)	3.072(6)	139.7(1)	132.8(1)	66.4(1)	63.2(1)
S17	5.833(8)	4.351(8)	3.546(7)	5.782(9)	3.087(6)	72.5(1)	74.4(1)	113.9(1)
S21	4.328(8)	5.930(7)	3.667(7)	5.677(8)	3.673(7)	3.123(5)	115.0(1)	72.3(1)
S16	5.833(7)	4.055(8)	5.950(8)	3.528(8)	3.903(8)	5.467(7)	3.356(5)	72.6(1)
S13	4.296(7)	5.983(8)	6.141(8)	3.475(7)	5.546(9)	3.936(9)	4.075(8)	3.523(6)

Pb6	S23	S24	S20	S13	S9	S11	S12	S25	S21
S23	2.775(6)	75.9(2)	69.7(1)	71.2(1)	76.3(1)	130.4(2)	121.1(1)	147.0(1)	131.0(1)
S24	3.518(7)	2.943(5)	87.4(1)	145.9(1)	78.9(1)	82.1(1)	129.2(1)	79.8(1)	141.2(1)
S20	3.328(8)	4.130(7)	3.034(5)	89.5(1)	145.6(1)	65.3(1)	142.6(1)	131.3(1)	79.9(1)
S13	3.410(8)	5.746(7)	4.296(7)	3.066(5)	84.8(1)	126.8(1)	64.9(1)	125.5(1)	71.0(1)
S9	3.674(7)	3.878(7)	5.911(8)	4.194(8)	3.154(6)	141.5(1)	62.8(1)	77.4(1)	129.0(1)
S11	5.530(9)	4.116(9)	3.433(8)	5.703(8)	6.104(9)	3.312(6)	107.3(1)	66.4(1)	59.3(1)
S12	5.460(7)	5.809(7)	6.173(7)	3.533(7)	3.467(8)	5.475(8)	3.483(5)	61.0(1)	66.4(1)
S25	6.080(7)	4.200(8)	6.013(7)	5.897(7)	4.210(8)	3.770(8)	3.578(7)	3.562(5)	81.5(1)
S21	5.869(9)	6.234(8)	4.328(8)	3.936(9)	6.157(9)	3.464(8)	3.915(8)	4.716(7)	3.662(6)

Pb7	S27	S24	S28	S29	S5	S9	S25	S8	S7
S27	2.878(6)	75.6(1)	70.1(1)	137.4(1)	70.0(1)	73.5(1)	151.8(1)	118.8(1)	133.9(1)
S24	3.621(8)	3.028(5)	90.1(1)	140.1(1)	144.6(1)	78.3(1)	84.3(1)	128.6(1)	81.3(1)
S28	3.402(7)	4.294(7)	3.041(5)	84.7(1)	86.2(1)	143.5(1)	130.3(1)	141.1(1)	70.7(1)
S29	5.577(8)	5.767(7)	4.144(8)	3.108(5)	74.7(1)	125.7(1)	69.8(1)	63.3(1)	59.6(1)
S5	3.439(7)	5.845(7)	4.204(7)	3.770(9)	3.108(6)	84.0(1)	123.9(1)	65.2(1)	129.7(1)
S9	3.593(8)	3.878(7)	5.847(7)	5.537(7)	4.164(7)	3.115(5)	83.2(1)	62.5(1)	139.1(1)
S25	5.920(9)	4.200(8)	5.687(8)	3.623(7)	5.590(9)	4.210(8)	3.225(6)	60.4(1)	59.7(1)
S8	5.416(8)	5.801(7)	6.082(7)	3.427(7)	3.521(8)	3.392(7)	3.343(8)	3.408(5)	106.9(1)
S7	6.165(9)	4.493(7)	4.011(9)	3.492(8)	6.269(8)	6.493(8)	3.538(7)	5.801(8)	3.809(6)

Pb8	S31	S28	S32	S5	S1	S3	S4	S29	S33
S31	2.867(6)	71.9(1)	75.8(1)	71.2(1)	74.1(1)	132.7(1)	121.4(1)	129.7(1)	144.7(1)
S28	3.452(8)	3.013(5)	87.7(1)	87.0(1)	145.4(1)	65.0(1)	140.9(1)	77.4(1)	127.7(1)
S32	3.616(7)	4.177(7)	3.018(5)	146.5(1)	78.5(1)	83.9(1)	130.1(1)	141.8(1)	76.3(1)
S5	3.472(8)	4.204(7)	5.850(7)	3.091(5)	87.4(1)	123.0(1)	66.9(1)	68.4(1)	131.2(1)
S1	3.637(7)	5.893(7)	3.911(7)	4.319(7)	3.159(6)	142.6(1)	65.1(1)	131.1(1)	79.7(1)
S3	5.839(9)	3.523(7)	4.373(9)	5.796(7)	6.309(8)	3.501(6)	104.5(1)	57.9(1)	64.1(1)
S4	5.574(8)	6.153(7)	5.925(7)	3.659(7)	3.604(8)	5.546(7)	3.514(5)	66.3(1)	64.9(1)
S29	5.841(9)	4.144(8)	6.233(8)	3.770(9)	6.132(9)	3.424(7)	3.877(8)	3.575(6)	85.4(1)
S33	6.178(7)	5.952(6)	4.119(7)	6.106(6)	4.351(7)	3.774(7)	3.823(6)	4.873(7)	3.611(4)

Pb9	S35	S32	S1	S32	S2	S1	S33	S35	S34
S35	2.889(4)	77.8(1)	69.5(1)	69.2(1)	135.4(1)	76.3(1)	155.5(1)	121.1(2)	129.7(1)
S32	3.682(7)	2.973(5)	88.9(1)	145.8(2)	138.5(1)	79.1(1)	82.8(1)	125.8(1)	81.4(1)
S1	3.372(6)	4.199(7)	3.023(5)	88.2(1)	84.0(1)	145.4(2)	125.4(1)	144.3(1)	64.7(1)
S32	3.405(6)	5.801(7)	4.258(7)	3.097(5)	74.9(1)	84.2(1)	125.6(1)	68.1(1)	127.2(1)
S2	5.579(7)	5.716(7)	4.123(8)	3.793(9)	3.139(5)	125.8(1)	68.9(1)	64.8(1)	58.6(1)
S1	3.745(7)	3.911(7)	5.908(7)	4.199(7)	5.611(7)	3.165(5)	85.5(1)	61.0(1)	142.7(1)
S33	5.998(7)	4.119(7)	5.572(7)	5.644(8)	3.612(8)	4.351(7)	3.248(5)	60.3(1)	60.6(1)
S35	5.538(7)	5.732(7)	6.174(7)	3.682(7)	3.547(7)	3.372(6)	3.377(7)	3.462(5)	108.3(1)
S34	6.096(9)	4.485(8)	3.733(10)	6.214(9)	3.466(8)	6.631(8)	3.609(7)	5.914(8)	3.832(7)

As1	S7	S3	S29	S6	S2	S31	S30
S7	2.273(5)	98.0(2)	98.9(2)	82.7(2)	157.8(2)	89.2(2)	68.7(2)
S3	3.456(7)	2.306(6)	95.5(2)	177.1(2)	75.6(2)	104.1(2)	63.5(2)
S29	3.492(8)	3.424(7)	2.321(6)	87.2(2)	102.8(2)	157.6(2)	152.3(2)
S6	3.472(8)	5.232(8)	3.646(9)	2.928(6)	102.7(2)	73.0(1)	114.4(1)
S2	5.430(7)	3.491(7)	4.398(7)	4.833(8)	3.257(6)	72.2(1)	89.7(1)
S31	4.053(8)	4.538(9)	5.602(8)	3.776(7)	3.918(8)	3.387(6)	49.9(1)
S30	4.117(7)	3.913(8)	6.501(8)	6.170(8)	5.423(8)	3.384(8)	4.356(6)

As2	S28	S3	S4	S7	S8	S29	S30
S28	2.252(6)	101.7(2)	99.9(2)	95.5(2)	81.6(2)	127.5(2)	167.9(2)
S3	3.523(7)	2.291(5)	95.7(2)	77.9(2)	146.3(2)	130.7(2)	75.6(2)
S4	3.517(6)	3.436(8)	2.343(6)	164.3(2)	117.0(2)	75.4(2)	92.1(2)
S7	4.011(9)	3.456(7)	5.402(8)	3.109(6)	68.4(1)	97.7(1)	72.5(1)
S8	3.764(7)	5.420(7)	4.893(7)	3.643(8)	3.362(5)	57.5(1)	94.2(1)
S29	5.410(7)	5.510(7)	3.877(8)	5.170(8)	3.427(7)	3.735(5)	56.9(1)
S30	6.015(8)	3.913(8)	4.532(9)	4.117(7)	5.252(7)	3.587(8)	3.794(6)

As3	S6	S25	S7	S27	S10	S11	S26
S6	2.303(5)	92.6(2)	96.1(2)	78.8(2)	93.2(2)	154.6(2)	129.0(2)
S25	3.342(7)	2.318(6)	98.2(2)	158.2(2)	87.6(2)	76.7(2)	138.4(2)
S7	3.472(8)	3.538(7)	2.365(6)	102.7(2)	168.8(2)	108.2(2)	79.4(2)
S27	3.474(8)	5.307(8)	4.280(9)	3.086(6)	73.1(1)	102.5(1)	53.7(1)
S10	4.106(8)	3.930(9)	5.612(8)	3.789(7)	3.274(6)	63.7(1)	90.0(1)
S11	5.718(8)	3.770(8)	4.842(8)	5.187(8)	3.609(8)	3.552(6)	65.1(1)
S26	5.781(7)	5.981(7)	4.294(8)	3.336(7)	5.205(7)	4.110(7)	4.047(6)

As4	S24	S8	S12	S11	S7	S26	S25
S24	2.247(6)	97.0(2)	98.2(2)	98.7(2)	107.1(2)	166.2(2)	137.2(2)
S8	3.370(7)	2.254(6)	99.3(2)	164.2(2)	79.8(2)	96.1(2)	55.3(2)
S12	3.444(8)	3.477(7)	2.309(5)	75.9(2)	154.7(2)	84.2(2)	61.2(2)
S11	4.116(9)	5.330(9)	3.403(8)	3.126(7)	98.0(2)	68.6(1)	110.2(1)
S7	4.493(7)	3.643(8)	5.464(7)	4.842(8)	3.287(5)	70.8(1)	99.6(1)
S26	6.250(9)	4.835(9)	4.450(8)	4.110(7)	4.294(8)	4.045(6)	55.5(1)
S25	5.914(7)	3.343(8)	3.578(7)	5.919(8)	5.635(7)	3.776(8)	4.063(5)

M5a	S11	S21	S15	S10	S23	S14	S22
S11	2.559(8)	81.5(2)	94.4(2)	84.1(2)	127.8(2)	154.9(2)	76.7(2)
S21	3.464(8)	2.741(7)	82.7(2)	86.9(2)	144.4(2)	73.8(2)	151.5(2)

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S15    3.943( 9) 3.667( 7) 2.808( 6) 169.6( 2) 110.5( 2)  87.1( 2)  80.8( 2)
S10    3.609( 8) 3.824( 7) 5.606( 7) 2.821( 6)  78.1( 2)  89.8( 2) 108.8( 2)
S23    4.896( 9) 5.362( 8) 4.682( 8) 3.600( 8) 2.890( 7)  74.1( 2)  63.9( 2)
S14    5.365( 9) 3.412( 9) 3.960( 8) 4.067( 8) 3.511( 7) 2.937( 7) 128.1( 2)
S22    3.859( 8) 6.087( 7) 4.151( 7) 5.184( 7) 3.443( 8) 5.827( 7) 3.536( 6)

M5b         S21       S11       S15       S10       S14       S23       S22
S21    2.371( 7)  90.3( 3)  90.7( 2)  94.0( 2)  80.5( 2) 147.3( 3) 155.1( 2)
S11    3.464( 8) 2.514( 9)  96.4( 2)  84.5( 2) 169.3( 3) 117.0( 2)  71.1( 2)
S15    3.667( 7) 3.943( 9) 2.769( 7) 175.3( 3)  89.1( 2) 102.8( 2)  75.6( 2)
S10    3.824( 7) 3.609( 8) 5.606( 7) 2.842( 7)  90.7( 2)  72.7( 2) 100.4( 2)
S14    3.412( 9) 5.365( 9) 3.960( 8) 4.067( 8) 2.875( 8)  70.2( 2) 119.3( 2)
S23    5.362( 8) 4.896( 9) 4.682( 8) 3.600( 8) 3.511( 7) 3.211( 8)  57.5( 1)
S22    6.087( 7) 3.859( 8) 4.151( 7) 5.184( 7) 5.827( 7) 3.443( 8) 3.854( 7)

As6         S20       S11       S12       S15       S22       S21
S20    2.245( 6)  99.5( 2)  98.8( 2)  85.6( 2) 158.9( 2) 128.2( 2)
S11    3.433( 8) 2.253( 6)  96.2( 2)  89.2( 2)  77.7( 2) 132.3( 2)
S12    3.466( 7) 3.403( 8) 2.321( 6) 172.4( 2) 102.4( 2)  77.3( 2)
S15    3.818( 9) 3.943( 9) 5.575( 8) 3.266( 7)  73.5( 1)  95.1( 1)
S22    5.802( 8) 3.859( 8) 4.727( 9) 4.151( 7) 3.651( 6)  58.6( 1)
S21    5.391( 7) 5.481( 8) 3.915( 8) 5.154( 7) 3.598( 7) 3.706( 6)

As7         S17       S15       S18       S14       S17       S19       S18
S17    2.291( 6) 101.1( 2)  95.3( 2)  82.1( 2)  86.5( 2) 139.5( 2) 162.3( 2)
S15    3.546( 7) 2.300( 6)  96.9( 2)  94.5( 2) 172.3( 2) 106.7( 2)  80.9( 2)
S18    3.446( 7) 3.493( 8) 2.369( 5) 168.6( 2)  83.3( 2) 109.7( 2)  67.0( 2)
S14    3.552( 7) 3.960( 8) 5.390( 7) 3.047( 5)  85.5( 1)  67.0( 1) 115.4( 1)
S17    3.944( 9) 5.639( 9) 3.871( 8) 4.349( 8) 3.352( 6)  66.3( 1)  92.2( 1)
S19    5.451( 8) 4.708( 9) 4.843( 8) 3.636( 8) 3.748( 7) 3.501( 6)  53.7( 1)
S18    6.107( 7) 4.187( 8) 3.676( 7) 5.874( 7) 5.224( 7) 3.352( 7) 3.883( 6)

As8         S16       S18       S19       S15       S17       S18
S16    2.254( 6) 100.9( 2) 100.8( 2)  91.6( 2) 137.5( 2) 158.7( 2)
S18    3.498( 9) 2.284( 6)  93.3( 2)  80.0( 2) 121.4( 2)  64.7( 2)
S19    3.528( 8) 3.352( 7) 2.326( 5) 166.8( 2)  73.8( 2)  95.9( 2)
S15    3.861( 8) 3.493( 8) 5.362( 7) 3.071( 5)  99.9( 1)  71.0( 1)
S17    5.532( 8) 5.224( 7) 3.748( 7) 5.167( 7) 3.658( 5)  60.4( 1)
S18    6.169( 9) 3.676( 7) 4.843( 8) 4.187( 8) 3.871( 8) 4.015( 6)

As9a        S14       S21       S22       S17       S18       S15
S14    2.292(13)  95.3( 6)  91.4( 5)  83.0( 4)  76.3( 4) 144.2( 6)
S21    3.412( 9) 2.323(16)  93.0( 5)  86.1( 5) 157.6( 6) 120.1( 5)
S22    3.529( 7) 3.598( 7) 2.627(16) 174.3( 6) 107.7( 5)  82.4( 4)
S17    3.552( 7) 3.673( 7) 5.626( 7) 3.006(16)  72.3( 3) 103.0( 4)
S18    3.714( 7) 5.732( 8) 4.989( 8) 3.871( 8) 3.516(18)  72.3( 3)
S15    5.604( 7) 5.154( 7) 4.151( 7) 5.167( 7) 4.187( 8) 3.582(13)

As9b        S14       S21       S17       S22       S18       S15
S14    2.183(11)  96.7( 5) 102.1( 5)  78.4( 4)  81.2( 4) 133.9( 5)
S21    3.412( 9) 2.380(13) 101.0( 5)  77.8( 3) 175.8( 5) 109.0( 4)
S17    3.552( 7) 3.673( 7) 2.381(12) 178.8( 5)  83.0( 4) 109.4( 4)
S22    3.529( 7) 3.598( 7) 5.626( 7) 3.246(12)  98.2( 3)  70.8( 3)
S18    3.714( 7) 5.732( 8) 3.871( 8) 4.989( 8) 3.356(13)  70.5( 2)
S15    5.604( 7) 5.154( 7) 5.167( 7) 4.151( 7) 4.187( 8) 3.864(15)

As10        S13       S23       S19       S22       S18       S15       S14
S13    2.234( 6)  99.3( 2)  99.0( 2)  99.7( 2)  99.0( 2) 161.7( 2) 140.4( 2)
S23    3.410( 8) 2.241( 5) 100.1( 2)  77.0( 2) 161.2( 2)  92.9( 2)  57.2( 2)
S19    3.475( 7) 3.508( 7) 2.335( 6) 161.3( 2)  73.1( 2)  92.2( 2)  60.3( 2)
S22    4.173( 9) 3.443( 8) 5.431( 8) 3.168( 6) 103.7( 1)  69.7( 1) 104.2( 1)
S18    4.161( 7) 5.348( 7) 3.352( 7) 4.989( 8) 3.177( 5)  70.3( 1) 105.2( 1)
S15    6.160( 8) 4.682( 8) 4.708( 9) 4.151( 7) 4.187( 8) 4.000( 6)  57.9( 1)
S14    6.067( 7) 3.511( 7) 3.636( 8) 5.827( 7) 5.874( 7) 3.960( 8) 4.176( 6)

As11        S10       S26       S22       S21       S25       S12       S11
S10    2.251( 6)  99.1( 2)  98.9( 2)  91.1( 2)  89.8( 2) 146.9( 2) 161.3( 2)
S26    3.469( 7) 2.308( 5)  93.7( 2) 169.7( 2)  84.3( 2)  98.4( 2)  72.3( 2)
S22    3.465( 7) 3.367( 7) 2.309( 6)  83.2( 2) 171.3( 2) 107.7( 2)  65.9( 2)
S21    3.824( 7) 5.334( 6) 3.598( 7) 3.047( 5)  97.4( 1)  73.4( 1)  97.5( 1)
S25    3.930( 9) 3.776( 8) 5.522( 8) 4.716( 7) 3.229( 6)  64.3( 1) 105.4( 1)
S12    5.506( 8) 4.450( 8) 4.727( 9) 3.915( 8) 3.579( 7) 3.481( 6)  51.8( 1)
S11    6.348( 8) 4.110( 7) 3.859( 8) 5.481( 8) 5.919( 8) 3.403( 8) 4.175( 6)
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As12	S9	S26	S27	S22	S23	S10	S11
S9	2.240(6)	99.7(2)	94.4(2)	91.6(2)	84.6(2)	132.5(2)	160.9(2)
S26	3.464(9)	2.291(6)	84.8(2)	83.7(2)	155.0(2)	123.7(2)	79.6(2)
S27	3.593(8)	3.336(7)	2.641(5)	167.8(2)	119.6(2)	73.4(2)	104.5(2)
S22	3.581(7)	3.367(7)	5.343(7)	2.733(5)	71.6(2)	109.9(2)	69.4(2)
S23	3.674(7)	5.296(8)	4.992(7)	3.443(8)	3.130(6)	64.6(1)	88.4(1)
S10	5.348(7)	5.205(7)	3.789(7)	5.184(7)	3.600(8)	3.573(5)	58.0(1)
S11	6.015(8)	4.110(7)	5.187(8)	3.859(8)	4.896(9)	3.609(8)	3.853(6)

M13a	S29	S6	S8	S25	S30	S26	S7
S29	2.615(9)	85.9(2)	79.4(2)	83.2(2)	76.5(2)	155.2(3)	121.6(3)
S6	3.646(9)	2.735(8)	145.3(3)	73.6(2)	79.4(2)	73.9(2)	139.7(3)
S8	3.427(7)	5.232(8)	2.746(8)	73.5(2)	126.2(3)	109.3(2)	73.5(2)
S25	3.623(7)	3.342(7)	3.343(8)	2.839(8)	147.2(3)	77.6(2)	133.3(3)
S30	3.587(8)	3.767(7)	5.252(7)	5.736(7)	3.139(8)	112.5(2)	79.5(2)
S26	5.653(8)	3.567(7)	4.835(9)	3.776(8)	5.249(7)	3.172(9)	83.2(2)
S7	5.170(8)	5.666(8)	3.643(8)	5.635(7)	4.117(7)	4.294(8)	3.297(9)

M13b	S25	S29	S8	S6	S26	S30	S7
S25	2.320(7)	101.3(3)	85.7(2)	83.8(2)	81.5(2)	155.2(3)	134.1(3)
S29	3.623(7)	2.367(8)	87.4(2)	92.6(2)	163.9(3)	71.5(2)	112.9(2)
S8	3.343(8)	3.427(7)	2.587(8)	169.3(3)	108.6(2)	116.9(2)	67.0(2)
S6	3.342(7)	3.646(9)	5.232(8)	2.668(8)	71.8(2)	73.1(2)	122.5(2)
S26	3.776(8)	5.653(8)	4.835(9)	3.567(7)	3.341(8)	99.2(2)	74.0(2)
S30	5.736(7)	3.587(8)	5.252(7)	3.767(7)	5.249(7)	3.547(7)	68.4(2)
S7	5.635(7)	5.170(8)	3.643(8)	5.666(8)	4.294(8)	4.117(7)	3.768(7)

As14	S5	S31	S27	S26	S30	S7	S6
S5	2.254(6)	100.2(2)	97.6(2)	100.8(2)	101.7(2)	172.7(2)	136.4(2)
S31	3.472(8)	2.273(5)	99.2(2)	158.4(2)	72.5(2)	82.6(2)	60.9(2)
S27	3.439(7)	3.494(7)	2.315(6)	72.6(2)	160.0(2)	88.5(2)	53.3(2)
S26	4.239(7)	5.372(7)	3.336(7)	3.193(5)	108.3(1)	77.3(1)	99.5(1)
S30	4.342(9)	3.384(8)	5.514(8)	5.249(7)	3.281(6)	72.5(1)	107.8(1)
S7	5.902(8)	4.053(8)	4.280(9)	4.294(8)	4.117(7)	3.660(6)	50.8(1)
S6	6.151(7)	3.776(7)	3.474(8)	5.781(7)	6.170(8)	3.472(8)	4.319(6)

As15	S34	S2	S30	S33	S29	S4	S3
S34	2.250(6)	99.3(2)	92.9(2)	86.2(2)	157.2(2)	91.7(2)	67.0(2)
S2	3.466(8)	2.299(6)	98.6(2)	85.8(2)	102.6(2)	155.3(2)	154.4(2)
S30	3.307(8)	3.498(7)	2.313(6)	175.5(2)	77.7(2)	102.9(2)	62.3(2)
S33	3.629(8)	3.645(8)	5.310(8)	3.001(5)	101.6(1)	72.8(1)	113.4(1)
S29	5.425(7)	4.398(7)	3.587(8)	4.873(7)	3.281(5)	70.7(1)	90.3(1)
S4	4.146(9)	5.588(8)	4.532(9)	3.823(6)	3.877(8)	3.416(6)	50.1(1)
S3	4.096(7)	6.561(7)	3.913(8)	6.245(7)	5.510(7)	3.436(8)	4.412(6)

As16	S1	S30	S34	S31	S35	S2	S3
S1	2.269(6)	100.0(2)	99.9(2)	93.6(2)	84.6(2)	128.1(2)	176.0(2)
S30	3.505(7)	2.307(5)	84.6(2)	84.6(2)	156.3(2)	127.3(2)	76.4(2)
S34	3.733(10)	3.307(8)	2.598(7)	163.9(2)	71.8(2)	104.2(2)	78.1(2)
S31	3.637(7)	3.384(8)	5.250(9)	2.704(6)	118.5(2)	73.5(1)	87.8(1)
S35	3.745(7)	5.394(7)	3.434(8)	5.082(7)	3.201(5)	61.3(1)	98.0(1)
S2	5.409(7)	5.423(8)	5.019(8)	3.918(8)	3.547(7)	3.706(5)	55.9(1)
S3	6.013(8)	3.913(8)	4.096(7)	4.538(9)	5.257(6)	3.491(7)	3.748(6)

As17	S33	S33	S2	S35	S34	S3	S34
S33	2.304(5)	87.4(2)	96.4(2)	81.7(2)	87.1(2)	156.9(2)	134.0(2)
S33	3.275(5)	2.436(5)	94.2(2)	168.3(2)	84.1(2)	76.8(1)	131.2(2)
S2	3.612(8)	3.645(8)	2.538(7)	82.7(2)	176.1(2)	68.6(2)	103.2(2)
S35	3.377(7)	5.230(6)	3.547(7)	2.822(5)	99.6(2)	112.2(1)	60.5(1)
S34	3.629(8)	3.609(7)	5.458(9)	4.388(9)	2.923(7)	107.5(2)	75.4(2)
S3	5.686(6)	3.774(7)	3.491(7)	5.257(6)	5.187(7)	3.494(5)	68.3(1)
S34	5.639(7)	5.696(8)	5.019(8)	3.434(8)	4.163(9)	4.096(7)	3.789(6)

As18	S35	S32	S4	S34	S3	S34	S33
S35	2.232(5)	98.2(2)	97.8(2)	75.2(2)	159.3(2)	90.3(2)	50.8(1)
S32	3.405(6)	2.273(6)	98.7(2)	107.5(2)	101.5(2)	171.3(2)	135.2(2)
S4	3.426(7)	3.479(8)	2.312(5)	153.5(2)	72.9(2)	82.3(2)	62.1(1)
S34	3.434(8)	4.485(8)	5.411(7)	3.243(6)	104.7(2)	72.4(2)	95.5(1)
S3	5.456(7)	4.373(9)	3.436(8)	5.187(7)	3.310(6)	70.4(1)	109.3(1)
S34	4.388(9)	6.024(10)	4.146(9)	4.163(9)	4.096(7)	3.767(8)	52.9(1)
S33	3.377(7)	6.137(7)	3.823(6)	5.639(7)	6.245(7)	3.629(8)	4.312(5)