Table S1

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Charge contributions: ()<0.1; []<0.01

CN - Coordination number

ECoN - Effective coordination number

EDEV - Deviation of ECoN from CNR

QX - Charge received by cations

qX - Oxidation number of cations

QA - Charge received by anions

qA - Oxidation number of anions

BVS - Bond valence sum

MAPDL - Mean absolute percentage deviation of QA for local ligands

MAPD - Mean absolute percentage deviation of QX, QA and BVS

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Cation Site population Bonding atoms CN ECoN EDEV qX QX qX/QX MAPDL BVS

Pb1 1.000.Pb S17,S18,S20,S30,S10,S23,S28 7 6.976 0.003 2.000 1.975 1.013 3.948 1.771

Pb2 1.000.Pb S30,S18,S17,S20,S52,S10,S23,(S59) 8 7.449 0.069 2.000 1.977 1.011 3.861 1.795

Pb3 1.000.Pb S51,S13,S27,S25,S45,S51',S9,S19 8 7.615 0.048 2.000 1.897 1.054 16.128 1.905

Pb4 1.000.Pb S53,S27,S13,S53',S25,S45,S4,S12 8 7.517 0.060 2.000 1.886 1.061 15.153 1.916

Pb5 1.000.Pb S50,S45,S25,S46,S35,S62,S39,(S12) 8 7.063 0.117 2.000 2.079 0.962 7.703 2.018

Pb6 1.000.Pb S61,S25,S45,S35,S46,S39,S62 7 6.619 0.054 2.000 2.095 0.955 7.326 2.010

Pb7 1.000.Pb S31,S47,S29,S44,S58,S41,S36 7 6.652 0.050 2.000 1.947 1.027 12.260 2.005

Pb8 1.000.Pb S11,S21,S58,S8,S56,S44,S64,(S55) 8 6.944 0.132 2.000 1.968 1.016 9.985 2.002

Pb9 1.000.Pb S57,S1,S29,S5,S10,S31,S20,(S60) 8 7.543 0.057 2.000 1.974 1.013 6.694 1.812

Pb10 1.000.Pb S36,S29,S5,S10,S31,S1,S20,S63 8 7.729 0.034 2.000 1.964 1.019 6.534 1.819

Pb11 1.000.Pb S40,S16,S22,S8,S38,S11,S7,S2 8 7.281 0.090 2.000 1.948 1.027 8.490 1.965

Me12 0.500.Pb:0.500.Tl S37,S3,S6,S17,S1,S30,S5,S34 8 7.856 0.018 1.500 1.487 1.008 7.768 1.845

Pb13 1.000.Pb S16,S40,S33,S32,S2,S8,S7,S11 8 7.298 0.088 2.000 1.910 1.047 7.941 1.881

Pb14 1.000.Pb S43,S31,S29,S44,S58,S55,S57 7 6.720 0.040 2.000 1.907 1.049 12.148 2.055

Pb15 1.000.Pb S3,S6,S54,S30,S5,S17,S1,S14 8 7.840 0.020 2.000 1.946 1.028 6.862 1.819

Pb16 1.000.Pb S8,S26,S58,S11,S44,S64,S56,(S41) 8 7.055 0.118 2.000 1.932 1.035 8.399 1.840

Pb17a 0.850.Pb S4,S27,S3,S6,S13,S14,(S66),(S65),[S66] 9 5.821 0.353 1.700 1.708 0.995 6.291 1.632

Pb17a 0.150.Pb (S13),(S3),(S27),(S4),(S14),(S6),(S65),(S66),(S66) 9 8.071 0.103 0.300 0.303 0.992 6.291 0.221

Pb18a 0.790.Pb S9,S6,S27,S13,S3,S34,(S66),(S65),[S65] 9 6.022 0.331 1.580 1.610 0.982 6.862 1.453

Pb18b 0.210.Pb (S27),(S13),(S6),(S9),(S34),(S3),(S66),(S65),(S65) 9 8.086 0.102 0.420 0.427 0.984 6.862 0.307

Me19 0.426.Pb:0.287.Ag:0.287.Sb S24,S55,S41,S42,S48,(S36) 6 4.405 0.266 2.000 1.990 1.005 5.507 2.204

Pb20 1.000.Pb S15,S55,S41,S48,S42,S57,(S36) 7 5.864 0.162 2.000 2.024 0.988 6.750 2.111

Me21a 0.898.Pb S62,S39,S19,S16,S40,S22,S49,(S59) 8 7.247 0.094 1.796 1.786 1.006 5.282 1.690

Me21b 0.102.As S19,(S39),(S62),[S40],[S16] 5 2.965 0.012 0.306 0.291 1.052 4.216 0.237

Me22a 0.731.Pb S2,S42,S33,S48,S38,(S54),(S37) 7 5.417 0.226 1.462 1.450 1.008 8.355 1.413

Me22b 0.269.Sb S2,S38,S33,(S48),(S42) 5 3.493 0.301 0.807 0.764 1.057 5.721 0.710

Sb1 1.000.Sb S20,S59,S63,S49,S60,(S32) 6 4.014 0.331 3.000 2.997 1.001 3.967 3.174

Sb2 1.000.Sb S45,S51,S50,S61,S53',S53,(S51') 7 5.421 0.226 3.000 3.039 0.987 32.473 2.915

Sb3 1.000.Sb S25,S53,S61,S50,S51',S51,(S53') 7 5.507 0.213 3.000 3.040 0.987 32.492 2.918

Sb4 1.000.Sb S49,S10,S59,(S60),(S63),(S22) 6 3.249 0.459 3.000 3.084 0.973 4.668 3.509

Sb5 1.000.Sb S18,S28,S52,S46,S35,S50 6 4.541 0.243 3.000 3.107 0.965 9.980 2.998

Sb6 1.000.Sb S30,S14,S34,S52,S28,[S51'],[S51] 7 3.640 0.480 3.000 3.053 0.983 17.493 2.986

Sb7 1.000.Sb S23,S52,S28,S35,S46,S61 6 4.747 0.209 3.000 3.083 0.973 9.447 2.908

Sb8 1.000.Sb S29,S43,S60,S47,S63,(S26) 6 3.899 0.350 3.000 3.040 0.987 8.967 2.756

Sb9 1.000.Sb S17,S34,S14,S28,S52,(S53),[S53'] 7 3.879 0.446 3.000 3.052 0.983 17.302 2.948

Sb10 1.000.Sb S31,S63,S60,(S43),(S47),[S21] 6 3.234 0.461 3.000 2.961 1.013 9.746 3.240

Sb11 1.000.Sb S40,S19,S12,(S38),(S33),[S4] 6 3.284 0.343 3.000 2.803 1.070 5.541 3.113

Sb12 1.000.Sb S44,S26,S21,S47,(S43),[S43] 6 3.336 0.444 3.000 3.121 0.961 13.169 3.066

Sb13 1.000.Sb S16,S19,S38,S33,S12,[S9] 6 4.387 0.269 3.000 2.953 1.016 5.884 2.480

Sb14 1.000.Sb S11,S32,S22,(S21),(S26),[S63] 6 3.096 0.484 3.000 2.986 1.005 7.674 3.244

Sb15 1.000.Sb S8,S32,S21,S22,S26,(S60) 6 3.993 0.335 3.000 3.077 0.975 7.192 2.737

Sb16 1.000.Sb S51',S13,S65,S66,S53,(S53'),(S51) 7 5.195 0.258 3.000 2.673 1.122 27.267 3.132

Sb17 1.000.Sb S3,S4,S9,(S37),(S54) 5 3.110 0.378 3.000 3.001 1.000 10.895 3.190

Sb18 1.000.Sb S58,S47,S43,S26,(S21),(S47) 6 3.772 0.371 3.000 3.158 0.950 13.468 2.900

Sb19 1.000.Sb S65,S53',S27,S66,S51,(S51'),(S53) 7 5.168 0.262 3.000 2.675 1.121 27.420 2.961

Sb20a 0.864.Sb S1,S36,S57,(S37),[S54] 5 3.042 0.392 2.592 2.835 0.914 12.174 2.855

Sb20b 0.136.Sb S1,S37,(S57),(S54),(S36) 5 3.781 0.244 0.408 0.452 0.904 12.174 0.333

Sb21a 0.730.Sb S42,S7,S15,S2,S24,(S64) 6 4.235 0.294 2.190 2.106 1.040 8.897 2.109

Sb21b 0.270.Sb S7,S42,S15,S2,S24 5 4.972 0.006 0.810 0.773 1.048 9.795 0.490

Sb22 1.000.Sb S6,S54,S37,S9,S4 5 4.276 0.145 3.000 3.196 0.939 10.157 2.892

Sb23a 0.841.Sb S5,S54,S37,S36,S57 5 3.665 0.267 2.523 2.742 0.920 12.593 2.445

Sb23b 0.159.Sb S5,S36,S57,(S54),(S37) 5 3.339 0.332 0.477 0.515 0.926 12.593 0.455

(Sb,As24 0.740.Sb:0.260.As S56,S55,S64,S24,(S15),[S24] 6 3.467 0.422 3.000 3.037 0.988 6.425 2.723

Sb25 1.000.Sb S64,S41,S15,S56,S24,(S15) 6 3.857 0.357 3.000 2.992 1.003 5.257 2.532

Sb26 1.000.Sb S48,S2,S24,S7,S15,(S56) 6 4.052 0.325 3.000 2.869 1.046 9.853 2.833

Me27a 0.859.Sb S62,S39,S12,(S40),(S16) 5 3.188 0.362 2.577 2.465 1.045 4.042 2.688

Me27b 0.141.Pb (S62),(S39),(S16),(S12),(S40),(S32),(S49),[S59] 8 6.356 0.206 0.282 0.275 1.025 4.521 0.279

Me28a 0.804.Sb S7,S33,S38,S42,(S48) 5 3.398 0.320 2.412 2.314 1.042 6.174 2.545

Me28b 0.196.Pb (S33),(S38),(S7),(S42),(S48),(S54),(S37) 7 5.757 0.178 0.392 0.394 0.995 8.679 0.446

Hg 0.767.Hg:0.233.Ag S46,S35,[S50],[S61],[S61],[S50] 6 2.057 0.657 1.767 1.646 1.073 15.392 1.811

Cu1 1.000.Cu S62,S23,S18,S49 4 3.991 0.002 1.000 1.015 0.985 3.965 0.928

Cu2 1.000.Cu S39,S23,S18,S59 4 3.970 0.008 1.000 0.985 1.015 1.779 0.950