Table S2

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CN - Coordination number

AV - Average distance

AVsd - Standard deviation of distances

Xo,Yo,Zo - Coordinates of centroid

I,J,K - Components of vector between central atom and centroid

Î” - Displacement of central atom from centroid

SRad - Radius of least-squares fitted circumsphere

SVol - Volume of least-squares fitted circumsphere

SAVsd - Standard deviation of distances to centroid

LEcc,VEcc - Linear and volume-based eccentricity

LSph,VSph - Linear and volume-based sphericity

PVol - Volume of coordination polyhedron

IPVol - Volume of ideal coordination polyhedron

PDist - Polyhedron volume distortion

Î”R - Distortion indexes - (Ba)ur, (Br)own

EDEV - Deviation of ECoN from CNR

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Cation CN AV AVsd Xo Yo Zo I J K Î” SRad SVol LEcc VEcc LSph VSph SAVsd PVol IPVol PDist Î”R(Ba) Î”R(Ba) EDEV Ideal polyhedron type

Pb1 7 3.051 0.034 0.9064 0.6625 0.1853 0.0003 0.0050 0.0001 0.041 3.051 119.011 0.020 0.013 0.040 0.993 0.980 39.496 37.873 0.043 0.009 0.001 0.003 monocapped trigonal prism

Pb2 8 3.121 0.176 0.9041 0.1682 0.1881 0.0031 0.0008 -0.0028 0.205 3.111 126.145 0.127 0.066 0.185 0.959 0.877 52.554 72.702 0.277 0.034 0.027 0.069 bicapped trigonal prism

Pb3 8 3.028 0.128 0.1384 0.7402 0.0972 -0.0026 -0.0034 -0.0050 0.169 3.056 119.518 0.059 0.055 0.157 0.981 0.942 41.427 38.034 0.089 0.031 0.021 0.048 monocapped trigonal prism

Pb4 8 3.029 0.146 0.1382 0.2431 0.0969 -0.0034 -0.0041 -0.0059 0.202 3.061 120.113 0.058 0.066 0.186 0.981 0.943 41.489 38.223 0.085 0.037 0.024 0.060 monocapped trigonal prism

Pb5 8 3.108 0.278 0.2354 0.2938 0.1001 0.0009 -0.0054 -0.0078 0.314 3.088 123.357 0.210 0.102 0.275 0.932 0.796 50.888 71.095 0.284 0.054 0.058 0.117 bicapped trigonal prism

Pb6 7 3.023 0.131 0.2388 0.7937 0.0990 -0.0033 -0.0062 -0.0062 0.211 3.038 117.423 0.016 0.069 0.194 0.995 0.984 38.794 37.367 0.038 0.030 0.020 0.054 monocapped trigonal prism

Pb7 7 3.022 0.133 0.0688 0.3737 0.4256 -0.0030 -0.0047 0.0017 0.174 3.025 115.964 0.078 0.058 0.163 0.974 0.923 39.119 36.903 0.060 0.032 0.018 0.050 monocapped trigonal prism

Pb8 8 3.114 0.273 0.1468 0.9712 0.5415 0.0001 -0.0068 0.0090 0.352 3.093 123.993 0.178 0.114 0.304 0.943 0.828 51.854 71.462 0.274 0.054 0.061 0.132 bicapped trigonal prism

Pb9 8 3.113 0.152 0.9934 0.7728 0.3047 0.0039 -0.0022 -0.0011 0.194 3.112 126.209 0.095 0.062 0.175 0.970 0.909 53.021 72.739 0.271 0.028 0.022 0.057 bicapped trigonal prism

Pb10 8 3.102 0.112 0.9934 0.2683 0.3036 0.0031 0.0027 -0.0001 0.135 3.102 125.051 0.074 0.043 0.125 0.976 0.928 52.519 72.072 0.271 0.021 0.013 0.034 bicapped trigonal prism

Pb11 8 3.095 0.167 0.2286 0.5827 0.6731 -0.0016 0.0002 0.0059 0.263 3.098 124.530 0.049 0.085 0.233 0.984 0.952 52.261 71.771 0.272 0.047 0.034 0.090 bicapped trigonal prism

Me12 8 3.093 0.077 0.0092 0.7209 0.1913 0.0023 0.0022 0.0008 0.091 3.092 123.876 0.054 0.029 0.086 0.982 0.947 52.129 71.394 0.270 0.020 0.007 0.018 bicapped trigonal prism

Pb13 8 3.111 0.166 0.2283 0.0795 0.6734 0.0020 0.0093 0.0079 0.272 3.111 126.143 0.048 0.087 0.240 0.985 0.954 52.949 72.701 0.272 0.043 0.034 0.088 bicapped trigonal prism

Pb14 7 3.009 0.116 0.0685 0.8598 0.4251 -0.0032 0.0006 0.0010 0.160 3.012 114.468 0.059 0.053 0.151 0.980 0.941 38.811 36.427 0.065 0.029 0.014 0.040 monocapped trigonal prism

Pb15 8 3.097 0.082 0.0093 0.2204 0.1914 0.0020 0.0022 0.0003 0.080 3.097 124.407 0.066 0.026 0.075 0.979 0.936 52.250 71.700 0.271 0.021 0.008 0.020 bicapped trigonal prism

Pb16 8 3.134 0.238 0.1481 0.4663 0.5416 -0.0016 -0.0015 0.0074 0.321 3.118 126.951 0.138 0.103 0.278 0.956 0.867 53.016 73.167 0.275 0.053 0.050 0.118 bicapped trigonal prism

Me17a 9 3.265 0.408 0.0315 0.1844 0.0835 0.0126 0.0113 0.0161 0.601 3.224 140.427 0.127 0.186 0.461 0.961 0.882 65.426 68.514 0.045 0.107 0.198 0.353 tricapped trigonal prism

Me17b 9 3.234 0.199 0.0315 0.1844 0.0835 0.0042 0.0186 0.0060 0.242 3.224 140.427 0.127 0.075 0.209 0.961 0.882 65.426 68.514 0.045 0.049 0.068 0.103 tricapped trigonal prism

Me18a 9 3.266 0.386 0.0315 0.6792 0.0839 0.0119 0.0159 0.0153 0.569 3.228 140.942 0.122 0.176 0.441 0.962 0.886 65.761 68.766 0.044 0.101 0.183 0.331 tricapped trigonal prism

Me18b 9 3.235 0.194 0.0315 0.6792 0.0839 0.0047 0.0188 0.0056 0.241 3.228 140.942 0.122 0.075 0.208 0.962 0.886 65.761 68.766 0.044 0.049 0.067 0.102 tricapped trigonal prism

Me19 6 2.901 0.316 0.1353 0.6227 0.3889 0.0108 0.0146 0.0144 0.530 2.966 109.329 0.051 0.179 0.446 0.983 0.949 28.937 34.801 0.168 0.088 0.092 0.266 octahedron

Pb20 7 3.043 0.243 0.1319 0.1274 0.3883 0.0095 0.0044 0.0085 0.386 3.065 120.561 0.044 0.126 0.333 0.986 0.957 39.195 38.366 0.022 0.063 0.058 0.162 monocapped trigonal prism

Me21a 8 3.113 0.188 0.2059 0.6242 0.7745 0.0054 -0.0052 0.0044 0.230 3.112 126.255 0.119 0.074 0.206 0.962 0.885 52.303 72.765 0.281 0.043 0.036 0.094 bicapped trigonal prism

Me21b 5 2.820 0.600 0.2134 0.6211 0.7768 0.0188 0.0289 0.0326 1.122 2.972 109.993 0.001 0.377 0.759 1.000 0.999 12.157 20.748 0.414 0.194 0.264 0.012 square pyramid

Me22a 7 3.105 0.311 0.3506 0.9110 0.7117 -0.0114 0.0001 -0.0109 0.481 3.151 131.042 0.072 0.153 0.392 0.977 0.932 41.165 41.701 0.013 0.080 0.088 0.226 monocapped trigonal prism

Me22a 5 2.797 0.263 0.3439 0.9047 0.7066 -0.0177 -0.0177 -0.0096 0.674 3.014 114.720 0.012 0.224 0.532 0.996 0.988 14.144 21.640 0.346 0.063 0.087 0.301 square pyramid

Sb1 6 2.815 0.328 0.8934 0.9474 0.2910 0.0050 0.0283 -0.0084 0.520 2.812 93.138 0.060 0.185 0.458 0.979 0.937 28.929 29.647 0.024 0.095 0.105 0.331 octahedron

Sb2 7 2.801 0.290 0.1432 0.9333 -0.0072 0.0098 0.0212 0.0126 0.476 2.850 97.001 0.206 0.167 0.422 0.928 0.783 14.475 18.297 0.209 0.076 0.150 0.226 square pyramid

Sb3 7 2.796 0.288 0.1437 0.4343 -0.0063 0.0093 0.0199 0.0111 0.435 2.832 95.183 0.213 0.154 0.393 0.925 0.774 14.622 17.954 0.186 0.075 0.146 0.213 square pyramid

Sb4 6 2.827 0.396 0.8999 0.4687 0.3008 -0.0028 -0.0023 -0.0189 0.671 2.851 97.072 0.062 0.236 0.553 0.978 0.935 29.499 30.899 0.045 0.126 0.154 0.459 octahedron

Sb5 6 2.804 0.262 0.8219 0.8243 0.0743 0.0078 0.0043 0.0116 0.414 2.812 93.149 0.013 0.147 0.380 0.995 0.986 29.265 29.650 0.013 0.077 0.073 0.243 octahedron

Sb6 7 2.959 0.422 0.9123 0.3701 0.0784 0.0149 0.0118 0.0172 0.670 2.923 104.596 0.061 0.229 0.542 0.979 0.937 33.475 33.294 0.005 0.121 0.243 0.480 octahedron

Sb7 6 2.810 0.254 0.8229 0.3248 0.0722 0.0046 0.0011 0.0118 0.401 2.824 94.290 0.017 0.142 0.368 0.994 0.981 29.488 30.013 0.018 0.058 0.068 0.209 octahedron

Sb8 6 2.883 0.358 0.9634 0.5304 0.3994 0.0102 0.0384 -0.0031 0.577 2.927 105.085 0.038 0.197 0.483 0.987 0.961 31.623 33.450 0.055 0.102 0.121 0.350 octahedron

Sb9 7 2.947 0.401 0.9138 0.8725 0.0789 0.0130 0.0084 0.0168 0.626 2.907 102.859 0.053 0.215 0.517 0.982 0.945 33.020 32.741 0.009 0.111 0.227 0.446 octahedron

Sb10 6 2.888 0.454 0.9718 0.0643 0.4089 0.0010 -0.0099 -0.0183 0.714 2.924 104.731 0.066 0.244 0.568 0.977 0.932 31.891 33.337 0.043 0.138 0.186 0.461 octahedron

Sb11 6 2.945 0.543 0.3223 0.9461 0.7915 -0.0212 -0.0234 -0.0032 0.867 3.032 116.740 0.111 0.286 0.636 0.963 0.890 30.910 37.160 0.168 0.159 0.228 0.343 octahedron

Sb12 6 2.896 0.435 0.0368 0.1263 0.5133 0.0179 0.0305 0.0065 0.708 2.948 107.278 0.031 0.240 0.562 0.989 0.968 32.145 34.147 0.059 0.126 0.173 0.444 octahedron

Sb13 6 2.932 0.419 0.3230 0.4415 0.7984 -0.0186 0.0022 -0.0129 0.732 3.054 119.353 0.145 0.240 0.561 0.953 0.858 30.429 37.991 0.199 0.098 0.131 0.269 octahedron

Sb14 6 2.911 0.480 0.1119 0.7302 0.6282 0.0199 0.0202 0.0104 0.760 2.946 107.135 0.029 0.258 0.591 0.990 0.971 32.452 34.102 0.048 0.147 0.210 0.484 octahedron

Sb15 6 2.883 0.354 0.1175 0.2578 0.6349 0.0117 -0.0232 -0.0003 0.558 2.903 102.465 0.045 0.192 0.473 0.984 0.953 31.467 32.615 0.035 0.094 0.118 0.335 octahedron

Sb16 7 2.705 0.289 0.4400 0.1041 0.0068 0.0057 -0.0023 -0.0045 0.358 2.672 79.952 0.224 0.134 0.351 0.916 0.748 13.863 15.081 0.081 0.091 0.121 0.258 square pyramid

Sb17 5 2.777 0.397 0.1142 0.5388 0.2177 -0.0099 -0.0162 -0.0210 0.709 2.917 103.917 0.034 0.243 0.566 0.988 0.965 13.353 19.602 0.319 0.124 0.136 0.378 square pyramid

Sb18 6 2.877 0.379 0.0436 0.6646 0.5222 0.0050 -0.0254 -0.0117 0.603 2.921 104.370 0.025 0.206 0.500 0.991 0.974 31.687 33.222 0.046 0.101 0.134 0.371 octahedron

Sb19 7 2.725 0.292 0.4393 0.6035 0.0050 0.0065 0.0007 -0.0035 0.360 2.681 80.726 0.224 0.134 0.351 0.917 0.750 14.326 15.227 0.059 0.091 0.119 0.262 square pyramid

Sb20a 5 2.793 0.449 0.0958 0.5689 0.3032 -0.0158 -0.0054 0.0046 0.776 2.933 105.708 0.006 0.265 0.602 0.998 0.994 13.296 19.940 0.333 0.141 0.166 0.392 square pyramid

Sb20b 5 2.810 0.256 0.0958 0.5689 0.3032 -0.0123 0.0131 -0.0114 0.544 2.933 105.708 0.006 0.186 0.460 0.998 0.994 13.572 19.940 0.319 0.072 0.072 0.244 square pyramid

Sb21a 6 2.852 0.341 0.2574 0.0587 0.5868 0.0152 0.0337 0.0127 0.626 2.940 106.464 0.070 0.213 0.513 0.976 0.929 28.239 33.889 0.167 0.088 0.107 0.294 octahedron

Sb21b 5 2.851 0.041 0.2621 0.0600 0.5903 0.0002 0.0060 0.0012 0.060 2.856 97.556 0.004 0.021 0.062 0.999 0.996 17.512 18.402 0.048 0.010 0.002 0.006 square pyramid

Sb22 5 2.719 0.195 0.1126 0.0355 0.2102 -0.0110 -0.0119 -0.0041 0.425 2.828 94.753 0.029 0.150 0.387 0.990 0.969 12.819 17.873 0.283 0.053 0.042 0.145 square pyramid

Sb23a 5 2.751 0.274 0.0937 0.0677 0.3088 -0.0114 -0.0056 -0.0149 0.554 2.881 100.166 0.006 0.192 0.473 0.998 0.994 12.903 18.894 0.317 0.081 0.076 0.267 square pyramid

Sb23b 5 2.782 0.329 0.0937 0.0677 0.3088 -0.0137 0.0053 0.0006 0.608 2.881 100.166 0.006 0.211 0.509 0.998 0.994 12.903 18.894 0.317 0.099 0.102 0.332 square pyramid

(Sb,As)24 6 2.880 0.412 0.2251 0.9777 0.5039 -0.0177 -0.0245 -0.0026 0.730 2.964 109.120 0.091 0.246 0.572 0.969 0.908 28.913 34.734 0.168 0.116 0.156 0.422 octahedron

Sb25 6 2.909 0.339 0.2259 0.4867 0.5075 -0.0147 -0.0469 -0.0072 0.633 3.008 113.960 0.082 0.211 0.508 0.973 0.918 29.974 36.275 0.174 0.099 0.116 0.357 octahedron

Sb26 6 2.858 0.330 0.2572 0.5604 0.5858 0.0136 0.0426 0.0138 0.623 2.952 107.747 0.064 0.211 0.509 0.978 0.935 28.110 34.297 0.180 0.093 0.106 0.325 octahedron

Me27a 5 2.776 0.388 0.2853 0.3820 0.2255 -0.0098 -0.0143 -0.0196 0.665 2.909 103.108 0.005 0.228 0.541 0.998 0.995 14.588 19.449 0.250 0.122 0.129 0.362 square pyramid

Me27b 8 3.135 0.259 0.2977 0.3877 0.2293 -0.0071 -0.0127 -0.0070 0.302 3.142 129.959 0.167 0.096 0.262 0.947 0.841 53.902 74.900 0.280 0.062 0.078 0.206 bicapped trigonal prism

Me28a 5 2.739 0.322 0.1613 0.0940 0.3013 0.0142 0.0179 0.0009 0.603 2.877 99.714 0.007 0.210 0.506 0.998 0.993 13.379 18.809 0.289 0.100 0.096 0.320 square pyramid

Me28a 7 3.020 0.256 0.1527 0.0868 0.2948 0.0092 0.0142 0.0038 0.359 3.040 117.697 0.099 0.118 0.314 0.967 0.902 38.498 37.454 0.028 0.067 0.063 0.178 monocapped trigonal prism

Hg 6 2.953 0.450 0.2500 1.0005 0.0001 0.0000 -0.0010 0.0001 0.009 2.953 107.909 0.449 0.003 0.009 0.848 0.543 32.045 34.349 0.067 0.131 0.238 0.657 octahedron

Cu1 4 2.352 0.022 0.8283 0.6231 0.1731 -0.0009 -0.0014 -0.0005 0.034 2.351 54.407 0.000 0.015 0.043 1.000 1.000 6.480 6.666 0.028 0.007 0.001 0.002 tetrahedron

Cu2 4 2.345 0.041 0.8308 0.1234 0.1737 -0.0016 -0.0013 -0.0015 0.065 2.341 53.713 0.000 0.028 0.081 1.000 1.000 6.426 6.581 0.024 0.011 0.002 0.008 tetrahedron

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