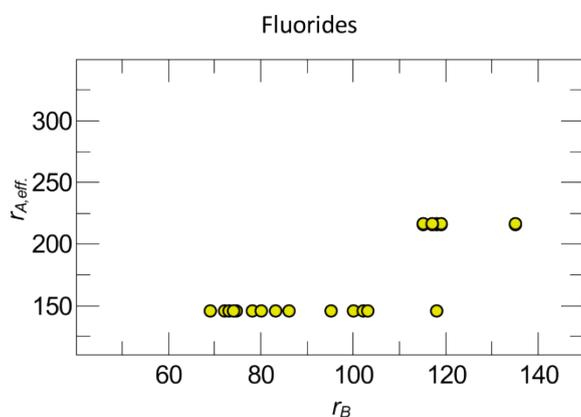


## SUPPORTING INFORMATION

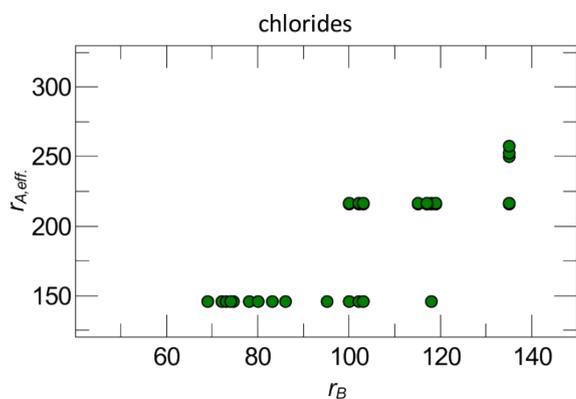
### An Extended Tolerance Factor Approach for Organic-Inorganic Perovskites

Gregor Kieslich, Shijing Sun and Anthony K. Cheetham\*

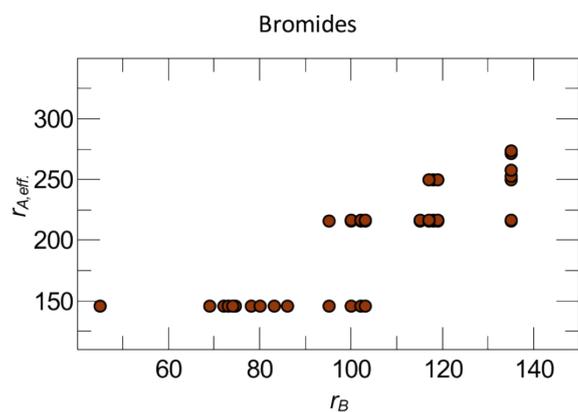
Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles  
Babbage Road, Cambridge CB3 0FS, UK



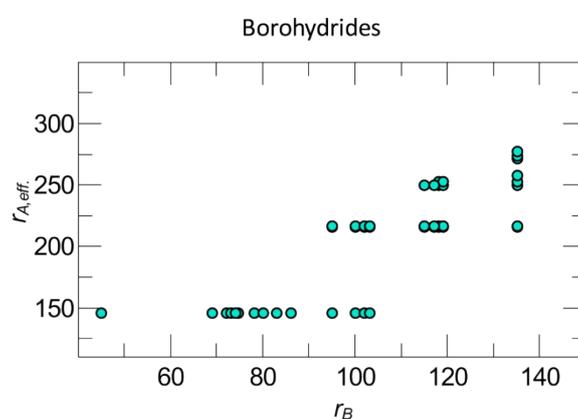
**SI-Figure 1.** Plotted are the effective radii of protonated amines  $r_{A,eff}$  vs ionic radii of the divalent metals  $r_B$  of potentially existing fluorides.



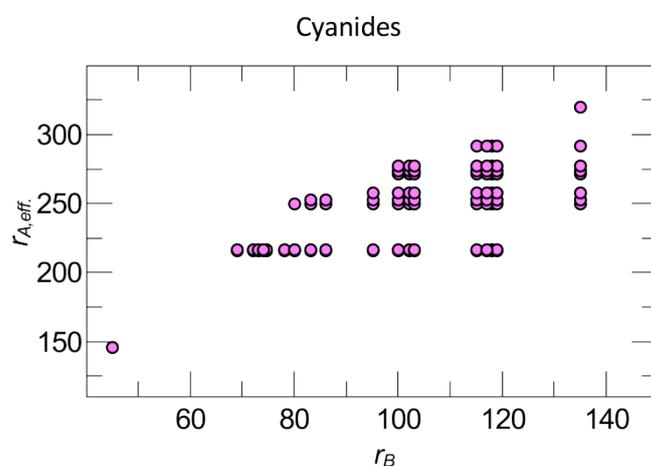
**SI-Figure 2.** Plotted are the effective radii of protonated amines  $r_{A,eff}$  vs ionic radii of the divalent metals  $r_B$  of potentially existing chlorides.



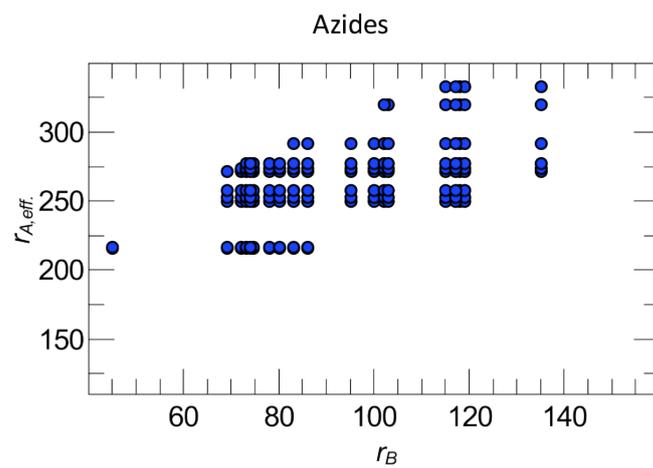
**SI-Figure 3.** Plotted are the effective radii of protonated amines  $r_{A,eff}$ . vs ionic radii of the divalent metals  $r_B$  of potentially existing bromides.



**SI-Figure 4.** Plotted are the effective radii of protonated amines  $r_{A,eff}$ . vs ionic radii of the divalent metals  $r_B$  of potentially existing borohydrides.



**SI-Figure 5.** Plotted are the effective radii of protonated amines  $r_{A,eff}$ . vs ionic radii of the divalent metals  $r_B$  of potentially existing cyanides.



**SI-Figure 6.** Plotted are the effective radii of protonated amines  $r_{A,eff}$  vs ionic radii of the divalent metals  $r_B$  of potentially existing azides.

**SI-Table 1.** Shown are Tolerance Factors of all 2352 amine-metal-anion permutations regarded in this work.

**Count**  
**TFs:** **2352.000**  
**0.8 < TF < 1:** **742.000**  
**0.8 < TF < 1 (organic anions):** **562.000**  
**0.8 < TF < 1 (halides only):** **180.000**

|                    |     | <b>Be</b> | <b>AmH-M-F</b> | <b>AmH-M-Cl</b> | <b>AmH-M-Br</b> | <b>AmH-M-I</b> | <b>AmH-M-BH4</b> | <b>AmH-M-HCOO</b> | <b>AmH-M-CN</b> | <b>AmH-M-N3</b> |
|--------------------|-----|-----------|----------------|-----------------|-----------------|----------------|------------------|-------------------|-----------------|-----------------|
| Ammonium           | 146 | 45        | 1.119          | 1.023           | 1.003           | 0.977          | 0.995            | 0.743             | 0.851           | 0.760           |
| Hydroxylammonium   | 216 | 45        | 1.404          | 1.242           | 1.209           | 1.163          | 1.195            | 0.927             | 1.056           | 0.943           |
| Methylammonium     | 217 | 45        | 1.408          | 1.245           | 1.212           | 1.166          | 1.198            | 0.930             | 1.058           | 0.945           |
| Hydrazinium        | 217 | 45        | 1.408          | 1.245           | 1.212           | 1.166          | 1.198            | 0.930             | 1.058           | 0.945           |
| Azetidinium        | 250 | 45        | 1.543          | 1.349           | 1.309           | 1.254          | 1.292            | 1.017             | 1.155           | 1.031           |
| Formamidinium      | 253 | 45        | 1.555          | 1.358           | 1.317           | 1.262          | 1.300            | 1.024             | 1.163           | 1.039           |
| Imidazolium        | 258 | 45        | 1.575          | 1.374           | 1.332           | 1.275          | 1.314            | 1.038             | 1.178           | 1.052           |
| Dimethylammonium   | 272 | 45        | 1.632          | 1.417           | 1.373           | 1.313          | 1.354            | 1.074             | 1.219           | 1.089           |
| Pyrrolinium        | 272 | 45        | 1.632          | 1.417           | 1.373           | 1.313          | 1.354            | 1.074             | 1.219           | 1.089           |
| Ethylammonium      | 274 | 45        | 1.640          | 1.424           | 1.379           | 1.318          | 1.360            | 1.080             | 1.225           | 1.094           |
| Guanidinium        | 278 | 45        | 1.657          | 1.436           | 1.391           | 1.329          | 1.371            | 1.090             | 1.236           | 1.104           |
| Tetramethylammoium | 292 | 45        | 1.714          | 1.480           | 1.432           | 1.366          | 1.411            | 1.127             | 1.277           | 1.141           |
| Thiazolium         | 320 | 45        | 1.828          | 1.568           | 1.514           | 1.441          | 1.491            | 1.201             | 1.359           | 1.214           |
| Tropylium          | 333 | 45        | 1.881          | 1.608           | 1.552           | 1.476          | 1.528            | 1.235             | 1.397           | 1.248           |

|                    |     | <b>Mg</b> |       |       |       |       |       |       |       |       |
|--------------------|-----|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | 72        | 0.968 | 0.914 | 0.902 | 0.886 | 0.897 | 0.675 | 0.766 | 0.692 |
| Hydroxylammonium   | 216 | 72        | 1.215 | 1.110 | 1.087 | 1.056 | 1.077 | 0.842 | 0.950 | 0.858 |
| Methylammonium     | 217 | 72        | 1.218 | 1.112 | 1.090 | 1.058 | 1.080 | 0.845 | 0.952 | 0.860 |
| Hydrazinium        | 217 | 72        | 1.218 | 1.112 | 1.090 | 1.058 | 1.080 | 0.845 | 0.952 | 0.860 |
| Azetidinium        | 250 | 72        | 1.335 | 1.205 | 1.177 | 1.138 | 1.165 | 0.924 | 1.039 | 0.938 |
| Formamidinium      | 253 | 72        | 1.345 | 1.213 | 1.185 | 1.145 | 1.173 | 0.931 | 1.047 | 0.945 |
| Imidazolium        | 258 | 72        | 1.363 | 1.227 | 1.198 | 1.158 | 1.185 | 0.943 | 1.060 | 0.957 |
| Dimethylammonium   | 272 | 72        | 1.412 | 1.266 | 1.235 | 1.191 | 1.221 | 0.976 | 1.097 | 0.990 |
| Pyrrolinium        | 272 | 72        | 1.412 | 1.266 | 1.235 | 1.191 | 1.221 | 0.976 | 1.097 | 0.990 |
| Ethylammonium      | 274 | 72        | 1.420 | 1.272 | 1.240 | 1.196 | 1.227 | 0.981 | 1.102 | 0.995 |
| Guanidinium        | 278 | 72        | 1.434 | 1.283 | 1.251 | 1.206 | 1.237 | 0.991 | 1.112 | 1.004 |
| Tetramethylammoium | 292 | 72        | 1.483 | 1.322 | 1.288 | 1.240 | 1.273 | 1.024 | 1.149 | 1.038 |
| Thiazolium         | 320 | 72        | 1.582 | 1.400 | 1.361 | 1.308 | 1.345 | 1.091 | 1.223 | 1.104 |
| Tropylium          | 333 | 72        | 1.628 | 1.437 | 1.396 | 1.339 | 1.378 | 1.122 | 1.257 | 1.135 |

## Ca

|                    |     |            |       |       |       |       |       |       |       |       |
|--------------------|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>100</b> | 0.849 | 0.823 | 0.817 | 0.809 | 0.814 | 0.616 | 0.694 | 0.632 |
| Hydroxylammonium   | 216 | <b>100</b> | 1.066 | 0.999 | 0.984 | 0.963 | 0.978 | 0.769 | 0.860 | 0.784 |
| Methylammonium     | 217 | <b>100</b> | 1.069 | 1.002 | 0.987 | 0.966 | 0.980 | 0.772 | 0.863 | 0.786 |
| Hydrazinium        | 217 | <b>100</b> | 1.069 | 1.002 | 0.987 | 0.966 | 0.980 | 0.772 | 0.863 | 0.786 |
| Azetidinium        | 250 | <b>100</b> | 1.171 | 1.085 | 1.065 | 1.039 | 1.057 | 0.844 | 0.941 | 0.858 |
| Formamidinium      | 253 | <b>100</b> | 1.181 | 1.092 | 1.073 | 1.045 | 1.064 | 0.850 | 0.948 | 0.864 |
| Imidazolium        | 258 | <b>100</b> | 1.196 | 1.105 | 1.085 | 1.056 | 1.076 | 0.861 | 0.960 | 0.875 |
| Dimethylammonium   | 272 | <b>100</b> | 1.239 | 1.140 | 1.118 | 1.087 | 1.109 | 0.892 | 0.994 | 0.905 |
| Pyrrolinium        | 272 | <b>100</b> | 1.239 | 1.140 | 1.118 | 1.087 | 1.109 | 0.892 | 0.994 | 0.905 |
| Ethylammonium      | 274 | <b>100</b> | 1.246 | 1.145 | 1.123 | 1.092 | 1.113 | 0.896 | 0.998 | 0.910 |
| Guanidinium        | 278 | <b>100</b> | 1.258 | 1.155 | 1.132 | 1.100 | 1.123 | 0.905 | 1.008 | 0.918 |
| Tetramethylammoium | 292 | <b>100</b> | 1.301 | 1.190 | 1.166 | 1.131 | 1.155 | 0.936 | 1.041 | 0.949 |
| Thiazolium         | 320 | <b>100</b> | 1.388 | 1.261 | 1.233 | 1.193 | 1.221 | 0.997 | 1.108 | 1.009 |
| Tropylium          | 333 | <b>100</b> | 1.428 | 1.293 | 1.264 | 1.222 | 1.251 | 1.025 | 1.139 | 1.037 |

## Sr

|                    |     |            |       |       |       |       |       |       |       |       |
|--------------------|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>118</b> | 0.787 | 0.773 | 0.770 | 0.766 | 0.769 | 0.584 | 0.654 | 0.599 |
| Hydroxylammonium   | 216 | <b>118</b> | 0.988 | 0.939 | 0.928 | 0.912 | 0.923 | 0.729 | 0.811 | 0.743 |
| Methylammonium     | 217 | <b>118</b> | 0.991 | 0.941 | 0.930 | 0.914 | 0.925 | 0.731 | 0.814 | 0.745 |
| Hydrazinium        | 217 | <b>118</b> | 0.991 | 0.941 | 0.930 | 0.914 | 0.925 | 0.731 | 0.814 | 0.745 |
| Azetidinium        | 250 | <b>118</b> | 1.086 | 1.019 | 1.004 | 0.983 | 0.998 | 0.799 | 0.888 | 0.813 |
| Formamidinium      | 253 | <b>118</b> | 1.094 | 1.026 | 1.011 | 0.990 | 1.004 | 0.805 | 0.894 | 0.819 |
| Imidazolium        | 258 | <b>118</b> | 1.109 | 1.038 | 1.022 | 1.000 | 1.016 | 0.816 | 0.905 | 0.829 |
| Dimethylammonium   | 272 | <b>118</b> | 1.149 | 1.071 | 1.054 | 1.029 | 1.046 | 0.845 | 0.937 | 0.858 |
| Pyrrolinium        | 272 | <b>118</b> | 1.149 | 1.071 | 1.054 | 1.029 | 1.046 | 0.845 | 0.937 | 0.858 |
| Ethylammonium      | 274 | <b>118</b> | 1.155 | 1.076 | 1.058 | 1.033 | 1.051 | 0.849 | 0.941 | 0.862 |
| Guanidinium        | 278 | <b>118</b> | 1.166 | 1.085 | 1.067 | 1.042 | 1.060 | 0.857 | 0.950 | 0.870 |
| Tetramethylammoium | 292 | <b>118</b> | 1.206 | 1.119 | 1.099 | 1.071 | 1.090 | 0.886 | 0.982 | 0.899 |
| Thiazolium         | 320 | <b>118</b> | 1.287 | 1.185 | 1.162 | 1.130 | 1.152 | 0.944 | 1.044 | 0.956 |
| Tropylium          | 333 | <b>118</b> | 1.324 | 1.216 | 1.191 | 1.157 | 1.181 | 0.971 | 1.074 | 0.983 |

## Ba

|                  |     |            |       |       |       |       |       |       |       |       |
|------------------|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium         | 146 | <b>135</b> | 0.737 | 0.732 | 0.731 | 0.729 | 0.730 | 0.556 | 0.621 | 0.571 |
| Hydroxylammonium | 216 | <b>135</b> | 0.924 | 0.888 | 0.880 | 0.868 | 0.877 | 0.694 | 0.770 | 0.708 |
| Methylammonium   | 217 | <b>135</b> | 0.927 | 0.891 | 0.882 | 0.870 | 0.879 | 0.696 | 0.772 | 0.710 |
| Hydrazinium      | 217 | <b>135</b> | 0.927 | 0.891 | 0.882 | 0.870 | 0.879 | 0.696 | 0.772 | 0.710 |
| Azetidinium      | 250 | <b>135</b> | 1.016 | 0.964 | 0.953 | 0.936 | 0.948 | 0.761 | 0.842 | 0.775 |
| Formamidinium    | 253 | <b>135</b> | 1.024 | 0.971 | 0.959 | 0.942 | 0.954 | 0.767 | 0.849 | 0.780 |
| Imidazolium      | 258 | <b>135</b> | 1.037 | 0.982 | 0.970 | 0.952 | 0.964 | 0.777 | 0.859 | 0.790 |

|                    |     |            |       |       |       |       |       |       |       |       |
|--------------------|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Dimethylammonium   | 272 | <b>135</b> | 1.075 | 1.014 | 1.000 | 0.980 | 0.994 | 0.805 | 0.889 | 0.818 |
| Pyrrolinium        | 272 | <b>135</b> | 1.075 | 1.014 | 1.000 | 0.980 | 0.994 | 0.805 | 0.889 | 0.818 |
| Ethylammonium      | 274 | <b>135</b> | 1.080 | 1.018 | 1.004 | 0.984 | 0.998 | 0.809 | 0.893 | 0.822 |
| Guanidinium        | 278 | <b>135</b> | 1.091 | 1.027 | 1.013 | 0.992 | 1.006 | 0.817 | 0.902 | 0.829 |
| Tetramethylammoium | 292 | <b>135</b> | 1.128 | 1.058 | 1.043 | 1.020 | 1.036 | 0.844 | 0.931 | 0.857 |
| Thiazolium         | 320 | <b>135</b> | 1.204 | 1.121 | 1.102 | 1.076 | 1.094 | 0.899 | 0.991 | 0.912 |
| Tropylium          | 333 | <b>135</b> | 1.238 | 1.150 | 1.130 | 1.101 | 1.121 | 0.925 | 1.019 | 0.937 |

### Mn

|                    |     |           |       |       |       |       |       |       |       |       |
|--------------------|-----|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>83</b> | 0.918 | 0.876 | 0.867 | 0.854 | 0.863 | 0.651 | 0.736 | 0.667 |
| Hydroxylammonium   | 216 | <b>83</b> | 1.152 | 1.063 | 1.044 | 1.017 | 1.036 | 0.812 | 0.913 | 0.827 |
| Methylammonium     | 217 | <b>83</b> | 1.155 | 1.066 | 1.047 | 1.020 | 1.038 | 0.814 | 0.915 | 0.829 |
| Hydrazinium        | 217 | <b>83</b> | 1.155 | 1.066 | 1.047 | 1.020 | 1.038 | 0.814 | 0.915 | 0.829 |
| Azetidinium        | 250 | <b>83</b> | 1.265 | 1.154 | 1.130 | 1.097 | 1.120 | 0.891 | 0.998 | 0.905 |
| Formamidinium      | 253 | <b>83</b> | 1.275 | 1.162 | 1.138 | 1.104 | 1.127 | 0.897 | 1.006 | 0.912 |
| Imidazolium        | 258 | <b>83</b> | 1.292 | 1.176 | 1.151 | 1.116 | 1.140 | 0.909 | 1.018 | 0.923 |
| Dimethylammonium   | 272 | <b>83</b> | 1.339 | 1.213 | 1.186 | 1.148 | 1.174 | 0.941 | 1.054 | 0.955 |
| Pyrrolinium        | 272 | <b>83</b> | 1.339 | 1.213 | 1.186 | 1.148 | 1.174 | 0.941 | 1.054 | 0.955 |
| Ethylammonium      | 274 | <b>83</b> | 1.346 | 1.219 | 1.191 | 1.153 | 1.179 | 0.946 | 1.059 | 0.960 |
| Guanidinium        | 278 | <b>83</b> | 1.359 | 1.229 | 1.201 | 1.162 | 1.189 | 0.955 | 1.069 | 0.969 |
| Tetramethylammoium | 292 | <b>83</b> | 1.406 | 1.267 | 1.237 | 1.195 | 1.224 | 0.987 | 1.104 | 1.001 |
| Thiazolium         | 320 | <b>83</b> | 1.499 | 1.342 | 1.308 | 1.260 | 1.293 | 1.052 | 1.175 | 1.065 |
| Tropylium          | 333 | <b>83</b> | 1.543 | 1.377 | 1.341 | 1.291 | 1.325 | 1.082 | 1.208 | 1.094 |

### Fe

|                    |     |           |       |       |       |       |       |       |       |       |
|--------------------|-----|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>78</b> | 0.940 | 0.893 | 0.883 | 0.868 | 0.878 | 0.661 | 0.749 | 0.678 |
| Hydroxylammonium   | 216 | <b>78</b> | 1.180 | 1.084 | 1.063 | 1.035 | 1.054 | 0.826 | 0.929 | 0.841 |
| Methylammonium     | 217 | <b>78</b> | 1.183 | 1.087 | 1.066 | 1.037 | 1.057 | 0.828 | 0.932 | 0.843 |
| Hydrazinium        | 217 | <b>78</b> | 1.183 | 1.087 | 1.066 | 1.037 | 1.057 | 0.828 | 0.932 | 0.843 |
| Azetidinium        | 250 | <b>78</b> | 1.296 | 1.177 | 1.151 | 1.115 | 1.140 | 0.905 | 1.016 | 0.920 |
| Formamidinium      | 253 | <b>78</b> | 1.306 | 1.185 | 1.159 | 1.122 | 1.147 | 0.912 | 1.024 | 0.927 |
| Imidazolium        | 258 | <b>78</b> | 1.323 | 1.199 | 1.172 | 1.134 | 1.160 | 0.924 | 1.037 | 0.938 |
| Dimethylammonium   | 272 | <b>78</b> | 1.371 | 1.237 | 1.208 | 1.167 | 1.195 | 0.957 | 1.073 | 0.971 |
| Pyrrolinium        | 272 | <b>78</b> | 1.371 | 1.237 | 1.208 | 1.167 | 1.195 | 0.957 | 1.073 | 0.971 |
| Ethylammonium      | 274 | <b>78</b> | 1.378 | 1.242 | 1.213 | 1.172 | 1.200 | 0.962 | 1.078 | 0.975 |
| Guanidinium        | 278 | <b>78</b> | 1.392 | 1.253 | 1.223 | 1.182 | 1.210 | 0.971 | 1.088 | 0.985 |
| Tetramethylammoium | 292 | <b>78</b> | 1.440 | 1.291 | 1.259 | 1.215 | 1.246 | 1.004 | 1.124 | 1.017 |
| Thiazolium         | 320 | <b>78</b> | 1.536 | 1.368 | 1.332 | 1.281 | 1.316 | 1.069 | 1.196 | 1.082 |
| Tropylium          | 333 | <b>78</b> | 1.580 | 1.403 | 1.365 | 1.312 | 1.349 | 1.100 | 1.229 | 1.112 |

## Co

|                    |     |             |       |       |       |       |       |       |       |       |
|--------------------|-----|-------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>74.5</b> | 0.956 | 0.905 | 0.894 | 0.879 | 0.889 | 0.669 | 0.759 | 0.686 |
| Hydroxylammonium   | 216 | <b>74.5</b> | 1.200 | 1.099 | 1.077 | 1.047 | 1.068 | 0.835 | 0.941 | 0.850 |
| Methylammonium     | 217 | <b>74.5</b> | 1.203 | 1.101 | 1.080 | 1.049 | 1.070 | 0.838 | 0.944 | 0.853 |
| Hydrazinium        | 217 | <b>74.5</b> | 1.203 | 1.101 | 1.080 | 1.049 | 1.070 | 0.838 | 0.944 | 0.853 |
| Azetidinium        | 250 | <b>74.5</b> | 1.318 | 1.193 | 1.166 | 1.128 | 1.154 | 0.916 | 1.029 | 0.930 |
| Formamidinium      | 253 | <b>74.5</b> | 1.329 | 1.201 | 1.174 | 1.136 | 1.162 | 0.923 | 1.037 | 0.937 |
| Imidazolium        | 258 | <b>74.5</b> | 1.346 | 1.215 | 1.187 | 1.148 | 1.175 | 0.935 | 1.050 | 0.949 |
| Dimethylammonium   | 272 | <b>74.5</b> | 1.395 | 1.254 | 1.223 | 1.181 | 1.210 | 0.968 | 1.087 | 0.982 |
| Pyrrolinium        | 272 | <b>74.5</b> | 1.395 | 1.254 | 1.223 | 1.181 | 1.210 | 0.968 | 1.087 | 0.982 |
| Ethylammonium      | 274 | <b>74.5</b> | 1.402 | 1.259 | 1.229 | 1.186 | 1.215 | 0.973 | 1.092 | 0.987 |
| Guanidinium        | 278 | <b>74.5</b> | 1.416 | 1.270 | 1.239 | 1.196 | 1.226 | 0.982 | 1.102 | 0.996 |
| Tetramethylammoium | 292 | <b>74.5</b> | 1.465 | 1.309 | 1.276 | 1.229 | 1.261 | 1.016 | 1.139 | 1.029 |
| Thiazolium         | 320 | <b>74.5</b> | 1.562 | 1.387 | 1.349 | 1.297 | 1.333 | 1.082 | 1.211 | 1.095 |
| Tropylium          | 333 | <b>74.5</b> | 1.608 | 1.423 | 1.383 | 1.328 | 1.366 | 1.113 | 1.245 | 1.125 |

## Ni

|                    |     |           |       |       |       |       |       |       |       |       |
|--------------------|-----|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>69</b> | 0.983 | 0.925 | 0.913 | 0.896 | 0.907 | 0.682 | 0.775 | 0.699 |
| Hydroxylammonium   | 216 | <b>69</b> | 1.233 | 1.123 | 1.099 | 1.067 | 1.089 | 0.851 | 0.960 | 0.866 |
| Methylammonium     | 217 | <b>69</b> | 1.237 | 1.126 | 1.102 | 1.069 | 1.092 | 0.853 | 0.963 | 0.869 |
| Hydrazinium        | 217 | <b>69</b> | 1.237 | 1.126 | 1.102 | 1.069 | 1.092 | 0.853 | 0.963 | 0.869 |
| Azetidinium        | 250 | <b>69</b> | 1.355 | 1.219 | 1.190 | 1.150 | 1.178 | 0.933 | 1.051 | 0.948 |
| Formamidinium      | 253 | <b>69</b> | 1.366 | 1.228 | 1.198 | 1.157 | 1.185 | 0.940 | 1.059 | 0.955 |
| Imidazolium        | 258 | <b>69</b> | 1.384 | 1.242 | 1.211 | 1.170 | 1.198 | 0.952 | 1.072 | 0.967 |
| Dimethylammonium   | 272 | <b>69</b> | 1.434 | 1.281 | 1.249 | 1.204 | 1.235 | 0.986 | 1.109 | 1.000 |
| Pyrrolinium        | 272 | <b>69</b> | 1.434 | 1.281 | 1.249 | 1.204 | 1.235 | 0.986 | 1.109 | 1.000 |
| Ethylammonium      | 274 | <b>69</b> | 1.441 | 1.287 | 1.254 | 1.209 | 1.240 | 0.991 | 1.114 | 1.005 |
| Guanidinium        | 278 | <b>69</b> | 1.455 | 1.298 | 1.265 | 1.218 | 1.250 | 1.001 | 1.125 | 1.015 |
| Tetramethylammoium | 292 | <b>69</b> | 1.506 | 1.338 | 1.302 | 1.253 | 1.287 | 1.035 | 1.162 | 1.048 |
| Thiazolium         | 320 | <b>69</b> | 1.606 | 1.417 | 1.377 | 1.321 | 1.360 | 1.102 | 1.236 | 1.115 |
| Tropylium          | 333 | <b>69</b> | 1.652 | 1.454 | 1.412 | 1.353 | 1.393 | 1.134 | 1.271 | 1.146 |

## Pd

|                  |     |           |       |       |       |       |       |       |       |       |
|------------------|-----|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium         | 146 | <b>86</b> | 0.905 | 0.866 | 0.858 | 0.846 | 0.854 | 0.644 | 0.728 | 0.661 |
| Hydroxylammonium | 216 | <b>86</b> | 1.136 | 1.051 | 1.033 | 1.008 | 1.025 | 0.804 | 0.903 | 0.819 |
| Methylammonium   | 217 | <b>86</b> | 1.139 | 1.054 | 1.036 | 1.010 | 1.028 | 0.806 | 0.905 | 0.821 |
| Hydrazinium      | 217 | <b>86</b> | 1.139 | 1.054 | 1.036 | 1.010 | 1.028 | 0.806 | 0.905 | 0.821 |
| Azetidinium      | 250 | <b>86</b> | 1.248 | 1.141 | 1.118 | 1.086 | 1.108 | 0.882 | 0.988 | 0.896 |
| Formamidinium    | 253 | <b>86</b> | 1.258 | 1.149 | 1.126 | 1.093 | 1.116 | 0.889 | 0.995 | 0.903 |
| Imidazolium      | 258 | <b>86</b> | 1.274 | 1.163 | 1.138 | 1.105 | 1.128 | 0.900 | 1.008 | 0.914 |
| Dimethylammonium | 272 | <b>86</b> | 1.320 | 1.200 | 1.173 | 1.137 | 1.162 | 0.932 | 1.043 | 0.946 |

|                    |     |           |       |       |       |       |       |       |       |       |
|--------------------|-----|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| Pyrrolinium        | 272 | <b>86</b> | 1.320 | 1.200 | 1.173 | 1.137 | 1.162 | 0.932 | 1.043 | 0.946 |
| Ethylammonium      | 274 | <b>86</b> | 1.327 | 1.205 | 1.179 | 1.142 | 1.167 | 0.937 | 1.048 | 0.950 |
| Guanidinium        | 278 | <b>86</b> | 1.340 | 1.216 | 1.189 | 1.151 | 1.177 | 0.946 | 1.058 | 0.959 |
| Tetramethylammoium | 292 | <b>86</b> | 1.386 | 1.253 | 1.224 | 1.183 | 1.211 | 0.978 | 1.092 | 0.991 |
| Thiazolium         | 320 | <b>86</b> | 1.478 | 1.327 | 1.294 | 1.248 | 1.280 | 1.042 | 1.162 | 1.054 |
| Tropylium          | 333 | <b>86</b> | 1.521 | 1.361 | 1.326 | 1.278 | 1.311 | 1.072 | 1.195 | 1.084 |

### Pt

|                    |     |           |       |       |       |       |       |       |       |       |
|--------------------|-----|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>80</b> | 0.931 | 0.886 | 0.876 | 0.863 | 0.872 | 0.657 | 0.744 | 0.674 |
| Hydroxylammonium   | 216 | <b>80</b> | 1.168 | 1.076 | 1.056 | 1.028 | 1.047 | 0.820 | 0.922 | 0.835 |
| Methylammonium     | 217 | <b>80</b> | 1.172 | 1.078 | 1.058 | 1.030 | 1.049 | 0.822 | 0.925 | 0.837 |
| Hydrazinium        | 217 | <b>80</b> | 1.172 | 1.078 | 1.058 | 1.030 | 1.049 | 0.822 | 0.925 | 0.837 |
| Azetidinium        | 250 | <b>80</b> | 1.284 | 1.168 | 1.143 | 1.108 | 1.132 | 0.899 | 1.009 | 0.914 |
| Formamidinium      | 253 | <b>80</b> | 1.294 | 1.176 | 1.150 | 1.115 | 1.139 | 0.906 | 1.017 | 0.921 |
| Imidazolium        | 258 | <b>80</b> | 1.311 | 1.189 | 1.163 | 1.127 | 1.152 | 0.918 | 1.029 | 0.932 |
| Dimethylammonium   | 272 | <b>80</b> | 1.358 | 1.227 | 1.199 | 1.160 | 1.187 | 0.951 | 1.065 | 0.964 |
| Pyrrolinium        | 272 | <b>80</b> | 1.358 | 1.227 | 1.199 | 1.160 | 1.187 | 0.951 | 1.065 | 0.964 |
| Ethylammonium      | 274 | <b>80</b> | 1.365 | 1.233 | 1.204 | 1.164 | 1.192 | 0.955 | 1.070 | 0.969 |
| Guanidinium        | 278 | <b>80</b> | 1.379 | 1.244 | 1.214 | 1.174 | 1.202 | 0.965 | 1.080 | 0.978 |
| Tetramethylammoium | 292 | <b>80</b> | 1.426 | 1.281 | 1.250 | 1.207 | 1.237 | 0.997 | 1.116 | 1.010 |
| Thiazolium         | 320 | <b>80</b> | 1.521 | 1.357 | 1.322 | 1.273 | 1.307 | 1.062 | 1.187 | 1.075 |
| Tropylium          | 333 | <b>80</b> | 1.565 | 1.393 | 1.355 | 1.303 | 1.339 | 1.093 | 1.221 | 1.105 |

### Cu

|                    |     |           |       |       |       |       |       |       |       |       |
|--------------------|-----|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>73</b> | 0.963 | 0.910 | 0.899 | 0.883 | 0.894 | 0.673 | 0.763 | 0.689 |
| Hydroxylammonium   | 216 | <b>73</b> | 1.209 | 1.105 | 1.083 | 1.052 | 1.073 | 0.839 | 0.946 | 0.855 |
| Methylammonium     | 217 | <b>73</b> | 1.212 | 1.108 | 1.086 | 1.055 | 1.076 | 0.842 | 0.949 | 0.857 |
| Hydrazinium        | 217 | <b>73</b> | 1.212 | 1.108 | 1.086 | 1.055 | 1.076 | 0.842 | 0.949 | 0.857 |
| Azetidinium        | 250 | <b>73</b> | 1.328 | 1.200 | 1.172 | 1.134 | 1.161 | 0.921 | 1.035 | 0.935 |
| Formamidinium      | 253 | <b>73</b> | 1.339 | 1.208 | 1.180 | 1.142 | 1.168 | 0.928 | 1.043 | 0.942 |
| Imidazolium        | 258 | <b>73</b> | 1.356 | 1.222 | 1.193 | 1.154 | 1.181 | 0.940 | 1.056 | 0.954 |
| Dimethylammonium   | 272 | <b>73</b> | 1.405 | 1.261 | 1.230 | 1.187 | 1.217 | 0.973 | 1.093 | 0.987 |
| Pyrrolinium        | 272 | <b>73</b> | 1.405 | 1.261 | 1.230 | 1.187 | 1.217 | 0.973 | 1.093 | 0.987 |
| Ethylammonium      | 274 | <b>73</b> | 1.412 | 1.267 | 1.235 | 1.192 | 1.222 | 0.978 | 1.098 | 0.992 |
| Guanidinium        | 278 | <b>73</b> | 1.426 | 1.278 | 1.246 | 1.202 | 1.232 | 0.987 | 1.108 | 1.001 |
| Tetramethylammoium | 292 | <b>73</b> | 1.476 | 1.317 | 1.283 | 1.236 | 1.268 | 1.021 | 1.145 | 1.034 |
| Thiazolium         | 320 | <b>73</b> | 1.574 | 1.395 | 1.356 | 1.303 | 1.340 | 1.087 | 1.218 | 1.100 |
| Tropylium          | 333 | <b>73</b> | 1.620 | 1.431 | 1.391 | 1.335 | 1.373 | 1.118 | 1.252 | 1.131 |

## Zn

|                    |     |           |       |       |       |       |       |       |       |       |
|--------------------|-----|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>74</b> | 0.959 | 0.907 | 0.896 | 0.880 | 0.891 | 0.670 | 0.760 | 0.687 |
| Hydroxylammonium   | 216 | <b>74</b> | 1.203 | 1.101 | 1.079 | 1.049 | 1.070 | 0.837 | 0.943 | 0.852 |
| Methylammonium     | 217 | <b>74</b> | 1.206 | 1.104 | 1.082 | 1.051 | 1.072 | 0.839 | 0.945 | 0.854 |
| Hydrazinium        | 217 | <b>74</b> | 1.206 | 1.104 | 1.082 | 1.051 | 1.072 | 0.839 | 0.945 | 0.854 |
| Azetidinium        | 250 | <b>74</b> | 1.322 | 1.195 | 1.168 | 1.130 | 1.156 | 0.917 | 1.031 | 0.932 |
| Formamidinium      | 253 | <b>74</b> | 1.332 | 1.203 | 1.176 | 1.138 | 1.164 | 0.925 | 1.039 | 0.939 |
| Imidazolium        | 258 | <b>74</b> | 1.350 | 1.217 | 1.189 | 1.150 | 1.177 | 0.936 | 1.052 | 0.951 |
| Dimethylammonium   | 272 | <b>74</b> | 1.399 | 1.256 | 1.226 | 1.183 | 1.213 | 0.970 | 1.089 | 0.984 |
| Pyrrrolinium       | 272 | <b>74</b> | 1.399 | 1.256 | 1.226 | 1.183 | 1.213 | 0.970 | 1.089 | 0.984 |
| Ethylammonium      | 274 | <b>74</b> | 1.405 | 1.262 | 1.231 | 1.188 | 1.218 | 0.975 | 1.094 | 0.988 |
| Guanidinium        | 278 | <b>74</b> | 1.419 | 1.273 | 1.241 | 1.198 | 1.228 | 0.984 | 1.104 | 0.998 |
| Tetramethylammoium | 292 | <b>74</b> | 1.468 | 1.312 | 1.278 | 1.231 | 1.264 | 1.017 | 1.141 | 1.031 |
| Thiazolium         | 320 | <b>74</b> | 1.566 | 1.389 | 1.351 | 1.299 | 1.335 | 1.084 | 1.214 | 1.097 |
| Tropylium          | 333 | <b>74</b> | 1.612 | 1.425 | 1.385 | 1.330 | 1.368 | 1.115 | 1.248 | 1.127 |

## Cd

|                    |     |           |       |       |       |       |       |       |       |       |
|--------------------|-----|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>95</b> | 0.868 | 0.838 | 0.831 | 0.822 | 0.828 | 0.626 | 0.706 | 0.642 |
| Hydroxylammonium   | 216 | <b>95</b> | 1.090 | 1.017 | 1.001 | 0.979 | 0.994 | 0.781 | 0.875 | 0.796 |
| Methylammonium     | 217 | <b>95</b> | 1.093 | 1.020 | 1.004 | 0.981 | 0.997 | 0.784 | 0.878 | 0.798 |
| Hydrazinium        | 217 | <b>95</b> | 1.093 | 1.020 | 1.004 | 0.981 | 0.997 | 0.784 | 0.878 | 0.798 |
| Azetidinium        | 250 | <b>95</b> | 1.197 | 1.104 | 1.084 | 1.055 | 1.075 | 0.857 | 0.957 | 0.871 |
| Formamidinium      | 253 | <b>95</b> | 1.207 | 1.112 | 1.091 | 1.062 | 1.082 | 0.864 | 0.965 | 0.878 |
| Imidazolium        | 258 | <b>95</b> | 1.223 | 1.125 | 1.103 | 1.073 | 1.094 | 0.875 | 0.977 | 0.889 |
| Dimethylammonium   | 272 | <b>95</b> | 1.267 | 1.161 | 1.137 | 1.104 | 1.127 | 0.906 | 1.010 | 0.919 |
| Pyrrrolinium       | 272 | <b>95</b> | 1.267 | 1.161 | 1.137 | 1.104 | 1.127 | 0.906 | 1.010 | 0.919 |
| Ethylammonium      | 274 | <b>95</b> | 1.273 | 1.166 | 1.142 | 1.109 | 1.132 | 0.910 | 1.015 | 0.924 |
| Guanidinium        | 278 | <b>95</b> | 1.286 | 1.176 | 1.152 | 1.118 | 1.141 | 0.919 | 1.025 | 0.933 |
| Tetramethylammoium | 292 | <b>95</b> | 1.330 | 1.212 | 1.186 | 1.149 | 1.175 | 0.950 | 1.059 | 0.963 |
| Thiazolium         | 320 | <b>95</b> | 1.419 | 1.284 | 1.254 | 1.212 | 1.241 | 1.012 | 1.127 | 1.025 |
| Tropylium          | 333 | <b>95</b> | 1.460 | 1.317 | 1.285 | 1.241 | 1.272 | 1.041 | 1.158 | 1.054 |

## Hg

|                  |     |            |       |       |       |       |       |       |       |       |
|------------------|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium         | 146 | <b>102</b> | 0.842 | 0.817 | 0.812 | 0.804 | 0.809 | 0.613 | 0.689 | 0.629 |
| Hydroxylammonium | 216 | <b>102</b> | 1.057 | 0.992 | 0.978 | 0.957 | 0.971 | 0.765 | 0.855 | 0.779 |
| Methylammonium   | 217 | <b>102</b> | 1.060 | 0.994 | 0.980 | 0.960 | 0.974 | 0.767 | 0.857 | 0.781 |
| Hydrazinium      | 217 | <b>102</b> | 1.060 | 0.994 | 0.980 | 0.960 | 0.974 | 0.767 | 0.857 | 0.781 |
| Azetidinium      | 250 | <b>102</b> | 1.161 | 1.077 | 1.058 | 1.032 | 1.050 | 0.839 | 0.935 | 0.852 |
| Formamidinium    | 253 | <b>102</b> | 1.170 | 1.084 | 1.065 | 1.039 | 1.057 | 0.845 | 0.942 | 0.859 |
| Imidazolium      | 258 | <b>102</b> | 1.186 | 1.097 | 1.077 | 1.050 | 1.069 | 0.856 | 0.954 | 0.870 |
| Dimethylammonium | 272 | <b>102</b> | 1.229 | 1.132 | 1.110 | 1.080 | 1.101 | 0.886 | 0.987 | 0.900 |

|                    |     |            |       |       |       |       |       |       |       |       |
|--------------------|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Pyrrolinium        | 272 | <b>102</b> | 1.229 | 1.132 | 1.110 | 1.080 | 1.101 | 0.886 | 0.987 | 0.900 |
| Ethylammonium      | 274 | <b>102</b> | 1.235 | 1.137 | 1.115 | 1.085 | 1.106 | 0.891 | 0.992 | 0.904 |
| Guanidinium        | 278 | <b>102</b> | 1.247 | 1.147 | 1.125 | 1.094 | 1.115 | 0.899 | 1.001 | 0.913 |
| Tetramethylammoium | 292 | <b>102</b> | 1.290 | 1.182 | 1.158 | 1.124 | 1.148 | 0.930 | 1.034 | 0.943 |
| Thiazolium         | 320 | <b>102</b> | 1.376 | 1.252 | 1.224 | 1.186 | 1.213 | 0.991 | 1.100 | 1.003 |
| Tropylium          | 333 | <b>102</b> | 1.416 | 1.284 | 1.255 | 1.214 | 1.243 | 1.019 | 1.131 | 1.031 |

## Ge

|                    |     |           |       |       |       |       |       |       |       |       |
|--------------------|-----|-----------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>73</b> | 0.963 | 0.910 | 0.899 | 0.883 | 0.894 | 0.673 | 0.763 | 0.689 |
| Hydroxylammonium   | 216 | <b>73</b> | 1.209 | 1.105 | 1.083 | 1.052 | 1.073 | 0.839 | 0.946 | 0.855 |
| Methylammonium     | 217 | <b>73</b> | 1.212 | 1.108 | 1.086 | 1.055 | 1.076 | 0.842 | 0.949 | 0.857 |
| Hydrazinium        | 217 | <b>73</b> | 1.212 | 1.108 | 1.086 | 1.055 | 1.076 | 0.842 | 0.949 | 0.857 |
| Azetidinium        | 250 | <b>73</b> | 1.328 | 1.200 | 1.172 | 1.134 | 1.161 | 0.921 | 1.035 | 0.935 |
| Formamidinium      | 253 | <b>73</b> | 1.339 | 1.208 | 1.180 | 1.142 | 1.168 | 0.928 | 1.043 | 0.942 |
| Imidazolium        | 258 | <b>73</b> | 1.356 | 1.222 | 1.193 | 1.154 | 1.181 | 0.940 | 1.056 | 0.954 |
| Dimethylammonium   | 272 | <b>73</b> | 1.405 | 1.261 | 1.230 | 1.187 | 1.217 | 0.973 | 1.093 | 0.987 |
| Pyrrolinium        | 272 | <b>73</b> | 1.405 | 1.261 | 1.230 | 1.187 | 1.217 | 0.973 | 1.093 | 0.987 |
| Ethylammonium      | 274 | <b>73</b> | 1.412 | 1.267 | 1.235 | 1.192 | 1.222 | 0.978 | 1.098 | 0.992 |
| Guanidinium        | 278 | <b>73</b> | 1.426 | 1.278 | 1.246 | 1.202 | 1.232 | 0.987 | 1.108 | 1.001 |
| Tetramethylammoium | 292 | <b>73</b> | 1.476 | 1.317 | 1.283 | 1.236 | 1.268 | 1.021 | 1.145 | 1.034 |
| Thiazolium         | 320 | <b>73</b> | 1.574 | 1.395 | 1.356 | 1.303 | 1.340 | 1.087 | 1.218 | 1.100 |
| Tropylium          | 333 | <b>73</b> | 1.620 | 1.431 | 1.391 | 1.335 | 1.373 | 1.118 | 1.252 | 1.131 |

## Sn

|                    |     |            |       |       |       |       |       |       |       |       |
|--------------------|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>115</b> | 0.797 | 0.781 | 0.778 | 0.773 | 0.776 | 0.589 | 0.661 | 0.605 |
| Hydroxylammonium   | 216 | <b>115</b> | 1.000 | 0.948 | 0.937 | 0.920 | 0.932 | 0.735 | 0.819 | 0.750 |
| Methylammonium     | 217 | <b>115</b> | 1.003 | 0.951 | 0.939 | 0.922 | 0.934 | 0.737 | 0.821 | 0.752 |
| Hydrazinium        | 217 | <b>115</b> | 1.003 | 0.951 | 0.939 | 0.922 | 0.934 | 0.737 | 0.821 | 0.752 |
| Azetidinium        | 250 | <b>115</b> | 1.099 | 1.030 | 1.014 | 0.992 | 1.007 | 0.806 | 0.896 | 0.820 |
| Formamidinium      | 253 | <b>115</b> | 1.108 | 1.037 | 1.021 | 0.998 | 1.014 | 0.813 | 0.903 | 0.826 |
| Imidazolium        | 258 | <b>115</b> | 1.122 | 1.049 | 1.032 | 1.009 | 1.025 | 0.823 | 0.914 | 0.837 |
| Dimethylammonium   | 272 | <b>115</b> | 1.163 | 1.082 | 1.064 | 1.038 | 1.056 | 0.852 | 0.946 | 0.866 |
| Pyrrolinium        | 272 | <b>115</b> | 1.163 | 1.082 | 1.064 | 1.038 | 1.056 | 0.852 | 0.946 | 0.866 |
| Ethylammonium      | 274 | <b>115</b> | 1.169 | 1.087 | 1.069 | 1.043 | 1.061 | 0.856 | 0.950 | 0.870 |
| Guanidinium        | 278 | <b>115</b> | 1.180 | 1.096 | 1.078 | 1.051 | 1.070 | 0.865 | 0.959 | 0.878 |
| Tetramethylammoium | 292 | <b>115</b> | 1.221 | 1.130 | 1.110 | 1.081 | 1.101 | 0.894 | 0.991 | 0.907 |
| Thiazolium         | 320 | <b>115</b> | 1.302 | 1.197 | 1.173 | 1.140 | 1.163 | 0.953 | 1.054 | 0.965 |
| Tropylium          | 333 | <b>115</b> | 1.340 | 1.228 | 1.203 | 1.167 | 1.192 | 0.980 | 1.084 | 0.992 |

**Pb**

|                    |     |            |       |       |       |       |       |       |       |       |
|--------------------|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>119</b> | 0.784 | 0.771 | 0.768 | 0.763 | 0.766 | 0.582 | 0.652 | 0.598 |
| Hydroxylammonium   | 216 | <b>119</b> | 0.984 | 0.936 | 0.925 | 0.909 | 0.920 | 0.727 | 0.809 | 0.741 |
| Methylammonium     | 217 | <b>119</b> | 0.987 | 0.938 | 0.927 | 0.912 | 0.922 | 0.729 | 0.811 | 0.743 |
| Hydrazinium        | 217 | <b>119</b> | 0.987 | 0.938 | 0.927 | 0.912 | 0.922 | 0.729 | 0.811 | 0.743 |
| Azetidinium        | 250 | <b>119</b> | 1.081 | 1.016 | 1.001 | 0.980 | 0.995 | 0.797 | 0.885 | 0.810 |
| Formamidinium      | 253 | <b>119</b> | 1.090 | 1.023 | 1.008 | 0.987 | 1.001 | 0.803 | 0.891 | 0.817 |
| Imidazolium        | 258 | <b>119</b> | 1.104 | 1.035 | 1.019 | 0.997 | 1.012 | 0.813 | 0.903 | 0.827 |
| Dimethylammonium   | 272 | <b>119</b> | 1.144 | 1.068 | 1.051 | 1.026 | 1.043 | 0.842 | 0.934 | 0.855 |
| Pyrrolinium        | 272 | <b>119</b> | 1.144 | 1.068 | 1.051 | 1.026 | 1.043 | 0.842 | 0.934 | 0.855 |
| Ethylammonium      | 274 | <b>119</b> | 1.150 | 1.072 | 1.055 | 1.030 | 1.047 | 0.846 | 0.938 | 0.860 |
| Guanidinium        | 278 | <b>119</b> | 1.161 | 1.082 | 1.064 | 1.039 | 1.056 | 0.855 | 0.947 | 0.868 |
| Tetramethylammoium | 292 | <b>119</b> | 1.201 | 1.115 | 1.095 | 1.068 | 1.087 | 0.884 | 0.979 | 0.896 |
| Thiazolium         | 320 | <b>119</b> | 1.281 | 1.181 | 1.158 | 1.126 | 1.148 | 0.941 | 1.041 | 0.954 |
| Tropylum           | 333 | <b>119</b> | 1.319 | 1.212 | 1.187 | 1.153 | 1.177 | 0.968 | 1.070 | 0.980 |

**Eu**

|                    |     |            |       |       |       |       |       |       |       |       |
|--------------------|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>117</b> | 0.791 | 0.776 | 0.773 | 0.768 | 0.771 | 0.586 | 0.657 | 0.601 |
| Hydroxylammonium   | 216 | <b>117</b> | 0.992 | 0.942 | 0.931 | 0.915 | 0.926 | 0.731 | 0.814 | 0.745 |
| Methylammonium     | 217 | <b>117</b> | 0.995 | 0.944 | 0.933 | 0.917 | 0.928 | 0.733 | 0.816 | 0.747 |
| Hydrazinium        | 217 | <b>117</b> | 0.995 | 0.944 | 0.933 | 0.917 | 0.928 | 0.733 | 0.816 | 0.747 |
| Azetidinium        | 250 | <b>117</b> | 1.090 | 1.023 | 1.008 | 0.986 | 1.001 | 0.802 | 0.890 | 0.815 |
| Formamidinium      | 253 | <b>117</b> | 1.099 | 1.030 | 1.014 | 0.992 | 1.008 | 0.808 | 0.897 | 0.821 |
| Imidazolium        | 258 | <b>117</b> | 1.113 | 1.042 | 1.026 | 1.003 | 1.019 | 0.818 | 0.908 | 0.832 |
| Dimethylammonium   | 272 | <b>117</b> | 1.154 | 1.075 | 1.057 | 1.032 | 1.050 | 0.847 | 0.940 | 0.860 |
| Pyrrolinium        | 272 | <b>117</b> | 1.154 | 1.075 | 1.057 | 1.032 | 1.050 | 0.847 | 0.940 | 0.860 |
| Ethylammonium      | 274 | <b>117</b> | 1.159 | 1.080 | 1.062 | 1.037 | 1.054 | 0.851 | 0.944 | 0.865 |
| Guanidinium        | 278 | <b>117</b> | 1.171 | 1.089 | 1.071 | 1.045 | 1.063 | 0.860 | 0.953 | 0.873 |
| Tetramethylammoium | 292 | <b>117</b> | 1.211 | 1.122 | 1.102 | 1.074 | 1.094 | 0.889 | 0.985 | 0.902 |
| Thiazolium         | 320 | <b>117</b> | 1.292 | 1.189 | 1.166 | 1.133 | 1.156 | 0.947 | 1.048 | 0.959 |
| Tropylum           | 333 | <b>117</b> | 1.329 | 1.220 | 1.195 | 1.160 | 1.184 | 0.974 | 1.077 | 0.986 |

**Tm**

|                  |     |            |       |       |       |       |       |       |       |       |
|------------------|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium         | 146 | <b>103</b> | 0.838 | 0.814 | 0.809 | 0.801 | 0.806 | 0.611 | 0.687 | 0.627 |
| Hydroxylammonium | 216 | <b>103</b> | 1.052 | 0.988 | 0.974 | 0.954 | 0.968 | 0.762 | 0.852 | 0.777 |
| Methylammonium   | 217 | <b>103</b> | 1.055 | 0.991 | 0.977 | 0.957 | 0.971 | 0.764 | 0.854 | 0.779 |
| Hydrazinium      | 217 | <b>103</b> | 1.055 | 0.991 | 0.977 | 0.957 | 0.971 | 0.764 | 0.854 | 0.779 |
| Azetidinium      | 250 | <b>103</b> | 1.156 | 1.073 | 1.055 | 1.029 | 1.047 | 0.836 | 0.932 | 0.850 |
| Formamidinium    | 253 | <b>103</b> | 1.165 | 1.081 | 1.062 | 1.035 | 1.054 | 0.842 | 0.939 | 0.856 |
| Imidazolium      | 258 | <b>103</b> | 1.181 | 1.093 | 1.074 | 1.046 | 1.065 | 0.853 | 0.951 | 0.867 |
| Dimethylammonium | 272 | <b>103</b> | 1.223 | 1.128 | 1.107 | 1.077 | 1.098 | 0.884 | 0.984 | 0.897 |

|                    |     |            |       |       |       |       |       |       |       |       |
|--------------------|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Pyrrolinium        | 272 | <b>103</b> | 1.223 | 1.128 | 1.107 | 1.077 | 1.098 | 0.884 | 0.984 | 0.897 |
| Ethylammonium      | 274 | <b>103</b> | 1.229 | 1.133 | 1.112 | 1.081 | 1.102 | 0.888 | 0.988 | 0.901 |
| Guanidinium        | 278 | <b>103</b> | 1.242 | 1.143 | 1.121 | 1.090 | 1.111 | 0.897 | 0.998 | 0.910 |
| Tetramethylammoium | 292 | <b>103</b> | 1.284 | 1.178 | 1.154 | 1.121 | 1.144 | 0.927 | 1.031 | 0.940 |
| Thiazolium         | 320 | <b>103</b> | 1.370 | 1.247 | 1.220 | 1.182 | 1.209 | 0.988 | 1.097 | 1.000 |
| Tropylium          | 333 | <b>103</b> | 1.410 | 1.280 | 1.251 | 1.211 | 1.239 | 1.016 | 1.127 | 1.028 |

## Yb

|                    |     |            |       |       |       |       |       |       |       |       |
|--------------------|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|
| Ammonium           | 146 | <b>102</b> | 0.842 | 0.817 | 0.812 | 0.804 | 0.809 | 0.613 | 0.689 | 0.629 |
| Hydroxylammonium   | 216 | <b>102</b> | 1.057 | 0.992 | 0.978 | 0.957 | 0.971 | 0.765 | 0.855 | 0.779 |
| Methylammonium     | 217 | <b>102</b> | 1.060 | 0.994 | 0.980 | 0.960 | 0.974 | 0.767 | 0.857 | 0.781 |
| Hydrazinium        | 217 | <b>102</b> | 1.060 | 0.994 | 0.980 | 0.960 | 0.974 | 0.767 | 0.857 | 0.781 |
| Azetidinium        | 250 | <b>102</b> | 1.161 | 1.077 | 1.058 | 1.032 | 1.050 | 0.839 | 0.935 | 0.852 |
| Formamidinium      | 253 | <b>102</b> | 1.170 | 1.084 | 1.065 | 1.039 | 1.057 | 0.845 | 0.942 | 0.859 |
| Imidazolium        | 258 | <b>102</b> | 1.186 | 1.097 | 1.077 | 1.050 | 1.069 | 0.856 | 0.954 | 0.870 |
| Dimethylammonium   | 272 | <b>102</b> | 1.229 | 1.132 | 1.110 | 1.080 | 1.101 | 0.886 | 0.987 | 0.900 |
| Pyrrolinium        | 272 | <b>102</b> | 1.229 | 1.132 | 1.110 | 1.080 | 1.101 | 0.886 | 0.987 | 0.900 |
| Ethylammonium      | 274 | <b>102</b> | 1.235 | 1.137 | 1.115 | 1.085 | 1.106 | 0.891 | 0.992 | 0.904 |
| Guanidinium        | 278 | <b>102</b> | 1.247 | 1.147 | 1.125 | 1.094 | 1.115 | 0.899 | 1.001 | 0.913 |
| Tetramethylammoium | 292 | <b>102</b> | 1.290 | 1.182 | 1.158 | 1.124 | 1.148 | 0.930 | 1.034 | 0.943 |
| Thiazolium         | 320 | <b>102</b> | 1.376 | 1.252 | 1.224 | 1.186 | 1.213 | 0.991 | 1.100 | 1.003 |
| Tropylium          | 333 | <b>102</b> | 1.416 | 1.284 | 1.255 | 1.214 | 1.243 | 1.019 | 1.131 | 1.031 |