Table 2

h j0 i form factors for the 5d electrons of transition atoms and ions from Hf to Re.

Atoms and ions

(electronic configuration) A0 a0 B0 b0 C0 c0 D0 d0 E0 e

Hf2þ (6s0 5d2 ) 0.4229 50.465 0.7333 23.865 0.3798 4.051 0.2252 2.497 0.0018 0.0080

Hf3þ (6s0 5d1 ) 0.3555 40.954 0.8483 21.726 0.4116 4.305 0.2101 2.349 0.0023 0.0051

Ta2þ (6s0 5d3 ) 0.3976 45.095 0.7746 21.028 0.6098 3.471 0.4395 2.570 0.0020 0.0077

Ta3þ (6s0 5d2 ) 0.3611 36.921 0.8579 19.195 0.4945 3.857 0.2781 2.303 0.0026 0.0057

Ta4þ (6s0 5d1 ) 0.3065 31.817 0.9611 17.749 0.5463 3.979 0.2816 2.232 0.0030 0.0050

W (6s0 5d6 ) 0.3990 73.810 0.7138 22.815 2.0436 2.710 1.9319 2.559 0.0023 0.0524

W (6s1 5d5 ) 0.3811 62.707 0.7523 21.434 12.5449 2.702 12.4130 2.674 0.0023 0.0365

W (6s2 5d4 ) 0.3653 53.965 0.7926 20.078 0.8142 3.030 0.6581 2.476 0.0023 0.0247

Wþ (6s0 5d5 ) 0.4077 51.367 0.7436 20.256 9.8283 2.780 9.6788 2.740 0.0021 0.0198

Wþ (6s1 5d4 ) 0.3834 46.233 0.7890 19.278 1.4650 2.947 1.2945 2.628 0.0022 0.0138

W2þ (6s0 5d4 ) 0.3876 40.340 0.8008 18.621 1.3911 2.995 1.2048 2.627 0.0023 0.0081

W3þ (6s0 5d3 ) 0.3610 33.519 0.8717 17.176 0.6183 3.445 0.3883 2.276 0.0028 0.0041

W4þ (6s0 5d2 ) 0.3221 29.047 0.9574 15.979 0.6287 3.597 0.3525 2.174 0.0033 0.0034

W5þ (6s0 5d1 ) 0.2725 25.966 1.0558 14.954 0.6990 3.643 0.3745 2.145 0.0037 0.0045

Re (6s0 5d7 ) 0.3807 63.042 0.7497 19.967 6.5300 2.501 6.4013 2.451 0.0028 0.0480

Re (6s1 5d6 ) 0.3691 53.934 0.7837 18.790 9.1491 2.558 8.9983 2.517 0.0027 0.0333

Re (6s2 5d5 ) 0.3548 47.108 0.8210 17.769 9.8674 2.599 9.6938 2.556 0.0027 0.0248

Reþ (6s0 5d6 ) 0.3944 45.427 0.7742 17.948 3.1692 2.653 3.0028 2.521 0.0026 0.0192

Reþ (6s1 5d5 ) 0.3736 41.151 0.8160 17.158 7.0396 2.642 6.8523 2.577 0.0026 0.0139

Re2þ (6s0 5d5 ) 0.3825 36.336 0.8218 16.636 8.7220 2.657 8.5201 2.601 0.0026 0.0083

Re3þ (6s0 5d4 ) 0.3585 30.671 0.8863 15.527 0.8682 3.047 0.6263 2.280 0.0030 0.0052

Re4þ (6s0 5d3 ) 0.2974 27.372 0.9826 14.807 1.8869 2.840 1.6100 2.476 0.0031 0.0036

Re5þ (6s0 5d2 ) 0.3143 23.522 1.0276 13.505 0.7438 3.393 0.4059 2.030 0.0041 0.0037

Re6þ (6s0 5d1 ) 0.2146 22.496 1.1616 13.064 1.0455 3.162 0.6734 2.196 0.0041 0.0035

Table 3

h j0 i form factors for the 5d electrons of transition atoms and ions from Os to Au.

Atoms and ions

(electronic configuration) A0 a0 B0 b0 C0 c0 D0 d0 E0 e

Os (6s0 5d8 ) 0.3676 54.835 0.7793 17.716 2.0669 2.418 1.9224 2.247 0.0034 0.0446

Os (6s1 5d7 ) 0.3571 47.458 0.8123 16.770 1.2072 2.556 1.0404 2.211 0.0033 0.0314

Os (6s2 5d6 ) 0.3467 41.778 0.8458 15.918 5.6370 2.459 5.4472 2.381 0.0032 0.0222

Osþ (6s0 5d7 ) 0.3837 40.665 0.8006 16.096 3.5305 2.487 3.3488 2.366 0.0030 0.0190

Osþ (6s1 5d6 ) 0.3666 36.997 0.8390 15.425 2.6944 2.537 2.4916 2.360 0.0031 0.0140

Os2þ (6s0 5d6 ) 0.3786 33.005 0.8412 14.990 7.0632 2.503 6.8462 2.433 0.0030 0.0098

Os3þ (6s0 5d5 ) 0.3557 28.222 0.9002 14.140 2.5972 2.601 2.3444 2.376 0.0032 0.0041

Os4þ (6s0 5d4 ) 0.3337 24.723 0.9655 13.288 0.9653 2.906 0.6698 2.117 0.0037 0.0050

Os5þ (6s0 5d3 ) 0.3055 22.152 1.0395 12.529 0.9158 3.016 0.5750 2.032 0.0042 0.0022

Os6þ (6s0 5d2 ) 0.2714 20.218 1.1211 11.851 0.9773 3.050 0.5894 2.005 0.0046 0.0021

Os7þ (6s0 5d1 ) 0.2101 19.108 1.2240 11.347 1.2543 2.933 0.8250 2.088 0.0048 0.0022

Ir (6s0 5d9 ) 0.3564 48.464 0.8049 15.923 2.5258 2.265 2.3675 2.121 0.0040 0.0420

Ir (6s1 5d8 ) 0.3492 42.195 0.8350 15.113 5.1496 2.279 4.9686 2.201 0.0038 0.0296

Ir (6s2 5d7 ) 0.3400 37.499 0.8675 14.402 2.3703 2.370 2.1661 2.177 0.0037 0.0214

Irþ (6s0 5d8 ) 0.3744 36.764 0.8240 14.576 8.8616 2.303 8.6664 2.255 0.0035 0.0191

Irþ (6s1 5d7 ) 0.3604 33.570 0.8597 13.993 2.1686 2.412 1.9518 2.188 0.0036 0.0142

Ir2þ (6s0 5d7 ) 0.3802 30.032 0.8550 13.567 1.6185 2.488 1.3866 2.162 0.0035 0.0094

Ir3þ (6s0 5d6 ) 0.3678 25.828 0.9065 12.788 0.8587 2.745 0.5883 1.960 0.0040 0.0049

Ir4þ (6s0 5d5 ) 0.3969 22.050 0.9310 11.768 0.7090 3.017 0.3857 1.778 0.0047 0.0045

Ir5þ (6s0 5d4 ) 0.3059 20.759 1.0432 11.622 1.3457 2.655 1.0008 2.066 0.0043 0.0043

Ir6þ (6s0 5d3 ) 0.2854 18.867 1.1123 10.982 1.1403 2.782 0.7475 1.959 0.0049 0.0035

Ptþ (6s0 5d9 ) 0.3664 33.503 0.8449 13.303 2.6192 2.227 2.4116 2.059 0.0041 0.0189

Pt2þ (6s0 5d8 ) 0.3701 27.799 0.8761 12.480 3.2959 2.258 3.0535 2.106 0.0040 0.0098

Pt3þ (6s0 5d7 ) 0.3606 24.052 0.9205 11.833 4.0612 2.271 3.7841 2.133 0.0041 0.0049

Pt4þ (6s0 5d6 ) 0.3429 21.358 0.9753 11.261 2.2859 2.357 1.9719 2.074 0.0043 0.0033

Pt5þ (6s0 5d5 ) 0.3649 18.762 1.0102 10.456 0.8785 2.765 0.5087 1.737 0.0053 0.0033

Pt6þ (6s0 5d4 ) 0.2877 17.780 1.1111 10.263 1.9416 2.432 1.5477 2.015 0.0049 0.0026

Auþ (6s1 5d9 ) 0.3475 28.294 0.8964 11.794 4.5383 2.086 4.2988 1.983 0.0047 0.0143

Au2þ (6s0 5d9 ) 0.3664 25.714 0.8919 11.488 1.7302 2.207 1.4763 1.908 0.0046 0.0102

Au3þ (6s0 5d8 ) 0.3639 22.330 0.9313 10.883 1.1359 2.355 0.8455 1.809 0.0048 0.0068

Au4þ (6s0 5d7 ) 0.3472 19.944 0.9807 10.424 3.8228 2.169 3.4995 2.009 0.0047 0.0040

Au 5þ (6s0 5d6 ) 0.3292 18.073 1.0376 9.957 2.2028 2.257 1.8410 1.938 0.0050 0.0035

Table 4

h j2 i form factors for the 5d electrons of transition atoms and ions from Hf to Re.

Atoms and ions

(electronic configuration) A2 a2 B2 b2 C2 c2 D2 d2 E2 e

Hf2þ (6s0 5d2 ) 9.6670 33.435 5.2429 13.529 0.5533 1.402 0.4934 1.254 0.0033 0.0448

Hf3þ (6s0 5d1 ) 7.5646 27.367 5.0743 12.402 0.4133 1.742 0.3163 1.437 0.0012 0.0251

Ta2þ (6s0 5d3 ) 8.1746 29.871 4.9405 12.188 1.1294 1.254 1.0658 1.181 0.0046 0.0411

Ta3þ (6s0 5d2 ) 6.5998 25.026 4.7913 11.303 0.7801 1.529 0.6820 1.382 0.0019 0.0239

Ta4þ (6s0 5d1 ) 5.5048 21.620 4.6734 10.556 0.2181 2.100 0.0810 1.049 0.0016 0.0154

W (6s0 5d6 ) 8.4216 64.652 7.6983 23.124 2.3605 8.583 0.3876 4.620 0.0033 0.0424

W (6s1 5d5 ) 6.9289 53.425 7.2157 20.016 5.7754 6.543 4.2114 5.854 0.0036 0.0398

W (6s2 5d4 ) 5.4017 47.110 6.9113 18.760 7.0586 6.363 5.4525 5.802 0.0040 0.0400

Wþ (6s0 5d5 ) 5.6854 44.743 6.8903 18.753 7.8523 6.308 6.3447 5.842 0.0038 0.0383

Wþ (6s1 5d4 ) 4.5118 41.281 6.7136 17.964 7.6331 6.269 6.0365 5.758 0.0042 0.0405

W2þ (6s0 5d4 ) 7.0301 26.990 4.6604 11.083 0.8220 1.145 0.7581 1.042 0.0068 0.0381

W3þ (6s0 5d3 ) 5.8036 22.969 4.5243 10.361 0.7897 1.388 0.6927 1.248 0.0031 0.0229

W4þ (6s0 5d2 ) 4.9006 20.117 4.4360 9.765 2.0009 1.497 1.8714 1.431 0.0014 0.0145

W5þ (6s0 5d1 ) 4.1973 17.967 4.3791 9.255 1.8830 1.603 1.7205 1.518 0.0004 0.0088

Re (6s0 5d7 ) 6.7574 55.529 6.7931 20.125 2.3113 7.529 0.5004 4.412 0.0037 0.0365

Re (6s1 5d6 ) 5.5830 46.852 6.4516 17.855 5.0609 6.037 3.5427 5.312 0.0040 0.0334

Re (6s2 5d5 ) 4.4322 41.798 6.2063 16.844 9.8763 5.751 8.3294 5.406 0.0043 0.0327

Reþ (6s0 5d6 ) 4.7231 40.130 6.2139 16.902 8.8240 5.766 7.3608 5.396 0.0042 0.0316

Reþ (6s1 5d5 ) 3.7875 37.254 6.0587 16.264 6.9896 5.786 5.4457 5.279 0.0045 0.0329

Re2þ (6s0 5d5 ) 3.0708 33.896 5.9941 15.817 6.7816 5.768 5.2056 5.231 0.0047 0.0343

Re3þ (6s0 5d4 ) 1.7870 31.248 5.9068 15.160 17.4262 5.551 15.6856 5.339 0.0053 0.0374

Re4þ (6s0 5d3 ) 4.4033 18.733 4.1971 9.047 2.3106 1.352 2.1866 1.299 0.0025 0.0158

Re5þ (6s0 5d2 ) 3.8162 16.843 4.1400 8.605 4.0882 1.443 3.9333 1.408 0.0012 0.0132

Re6þ (6s0 5d1 ) 3.3349 15.341 4.1015 8.213 2.3511 1.531 2.1651 1.459 0.0003 0.0067

Table 5

h j2 i form factors for the 5d electrons of transition atoms and ions from Os to Au.

Atoms and ions

(electronic configuration) A2 a2 B2 b2 C2 c2 D2 d2 E2 e

Os (6s0 5d8 ) 5.5418 48.893 6.0803 17.984 2.2542 6.853 0.5285 4.095 0.0040 0.0303

Os (6s1 5d7 ) 4.6511 41.610 5.8194 16.062 6.7172 5.447 5.2689 4.986 0.0043 0.0274

Os (6s2 5d6 ) 3.7421 37.491 5.6137 15.256 10.0488 5.293 8.5683 4.991 0.0046 0.0259

Osþ (6s0 5d7 ) 4.0236 36.272 5.6349 15.338 8.6568 5.318 7.2505 4.980 0.0044 0.0253

Osþ (6s1 5d6 ) 3.2611 33.818 5.4945 14.808 5.7610 5.391 4.2811 4.827 0.0048 0.0261

Os2þ (6s0 5d6 ) 2.7289 30.900 5.4357 14.396 18.6546 5.151 17.1708 4.993 0.0050 0.0268

Os3þ (6s0 5d5 ) 4.5913 19.692 4.0615 8.862 0.9950 1.086 0.9081 0.986 0.0077 0.0206

Os4þ (6s0 5d4 ) 3.9724 17.514 3.9817 8.421 0.7719 1.264 0.6552 1.107 0.0042 0.0131

Os5þ (6s0 5d3 ) 3.4764 15.826 3.9241 8.032 0.6854 1.397 0.5394 1.184 0.0024 0.0098

Os6þ (6s0 5d2 ) 3.0642 14.479 3.8847 7.686 4.7235 1.384 4.5485 1.352 0.0012 0.0063

Os7þ (6s0 5d1 ) 2.7164 13.366 3.8554 7.370 5.0211 1.439 4.8166 1.405 0.0004 0.0064

Ir (6s0 5d9 ) 4.6102 43.878 5.4892 16.394 2.1707 6.423 0.4761 3.722 0.0043 0.0254

Ir (6s1 5d8 ) 3.9372 37.508 5.2846 14.661 3.7267 5.263 2.3158 4.416 0.0045 0.0217

Ir (6s2 5d7 ) 3.2263 33.922 5.1086 13.921 6.5993 4.978 5.1841 4.549 0.0048 0.0203

Irþ (6s0 5d8 ) 3.4956 32.991 5.1369 13.998 8.3991 4.924 7.0561 4.612 0.0047 0.0196

Irþ (6s1 5d7 ) 2.8732 30.809 5.0094 13.522 6.8656 4.933 5.4669 4.526 0.0050 0.0199

Ir2þ (6s0 5d7 ) 2.4419 28.356 4.9470 13.222 4.7478 5.029 3.3259 4.393 0.0052 0.0208

Ir3þ (6s0 5d6 ) 1.5883 25.969 4.8472 12.711 5.6507 4.949 4.1190 4.388 0.0056 0.0218

Ir4þ (6s0 5d5 ) 3.5964 16.439 3.7872 7.873 1.2303 1.092 1.1232 1.003 0.0068 0.0127

Ir5þ (6s0 5d4 ) 3.1710 14.923 3.7320 7.529 1.5400 1.200 1.4048 1.119 0.0040 0.0091

Ir6þ (6s0 5d3 ) 2.8163 13.697 3.6906 7.219 5.2957 1.254 5.1328 1.228 0.0024 0.0109

Ptþ (6s0 5d9 ) 3.0783 30.198 4.7065 12.857 5.7270 4.650 4.4425 4.222 0.0048 0.0156

Pt2þ (6s0 5d8 ) 2.2407 26.003 4.5300 12.118 6.7189 4.557 5.3954 4.187 0.0053 0.0147

Pt3þ (6s0 5d7 ) 1.5391 23.689 4.4263 11.645 8.5673 4.482 7.1591 4.181 0.0057 0.0160

Pt4þ (6s0 5d6 ) 0.9477 22.775 4.3337 11.319 7.2374 4.500 5.7086 4.106 0.0062 0.0166

Pt5þ (6s0 5d5 ) 0.5132 23.124 4.1835 11.009 7.4312 4.478 5.7759 4.065 0.0066 0.0176

Pt6þ (6s0 5d4 ) 2.5907 12.991 3.5155 6.801 0.7511 1.206 0.6014 1.022 0.0043 0.0070

Auþ (6s1 5d9 ) 2.3189 25.954 4.2267 11.444 9.0997 4.215 7.8523 3.981 0.0052 0.0120

Au2þ (6s0 5d9 ) 2.0676 23.960 4.1678 11.164 13.3827 4.151 12.1447 3.996 0.0054 0.0130

Au3þ (6s0 5d8 ) 1.4776 21.784 4.0585 10.746 5.9059 4.242 4.5905 3.842 0.0058 0.0116

Au4þ (6s0 5d7 ) 2.9775 14.632 3.4472 6.956 1.9784 0.794 1.8980 0.745 0.0182 0.0123

Au 5þ (6s0 5d6 ) 0.5763 20.517 3.8572 10.171 6.0222 4.213 4.5020 3.760 0.0067 0.0129

Table 6

h j4 i form factors for the 5d electrons of transition atoms and ions from Hf to Re.

Atoms and ions

(electronic configuration) A4 a4 B4 b4 C4 c4 D4 d4 E4 e

Hf2þ (6s0 5d2 ) 2.5342 43.826 1.8466 10.393 0.7761 4.888 0.0327 1.589 0.0017 0.0046

Hf3þ (6s0 5d1 ) 2.3574 32.651 1.8717 8.476 0.6367 3.953 0.1133 2.169 0.0017 0.0048

Ta2þ (6s0 5d3 ) 2.1974 38.294 1.6220 8.838 0.6836 4.212 0.0539 1.746 0.0016 0.0069

Ta3þ (6s0 5d2 ) 2.0884 29.531 1.7145 7.385 1.1809 2.994 0.7705 2.577 0.0016 0.0066

Ta4þ (6s0 5d1 ) 2.0226 24.035 1.7084 6.594 1.1799 2.775 0.8384 2.430 0.0020 0.0053

W (6s0 5d6 ) 2.1307 79.955 1.4055 11.876 0.8808 4.969 0.0120 0.419 0.0051 0.0085

W (6s1 5d5 ) 1.9667 60.069 1.3446 9.992 0.7861 4.554 0.0197 1.087 0.0021 0.0083

W (6s2 5d4 ) 1.8575 47.554 1.3868 8.437 0.6537 3.939 0.0570 1.722 0.0015 0.0092

Wþ (6s0 5d5 ) 2.0231 46.962 1.3937 9.263 0.7420 4.332 0.0288 1.327 0.0018 0.0062

Wþ (6s1 5d4 ) 1.9122 39.952 1.4385 8.019 0.6336 3.725 0.0819 1.868 0.0015 0.0073

W2þ (6s0 5d4 ) 1.9355 33.935 1.5020 7.541 0.6453 3.375 0.1601 2.110 0.0015 0.0063

W3þ (6s0 5d3 ) 1.8752 26.706 1.5440 6.585 5.9785 2.575 5.6111 2.516 0.0018 0.0061

W4þ (6s0 5d2 ) 1.8309 22.142 1.5605 5.935 1.4898 2.482 1.1930 2.266 0.0022 0.0066

W5þ (6s0 5d1 ) 1.7958 18.987 1.5913 5.419 2.0498 2.278 1.8262 2.156 0.0026 0.0050

Re (6s0 5d7 ) 1.8013 63.944 1.1773 9.808 0.7912 4.380 0.0155 0.795 0.0027 0.0080

Re (6s1 5d6 ) 1.7056 49.628 1.2209 8.231 0.6637 3.836 0.0443 1.514 0.0015 0.0088

Re (6s2 5d5 ) 1.6402 40.319 1.3192 7.064 0.8659 2.901 0.4299 2.306 0.0013 0.0098

Reþ (6s0 5d6 ) 1.7723 40.683 1.2795 7.798 0.6385 3.630 0.0656 1.686 0.0015 0.0084

Reþ (6s1 5d5 ) 1.6968 34.939 1.3535 6.851 1.7292 2.681 1.3118 2.445 0.0014 0.0084

Re2þ (6s0 5d5 ) 1.7305 30.305 1.3808 6.606 1.5787 2.630 1.1785 2.378 0.0015 0.0079

Re3þ (6s0 5d4 ) 1.6969 24.325 1.4088 5.901 1.5067 2.424 1.1834 2.209 0.0019 0.0069

Re4þ (6s0 5d3 ) 1.6679 20.454 1.4439 5.357 0.8175 2.321 0.5685 1.976 0.0024 0.0056

Re5þ (6s0 5d2 ) 1.6427 17.722 1.4880 4.916 0.5419 2.189 0.3694 1.781 0.0029 0.0050

Re6þ (6s0 5d1 ) 1.6211 15.673 1.5419 4.548 1.9205 1.833 1.8287 1.766 0.0034 0.0055

Table 7

h j4 i form factors for the 5d electrons of transition atoms and ions from Os to Au.

Atoms and ions

(electronic configuration) A4 a4 B4 b4 C4 c4 D4 d4 E4 e

Os (6s0 5d8 ) 1.5677 53.075 1.0631 8.143 0.6808 3.771 0.0308 1.243 0.0017 0.0095

Os (6s1 5d7 ) 1.5109 42.193 1.1910 6.850 2.4597 2.602 2.0163 2.444 0.0011 0.0100

Os (6s2 5d6 ) 1.4734 34.814 1.2105 6.165 0.9468 2.534 0.5773 2.131 0.0015 0.0108

Osþ (6s0 5d7 ) 1.5777 35.746 1.2222 6.650 1.7260 2.590 1.2942 2.360 0.0012 0.0081

Osþ (6s1 5d6 ) 1.5274 30.891 1.2364 6.044 1.4100 2.431 1.0480 2.188 0.0016 0.0086

Os2þ (6s0 5d6 ) 1.5637 27.292 1.2627 5.880 1.3526 2.393 1.0026 2.146 0.0017 0.0071

Os3þ (6s0 5d5 ) 1.5453 22.300 1.3058 5.301 0.7208 2.294 0.4480 1.881 0.0022 0.0071

Os4þ (6s0 5d4 ) 1.5267 18.972 1.3619 4.834 3.0121 1.938 2.8240 1.877 0.0027 0.0091

Os5þ (6s0 5d3 ) 1.5094 16.573 1.4158 4.458 0.8448 1.797 0.7349 1.638 0.0033 0.0058

Os6þ (6s0 5d2 ) 1.4938 14.751 1.4678 4.149 0.8091 1.535 0.7720 1.442 0.0041 0.0048

Os7þ (6s0 5d1 ) 0.0341 37.994 1.4680 13.159 1.5216 3.898 0.0308 0.550 0.0083 0.0044

Ir (6s0 5d9 ) 1.3913 45.243 1.0627 6.722 2.5141 2.534 2.0510 2.383 0.0009 0.0099

Ir (6s1 5d8 ) 1.3605 36.399 1.0953 5.990 1.7223 2.353 1.3416 2.162 0.0014 0.0111

Ir (6s2 5d7 ) 1.3382 30.628 1.1376 5.420 1.4261 2.160 1.1282 1.974 0.0019 0.0115

Irþ (6s0 5d8 ) 1.4233 31.680 1.1221 5.872 2.2721 2.301 1.8973 2.163 0.0015 0.0108

Irþ (6s1 5d7 ) 1.3875 27.660 1.1508 5.362 0.6586 2.302 0.3554 1.810 0.0020 0.0094

Ir2þ (6s0 5d7 ) 1.4233 24.796 1.1799 5.246 3.2548 2.072 2.9649 1.997 0.0020 0.0099

Ir3þ (6s0 5d6 ) 1.4149 20.563 1.2388 4.761 1.1780 1.928 0.9708 1.761 0.0026 0.0071

Ir4þ (6s0 5d5 ) 1.4039 17.664 1.2993 4.371 3.5599 1.661 3.4340 1.625 0.0033 0.0065

Ir5þ (6s0 5d4 ) 1.3927 15.539 1.3536 4.057 0.2946 1.554 0.2412 1.266 0.0043 0.0061

Ir6þ (6s0 5d3 ) 0.0364 41.929 1.3662 13.771 1.4130 3.784 0.0384 0.190 0.0241 0.0043

Ptþ (6s0 5d9 ) 1.2955 28.407 1.0534 5.206 1.2452 2.096 0.9336 1.881 0.0018 0.0104

Pt2þ (6s0 5d8 ) 1.3038 22.692 1.1238 4.691 3.2444 1.814 3.0209 1.757 0.0025 0.0100

Pt3þ (6s0 5d7 ) 1.3019 19.052 1.1904 4.286 3.3886 1.592 3.2484 1.554 0.0034 0.0087

Pt4þ (6s0 5d6 ) 1.2964 16.503 1.2497 3.964 1.7648 1.350 1.6992 1.305 0.0046 0.0066

Pt5þ (6s0 5d5 ) 1.2902 14.600 1.2945 3.709 0.5190 1.033 0.5122 0.963 0.0067 0.0054

Pt6þ (6s0 5d4 ) 0.0482 33.010 1.2661 12.839 1.3254 3.545 0.0455 0.144 0.0315 0.0027

Auþ (6s1 5d9 ) 1.1686 22.808 1.0729 4.243 0.9462 1.573 0.7943 1.428 0.0036 0.0104

Au2þ (6s0 5d9 ) 1.2005 20.888 1.0879 4.203 0.8896 1.584 0.7371 1.428 0.0036 0.0109

Au3þ (6s0 5d8 ) 1.2033 17.722 1.1507 3.874 0.2426 1.455 0.1649 1.049 0.0053 0.0080

Au4þ (6s0 5d7 ) 1.2021 15.459 1.2003 3.615 0.6189 0.952 0.6028 0.886 0.0081 0.0074

Au 5þ (6s0 5d6 ) 1.2007 13.734 1.2262 3.424 0.5164 0.401 0.5461 0.379 0.0216 0.0060