

## Radial integrals for the magnetic form factor of 5d transition elements

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The radial integrals,  $\langle j_L \rangle$ , where  $L = 0, 2, 4$ , for several electronic configurations in the 5d electrons of transition metal atoms and ions are calculated using radial wavefunctions from the pseudo-relativistic Hartree–Fock method in the Cowan program. The resultant values are fitted to Gaussian analytical expressions with four exponential terms, and the fitted coefficients are tabulated. This table can be used to interpret the magnetic form factor measurements for 5d transition metals.

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## 1. Introduction

Magnetic compounds, including 5d transition metals, have attracted much attention in both research and industry. Various kinds of magnetic orders, such as ferromagnetic and antiferromagnetic orders, are observed for the compounds because of the effects of partially filled electronic shells in the constituent atoms. 3d electrons in Fe are influenced by the crystal field to the extent that the orbital angular momentum is almost quenched. On the other hand, the 5d electrons of transition metals are influenced not only by the crystal field but also by spin–orbit coupling; competition between these two interactions may introduce new fascinating properties to 5d electron systems.

Compounds of 5d transition metals have exhibited a variety of magnetic properties, and therefore they have attracted much research attention (Shiga, 1986; Franse & Gersdorf, 1986; Booth, 1988). The magnetic moments of Pt in several Pt alloys were estimated in polarized neutron diffraction experiments (Antonini *et al.*, 1969; Menzinger & Paoletti, 1966; Ito *et al.*, 1974). Additionally, a magnetic thin film of Co/Pt multilayers was shown to have perpendicular magnetic anisotropy owing to its magnetic quantum number (Ota *et al.*, 2010). Although bulk Au is usually diamagnetic, Au nanoparticles exhibited intrinsic ferromagnetic spin polarization (Crespo *et al.*, 2004; Yamamoto *et al.*, 2004). Regarding Ir compounds, BaIrO<sub>3</sub> acted like a weak ferromagnetic insulator below the Curie temperature,  $T_C = 180$  K (Lindsay *et al.*, 1993); the ferrimagnetism of Ir-doped CaMnO<sub>3</sub> was discussed using the orbital magnetic moment resulting from the localized 5d electrons of Ir<sup>4+</sup> ions (Mizusaki *et al.*, 2008, 2009). The Ir magnetic moment in Co–Ir alloys exhibited a violation of Hund's third rule owing to the hybridization between Co and Ir states (Krishnamurthy *et al.*, 2006). The ferromagnetism in double-perovskite Ba<sub>2</sub>NaOsO<sub>6</sub> below  $T_C = 6.8 \pm 0.3$  K could be caused by the orbital ordering of Os 5d<sup>1</sup> electrons (Stitzer

*et al.*, 2002; Erickson *et al.*, 2007); an antiferromagnetic order below the Neel temperature,  $T_N = 40$  K, of Li<sub>3</sub>OsO<sub>6</sub> could be caused by unpaired electrons influenced by a strong Jahn–Teller distortion (Derakhshan *et al.*, 2008).

One of the experimentally observed quantities relevant to magnetic properties is the magnetic form factor. Polarized neutron diffraction (PND) experiments have provided a traditional tool with which the magnetic form factor can be investigated (Bacon, 1975; Lovesey, 1986; Williams, 1988). Recently, the availability of brilliant X-ray sources has enabled us to obtain the magnetic form factor using X-ray magnetic diffraction (XMD) (Blume, 1985; Lovesey, 1987; Blume & Gibbs, 1988). This technique can measure the spin and orbital contributions to the form factor separately. Using elliptically polarized white X-ray beams, the experimental accuracy of XMD has become comparable with that of PND (Laundy *et al.*, 1991; Collins *et al.*, 1992; Ito *et al.*, 1995, 2004; Suzuki *et al.*, 2009).

When the experimental form factor is analyzed for the purpose of estimating the magnetic moment, the atomic model can be used if the magnetic electrons are well localized. In such a case the radial integrals,  $\langle j_L \rangle$ , are used for the interpretation of the experimental results. For practical applications, approximated Gaussian analytical expressions for  $\langle j_L \rangle$ , whose functional forms are parameterized by several fitting parameters, are widely used. The fitted coefficients of the Gaussian analytical expressions of these radial integrals for the 3d and 4d electrons of transition metal atoms and ions, the 4f electrons of rare earth ions, and the 5f electrons of actinide ions were tabulated (Brown, 2004). The values of the radial integrals were calculated based on Slater-type wavefunctions derived from the Hartree–Fock method for the 3d and 4d electrons (Clementi & Roetti, 1974). The coefficients were fitted to the values of radial integrals using the wavefunctions of Dirac–Fock (DF) theory for the 4f electrons and 5f electrons (Freeman & Desclaux, 1979; Desclaux & Freeman,

1978). However, a table of radial integrals for the 5*d* electrons of transition metal atoms and ions is absent, and the magnetic form factor study of 5*d* metals has been limited (Cromer *et al.*, 1964; Menzinger & Paoletti, 1966; Ito *et al.*, 1974).

The purpose of the present paper is both to calculate  $\langle j_L \rangle$  values and to present fitted coefficients in the Gaussian analytical expressions required to describe the magnetic form factor of the 5*d* transition metals.  $\langle j_L \rangle$  values are important when determining the magnetic contributions from individual atoms in a compound.

The remainder of this paper is organized as follows. In §2, the formalism of the calculation and fitting method is described. In §3, our results regarding the radial integrals of the 5*d* electrons of transition metal atoms and ions are presented, and fitted parameters are tabulated.

## 2. Method of calculation

The magnetic form factor in the non-relativistic framework for *d* electrons is expressed as

$$\mu f(\mathbf{k}) = \mu [ \langle j_0(k) \rangle + c_2 \langle j_2(k) \rangle + c_4 \langle j_4(k) \rangle ], \quad (1)$$

where  $\mathbf{k}$  is the scattering vector and  $\mu$  is the total magnetic moment. The coefficients  $c_2$  and  $c_4$  generally depend on electronic configurations, experimental conditions and crystal-field interactions (Freeman *et al.*, 1976). When the radial wavefunction  $R_{nl}(r)$  of unpaired electrons with quantum number  $nl$  is normalized as  $\int_0^\infty R_{nl}^2(r)r^2 dr = 1$ , the radial integrals are defined by

$$\langle j_L(s = k/4\pi) \rangle = \int_0^\infty R_{nl}^2(r) j_L(kr) r^2 dr, \quad (2)$$

where  $j_L(kr)$  is the spherical Bessel function of *L*th order and *L* can take on the following values: 0, 2, ..., 2*l*. The length of the scattering vector is denoted by  $k = 4\pi s = (4\pi \sin \theta)/\lambda$ .

We employ the Hartree–Fock relativistic (HFR) version of the Cowan program (Cowan, 1981) to generate the radial wavefunctions used in the following calculations. For the HFR method the relativistic interactions other than the spin–orbit term are included as a correction to the Hartree–Fock Hamiltonian; this is a reasonable approximation for valence electrons. Equation (2) is used to compute radial integrals for several possible electronic configurations.

In the fully relativistic counterpart, the DF equations can be employed. The term with  $nl$  ( $l \geq 1$ ) is split into two states with the total angular momentum  $j = l + 1/2$  and  $j = l - 1/2$  as a result of

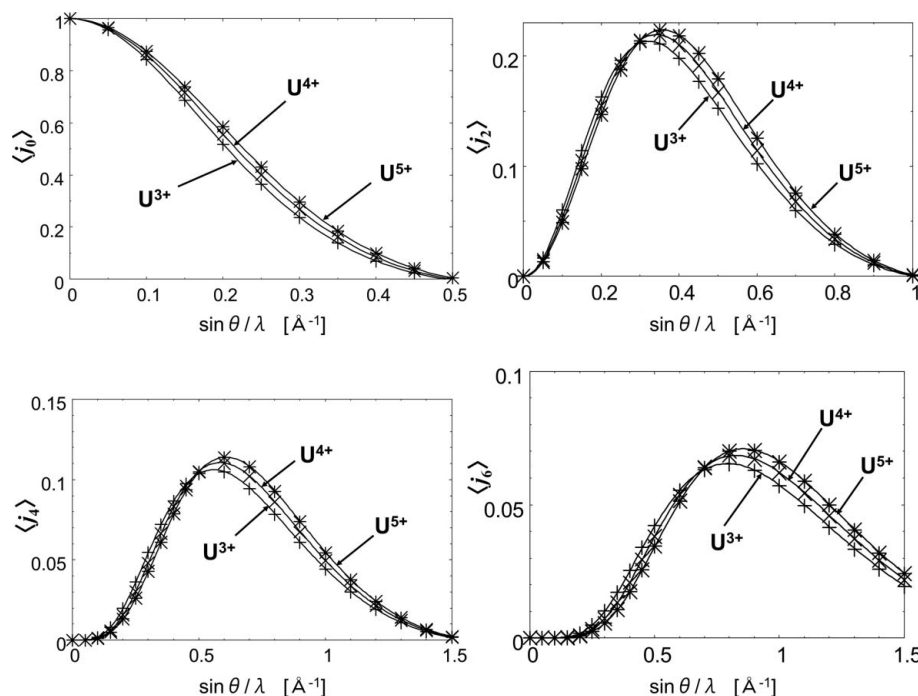
spin–orbit coupling; thus, the state is characterized by  $nlj$ . The state with  $nlj$  has two radial wavefunctions:  $P_{nlj}(r)$ , a large component, and  $Q_{nlj}(r)$ , a small component. Although the relativistic formulation (Stassis & Deckman, 1976; Stassis *et al.*, 1977) is a candidate for the relativistic wavefunctions, the formulation of the non-relativistic equation (1) is generally used because of its greater simplicity and because relativistic effects are less important for valence electrons. The radial integrals of the state with  $nlj$  in the DF theory become

$$\langle j_L^{\text{DF}}(s) \rangle_j = \int_0^\infty [P_{nlj}^2(r) + Q_{nlj}^2(r)] j_L(kr) dr. \quad (3)$$

A weighted average for *j* is used so as to take degeneracy into account. For example, as a result of spin–orbit coupling, the *d* state is split into four orbitals of  $j = 3/2$  and six orbitals of  $j = 5/2$ . Thus, the degeneracy-weighted average of the radial integrals becomes

$$\langle j_L(s) \rangle^{\text{DF}} = \frac{4}{10} \langle j_L^{\text{DF}}(s) \rangle_{j=3/2} + \frac{6}{10} \langle j_L^{\text{DF}}(s) \rangle_{j=5/2}. \quad (4)$$

To justify the use of the HFR version of the Cowan program instead of the DF equations, we calculate the radial integrals for U ions using the HFR method. Fig. 1 compares the radial integrals from the radial wavefunction of the HFR method with those of the fully relativistic DF equations for  $U^{3+}$  ( $5f^3$ ),  $U^{4+}$  ( $5f^2$ ), and  $U^{5+}$  ( $5f^1$ ), as found by Freeman *et al.* (1976). For the DF equations the degeneracy of the 5*f* electrons is split into six orbitals of  $j = 5/2$  and eight orbitals of  $j = 7/2$ . As a result, the degeneracy-weighted average is calculated as



**Figure 1** Comparison of  $\langle j_L \rangle$  between Cowan's HFR (+, x, \*) and DF (lines) for  $U^{3+}$ ,  $U^{4+}$  and  $U^{5+}$ , respectively. Note that different scales are used in the figures to give a clear view of the differences.

**Table 1**

The values,  $\varepsilon$ , of the difference between DF and HFR and the fitting error values,  $e$ , from Brown (2004) in parentheses.

	$\varepsilon(e)$			
	$\langle j_0 \rangle$	$\langle j_2 \rangle$	$\langle j_4 \rangle$	$\langle j_6 \rangle$
U <sup>3+</sup>	0.1102 (0.1507)	0.0527 (0.0822)	0.0299 (0.0599)	0.0218 (0.0345)
U <sup>4+</sup>	0.0950 (0.1757)	0.0471 (0.0928)	0.0305 (0.0471)	0.0202 (0.0472)
U <sup>5+</sup>	0.0842 (0.1750)	0.0447 (0.0477)	0.0294 (0.0493)	0.0194 (0.0444)

$$\langle j_L(s) \rangle^{\text{DF}} = \frac{6}{14} \langle j_L^{\text{DF}}(s) \rangle_{j=5/2} + \frac{8}{14} \langle j_L^{\text{DF}}(s) \rangle_{j=7/2}, \quad (5)$$

where  $L = 0, 2, 4, 6$  is taken for the  $f$  orbitals. These figures indicate good agreement between the two calculations, and this supports our justification of the use of the *Cowan* code.

To evaluate the agreement quantitatively, we introduce the quantity  $\varepsilon$ , defined by

$$\varepsilon = 100 \left[ \sum_{i=1}^N (\langle j_L(s_i) \rangle^{\text{DF}} - \langle j_L(s_i) \rangle^{\text{HFR}})^2 / N \right]^{1/2}, \quad (6)$$

for each  $L = 0, 2, 4, 6$ , where the sum is over the computed points used, which are the same as the computed points of Freeman *et al.* (1976);  $N$  is the number of computed points;  $\langle j_L(s_i) \rangle^{\text{DF}}$  and  $\langle j_L(s_i) \rangle^{\text{HFR}}$  are the computed values of the radial integrals using DF and HFR, respectively. Table 1 shows these  $\varepsilon$  values for each value of  $L$ . Moreover, for comparison, the accuracy at which the Gaussian analytical expressions with three exponential terms fit the computed radial integrals using DF is listed from Brown (2004). This accuracy is defined as

$$e = 100 \left\{ \sum_{i=1}^N [\langle j_L(s_i) \rangle^{\text{DF}} - f(s_i)]^2 / N \right\}^{1/2}, \quad (7)$$

where  $f(s_i)$  are the values of the fitted analytical expressions. Because the  $\varepsilon$  values are smaller than the  $e$  values, the difference between HFR and DF can be smaller than the fitting accuracy of the analytical expressions used.

The values of the radial integrals from the HFR calculation are fitted to Gaussian-type analytical expressions. Although three exponential terms were used by Brown (2004), an additional exponential term is included to increase the accuracy. For example, the calculated values for  $\langle j_L \rangle$  for  $L = 0$  are fitted to the analytical expression

$$\langle j_0(s) \rangle = A_0 \exp(-a_0 s^2) + B \exp(-b_0 s^2) + C_0 \exp(-c_0 s^2) + D_0 \exp(-d_0 s^2) + E_0, \quad (8)$$

where  $A_0, a_0, B_0, b_0, C_0, c_0, D_0, d_0, E_0$  are fitting parameters. Additionally,  $\langle j_L \rangle$  for  $L = 2$  and 4 are fitted to the analytical expressions

$$\langle j_L(s) \rangle = s^2 [A_L \exp(-a_L s^2) + B_L \exp(-b_L s^2) + C_L \exp(-c_L s^2) + D_L \exp(-d_L s^2) + E_L], \quad (9)$$

where  $A_L, a_L, B_L, b_L, C_L, c_L, D_L, d_L, E_L$  are the fitting parameters for each value of  $L$ . These expressions were used to express the computed atomic scattering factors (Cromer & Waber, 1965). The values of  $A_L, a_L, B_L, b_L, C_L, c_L, D_L, d_L, E_L$  for  $L = 0, 2$  and 4 are determined by minimizing the following

value, which has the same definition as is found in equation (7),

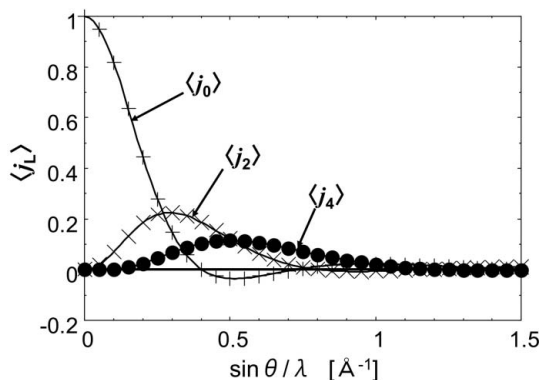
$$e = 100 \times \left\{ \sum_{i=1}^N [\langle j_L(s_i) \rangle^{\text{HFR}} - f(s_i, A_L, a_L, B_L, b_L, C_L, c_L, D_L, d_L, E_L)]^2 / N \right\}^{1/2}, \quad (10)$$

where the parameter dependence is expressed explicitly for  $f(s_i, A_L, a_L, B_L, b_L, C_L, c_L, D_L, d_L, E_L)$ .

The radial integrals from the HFR method are calculated from 0 to  $1.5 \text{ \AA}^{-1}$  for  $s = \sin \theta / \lambda$  at an interval of  $0.01 \text{ \AA}^{-1}$ . Note that this range is the same as that adopted by Brown (2004) for the  $3d$  and  $4d$  electrons of transition metal atoms and ions. Although in the above literature numerical data at an interval of  $0.05 \text{ \AA}^{-1}$  were used, we chose  $0.01 \text{ \AA}^{-1}$  for the following treatment so as to obtain a better fit.

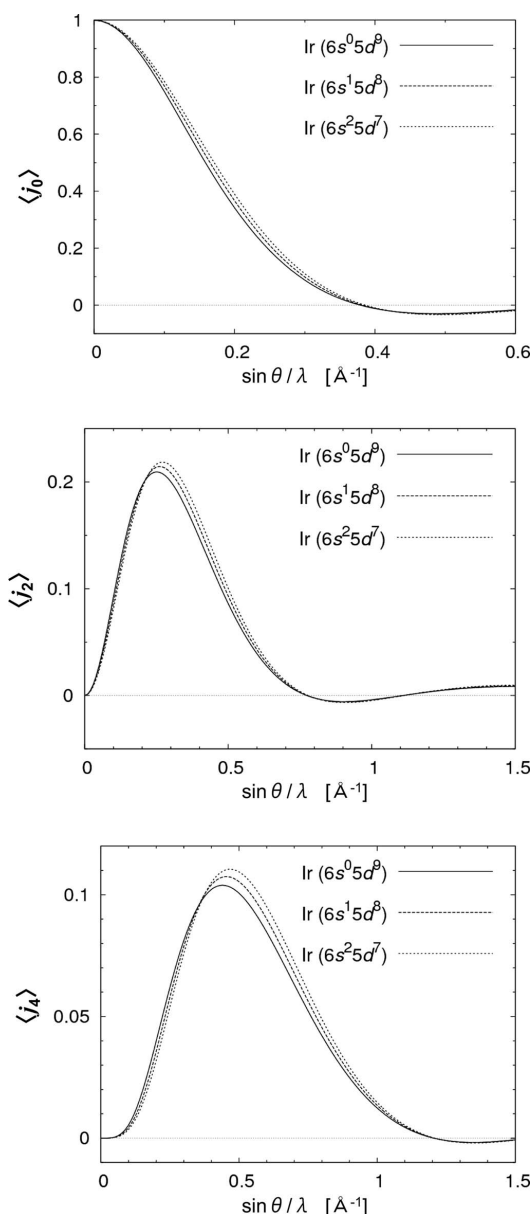
### 3. Results and summary

First, the fitting quality of the Gaussian analytical expressions, equation (8) for  $L = 0$  and equation (9) for  $L = 2$  and 4, is examined. In Fig. 2 the calculated values of the radial integrals at an interval of  $0.05 \text{ \AA}^{-1}$  and fitted Gaussian analytical expressions are compared for Pt<sup>2+</sup> in the  $(6s^0 5d^8)$  configuration. In the radial integrals, the values of the Gaussian analytical expression agree well with the computed values.  $\langle j_0 \rangle$  rapidly decreases from 1.0 at  $s = 0 \text{ \AA}^{-1}$ , crosses the baseline twice, and approaches zero from the positive side with increasing  $s$ . On the other hand,  $\langle j_2 \rangle$  and  $\langle j_4 \rangle$  start at 0 at  $s = 0 \text{ \AA}^{-1}$ , have a peak, and cross zero with increasing  $s$ . They approach zero smoothly after crossing zero several times after  $s = 1.5 \text{ \AA}^{-1}$ . The maximum value of  $\langle j_0 \rangle$  is 1.0 at  $s = 0 \text{ \AA}^{-1}$ ; the maximum values of  $\langle j_2 \rangle$  and  $\langle j_4 \rangle$  are approximately 0.225 at  $s = 0.29 \text{ \AA}^{-1}$  and  $0.115$  at  $s = 0.50 \text{ \AA}^{-1}$ , respectively. The  $s$  value at the peak of  $\langle j_4 \rangle$  is larger than that of  $\langle j_2 \rangle$ . These trends for the radial integrals appear for all  $5d$  electrons of transition metal atoms and ions. The Gaussian analytical expressions can describe the plots sufficiently well.


**Figure 2**

Comparison between the Gaussian analytical expressions using the coefficients in the table (lines) and the calculated values (+ for  $\langle j_0 \rangle$ , × for  $\langle j_2 \rangle$ , • for  $\langle j_4 \rangle$ ) of the radial integrals for Pt<sup>2+</sup> in the  $(6s^0 5d^8)$  configuration. The calculated values are plotted at an interval of  $0.05 \text{ \AA}^{-1}$ .

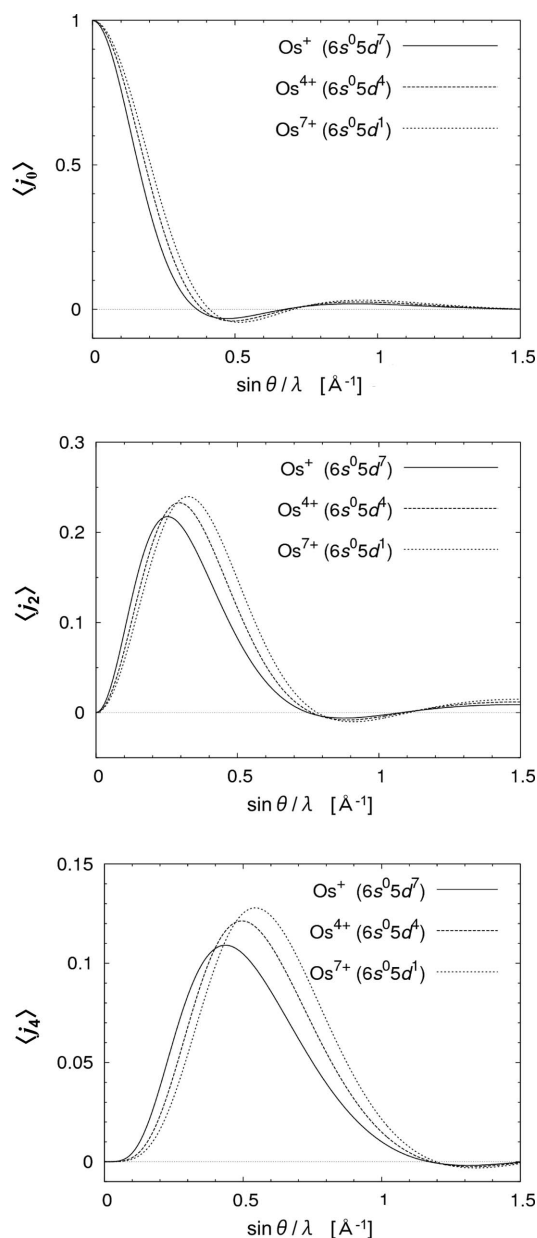
Second, to demonstrate the effect of different electronic configurations, Fig. 3 presents a comparison of the radial integrals of a neutral Ir atom for the following electronic configurations:  $(6s^05d^9)$ ,  $(6s^15d^8)$  and  $(6s^25d^7)$ . In  $\langle j_0 \rangle$ , there is a difference for  $0 < s < 0.5 \text{ \AA}^{-1}$ , and these lines approach the same line for  $s \geq 0.5 \text{ \AA}^{-1}$ . On the other hand, for  $\langle j_2 \rangle$  and  $\langle j_4 \rangle$ , the differences appear up to the point at which the radial integrals cross zero, e.g.  $s \simeq 0.8 \text{ \AA}^{-1}$  for  $\langle j_2 \rangle$  and  $s \simeq 1.2 \text{ \AA}^{-1}$  for  $\langle j_4 \rangle$ . The peak height and position of  $\langle j_2 \rangle$  are moved from 0.210 at  $s = 0.25 \text{ \AA}^{-1}$  for Ir  $(6s^05d^9)$  to 0.215 at  $s = 0.26 \text{ \AA}^{-1}$  for Ir  $(6s^15d^8)$ , and then on to 0.219 at  $s = 0.27 \text{ \AA}^{-1}$  for Ir  $(6s^25d^7)$ . Similarly, the peak height and position of  $\langle j_4 \rangle$  are moved from 0.104 at  $s = 0.44 \text{ \AA}^{-1}$  for Ir  $(6s^05d^9)$  to 0.107 at  $s = 0.45 \text{ \AA}^{-1}$  for Ir  $(6s^15d^8)$ , and then on to 0.111 at  $s = 0.47 \text{ \AA}^{-1}$  for Ir  $(6s^25d^7)$ .



**Figure 3**  
Comparison of the values of  $\langle j_L \rangle$  for a neutral Ir atom for different electronic configurations: Ir  $(6s^05d^9)$ , Ir  $(6s^15d^8)$  and Ir  $(6s^25d^7)$ . Note that different scales are used for the figures to give a clear view of the differences.

When electrons occupy  $6s$  orbitals,  $5d$  electrons feel less potential from the positive core, and the  $5d$  orbitals tend to spread because of this screening. As a result, the radial integrals of the  $(6s^05d^9)$  electronic configuration are the most squeezed in the  $k$ -space among the three configurations considered.

Next, the influence of valence numbers on the radial integrals is considered for Os ions, which can take valence numbers from  $-2$  to  $+8$  in the oxides. In Fig. 4 the radial integrals of  $\text{Os}^+$   $(6s^05d^7)$ ,  $\text{Os}^{4+}$   $(6s^05d^4)$  and  $\text{Os}^{7+}$   $(6s^05d^1)$  are plotted. The plots of  $\langle j_0 \rangle$  show differences in the region  $0 \leq s \leq 0.5 \text{ \AA}^{-1}$ . On the other hand, the first peaks of both  $\langle j_2 \rangle$  and  $\langle j_4 \rangle$  are noticeably shifted. For example, in  $\langle j_2 \rangle$  the peak position of  $\text{Os}^+$  at  $s = 0.25 \text{ \AA}^{-1}$  shifts to  $s = 0.29 \text{ \AA}^{-1}$  for



**Figure 4**  
Comparison of the values of  $\langle j_L \rangle$  for  $\text{Os}^+$   $(6s^05d^7)$ ,  $\text{Os}^{4+}$   $(6s^05d^4)$  and  $\text{Os}^{7+}$   $(6s^05d^1)$ , respectively. Note that different scales are used for the figures to give a clear view of the differences.

**Table 2**  
 $\langle j_0 \rangle$  form factors for the  $5d$  electrons of transition atoms and ions from Hf to Re.

Atoms and ions (electronic configuration)	$A_0$	$a_0$	$B_0$	$b_0$	$C_0$	$c_0$	$D_0$	$d_0$	$E_0$	$e$
Hf <sup>2+</sup> ( $6s^0 5d^2$ )	0.4229	50.465	0.7333	23.865	-0.3798	4.051	0.2252	2.497	-0.0018	0.0080
Hf <sup>3+</sup> ( $6s^0 5d^1$ )	0.3555	40.954	0.8483	21.726	-0.4116	4.305	0.2101	2.349	-0.0023	0.0051
Ta <sup>2+</sup> ( $6s^0 5d^3$ )	0.3976	45.095	0.7746	21.028	-0.6098	3.471	0.4395	2.570	-0.0020	0.0077
Ta <sup>3+</sup> ( $6s^0 5d^2$ )	0.3611	36.921	0.8579	19.195	-0.4945	3.857	0.2781	2.303	-0.0026	0.0057
Ta <sup>4+</sup> ( $6s^0 5d^1$ )	0.3065	31.817	0.9611	17.749	-0.5463	3.979	0.2816	2.232	-0.0030	0.0050
W ( $6s^0 5d^6$ )	0.3990	73.810	0.7138	22.815	-2.0436	2.710	1.9319	2.559	-0.0023	0.0524
W ( $6s^1 5d^5$ )	0.3811	62.707	0.7523	21.434	-12.5449	2.702	12.4130	2.674	-0.0023	0.0365
W ( $6s^2 5d^4$ )	0.3653	53.965	0.7926	20.078	-0.8142	3.030	0.6581	2.476	-0.0023	0.0247
W <sup>+</sup> ( $6s^0 5d^5$ )	0.4077	51.367	0.7436	20.256	-9.8283	2.780	9.6788	2.740	-0.0021	0.0198
W <sup>+</sup> ( $6s^1 5d^4$ )	0.3834	46.233	0.7890	19.278	-1.4650	2.947	1.2945	2.628	-0.0022	0.0138
W <sup>2+</sup> ( $6s^0 5d^4$ )	0.3876	40.340	0.8008	18.621	-1.3911	2.995	1.2048	2.627	-0.0023	0.0081
W <sup>3+</sup> ( $6s^0 5d^3$ )	0.3610	33.519	0.8717	17.176	-0.6183	3.445	0.3883	2.276	-0.0028	0.0041
W <sup>4+</sup> ( $6s^0 5d^2$ )	0.3221	29.047	0.9574	15.979	-0.6287	3.597	0.3525	2.174	-0.0033	0.0034
W <sup>5+</sup> ( $6s^0 5d^1$ )	0.2725	25.966	1.0558	14.954	-0.6990	3.643	0.3745	2.145	-0.0037	0.0045
Re ( $6s^0 5d^7$ )	0.3807	63.042	0.7497	19.967	-6.5300	2.501	6.4013	2.451	-0.0028	0.0480
Re ( $6s^1 5d^6$ )	0.3691	53.934	0.7837	18.790	-9.1491	2.558	8.9983	2.517	-0.0027	0.0333
Re ( $6s^2 5d^5$ )	0.3548	47.108	0.8210	17.769	-9.8674	2.599	9.6938	2.556	-0.0027	0.0248
Re <sup>+</sup> ( $6s^0 5d^6$ )	0.3944	45.427	0.7742	17.948	-3.1692	2.653	3.0028	2.521	-0.0026	0.0192
Re <sup>+</sup> ( $6s^1 5d^5$ )	0.3736	41.151	0.8160	17.158	-7.0396	2.642	6.8523	2.577	-0.0026	0.0139
Re <sup>2+</sup> ( $6s^0 5d^5$ )	0.3825	36.336	0.8218	16.636	-8.7220	2.657	8.5201	2.601	-0.0026	0.0083
Re <sup>3+</sup> ( $6s^0 5d^4$ )	0.3585	30.671	0.8863	15.527	-0.8682	3.047	0.6263	2.280	-0.0030	0.0052
Re <sup>4+</sup> ( $6s^0 5d^3$ )	0.2974	27.372	0.9826	14.807	-1.8869	2.840	1.6100	2.476	-0.0031	0.0036
Re <sup>5+</sup> ( $6s^0 5d^2$ )	0.3143	23.522	1.0276	13.505	-0.7438	3.393	0.4059	2.030	-0.0041	0.0037
Re <sup>6+</sup> ( $6s^0 5d^1$ )	0.2146	22.496	1.1616	13.064	-1.0455	3.162	0.6734	2.196	-0.0041	0.0035

**Table 3**  
 $\langle j_0 \rangle$  form factors for the  $5d$  electrons of transition atoms and ions from Os to Au.

Atoms and ions (electronic configuration)	$A_0$	$a_0$	$B_0$	$b_0$	$C_0$	$c_0$	$D_0$	$d_0$	$E_0$	$e$
Os ( $6s^0 5d^8$ )	0.3676	54.835	0.7793	17.716	-2.0669	2.418	1.9224	2.247	-0.0034	0.0446
Os ( $6s^1 5d^7$ )	0.3571	47.458	0.8123	16.770	-1.2072	2.556	1.0404	2.211	-0.0033	0.0314
Os ( $6s^2 5d^6$ )	0.3467	41.778	0.8458	15.918	-5.6370	2.459	5.4472	2.381	-0.0032	0.0222
Os <sup>+</sup> ( $6s^0 5d^7$ )	0.3837	40.665	0.8006	16.096	-3.5305	2.487	3.3488	2.366	-0.0030	0.0190
Os <sup>+</sup> ( $6s^1 5d^6$ )	0.3666	36.997	0.8390	15.425	-2.6944	2.537	2.4916	2.360	-0.0031	0.0140
Os <sup>2+</sup> ( $6s^0 5d^6$ )	0.3786	33.005	0.8412	14.990	-7.0632	2.503	6.8462	2.433	-0.0030	0.0098
Os <sup>3+</sup> ( $6s^0 5d^5$ )	0.3557	28.222	0.9002	14.140	-2.5972	2.601	2.3444	2.376	-0.0032	0.0041
Os <sup>4+</sup> ( $6s^0 5d^4$ )	0.3337	24.723	0.9655	13.288	-0.9653	2.906	0.6698	2.117	-0.0037	0.0050
Os <sup>5+</sup> ( $6s^0 5d^3$ )	0.3055	22.152	1.0395	12.529	-0.9158	3.016	0.5750	2.032	-0.0042	0.0022
Os <sup>6+</sup> ( $6s^0 5d^2$ )	0.2714	20.218	1.1211	11.851	-0.9773	3.050	0.5894	2.005	-0.0046	0.0021
Os <sup>7+</sup> ( $6s^0 5d^1$ )	0.2101	19.108	1.2240	11.347	-1.2543	2.933	0.8250	2.088	-0.0048	0.0022
Ir ( $6s^0 5d^9$ )	0.3564	48.464	0.8049	15.923	-2.5258	2.265	2.3675	2.121	-0.0040	0.0420
Ir ( $6s^1 5d^8$ )	0.3492	42.195	0.8350	15.113	-5.1496	2.279	4.9686	2.201	-0.0038	0.0296
Ir ( $6s^2 5d^7$ )	0.3400	37.499	0.8675	14.402	-2.3703	2.370	2.1661	2.177	-0.0037	0.0214
Ir <sup>+</sup> ( $6s^0 5d^8$ )	0.3744	36.764	0.8240	14.576	-8.8616	2.303	8.6664	2.255	-0.0035	0.0191
Ir <sup>+</sup> ( $6s^1 5d^7$ )	0.3604	33.570	0.8597	13.993	-2.1686	2.412	1.9518	2.188	-0.0036	0.0142
Ir <sup>2+</sup> ( $6s^0 5d^7$ )	0.3802	30.032	0.8550	13.567	-1.6185	2.488	1.3866	2.162	-0.0035	0.0094
Ir <sup>3+</sup> ( $6s^0 5d^6$ )	0.3678	25.828	0.9065	12.788	-0.8587	2.745	0.5883	1.960	-0.0040	0.0049
Ir <sup>4+</sup> ( $6s^0 5d^5$ )	0.3969	22.050	0.9310	11.768	-0.7090	3.017	0.3857	1.778	-0.0047	0.0045
Ir <sup>5+</sup> ( $6s^0 5d^4$ )	0.3059	20.759	1.0432	11.622	-1.3457	2.655	1.0008	2.066	-0.0043	0.0043
Ir <sup>6+</sup> ( $6s^0 5d^3$ )	0.2854	18.867	1.1123	10.982	-1.1403	2.782	0.7475	1.959	-0.0049	0.0035
Pt <sup>+</sup> ( $6s^0 5d^9$ )	0.3664	33.503	0.8449	13.303	-2.6192	2.227	2.4116	2.059	-0.0041	0.0189
Pt <sup>2+</sup> ( $6s^0 5d^8$ )	0.3701	27.799	0.8761	12.480	-3.2959	2.258	3.0535	2.106	-0.0040	0.0098
Pt <sup>3+</sup> ( $6s^0 5d^7$ )	0.3606	24.052	0.9205	11.833	-4.0612	2.271	3.7841	2.133	-0.0041	0.0049
Pt <sup>4+</sup> ( $6s^0 5d^6$ )	0.3429	21.358	0.9753	11.261	-2.2859	2.357	1.9719	2.074	-0.0043	0.0033
Pt <sup>5+</sup> ( $6s^0 5d^5$ )	0.3649	18.762	1.0102	10.456	-0.8785	2.765	0.5087	1.737	-0.0053	0.0033
Pt <sup>6+</sup> ( $6s^0 5d^4$ )	0.2877	17.780	1.1111	10.263	-1.9416	2.432	1.5477	2.015	-0.0049	0.0026
Au <sup>+</sup> ( $6s^1 5d^9$ )	0.3475	28.294	0.8964	11.794	-4.5383	2.086	4.2988	1.983	-0.0047	0.0143
Au <sup>2+</sup> ( $6s^0 5d^9$ )	0.3664	25.714	0.8919	11.488	-1.7302	2.207	1.4763	1.908	-0.0046	0.0102
Au <sup>3+</sup> ( $6s^0 5d^8$ )	0.3639	22.330	0.9313	10.883	-1.1359	2.355	0.8455	1.809	-0.0048	0.0068
Au <sup>4+</sup> ( $6s^0 5d^7$ )	0.3472	19.944	0.9807	10.424	-3.8228	2.169	3.4995	2.009	-0.0047	0.0040
Au <sup>5+</sup> ( $6s^0 5d^6$ )	0.3292	18.073	1.0376	9.957	-2.2028	2.257	1.8410	1.938	-0.0050	0.0035

**Table 4**  
 $\langle j_2 \rangle$  form factors for the 5d electrons of transition atoms and ions from Hf to Re.

Atoms and ions (electronic configuration)	$A_2$	$a_2$	$B_2$	$b_2$	$C_2$	$c_2$	$D_2$	$d_2$	$E_2$	$e$
Hf <sup>2+</sup> (6s <sup>0</sup> 5d <sup>2</sup> )	9.6670	33.435	5.2429	13.529	-0.5533	1.402	0.4934	1.254	-0.0033	0.0448
Hf <sup>3+</sup> (6s <sup>0</sup> 5d <sup>1</sup> )	7.5646	27.367	5.0743	12.402	-0.4133	1.742	0.3163	1.437	-0.0012	0.0251
Ta <sup>2+</sup> (6s <sup>0</sup> 5d <sup>3</sup> )	8.1746	29.871	4.9405	12.188	-1.1294	1.254	1.0658	1.181	-0.0046	0.0411
Ta <sup>3+</sup> (6s <sup>0</sup> 5d <sup>2</sup> )	6.5998	25.026	4.7913	11.303	-0.7801	1.529	0.6820	1.382	-0.0019	0.0239
Ta <sup>4+</sup> (6s <sup>0</sup> 5d <sup>1</sup> )	5.5048	21.620	4.6734	10.556	-0.2181	2.100	0.0810	1.049	-0.0016	0.0154
W (6s <sup>0</sup> 5d <sup>6</sup> )	8.4216	64.652	7.6983	23.124	2.3605	8.583	-0.3876	4.620	0.0033	0.0424
W (6s <sup>1</sup> 5d <sup>5</sup> )	6.9289	53.425	7.2157	20.016	5.7754	6.543	-4.2114	5.854	0.0036	0.0398
W (6s <sup>2</sup> 5d <sup>4</sup> )	5.4017	47.110	6.9113	18.760	7.0586	6.363	-5.4525	5.802	0.0040	0.0400
W <sup>+</sup> (6s <sup>0</sup> 5d <sup>5</sup> )	5.6854	44.743	6.8903	18.753	7.8523	6.308	-6.3447	5.842	0.0038	0.0383
W <sup>+</sup> (6s <sup>1</sup> 5d <sup>4</sup> )	4.5118	41.281	6.7136	17.964	7.6331	6.269	-6.0365	5.758	0.0042	0.0405
W <sup>2+</sup> (6s <sup>0</sup> 5d <sup>4</sup> )	7.0301	26.990	4.6604	11.083	-0.8220	1.145	0.7581	1.042	-0.0068	0.0381
W <sup>3+</sup> (6s <sup>0</sup> 5d <sup>3</sup> )	5.8036	22.969	4.5243	10.361	-0.7897	1.388	0.6927	1.248	-0.0031	0.0229
W <sup>4+</sup> (6s <sup>0</sup> 5d <sup>2</sup> )	4.9006	20.117	4.4360	9.765	-2.0009	1.497	1.8714	1.431	-0.0014	0.0145
W <sup>5+</sup> (6s <sup>0</sup> 5d <sup>1</sup> )	4.1973	17.967	4.3791	9.255	-1.8830	1.603	1.7205	1.518	-0.0004	0.0088
Re (6s <sup>0</sup> 5d <sup>7</sup> )	6.7574	55.529	6.7931	20.125	2.3113	7.529	-0.5004	4.412	0.0037	0.0365
Re (6s <sup>1</sup> 5d <sup>6</sup> )	5.5830	46.852	6.4516	17.855	5.0609	6.037	-3.5427	5.312	0.0040	0.0334
Re (6s <sup>2</sup> 5d <sup>5</sup> )	4.4322	41.798	6.2063	16.844	9.8763	5.751	-8.3294	5.406	0.0043	0.0327
Re <sup>+</sup> (6s <sup>0</sup> 5d <sup>6</sup> )	4.7231	40.130	6.2139	16.902	8.8240	5.766	-7.3608	5.396	0.0042	0.0316
Re <sup>+</sup> (6s <sup>1</sup> 5d <sup>5</sup> )	3.7875	37.254	6.0587	16.264	6.9896	5.786	-5.4457	5.279	0.0045	0.0329
Re <sup>2+</sup> (6s <sup>0</sup> 5d <sup>5</sup> )	3.0708	33.896	5.9941	15.817	6.7816	5.768	-5.2056	5.231	0.0047	0.0343
Re <sup>3+</sup> (6s <sup>0</sup> 5d <sup>4</sup> )	1.7870	31.248	5.9068	15.160	17.4262	5.551	-15.6856	5.339	0.0053	0.0374
Re <sup>4+</sup> (6s <sup>0</sup> 5d <sup>3</sup> )	4.4033	18.733	4.1971	9.047	-2.3106	1.352	2.1866	1.299	-0.0025	0.0158
Re <sup>5+</sup> (6s <sup>0</sup> 5d <sup>2</sup> )	3.8162	16.843	4.1400	8.605	-4.0882	1.443	3.9333	1.408	-0.0012	0.0132
Re <sup>6+</sup> (6s <sup>0</sup> 5d <sup>1</sup> )	3.3349	15.341	4.1015	8.213	-2.3511	1.531	2.1651	1.459	-0.0003	0.0067

**Table 5**  
 $\langle j_2 \rangle$  form factors for the 5d electrons of transition atoms and ions from Os to Au.

Atoms and ions (electronic configuration)	$A_2$	$a_2$	$B_2$	$b_2$	$C_2$	$c_2$	$D_2$	$d_2$	$E_2$	$e$
Os (6s <sup>0</sup> 5d <sup>8</sup> )	5.5418	48.893	6.0803	17.984	2.2542	6.853	-0.5285	4.095	0.0040	0.0303
Os (6s <sup>1</sup> 5d <sup>7</sup> )	4.6511	41.610	5.8194	16.062	6.7172	5.447	-5.2689	4.986	0.0043	0.0274
Os (6s <sup>2</sup> 5d <sup>6</sup> )	3.7421	37.491	5.6137	15.256	10.0488	5.293	-8.5683	4.991	0.0046	0.0259
Os <sup>+</sup> (6s <sup>0</sup> 5d <sup>7</sup> )	4.0236	36.272	5.6349	15.338	8.6568	5.318	-7.2505	4.980	0.0044	0.0253
Os <sup>+</sup> (6s <sup>1</sup> 5d <sup>6</sup> )	3.2611	33.818	5.4945	14.808	5.7610	5.391	-4.2811	4.827	0.0048	0.0261
Os <sup>2+</sup> (6s <sup>0</sup> 5d <sup>6</sup> )	2.7289	30.900	5.4357	14.396	18.6546	5.151	-17.1708	4.993	0.0050	0.0268
Os <sup>3+</sup> (6s <sup>0</sup> 5d <sup>5</sup> )	4.5913	19.692	4.0615	8.862	-0.9950	1.086	0.9081	0.986	-0.0077	0.0206
Os <sup>4+</sup> (6s <sup>0</sup> 5d <sup>4</sup> )	3.9724	17.514	3.9817	8.421	-0.7719	1.264	0.6552	1.107	-0.0042	0.0131
Os <sup>5+</sup> (6s <sup>0</sup> 5d <sup>3</sup> )	3.4764	15.826	3.9241	8.032	-0.6854	1.397	0.5394	1.184	-0.0024	0.0098
Os <sup>6+</sup> (6s <sup>0</sup> 5d <sup>2</sup> )	3.0642	14.479	3.8847	7.686	-4.7235	1.384	4.5485	1.352	-0.0012	0.0063
Os <sup>7+</sup> (6s <sup>0</sup> 5d <sup>1</sup> )	2.7164	13.366	3.8554	7.370	-5.0211	1.439	4.8166	1.405	-0.0004	0.0064
Ir (6s <sup>0</sup> 5d <sup>9</sup> )	4.6102	43.878	5.4892	16.394	2.1707	6.423	-0.4761	3.722	0.0043	0.0254
Ir (6s <sup>1</sup> 5d <sup>8</sup> )	3.9372	37.508	5.2846	14.661	3.7267	5.263	-2.3158	4.416	0.0045	0.0217
Ir (6s <sup>2</sup> 5d <sup>7</sup> )	3.2263	33.922	5.1086	13.921	6.5993	4.978	-5.1841	4.549	0.0048	0.0203
Ir <sup>+</sup> (6s <sup>0</sup> 5d <sup>8</sup> )	3.4956	32.991	5.1369	13.998	8.3991	4.924	-7.0561	4.612	0.0047	0.0196
Ir <sup>+</sup> (6s <sup>1</sup> 5d <sup>7</sup> )	2.8732	30.809	5.0094	13.522	6.8656	4.933	-5.4669	4.526	0.0050	0.0199
Ir <sup>2+</sup> (6s <sup>0</sup> 5d <sup>7</sup> )	2.4419	28.356	4.9470	13.222	4.7478	5.029	-3.3259	4.393	0.0052	0.0208
Ir <sup>3+</sup> (6s <sup>0</sup> 5d <sup>6</sup> )	1.5883	25.969	4.8472	12.711	5.6507	4.949	-4.1190	4.388	0.0056	0.0218
Ir <sup>4+</sup> (6s <sup>0</sup> 5d <sup>5</sup> )	3.5964	16.439	3.7872	7.873	-1.2303	1.092	1.1232	1.003	-0.0068	0.0127
Ir <sup>5+</sup> (6s <sup>0</sup> 5d <sup>4</sup> )	3.1710	14.923	3.7320	7.529	-1.5400	1.200	1.4048	1.119	-0.0040	0.0091
Ir <sup>6+</sup> (6s <sup>0</sup> 5d <sup>3</sup> )	2.8163	13.697	3.6906	7.219	-5.2957	1.254	5.1328	1.228	-0.0024	0.0109
Pt <sup>+</sup> (6s <sup>0</sup> 5d <sup>9</sup> )	3.0783	30.198	4.7065	12.857	5.7270	4.650	-4.4425	4.222	0.0048	0.0156
Pt <sup>2+</sup> (6s <sup>0</sup> 5d <sup>8</sup> )	2.2407	26.003	4.5300	12.118	6.7189	4.557	-5.3954	4.187	0.0053	0.0147
Pt <sup>3+</sup> (6s <sup>0</sup> 5d <sup>7</sup> )	1.5391	23.689	4.4263	11.645	8.5673	4.482	-7.1591	4.181	0.0057	0.0160
Pt <sup>4+</sup> (6s <sup>0</sup> 5d <sup>6</sup> )	0.9477	22.775	4.3337	11.319	7.2374	4.500	-5.7086	4.106	0.0062	0.0166
Pt <sup>5+</sup> (6s <sup>0</sup> 5d <sup>5</sup> )	0.5132	23.124	4.1835	11.009	7.4312	4.478	-5.7759	4.065	0.0066	0.0176
Pt <sup>6+</sup> (6s <sup>0</sup> 5d <sup>4</sup> )	2.5907	12.991	3.5155	6.801	-0.7511	1.206	0.6014	1.022	-0.0043	0.0070
Au <sup>+</sup> (6s <sup>1</sup> 5d <sup>9</sup> )	2.3189	25.954	4.2267	11.444	9.0997	4.215	-7.8523	3.981	0.0052	0.0120
Au <sup>2+</sup> (6s <sup>0</sup> 5d <sup>9</sup> )	2.0676	23.960	4.1678	11.164	13.3827	4.151	-12.1447	3.996	0.0054	0.0130
Au <sup>3+</sup> (6s <sup>0</sup> 5d <sup>8</sup> )	1.4776	21.784	4.0585	10.746	5.9059	4.242	-4.5905	3.842	0.0058	0.0116
Au <sup>4+</sup> (6s <sup>0</sup> 5d <sup>7</sup> )	2.9775	14.632	3.4472	6.956	-1.9784	0.794	1.8980	0.745	-0.0182	0.0123
Au <sup>5+</sup> (6s <sup>0</sup> 5d <sup>6</sup> )	0.5763	20.517	3.8572	10.171	6.0222	4.213	-4.5020	3.760	0.0067	0.0129

**Table 6**  
 $\langle j_4 \rangle$  form factors for the 5d electrons of transition atoms and ions from Hf to Re.

Atoms and ions (electronic configuration)	$A_4$	$a_4$	$B_4$	$b_4$	$C_4$	$c_4$	$D_4$	$d_4$	$E_4$	$e$
Hf <sup>2+</sup> (6s <sup>0</sup> 5d <sup>2</sup> )	-2.5342	43.826	1.8466	10.393	0.7761	4.888	-0.0327	1.589	0.0017	0.0046
Hf <sup>3+</sup> (6s <sup>0</sup> 5d <sup>1</sup> )	-2.3574	32.651	1.8717	8.476	0.6367	3.953	-0.1133	2.169	0.0017	0.0048
Ta <sup>2+</sup> (6s <sup>0</sup> 5d <sup>3</sup> )	-2.1974	38.294	1.6220	8.838	0.6836	4.212	-0.0539	1.746	0.0016	0.0069
Ta <sup>3+</sup> (6s <sup>0</sup> 5d <sup>2</sup> )	-2.0884	29.531	1.7145	7.385	1.1809	2.994	-0.7705	2.577	0.0016	0.0066
Ta <sup>4+</sup> (6s <sup>0</sup> 5d <sup>1</sup> )	-2.0226	24.035	1.7084	6.594	1.1799	2.775	-0.8384	2.430	0.0020	0.0053
W (6s <sup>0</sup> 5d <sup>6</sup> )	-2.1307	79.955	1.4055	11.876	0.8808	4.969	-0.0120	0.419	0.0051	0.0085
W (6s <sup>1</sup> 5d <sup>5</sup> )	-1.9667	60.069	1.3446	9.992	0.7861	4.554	-0.0197	1.087	0.0021	0.0083
W (6s <sup>2</sup> 5d <sup>4</sup> )	-1.8575	47.554	1.3868	8.437	0.6537	3.939	-0.0570	1.722	0.0015	0.0092
W <sup>+</sup> (6s <sup>0</sup> 5d <sup>5</sup> )	-2.0231	46.962	1.3937	9.263	0.7420	4.332	-0.0288	1.327	0.0018	0.0062
W <sup>+</sup> (6s <sup>1</sup> 5d <sup>4</sup> )	-1.9122	39.952	1.4385	8.019	0.6336	3.725	-0.0819	1.868	0.0015	0.0073
W <sup>2+</sup> (6s <sup>0</sup> 5d <sup>4</sup> )	-1.9355	33.935	1.5020	7.541	0.6453	3.375	-0.1601	2.110	0.0015	0.0063
W <sup>3+</sup> (6s <sup>0</sup> 5d <sup>3</sup> )	-1.8752	26.706	1.5440	6.585	5.9785	2.575	-5.6111	2.516	0.0018	0.0061
W <sup>4+</sup> (6s <sup>0</sup> 5d <sup>2</sup> )	-1.8309	22.142	1.5605	5.935	1.4898	2.482	-1.1930	2.266	0.0022	0.0066
W <sup>5+</sup> (6s <sup>0</sup> 5d <sup>1</sup> )	-1.7958	18.987	1.5913	5.419	2.0498	2.278	-1.8262	2.156	0.0026	0.0050
Re (6s <sup>0</sup> 5d <sup>7</sup> )	-1.8013	63.944	1.1773	9.808	0.7912	4.380	-0.0155	0.795	0.0027	0.0080
Re (6s <sup>1</sup> 5d <sup>6</sup> )	-1.7056	49.628	1.2209	8.231	0.6637	3.836	-0.0443	1.514	0.0015	0.0088
Re (6s <sup>2</sup> 5d <sup>5</sup> )	-1.6402	40.319	1.3192	7.064	0.8659	2.901	-0.4299	2.306	0.0013	0.0098
Re <sup>+</sup> (6s <sup>0</sup> 5d <sup>6</sup> )	-1.7723	40.683	1.2795	7.798	0.6385	3.630	-0.0656	1.686	0.0015	0.0084
Re <sup>+</sup> (6s <sup>1</sup> 5d <sup>5</sup> )	-1.6968	34.939	1.3535	6.851	1.7292	2.681	-1.3118	2.445	0.0014	0.0084
Re <sup>2+</sup> (6s <sup>0</sup> 5d <sup>5</sup> )	-1.7305	30.305	1.3808	6.606	1.5787	2.630	-1.1785	2.378	0.0015	0.0079
Re <sup>3+</sup> (6s <sup>0</sup> 5d <sup>4</sup> )	-1.6969	24.325	1.4088	5.901	1.5067	2.424	-1.1834	2.209	0.0019	0.0069
Re <sup>4+</sup> (6s <sup>0</sup> 5d <sup>3</sup> )	-1.6679	20.454	1.4439	5.357	0.8175	2.321	-0.5685	1.976	0.0024	0.0056
Re <sup>5+</sup> (6s <sup>0</sup> 5d <sup>2</sup> )	-1.6427	17.722	1.4880	4.916	0.5419	2.189	-0.3694	1.781	0.0029	0.0050
Re <sup>6+</sup> (6s <sup>0</sup> 5d <sup>1</sup> )	-1.6211	15.673	1.5419	4.548	1.9205	1.833	-1.8287	1.766	0.0034	0.0055

**Table 7**  
 $\langle j_4 \rangle$  form factors for the 5d electrons of transition atoms and ions from Os to Au.

Atoms and ions (electronic configuration)	$A_4$	$a_4$	$B_4$	$b_4$	$C_4$	$c_4$	$D_4$	$d_4$	$E_4$	$e$
Os (6s <sup>0</sup> 5d <sup>8</sup> )	-1.5677	53.075	1.0631	8.143	0.6808	3.771	-0.0308	1.243	0.0017	0.0095
Os (6s <sup>1</sup> 5d <sup>7</sup> )	-1.5109	42.193	1.1910	6.850	2.4597	2.602	-2.0163	2.444	0.0011	0.0100
Os (6s <sup>2</sup> 5d <sup>6</sup> )	-1.4734	34.814	1.2105	6.165	0.9468	2.534	-0.5773	2.131	0.0015	0.0108
Os <sup>+</sup> (6s <sup>0</sup> 5d <sup>7</sup> )	-1.5777	35.746	1.2222	6.650	1.7260	2.590	-1.2942	2.360	0.0012	0.0081
Os <sup>+</sup> (6s <sup>1</sup> 5d <sup>6</sup> )	-1.5274	30.891	1.2364	6.044	1.4100	2.431	-1.0480	2.188	0.0016	0.0086
Os <sup>2+</sup> (6s <sup>0</sup> 5d <sup>6</sup> )	-1.5637	27.292	1.2627	5.880	1.3526	2.393	-1.0026	2.146	0.0017	0.0071
Os <sup>3+</sup> (6s <sup>0</sup> 5d <sup>5</sup> )	-1.5453	22.300	1.3058	5.301	0.7208	2.294	-0.4480	1.881	0.0022	0.0071
Os <sup>4+</sup> (6s <sup>0</sup> 5d <sup>4</sup> )	-1.5267	18.972	1.3619	4.834	3.0121	1.938	-2.8240	1.877	0.0027	0.0091
Os <sup>5+</sup> (6s <sup>0</sup> 5d <sup>3</sup> )	-1.5094	16.573	1.4158	4.458	0.8448	1.797	-0.7349	1.638	0.0033	0.0058
Os <sup>6+</sup> (6s <sup>0</sup> 5d <sup>2</sup> )	-1.4938	14.751	1.4678	4.149	0.8091	1.535	-0.7720	1.442	0.0041	0.0048
Os <sup>7+</sup> (6s <sup>0</sup> 5d <sup>1</sup> )	-0.0341	37.994	-1.4680	13.159	1.5216	3.898	-0.0308	0.550	0.0083	0.0044
Ir (6s <sup>0</sup> 5d <sup>9</sup> )	-1.3913	45.243	1.0627	6.722	2.5141	2.534	-2.0510	2.383	0.0009	0.0099
Ir (6s <sup>1</sup> 5d <sup>8</sup> )	-1.3605	36.399	1.0953	5.990	1.7223	2.353	-1.3416	2.162	0.0014	0.0111
Ir (6s <sup>2</sup> 5d <sup>7</sup> )	-1.3382	30.628	1.1376	5.420	1.4261	2.160	-1.1282	1.974	0.0019	0.0115
Ir <sup>+</sup> (6s <sup>0</sup> 5d <sup>8</sup> )	-1.4233	31.680	1.1221	5.872	2.2721	2.301	-1.8973	2.163	0.0015	0.0108
Ir <sup>+</sup> (6s <sup>1</sup> 5d <sup>7</sup> )	-1.3875	27.660	1.1508	5.362	0.6586	2.302	-0.3554	1.810	0.0020	0.0094
Ir <sup>2+</sup> (6s <sup>0</sup> 5d <sup>7</sup> )	-1.4233	24.796	1.1799	5.246	3.2548	2.072	-2.9649	1.997	0.0020	0.0099
Ir <sup>3+</sup> (6s <sup>0</sup> 5d <sup>6</sup> )	-1.4149	20.563	1.2388	4.761	1.1780	1.928	-0.9708	1.761	0.0026	0.0071
Ir <sup>4+</sup> (6s <sup>0</sup> 5d <sup>5</sup> )	-1.4039	17.664	1.2993	4.371	3.5599	1.661	-3.4340	1.625	0.0033	0.0065
Ir <sup>5+</sup> (6s <sup>0</sup> 5d <sup>4</sup> )	-1.3927	15.539	1.3536	4.057	0.2946	1.554	-0.2412	1.266	0.0043	0.0061
Ir <sup>6+</sup> (6s <sup>0</sup> 5d <sup>3</sup> )	-0.0364	41.929	-1.3662	13.771	1.4130	3.784	-0.0384	0.190	0.0241	0.0043
Pt <sup>+</sup> (6s <sup>0</sup> 5d <sup>9</sup> )	-1.2955	28.407	1.0534	5.206	1.2452	2.096	-0.9336	1.881	0.0018	0.0104
Pt <sup>2+</sup> (6s <sup>0</sup> 5d <sup>8</sup> )	-1.3038	22.692	1.1238	4.691	3.2444	1.814	-3.0209	1.757	0.0025	0.0100
Pt <sup>3+</sup> (6s <sup>0</sup> 5d <sup>7</sup> )	-1.3019	19.052	1.1904	4.286	3.3886	1.592	-3.2484	1.554	0.0034	0.0087
Pt <sup>4+</sup> (6s <sup>0</sup> 5d <sup>6</sup> )	-1.2964	16.503	1.2497	3.964	1.7648	1.350	-1.6992	1.305	0.0046	0.0066
Pt <sup>5+</sup> (6s <sup>0</sup> 5d <sup>5</sup> )	-1.2902	14.600	1.2945	3.709	0.5190	1.033	-0.5122	0.963	0.0067	0.0054
Pt <sup>6+</sup> (6s <sup>0</sup> 5d <sup>4</sup> )	-0.0482	33.010	-1.2661	12.839	1.3254	3.545	-0.0455	0.144	0.0315	0.0027
Au <sup>+</sup> (6s <sup>1</sup> 5d <sup>9</sup> )	-1.1686	22.808	1.0729	4.243	0.9462	1.573	-0.7943	1.428	0.0036	0.0104
Au <sup>2+</sup> (6s <sup>0</sup> 5d <sup>9</sup> )	-1.2005	20.888	1.0879	4.203	0.8896	1.584	-0.7371	1.428	0.0036	0.0109
Au <sup>3+</sup> (6s <sup>0</sup> 5d <sup>8</sup> )	-1.2033	17.722	1.1507	3.874	0.2426	1.455	-0.1649	1.049	0.0053	0.0080
Au <sup>4+</sup> (6s <sup>0</sup> 5d <sup>7</sup> )	-1.2021	15.459	1.2003	3.615	0.6189	0.952	-0.6028	0.886	0.0081	0.0074
Au <sup>5+</sup> (6s <sup>0</sup> 5d <sup>6</sup> )	-1.2007	13.734	1.2262	3.424	0.5164	0.401	-0.5461	0.379	0.0216	0.0060

Os<sup>4+</sup>, and then on to  $s = 0.32 \text{ \AA}^{-1}$  for Os<sup>7+</sup>. At the same time the peak height increases from 0.218 for Os<sup>+</sup> to 0.233 for Os<sup>4+</sup>, and then on to 0.240 for Os<sup>7+</sup>. The shifts of the peak position and height of  $\langle j_4 \rangle$  are more noticeable than those of  $\langle j_2 \rangle$ . In the dipole approximation the magnetic form factor is approximated by

$$\mu_{\text{dipole}}^f(\mathbf{k}) = \mu[\langle j_0(k) \rangle + \tilde{c}_2 \langle j_2(k) \rangle], \quad (11)$$

where  $\tilde{c}_2$  is an isotropic contribution of  $c_2$  in equation (1) (Balcar & Lovesey, 1989). Therefore, the differences in  $\langle j_2 \rangle$  as well as the inclusion of  $\langle j_4 \rangle$  may significantly affect the analysis of the magnetic structure of 5d transition metals, whose orbital moment might not be quenched.

Lastly, the results shown in Figs. 3 and 4 indicate that the electronic configuration and/or valence number can influence the shape of form factors; therefore, the fitted coefficients of the calculated radial integrals of possible electronic configurations and valence numbers of 5d transition metals in compounds have been tabulated for the preparation of experimental analysis. Tables 2 and 3 give the fitting parameters in equation (8) for  $\langle j_0 \rangle$ . Tables 4 and 5 and Tables 6 and 7 show the fitting parameters in equation (9) for  $\langle j_2 \rangle$  and  $\langle j_4 \rangle$ , respectively. Moreover,  $e$  values, defined by equation (10), are tabulated. As the valence number increases, the fitting parameter  $e$  decreases. Therefore, the states with a high valence number may be described more correctly by the Gaussian analytical expressions.

In summary, the radial integrals for the 5d electrons of transition metal atoms and ions were calculated using the HFR method of the Cowan program, and the fitted coefficients of these integral values in the Gaussian analytical expressions were tabulated. This table can be used for the interpretation of magnetic form factor measurements for compounds that include 5d transition elements.

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