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Electric field gradient in transition metal: Scandium

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Abstract. Corrections to results of electric field gradient (EFG) already published [*Pramaṇa – J. Phys.* **41**, 443 (1993)] are reported. The corrected net EFG is: $q = -8{\cdot}01 \times 10^{13}$ esu/cm^3 against the published value $q = 16{\cdot}06 \times 10^{13}$ esu/cm^3. The present result agrees reasonably well with the experimental result, $|q_{expt}| = 13 \times 10^{13}$ esu/cm^3.

Recently, a computational error is detected, which modifies the results of EFG, we have already published [1]. The error was committed mainly in the part that evaluated the p–p contribution [1] to EFG by the conduction electrons. The corrected results are summarized in table 1 which must replace the table 1 of the published work [1].

In addition, the lattice parameters as well as the temperature were also misquoted in the previous work [1]. The right parameters are: $a = 6{\cdot}25311$ au and $c = 9{\cdot}96509$ au. The temperature at which EFG's are calculated is 293 K instead of 11 K as reported before [1].

The discussions and conclusions made in the published work [1] remain almost unchanged except that they now refer to the corrected numbers. Although the corrected net EFG suffers a sign reversal from the one already published [1], the agreement with experiment is still considered reasonably good because the sign of experimental EFG is not determined. The computational error however does not affect the introduction and theory section of the published work [1].

References

[1] B B Panigrahi and N C Mohapatra, *Pramana – J. Phys.* **41**, 443 (1993)
[2] P Blaha, K Schwartz and P H Dederichs, *Phys. Rev.* **B37**, 2792 (1988)

Table 1. Various components of EFG in hcp scandium metal. All the EFG's are expressed in units of 10^{13} esu/cm^3.

	Present work											
	q_{el}											
q_{latt}	PW–PW unshielded	PW–PW shielded	s–d	p–p	p–f	dist.	Total (unshielded)	Total (shielded)	Net q Colm. 1 + Colm. 8	Net q Colm. 1 + Colm. 9	Other work [2] q	Expt. $\|q\|$
122·17	−0·45	−5·72	−4·81	−118·23	−1·32	−0·10	−124·91	−130·18	−2·74	−8·01	32·0	13·0