The corrected crystal field matrix elements are tabulated in an accompanying erratum.[7] The corrected matrices formed, when diagonalized without spin–orbit interaction give eigenvalues identical to those of the Tanabe–Sugano matrices[8] except for degeneracy.

The errors in the spin–orbit elements are all systematic and are caused by a failure to recognize that no spin–orbit interaction can exist between linearly independent terms of the same classification. Clearly, this would split the degeneracy of a J state even in the absence of a crystal field, contrary to the $\mathbf{S}\cdot\mathbf{L}$ coupling scheme. If spin–orbit elements between the pairs of states listed in the erratum[9] are deleted, the spin–orbit part is correct. This was confirmed by direct diagonalization of the spin–orbit part (i.e., crystal field set equal to zero) and comparison of the eigenvalues with the eigenvalues of d^4 in a simple jj coupling scheme. They are of course identical except for degeneracy in the absence of electronic repulsion terms.

It should be noted that when using these matrices to assign spectra, the electronic repulsion integrals, corresponding to the free-ion energies, must be added in the correct way as outlined previously.[1] This may be checked against the strong field spin orbit matrices[9] for consistency.

[1] J. Ferguson, H. J. Guggenheim, and E. R. Krausz, Australian J. Chem. **22**, 1809 (1969).
[2] T. M. Dunn and W.-K. Li, J. Chem. Phys. **47**, 3783 (1967).
[3] C. W. Nielson and G. F. Koster, *Spectroscopic Coefficients for the p^n, d^n and f^n Configuration* (M.I.T. Press, Cambridge, Mass., 1963).
[4] M. Rotenberg, R. Bivens, N. Metropolis, and J. K. Wooten, Jr., *The 3j and 6j Symbols* (Technology, Cambridge, Mass., 1969).
[5] G. Racah, Phys. Rev. **62**, 438 (1942).
[6] Contrary to what Rotenberg *et al.*[4] indicate, there is no phase difference between a Racah and Condon and Shortley matrix element, in fact

$$\langle L' \,||\, F_k \,||\, L\rangle_{\mathrm{R}} = \langle L' \,||\, F_k \,||\, L\rangle_{\mathrm{C\text{-}S}}(2L'+1)^{1/2}.$$

Using this and Eq. (5.23) (p. 85) in D. M. Brink and G. R. Satchler, *Angular Momentum* (Oxford U. P., London, 1962), the factor may be determined.
[7] T. M. Dunn and W.-K. Li, J. Chem. Phys. **53**, 2132 (1970) (following paper).
[8] Y. Tanabe and S. Sugano, J. Phys. Soc. Japan **9**, 753 (1954).
[9] K. A. Schroeder, J. Chem. Phys. **37**, 2553 (1962).

Errata

Erratum: Matrix Elements for Configuration d^4 in a Weak Octahedral Field Using Racah Methods

[J. Chem. Phys. **47**, 3783 (1967)]

T. M. Dunn and Wai-Kee Li
Chemistry Department, University of Michigan, Ann Arbor, Michigan 48104

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It has been pointed out to us[1] that the list of matrix elements published by us contain some errors. These errors occur in Tables IV and V and include some errors of both the crystal-field and spin–orbit elements.

Crystal-Field Elements:

Γ_4		Original	Corrected
$^3{}_4H_4$	$^3{}_4P_1$	$-4(770)^{1/2}i/105$	$4(770)^{1/2}i/105$
$^3{}_4H_5$	$^3{}_4F_4$	$-(105)^{1/2}/14$	$-(105)^{1/2}i/14$
$^3G_3$	$^3G_3$	$-33/14$	$-39/14$
$^3D_3$	$^3D_3$	$22/21$	$-22/21$
Γ_5			
$^3{}_4G_3$	$^3{}_4F_2$	$-11i/22$	$-11i/21$

Spin–Orbit Elements:

All off-Diagonal elements between primed and unprimed irreducible representations should be zero, i.e.,

$$^3{}_4H_5/{}^3{}_4H_5' \equiv {}^3{}_4H_5/{}^3{}_4G_5' \equiv {}^3{}_4H_5'/{}^3{}_4G_5 \equiv {}^3{}_4G_5/{}^3{}_4G_5' \equiv 0 \quad (\text{all } \Gamma_4)$$

and

$$^3{}_4H_6/{}^3{}_4H_6' \equiv {}^3{}_4H_6/{}^1{}_4I_6' \equiv {}^3{}_4H_6'/{}^1{}_4I_6 \equiv 0_6 \quad (\text{all } \Gamma_5).$$

We are indebted to Dr. Krausz for pointing out these errors.

[1] E. R. Krausz, J. Chem. Phys. **53**, 2132 (1970) (preceding paper).