

The results obtained show a root-mean-square deviation of $\pm 249 \text{ cm}^{-1}$ compared to Racah's $\pm 332 \text{ cm}^{-1}$. Certainly, one more application of the perturbation method and the inclusion of the 2P matrix in obtaining our normal equations would yield still better values.

An error in the calculation of the 2P terms occurs because of the uncertainty in the value of $W(d^2 \text{ } {}^1S)$.

The writer wishes to express his sincere gratitude to Dr. C. W. Ufford for suggesting this topic and for guiding him in all phases of the work.

Electrostatic Energy Matrices of the Configuration f^4

EDITH F. REILLY

University of Pennsylvania, Philadelphia, Pennsylvania

(Received February 17, 1953)

The electrostatic energy matrices of the configuration f^4 are computed by the Racah method, which separates terms of the same kind. The diagonal sums of these matrices are checked by the Slater diagonal sum rule. Three of the matrices are checked by a method developed by Innes.

RACAH¹ has developed a method for computing the electrostatic energy matrices of the configuration f^4 . This method enables one to separate terms of the same kind which occur in a given configuration, whereas Slater's method² finds only the sum, or average, of the terms of the same kind. Hence, the latter method is a partial check on the former. Both methods have been applied to the f^4 configuration and the results of Racah's method are given in Table I. The eigenvalues of the two-by-two matrices are given in Table II. The multiplicity of the term r is the left superscript, the seniority number v is the left subscript, and in place of J , the right subscript, the quantum numbers U have been inserted. These quantum numbers are found in Table I

of reference 1, and serve to distinguish terms of the same L , S , and v .

The parameters E^0 , E^1 , E^2 , and E^3 are defined in terms of Slater's F 's in reference 1, Eq. (66) as follows:

$$\begin{aligned} E^0 &= F_0 - 10F_2 - 33F_4 - 286F_6, \\ E^1 &= (70/9)F_2 + (231/9)F_4 + (2002/9)F_6, \\ E^2 &= (1/9)F_2 - (1/3)F_4 + (7/9)F_6, \\ E^3 &= (5/3)F_2 + 2F_4 - (91/3)F_6. \end{aligned} \quad (1)$$

As a further check on the interpretation of the Racah method, matrix elements for three typical matrices (1S , a two-by-two matrix, 3P , a three-by-three matrix, and 3F , a four-by-four matrix) have been checked by a

TABLE I. Electrostatic energy matrices of the configuration f^4 .

${}^4F_{21} = 6E^0 + 6E^1 - 195E^2 + 33E^3$									
${}^4K_{21} = 6E^0 + 6E^1 - 129E^2 - 11E^3$									
${}^4N_{22} = 6E^0 + 6E^1 + 60E^2 - 11E^3$									
${}^4L_{21} = 6E^0 + 4E^1 - 85E^2 - 19E^3$									
${}^4M_{30} = 6E^0 + 4E^1 + 50E^2 - 19E^3$									
${}^4S_{00} = 6E^0$									
${}^4D_{20} = 6E^0 + 33E^3$									
${}^4F_{10} = 6E^0$									
${}^4G_{20} = 6E^0 + 12E^3$									
${}^4I_{20} = 6E^0 - 21E^3$									
	<table border="1"> <thead> <tr> <th>${}^0S_{00}$</th> <th>${}^4S_{22}$</th> </tr> </thead> <tbody> <tr> <td>${}^0S_{00}$</td> <td>$6E^0 + 18E^1$</td> </tr> <tr> <td>${}^4S_{22}$</td> <td>$-12(22)^{1/2}E^3$</td> </tr> <tr> <td></td> <td>$6E^0 + 6E^1 + 390E^2 + 66E^3$</td> </tr> </tbody> </table>	${}^0S_{00}$	${}^4S_{22}$	${}^0S_{00}$	$6E^0 + 18E^1$	${}^4S_{22}$	$-12(22)^{1/2}E^3$		$6E^0 + 6E^1 + 390E^2 + 66E^3$
${}^0S_{00}$	${}^4S_{22}$								
${}^0S_{00}$	$6E^0 + 18E^1$								
${}^4S_{22}$	$-12(22)^{1/2}E^3$								
	$6E^0 + 6E^1 + 390E^2 + 66E^3$								

¹ G. Racah, Phys. Rev. **76**, 1352 (1949).

² J. C. Slater, Phys. Rev. **34**, 1293 (1929).

TABLE I.—(Continued).

	4^1H_{21}		4^1H_{22}	
4^1H_{21}	$6E^0+6E^1+183E^2-24E^3$		$-36(78)^{\frac{1}{2}}E^2$	
4^1H_{22}	$-36(78)^{\frac{1}{2}}E^2$		$6E^0+6E^1+156E^2+33E^3$	
	4^1L_{21}		4^1L_{22}	
4^1L_{21}	$6E^0+6E^1+15E^2-3E^3$		$-24(95)^{\frac{1}{2}}E^2$	
4^1L_{22}	$-24(95)^{\frac{1}{2}}E^2$		$6E^0+6E^1-54E^2-30E^3$	
	4^3D_{20}		4^3D_{21}	
4^3D_{20}	$6E^0+4E^1-(1144/7)E^2+(11/7)E^3$		$-(4/7)(66)^{\frac{1}{2}}(39E^2+4E^3)$	
4^3D_{21}	$-(4/7)(66)^{\frac{1}{2}}(39E^2+4E^3)$		$6E^0+4E^1+(1781/7)E^2+(164/7)E^3$	
	4^3I_{20}		4^3I_{30}	
4^3I_{20}	$6E^0+4E^1-40E^2-E^3$		$4(3)^{\frac{1}{2}}(30E^2+E^3)$	
4^3I_{30}	$4(3)^{\frac{1}{2}}(30E^2+E^3)$		$6E^0+4E^1+50E^2+17E^3$	
	4^3K_{21}		4^3K_{30}	
4^3K_{21}	$6E^0+4E^1+219E^2-(17/3)E^3$		$-(8/3)(17)^{\frac{1}{2}}(3E^2-2E^3)$	
4^3K_{30}	$-(8/3)(17)^{\frac{1}{2}}(3E^2-2E^3)$		$6E^0+4E^1-188E^2-(40/3)E^3$	
	2^1I_{20}	4^1I_{20}	4^1I_{22}	
2^1I_{20}	$6E^0+11E^1+70E^2-(49/5)E^3$	$\frac{3}{5}(21)^{\frac{1}{2}}E^3$	$-3(51)^{\frac{1}{2}}E^3$	
4^1I_{20}	$\frac{3}{5}(21)^{\frac{1}{2}}E^3$	$6E^0+6E^1+15/2E^2+81/20E^3$	$-\frac{3}{5}(119)^{\frac{1}{2}}(30E^2+E^3)$	
4^1I_{22}	$-3(51)^{\frac{1}{2}}E^3$	$-\frac{3}{5}(119)^{\frac{1}{2}}(30E^2+E^3)$	$6E^0+6E^1-543/2E^2+75/4E^3$	
	2^3P_{11}	4^3P_{11}	4^3P_{30}	
2^3P_{11}	$6E^0+9E^1+(33/5)E^3$	$-(66/5)E^3$	$6(11)^{\frac{1}{2}}E^3$	
4^3P_{11}	$-(66/5)E^3$	$6E^0+4E^1-(154/15)E^3$	$-\frac{1}{3}(11)^{\frac{1}{2}}(390E^2+E^3)$	
4^3P_{30}	$6(11)^{\frac{1}{2}}E^3$	$-\frac{1}{3}(11)^{\frac{1}{2}}(390E^2+E^3)$	$6E^0+4E^1-104E^2+(152/3)E^3$	
	4^3G_{20}	4^3G_{21}	4^3G_{30}	
4^3G_{20}	$6E^0+4E^1+(1040/7)E^2+(4/7)E^3$	$(8/21)(2145)^{\frac{1}{2}}(6E^2-E^3)$	$-(4/3)(15)^{\frac{1}{2}}(39E^2-2E^3)$	
4^3G_{21}	$(8/21)(2145)^{\frac{1}{2}}(6E^2-E^3)$	$6E^0+4E^1-(1089/7)E^2+(121/21)E^3$	$(4/3)(143)^{\frac{1}{2}}(12E^2+E^3)$	
4^3G_{30}	$-(4/3)(15)^{\frac{1}{2}}(39E^2-2E^3)$	$(4/3)(143)^{\frac{1}{2}}(12E^2+E^3)$	$6E^0+4E^1-104E^2+(62/3)E^3$	
	2^1D_{20}	4^1D_{20}	4^1D_{21}	4^1D_{22}
2^1D_{20}	$6E^0+11E^1+286E^2+77/5E^3$	$-(33/35)(21)^{\frac{1}{2}}E^3$	$-(24/35)(2310)^{\frac{1}{2}}E^3$	$-(9/5)(715)^{\frac{1}{2}}E^3$
4^1D_{20}	$-(33/35)(21)^{\frac{1}{2}}E^3$	$6E^0+6E^1+429/14E^2-(891/140)E^3$	$-(3/35)(110)^{\frac{1}{2}}(195E^2-16E^3)$	$-(3/140)(15015)^{\frac{1}{2}}(30E^2+7E^3)$
4^1D_{21}	$-(24/35)(2310)^{\frac{1}{2}}E^3$	$-(3/35)(110)^{\frac{1}{2}}(195E^2-16E^3)$	$6E^0+6E^1-(2535/7)E^2+(12/7)E^3$	$(135/7)(546)^{\frac{1}{2}}E^2$
4^1D_{22}	$-(9/5)(715)^{\frac{1}{2}}E^3$	$-(3/140)(15015)^{\frac{1}{2}}(30E^2+7E^3)$	$(135/7)(546)^{\frac{1}{2}}E^2$	$6E^0+6E^1-(75/2)E^2+(177/4)E^3$
	2^1G_{20}	4^1G_{20}	4^1G_{21}	4^1G_{22}
2^1G_{20}	$6E^0+11E^1-260E^2+28/5E^3$	$-(12/35)(21)^{\frac{1}{2}}E^3$	$-(4/7)(3003)^{\frac{1}{2}}E^3$	$-4(39)^{\frac{1}{2}}E^3$
4^1G_{20}	$-(12/35)(21)^{\frac{1}{2}}E^3$	$6E^0+6E^1-(195/7)E^2-(81/35)E^3$	$(4/7)(143)^{\frac{1}{2}}(15E^2+2E^3)$	$(1/7)(91)^{\frac{1}{2}}(285E^2-7E^3)$
4^1G_{21}	$-(4/7)(3003)^{\frac{1}{2}}E^3$	$(4/7)(143)^{\frac{1}{2}}(15E^2+2E^3)$	$6E^0+6E^1+(2211/7)E^2+(187/7)E^3$	$(36/7)(77)^{\frac{1}{2}}E^2$
4^1G_{22}	$-4(39)^{\frac{1}{2}}E^3$	$(1/7)(91)^{\frac{1}{2}}(285E^2-7E^3)$	$(36/7)(77)^{\frac{1}{2}}E^2$	$6E^0+6E^1+141E^2-17E^3$
	2^3F_{10}	4^3F_{10}	4^3F_{21}	4^3F_{30}
2^3F_{10}	$6E^0+9E^1$	0	$-(12/5)(165)^{\frac{1}{2}}E^3$	0
4^3F_{10}	0	$6E^0+4E^1$	$(8/15)(165)^{\frac{1}{2}}E^3$	$-20(143)^{\frac{1}{2}}E^2$
4^3F_{21}	$-(12/5)(165)^{\frac{1}{2}}E^3$	$(8/15)(165)^{\frac{1}{2}}E^3$	$6E^0+4E^1+65E^2+9E^3$	$\frac{1}{3}(195)^{\frac{1}{2}}(72E^2-4E^3)$
4^3F_{30}	0	$-20(143)^{\frac{1}{2}}E^2$	$\frac{1}{3}(195)^{\frac{1}{2}}(72E^2-4E^3)$	$6E^0+4E^1+76E^2-6E^3$
	2^3H_{11}	4^3H_{11}	4^3H_{21}	4^3H_{30}
2^3H_{11}	$6E^0+9E^1-9/5E^3$	$18/5E^3$	0	$6(39)^{\frac{1}{2}}E^3$
4^3H_{11}	$(18/5)E^3$	$6E^0+4E^1+(14/5)E^3$	$10(182)^{\frac{1}{2}}E^2$	$\frac{1}{3}(39)^{\frac{1}{2}}(30E^2-E^3)$
4^3H_{21}	0	$10(182)^{\frac{1}{2}}E^2$	$6E^0+4E^1-197E^2+16E^3$	$\frac{2}{3}(42)^{\frac{1}{2}}(33E^2+4E^3)$
4^3H_{30}	$6(39)^{\frac{1}{2}}E^3$	$\frac{1}{3}(39)^{\frac{1}{2}}(30E^2-E^3)$	$\frac{2}{3}(42)^{\frac{1}{2}}(33E^2+4E^3)$	$6E^0+4E^1+176E^2+4E^3$

TABLE II. Eigenvalues of the two-by-two electrostatic energy matrices of the configuration f^4 .

${}^1S = 6E^0 + 12E^1 + 195E^2 + 33E^3 \pm \frac{1}{2}[144(E^1)^2 + 152100(E^2)^2 + 17028(E^3)^2 - 9360E^1E^2 - 1584E^1E^3 + 51480E^2E^3]^{\frac{1}{2}}$
${}^1H = 6E^0 + 6E^1 + (339/2)E^2 + (9/2)E^3 \pm \frac{1}{2}[405081(E^2)^2 - 3078E^2E^3 + 3249(E^3)^2]^{\frac{1}{2}}$
${}^1L = 6E^0 + 6E^1 - (39/2)E^2 - 33/2E^3 \pm \frac{1}{2}[223641(E^2)^2 + 3726E^2E^3 + 729(E^3)^2]^{\frac{1}{2}}$
${}^3D = 6E^0 + 4E^1 + (91/2)E^2 + (25/2)E^3 \pm \frac{1}{2}[305721(E^2)^2 + 45162E^2E^3 + 1857(E^3)^2]^{\frac{1}{2}}$
${}^3I = 6E^0 + 4E^1 + 5E^2 + 8E^3 \pm \frac{1}{2}[180900(E^2)^2 + 14760E^2E^3 + 516(E^3)^2]^{\frac{1}{2}}$
${}^3K = 6E^0 + 4E^1 + (31/2)E^2 - (19/2)E^3 \pm \frac{1}{2}[170001(E^2)^2 + 438E^2E^3 + 1993(E^3)^2]^{\frac{1}{2}}$

formula developed by Innes:³

$$\begin{aligned}
 \langle l^{n\nu}USL | Q^{(t)} | l^{n\nu'}U'SL \rangle &= \frac{\frac{1}{2}(l \| C^{(t)} \| l)^2}{(2L+1)} \\
 &\times \sum_{v''U''L''} (-)^{L-L''} \langle l^{n\nu}USL \| U^{(t)} \| l^{n\nu'}U''SL'' \rangle \\
 &\times \langle l^{n\nu'}U''SL'' \| U^{(t)} \| l^{n\nu'}U'SL \rangle - \frac{1}{2} \frac{n(l \| C^{(t)} \| l)^2}{2L+1} \\
 &\times \delta(v\nu')\delta(UU'), \quad (2)
 \end{aligned}$$

where

$$\begin{aligned}
 &\langle l^{n\nu}USL \| U^{(t)} \| l^{n\nu'}U''SL'' \rangle \\
 &= n(-)^{t-L-L''} [(2L+1)(2L''+1)]^{\frac{1}{2}} \\
 &\times \sum_{v_1U_1S_1L_1} (-)^{L_1} \langle l^{n\nu}USL \| [l^{n-1}(v_1U_1S_1L_1)lSL] \\
 &\times \langle l^{n-1}(v_1U_1S_1L_1)lSL'' \| [l^{n\nu'}U''SL''] W(lLL''; L_1t) \rangle.
 \end{aligned}$$

³ F. R. Innes, Phys. Rev. **91**, 31 (1953), Eq. (13).

The second part of (2) involves the coefficients of fractional parentage⁴ for the configuration f^4 . These are computed by Racah,¹ Eq. (34) and checked by the use of Racah,⁵ Eq. (13). The W 's are tabulated by Biedenharn.⁶

K. S. Rao^{7,8} has given term values for the configuration f^4 , which he computed by the Slater method.² Many of his results do not agree with those in Table I (computed by two independent methods, as stated above).

I wish to express my gratitude to Dr. C. W. Ufford for suggesting this problem to me and for his helpful discussion of the problem.

⁴ The coefficients of fractional parentage for the configurations f^2 , f^3 , and f^4 are in the physics dissertation of E. F. Reilly, which is in the Math-Physics Library of the University of Pennsylvania.

⁵ G. Racah, Phys. Rev. **63**, 367 (1943).

⁶ Oak Ridge National Laboratory Report ORNL-1098, 1952 (unpublished).

⁷ K. S. Rao, Indian J. Phys. **26**, 427 (1952).

⁸ K. S. Rao, Indian J. Phys. **24**, 51 (1950); V. R. Rao, Current Sci. (India) **19**, 8 (1950); G. Racah, Current Sci. (India) **21**, 67 (1952).