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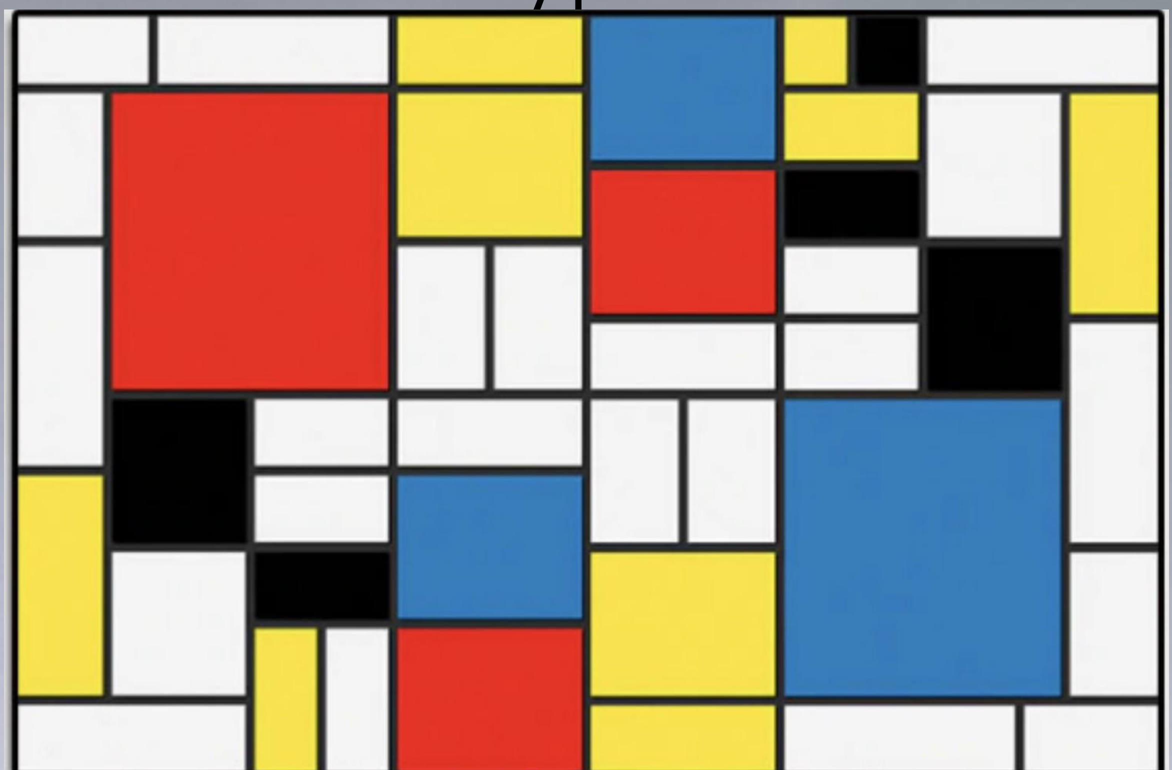
Orthogonal Operators: Extension to hyperfine structure



ASOS23, Paris

Orthogonal operators, short story

$$u : v = \sum_{\Psi, \Psi'} \langle \Psi \mid u \mid \Psi' \rangle \langle \Psi' \mid v \mid \Psi \rangle$$

Orthogonal operators, like it was 25 years ago:

- p-shell: 2p, 3p …… hardly
- d-shell: 3d,4d,5d…. mostly III,IV, V and VI spectra (plus Fe II and Co II)
- E1, M1 and E2 transition probabilities.
- f-shell: 4f,5f…. no.
- g-factors: no.
- hyperfine structure: no.

Orthogonal operators, like it is now:

- p-shell: 2p, 3p …… Yes.
- d-shell: 3d,4d,5d…. neutral to 10+ spectra.
- E1, M1, E2 and M2 transition probabilities.
- f-shell: 4f,5f…. Yes.
- g-factors: Yes.
- hyperfine structure: Yes.

Use eigenvectors to:

- Calculate transition probabilities from the model space

$$S_{if} = \left| \sum_{SL\nu S'L'\nu'} (i|SL\nu\, J)\; S^{\frac{1}{2}}(SL\nu\, J, S'L'\nu'\, J')\; (S'L'\nu'\, J'|f) \right|^2$$

Use eigenvectors to:

- Calculate transition probabilities from the model space

$$S_{if} = \left| \sum_{SL\nu S'L'\nu'} (i|SL\nu\, J)\ S^{\frac{1}{2}}(SL\nu\, J, S'L'\nu'\, J')\ (S'L'\nu'\, J'|f) \right|^2$$

- Calculate hyperfine structure A and B constants

$$A_J(E_J) = \sum_{SL\gamma, S'L'\gamma'} (E_J|SL\gamma J) \cdot A_J(SL\gamma J, S'L'\gamma' J') \cdot (S'L'\gamma' J|E_J)$$

Use eigenvectors to:

- Calculate transition probabilities from the model space

$$S_{if} = \left| \sum_{SL\nu S'L'\nu'} (i|SL\nu\, J)\; S^{\frac{1}{2}}(SL\nu\, J, S'L'\nu'\, J')\; (S'L'\nu'\, J'|f) \right|^2$$

- Calculate hyperfine structure A and B constants

$$A_J(E_J) = \sum_{SL\gamma, S'L'\gamma'} (E_J|SL\gamma J) \cdot A_J(SL\gamma J, S'L'\gamma' J') \cdot (S'L'\gamma' J|E_J)$$

- Calculate g-factors

$$g_J(E_J) = \sum_{SL\nu} (E_J|SL\nu J) \cdot g_J(SL) \cdot (SL\nu J|E_J)$$

Model space large enough?

Include core and valence excitations:

$3s \rightarrow 3d$ and $3p^2 \rightarrow 3\mathrm{d}^2$

or:

$5d \rightarrow 6s$

A simple example with $\langle\alpha'| = \langle 5d^9|$, $|\alpha\rangle = |5d^8 6p\rangle$ and $|\gamma\rangle = |5d^8 6s\rangle$ would be:

$$\langle\Psi'|\,\mathbf{r}\,|\Psi\rangle \approx \left\langle 5d^9\right|\mathbf{r}\left|5d^8 6p\right\rangle + \frac{\langle 5d^9|V|5d^8 6s\rangle\,\langle 5d^8 6s|\,\mathbf{r}\,|5d^8 6p\rangle}{E_{5d} - E_{6s}} \tag{18.30}$$

The results turn out to be in quite good agreement with the results from the full diagonalization procedure:

$$\langle\Psi'|\,\mathbf{r}\,|\Psi\rangle \approx \left\langle 5d^9 + 5d^8 6s\right|\mathbf{r}\left|5d^8 6p\right\rangle \tag{18.31}$$

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Astronomy & Astrophysics

The CARMENES search for exoplanets around M dwarfs

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Our investigation underlines the fact that HFS can have a dramatic impact on line profiles and on abundance measurements. We suggest that this quantum effect could play an important role in cool star spectroscopy where a number of elements appear to exhibit stronger and wider splitting patterns than in Sun-like stars. We have exploited this property to provide a reasonable assessment of V abundance in the cool photospheres of the most abundant type of stars in the Galaxy. This type of study is made possible with the accessibility of constantly improving laboratory measurements, which are essential and powerful tools for interpreting increasingly complex stellar spectra in new temperature and wavelength regimes.

$$E_F = E_J + \tfrac{1}{2}A_J \cdot C + \tfrac{1}{2}B_J \cdot \frac{\tfrac{3}{4}C(C+1) - J(J+1)I(I+1)}{I(2I-1)J(2J-1)}$$

where E_J is the energy of the fine structure level of quantum number J and $C = F(F+1) - J(J+1) - I(I+1)$.

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where E_J is the energy of the fine structure level of quantum number J and $C = F(F+1) - J(J+1) - I(I+1)$.

$$A_J(E_J) = \sum_{SL\gamma, S'L'\gamma'} (E_J|SL\gamma J) \cdot A_J(SL\gamma J, S'L'\gamma' J') \cdot (S'L'\gamma' J|E_J)$$

$$\left\langle \gamma(SL)JF|H^D_{\mathrm{hfs}}|\gamma'(S'L')J'F\right\rangle = \sqrt{I(I+1)(2I+1)} \cdot (-1)^{J'+I+F} \cdot \begin{Bmatrix} J' & I & F \\ I & J & 1 \end{Bmatrix}$$

$$\cdot \sum_{\kappa k, nl} [J, J', 1]^{\frac{1}{2}} \cdot \begin{Bmatrix} S & S' & \kappa \\ L & L' & k \\ J & J' & 1 \end{Bmatrix} \cdot a^{\kappa k}_{nl} \cdot f^{\kappa k} \cdot \left\langle \gamma(SL) \parallel \left(\mathbf{a}^\dagger \mathbf{a}\right)^{(\kappa k)} \parallel \gamma'(S'L')\right\rangle \qquad (5.67a)$$

It follows directly from comparison with equation (3.94):

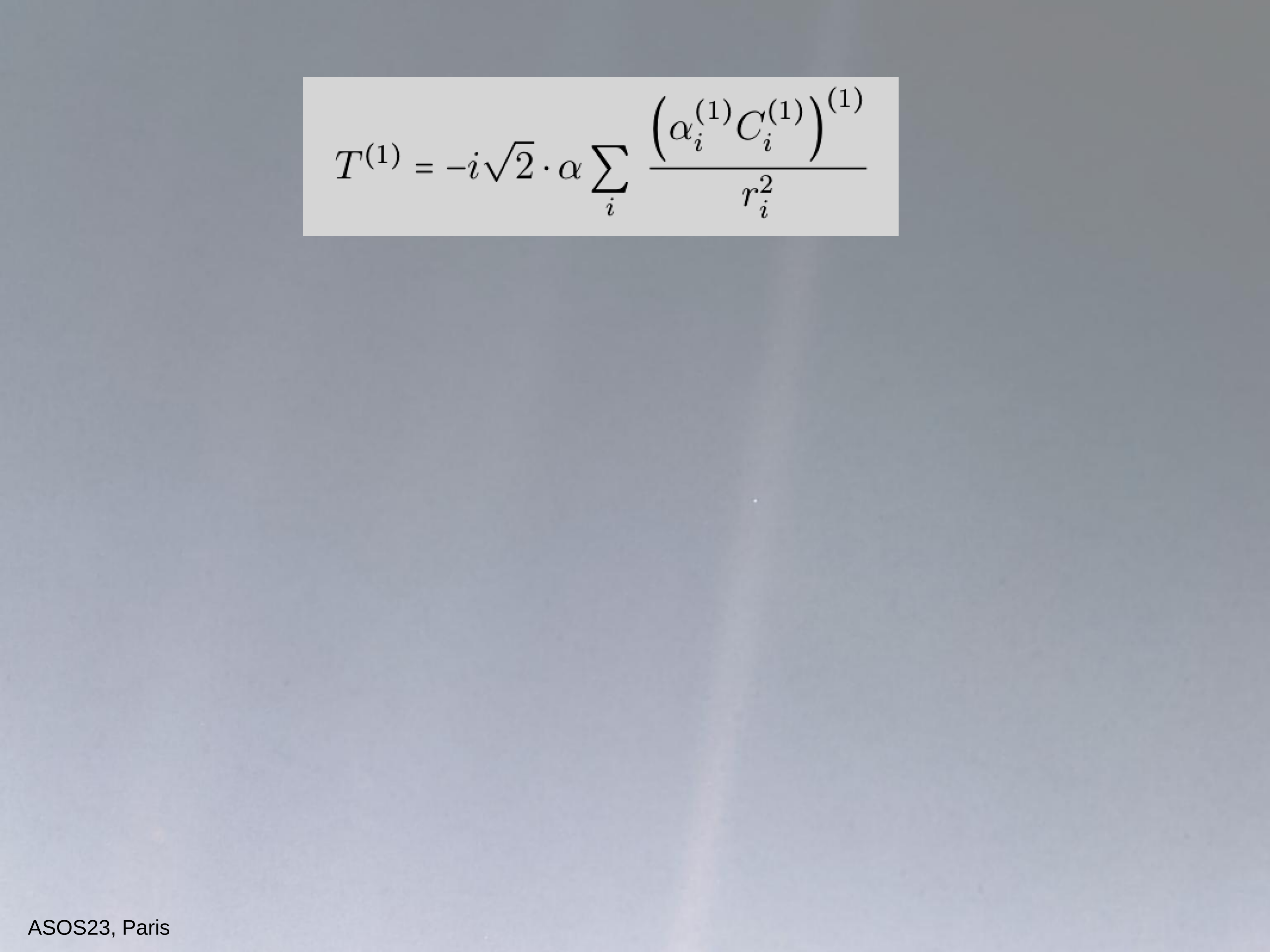
$$A_J(SL\gamma J, S'L'\gamma' J') = \left[\frac{3(2J+1)}{J(J+1)}\right]^{\frac{1}{2}}$$

$$\sum_{\kappa k, nl} \begin{Bmatrix} S & S' & \kappa \\ L & L' & k \\ J & J & 1 \end{Bmatrix} \cdot a^{\kappa k}_{nl} \cdot f^{\kappa k} \cdot \left\langle \gamma(SL) \parallel \left(\mathbf{a}^\dagger \mathbf{a}\right)^{(\kappa k)} \parallel \gamma'(S'L')\right\rangle \qquad (5.67b)$$

Transformation of a fully relativistic expression to *SL*-coupling:

$$S(a,b) = [t]^{-\frac{1}{2}} \sum_{j,j'} [j,j',\kappa,k]^{\frac{1}{2}} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & \kappa \\ l & l' & k \\ j & j' & t \end{Bmatrix} \left(p \parallel \hat{F}^{(t)} \parallel q\right)$$

Correct weighting procedure over j and j'!



$$T^{(1)} = -i\sqrt{2}\cdot\alpha\sum_i \frac{\left(\alpha_i^{(1)} C_i^{(1)}\right)^{(1)}}{r_i^2}$$

$$T^{(1)} = -i\sqrt{2} \cdot \alpha \sum_i \frac{\left(\alpha_i^{(1)} C_i^{(1)}\right)^{(1)}}{r_i^2}$$

$$T^{(1)} = -\sum_{\kappa k} S_{nl}^{\kappa k} \left(\mathbf{a}^\dagger \mathbf{a}\right)^{(\kappa k)1} \qquad \text{with } \kappa + k \text{ odd}$$

After application of equation (21.7), one arrives for the magnetic dipole

$$S_{nl}^{\kappa k} = \tfrac{1}{3}\sqrt{6} \cdot \alpha \sum_{jj'} [j, j'] \cdot [\kappa, k]^{\frac{1}{2}} \cdot \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & \kappa \\ l & l & k \\ j & j' & 1 \end{Bmatrix} (-1)^l \cdot \begin{pmatrix} j & j' & 1 \\ -\frac{1}{2} & -\frac{1}{2} & 1 \end{pmatrix} \cdot P_{jj'}$$

$$P_{jj'} = \int_0^\infty \frac{F_{nlj}\, G_{nlj'} + G_{nlj}\, F_{nlj'}}{r^2}\, \mathrm{d}r$$

Co I: A-values even system

J= 5.5

A(obs.)	A(calc.)	Delta	E-value	Composition
-	6.027	-	59850.407	69% 8|4F)3D2H + 18% 8|4F)3D4H + 13% 8|4F)1D4H
-	6.243	-	59664.827	61% 8|4F)3D4G + 30% 8|4F)1D4G + 5% 8|4F)3D4H
-	11.703	-	57578.514	64% 6|3F)4H + 26% 6|3F)2H + 10% 6|3F)4G
-	10.459	-	56649.502	83% 6|3F)4G + 16% 6|3F)2H + 1% 6|3F)4H
-	11.538	-	56635.917	59% 6|3F)2H + 35% 6|3F)4H + 7% 6|3F)4G
13.900	14.583	-0.683	54947.632*	69% 8|4F)3D6H + 17% 8|4F)3D6G + 9% 8|4F)1D4H
20.860	21.327	-0.467	54367.332*	44% 8|4F)3D6G + 23% 8|4F)3D6H + 23% 8|4F)3D6F
20.400	20.949	-0.549	54315.611*	49% 8|4F)1D4H + 28% 8|4F)3D4H + 9% 8|4F)3D6G
29.100	28.847	0.253	53660.238*	71% 8|4F)3D6F + 27% 8|4F)3D6G + 2% 8|4F)3D6H
-	28.344	-	53511.734*	55% 8|4F)1D4G + 29% 8|4F)3D4G + 7% 8|4F)1D4H
10.600	10.332	0.268	52113.842*	62% 4|3F)4H + 26% 4|3F)2H + 11% 4|3F)4G
8.100	9.315	-1.215	51203.690*	87% 4|3F)4G + 9% 4|3F)2H + 4% 4|3F)4H
8.900	10.176	-1.276	51174.230*	65% 4|3F)2H + 33% 4|3F)4H + 2% 4|3F)4G
33.470	33.931	-0.461	45675.937*	100% 9|4F)3S6F + 0% 9|2G)3S4G + 0% 8|4F)3D6F
22.600	23.008	-0.408	21780.442*	100% 3|2H)2H + 0% 9|2H)3S2H + 0% 4|3F)2H

J= 6.5

A(obs.)	A(calc.)	Delta	E-value	Composition
-	5.974	-	59807.746	66% 8|4F)3D4H + 33% 8|4F)1D4H + 0% 8|4F)3D6H
-	9.774	-	56626.829	100% 6|3F)4H + 0% 6|1G)2I + 0% 8|4F)3D4H
18.700	18.851	-0.151	54452.305*	82% 8|4F)3D6H + 11% 8|4F)3D6G + 5% 8|4F)1D4H
25.800	25.529	0.271	53728.230*	85% 8|4F)3D6G + 14% 8|4F)3D6H + 1% 8|4F)1D4H
25.000	25.536	-0.536	53617.983*	61% 8|4F)1D4H + 32% 8|4F)3D4H + 4% 8|4F)3D6G
7.600	8.648	-1.048	51142.456*	100% 4|3F)4H + 0% 4|1G)2I + 0% 8|2F)3D4H

11100.596	11098.603	1.993	1.111	96% 3|2G)2G + 2% B|2G1S)2G + 1% 1|2G1)
2424.809	2427.200	-2.391	1.557	97% 2|5D)6D + 1% 8|4F)3D6D + 1% 8|4P)3D6D
552.955	556.852	-3.897	1.334	97% 3|4F)4F + 2% B|4F1S)4F + 1% 1|4F)

Vanadium I: energy fit

J= 5.5

E(obs.)	E(calc.)	Delta	Mixd.g-fac.	Composition
-	50340.322	-	1.421	71% A|4F)3D6F + 27% A|4F)3D6G + 2% A|4F)3D6H
-	50141.634	-	1.344	52% A|4F)3D6G + 26% A|4F)3D6F + 19% A|4F)3D6H
50114.450	50117.380	-2.930	1.271	63% 9|2G)3S4G + 17% 5|3G)4G + 9% 8|4F)3D4G
49951.709	49961.871	-10.162	1.234	77% A|4F)3D6H + 19% A|4F)3D6G + 2% A|4F)3D6F
-	49747.541	-	1.228	37% 6|5D)4G + 9% 5|3H)4H + 9% A|4F)1D4G
49717.572	49727.490	-9.918	1.175	30% 6|5D)4G + 30% 5|3H)4H + 12% 5|3H)2H
-	49658.710	-	1.264	28% 6|5D)4G + 21% 8|4F)3D4G + 20% A|4F)1D4G
-	49600.249	-	1.103	60% 5|3H)2H + 14% 5|3H)4H + 14% 8|4F)3D2H
-	49249.524	-	1.138	29% A|4F)1D4H + 26% 8|4F)3D4H + 19% 5|3H)4H
-	49147.622	-	1.444	88% 6|5D)6F + 9% 6|5D)6G + 2% B|4F3P)6F
-	48985.875	-	1.354	88% 6|5D)6G + 9% 6|5D)6F + 1% 4|5D)6G
44746.714	44686.750	59.964	1.273	48% 4|5D)4G + 31% 8|4F)1D4G + 14% 8|4F)3D4G
-	44389.992	-	1.278	45% 4|5D)4G + 28% 8|4F)1D4G + 12% 8|4F)3D4G
44326.651	44334.170	-7.519	1.409	62% 8|4F)3D6F + 32% 8|4F)3D6G + 2% 4|5D)4G
44193.427	44173.592	19.835	1.199	47% 8|4F)1D4H + 20% 8|4F)3D4H + 16% 8|4F)3D6G
44139.591	44132.936	6.655	1.311	42% 8|4F)3D6G + 22% 8|4F)3D6F + 12% 8|4F)1D4H
43894.149	43890.623	3.526	1.212	87% 8|4F)3D6H + 7% 8|4F)3D6G + 2% 8|4F)1D4H
42578.093	42574.255	3.838	1.452	95% 4|5D)6F + 3% 4|5D)6G + 1% 6|5D)6F
42257.394	42258.703	-1.309	1.347	95% 4|5D)6G + 3% 4|5D)6F + 1% 8|4F)3D6G
-	40664.827	-	1.089	93% 1|2H) + 2% 3|2H)2H + 1% B|2H1S)2H
-	38221.912	-	0.925	98% 1|2I) + 1% 1|2H) + 0% B|2H3P)2I
37931.460	37910.403	21.057	1.456	99% 9|4F)3S6F + 0% 4|5D)6F + 0% 8|4F)3D6F
32417.169	32411.187	5.982	1.273	97% 1|4G) + 1% B|4F1D)4G + 0% 4|5D)4G
22496.546	22502.257	-5.711	0.923	97% 2|1I)2I + 1% 8|2H)3D2I + 1% B|2H1D)2I
19145.148	19144.516	0.632	1.091	93% 2|3H)2H + 3% 3|2H)2H + 1% B|2H1D)2H
17242.070	17242.115	-0.045	1.273	97% 2|3G)4G + 1% B|4F1D)4G + 0% 2|3H)4H
15264.832	15266.668	-1.836	1.091	93% 3|2H)2H + 3% 2|3H)2H + 2% 1|2H)
15000.937	14997.904	3.033	1.134	97% 2|3H)4H + 1% 8|2H)3D4H + 1% B|4F1D)4H

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    8.754          8.396          0.358     14949.359*   97% 2|3H )4H    +  1% 8|2H )3D4H +  1% B|4F1D)4H
    9.960         10.208         -0.248     11100.596*   96% 3|2G )2G    +  2% B|2G1S)2G  +  1% 1|2G1)
   13.571         14.593         -1.022      2424.809*   97% 2|5D )6D    +  1% 8|4F )3D6D +  1% 8|4P )3D6D
    7.576          8.027         -0.451       552.955*   97% 3|4F )4F    +  2% B|4F1S)4F  +  1% 1|4F )
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Vanadium I: A-values (mK)

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J= 5.5

  A(obs.)      A(calc.)        Delta    E-value                        Composition
..............................................................................................................

      -           11.674          -     49951.709*   77% A|4F )3D6H + 19% A|4F )3D6G +  2% A|4F )3D6F
      -            7.124          -     49747.541    37% 6|5D )4G    +  9% 5|3H )4H    +  9% A|4F )1D4G
    8.072          5.855        2.217   49717.572*   30% 6|5D )4G    + 30% 5|3H )4H    + 12% 5|3H )2H
      -            8.063          -     49658.710    28% 6|5D )4G    + 21% 8|4F )3D4G + 20% A|4F )1D4G
      -            8.803          -     49600.249    60% 5|3H )2H    + 14% 5|3H )4H    + 14% 8|4F )3D2H
      -            8.899          -     49249.524    29% A|4F )1D4H + 26% 8|4F )3D4H + 19% 5|3H )4H
      -            3.686          -     49147.622    88% 6|5D )6F    +  9% 6|5D )6G    +  2% B|4F3P)6F
      -            2.812          -     48985.875    88% 6|5D )6G    +  9% 6|5D )6F    +  1% 4|5D )6G
   15.110         10.616        4.494   44746.714*   48% 4|5D )4G    + 31% 8|4F )1D4G + 14% 8|4F )3D4G
      -           10.903          -     44389.992    45% 4|5D )4G    + 28% 8|4F )1D4G + 12% 8|4F )3D4G
      -           18.491          -     44326.651*   62% 8|4F )3D6F + 32% 8|4F )3D6G +  2% 4|5D )4G
      -           12.833          -     44193.427*   47% 8|4F )1D4H + 20% 8|4F )3D4H + 16% 8|4F )3D6G
      -           14.534          -     44139.591*   42% 8|4F )3D6G + 22% 8|4F )3D6F + 12% 8|4F )1D4H
   11.875         10.264        1.611   43894.149*   87% 8|4F )3D6H +  7% 8|4F )3D6G +  2% 8|4F )1D4H
      -            3.453          -     42578.093*   95% 4|5D )6F    +  3% 4|5D )6G    +  1% 6|5D )6F
    2.135          3.192       -1.057   42257.394*   95% 4|5D )6G    +  3% 4|5D )6F    +  1% 8|4F )3D6G
      -            7.906          -     40664.827    93% 1|2H )      +  2% 3|2H )2H    +  1% B|2H1S)2H
      -            8.382          -     38221.912    98% 1|2I )      +  1% 1|2H )      +  0% B|2H3P)2I
   20.991         21.051       -0.060   37931.460*   99% 9|4F )3S6F +  0% 4|5D )6F    +  0% 8|4F )3D6F
    3.282          6.903       -3.621   32417.169*   97% 1|4G )      +  1% B|4F1D)4G  +  0% 4|5D )4G
      -            3.333          -     22496.546*   97% 2|1I )2I    +  1% 8|2H )3D2I +  1% B|2H1D)2I
    5.370          6.446       -1.076   19145.148*   93% 2|3H )2H    +  3% 3|2H )2H    +  1% B|2H1D)2H
   15.468         14.860        0.608   17242.070*   97% 2|3G )4G    +  1% B|4F1D)4G  +  0% 2|3H )4H
    9.930         10.467       -0.537   15264.832*   93% 3|2H )2H    +  3% 2|3H )2H    +  2% 1|2H )
   12.497         12.161        0.336   15000.937*   97% 2|3H )4H    +  1% 8|2H )3D4H +  1% B|4F1D)4H
```

Vanadium I: two levels, good case

Table 1: Energy levels in cm^{-1} and % composition of two $3d^4 4s^2$ J=$\frac{3}{2}$ levels in V I.

$E_e(\text{cm}^{-1})$	$E_c(\text{cm}^{-1})$	$E_o(\text{cm}^{-1})$	Δ_{ec}	Δ_{eo}	^{2}P	^{2}D1	^{2}D2
13801.551	13616.6	13807.930	185.0	-6.4	79|69	–|6	6|18
14514.756	14610.8	14499.834	-96.0	14.9	7|23	20|16	64|53

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13801.551	13616.6	13807.930	185.0	-6.4	79|69	–|6	6|18
14514.756	14610.8	14499.834	-96.0	14.9	7|23	20|16	64|53

Table 2: Landé g_J-factors and A-values of two $3d^4 4s^2$ J=$\frac{3}{2}$ levels in V I.

$E_e(\mathrm{cm}^{-1})$	g_e	g_c	g_o	Δ_{ec}	Δ_{eo}	A_e(mK)	A_o(mK)
13801.551	1.20	1.292	1.201	-0.092	-0.001	11.120	10.494
14514.756	0.97	0.844	0.936	0.126	0.034	11.392	11.183

1	$3d^5$
2	$3d^4$ 4s
3	$3d^3$ $4s^2$
4	$3d^4$ 4d
5	$3d^4$ 5s
6	$3d^4$ 5d
7	$3d^4$ 6s
8	$3d^3$ 4s 4d
9	$3d^3$ 4s 5s
A	$3d^3$ 4s 5d
B	$3d^3$ $4p^2$

Vanadium I: two levels, bad case

Table 4: Energy levels in cm^{-1} and % composition of two $3d^4 4s^2$ J=$\frac{1}{2}$ levels in V I.

$E_e(cm^{-1})$	$E_c(cm^{-1})$	$E_o(cm^{-1})$	Δ_{ec}	Δ_{eo}	$2\|^4D$	$2\|^6D$	$8\|^6D$	$8\|^4D$	$B\|^4D$
2112.282	2044.9	2108.953	67.4	3.3	0| 0	100|97	0| 2	0| 0	0| 0
8413.009	8364.1	8403.516	48.9	9.5	97|95	0| 0	0| 0	0| 2	2| 2

1	$3d^5$
2	$3d^4$ 4s
3	$3d^3$ $4s^2$
4	$3d^4$ 4d
5	$3d^4$ 5s
6	$3d^4$ 5d
7	$3d^4$ 6s
8	$3d^3$ 4s 4d
9	$3d^3$ 4s 5s
A	$3d^3$ 4s 5d
B	$3d^3$ $4p^2$

Vanadium I: two levels, bad case

Table 4: Energy levels in cm^{-1} and % composition of two $3d^4 4s^2$ J=$\frac{1}{2}$ levels in V I.

$E_e(cm^{-1})$	$E_c(cm^{-1})$	$E_o(cm^{-1})$	Δ_{ec}	Δ_{eo}	$2\|^4D$	$2\|^6D$	$8\|^6D$	$8\|^4D$	$B\|^4D$
2112.282	2044.9	2108.953	67.4	3.3	0| 0	100|97	0| 2	0| 0	0| 0
8413.009	8364.1	8403.516	48.9	9.5	97|95	0| 0	0| 0	0| 2	2| 2

Table 5: Landé g_J-factors and A-values of two $3d^4 4s^2$ J=$\frac{1}{2}$ levels in V I.

$E_e(cm^{-1})$	g_e	g_c	g_o	Δ_{ec}	Δ_{eo}	A_e(mK)	A_o(mK)
2112.282	3.338	3.338	3.338	0.000	0.000	25.077	31.667
8413.009	0.00	-0.001	-0.001	0.001	0.001	42.650	30.118

Vanadium I: lowest levels

1	$3d^5$
2	$3d^4\ 4s$
3	$3d^3\ 4s^2$
4	$3d^4\ 4d$
5	$3d^4\ 5s$
6	$3d^4\ 5d$
7	$3d^4\ 6s$
8	$3d^3\ 4s\ 4d$
9	$3d^3\ 4s\ 5s$
A	$3d^3\ 4s\ 5d$
B	$3d^3\ 4p^2$

J=4.5							
	13.571	14.593	-1.022	2424.809*	97% 2|5D)6D	+	1% 8|4F)3D6D
	7.576	8.027	-0.451	552.955*	97% 3|4F)4F	+	2% B|4F1S)4F
J=3.5							
	12.754	13.824	-1.070	2311.369*	97% 2|5D)6D	+	1% 8|4F)3D6D
	8.331	8.642	-0.311	323.432*	97% 3|4F)4F	+	2% B|4F1S)4F
J=2.5							
	12.462	13.703	-1.241	2220.156*	97% 2|5D)6D	+	1% 8|4F)3D6D
	10.715	10.619	0.096	137.383*	97% 3|4F)4F	+	2% B|4F1S)4F
J=1.5							
	13.530	15.410	-1.880	2153.221*	97% 2|5D)6D	+	1% 8|4F)3D6D
	18.682	17.247	1.435	0.000*	97% 3|4F)4F	+	2% B|4F1S)4F
J=0.5							
	42.650	30.121	12.529	8413.009*	95% 2|5D)4D	+	2% B|4F1D)4D
	25.077	31.666	-6.589	2112.282*	97% 2|5D)6D	+	1% 8|4F)3D6D

Scope Orthogonal operators: Lanthanides & Actinides

- Configurations: $f^n + f^{n-1}(s + p + d) + \ ...$
- Core excited: $p^5 f^{n+1} + p^5 f^n (s + p + d) \ldots$

	Pr III(f^3)	DHF	B-spl	Pr IV(f^2)	B-spl	Nd IV(f^3)	DHF	B-spl	Nd V(f^2)	B-spl
E_{av}	19709.2			10202.8		24892.1			12248.6	
E'_1	4924.8			60446.9		6393.5			7101.1	
E_2	2191.5			2526.1		2671.0			2915.5	
E_3	4942.9			5899.7		6197.9			6835.0	
E'_α	301.7			236.7		224.5			225.6	
E'_β	0			6.0		7.6			8.0*	
E'_γ	448.1			290.0		261.0			250*	
T'_2	122.7					64.4				
T_3	14.7					14.8				
T_4	24.5					16.0				
T_6	-49.5					-54.7				
T_7	60.3					60.2				
T_8	51.7					53.0				
ζ_f	660.7	609.2	711.4	764.6	813.4	892.4	843.0	944.0	998.4	1047.7
A_5	-2.7	-2.9	-2.7	-2.4	-2.0	-3.8	-2.9	-2.6	-3.7	-2.2
A_6	4.5	4.3	4.5	4.2	3.6	4.4	4.6	4.5	4.4	4.1
A_7	-2.3	-2.5	-2.3	-2.8	-2.4	-0.8	-3.0	-2.8	0	-3.0
A_8	4.6	5.2	4.6	5.7	5.0	5.1	6.4	5.8	5.7	6.3
A_9	1.3	0.5	1.3	5.4	5.1	4.3	3.9	4.8	5.9	7.8
A_{10}	-3.8	-4.3	-3.8	-2.6	-2.2	-2.8	-3.6	-3.0	-2.3	-2.0
A_{11}	-5.1	-5.6	-5.1	-4.2	-3.5	-3.8	-5.4	-4.6	-3.5	-3.7
A'_{12}	-10.5	-10.6	-9.0	-6.0	-4.8	-8.2	-8.6	-7.0	-6.7	-4.1
A_1	0.2	-0.5	0.2	0.3	0.3	0.3	0.7	0.3	0.4	0.3
A_2	-0.6	-0.4	-0.6	-0.8	-0.7	-0.8	-0.3	-0.8	-1.0	-0.9
A_3	0.1	0.5	0.1	0.1	0.1	0.1	0.1	0.3	0.1	0.1
A_4	-1.2	-0.0	-1.2	-1.7	-1.5	-1.7	0.1	-1.7	-2.2	-2.0
σ	14.2			6.9		7.6			3.8	

Some Lanthanide parameters

Nd IV, $4f^3$

J= 5.5

E(obs.)	E(calc.)	Delta	Mixd.g-fac.	Composition		
35136.610	35135.380	1.230	1.065	68% 1|2H1)	+ 16% 1|2I)	+ 14% 1|2H2)
30179.930	30182.298	-2.368	0.952	83% 1|2I)	+ 15% 1|2H1)	+ 1% 1|2H2)
22047.390	22044.330	3.060	1.261	93% 1|4G)	+ 4% 1|2H1)	+ 3% 1|2H2)
16161.530	16161.950	-0.420	1.099	80% 1|2H2)	+ 13% 1|2H1)	+ 5% 1|4G)
1897.110	1894.913	2.197	0.966	99% 1|4I)	+ 1% 1|2H2)	+ 0% 1|2H1)

J= 6.5

E(obs.)	E(calc.)	Delta	Mixd.g-fac.	Composition		
31582.850	31582.430	0.420	1.076	99% 1|2I)	+ 1% 1|2K)	+ 0% 1|4I)
20005.220	20011.260	-6.040	0.935	99% 1|2K)	+ 1% 1|2I)	+ 0% 1|4I)
3907.430	3909.988	-2.558	1.107	100% 1|4I)	+ 0% 1|2K)	+ 0% 1|2I)

J= 7.5

E(obs.)	E(calc.)	Delta	Mixd.g-fac.	Composition		
31036.000	31037.304	-1.304	0.946	96% 1|2L)	+ 4% 1|2K)	+ 0% 1|4I)
22043.770	22042.141	1.629	1.063	95% 1|2K)	+ 4% 1|2L)	+ 1% 1|4I)
5988.510	5993.501	-4.991	1.199	99% 1|4I)	+ 1% 1|2K)	+ 0% 1|2L)

Er IV, $4f^{11} + 4f^{10}6p$

J= 7.5

E(obs.)	E(calc.)	Delta	Mixd.g-fac.	Composition			
-	176633.644	-	0.993	33% 2|3K2)4L	+ 12% 2|3K2)4K	+ 12% 2|3K2)2L	+ 10% 2|3K1)4L
170771.010	170787.321	-16.311	1.136	35% 2|3K2)4I	+ 11% 2|3K1)4I	+ 9% 2|3K2)2K	+ 9% 2|3K2)4K
165670.200	165683.409	-13.209	1.120	54% 2|5I)6K	+ 37% 2|5I)4K	+ 2% 2|3H4)4I	+ 2% 2|5I)6I
161112.630	161111.297	1.333	1.183	53% 2|5I)6I	+ 28% 2|5I)4K	+ 7% 2|5I)4I	+ 7% 2|5I)6K
155801.730	155802.751	-1.021	1.233	61% 2|5I)4I	+ 29% 2|5I)6H	+ 3% 2|5I)6I	+ 3% 2|3K2)2K
153525.140	153536.379	-11.239	1.153	34% 2|5I)6K	+ 30% 2|5I)4K	+ 23% 2|5I)6I	+ 6% 2|5I)4I
147031.140	147027.318	3.822	1.279	57% 2|5I)6H	+ 18% 2|5I)4I	+ 15% 2|5I)6I	+ 4% 2|3K2)4I
-	48803.581	-	0.948	95% 1|2L)	+ 5% 1|2K)	+ 0% 1|4I)	+ 0% 2|3M)2L
28312.440	28275.654	36.786	1.064	92% 1|2K)	+ 5% 1|2L)	+ 3% 1|4I)	+ 0% 2|1L1)2K
0.000	-49.982	49.982	1.197	97% 1|4I)	+ 3% 1|2K)	+ 0% 1|2L)	+ 0% 2|3K1)4I

J= 8.5

E(obs.)	E(calc.)	Delta	Mixd.g-fac.	Composition			
171139.220	171128.295	10.925	1.081	22% 2|3K2)2L	+ 17% 2|3K2)4K	+ 16% 2|3K2)4L	+ 7% 2|3K1)2L
161334.420	161347.885	-13.465	1.200	76% 2|5I)6K	+ 18% 2|5I)4K	+ 2% 2|5I)6I	+ 1% 2|3K2)4L
155006.200	154995.488	10.712	1.240	56% 2|5I)6I	+ 34% 2|5I)4K	+ 3% 2|3K2)4K	+ 3% 2|5I)6K
147457.990	147445.611	12.379	1.219	40% 2|5I)4K	+ 36% 2|5I)6I	+ 17% 2|5I)6K	+ 2% 2|3K2)2L
42580.900	42565.349	15.551	1.059	100% 1|2L)	+ 0% 2|3K1)2L	+ 0% 2|3M)2L	+ 0% 2|3L)2L

Yb V, $4f^{11}6p$, DHF

J= 8.0

E(obs.)	E(calc.)	Delta	Mixd.g-fac.	Composition		
80127.010	80130.881	-3.871	0.995	42% 1|2L)3L	+ 39% 1|2L)1L	+ 14% 1|2L)3M
72687.310	72686.440	0.870	1.082	48% 1|2I)3K	+ 21% 1|2L)1L	+ 15% 1|2L)3K
70989.660	70990.832	-1.172	1.063	43% 1|2I)3K	+ 26% 1|2L)1L	+ 22% 1|2L)3L
66559.670	66559.708	-0.038	0.914	80% 1|2L)3M	+ 8% 1|2L)3L	+ 6% 1|2L)1L
58490.410	58490.586	-0.176	1.100	77% 1|2L)3K	+ 12% 1|2L)3L	+ 7% 1|2L)1L
55164.010	55165.716	-1.706	1.021	46% 1|2K)3L	+ 42% 1|2K)1L	+ 7% 1|2I)3K
49947.580	49950.607	-3.027	1.096	72% 1|2K)3K	+ 16% 1|2K)1L	+ 5% 1|2K)3L
38002.090	37999.398	2.692	1.030	40% 1|2K)3L	+ 33% 1|2K)1L	+ 19% 1|2K)3K
19203.420	19205.866	-2.446	1.149	74% 1|4I)5K	+ 22% 1|4I)3K	+ 3% 1|4I)5I
11383.350	11383.821	-0.471	1.209	68% 1|4I)5I	+ 28% 1|4I)3K	+ 2% 1|2K)3K
578.210	571.792	6.418	1.163	47% 1|4I)3K	+ 27% 1|4I)5I	+ 23% 1|4I)5K

J= 9.0

E(obs.)	E(calc.)	Delta	Mixd.g-fac.	Composition		
76511.210	76512.294	-1.084	1.012	49% 1|2L)3M	+ 45% 1|2L)1M	+ 5% 1|2K)3L
71742.850	71743.171	-0.321	1.092	82% 1|2L)3L	+ 13% 1|2L)1M	+ 4% 1|2L)3M
58676.690	58674.390	2.300	1.023	44% 1|2L)3M	+ 39% 1|2L)1M	+ 17% 1|2L)3L
47727.100	47727.277	-0.177	1.109	93% 1|2K)3L	+ 3% 1|2L)3M	+ 3% 1|4I)5K
10305.360	10303.043	2.317	1.220	97% 1|4I)5K	+ 3% 1|2K)3L	+ 0% 1|2L)3M

Yb V, $4f^{12} + 4f^{11}6p$

```
J= 7.0

  E(obs.)      E(calc.)         Delta    Mixd.g-fac.                             Composition
.....................................................................................................

      -        284318.314         -          1.119   52% 2|2K )3I   + 12% 2|2K )3K   + 10% 2|4G )5H
      -        283415.991         -          1.156   33% 2|2H2)3I   + 27% 2|4G )5H   + 13% 2|2K )3I
 273216.250    273210.150       6.100        1.070   36% 2|4I )5K   + 35% 2|4I )3K   + 21% 2|2H2)3I
 269233.490    269236.980      -3.490        1.130   58% 2|4I )5I   + 23% 2|4I )3K   + 11% 2|4I )3I
 260750.180    260749.765       0.415        1.180   64% 2|4I )3I   + 26% 2|4I )5H   +  7% 2|4I )5I
 257348.770    257349.454      -0.684        1.077   43% 2|4I )5K   + 29% 2|4I )3K   + 18% 2|4I )5I
 247890.510    247895.864      -5.354        1.240   65% 2|4I )5H   + 16% 2|4I )3I   + 14% 2|4I )5I
```

```
J= 8.0

  E(obs.)      E(calc.)         Delta    Mixd.g-fac.                             Composition
.....................................................................................................

      -        284400.720         -          1.031   39% 2|2K )3L   + 32% 2|2K )1L   + 21% 2|2K )3K
 268532.230    268534.752      -2.522        1.148   74% 2|4I )5K   + 22% 2|4I )3K   +  3% 2|4I )5I
 260218.140    260226.054      -7.914        1.208   67% 2|4I )5I   + 28% 2|4I )3K   +  2% 2|2K )3K
 248573.040    248576.376      -3.336        1.164   46% 2|4I )3K   + 28% 2|4I )5I   + 23% 2|4I )5K
```

```
J= 9.0

  E(obs.)      E(calc.)         Delta    Mixd.g-fac.                             Composition
.....................................................................................................

 259305.050    259308.268      -3.218        1.219   97% 2|4I )5K   +  3% 2|2K )3L   +  0% 2|2L )3M
```