**f\_electron Test Data**

It is remarkably difficult to find reliable test data in the literature to compare to the calculations from this program. This is despite the many hundreds of publications with tables of energy levels that one should be able to reproduce exactly. There are several reasons for this.

1. Round-off errors. Usually a publication has made a least-squares fit to experimental data by varying *Np* parameters. The parameters and calculated energy levels are only reported to a certain number of decimal places. A small change in a parameter value can result in a larger change in the calculated energy levels. In other words, the energies given have not been recalculated using the reported values and will therefore differ.
2. The widely used suite of programs by Michael Reid was found to have errors in a file “fncross” that contained tables of reduced matrix elements [1], [2]. Literature results that have these errors can be reproduced by including the appropriate errors (obtained from the fncross file provided by M Reid ~ 2005). While there is no guarantee that exactly the same errors are reproduced in this way, as different errors may have been introduced at a number of different points in time, in practice many of the published literature results can be reproduced this way. These types of errors can be reproduced by using the FNCR command.
3. The matrices for the three electron parameter T2 has often not been treated correctly for the complementary configuration f8-f11. These matrices are not just the negative of the f3-f6 matrices as there is some one-electron character that must be correctly taken into account [2]. This type of error can be reproduced by setting FNCR(7).
4. The Marvin integrals *M0, M2, M4* can also be used to take the spin-spin interactions, Hss,into account. Some authors include Hss and some do not [2]. This program includes Hss by default, but it can be also be excluded by setting OPTN(5) to true.
5. For the larger systems f4-f9, computer limitations in earlier studies suffer from truncation errors. This was often not a simple truncation of the free ion states in the basis set. Typically, a calculation using atomic parameters only was made, and then the eigenvectors from a truncated set of the resulting atomic multiplets would be used as a basis set, resulting in a smaller matrix. The f\_electron program also allows you to reproduce this type of truncation error using the PRED ("prediagonalise") command.
6. Some papers shift the bari-centres of the atomic multiplets to match experiment. For references that report the values of these energy shifts the energies can be reproduced using the OFFS ("offset") command.

Here we list a series of calculations in the literature whose published *Nc* calculated energy levels *Ec* results can be reproduced using the published parameters given in the paper. σ =

**Table 1 Some reliable f electron literature calculations**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| fn | System | Ref | Sym | Type | Hss? | Nc | σ | Comments |
| 1 | Ce(III)/LaCl3 | [3] | C3h | E | - | 5 | 0.082 |  |
| 2 | Pr (III)/LaCl3 | [2] | C3h | E, g-val | yes | 61 |  |  |
| 3 | Nd(III)/LaCl3 | [2] | C3h | E, g-val | yes | 166 |  |  |
| 4 | Cs2YPmCl6 | [4] | Oh | E | no | 376 | 0.023 | E given to 3 dec.pl. |
| 5 | Sm |  |  |  |  |  |  |  |
| 6 | EuCl3.6H2O | [5] |  | E | no | 74 | 1.54 | NPRED 700, σ=0.49 |
| 7 | Gd |  |  |  |  |  |  |  |
| 8 | Tb |  |  |  |  |  |  |  |
| 9 | Dy(III)/LaCl3 | [6] | C3h | E, WFs | no | 210 | 0.35 |  |
| 10 | Cs2NaHoF6 | [7] | Oh | E, Int |  |  |  |  |
| 11 | Er(III)/LaCl3 | [2] | C3h | E, g-val | yes | 134 | 0.166 | Eave=35,544.5 cm-1 |
| 12 | Tm(III)/LaCl3 | [8] | C3h | E | - | 61 | 0.365 |  |
| 13 | Cs2NaYbCl6 | [9] | Oh | E | - | 5 | 0.530 |  |

**References:**

[1] X. Chen, G. Liu, J. Margerie, M. F. Reid, *J. Lumin*., 128, 421, (2008).

[2] Y. Y. Yeung, P. A. Tanner, *J. Alloy & Compounds*, 575, 54, (2013).

[3] Bagguley, et al, *J. Chem. Phys*., 39, 973, (1968).

[4] C.-K. Duan, P. A. Tanner, *J. Phys. Chem. A*, 114, 6055, (2010) (Supp.Mat.).

[5] K. Binnemans, C. Görller-Walrand, *J. Alloys & Compounds*, 250, 326, (1997).

[6] R. S. Rana, *et al*., *J. Chem. Phys*., 88, 2242, (1988).  
[7] P. A. Tanner, M. D. Faucher, X. Zhou, *J. Phys. Chem. A*, 115, 2557, (2011).

[8] J. B. Gruber, *et al*, *J. Chem. Phys*.,74, 2705, (1981).

[9] F. S. Richardson *et al*, *J. Chem. Phys*., 83, 3813, (1985).

**Table 1 Notes**

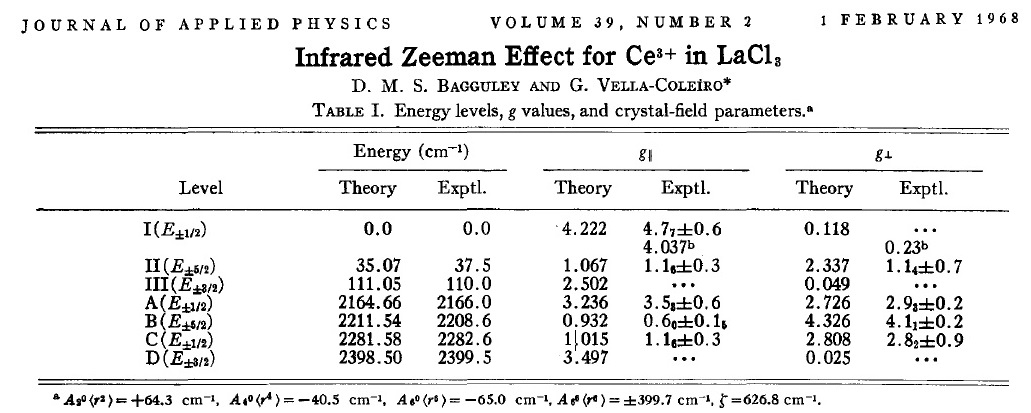
**EuCl3.6H2O**

Although truncation is not mentioned, the agreement is better (σ =0.486 cm-1) when a basis of 700 atomic states are used, and one energy level (32953.0 cm-1), that is calculated to be 9.5 cm-1 different, is not included in calculation of σ

**Tm(III)/LaCl3**

The baricentre of the multiplets are used as parameters in this paper [8]. To reproduce in the f\_electron program, use PRED to do a “prediagonalisation” in a |SLJ> basis and then shift these terms before applying ligand field using OFFS. Note: In this calculation the Mn and Tn parameters are all zero, so these are not tested.

Ce(III)/LaCl3



TITL Test input for Ce(III)/LaCl3 Bagguley, JCP,39,973,(1968).

echo F

Conf 3 1

OPTN T F T F F T F F F F

GEXS 0 1 14

ZETA 626.8

SYML C3h 1 0

CF

128.6 ! B20 2x 64.3

0 0

0 0

-324.0 ! B40 8x -40.5

0 0

0 0

0 0

0 0 ! B44, B44'

-1040.0 ! B60 16x -65.0

0 0

0 0

0 0

0 0 ! B64, B64'

0 0

420.773268 0 ! B66, B66' 16/sqrt(231)x 399.7

EXPE 7 1

0.00 1.0 1

35.07 1.0 3

111.05 1.0 5

2164.66 1.0 7

2211.54 1.0 9

2281.58 1.0 11

2398.50 1.0 13

EXPG 7

0.118 1.0 0.118 1.0 4.222 1.0 1

1.067 1.0 2.337 1.0 2.337 1.0 3

0.049 1.0 0.049 1.0 2.502 1.0 5

2.726 1.0 2.726 1.0 3.236 1.0 7

0.932 1.0 4.326 1.0 4.326 1.0 9

1.015 1.0 2.808 1.0 2.808 1.0 11

0.025 1.0 0.025 1.0 3.497 1.0 13

end

F-ELECTRON version:1.53.1; compile date: 13th March 2020; this run:(16/03/2020) 16:15

Title: Test input for Ce(III)/LaCl3 Bagguley, JCP,39,973,(1968).

Input from file:Ce\_LaCl3.in

Calculation: f^ 1 electrons

Calculation Options: OPTN(1-10) = T F T F F T F F F F

Energies relative to lowest energy=0.

Calculate % of free ion terms (short 40 char).

The Hss spin-spin interactions (using the Mn parameters) were included.

Calculate % of MJ (short 40 char).

Experimental data provided:

A comparison of calculated and given g-values will be made.

---------------------------------------------------------------------------------------------------------

Atomic Parameters: (L:LINKed; F:formula)

---------------------------------------------------------------------------------------------------------

Offset: 1 EAVE= 0.0000 |

E-E parameters: 2 F2= 0.0000 3 F4= 0.0000 4 F6= 0.0000 |

SOC parameter: 5 ZETA= 626.8000 |

E-E CI parameters: 6 ALPHA= 0.0000 7 BETA= 0.0000 8 GAMMA= 0.0000 |

soo parameters: 9 M0= 0.0000 10 M2= 0.0000 11 M4= 0.0000 |

ec-so parameters: 12 P2= 0.0000 13 P4= 0.0000 14 P6= 0.0000 |

3 body parameters: 15 T2= 0.0000 16 T3= 0.0000 17 T4= 0.0000 |

18 T6= 0.0000 19 T7= 0.0000 20 T8= 0.0000 |

Ligand Field Parameters:

---------------------------------------------------------------------------------------------------------

21 B20 128.600000

22 B21 0.000000 42 B21' 0.000000

23 B22 0.000000 43 B22' 0.000000

24 B40 -324.000000

25 B41 0.000000 45 B41' 0.000000

26 B42 0.000000 46 B42' 0.000000

27 B43 0.000000 47 B43' 0.000000

28 B44 0.000000 48 B44' 0.000000

29 B60 -1040.000000

30 B61 0.000000 50 B61' 0.000000

31 B62 0.000000 51 B62' 0.000000

32 B63 0.000000 52 B63' 0.000000

33 B64 0.000000 53 B64' 0.000000

34 B65 0.000000 54 B65' 0.000000

35 B66 420.773268 55 B66' 0.000000

Nv/sqrt(4pi)= 354.13 The ligand field is real

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Energy relative to lowest calculated E0= -1314.7

| C3h group |

Level Rel.Eng. (deg)| - Exp del | Symmetry | MJ projections | Free Ion %

---------------------------------------------------------------------------------------------------------

13- 14 2398.6 ( 2)| - 2398.5 0.1 | G11 G12| 99\*(-3/2) | 99\*2F(7/2)

11- 12 2281.7 ( 2)| - 2281.6 0.1 | G7 G8 | 67\*(-5/2) +32\*(7/2) | 99\*2F(7/2)

9- 10 2211.6 ( 2)| - 2211.5 0.1 | G9 G10| 88\*(-1/2) +11\*(1/2) | 98\*2F(7/2)

7- 8 2164.8 ( 2)| - 2164.7 0.1 | G7 G8 | 66\*(-7/2) +33\*(5/2) | 99\*2F(7/2)

5- 6 111.1 ( 2)| - 111.0 0.0 | G11 G12| 99\*(3/2) | 99\*2F(5/2)

3- 4 35.0 ( 2)| - 35.1 -0.0 | G9 G10| 92\*(1/2) + 7\*(-1/2) | 98\*2F(5/2)

1- 2 0.0 ( 2)| - 0.0 0.0 | G7 G8 | 99\*(5/2) | 99\*2F(5/2)

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sqrt(sum(Ec-Eex)^2/Nex)= | 0.82576E-01 |

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g-Values

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States Energy | g1(calc) g1(exp) diff | g2(calc) g2(exp) diff | g3(calc) g3(exp) diff |

---------------------------------------------------------------------------------------------------------

1- 2 0.0 | 0.1207 0.1180 0.0027 | 0.1207 0.1180 0.0027 | 4.2210 4.2220 -0.0010 |

3- 4 35.0 | 1.0697 1.0670 0.0027 | 2.3849 2.3370 0.0479 | 2.3849 2.3370 0.0479 |

5- 6 111.1 | 0.0000 0.0490 -0.0490 | 0.0000 0.0490 -0.0490 | 2.4997 2.5020 -0.0023 |

7- 8 2164.8 | 2.7504 2.7260 0.0244 | 2.7504 2.7260 0.0244 | 3.3870 3.2360 0.1510 |

9- 10 2211.6 | 0.9303 0.9320 -0.0017 | 4.3872 4.3260 0.0612 | 4.3872 4.3260 0.0612 |

11- 12 2281.7 | 1.1637 1.0150 0.1487 | 2.8711 2.8080 0.0631 | 2.8711 2.8080 0.0631 |

13- 14 2398.6 | 0.0000 0.0250 -0.0250 | 0.0000 0.0250 -0.0250 | 3.5003 3.4970 0.0033 |

---------------------------------------------------------------------------------------------------------

sqrt(sum(Gc-Gex)^2/Nex)= | 0.58659E-01 |

---------------------------------------------------------------------------------------------------------

total CPU time: 0.05 secs

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Notes:

1. The A<r> CF parameters are converted into Bkq parameters of the Wybourne convention using the expressions in the appendix of the manual.

2. The Γ11, Γ12 Kramers doublets (labelled E±3/2 in the paper) have g⊥ = 0 by symmetry and g|| = J.

Pr(III)/LaCl3

[2] Y. Y. Yeung, P. A. Tanner, *J.Alloy& Compounds*, 575, 54, (2013).

Supplemental Material

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No. | *SLJ* | μ | *C*3h irrep | *E*obs | *E*calc | Δ | |*s*|obs | |*s*(1)|calc | |*s*(1)+*s*(2)|calc |
| 1 | 3H4 | 2 | E' | 0.0 | -0.6 | 0.6 | 1.00 | 1.29 | 1.24 |
| 2 |  | 3 | A'' | 33.1 | 27.1 | 6.0 | 0.00 | 0.00 | 0.00 |
| 3 |  | 2' | E' | 96.4 | 100.4 | -4.0 | 4.33 | 4.52 | 4.51 |
| 4 |  | 1 | E'' | 130.2 | 124.5 | 5.7 |  | 1.60 | 1.47 |
| 5 |  | 3' | A'' | 137.0 | 147.6 | -10.6 |  | 0.00 | 0.00 |
| 6 |  | 0 | A' | 199.5 | 206.3 | -6.8 |  | 0.00 | 0.00 |
| 7 | 3H5 | 3 | A'' | 2137.2 | 2131.4 | 5.8 | 0.00 | 0.00 | 0.00 |
| 8 |  | 2 | E' | 2169.8 | 2162.7 | 7.1 | 0.0 | 0.11 | 0.14 |
| 9 |  | 1 | E'' | 2188.5 | 2190.1 | -1.6 | 9.42 | 10.04 | 10.01 |
| 10 |  | 3' | A'' | 2202.2 | 2199.0 | 3.2 | 0.00 | 0.00 | 0.00 |

Input:

TITL Test input for f^2 Pr(III)/LaCl3 Yeung, JAlloyComp,575,54,(2013). Table 5 & S6

ECHO F

OPTN F F F T F F F F F F

CONF 3 2

GEXS 0 -1 2 4 5 6 7 11 12 13 14

ROTL 0 0 0

SYML C3h 1 0

MFLD 0. 0. 0.0

MDIP 1 5 1 6 3 1 1.0

EAVE 9931

F2 68439

F4 50226

F6 32973

ZETA 748.0

ALPH 22.8

BETA -676.0

GAMM 1452.5

M0 1.71

M2 0.9576 ! 0.56 M0

M4 0.6498 ! 0.38 M0

P2 265.7

P4 199.275 ! 0.75 P2

P6 132.85 ! 0.50 P2

CF ! Bkq

106.3 ! B20

0.0000 0.0000

0.0000 0.0000

-332.7 ! B40

0.0000 0.0000

0.0000 0.0000

0.0000 0.0000 ! B43

0.0000 0.0000

-651.8 ! B60

0.0000 0.0000

0.0000 0.0000

0.0000 0.0000 ! B63

0.0000 0.0000

0.0000 0.0000

447.0 0.00 ! B66 B66'

EXPE 61 1

-0.6 1.0 1

27.1 1.0 3

100.4 1.0 4

124.5 1.0 6

147.6 1.0 8

206.3 1.0 9

2131.4 1.0 10

2162.7 1.0 11

2190.1 1.0 13

2199.0 1.0 15

2225.8 1.0 16

2257.4 1.0 18

2289.3 1.0 20

4234.8 1.0 21

4294.8 1.0 22

4348.9 1.0 24

4365.7 1.0 25

4385.5 1.0 26

4419.9 1.0 27

4430.9 1.0 29

4514.5 1.0 31

4526.8 1.0 33

4924.6 1.0 34

4945.5 1.0 36

4950.7 1.0 37

6284.5 1.0 39

6307.6 1.0 40

6308.1 1.0 42

6348.0 1.0 43

6375.2 1.0 45

6707.5 1.0 46

6750.8 1.0 47

6768.7 1.0 48

6776.2 1.0 50

6783.6 1.0 51

6812.1 1.0 53

9583.2 1.0 55

9743.9 1.0 56

9756.5 1.0 57

9778.9 1.0 58

9812.9 1.0 60

9915.9 1.0 62

16644.5 1.0 64

16742.2 1.0 65

16755.9 1.0 67

20471.3 1.0 69

21068.9 1.0 70

21101.5 1.0 72

21299.5 1.0 73

21304.4 1.0 74

21373.2 1.0 75

21387.1 1.0 77

21416.8 1.0 78

21439.5 1.0 80

21468.7 1.0 82

21493.6 1.0 83

21522.8 1.0 85

22204.0 1.0 86

22222.6 1.0 87

22248.5 1.0 89

46450.6 1.0 91

EXPG 5

0.0 1.0 0.0 1.0 1.24 1.0 1

0.0 1.0 0.0 1.0 4.51 1.0 4

0.0 1.0 0.0 1.0 1.47 1.0 6

0.0 1.0 0.0 1.0 0.14 1.0 11

0.0 1.0 0.0 1.0 10.01 1.0 13

end

Output:

F-ELECTRON version:1.53.1; compile date: 13th March 2020; this run:(16/03/2020) 18:46

Title: Test input for f^2 Pr(III)/LaCl3 Yeung, JAlloyComp,575,54,(2013). Table 5 & S6

\*\*\*WARNING: more than one of EXPB,EXPE,EXPG,EXPM,EXP1.

Input from file:Pr\_LaCl3.in

Calculation: f^ 2 electrons

Calculation Options: OPTN(1-10) = F F F T F F F F F F

Calculate % of free ion terms (long 80 char).

The Hss spin-spin interactions (using the Mn parameters) were included.

Experimental data provided:

A comparison of calculated and given g-values will be made.

-------------------------------------------------------------------------------------------------

\*\*\*WARNING: fitting g-values for even electron systems

Atomic Parameters: (L:LINKed; F:formula)

-------------------------------------------------------------------------------------------------

Offset: 1 EAVE= 9931.0000 |

E-E parameters: 2 F2= 68439.0000 3 F4= 50226.0000 4 F6= 32973.0000 |

SOC parameter: 5 ZETA= 748.0000 |

E-E CI parameters: 6 ALPHA= 22.8000 7 BETA= -676.0000 8 GAMMA= 1452.5000 |

soo parameters: 9 M0= 1.7100 10 M2= 0.9576 11 M4= 0.6498 |

ec-so parameters: 12 P2= 265.7000 13 P4= 199.2750 14 P6= 132.8500 |

3 body parameters: 15 T2= 0.0000 16 T3= 0.0000 17 T4= 0.0000 |

18 T6= 0.0000 19 T7= 0.0000 20 T8= 0.0000 |

Ligand Field Parameters:

----------------------------------------------------------------------------------------------

21 B20 106.300000

22 B21 0.000000 42 B21' 0.000000

23 B22 0.000000 43 B22' 0.000000

24 B40 -332.700000

25 B41 0.000000 45 B41' 0.000000

26 B42 0.000000 46 B42' 0.000000

27 B43 0.000000 47 B43' 0.000000

28 B44 0.000000 48 B44' 0.000000

29 B60 -651.800000

30 B61 0.000000 50 B61' 0.000000

31 B62 0.000000 51 B62' 0.000000

32 B63 0.000000 52 B63' 0.000000

33 B64 0.000000 53 B64' 0.000000

34 B65 0.000000 54 B65' 0.000000

35 B66 447.000000 55 B66' 0.000000

Nv/sqrt(4pi)= 279.25 The ligand field is real

----------------------------------------------------------------------------------------------

| C3h group |

Level Rel.Eng. (deg)| - Exp del | Symmetry | Free Ion %

----------------------------------------------------------------------------------------------

91 46450.8 | - 46450.6 0.2 | G1 | 99\*1S(0)

89- 90 22248.9 ( 2)| - 22248.5 0.4 | G2 G3 | 90\*3P(2) + 8\*1D(2)

87- 88 22223.1 ( 2)| - 22222.6 0.5 | G6 G5 | 90\*3P(2) + 8\*1D(2)

86 22204.4 | - 22204.0 0.4 | G1 | 90\*3P(2) + 8\*1D(2)

85 21522.7 | - 21522.8 -0.1 | G4 | 99\*1I(6)

83- 84 21493.6 ( 2)| - 21493.6 -0.0 | G3 G2 | 99\*1I(6)

82 21468.6 | - 21468.7 -0.1 | G4 | 99\*1I(6)

80- 81 21439.5 ( 2)| - 21439.5 -0.0 | G2 G3 | 99\*1I(6)

78- 79 21416.7 ( 2)| - 21416.8 -0.1 | G5 G6 | 99\*1I(6)

77 21387.0 | - 21387.1 -0.1 | G1 | 99\*1I(6)

75- 76 21373.1 ( 2)| - 21373.2 -0.1 | G6 G5 | 99\*1I(6)

74 21304.4 | - 21304.4 -0.0 | G1 | 98\*1I(6)

73 21299.5 | - 21299.5 -0.0 | G1 | 99\*1I(6)

72 21101.7 | - 21101.5 0.2 | G1 | 99\*3P(1)

70- 71 21069.1 ( 2)| - 21068.9 0.2 | G5 G6 | 99\*3P(1)

69 20471.5 | - 20471.3 0.2 | G1 | 98\*3P(0)

67- 68 16756.1 ( 2)| - 16755.9 0.2 | G6 G5 | 88\*1D(2) + 8\*3P(2)

65- 66 16742.4 ( 2)| - 16742.2 0.2 | G3 G2 | 88\*1D(2) + 8\*3P(2)

64 16644.7 | - 16644.5 0.2 | G1 | 88\*1D(2) + 8\*3P(2)

62- 63 9916.0 ( 2)| - 9915.9 0.1 | G3 G2 | 67\*1G(4) + 31\*3F(4)

60- 61 9813.1 ( 2)| - 9812.9 0.2 | G5 G6 | 65\*1G(4) + 33\*3F(4)

58- 59 9779.0 ( 2)| - 9778.9 0.1 | G3 G2 | 64\*1G(4) + 34\*3F(4)

57 9756.6 | - 9756.5 0.1 | G4 | 64\*1G(4) + 34\*3F(4)

56 9744.0 | - 9743.9 0.1 | G1 | 63\*1G(4) + 35\*3F(4)

55 9583.4 | - 9583.2 0.2 | G4 | 60\*1G(4) + 38\*3F(4)

53- 54 6812.1 ( 2)| - 6812.1 0.0 | G2 G3 | 67\*3F(4) + 31\*1G(4)

51- 52 6783.7 ( 2)| - 6783.6 0.1 | G6 G5 | 66\*3F(4) + 31\*1G(4)

50 6776.3 | - 6776.2 0.1 | G1 | 64\*3F(4) + 33\*1G(4)

48- 49 6768.7 ( 2)| - 6768.7 0.0 | G3 G2 | 66\*3F(4) + 32\*1G(4)

47 6750.9 | - 6750.8 0.1 | G4 | 65\*3F(4) + 32\*1G(4)

46 6707.5 | - 6707.5 0.0 | G4 | 60\*3F(4) + 36\*1G(4)

45 6375.3 | - 6375.2 0.1 | G4 | 99\*3F(3)

43- 44 6348.1 ( 2)| - 6348.0 0.1 | G6 G5 | 99\*3F(3)

42 6308.2 | - 6308.1 0.1 | G4 | 99\*3F(3)

40- 41 6307.7 ( 2)| - 6307.6 0.1 | G2 G3 | 99\*3F(3)

39 6284.6 | - 6284.5 0.1 | G1 | 99\*3F(3)

37- 38 4950.7 ( 2)| - 4950.7 0.0 | G2 G3 | 95\*3F(2)

36 4945.5 | - 4945.5 -0.0 | G1 | 92\*3F(2) + 5\*3H(6)

34- 35 4924.6 ( 2)| - 4924.6 -0.0 | G6 G5 | 96\*3F(2)

33 4526.9 | - 4526.8 0.1 | G1 | 96\*3H(6)

31- 32 4514.6 ( 2)| - 4514.5 0.1 | G5 G6 | 98\*3H(6)

29- 30 4431.0 ( 2)| - 4430.9 0.1 | G2 G3 | 98\*3H(6)

27- 28 4420.0 ( 2)| - 4419.9 0.1 | G5 G6 | 98\*3H(6)

26 4385.6 | - 4385.5 0.1 | G4 | 99\*3H(6)

25 4365.8 | - 4365.7 0.1 | G1 | 99\*3H(6)

24 4349.0 | - 4348.9 0.1 | G1 | 97\*3H(6)

22- 23 4294.8 ( 2)| - 4294.8 0.0 | G2 G3 | 98\*3H(6)

21 4234.8 | - 4234.8 0.0 | G4 | 98\*3H(6)

20 2289.2 | - 2289.3 -0.1 | G1 | 99\*3H(5)

18- 19 2257.3 ( 2)| - 2257.4 -0.1 | G5 G6 | 99\*3H(5)

16- 17 2225.7 ( 2)| - 2225.8 -0.1 | G3 G2 | 99\*3H(5)

15 2199.0 | - 2199.0 -0.0 | G4 | 99\*3H(5)

13- 14 2190.0 ( 2)| - 2190.1 -0.1 | G6 G5 | 99\*3H(5)

11- 12 2162.6 ( 2)| - 2162.7 -0.1 | G3 G2 | 99\*3H(5)

10 2131.3 | - 2131.4 -0.1 | G4 | 99\*3H(5)

9 206.1 | - 206.3 -0.2 | G1 | 96\*3H(4)

8 147.4 | - 147.6 -0.2 | G4 | 96\*3H(4)

6- 7 124.3 ( 2)| - 124.5 -0.2 | G5 G6 | 96\*3H(4)

4- 5 100.2 ( 2)| - 100.4 -0.2 | G2 G3 | 96\*3H(4)

3 26.9 | - 27.1 -0.2 | G4 | 96\*3H(4)

1- 2 -0.8 ( 2)| - -0.6 -0.2 | G2 G3 | 97\*3H(4)

-------------------------------------------------------------------------------------------------

sqrt(sum(Ec-Eex)^2/Nex)= | 0.15946E+00 |

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g-Values

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States Energy | g1(calc) g1(exp) diff | g2(calc) g2(exp) diff | g3(calc) g3(exp) diff |

------------------------------------------------------------------------------------------------

1- 2 -0.8 | 0.0000 0.0000 0.0000 | 0.0000 0.0000 0.0000 | 1.2395 1.2400 -0.0005 |

4- 5 100.2 | 0.0000 0.0000 0.0000 | 0.0000 0.0000 0.0000 | 4.5121 4.5100 0.0021 |

6- 7 124.3 | 0.0000 0.0000 0.0000 | 0.0000 0.0000 0.0000 | 1.4705 1.4700 0.0005 |

11- 12 2162.6 | 0.0000 0.0000 0.0000 | 0.0000 0.0000 0.0000 | 0.1344 0.1400 -0.0056 |

13- 14 2190.0 | 0.0000 0.0000 0.0000 | 0.0000 0.0000 0.0000 | 10.0083 10.0100 -0.0017 |

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sqrt(sum(Gc-Gex)^2/Nex)= | 0.16157E-02 |

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Magnetic Dipole Transitions

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kx=1.0000 ky=1.0000 kz=1.0000

Energy(deg.) Mag.Dipole Amplitude(Bohr Mag.)

deltaE <Mx> <My>/i <Mz>

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0.0 ( 1) -->

0.0 ( 1) 0.0 -0.0000 0.0000 0.0000 0.0000 -0.5296 0.0000

0.0 ( 1) 0.0 0.0000 0.0000 -0.0000 0.0000 0.3218 0.0000

27.7 ( 1) 27.7 0.8827 0.0000 -1.5693 0.0000 0.0000 0.0000

101.0 ( 1) 101.0 0.0000 0.0000 0.0000 0.0000 -1.7294 0.0000

101.0 ( 1) 101.0 -0.0000 0.0000 -0.0000 0.0000 -0.8001 0.0000

125.1 ( 1) 125.1 0.1741 0.0000 0.9306 0.0000 0.0000 0.0000

0.0 ( 1) -->

0.0 ( 1) 0.0 0.0000 0.0000 0.0000 0.0000 0.3218 0.0000

0.0 ( 1) 0.0 -0.0000 0.0000 0.0000 0.0000 0.5296 0.0000

27.7 ( 1) 27.7 -1.5693 0.0000 -0.8827 0.0000 0.0000 0.0000

101.0 ( 1) 101.0 -0.0000 0.0000 -0.0000 0.0000 0.8001 0.0000

101.0 ( 1) 101.0 -0.0000 0.0000 0.0000 0.0000 -1.7294 0.0000

125.1 ( 1) 125.1 -1.5055 0.0000 1.1962 0.0000 0.0000 0.0000

27.7 ( 1) -->

0.0 ( 1) 27.7 0.8827 0.0000 1.5693 0.0000 0.0000 0.0000

0.0 ( 1) 27.7 -1.5693 0.0000 0.8827 0.0000 0.0000 0.0000

27.7 ( 1) 0.0 0.0000 0.0000 -0.0000 0.0000 0.0000 0.0000

101.0 ( 1) 73.3 -0.2317 0.0000 -0.3210 0.0000 -0.0000 0.0000

101.0 ( 1) 73.3 -0.3210 0.0000 0.2317 0.0000 -0.0000 0.0000

125.1 ( 1) 97.5 0.0000 0.0000 -0.0000 0.0000 -0.0000 0.0000

101.0 ( 1) -->

0.0 ( 1) 101.0 0.0000 0.0000 -0.0000 0.0000 -1.7294 0.0000

0.0 ( 1) 101.0 -0.0000 0.0000 0.0000 0.0000 0.8001 0.0000

27.7 ( 1) 73.3 -0.2317 0.0000 0.3210 0.0000 -0.0000 0.0000

101.0 ( 1) 0.0 0.0000 0.0000 0.0000 0.0000 2.1411 0.0000

101.0 ( 1) 0.0 -0.0000 0.0000 -0.0000 0.0000 0.7109 0.0000

125.1 ( 1) 24.2 0.1778 0.0000 0.4103 0.0000 -0.0000 0.0000

101.0 ( 1) -->

0.0 ( 1) 101.0 -0.0000 0.0000 0.0000 0.0000 -0.8001 0.0000

0.0 ( 1) 101.0 -0.0000 0.0000 -0.0000 0.0000 -1.7294 0.0000

27.7 ( 1) 73.3 -0.3210 0.0000 -0.2317 0.0000 -0.0000 0.0000

101.0 ( 1) 0.0 -0.0000 0.0000 0.0000 0.0000 0.7109 0.0000

101.0 ( 1) 0.0 -0.0000 0.0000 -0.0000 0.0000 -2.1411 0.0000

125.1 ( 1) 24.2 0.7667 0.0000 -0.6716 0.0000 0.0000 0.0000

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total CPU time: 0.11 secs

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Notes:

1. Non Kramers ion. The g-values only calculated for degenerate pairs as if they are S=1/2 doublets. The Γ2, Γ3 and Γ5, Γ6 pairs (labelled E’ and E’’ in ref [2]) have to have g⊥ = 0 by symmetry.