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 N_p 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 T_2 has often not been treated correctly for the complementary configuration f^8-f^{11}. These matrices are not just the negative of the f^3-f^6 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 M^0, M^2, M^4 can also be used to take the spin-spin interactions, H_{ss}, into account. Some authors include H_{ss} and some do not [2]. This program includes H_{ss} by default, but it can be also be excluded by setting OPTN(5) to true.

5) For the larger systems f^4-f^9, 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 N_c calculated energy levels E_c results can be reproduced using the published parameters given in the paper. $\sigma = \sqrt{\sum(E - E_c)^2/N_c}$

Table 1 Some reliable f electron literature calculations

f^n	System	Ref	Sym	Type	H_{ss}?	N_c	σ	Comments
1	$Ce(III)/LaCl_3$	[3]	C_{3h}	E	-	5	0.082	
2	$Pr(III)/LaCl_3$	[2]	C_{3h}	E, g-val	yes	61		
3	$Nd(III)/LaCl_3$	[2]	C_{3h}	E, g-val	yes	166		
4	Cs_2YPmCl_6	[4]	O_h	E	no	376	0.023	E given to 3 dec.pl.
5	Sm							
6	$EuCl_3.6H_2O$	[5]		E	no	74	1.54	NPRED 700, σ=0.49
7	Gd							
8	Tb							
9	$Dy(III)/LaCl_3$	[6]	C_{3h}	E, WFs	no	210	0.35	
10	Cs_2NaHoF_6	[7]	O_h	E, Int				
11	$Er(III)/LaCl_3$	[2]	C_{3h}	E, g-val	yes	134	0.166	E_{ave}=35,544.5 cm^{-1}
12	$Tm(III)/LaCl_3$	[8]	C_{3h}	E	-	61	0.365	
13	$Cs_2NaYbCl_6$	[9]	O_h	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

$EuCl_3.6H_2O$

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

$Tm(III)/LaCl_3$

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)/$LaCl_3$

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Infrared Zeeman Effect for Ce^{3+} in $LaCl_3$

D. M. S. Bagguley and G. Vella-Coleiro*

Table I. Energy levels, g values, and crystal-field parameters.[a]

Level	Energy (cm^{-1}) Theory	Energy (cm^{-1}) Exptl.	$g_\parallel$ Theory	$g_\parallel$ Exptl.	$g_\perp$ Theory	$g_\perp$ Exptl.
$I(E_{\pm 1/2})$	0.0	0.0	4.222	$4.7_7 \pm 0.6$	0.118	...
				4.037[b]		0.23[b]
$II(E_{\pm 5/2})$	35.07	37.5	1.067	$1.1_6 \pm 0.3$	2.337	$1.1_4 \pm 0.7$
$III(E_{\pm 3/2})$	111.05	110.0	2.502	...	0.049	...
$A(E_{\pm 1/2})$	2164.66	2166.0	3.236	$3.5_8 \pm 0.6$	2.726	$2.9_3 \pm 0.2$
$B(E_{\pm 5/2})$	2211.54	2208.6	0.932	$0.6_0 \pm 0.1_6$	4.326	$4.1_1 \pm 0.2$
$C(E_{\pm 1/2})$	2281.58	2282.6	1.015	$1.1_6 \pm 0.3$	2.808	$2.8_2 \pm 0.9$
$D(E_{\pm 3/2})$	2398.50	2399.5	3.497	...	0.025	...

[a] $A_2^0\langle r^2\rangle = +64.3$ cm^{-1}, $A_4^0\langle r^4\rangle = -40.5$ cm^{-1}, $A_6^0\langle r^6\rangle = -65.0$ cm^{-1}, $A_6^6\langle r^6\rangle = \pm 399.7$ cm^{-1}, $\zeta = 626.8$ cm^{-1}.

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

g-Values
-------------------------------------------------------------------------------------------------------------
 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
-------------------------------------------------------------------------------------------------------------
```

Notes:

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

2. The Γ_{11}, Γ_{12} Kramers doublets (labelled $E_{\pm 3/2}$ in the paper) have $g_{\perp} = 0$ by symmetry and $g_{\parallel} = J$.

Pr(III)/$LaCl_3$

[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	$^3H_4$	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	$^3H_5$	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

g-Values

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

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

Magnetic Dipole Transitions

kx=1.0000 ky=1.0000 kz=1.0000

Energy(deg.)	deltaE	<Mx>		<My>/i		<Mz>	
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
-------------------------------------------------------------------------------------------------
              total CPU time:    0.11 secs
-------------------------------------------------------------------------------------------------
```

Notes:

1. Non Kramers ion. The g-values only calculated for degenerate pairs as if they are S=1/2 doublets. The Γ_2, Γ_3 and Γ_5, Γ_6 pairs (labelled E’ and E’’ in ref [2]) have to have $g_\perp = 0$ by symmetry.