Supplementary Materials for *Finite-Field Calculations of Transition Properties by the Fock Space Relativistic Coupled Cluster Method: Transitions between Different Fock Space Sectors*

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Table 1: FS RCC excitation energy ΔE and finite-field estimate of transition dipole moment D^{FF}_{X-B} for the $X0^+_g - B0^+_u$ transition in I_2 as functions of the internuclear separation R.

R, a.u.	ΔE, cm^{-1}	$\lvert D^{\mathrm{FF}}_{X-B}\rvert$, a.u.
4.450	27 962	0.2943
4.600	25 325	0.3120
4.850	21 411	0.3455
5.034	18 934	0.3719
5.250	16 462	0.4028
5.480	14 328	0.4328
5.715	12 644	0.4554
5.950	11 427	0.4627
6.200	10 603	0.4428
6.450	10 217	0.3824

Table 2: FS RCC excitation energy ΔE and finite-field estimate of transition dipole moment $D^{\rm FF}_{X-B}$ for the $X0^+ - B1$ transition in TlF as functions of the internuclear separation R.

R, a.u.	ΔE, cm^{-1}	$\lvert D^{\rm FF}_{X-B}\rvert$, a.u.
3.2006319	32 447	0.3057
3.3506319	34 013	0.2998
3.5556319	35 586	0.2962
3.7806319	36 629	0.2962
3.9306319	36 936	0.2967
4.0806319	36 919	0.2957
4.2506319	36 491	0.2901
4.4506319	35 435	0.2734
4.5506319	34 705	0.2604
4.7306319	33 124	0.2312
4.8506319	31 935	0.2096
5.0006319	30 362	0.1825

Table 3: Contracted Gaussian basis set for xenon. The DIRAC mol format is assumed

```
# s functions
F  11   2
   71.92137   0.0034852929    0.0014694470
   38.14097  -0.0099360414   -0.0038630017
   12.04919   0.6908335000    0.3730172368
    9.26456  -1.0824656657   -0.6916452826
    5.80173  -0.7120418275   -0.0335479143
    4.46287   0.7234964245    0.1698775686
    1.95239   0.9338491268    0.7058952035
    0.98282   0.2431078161    0.2496623023
    0.42332   0.0082483974   -0.6112798178
    0.19740  -0.0003125896   -0.6177426204
    0.09002   0.0003325679   -0.1318423562
F 10   0
      0.8606790
      0.4422460
      0.2081820
      0.0948280
          0.0368000
              0.017
              0.008
              0.004
      2.44490
      1.53520
# p functions
F  11   4
 100.58730    0.0000360921 -0.0010870678 -0.0000477194  0.0004160233
  45.15077   -0.0028302412 -0.0030147747 -0.0008403590  0.0006742758
  11.74875    0.0252946899 -0.2788579681 -0.0016159708  0.1162355977
   7.33945   -0.8686533994 -1.3986132151 -0.3234185450  0.3351961851
   6.06118    0.8293467851  2.5538164490  0.3402510936 -0.7414807462
   2.42472    0.6657825526  0.2084334024  0.3129952930 -0.2198344846
   1.21256    0.2817594987 -0.9385645182  0.1190338707  0.5188889383
   0.55607    0.0324287200 -0.1681367805 -0.3295838493  0.6504444639
   0.26305   -0.0026083565 -0.0208745590 -0.5073393413  0.0769000055
   0.12254    0.0016880153  0.0069196619 -0.3105302267 -0.5280823544
   0.05611   -0.0004449089 -0.0023993471 -0.0526849061 -0.3493910025
F  9   0
      0.3873040
      0.1715660
      0.0726410
          0.0288000
             0.014
             0.008
             0.004
      5.3238
      1.6251
# d functions
F  7   2
  69.10128     -0.0015119309    0.0109174617
  17.97744     -0.0113555518   -0.0380131427
  4.55014       0.2995543540   -1.0449679992
  2.29422       0.4446057944    0.3548691891
  1.14945       0.3077648884    0.2731100919
  0.54294       0.0886806138    0.4711265656
  0.19872       0.0064656205    0.0060618352
F  9   0
      0.6818480
      0.3807270
      0.1676000
          0.0639000
              0.032
              0.016
              0.008
      2.52010
      1.25480
# f
F  6   0
      0.6619000
      0.2979000
           0.1591000
           0.08
      5.61580
      1.61480
# g
F  3   0
      0.5278000
           0.2659000
      1.75300
```

Table 4: Gaussian basis set for mercury

```
# s functions
F  11  0
    19.3627
    13.0438
    10.0337
     5.95836
     1.74538
     0.96492
     0.49186
     0.21148
     0.091381
     0.039661
     0.01720
# p functions
F  11  0
    24.4363
    6.98179
    5.37060
    2.07047
    1.02149
    0.55188
    0.29270
    0.13049
    0.058613
    0.026097
    0.01160
#  d functions
F  10  0
    28.2740
    10.3059
    5.45000
    1.98137
    1.13496
    0.66097
    0.34888
    0.17706
    0.084258
    0.040100
#  f functions
F  5  0
    2.7709000
    1.6429000
    0.9741000
    0.3804000
    0.1486000
#  g functions
F  4  0
    3.2698000
    1.7219000
    0.7880000
    0.3606000
#  h functions
F  3  0
    1.3867000
    2.9400000
    0.6541000
```

Table 5: Contracted Gaussian basis set for iodine.

```
# s functions
F   9   1
 9.7839     0.1899779986
 6.9885    -1.6697136592
 4.9918     3.5664149367
 3.5656    -1.7757676150
 1.1606    -0.9777005679
 0.46635   -0.1356045830
 0.22952    0.0106290721
 0.10407   -0.0032042468
 .046125    0.0006225541
F   8   0
      5.539400
      2.454400
      1.087500
      0.466351
      0.229518
      0.104071
      0.046125
      0.01590
# p functions
F  10   2
 17.692   0.0008106277  0.0478444798
 6.3639   0.1116635250 -1.1341938008
 4.5457  -0.7851176421  0.6273377817
 3.2466   0.6761442601  1.4497047807
 1.3023   0.6719126924 -0.1583229394
 0.59801  0.2537263196 -0.7311502651
 0.30034  0.0200826776 -0.0917643372
 0.12978  0.0052868709 -0.0286357178
 .056435 -0.0015174829  0.0096151438
 .024493  0.0004462145 -0.0029226262
F   8   0
      2.7136
      1.3733
      0.6950
      0.300337
      0.129777
      0.056435
      0.024493
      0.0081000
# d functions
F   8   1
    12.005   0.0133774167
    3.7743   0.0635548761
    2.1181  -0.3391740075
    1.0043  -0.4366994855
    0.48733 -0.2958548464
    0.27632 -0.0989526264
    0.15227 -0.0446435566
    0.0677   0.0006426983
F   7   0
      0.276316
      0.152266
      0.06770
      2.9853
      1.3985
      0.6552
      0.0237000
# f functions
F   6   0
      0.42630
      0.16900
      2.75470
      1.59280
      0.92090
      0.06050
# g functions
F   4   0
     0.369
     3.0293
     0.9881
     0.1527
# h functions
F   1   0
   0.9331
```

Table 6: Contracted Gaussian basis set for thallium

```
# s functions
F  11  7
 30.34208        -0.0785616310 -0.0204548645 0. 0. 0. 0. 0.
 22.48117         0.2588283520  0.0654936632 0. 0. 0. 0. 0.
 14.35141        -0.6564469355 -0.2106304360 0. 0. 0. 0. 0.
  8.57320         1.0792272610  0.4378488048 0. 0. 0. 0. 0.
  2.44543        -0.7189360393 -0.4207039365 0. 0. 0. 0. 0.
      1.351130   -0.6047779298 -0.5102631566 0. 0. 0. 0. 0.
      0.616379   -0.0916005612 -0.1083919333 1. 0. 0. 0. 0.
      0.383455    0.0127531977  0.6020195562 0. 1. 0. 0. 0.
      0.180056   -0.0026686298  0.6138122015 0. 0. 1. 0. 0.
      0.082327    0.0002423606  0.1527413060 0. 0. 0. 1. 0.
      0.003310    0.            0.           0. 0. 0. 0. 1.
F   2  0
   2.1767
   1.3661
# p functions
F  11  8
 19.95984    0.0388055942  0.0293122681 0. 0. 0. 0. 0. -0.0107426327
 14.93694   -0.0777775535  0.0777178718 0. 0. 0. 0. 0.  0.0192802860
 7.09087     0.7449659048  1.5920865182 0. 0. 0. 0. 0. -0.2673280324
 5.64870    -0.6635868223 -2.6803153566 0. 0. 0. 0. 0.  0.2608922666
 2.48653    -0.4525199216 -0.1043694459 0. 0. 0. 0. 0.  0.1822354434
   1.559500 -0.4030574169  0.4512311292 0. 0. 0. 0. 0.  0.2045896133
   0.768911 -0.1518143723  0.5975092409 1. 0. 0. 0. 0. -0.0313428471
   0.354814  0.0024244588 -0.0065797555 0. 1. 0. 0. 0. -0.4564330636
   0.154766 -0.0048656975  0.0272655439 0. 0. 1. 0. 0. -0.4999069824
   0.064699  0.0007830146 -0.0047101797 0. 0. 0. 1. 0. -0.1764351481
   0.025700  0.            0.           0. 0. 0. 0. 1.  0.
F   2  0
   4.9530
   1.4243
# d functions
F 10  6
  78.66904     -0.0009266998 0. 0. 0. 0. -0.0000487618
  23.08570     -0.0065713369 0. 0. 0. 0. -0.0352448519
  8.60547      -0.0077922017 0. 0. 0. 0.  0.1649754719
  4.14773       0.3176181736 0. 0. 0. 0.  0.8441294318
      1.984230  0.4446719129 0. 0. 0. 0. -0.2433315819
      1.152540  0.2066244692 0. 0. 0. 0. -0.0990735880
      0.651017  0.1617018631 1. 0. 0. 0. -0.5573463082
      0.347445  0.0190297144 0. 1. 0. 0. -0.0666618792
      0.154700  0.0063299664 0. 0. 1. 0. -0.0439588014
      0.064     0.           0. 0. 0. 1.  0.
F   2   0
        2.2773
        1.1010
# f functions
F   5   0
        4.8671
        1.3925
      0.58650
      0.24940
      0.12700
# g functions
F   3   0
        1.5444
      0.4730
      0.2338
```