Electronic supplementary material: Coupled-cluster calculations of the lowest 0–0 bands of the electronic excitation spectrum of naphthalene †

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1 Molecular structures

Carthesian coordinates in Å for optimized napthalene ground state structures on DFT, MP2 and CC2 levels of theory as well as optimized excited state structures. Ground state as well as excited state energies are reported in Hartree. If not otherwise stated the same basis set has been chosen as auxiliary basis for the CC2 calculations. In case the auxiliary basis differs from the orbital basis this is stated in parenthesis. We also include the optimized B3LYP/DZ(d) structure taken from Hsu and co-worker[1].

1.1 Ground state structure of Ref.[1]

```
Energy = -385.917487967
  C          -1.247231   -1.408472    0.000000
  C          -2.442246   -0.711801    0.000000
  C          -2.442246    0.711801    0.000000
  C          -1.247231    1.408472    0.000000
  C           0.000000    0.717709    0.000000
  C           0.000000   -0.717709    0.000000
  C           1.247231   -1.408472    0.000000
  C           2.442246   -0.711801    0.000000
  C           2.442246    0.711801    0.000000
  C           1.247231    1.408472    0.000000
  H          -1.245160   -2.498925    0.000000
  H          -3.389646   -1.249013    0.000000
  H          -3.389646    1.249013    0.000000
  H          -1.245160    2.498925    0.000000
  H           1.245160   -2.498925    0.000000
  H           3.389646   -1.249013    0.000000
  H           3.389646    1.249013    0.000000
  H           1.245160    2.498925    0.000000
```

1.2 Ground state structure B3LYP/def2-TZVP

```
Energy = -385.7826748712
C    -1.2412362   -1.3975273    0.0000000
C    -2.4250759   -0.7061111    0.0000000
C    -2.4250759    0.7061111    0.0000000
C    -1.2412362    1.3975273    0.0000000
C     0.0000000    0.7142865    0.0000000
C     0.0000000   -0.7142865    0.0000000
C     1.2412362   -1.3975273    0.0000000
C     2.4250759   -0.7061111    0.0000000
C     2.4250759    0.7061111    0.0000000
C     1.2412362    1.3975273    0.0000000
H    -1.2400201   -2.4816135    0.0000000
H    -3.3667265   -1.2412553    0.0000000
```

```
H    -3.3667265    1.2412553    0.0000000
H    -1.2400201    2.4816135    0.0000000
H     1.2400201   -2.4816135    0.0000000
H     3.3667265   -1.2412553    0.0000000
H     3.3667265    1.2412553    0.0000000
H     1.2400201    2.4816135    0.0000000
```

1.3 Ground state structure B3LYP/def2-TZVPD

```
Energy = -385.7838304174
C    -1.2412860   -1.3977487    0.0000000
C    -2.4252618   -0.7061860    0.0000000
C    -2.4252618    0.7061860    0.0000000
C    -1.2412860    1.3977487    0.0000000
C     0.0000000    0.7143598    0.0000000
C     0.0000000   -0.7143598    0.0000000
C     1.2412860   -1.3977487    0.0000000
C     2.4252618   -0.7061860    0.0000000
C     2.4252618    0.7061860    0.0000000
C     1.2412860    1.3977487    0.0000000
H    -1.2401847   -2.4818446    0.0000000
H    -3.3669082   -1.2413591    0.0000000
H    -3.3669082    1.2413591    0.0000000
H    -1.2401847    2.4818446    0.0000000
H     1.2401847   -2.4818446    0.0000000
H     3.3669082   -1.2413591    0.0000000
H     3.3669082    1.2413591    0.0000000
H     1.2401847    2.4818446    0.0000000
```

1.4 Ground state structure MP2/def2-TZVP

```
Energy = -385.0272329528
C    -1.2375270   -1.4008570    0.0000000
C    -2.4261154   -0.7055511    0.0000000
C    -2.4261154    0.7055511    0.0000000
C    -1.2375270    1.4008570    0.0000000
C     0.0000000    0.7150300    0.0000000
C     0.0000000   -0.7150300    0.0000000
C     1.2375270   -1.4008570    0.0000000
C     2.4261154   -0.7055511    0.0000000
C     2.4261154    0.7055511    0.0000000
C     1.2375270    1.4008570    0.0000000
H    -1.2351665   -2.4867626    0.0000000
H    -3.3678721   -1.2430708    0.0000000
H    -3.3678721    1.2430708    0.0000000
```

```
H    -1.2351665    2.4867626    0.0000000
H     1.2351665   -2.4867626    0.0000000
H     3.3678721   -1.2430708    0.0000000
H     3.3678721    1.2430708    0.0000000
H     1.2351665    2.4867626    0.0000000
```

1.5 Ground state structure CC2/def2-TZVPP

```
Energy = -385.0673060768
C    -1.2390077   -1.4024612    0.0000000
C    -2.4294803   -0.7065321    0.0000000
C    -2.4294803    0.7065321    0.0000000
C    -1.2390077    1.4024612    0.0000000
C     0.0000000    0.7154550    0.0000000
C     0.0000000   -0.7154550    0.0000000
C     1.2390077   -1.4024612    0.0000000
C     2.4294803   -0.7065321    0.0000000
C     2.4294803    0.7065321    0.0000000
C     1.2390077    1.4024612    0.0000000
H    -1.2356612   -2.4863195    0.0000000
H    -3.3693917   -1.2429786    0.0000000
H    -3.3693917    1.2429786    0.0000000
H    -1.2356612    2.4863195    0.0000000
H     1.2356612   -2.4863195    0.0000000
H     3.3693917   -1.2429786    0.0000000
H     3.3693917    1.2429786    0.0000000
H     1.2356612    2.4863195    0.0000000
```

1.6 Ground state structure CC2/def2-SVP

```
Energy = -384.3791473545
C    -1.2456737   -1.4083699    0.0000000
C    -2.4420002   -0.7097061    0.0000000
C    -2.4420002    0.7097061    0.0000000
C    -1.2456737    1.4083699    0.0000000
C     0.0000000    0.7185354    0.0000000
C     0.0000000   -0.7185354    0.0000000
C     1.2456737   -1.4083699    0.0000000
C     2.4420002   -0.7097061    0.0000000
C     2.4420002    0.7097061    0.0000000
C     1.2456737    1.4083699    0.0000000
H    -1.2434585   -2.5029287    0.0000000
H    -3.3913882   -1.2519669    0.0000000
H    -3.3913882    1.2519669    0.0000000
H    -1.2434585    2.5029287    0.0000000
```

```
H     1.2434585   -2.5029287    0.0000000
H     3.3913882   -1.2519669    0.0000000
H     3.3913882    1.2519669    0.0000000
H     1.2434585    2.5029287    0.0000000
```

1.7 Ground state structure CC2/def2-TZVPD(aug-cc-pVTZ)

```
Energy = -385.0515052229
C    -1.2389935   -1.4027978    0.0000000
C    -2.4296752   -0.7066357    0.0000000
C    -2.4296752    0.7066357    0.0000000
C    -1.2389935    1.4027978    0.0000000
C    -0.0000000    0.7156205    0.0000000
C    -0.0000000   -0.7156205    0.0000000
C     1.2389935   -1.4027978    0.0000000
C     2.4296752   -0.7066357    0.0000000
C     2.4296752    0.7066357    0.0000000
C     1.2389935    1.4027978    0.0000000
H    -1.2362889   -2.4899155    0.0000000
H    -3.3726183   -1.2442615    0.0000000
H    -3.3726183    1.2442615    0.0000000
H    -1.2362889    2.4899155    0.0000000
H     1.2362889   -2.4899155    0.0000000
H     3.3726183   -1.2442615    0.0000000
H     3.3726183    1.2442615    0.0000000
H     1.2362889    2.4899155    0.0000000
```

1.8 1 B_{3u} excited state structure B3LYP/def2-TZVPD

```
Energy = -385.6242121395
C    -1.2402717   -1.4114076    0.0000000
C    -2.4486868   -0.7112128    0.0000000
C    -2.4486868    0.7112128    0.0000000
C    -1.2402717    1.4114076    0.0000000
C     0.0000000    0.7416677    0.0000000
C     0.0000000   -0.7416677    0.0000000
C     1.2402717   -1.4114076    0.0000000
C     2.4486868   -0.7112128    0.0000000
C     2.4486868    0.7112128    0.0000000
C     1.2402717    1.4114076    0.0000000
H    -1.2471339   -2.4951781    0.0000000
H    -3.3865225   -1.2501444    0.0000000
H    -3.3865225    1.2501444    0.0000000
H    -1.2471339    2.4951781    0.0000000
H     1.2471339   -2.4951781    0.0000000
```

```
H     3.3865225   -1.2501444    0.0000000
H     3.3865225    1.2501444    0.0000000
H     1.2471339    2.4951781    0.0000000
```

1.9 1 B_{2u} excited state structure B3LYP/def2-TZVPD

```
Energy = -385.6343980436
C    -1.2383875   -1.3924007    0.0000000
C    -2.4765643   -0.6860959    0.0000000
C    -2.4765643    0.6860959    0.0000000
C    -1.2383875    1.3924007    0.0000000
C     0.0000000    0.7175729    0.0000000
C     0.0000000   -0.7175729    0.0000000
C     1.2383875   -1.3924007    0.0000000
C     2.4765643   -0.6860959    0.0000000
C     2.4765643    0.6860959    0.0000000
C     1.2383875    1.3924007    0.0000000
H    -1.2450046   -2.4760163    0.0000000
H    -3.4060617   -1.2403012    0.0000000
H    -3.4060617    1.2403012    0.0000000
H    -1.2450046    2.4760163    0.0000000
H     1.2450046   -2.4760163    0.0000000
H     3.4060617   -1.2403012    0.0000000
H     3.4060617    1.2403012    0.0000000
H     1.2450046    2.4760163    0.0000000
```

1.10 1 B_{3u} excited state structure CC2/def2-TZVPP

```
Energy = -384.9101433163
C    -1.2386852   -1.4186039    0.0000000
C    -2.4562395   -0.7119769    0.0000000
C    -2.4562395    0.7119769    0.0000000
C    -1.2386852    1.4186039    0.0000000
C     0.0000000    0.7458163    0.0000000
C     0.0000000   -0.7458163    0.0000000
C     1.2386852   -1.4186039    0.0000000
C     2.4562395   -0.7119769    0.0000000
C     2.4562395    0.7119769    0.0000000
C     1.2386852    1.4186039    0.0000000
H    -1.2426973   -2.5025931    0.0000000
H    -3.3931645   -1.2519186    0.0000000
H    -3.3931645    1.2519186    0.0000000
H    -1.2426973    2.5025931    0.0000000
H     1.2426973   -2.5025931    0.0000000
H     3.3931645   -1.2519186    0.0000000
```

```
H     3.3931645    1.2519186    0.0000000
H     1.2426973    2.5025931    0.0000000
```

1.11 1 B_{2u} excited state structure CC2/def2-TZVPP

```
Energy = -384.9014973736
C    -1.2361378   -1.3954537    0.0000000
C    -2.4805709   -0.6872395    0.0000000
C    -2.4805709    0.6872395    0.0000000
C    -1.2361378    1.3954537    0.0000000
C     0.0000000    0.7218101    0.0000000
C     0.0000000   -0.7218101    0.0000000
C     1.2361378   -1.3954537    0.0000000
C     2.4805709   -0.6872395    0.0000000
C     2.4805709    0.6872395    0.0000000
C     1.2361378    1.3954537    0.0000000
H    -1.2383585   -2.4801346    0.0000000
H    -3.4088500   -1.2427880    0.0000000
H    -3.4088500    1.2427880    0.0000000
H    -1.2383585    2.4801346    0.0000000
H     1.2383585   -2.4801346    0.0000000
H     3.4088500   -1.2427880    0.0000000
H     3.4088500    1.2427880    0.0000000
H     1.2383585    2.4801346    0.0000000
```

1.12 1 B_{3u} excited state structure B3LYP/def2-TZVP

```
Energy = -385.6226331061
C    -1.2403431   -1.4112699    0.0000000
C    -2.4485892   -0.7111560    0.0000000
C    -2.4485892    0.7111560    0.0000000
C    -1.2403431    1.4112699    0.0000000
C     0.0000000    0.7417344    0.0000000
C     0.0000000   -0.7417344    0.0000000
C     1.2403431   -1.4112699    0.0000000
C     2.4485892   -0.7111560    0.0000000
C     2.4485892    0.7111560    0.0000000
C     1.2403431    1.4112699    0.0000000
H    -1.2469534   -2.4950286    0.0000000
H    -3.3863920   -1.2500350    0.0000000
H    -3.3863920    1.2500350    0.0000000
H    -1.2469534    2.4950286    0.0000000
H     1.2469534   -2.4950286    0.0000000
H     3.3863920   -1.2500350    0.0000000
H     3.3863920    1.2500350    0.0000000
```

```
H     1.2469534    2.4950286    0.0000000
```

1.13 1 B_{2u} excited state structure B3LYP/def2-TZVP

```
Energy = -385.6327098617
C    -1.2383258   -1.3922335    0.0000000
C    -2.4765690   -0.6859082    0.0000000
C    -2.4765690    0.6859082    0.0000000
C    -1.2383258    1.3922335    0.0000000
C    -0.0000000    0.7175940    0.0000000
C    -0.0000000   -0.7175940    0.0000000
C     1.2383258   -1.3922335    0.0000000
C     2.4765690   -0.6859082    0.0000000
C     2.4765690    0.6859082    0.0000000
C     1.2383258    1.3922335    0.0000000
H    -1.2449504   -2.4758007    0.0000000
H    -3.4056740   -1.2407292    0.0000000
H    -3.4056740    1.2407292    0.0000000
H    -1.2449504    2.4758007    0.0000000
H     1.2449504   -2.4758007    0.0000000
H     3.4056740   -1.2407292    0.0000000
H     3.4056740    1.2407292    0.0000000
H     1.2449504    2.4758007    0.0000000
```

1.14 1 B_{3u} excited state structure CC2/def2-SVP

```
Energy = -384.2204359259
C    -1.2454768   -1.4249563    0.0000000
C    -2.4684827   -0.7146481    0.0000000
C    -2.4684827    0.7146481    0.0000000
C    -1.2454768    1.4249563    0.0000000
C     0.0000000    0.7499663    0.0000000
C     0.0000000   -0.7499663    0.0000000
C     1.2454768   -1.4249563    0.0000000
C     2.4684827   -0.7146481    0.0000000
C     2.4684827    0.7146481    0.0000000
C     1.2454768    1.4249563    0.0000000
H    -1.2511054   -2.5196803    0.0000000
H    -3.4151299   -1.2603716    0.0000000
H    -3.4151299    1.2603716    0.0000000
H    -1.2511054    2.5196803    0.0000000
H     1.2511054   -2.5196803    0.0000000
H     3.4151299   -1.2603716    0.0000000
H     3.4151299    1.2603716    0.0000000
H     1.2511054    2.5196803    0.0000000
```

1.15 1 B_{2u} excited state structure CC2/def2-SVP

```
Energy = -384.2057031845
C    -1.4026476    0.0062194   -1.2423695
C    -0.6909972   -0.0048996   -2.4902105
C     0.6909973    0.0048907   -2.4902103
C     1.4026475   -0.0062083   -1.2423690
C     0.7265565    0.0111912    0.0000001
C    -0.7265571   -0.0111697    0.0000001
C    -1.4026478    0.0062281    1.2423694
C    -0.6909973   -0.0048806    2.4902105
C     0.6909975    0.0048719    2.4902104
C     1.4026477   -0.0062176    1.2423690
H    -2.4980466    0.0039721   -1.2458297
H    -1.2521515   -0.0015301   -3.4283027
H     1.2521518    0.0015089   -3.4283023
H     2.4980465   -0.0039631   -1.2458289
H    -2.4980468    0.0039768    1.2458296
H    -1.2521514   -0.0014505    3.4283026
H     1.2521518    0.0014303    3.4283023
H     2.4980466   -0.0039701    1.2458289
```

1.16 1 B_{3u} excited state structure CC2/def2-TZVPD(aug-cc-pVTZ)

```
Energy = -384.8948117227
C    -1.2385002   -1.4186802   -0.0208853
C    -2.4563072   -0.7120193   -0.0110622
C    -2.4563069    0.7120192    0.0110576
C    -1.2385007    1.4186807    0.0208780
C     0.0000001    0.7457601    0.0000196
C    -0.0000001   -0.7457597    0.0000228
C     1.2385004   -1.4186807    0.0208902
C     2.4563073   -0.7120197    0.0110637
C     2.4563070    0.7120193   -0.0110470
C     1.2385006    1.4186803   -0.0208777
H    -1.2433420   -2.5058976   -0.0327426
H    -3.3962812   -1.2530949   -0.0216119
H    -3.3962810    1.2530945    0.0216268
H    -1.2433435    2.5058989    0.0326629
H     1.2433423   -2.5058986    0.0327003
H     3.3962813   -1.2530954    0.0216121
H     3.3962810    1.2530954   -0.0215810
H     1.2433428    2.5058978   -0.0327263
```

1.17 1 B_{2u} excited state structure CC2/def2-TZVPD(aug-cc-pVTZ)

```
Energy = -384.8866718547
C    -1.2361213   -1.3956161    0.0166117
C    -2.4807642   -0.6874120    0.0072095
C    -2.4807584    0.6874062   -0.0072148
C    -1.2361172    1.3956144   -0.0166015
C     0.0000023    0.7218022    0.0000075
C    -0.0000021   -0.7218019    0.0000233
C     1.2361170   -1.3956145   -0.0165990
C     2.4807583   -0.6874064   -0.0072080
C     2.4807643    0.6874118    0.0072086
C     1.2361216    1.3956165    0.0166015
H    -1.2392064   -2.4835113    0.0322930
H    -3.4120720   -1.2441077    0.0159570
H    -3.4120646    1.2441047   -0.0159677
H    -1.2392043    2.4835095   -0.0322919
H     1.2392037   -2.4835090   -0.0323261
H     3.4120644   -1.2441054   -0.0159415
H     3.4120722    1.2441075    0.0159487
H     1.2392067    2.4835115    0.0322898
```

2 Vibrational frequencies

Harmonic frequencies and zero point vibrational energies ZPVE (in Hartree) for the investigated molecular structures of napthalene. If not stated otherwise the geometry has been optimized on the same level of theory.

2.1 B3LYP/def2-TZVP frequencies for the optimized ground state structure

```
ZPVE = 0.1468154
#  mode     symmetry     wave number   IR intensity
#                         cm**(-1)        km/mol
     1                        0.00         0.00000
     2                        0.00         0.00000
     3                        0.00         0.00000
     4                        0.00         0.00000
     5                        0.00         0.00000
     6                        0.00         0.00000
     7        b1u           172.84         2.61692
     8        au            186.49         0.00000
     9        b2u           365.76         1.42941
    10        b2g           396.07         0.00000
    11        b3g           480.91         0.00000
    12        b1u           488.29        22.92877
```

13	b1g	518.66	0.00000
14	ag	520.26	0.00000
15	au	631.95	0.00000
16	b3u	636.20	3.30337
17	b2g	728.26	0.00000
18	ag	774.45	0.00000
19	b3g	787.79	0.00000
20	b1u	799.23	116.89782
21	b2u	810.01	0.21123
22	au	847.24	0.00000
23	b3g	900.64	0.00000
24	b2g	945.20	0.00000
25	b1g	953.85	0.00000
26	b1u	961.12	2.58959
27	au	966.65	0.00000
28	b3g	972.49	0.00000
29	b3u	1036.09	7.81452
30	ag	1046.47	0.00000
31	b2u	1152.68	4.70504
32	b3u	1169.92	0.76968
33	b1g	1172.81	0.00000
34	ag	1186.35	0.00000
35	b3u	1232.77	0.70753
36	b1g	1273.23	0.00000
37	b2u	1289.81	6.62459
38	b3u	1391.65	0.74730
39	ag	1395.89	0.00000
40	b2u	1422.75	4.30303
41	b1g	1493.76	0.00000
42	ag	1494.80	0.00000
43	b3u	1549.28	8.59546
44	ag	1612.22	0.00000
45	b2u	1640.12	3.83986
46	b1g	1667.73	0.00000
47	b1g	3157.40	0.00000
48	b2u	3159.18	5.51435
49	b3u	3161.35	0.72805
50	ag	3164.70	0.00000
51	b1g	3175.41	0.00000
52	b2u	3176.61	51.95513
53	b3u	3188.12	38.42347
54	ag	3189.06	0.00000

2.2 MP2/def2-TZVP frequencies for the optimized ground state structure

ZPVE = 0.1549321

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	au	220.75	0.00000
8	b1u	235.86	2.89398
9	b2u	406.38	2.16221
10	b2g	461.99	0.00000
11	b3g	544.23	0.00000
12	ag	547.33	0.00000
13	b1g	551.04	0.00000
14	b1u	557.55	20.83089
15	b3u	671.17	4.26894
16	au	693.27	0.00000
17	ag	811.90	0.00000
18	b2u	855.01	2.10513
19	b2g	858.63	0.00000
20	b3g	861.10	0.00000
21	b1u	921.57	147.55860
22	au	978.36	0.00000
23	b3g	1019.95	0.00000
24	b1g	1020.07	0.00000
25	b3u	1038.74	1.54568
26	b2g	1094.72	0.00000
27	ag	1105.09	0.00000
28	b3u	1110.36	4.43512
29	b1u	1111.66	3.22295
30	au	1113.77	0.00000
31	b3g	1117.84	0.00000
32	b2u	1224.77	3.34018
33	b1g	1240.58	0.00000
34	ag	1279.82	0.00000
35	b3u	1305.67	0.31378
36	b1g	1369.92	0.00000
37	b2u	1380.35	5.64191
38	ag	1400.00	0.00000
39	b3u	1417.02	1.33583
40	b2u	1541.19	3.61459

41	b1g	1599.00	0.00000
42	ag	1611.26	0.00000
43	b3u	1668.62	13.63637
44	ag	1710.85	0.00000
45	b2u	1723.94	8.37673
46	b1g	1782.79	0.00000
47	b1g	3213.29	0.00000
48	b2u	3216.60	4.16077
49	b3u	3217.16	0.56059
50	ag	3223.23	0.00000
51	b1g	3234.44	0.00000
52	b2u	3236.55	61.33126
53	b3u	3250.37	50.91482
54	ag	3251.52	0.00000

2.3 CC2/def2-TZVPP frequencies for the optimized ground state structure

ZPVE = 0.1461732

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	b1u	191.54	2.38162
8	au	199.84	0.00000
9	b2u	355.82	1.18511
10	b2g	394.84	0.00000
11	b3g	469.42	0.00000
12	b1u	490.85	18.11094
13	b1g	504.85	0.00000
14	ag	511.83	0.00000
15	au	559.88	0.00000
16	b3g	598.75	0.00000
17	b3u	616.56	3.21156
18	b2g	742.62	0.00000
19	ag	766.34	0.00000
20	b2u	798.08	0.09363
21	b1u	799.06	121.67162
22	au	840.82	0.00000
23	b3g	857.26	0.00000
24	au	918.62	0.00000
25	b2g	927.03	0.00000

26	b1g	934.54	0.00000
27	b1u	935.88	1.06602
28	b3g	938.68	0.00000
29	b3u	1034.50	6.51887
30	ag	1043.55	0.00000
31	b2u	1136.51	3.55090
32	b1g	1162.50	0.00000
33	ag	1176.83	0.00000
34	b3u	1178.29	0.23844
35	b3u	1250.23	1.45641
36	b1g	1257.67	0.00000
37	b2u	1279.10	7.67442
38	b2u	1405.95	5.04589
39	ag	1434.90	0.00000
40	b3u	1453.70	0.74477
41	b1g	1475.65	0.00000
42	ag	1480.39	0.00000
43	b3u	1544.26	8.23131
44	ag	1599.09	0.00000
45	b2u	1613.78	3.42365
46	b1g	1659.26	0.00000
47	b2u	3187.72	12.00219
48	b1g	3188.38	0.00000
49	b3u	3192.11	0.01363
50	ag	3193.13	0.00000
51	b2u	3208.08	33.63404
52	b1g	3208.86	0.00000
53	b3u	3222.14	28.64854
54	ag	3222.91	0.00000

2.4 CC2/def2-SVP frequencies for the optimized ground state structure

ZPVE = 0.1462850

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	b1u	172.66	2.25841
8	au	180.85	0.00000
9	b2u	359.68	1.18074
10	b2g	367.76	0.00000

11	b3g	393.57	0.00000
12	b3g	439.31	0.00000
13	b1u	461.65	15.19744
14	au	490.54	0.00000
15	b1g	510.66	0.00000
16	ag	517.67	0.00000
17	b3u	625.71	3.31124
18	b2g	722.20	0.00000
19	ag	774.62	0.00000
20	b1u	780.16	101.90033
21	b2u	803.78	0.08179
22	au	832.37	0.00000
23	b3g	846.55	0.00000
24	b2g	932.83	0.00000
25	b1g	936.89	0.00000
26	b1u	939.44	0.49739
27	au	940.94	0.00000
28	b3g	956.55	0.00000
29	b3u	1043.13	5.11320
30	ag	1052.58	0.00000
31	b2u	1141.84	3.71491
32	b1g	1162.13	0.00000
33	b3u	1172.94	0.34924
34	ag	1173.53	0.00000
35	b3u	1255.52	2.69099
36	b1g	1261.64	0.00000
37	b2u	1282.46	7.92750
38	b2u	1412.32	6.46896
39	ag	1460.84	0.00000
40	b3u	1475.83	1.52838
41	b1g	1492.03	0.00000
42	ag	1493.14	0.00000
43	b3u	1568.13	6.94801
44	ag	1632.21	0.00000
45	b2u	1643.04	4.74104
46	b1g	1697.51	0.00000
47	b1g	3211.09	0.00000
48	b2u	3212.10	8.66540
49	b3u	3214.86	0.00353
50	ag	3216.63	0.00000
51	b1g	3231.27	0.00000
52	b2u	3231.60	35.39634
53	b3u	3243.17	30.96530
54	ag	3243.79	0.00000

2.5 CC2/def2-TZVPD(aug-cc-pVTZ) frequencies for the optimized ground state structure

ZPVE = 0.1447542

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	au	92.68	0.00000
8	b1u	175.37	2.41255
9	b2u	353.68	1.22005
10	b2g	380.44	0.00000
11	b3g	452.49	0.00000
12	au	475.28	0.00000
13	b1u	476.42	20.53579
14	b3g	486.21	0.00000
15	b1g	503.04	0.00000
16	ag	512.37	0.00000
17	b3u	616.12	3.04178
18	b2g	727.41	0.00000
19	ag	765.85	0.00000
20	b1u	794.50	116.87430
21	b2u	796.85	0.06633
22	au	814.89	0.00000
23	b3g	844.61	0.00000
24	b1g	931.78	0.00000
25	b2g	934.30	0.00000
26	au	938.47	0.00000
27	b1u	951.60	2.85401
28	b3g	959.89	0.00000
29	b3u	1032.19	7.23540
30	ag	1041.03	0.00000
31	b2u	1133.03	3.40803
32	b1g	1157.73	0.00000
33	b3u	1171.32	0.21369
34	ag	1171.77	0.00000
35	b3u	1244.99	1.07741
36	b1g	1246.01	0.00000
37	b2u	1273.49	7.31674
38	b2u	1394.60	5.29022
39	ag	1433.50	0.00000
40	b3u	1446.85	0.56910

41	b1g	1466.26	0.00000
42	ag	1474.38	0.00000
43	b3u	1539.40	7.57300
44	ag	1595.82	0.00000
45	b2u	1608.81	2.58081
46	b1g	1654.67	0.00000
47	b1g	3168.37	0.00000
48	b2u	3168.81	9.40667
49	b3u	3172.13	0.00000
50	ag	3173.53	0.00000
51	b1g	3189.99	0.00000
52	b2u	3190.07	32.66447
53	b3u	3203.09	28.70735
54	ag	3203.67	0.00000

2.6 1 B_{3u} excited state CC2/def2-TZVPP

ZPVE = 0.1409144

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	au	130.95	0.00000
8	b1u	171.00	2.45593
9	b2g	323.11	0.00000
10	b2u	350.73	0.12201
11	b3g	364.04	0.00000
12	b1u	395.80	14.11221
13	au	402.86	0.00000
14	b1g	404.20	0.00000
15	b3g	476.66	0.00000
16	ag	501.13	0.00000
17	b3u	586.20	2.50278
18	b2g	651.77	0.00000
19	b1u	664.74	120.23691
20	ag	708.79	0.00000
21	au	714.16	0.00000
22	b3g	744.34	0.00000
23	au	765.32	0.00000
24	b2u	771.22	0.54314
25	b3g	809.65	0.00000

26	b2g	813.61	0.00000
27	b1u	827.88	15.28212
28	b1g	900.50	0.00000
29	b3u	949.23	6.75027
30	ag	999.48	0.00000
31	b2u	1095.09	3.74823
32	b1g	1117.98	0.00000
33	b3u	1156.58	1.09743
34	ag	1160.21	0.00000
35	b3u	1231.83	3.75256
36	b2u	1243.23	2.95323
37	b1g	1247.37	0.00000
38	b2u	1385.51	0.63262
39	ag	1425.96	0.00000
40	b1g	1431.09	0.00000
41	ag	1464.12	0.00000
42	b3u	1465.13	7.05969
43	b2u	1487.08	5.63148
44	ag	1556.98	0.00000
45	b1g	1632.92	0.00000
46	b3u	1674.91	3.38364
47	b2u	3187.82	27.21538
48	b1g	3189.50	0.00000
49	b3u	3192.17	0.16591
50	ag	3192.24	0.00000
51	b1g	3213.42	0.00000
52	b2u	3215.15	16.55013
53	b3u	3229.14	23.57660
54	ag	3231.44	0.00000

2.7 1 B_{2u} excited state CC2/def2-TZVPP

ZPVE = 0.1426821

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	au	165.10	0.00000
8	b1u	186.01	2.28482
9	b2g	259.10	0.00000
10	b2u	341.68	4.45656

11	b3g	345.99	0.00000
12	b1u	369.12	7.11276
13	au	399.93	0.00000
14	b3g	479.18	0.00000
15	ag	497.32	0.00000
16	b3u	534.50	228.56820
17	au	645.07	0.00000
18	b1g	671.26	0.00000
19	b1u	705.99	141.57704
20	b2g	708.92	0.00000
21	ag	747.28	0.00000
22	b2u	774.31	7.35261
23	b3g	781.03	0.00000
24	b2g	796.16	0.00000
25	b1u	803.87	8.09310
26	au	861.46	0.00000
27	b3g	870.37	0.00000
28	b3u	1003.44	50.86038
29	b1g	1004.74	0.00000
30	ag	1047.94	0.00000
31	b2u	1072.80	1.41021
32	b1g	1130.32	0.00000
33	ag	1168.36	0.00000
34	b3u	1172.50	2.69213
35	b3u	1237.32	1.75995
36	b1g	1254.45	0.00000
37	b2u	1276.72	15.81732
38	b2u	1393.87	18.74775
39	b1g	1409.29	0.00000
40	ag	1450.45	0.00000
41	ag	1478.10	0.00000
42	b2u	1480.03	8.20089
43	b3u	1568.64	45.33410
44	b3u	1587.79	16.39472
45	ag	1620.02	0.00000
46	b1g	1678.16	0.00000
47	b2u	3182.08	28.23349
48	b3u	3186.50	28.94424
49	ag	3188.23	0.00000
50	b1g	3188.78	0.00000
51	b2u	3209.03	10.36476
52	b3u	3227.58	33.93089
53	ag	3228.40	0.00000
54	b1g	3241.00	0.00000

2.8 1 B_{3u} excited state B3LYP/def2-TZVP

ZPVE = 0.1425817

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	b1g	126.39	0.00000
8	b1u	162.28	1.26675
9	au	245.55	0.00000
10	b2g	293.19	0.00000
11	b2u	354.27	2.09914
12	b1u	444.91	6.17239
13	ag	503.23	0.00000
14	b3g	506.00	0.00000
15	au	522.03	0.00000
16	b3u	554.30	161.38315
17	ag	705.31	0.00000
18	b3g	761.22	0.00000
19	b1u	776.24	142.84687
20	b2g	776.29	0.00000
21	au	803.40	0.00000
22	b2u	812.84	7.16657
23	b1g	841.66	0.00000
24	b2g	885.62	0.00000
25	b3g	902.50	0.00000
26	b1u	905.63	16.89909
27	au	915.82	0.00000
28	b3g	918.42	0.00000
29	b3u	994.85	20.29189
30	ag	1007.22	0.00000
31	b1g	1072.25	0.00000
32	b2u	1113.55	2.63300
33	ag	1159.46	0.00000
34	b3u	1171.19	2.20611
35	b3u	1241.27	1.26612
36	b1g	1259.39	0.00000
37	b2u	1285.38	13.16884
38	ag	1336.97	0.00000
39	b2u	1411.01	9.91257
40	b3u	1419.32	26.90533

41	b1g	1420.79	0.00000
42	b1g	1456.73	0.00000
43	ag	1478.99	0.00000
44	ag	1508.63	0.00000
45	b3u	1534.70	32.15252
46	b2u	1548.21	3.70226
47	b2u	3162.13	75.00004
48	b1g	3162.86	0.00000
49	b3u	3168.40	62.63647
50	ag	3172.83	0.00000
51	b1g	3182.45	0.00000
52	b2u	3189.98	14.30860
53	b3u	3204.12	28.36776
54	ag	3206.36	0.00000

2.9 1 B_{2u} excited state B3LYP/def2-TZVP

ZPVE = 0.1448681

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	b1u	224.06	2.33190
8	au	249.38	0.00000
9	b2g	348.84	0.00000
10	b2u	358.65	1.02609
11	b1u	466.91	5.86630
12	b1g	482.63	0.00000
13	ag	505.86	0.00000
14	b3g	518.03	0.00000
15	au	552.48	0.00000
16	b3u	566.74	186.95292
17	ag	758.25	0.00000
18	b3g	766.00	0.00000
19	b2g	784.94	0.00000
20	b1u	785.40	141.42497
21	b2u	798.22	7.82879
22	au	816.27	0.00000
23	b2g	887.16	0.00000
24	b1u	907.05	15.98194
25	b3g	908.64	0.00000

26	b1g	922.58	0.00000
27	au	941.21	0.00000
28	b3g	942.31	0.00000
29	b3u	1010.14	38.97924
30	b1g	1044.69	0.00000
31	ag	1058.32	0.00000
32	b2u	1084.82	0.50304
33	ag	1180.14	0.00000
34	b3u	1180.25	0.99379
35	b3u	1232.53	0.80920
36	b1g	1255.18	0.00000
37	b2u	1289.21	12.33750
38	ag	1395.65	0.00000
39	b2u	1413.81	11.59906
40	b1g	1425.19	0.00000
41	b3u	1438.72	0.19360
42	ag	1483.10	0.00000
43	b2u	1489.83	5.18554
44	b1g	1493.13	0.00000
45	b3u	1575.11	46.30235
46	ag	1607.50	0.00000
47	b1g	3165.05	0.00000
48	b3u	3167.19	44.45418
49	b2u	3168.34	18.14337
50	ag	3172.01	0.00000
51	b1g	3182.29	0.00000
52	b2u	3184.22	26.18126
53	b3u	3199.56	33.49964
54	ag	3200.67	0.00000

2.10 1 B_{3u} excited state CC2/def2-SVP

ZPVE = 0.1411378

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	au	107.81	0.00000
8	b1u	162.66	2.34935
9	b3g	168.92	0.00000
10	b2g	302.70	0.00000

11	au	321.22	0.00000
12	b3g	346.15	0.00000
13	b2u	354.49	0.12876
14	b1u	365.96	10.91504
15	b1g	430.99	0.00000
16	ag	506.56	0.00000
17	b3u	595.85	2.15934
18	b2g	645.94	0.00000
19	b1u	661.93	107.86530
20	ag	716.38	0.00000
21	au	722.43	0.00000
22	b3g	752.16	0.00000
23	b2u	778.95	0.40773
24	au	793.54	0.00000
25	b2g	820.99	0.00000
26	b3g	827.66	0.00000
27	b1u	828.81	10.08560
28	b1g	907.76	0.00000
29	b3u	960.19	3.18418
30	ag	1011.01	0.00000
31	b2u	1103.38	3.48294
32	b1g	1122.33	0.00000
33	ag	1157.20	0.00000
34	b3u	1158.68	1.31890
35	b3u	1234.50	5.53518
36	b1g	1249.15	0.00000
37	b2u	1254.68	3.54942
38	b2u	1392.62	1.53933
39	ag	1431.79	0.00000
40	b1g	1444.91	0.00000
41	ag	1489.99	0.00000
42	b3u	1490.09	6.12481
43	b2u	1514.37	5.78924
44	ag	1596.07	0.00000
45	b1g	1673.97	0.00000
46	b3u	1722.87	5.97601
47	b1g	3211.29	0.00000
48	b2u	3213.48	19.90658
49	b3u	3213.78	0.14396
50	ag	3214.93	0.00000
51	b1g	3235.20	0.00000
52	b2u	3236.91	19.75810
53	b3u	3248.53	27.06586
54	ag	3250.57	0.00000

2.11 1 B_{2u} excited state CC2/def2-SVP

ZPVE = 0.1419189

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	a	116.94	0.06623
8	a	157.27	2.80351
9	a	227.06	0.00000
10	a	242.58	0.00000
11	a	336.44	5.33530
12	a	346.30	0.10844
13	a	346.55	5.07518
14	a	430.49	0.00000
15	a	504.65	0.00000
16	a	547.77	237.33520
17	a	576.49	0.00000
18	a	658.22	1.29854
19	a	672.26	123.64033
20	a	673.88	0.00070
21	a	754.61	0.00000
22	a	780.85	8.20042
23	a	781.18	0.00004
24	a	798.40	0.00000
25	a	800.73	8.19921
26	a	884.90	0.41900
27	a	890.22	0.00000
28	a	955.27	0.00000
29	a	1017.53	30.55041
30	a	1056.38	0.00000
31	a	1064.62	0.00000
32	a	1083.62	0.57785
33	a	1165.64	0.00001
34	a	1170.96	5.41036
35	a	1239.95	7.84317
36	a	1241.89	0.00000
37	a	1281.10	18.48643
38	a	1402.12	25.29914
39	a	1421.34	0.00000
40	a	1463.28	0.00000

41	a	1498.54	0.00000
42	a	1506.74	9.57249
43	a	1530.77	0.00000
44	a	1598.50	46.47640
45	a	1616.16	3.25079
46	a	1653.62	0.00000
47	a	3208.62	15.95990
48	a	3209.05	0.00000
49	a	3209.11	25.35292
50	a	3211.86	0.00000
51	a	3230.49	12.12304
52	a	3235.91	0.00000
53	a	3246.82	45.84585
54	a	3247.50	0.00056

2.12 1 B_{3u} excited state CC2/def2-TZVPD(aug-cc-pVTZ)

ZPVE = 0.1397710

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	a	97.05	1.56055
8	a	113.92	0.00001
9	a	198.13	0.02249
10	a	337.03	3.83127
11	a	352.17	15.77000
12	a	375.89	0.05546
13	a	416.17	0.00000
14	a	496.65	0.00001
15	a	522.89	235.01693
16	a	548.11	0.22294
17	a	560.88	0.84475
18	a	653.31	0.02082
19	a	659.98	132.21969
20	a	664.26	0.00000
21	a	692.60	0.00001
22	a	786.01	0.97612
23	a	791.92	12.92042
24	a	801.33	0.31075
25	a	828.76	14.20795

26	a	857.56	0.00013
27	a	857.76	0.01909
28	a	929.62	0.03270
29	a	983.77	40.82625
30	a	997.47	0.00000
31	a	1061.76	0.01919
32	a	1092.21	1.09991
33	a	1143.54	0.00000
34	a	1156.70	0.56059
35	a	1219.90	0.04616
36	a	1228.26	0.03121
37	a	1265.90	20.54936
38	a	1377.36	21.07923
39	a	1379.43	0.00001
40	a	1417.77	0.01442
41	a	1431.68	0.17443
42	a	1455.60	0.00003
43	a	1456.10	49.27532
44	a	1519.84	0.00000
45	a	1521.09	4.41713
46	a	1601.33	22.44468
47	a	3167.89	0.00711
48	a	3169.45	20.00931
49	a	3169.80	25.40024
50	a	3171.98	0.00007
51	a	3196.86	0.00048
52	a	3199.07	6.96611
53	a	3212.43	29.05518
54	a	3213.20	0.00003

2.13 1 B_{2u} excited state CC2/def2-TZVPD(aug-cc-pVTZ)

ZPVE = 0.1408806

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	a	123.92	204.51246
8	a	184.02	0.00836
9	a	297.70	73.69241
10	a	332.10	74.25392

11	a	385.64	1.04413
12	a	399.16	0.97569
13	a	452.09	5.82895
14	a	462.11	0.00801
15	a	496.07	0.00017
16	a	544.32	0.05549
17	a	581.61	19.08903
18	a	724.69	44.85764
19	a	725.24	0.20606
20	a	759.31	0.00020
21	a	770.48	1.05219
22	a	804.22	0.00729
23	a	855.42	3.43278
24	a	884.20	15.00313
25	a	941.95	2.70161
26	a	942.73	0.40727
27	a	943.85	163.14219
28	a	946.83	0.25626
29	a	997.27	39.10418
30	a	997.83	24.88358
31	a	1010.97	8.24046
32	a	1038.87	0.00021
33	a	1088.86	0.42027
34	a	1144.36	4.22301
35	a	1148.08	0.00292
36	a	1181.12	200.81137
37	a	1206.00	20.24525
38	a	1317.12	146.90748
39	a	1330.84	5.38678
40	a	1413.83	0.00025
41	a	1446.85	76.12609
42	a	1463.61	27.97973
43	a	1463.69	103.05130
44	a	1500.77	214.62636
45	a	1543.67	707.10232
46	a	1600.02	0.00017
47	a	3155.60	328.89668
48	a	3155.74	918.86636
49	a	3158.00	0.01206
50	a	3161.56	0.27285
51	a	3186.57	185.40404
52	a	3189.80	1.74991
53	a	3190.19	0.30918
54	a	3190.57	1010.13556

2.14 1 B_{3u} excited state B3LYP/def2-TZVPD

ZPVE = 0.1416968

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	b1u	111.09	1.76306
8	au	197.04	0.00000
9	b2g	245.96	0.00000
10	b1g	246.64	0.00000
11	b2u	355.29	1.42501
12	b1u	398.56	13.20986
13	au	497.44	0.00000
14	b3g	499.10	0.00000
15	ag	504.72	0.00000
16	b3u	553.22	181.37474
17	b2g	699.89	0.00000
18	b1u	705.21	133.27795
19	ag	705.28	0.00000
20	b3g	741.96	0.00000
21	au	757.81	0.00000
22	b2u	813.36	11.33523
23	b1g	843.08	0.00000
24	b2g	854.54	0.00000
25	b3g	872.84	0.00000
26	b1u	885.33	13.13932
27	au	933.07	0.00000
28	b3g	936.26	0.00000
29	b3u	992.88	25.39514
30	ag	1007.14	0.00000
31	b1g	1076.63	0.00000
32	b2u	1112.99	0.65037
33	ag	1158.06	0.00000
34	b3u	1169.27	3.22720
35	b3u	1236.19	0.00173
36	b1g	1253.46	0.00000
37	b2u	1285.63	15.57247
38	ag	1337.41	0.00000
39	b2u	1408.17	13.16699
40	b3u	1419.23	23.11688

41	b1g	1422.37	0.00000
42	b1g	1449.17	0.00000
43	ag	1478.26	0.00000
44	ag	1508.06	0.00000
45	b3u	1535.14	31.99130
46	b2u	1548.66	2.95566
47	b1g	3160.10	0.00000
48	b3u	3163.81	34.35051
49	b2u	3166.43	31.14049
50	ag	3168.56	0.00000
51	b1g	3182.44	0.00000
52	b2u	3190.77	14.46146
53	b3u	3204.02	29.60570
54	ag	3205.17	0.00000

2.15 Ground state B3LYP/def2-TZVPD

ZPVE = 0.1470201

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	b1u	172.52	2.49534
8	au	184.92	0.00000
9	b2u	354.01	1.54225
10	b2g	397.15	0.00000
11	b3g	481.44	0.00000
12	b1u	488.74	21.67122
13	b1g	515.62	0.00000
14	ag	519.88	0.00000
15	b3u	635.06	3.15461
16	au	637.62	0.00000
17	b2g	731.04	0.00000
18	ag	773.94	0.00000
19	b3g	790.66	0.00000
20	b1u	802.60	111.51757
21	b2u	808.65	0.26282
22	au	851.28	0.00000
23	b3g	904.44	0.00000
24	b1g	950.56	0.00000
25	b2g	968.79	0.00000

26	b1u	988.89	3.56269
27	au	1002.74	0.00000
28	b3g	1008.04	0.00000
29	b3u	1035.55	8.29162
30	ag	1045.89	0.00000
31	b2u	1150.42	4.12582
32	b3u	1168.79	0.67921
33	b1g	1171.39	0.00000
34	ag	1185.14	0.00000
35	b3u	1232.05	0.51192
36	b1g	1268.57	0.00000
37	b2u	1287.82	6.21041
38	b3u	1391.20	0.47218
39	ag	1395.10	0.00000
40	b2u	1418.50	3.96036
41	b1g	1489.97	0.00000
42	ag	1493.65	0.00000
43	b3u	1548.10	7.95421
44	ag	1611.07	0.00000
45	b2u	1638.69	2.74961
46	b1g	1665.48	0.00000
47	b1g	3156.93	0.00000
48	b2u	3158.68	5.52811
49	b3u	3160.90	0.76237
50	ag	3164.22	0.00000
51	b1g	3175.01	0.00000
52	b2u	3176.18	50.48274
53	b3u	3187.75	37.66376
54	ag	3188.68	0.00000

2.16 1 B_{2u} excited state B3LYP/def2-TZVPD

ZPVE = 0.1428363

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol
1		0.00	0.00000
2		0.00	0.00000
3		0.00	0.00000
4		0.00	0.00000
5		0.00	0.00000
6		0.00	0.00000
7	au	153.87	0.00000
8	b1u	158.93	3.08276
9	b2g	261.41	0.00000
10	b2u	359.33	1.83049

11	b1u	384.57	13.04921
12	b3g	475.73	0.00000
13	b1g	482.72	0.00000
14	au	488.98	0.00000
15	ag	505.68	0.00000
16	b3u	565.81	191.12022
17	b2g	685.43	0.00000
18	b1u	691.65	127.68624
19	b3g	733.01	0.00000
20	au	748.18	0.00000
21	ag	758.37	0.00000
22	b2u	801.20	8.13893
23	b2g	838.12	0.00000
24	b3g	860.03	0.00000
25	b1u	867.59	11.97232
26	b1g	923.69	0.00000
27	au	940.83	0.00000
28	b3g	942.06	0.00000
29	b3u	1009.25	47.20984
30	b1g	1045.89	0.00000
31	ag	1058.42	0.00000
32	b2u	1085.12	0.81193
33	ag	1178.98	0.00000
34	b3u	1179.16	0.32494
35	b3u	1229.07	0.00081
36	b1g	1250.30	0.00000
37	b2u	1288.88	9.60782
38	ag	1395.62	0.00000
39	b2u	1410.27	12.89121
40	b1g	1423.86	0.00000
41	b3u	1436.90	0.14364
42	ag	1482.71	0.00000
43	b1g	1486.94	0.00000
44	b2u	1490.65	4.47399
45	b3u	1573.29	43.99471
46	ag	1606.31	0.00000
47	b1g	3165.60	0.00000
48	b3u	3167.39	37.10745
49	b2u	3167.68	23.85855
50	ag	3172.11	0.00000
51	b1g	3182.74	0.00000
52	b2u	3183.72	26.21935
53	b3u	3199.45	33.58463
54	ag	3200.41	0.00000

References

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