**Supplementary Material**

**Table S1. The potential energies, electric dipole moments, and the transition dipole moments at selected internuclear separations of the X3Σ**–**0+, a1Δ2, b1Σ+0+,and b1Σ+0+**–**X3Σ**–**0+ of the SO radical.**

**X3Σ-0+ a1Δ2 b1Σ+0+ a1Δ2 b1Σ+0+ b1Σ+0+ - X3Σ-0+**

***R*/Å *E*/hartree *E*/hartree *E*/hartree *μ*/a.u. *μ*/a.u. *μ*/a.u.**

1.2 -472.9065324 -472.8753905 -472.8503145 -0.16479494 -0.13659122 -0.00174400

1.3 -473.0009132 -472.9712165 -472.9472623 -0.31915740 -0.28577655 -0.00207100

1.4 -473.0378594 -473.0109023 -472.9880614 -0.44770626 -0.39792322 -0.00229100

1.5 -473.0434215 -473.0180352 -472.9973499 -0.52804611 -0.47669884 -0.00236900

1.6 -473.0323186 -473.0086639 -472.9902126 -0.58018537 -0.52869123 -0.00231300

1.7 -473.0127510 -472.9909867 -472.9747926 -0.60459451 -0.55343184 -0.00217100

1.8 -472.9893451 -472.9696804 -472.9557708 -0.60248643 -0.55214639 -0.00203000

1.9 -472.9649593 -472.9476706 -472.9360521 -0.57759895 -0.52892090 -0.00200400

2.0 -472.9411428 -472.9265527 -472.9171842 -0.52715102 -0.48174152 -0.00224000

2.1 -472.9189883 -472.9071237 -472.9000523 -0.44188709 -0.41186620 -0.00290300

2.2 -472.8998458 -472.8914034 -472.8861146 -0.37513144 -0.34854745 -0.00413100

2.3 -472.8836834 -472.8786181 -472.8747970 -0.30399456 -0.28209173 -0.00594500

2.4 -472.8710038 -472.8689065 -472.8662070 -0.23948526 -0.22268224 -0.00807000

2.5 -472.8616139 -472.8617267 -472.8598295 -0.18380981 -0.17163900 -0.00877500

2.6 -472.8551529 -472.8565466 -472.8552093 -0.13879005 -0.13023032 -0.00315485

2.7 -472.8509791 -472.8528590 -472.8518999 -0.10393945 -0.09796549 -0.00302540

2.8 -472.8483813 -472.8502364 -472.8495376 -0.07764331 -0.07343591 -0.00566574

2.9 -472.8467702 -472.8483644 -472.8478426 -0.05803432 -0.05500990 -0.00648691

3.0 -472.8457475 -472.8470142 -472.8466192 -0.04347139 -0.04127022 -0.00633774

3.1 -472.8450709 -472.8460425 -472.8457263 -0.03266392 -0.03103096 -0.00565580

3.2 -472.8446024 -472.8453307 -472.8450665 -0.02460956 -0.02339459 -0.00472922

3.3 -472.8442628 -472.8448060 -472.8445738 -0.01859148 -0.01768800 -0.00380021

3.4 -472.8440066 -472.8444160 -472.8442013 -0.01408598 -0.01341379 -0.00296832

3.5 -472.8438074 -472.8441233 -472.8439196 -0.01071411 -0.01020510 -0.00228014

3.6 -472.8436485 -472.8439008 -472.8436959 -0.00820391 -0.00779853 -0.00172364

3.7 -472.8435246 -472.8437365 -472.8435297 -0.00633063 -0.00599031 -0.00128796

3.8 -472.8433509 -472.8435626 -472.8434077 -0.00518779 -0.00484948 -0.00095301

3.9 -472.8433324 -472.8435120 -472.8432858 -0.00420208 -0.00386325 -0.00069886

4.0 -472.8432669 -472.8434325 -472.8432014 -0.00341981 -0.00308157 -0.00050743

4.1 -472.8432077 -472.8433659 -472.8431333 -0.00282388 -0.00249083 -0.00036417

4.2 -472.8431602 -472.8433126 -472.8430795 -0.00236785 -0.00204777 -0.00025776

4.3 -472.8431213 -472.8432706 -472.8430358 -0.00201482 -0.00171635 -0.00017934

4.4 -472.8430888 -472.8432357 -472.8430002 -0.00173975 -0.00147014 -0.00012203

4.5 -472.8430630 -472.8432069 -472.8429734 -0.00152740 -0.00128585 -0.00008026

4.6 -472.8430433 -472.8431845 -472.8429495 -0.00135824 -0.00114990 -0.00005012

**Table S2. Rotational transitions of the R branch for the 2 – 2 and 3 – 3 bands of the a 1Δ2 state.**

 *ṽ*/cm–1 *ṽ*/cm–1

 2–2 Exp. [17] *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D 3–3 Exp. [17] *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D

R(2) 4.21 --- 9.85E-6 1.17E-6 -1.328 4.18 --- 9.85E-6 1.16E-6 -1.332

R(3) 5.62 --- 3.27E-5 2.00E-6 -1.328 5.57 --- 3.27E-5 1.99E-6 -1.332

R(4) 7.02 --- 7.31E-5 2.72E-6 -1.328 6.96 --- 7.31E-5 2.71E-6 -1.332

R(5) 8.43 --- 1.36E-4 3.39E-6 -1.328 8.35 --- 1.36E-4 3.38E-6 -1.332

R(6) 9.83 --- 2.25E-4 4.03E-6 -1.328 9.74 --- 2.25E-4 4.03E-6 -1.332

R(7) 11.24 11.17*a* 3.46E-4 4.65E-6 -1.328 11.14 11.07*a* 3.46E-4 4.64E-6 -1.332

R(8) 12.64 12.57*a*,*b* 5.03E-4 5.28E-6 -1.328 12.53 12.46*a*,*b* 5.03E-4 5.25E-6 -1.332

R(9) 14.04 --- 7.00E-4 5.88E-6 -1.328 13.92 --- 7.00E-4 5.87E-6 -1.332

R(10) 15.45 15.36 9.43E-4 6.49E-6 -1.328 15.31 15.22 9.43E-4 6.47E-6 -1.332

R(11) 16.85 --- 1.24E-3 7.12E-6 -1.328 16.70 --- 1.24E-3 7.07E-6 -1.332

R(12) 18.25 --- 1.58E-3 7.68E-6 -1.328 18.09 --- 1.58E-3 7.67E-6 -1.332

R(13) 19.66 19.54*c* 1.99E-3 8.29E-6 -1.328 19.48 19.37*c* 1.99E-3 8.27E-6 -1.332

R(14) 21.06 20.93*c* 2.46E-3 8.89E-6 -1.328 20.87 --- 2.46E-3 8.83E-6 -1.332

R(15) 22.46 22.33*c* 2.99E-3 9.46E-6 -1.329 22.26 22.13*c* 2.99E-3 9.44E-6 -1.333

R(16) 23.86 23.72*c* 3.60E-3 1.01E-5 -1.329 23.65 23.51*c* 3.60E-3 1.00E-5 -1.333

R(17) 25.26 --- 4.29E-3 1.07E-5 -1.329 25.04 --- 4.29E-3 1.06E-5 -1.333

R(18) 26.66 26.50 5.06E-3 1.12E-5 -1.329 26.42 26.27 5.06E-3 1.12E-5 -1.333

R(19) 28.06 27.89 5.91E-3 1.18E-5 -1.329 27.81 27.65 5.91E-3 1.18E-5 -1.333

R(20) 29.46 29.28 6.86E-3 1.24E-5 -1.329 29.20 29.03 6.86E-3 1.24E-5 -1.333

R(21) 30.86 30.67 7.90E-3 1.30E-5 -1.329 30.58 30.41 7.90E-3 1.30E-5 -1.333

R(25) 36.45 1.31E-2 1.54E-5 -1.330 36.12 1.31E-2 1.53E-5 -1.334

R(30) 43.41 2.23E-2 1.83E-5 -1.331 43.02 2.23E-2 1.82E-5 -1.335

R(35) 50.36 3.50E-2 2.13E-5 -1.333 49.91 3.50E-2 2.12E-5 -1.337

R(40) 57.28 5.17E-2 2.42E-5 -1.334 56.76 5.17E-2 2.41E-5 -1.338

**Note**: (a) Ref. [15]; (b) Ref. [17]; (c) Ref. [25].

**Table S3. Rotational transitions of the R branch for the 4 – 4 and 6 – 6 bands of the a1Δ2 state.**

 *ṽ*/cm–1 *ṽ*/cm–1

 4–4 Exp. [17] *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D 6–6 Exp. [17] *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D

R(2) 4.14 --- 9.44E-6 1.16E-6 -1.335 4.07 --- 9.00E-6 1.14E-6 -1.339

R(3) 5.52 --- 3.13E-5 1.98E-6 -1.335 5.42 --- 2.99E-5 1.96E-6 -1.339

R(4) 6.90 --- 7.01E-5 2.70E-6 -1.335 6.78 --- 6.68E-5 2.66E-6 -1.339

R(5) 8.28 --- 1.30E-4 3.36E-6 -1.335 8.13 --- 1.24E-4 3.32E-6 -1.339

R(6) 9.66 --- 2.16E-4 4.00E-6 -1.335 9.49 --- 2.06E-4 3.96E-6 -1.339

R(7) 11.04 10.98*a* 3.31E-4 4.61E-6 -1.335 10.84 12.13 3.16E-4 4.57E-6 -1.340

R(8) 12.42 12.35*a* 4.82E-4 5.24E-6 -1.335 12.20 --- 4.60E-4 5.18E-6 -1.340

R(9) 13.79 --- 6.71E-4 5.85E-6 -1.335 13.55 14.82 6.40E-4 5.78E-6 -1.340

R(10) 15.17 15.07 9.03E-4 6.44E-6 -1.335 14.90 --- 8.62E-4 6.38E-6 -1.340

R(11) 16.55 --- 1.18E-3 7.02E-6 -1.335 16.26 --- 1.13E-3 6.96E-6 -1.340

R(12) 17.93 --- 1.51E-3 7.60E-6 -1.335 17.61 --- 1.45E-3 7.57E-6 -1.340

R(13) 19.31 19.20*b* 1.90E-3 8.21E-6 -1.335 18.96 --- 1.82E-3 8.15E-6 -1.340

R(14) 20.68 --- 2.35E-3 8.81E-6 -1.336 20.32 --- 2.24E-3 8.69E-6 -1.340

R(15) 22.06 21.94*b* 2.87E-3 9.41E-6 -1.336 21.67 --- 2.73E-3 9.28E-6 -1.340

R(16) 23.44 23.31*b* 3.45E-3 9.98E-6 -1.336 23.02 22.90*a* 3.29E-3 9.87E-6 -1.340

R(17) 24.81 --- 4.11E-3 1.06E-5 -1.336 24.37 --- 3.92E-3 1.05E-5 -1.340

R(18) 26.19 26.04 4.84E-3 1.12E-5 -1.336 25.72 --- 4.62E-3 1.10E-5 -1.341

R(19) 27.56 27.41 5.66E-3 1.17E-5 -1.336 27.07 --- 5.40E-3 1.16E-5 -1.341

R(20) 28.94 28.78 6.57E-3 1.23E-5 -1.336 28.42 --- 6.26E-3 1.22E-5 -1.341

R(21) 30.31 30.14 7.56E-3 1.29E-5 -1.337 29.77 29.61 7.21E-3 1.28E-5 -1.341

R(25) 35.80 1.25E-2 1.52E-5 -1.337 35.16 1.20E-2 1.51E-5 -1.342

R(30) 42.64 2.13E-2 1.81E-5 -1.338 41.88 2.03E-2 1.79E-5 -1.343

R(35) 49.46 3.35E-2 2.11E-5 -1.340 48.58 3.19E-2 2.08E-5 -1.344

R(40) 56.26 4.95E-2 2.40E-5 -1.341 55.25 4.72E-2 2.38E-5 -1.345

**References**: (a) Ref. [15]; (b) Ref. [25].

**Table S4. Rotational transitions of the R branch for the 7 – 7 and 8 – 8 bands of the a1Δ2 state.**

 *ṽ*/cm–1 *ṽ*/cm–1

 7–7 Exp. [17] *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D 8–8 Exp. [17] *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D

R(2) 4.03 --- 8.78E-6 1.13E-6 -1.341 3.99 --- 8.56E-6 1.13E-6 -1.341

R(3) 5.37 --- 2.91E-5 1.95E-6 -1.341 5.33 --- 2.84E-5 1.93E-6 -1.341

R(4) 6.72 --- 6.52E-5 2.65E-6 -1.341 6.66 --- 6.35E-5 2.62E-6 -1.341

R(5) 8.06 --- 1.21E-4 3.30E-6 -1.341 7.99 --- 1.18E-4 3.27E-6 -1.341

R(6) 9.40 --- 2.01E-4 3.94E-6 -1.341 9.32 --- 1.96E-4 3.90E-6 -1.342

R(7) 10.74 --- 3.09E-4 4.55E-6 -1.341 10.65 --- 3.01E-4 4.51E-6 -1.342

R(8) 12.09 12.02 4.48E-4 5.14E-6 -1.341 11.98 11.91 4.37E-4 5.10E-6 -1.342

R(9) 13.43 --- 6.24E-4 5.73E-6 -1.341 13.31 --- 6.08E-4 5.69E-6 -1.342

R(10) 14.77 --- 8.40E-4 6.32E-6 -1.341 14.64 14.56 8.19E-4 6.27E-6 -1.342

R(15) 21.47 --- 2.67E-3 9.24E-6 -1.342 21.28 --- 2.60E-3 9.16E-6 -1.342

R(16) 22.81 22.69*a* 3.21E-3 9.81E-6 -1.342 22.61 --- 3.13E-3 9.74E-6 -1.342

R(17) 24.15 --- 3.82E-3 1.04E-5 -1.342 23.94 --- 3.72E-3 1.03E-5 -1.342

R(18) 25.49 --- 4.51E-3 1.10E-5 -1.342 25.26 --- 4.39E-3 1.09E-5 -1.343

R(19) 26.83 --- 5.27E-3 1.15E-5 -1.342 26.59 --- 5.13E-3 1.14E-5 -1.343

R(20) 28.17 28.01 6.11E-3 1.21E-5 -1.342 27.91 27.76 5.95E-3 1.20E-5 -1.343

R(21) 29.50 29.34 7.03E-3 1.27E-5 -1.342 29.24 29.08 6.85E-3 1.26E-5 -1.343

R(25) 34.84 1.17E-2 1.50E-5 -1.343 34.53 1.14E-2 1.49E-5 -1.344

R(30) 41.50 1.98E-2 1.78E-5 -1.344 41.13 1.93E-2 1.77E-5 -1.344

R(35) 48.14 3.11E-2 2.07E-5 -1.345 47.71 3.03E-2 2.05E-5 -1.345

R(40) 54.75 4.60E-2 2.36E-5 -1.346 54.26 4.48E-2 2.34E-5 -1.347

**Note**: (a) Ref. [25].

**Table S5. Rotational transitions of the R branch for the 8 – 8 and 10 – 10 bands of the a 1Δ2 state.**

 *ṽ*/cm–1 *ṽ*/cm–1

 8–8 Exp. [17] *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D 10–10 Exp. [17] *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D

R(2) 3.96 --- 8.33E-6 1.11E-6 -1.341 3.92 --- 8.11E-6 1.11E-6 -1.341

R(3) 5.2 --- 2.77E-5 1.92E-6 -1.341 5.23 --- 2.69E-5 1.90E-6 -1.341

R(4) 6.60 --- 6.19E-5 2.60E-6 -1.341 6.54 --- 6.02E-5 2.58E-6 -1.341

R(5) 7.92 --- 1.15E-4 3.25E-6 -1.341 7.85 --- 1.12E-4 3.22E-6 -1.341

R(6) 9.24 --- 1.91E-4 3.87E-6 -1.341 9.15 --- 1.85E-4 3.82E-6 -1.341

R(7) 10.55 --- 2.93E-4 4.47E-6 -1.342 10.46 --- 2.85E-4 4.43E-6 -1.341

R(8) 11.87 1.80 4.25E-4 5.05E-6 -1.342 11.77 11.69 4.14E-4 5.01E-6 -1.341

R(9) 13.19 --- 5.92E-4 5.64E-6 -1.342 13.08 --- 5.76E-4 5.58E-6 -1.341

R(10) 14.51 14.42 7.97E-4 6.22E-6 -1.342 14.38 --- 7.76E-4 6.16E-6 -1.341

R(11) 15.83 --- 1.04E-3 6.76E-6 -1.342 15.69 --- 1.02E-3 6.75E-6 -1.341

R(12) 17.14 --- 1.34E-3 7.39E-6 -1.342 16.99 --- 1.30E-3 7.29E-6 -1.341

R(13) 18.46 --- 1.68E-3 7.94E-6 -1.342 18.30 --- 1.63E-3 7.84E-6 -1.341

R(14) 19.78 --- 2.08E-3 8.52E-6 -1.342 19.60 --- 2.02E-3 8.43E-6 -1.341

R(15) 21.09 --- 2.53E-3 9.08E-6 -1.342 20.91 --- 2.46E-3 8.98E-6 -1.341

R(16) 22.41 --- 3.05E-3 9.66E-6 -1.342 22.21 --- 2.96E-3 9.54E-6 -1.341

R(17) 23.73 --- 3.63E-3 1.02E-5 -1.342 23.52 --- 3.53E-3 1.01E-5 -1.342

R(18) 25.04 --- 4.27E-3 1.08E-5 -1.342 24.82 --- 4.16E-3 1.07E-5 -1.342

R(19) 26.35 --- 5.00E-3 1.13E-5 -1.343 26.12 27.25 4.86E-3 1.12E-5 -1.342

R(20) 27.67 27.50 5.79E-3 1.19E-5 -1.343 27.42 28.54 5.64E-3 1.18E-5 -1.342

R(21) 28.98 28.81 6.67E-3 1.25E-5 -1.343 28.73 6.49E-3 1.23E-5 -1.342

R(25) 34.23 1.11E-2 1.48E-5 -1.343 33.92 1.08E-2 1.46E-5 -1.343

R(30) 40.77 1.88E-2 1.75E-5 -1.344 40.41 1.83E-2 1.74E-5 -1.343

R(40) 53.78 4.36E-2 2.32E-5 -1.346 53.30 4.23E-2 2.29E-5 -1.345

**Table S6. Rovibrational transitions of the P branch for the 2 – 1 band of of the a 1Δ2 state.**

 *ṽ*/cm–1 *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D

 This work Exp. [16] This work This work This work

 P(3) 1088.34 --- 1.10E+00 9.94E-07 -9.04E-02

 P(4) 1086.88 --- 1.41E+00 1.39E-06 -9.05E-02

 P(5) 1085.41 --- 1.54E+00 1.60E-06 -9.06E-02

 P(6) 1083.93 1079.15 1.59E+00 1.72E-06 -9.07E-02

 P(7) 1082.44 1077.67 1.62E+00 1.80E-06 -9.08E-02

 P(8) 1080.94 --- 1.64E+00 1.86E-06 -9.09E-02

 P(9) 1079.42 1074.68 1.65E+00 1.90E-06 -9.11E-02

 P(10) 1077.89 1073.16 1.65E+00 1.93E-06 -9.12E-02

 P(11) 1076.35 --- 1.65E+00 1.95E-06 -9.13E-02

 P(12) 1074.79 1070.09 1.65E+00 1.97E-06 -9.14E-02

 P(13) 1073.23 --- 1.65E+00 1.99E-06 -9.15E-02

 P(15) 1070.06 1065.40 1.64E+00 2.01E-06 -9.17E-02

 P(20) 1061.92 1057.36 1.62E+00 2.05E-06 -9.22E-02

 P(30) 1044.74 1.57E+00 2.09E-06 -9.30E-02

 P(40) 1026.39 1.51E+00 2.10E-06 -9.37E-02

**Table S7. Rovibrational transitions of the R branch for the 2 – 1 band of the a 1Δ2 state.**

 *ṽ*/cm–1 *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D

 This work Exp. [16] This work This work This work

 R(2) 1096.80 1091.94 7.92E-01 1.38E-06 -8.96E-02

 R(3) 1098.17 --- 1.11E+00 1.77E-06 -8.95E-02

 R(4) 1099.52 --- 1.27E+00 1.92E-06 -8.94E-02

 R(5) 1100.87 --- 1.37E+00 2.00E-06 -8.92E-02

 R(6) 1102.20 --- 1.43E+00 2.04E-06 -8.91E-02

 R(7) 1103.51 1098.62 1.47E+00 2.05E-06 -8.90E-02

 R(8) 1104.81 --- 1.50E+00 2.06E-06 -8.88E-02

 R(9) 1106.10 --- 1.53E+00 2.07E-06 -8.87E-02

 R(10) 1107.38 1102.48 1.54E+00 2.06E-06 -8.86E-02

 R(11) 1108.65 --- 1.56E+00 2.07E-06 -8.84E-02

 R(12) 1109.90 1104.99 1.57E+00 2.06E-06 -8.83E-02

 R(15) 1113.57 1.59E+00 2.05E-06 -8.78E-02

 R(20) 1119.44 1.61E+00 2.02E-06 -8.71E-02

 R(30) 1130.18 1.62E+00 1.96E-06 -8.54E-02

 R(40) 1139.56 1.60E+00 1.89E-06 -8.36E-02

**Table S8. Rovibrational transitions of the R and P branches for the 3 – 2 band of the a 1Δ2 state.**

 *ṽ*/cm–1 *ṽ*/cm–1

 *J* P Exp. [16] *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D R Exp.[16] *AJ'*→*J*″/s–1  *fJ'*→*J*″ TDMMEs/D

 2 1084.13 --- 1.10 1.96E-6 -0.1076

 3 1075.74 1069.97 1.53 1.42E-6 -0.1085 1085.49 1079.66 1.54 2.52E-6 -0.1074

 4 1074.30 --- 1.97 1.99E-6 -0.1086 1086.83 1080.99 1.77 2.75E-6 -0.1073

 5 1072.84 --- 2.14 2.28E-6 -0.1088 1088.16 --- 1.90 2.84E-6 -0.1071

 6 1071.38 1065.63 2.22 2.45E-6 -0.1089 1089.47 1083.63 1.99 2.90E-6 -0.1069

 7 1069.90 --- 2.26 2.57E-6 -0.1091 1090.78 --- 2.05 2.93E-6 -0.1068

 8 1068.40 1062.68 2.28 2.64E-6 -0.1092 1092.07 --- 2.09 2.94E-6 -0.1066

 9 1066.90 2.29 2.70E-6 -0.1093 1093.35 --- 2.12 2.94E-6 -0.1064

10 1065.38 2.30 2.75E-6 -0.1095 1094.61 1088.75 2.15 2.95E-6 -0.1062

11 1063.85 2.30 2.78E-6 -0.1096 1095.86 --- 2.17 2.94E-6 -0.1061

12 1062.31 2.30 2.81E-6 -0.1097 1097.10 1091.24 2.18 2.93E-6 -0.1059

13 1060.76 2.29 2.83E-6 -0.1099 1098.33 1092.46 2.20 2.94E-6 -0.1057

15 1057.61 2.29 2.87E-6 -0.1101 1100.74 --- 2.21 2.91E-6 -0.1053

16 1056.02 2.28 2.88E-6 -0.1102 1101.93 1096.06 2.22 2.91E-6 -0.1052

20 1049.54 2.26 2.93E-6 -0.1107 1106.55 1100.68 2.24 2.88E-6 -0.1044

21 1047.89 2.25 2.93E-6 -0.1108 1107.67 --- 2.24 2.86E-6 -0.1042

22 1046.23 2.24 2.93E-6 -0.1109 1108.78 1102.92 2.24 2.85E-6 -0.1040

30 1032.50 2.18 2.97E-6 -0.1117 1117.17 2.24 2.78E-6 -0.1023

40 1014.30 2.09 2.97E-6 -0.1126 1126.46 2.21 2.68E-6 -0.1000

**Table S9. Rovibrational transitions of the R and P branches for the 2 – 0 band of b1Σ+0+ state.**

 R branch P branch

*J*″ *ṽ*/cm–1 *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D *ṽ*/cm–1 *AJ'*→*J*″/s–1 *fJ'*→*J*″  TDMMEs/D

0 2093.62 1.12E-01 1.15E-07 1.08E-02

1 2094.97 1.34E-01 7.63E-08 1.08E-02 2090.83 3.33E-01 3.81E-08 1.08E-02

2 2096.30 1.44E-01 6.88E-08 1.08E-02 2089.40 2.22E-01 4.57E-08 1.08E-02

3 2097.61 1.50E-01 6.57E-08 1.08E-02 2087.94 1.99E-01 4.89E-08 1.08E-02

4 2098.88 1.54E-01 6.41E-08 1.08E-02 2086.46 1.89E-01 5.06E-08 1.08E-02

5 2100.14 1.56E-01 6.27E-08 1.08E-02 2084.96 1.83E-01 5.16E-08 1.08E-02

6 2101.37 1.58E-01 6.19E-08 1.08E-02 2083.42 1.80E-01 5.26E-08 1.08E-02

7 2102.57 1.60E-01 6.15E-08 1.08E-02 2081.87 1.77E-01 5.31E-08 1.08E-02

8 2103.75 1.61E-01 6.10E-08 1.08E-02 2080.28 1.75E-01 5.35E-08 1.08E-02

9 2104.90 1.62E-01 6.06E-08 1.08E-02 2078.68 1.73E-01 5.37E-08 1.08E-02

10 2106.02 1.63E-01 6.03E-08 1.08E-02 2077.05 1.72E-01 5.41E-08 1.08E-02

20 2115.86 1.69E-01 5.94E-08 1.08E-02 2059.35 1.63E-01 5.48E-08 1.08E-02

25 2119.81 1.71E-01 5.93E-08 1.08E-02 2049.58 1.59E-01 5.45E-08 1.08E-02

40 2127.74 1.75E-01 5.94E-08 1.08E-02 2016.58 1.50E-01 5.39E-08 1.07E-02

**Table S10. Rovibrational transitions of the R and P branches for the 2 – 1 band of the b 1Σ+0+ state.**

R branch P branch

*J*″ *ṽ*/cm–1 *AJ'*→*J*″/s–1 *fJ'*→*J*″ TDMMEs/D *ṽ*/cm–1 *AJ'*→*J*″/s–1 *fJ'*→*J*″  TDMMEs/D

0 1041.85 8.78E-01 3.64E-06 -8.62E-02

1 1043.22 1.05E+00 2.41E-06 -8.60E-02 1039.08 2.63E+00 1.22E-06 -8.64E-02

2 1044.58 1.13E+00 2.17E-06 -8.59E-02 1037.67 1.75E+00 1.46E-06 -8.65E-02

3 1045.92 1.17E+00 2.06E-06 -8.58E-02 1036.26 1.57E+00 1.57E-06 -8.66E-02

4 1047.25 1.20E+00 2.00E-06 -8.57E-02 1034.83 1.49E+00 1.62E-06 -8.67E-02

5 1048.57 1.22E+00 1.97E-06 -8.55E-02 1033.38 1.45E+00 1.67E-06 -8.69E-02

6 1049.87 1.24E+00 1.95E-06 -8.54E-02 1031.93 1.42E+00 1.69E-06 -8.70E-02

7 1051.16 1.25E+00 1.92E-06 -8.53E-02 1030.46 1.40E+00 1.71E-06 -8.71E-02

8 1052.44 1.26E+00 1.91E-06 -8.52E-02 1028.98 1.39E+00 1.74E-06 -8.72E-02

9 1053.70 1.26E+00 1.88E-06 -8.50E-02 1027.49 1.37E+00 1.74E-06 -8.73E-02

10 1054.96 1.27E+00 1.87E-06 -8.49E-02 1025.98 1.36E+00 1.75E-06 -8.74E-02

20 1066.77 1.29E+00 1.78E-06 -8.34E-02 1010.26 1.29E+00 1.80E-06 -8.84E-02

30 1077.25 1.29E+00 1.72E-06 -8.18E-02 993.33 1.24E+00 1.82E-06 -8.92E-02

40 1086.37 1.27E+00 1.65E-06 -8.01E-02 975.22 1.19E+00 1.83E-06 -8.99E-02