**Supplementary Material**

**Table S1. Rotational transitions of the R branch of the 4–4 and 5–5 bands of the X 1Σ+0+ state.**

 *ṽ*/cm-1 *ṽ*/cm-1

 4–4 Exp.[21] *AJ'*→*J*″/s-1 *fJ'*→*J*″ TDMMEs/D 5–5 Exp.[21] *AJ'*→*J*″/s-1 *fJ'*→*J*″ TDMMEs/D

 R(0) 1.59 1.59 1.43×10-6 2.55×10-6 1.8488 1.58 1.57 1.35×10-3 2.44×10-3 1.8180

 R(1) 3.18 3.17*a* 1.37×10-5 3.39×10-3 1.8488 3.15 3.15*a* 1.30×10-5 3.27×10-6 1.8180

 R(2) 4.76 4.76*a* 4.97×10-5 4.60×10-6 1.8488 4.73 4.72*a* 4.70×10-5 4.40×10-6 1.8179

 R(3) 6.35 6.35*a* 1.22×10-4 5.84×10-6 1.8487 6.30 6.30*a* 1.15×10-4 5.60×10-6 1.8179

 R(4) 7.94 7.93*a* 2.44×10-4 7.09×10-6 1.8486 7.88 --- 2.30×10-4 6.80×10-6 1.8178

 R(5) 9.53 9.52*a* 4.28×10-4 8.34×10-6 1.8485 9.46 9.45*a* 4.04×10-4 8.00×10-6 1.8177

 R(6) 11.11 --- 6.87×10-4 9.62×10-6 1.8484 11.03 --- 6.49×10-4 9.23×10-6 1.8175

 R(7) 12.70 --- 1.03×10-3 1.09×10-5 1.8482 12.61 --- 9.77×10-4 1.04×10-5 1.8174

 R(8) 14.29 --- 1.48×10-3 1.21×10-5 1.8481 14.18 --- 1.40×10-3 1.17×10-5 1.8172

 R(9) 15.88 --- 2.04×10-3 1.34×10-5 1.8479 15.76 --- 1.93×10-3 1.29×10-5 1.8170

R(10) 17.46 --- 2.73×10-3 1.47×10-5 1.8477 17.33 --- 2.58×10-3 1.41×10-5 1.8168

R(11) 19.05 --- 3.55×10-3 1.59×10-5 1.8475 18.90 --- 3.36×10-3 1.53×10-5 1.8166

R(12) 20.63 20.62*b* 4.53×10-3 1.72×10-5 1.8472 20.48 20.46*b* 4.28×10-3 1.65×10-5 1.8164

R(13) 22.22 22.20*b* 5.66×10-3 1.85×10-5 1.8469 22.05 22.03*b* 5.35×10-3 1.77×10-5 1.8161

R(14) 23.80 --- 6.98×10-3 1.97×10-5 1.8467 23.62 --- 6.60×10-3 1.89×10-5 1.8158

R(15) 25.39 --- 8.48×10-3 2.10×10-5 1.8464 25.20 --- 8.02×10-3 2.01×10-5 1.8155

R(16) 26.97 --- 1.02×10-2 2.23×10-5 1.8460 26.77 --- 9.63×10-3 2.14×10-5 1.8152

R(17) 28.55 --- 1.21×10-2 2.35×10-5 1.8457 28.34 --- 1.14×10-2 2.26×10-5 1.8148

R(18) 30.14 30.11*b* 1.42×10-2 2.48×10-5 1.8453 29.91 29.89*b* 1.35×10-2 2.38×10-5 1.8145

R(19) 31.72 31.69*b* 1.66×10-2 2.60×10-5 1.8450 31.48 31.46*b* 1.57×10-2 2.50×10-5 1.8141

R(20) 33.30 --- 1.92×10-2 2.73×10-5 1.8446 33.05 --- 1.82×10-2 2.62×10-5 1.8137

R(21) 34.88 34.85*b* 2.21×10-2 2.85×10-5 1.8441 34.62 34.59*b* 2.09×10-2 2.74×10-5 1.8133

R(25) 41.20 3.65×10-2 3.35×10-5 1.8423 40.89 3.45×10-2 3.21×10-5 1.8114

R(35) 56.92 9.62×10-2 4.58×10-5 1.8362 56.49 9.09×10-2 4.39×10-5 1.8053

R(36) 58.49 1.04×10-1 4.70×10-5 1.8355 58.05 9.85×10-2 4.50×10-5 1.8046

R(37) 60.05 1.13×10-1 4.82×10-5 1.8347 59.60 1.07×10-1 4.62×10-5 1.8039

R(40) 64.74 1.41×10-1 5.17×10-5 1.8324 64.26 1.33×10-1 4.96×10-5 1.8015

**Note**: *a*Ref. [18]; *b*Ref. [20].

**Table S2. Rotational transitions of the R branch of the 8 – 8 and 9 – 9 bands of the X 1Σ+0+ state.**

 *ṽ*/cm-1 *ṽ*/cm-1

 8–8 Exp.[21] *AJ'*→*J*″/s-1 *fJ'*→*J*″ TDMMEs/D 9–9 Exp.[21] *AJ'*→*J*″/s-1 *fJ'*→*J*″ TDMMEs/D

 R(0) 1.54 1.54 1.14×10-6 2.15×10-6 1.7250 1.53 1.53 1.07×10-6 2.06×10-6 1.6949

 R(1) 3.08 3.08*a* 1.09×10-5 2.87×10-6 1.7250 3.06 3.05*a* 1.03×10-5 2.75×10-6 1.6949

 R(2) 4.62 4.62*a* 3.94×10-5 3.88×10-6 1.7250 4.59 4.58*a* 3.72×10-5 3.71×10-6 1.6948

 R(3) 6.16 --- 9.69×10-5 4.92×10-6 1.7249 6.11 --- 9.15×10-5 4.72×10-6 1.6947

 R(4) 7.70 --- 1.94×10-4 5.98×10-6 1.7248 7.64 --- 1.83×10-4 5.74×10-6 1.6947

 R(5) 9.24 9.23*b* 3.40×10-4 7.05×10-6 1.7247 9.17 9.16*b* 3.20×10-4 6.75×10-6 1.6945

 R(6) 10.78 10.77*b* 5.45×10-4 8.11×10-6 1.7245 10.70 10.70*b* 5.14×10-4 7.77×10-6 1.6944

 R(7) 12.32 --- 8.20×10-4 9.18×10-5 1.7244 12.23 --- 7.74×10-4 8.79×10-6 1.6943

 R(8) 13.86 --- 1.17×10-3 1.02×10-5 1.7242 13.75 --- 1.11×10-3 9.83×10-6 1.6941

 R(9) 15.39 --- 1.62×10-3 1.13×10-5 1.7240 15.28 --- 1.53×10-3 1.08×10-5 1.6939

R(10) 16.93 --- 2.16×10-3 1.24×10-5 1.7238 16.81 --- 2.04×10-3 1.19×10-5 1.6937

R(15) 24.62 --- 6.73×10-3 1.77×10-5 1.7225 24.43 --- 6.35×10-3 1.70×10-5 1.6923

R(16) 26.15 --- 8.08×10-3 1.88×10-5 1.7221 25.96 --- 7.63×10-3 1.80×10-5 1.6919

R(17) 27.69 --- 9.60×10-3 1.98×10-5 1.7218 27.48 --- 9.06×10-3 1.90×10-5 1.6916

R(18) 29.22 --- 1.13×10-2 2.09×10-5 1.7214 29.00 --- 1.07×10-2 2.00×10-5 1.6912

R(19) 30.76 30.74*b* 1.32×10-3 2.20×10-5 1.7210 30.53 30.51*b* 1.24×10-2 2.10×10-5 1.6908

R(20) 32.29 --- 1.53×10-2 2.30×10-5 1.7206 32.05 32.03*b* 1.44×10-2 2.20×10-5 1.6904

R(21) 33.82 33.81*b* 1.76×10-3 2.41×10-5 1.7201 33.57 33.55*b* 1.66×10-2 2.31×10-5 1.6899

R(22) 35.35 35.34*b* 2.01×10-3 2.51×10-5 1.7197 35.09 1.89×10-2 2.41×10-5 1.6895

R(25) 39.95 2.90×10-2 2.83×10-5 1.7182 39.64 2.73×10-2 2.71×10-5 1.6879

R(30) 47.58 4.89×10-2 3.35×10-5 1.7153 47.22 4.61×10-2 3.20×10-5 1.6850

R(38) 59.74 9.65×10-2 4.16×10-5 1.7097 59.29 9.10×10-2 3.98×10-5 1.6792

R(39) 61.26 1.04×10-1 4.26×10-5 1.7089 60.79 9.80×10-2 4.08×10-5 1.6784

R(40) 62.77 1.12×10-1 4.36×10-5 1.7080 62.29 1.05×10-1 4.17×10-5 1.6775

**Note**: *a*Ref. [18]; *b*Ref. [20].

**Table S3. Rotational line lists of the R and P branches for the 3 – 2 band in the X 1Σ+0+ state.**

 *ṽ*/cm-1 *AJ'*→*J*″/s-1  *ṽ*/cm-1 *AJ'*→*J*″/s-1

 This work Exp.[19] Exp.[22] This work This work Exp.[19] Exp.[22] This work

 R(0) 1253.19 --- --- 13.2 P(1) 1249.98 --- --- 39.0

 R(1) 1254.78 1249.43 1249.43 15.9 P(2) 1248.35 1243.01 1243.01 25.9

 R(2) 1256.35 1251.00 1251.00 17.1 P(3) 1246.72 1241.37 --- 23.2

 R(3) 1257.92 1252.57 --- 17.8 P(4) 1245.07 1239.73 1239.73 21.9

 R(4) 1259.47 1254.12 1254.12 18.3 P(5) 1243.41 1238.07 1238.07 21.2

 R(5) 1261.01 1255.66 1255.66 18.7 P(6) 1241.74 1236.41 1236.40 20.7

 R(6) 1262.54 1257.19 1257.18 19.0 P(7) 1240.06 1234.72 1234.72 20.3

 R(7) 1264.06 1258.70 1258.70 19.3 P(8) 1238.37 1233.03 1233.03 20.0

R(8) 1265.56 1260.20 1260.20 19.5 P(9) 1236.66 1231.33 1231.33 19.7

R(9) 1267.05 1261.69 1261.69 19.7 P(10) 1234.95 1229.61 1229.61 19.5

R(10) 1268.53 1263.17 1263.17 19.9 P(11) 1233.22 1227.88 1227.88 19.3

R(11) 1270.00 1264.64 1264.64 20.1 P(12) 1231.48 1226.14 1226.14 19.1

R(12) 1271.46 1266.09 1266.09 20.3 P(13) 1229.73 1224.40 1224.40 18.9

R(13) 1272.90 1267.53 1267.53 20.4 P(14) 1227.97 1222.63 1222.63 18.8

R(14) 1274.34 1268.96 1268.96 20.6 P(15) 1226.20 1220.86 1220.86 18.6

R(15) 1275.75 1270.38 1270.38 20.7 P(16) 1224.41 1219.08 1219.08 18.5

R(16) 1277.16 --- --- 20.9 P(17) 1222.62 1217.28 1217.28 18.3

R(17) 1278.56 1273.17 1273.17 21.0 P(18) 1220.81 1215.47 1215.47 18.2

R(18) 1279.94 1274.56 1274.56 21.1 P(19) 1218.99 1213.66 1213.66 18.0

R(19) 1281.31 1275.92 1275.92 21.3 P(20) 1217.17 1211.83 1211.83 17.9

R(20) 1282.67 1277.28 1277.28 21.4 P(25) 1207.85 1202.51 1202.51 17.3

R(25) 1289.27 1283.86 1283.86 22.0 P(30) 1198.27 1192.92 1192.92 16.7

R(30) 1295.56 1290.13 1290.13 22.6 P(35) 1188.42 1183.05 1183.05 16.1

R(35) 1301.53 1296.08 1296.08 23.2 P(39) 1180.34 1174.97 1174.97 15.7

R(40) 1307.18 1301.70 --- 23.7 P(40) 1178.29 1172.92 1172.92 15.6

**Table S4. Ro-vibrational transitions of the R and P branches for the 4 – 3 band in the X1Σ+0+ state.**

 *ṽ*/cm-1 *AJ'*→*J*″/s-1  *ṽ*/cm-1 *AJ'*→*J*″/s-1

 This work Exp. [19] Exp. [22] This work This work Exp. [19] Exp. [22] This work

 R(0) 1240.30 --- --- 16.9

 R(1) 1241.88 --- 1236.48 20.4 P(1) 1237.11 --- 1231.72 50.2

 R(2) 1243.44 1238.04 1238.04 22.0 P(2) 1235.50 1230.11 1230.11 33.3

 R(3) 1245.00 1239.59 1239.60 22.9 P(3) 1233.88 1228.49 1228.49 29.8

 R(4) 1246.54 1241.14 1241.13 23.6 P(4) 1232.24 1226.85 1226.86 28.2

 R(5) 1248.06 1242.66 1242.66 24.1 P(5) 1230.60 1225.21 1225.21 27.3

 R(6) 1249.58 1244.18 --- 24.5 P(6) 1228.94 1223.55 1223.55 26.6

 R(7) 1251.09 1245.68 1245.68 24.8 P(7) 1227.27 1221.88 1221.88 26.2

R(8) 1252.58 1247.17 1247.17 25.1 P(8) 1225.59 1220.20 1220.20 25.8

R(9) 1254.06 1248.65 1248.65 25.4 P(9) 1223.89 1218.51 1218.51 25.4

R(10) 1255.53 1250.11 1250.11 25.6 P(10) 1222.19 1216.81 1216.80 25.1

R(11) 1256.98 1251.57 1251.57 25.9 P(11) 1220.47 1215.09 1215.09 24.9

R(12) 1258.43 1253.01 1253.01 26.1 P(12) 1218.74 1213.36 1213.36 24.6

R(13) 1259.86 1254.44 1254.44 26.3 P(13) 1217.01 1211.62 1211.62 24.4

R(14) 1261.28 1255.86 1255.86 26.5 P(14) 1215.25 1209.87 1209.87 24.2

R(15) 1262.68 1257.26 1257.26 26.7 P(15) 1213.49 1208.11 1208.11 24.0

R(16) 1264.08 1258.66 1258.66 26.8 P(16) 1211.72 1206.34 1206.34 23.8

R(17) 1265.46 1260.04 1260.04 27.0 P(17) 1209.93 1204.56 1204.56 23.6

R(18) 1266.83 1261.40 1261.40 27.2 P(18) 1208.14 1202.76 1202.76 23.4

R(19) 1268.19 1262.76 1262.76 27.4 P(19) 1206.33 1200.96 1200.95 23.2

R(20) 1269.53 1264.10 1264.10 27.5 P(20) 1204.51 1199.14 1199.14 23.1

R(25) 1276.07 1270.63 1270.63 28.3 P(25) 1195.25 1189.88 1189.88 22.2

R(30) 1282.29 1276.83 1276.84 29.1 P(30) 1185.72 1180.35 1180.35 21.5

R(34) 1287.04 1281.57 1281.57 29.7 P(34) 1177.90 1172.52 1172.52 20.9

R(39) 1292.68 1287.20 1287.20 30.4 P(39) 1167.88 1162.50 1162.50 20.2

R(40) 1293.77 --- 1288.28 30.5 P(40) 1165.84 1160.47 1160.47 20.0

**Table S5. Rotational transitions for the 2–2 and 3–3 bands in the A 1Π state.**

2-2 3-3

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

R(1) 3.10 1.29×10-6 3.35×10-7 0.67983 3.03 1.10×10-6 2.99×10-7 0.64923

 R(2) 4.64 5.53×10-6 5.39×10-7 0.67984 4.54 4.71×10-6 4.79×10-7 0.64927

 R(3) 6.19 1.43×10-5 7.21×10-7 0.67985 6.05 1.22×10-5 6.43×10-7 0.64933

 R(4) 7.74 2.93×10-5 8.96×10-7 0.67986 7.56 2.50×10-5 8.00×10-7 0.64941

 R(5) 9.28 5.21×10-5 1.07×10-6 0.67988 9.07 4.44×10-5 9.56×10-7 0.64950

 R(6) 10.83 8.42×10-5 1.24×10-6 0.67990 10.59 7.18×10-5 1.11×10-6 0.64961

 R(7) 12.38 1.27×10-4 1.41×10-6 0.67993 12.10 1.09×10-4 1.26×10-6 0.64974

 R(8) 13.92 1.83×10-4 1.58×10-6 0.67995 13.61 1.56×10-4 1.41×10-6 0.64988

 R(9) 15.47 2.53×10-4 1.75×10-6 0.67998 15.12 2.16×10-4 1.57×10-6 0.65004

R(10) 17.02 3.39×10-4 1.92×10-6 0.68002 16.63 2.89×10-4 1.72×10-6 0.65022

R(11) 18.56 4.42×10-4 2.09×10-6 0.68006 18.14 3.78×10-4 1.87×10-6 0.65042

R(12) 20.10 5.64×10-4 2.26×10-6 0.68010 19.65 4.82×10-4 2.02×10-6 0.65064

R(13) 21.65 7.07×10-4 2.43×10-6 0.68015 21.16 6.05×10-4 2.17×10-6 0.65087

R(14) 23.19 8.72×10-4 2.60×10-6 0.68020 22.67 7.46×10-4 2.33×10-6 0.65112

R(15) 24.73 1.06×10-3 2.77×10-6 0.68026 24.18 9.08×10-4 2.48×10-6 0.65139

R(16) 26.28 1.27×10-3 2.93×10-6 0.68032 25.68 1.09×10-3 2.63×10-6 0.65168

R(17) 27.82 1.52×10-3 3.10×10-6 0.68039 27.19 1.30×10-3 2.79×10-6 0.65199

R(18) 29.36 1.79×10-3 3.27×10-6 0.68046 28.70 1.53×10-3 2.94×10-6 0.65232

R(19) 30.90 2.09×10-3 3.44×10-6 0.68054 30.20 1.79×10-3 3.09×10-6 0.65266

R(20) 32.44 2.42×10-3 3.61×10-6 0.68063 31.71 2.08×10-3 3.25×10-6 0.65303

R(25) 40.12 4.60×10-3 4.46×10-6 0.68116 39.21 3.98×10-3 4.03×10-6 0.65517

R(30) 47.78 7.82×10-3 5.30×10-6 0.68191 46.69 6.79×10-3 4.82×10-6 0.65783

R(32) 50.83 9.44×10-3 5.64×10-6 0.68229 49.68 8.22×10-3 5.15×10-6 0.65905

R(33) 52.36 1.03×10-2 5.81×10-6 0.68249 51.17 9.00×10-3 5.31×10-6 0.65969

R(34) 53.88 1.13×10-2 5.98×10-6 0.68271 52.66 9.84×10-3 5.47×10-6 0.66035

R(35) 55.40 1.23×10-2 6.16×10-6 0.68293 54.14 1.07×10-2 5.64×10-6 0.66104

R(40) 62.99 1.81×10-2 7.02×10-6 0.68429 61.56 1.60×10-2 6.47×10-6 0.66478

**Table S6. Rotational transitions for the 2 – 1 band in the A 1Π 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

1 1046.91 0.121 2.75×10-7 3.34×10-2

2 1048.41 0.153 2.93×10-7 3.34×10-2 1040.76 0.202 3.91×10-7 3.38×10-2

3 1049.89 0.168 2.94×10-7 3.33×10-2 1039.18 0.216 3.85×10-7 3.39×10-2

4 1051.35 0.176 2.92×10-7 3.33×10-2 1037.58 0.217 3.69×10-7 3.40×10-2

5 1052.79 0.182 2.90×10-7 3.33×10-2 1035.96 0.217 3.58×10-7 3.41×10-2

6 1054.21 0.186 2.89×10-7 3.32×10-2 1034.32 0.216 3.50×10-7 3.43×10-2

7 1055.62 0.189 2.88×10-7 3.32×10-2 1032.67 0.216 3.44×10-7 3.44×10-2

8 1057.00 0.191 2.87×10-7 3.32×10-2 1031.00 0.216 3.40×10-7 3.46×10-2

9 1058.37 0.194 2.86×10-7 3.32×10-2 1029.31 0.216 3.38×10-7 3.47×10-2

10 1059.72 0.196 2.86×10-7 3.32×10-2 1027.61 0.216 3.36×10-7 3.49×10-2

11 1061.06 0.198 2.86×10-7 3.33×10-2 1025.89 0.217 3.36×10-7 3.51×10-2

12 1062.37 0.200 2.86×10-7 3.33×10-2 1024.15 0.217 3.36×10-7 3.53×10-2

13 1063.67 0.202 2.87×10-7 3.33×10-2 1022.39 0.218 3.36×10-7 3.55×10-2

14 1064.94 0.204 2.88×10-7 3.34×10-2 1020.62 0.219 3.37×10-7 3.57×10-2

15 1066.20 0.205 2.88×10-7 3.35×10-2 1018.83 0.220 3.39×10-7 3.59×10-2

20 1072.21 0.216 2.95×10-7 3.39×10-2 1009.61 0.228 3.51×10-7 3.71×10-2

25 1077.74 0.228 3.06×10-7 3.45×10-2 999.95 0.237 3.70×10-7 3.85×10-2

30 1082.76 0.242 3.20×10-7 3.52×10-2 989.84 0.248 3.92×10-7 4.01×10-2

35 1087.26 0.257 3.35×10-7 3.59×10-2 979.29 0.260 4.18×10-7 4.17×10-2

40 1091.22 0.271 3.50×10-7 3.67×10-2 968.26 0.271 4.44×10-7 4.34×10-2

**Table S7. Rovibrational transitions of the P branch for the 0 – 0 and 1 – 1 vibronic bands of the A 1Π1 – X 1Σ+0+ system.**

0 − 0 1 − 1

 *ṽ*/cm-1 *AJ'*→*J*″/s-1 *fJ'*→*J*″ FC factor *ṽ*/cm-1 *AJ'*→*J*″/s-1 *fJ'*→*J*″ FC factor

P(2) 38795.03 2.10×106 1.25×10-3 0.8394 38572.83 1.28×106 7.74×10-4 0.5442

 P(3) 38793.25 2.52×106 1.79×10-3 0.8395 38571.05 1.54×106 1.11×10-3 0.5442

 P(4) 38791.41 2.70×106 2.09×10-3 0.8395 38569.20 1.64×106 1.29×10-3 0.5442

 P(5) 38789.50 2.80×106 2.28×10-3 0.8394 38567.28 1.71×106 1.41×10-3 0.5442

 P(6) 38787.52 2.86×106 2.41×10-3 0.8394 38565.27 1.74×106 1.49×10-3 0.5441

 P(7) 38785.47 2.90×106 2.51×10-3 0.8394 38563.20 1.77×106 1.55×10-3 0.5440

 P(8) 38783.35 2.93×106 2.58×10-3 0.8393 38561.04 1.79×106 1.59×10-3 0.5439

 P(9) 38781.16 2.96×106 2.64×10-3 0.8393 38558.81 1.80×106 1.63×10-3 0.5438

P(10) 38778.90 2.98×106 2.68×10-3 0.8392 38556.51 1.81×106 1.65×10-3 0.5436

P(15) 38766.56 3.03×106 2.82×10-3 0.8386 38543.85 1.84×106 1.74×10-3 0.5422

P(20) 38752.48 3.04×106 2.89×10-3 0.8386 38529.28 1.84×106 1.77×10-3 0.5340

P(30) 38719.02 3.04×106 2.94×10-3 0.8346 38494.38 1.82×106 1.79×10-3 0.5331

P(40) 38678.32 3.02×106 2.95×10-3 0.8300 38451.64 1.78×106 1.76×10-3 0.5229

P(70) 38509.40 2.84×106 2.83×10-3 0.8059 38273.32 1.55×106 1.56×10-3 0.4703

P(100) 38258.31 2.54×106 2.58×10-3 0.7619 38008.16 1.18×106 1.21×10-3 0.3796

P(149) 18255.87 1.76×106 1.86×10-3 0.6229 37305.81 3.91×105 4.18×10-4 0.1484

**Table S8. Rovibrational transitions of the R branch for the 0 – 0 and 2 – 1 bands of the A 1Π1 – X 1Σ+0+ system.**

0−0 2−1

 *ṽ*/cm-1 *AJ'*→*J*″/s-1 *fJ'*→*J*″ FC factor *ṽ*/cm-1 *AJ'*→*J*″/s-1 *fJ'*→*J*″ FC factor

R(0) 38799.93 4.20×106 0.0125 0.8393 39621.55 1.67×106 4.77×10-3 0.2712

 R(1) 38801.43 3.78×106 0.0063 0.8392 39622.99 1.50×106 2.39×10-3 0.2712

 R(2) 38802.86 3.60×106 0.0050 0.8392 39624.33 1.43×106 1.91×10-3 0.2713

 R(3) 38804.21 3.50×106 0.0045 0.8391 39625.58 1.39×106 1.71×10-3 0.2714

 R(4) 38805.50 3.43×106 0.0042 0.8389 39626.74 1.36×106 1.59×10-3 0.2715

 R(5) 38806.72 3.39×106 0.0040 0.8388 39627.80 1.35×106 1.52×10-3 0.2716

 R(6) 38807.87 3.36×106 0.0039 0.8387 39628.77 1.34×106 1.47×10-3 0.2717

 R(7) 38808.95 3.33×106 0.0038 0.8385 39629.64 1.33×106 1.43×10-3 0.2719

 R(8) 38809.96 3.31×106 0.0037 0.8383 39630.42 1.32×106 1.41×10-3 0.2720

 R(9) 38810.90 3.29×106 0.0036 0.8382 39631.11 1.31×106 1.39×10-3 0.2722

R(10) 38811.76 3.28×106 0.0036 0.8380 39631.70 1.31×106 1.37×10-3 0.2724

R(20) 38816.56 3.20×106 0.0033 0.8352 39632.39 1.29×106 1.29×10-3 0.2749

R(30) 38814.15 3.15×106 0.0032 0.8310 39623.39 1.29×106 1.27×10-3 0.2786

R(40) 38804.25 3.10×106 0.0032 0.8252 39604.34 1.30×106 1.27×10-3 0.2831

R(70) 38725.37 2.90×106 0.0029 0.7969 39481.63 1.33×106 1.30×10-3 0.3045

R(100) 38558.98 2.58×106 0.0026 0.7478 39245.90 1.35×106 1.33×10-3 0.3322

R(149) 38021.21 1.76×106 0.0018 0.4507 38540.87 1.11×105 1.12×10-3 0.3290

**Table S9. Rotational lines of the P branch for the 2–1 and 2–2 bands of the A1Π1 – X1Σ+0+ system.**

2-1 2-2

 *ṽ*/cm-1 *AJ'*→*J*″/s-1 *fJ'*→*J*″ FC factor *ṽ*/cm-1 *AJ'*→*J*″/s-1 *fJ'*→*J*″ FC factor

P(2) 39616.68 8.32×105 4.77×10-4 0.2710 38352.09 6.66×105 4.07×10-4 0.2963

 P(3) 39614.87 9.98×105 6.81×10-4 0.2710 38350.32 7.99×105 5.82×10-4 0.2964

 P(4) 39612.97 1.07×105 7.95×10-4 0.2710 38348.46 8.56×105 6.79×10-4 0.2964

 P(5) 39610.97 1.11×105 8.67×10-4 0.2710 38346.52 8.88×105 7.40×10-4 0.2963

 P(6) 39608.88 1.13×105 9.17×10-4 0.2710 38344.50 9.07×105 7.83×10-4 0.2963

 P(7) 39606.70 1.15×105 9.54×10-4 0.2710 38342.40 9.21×105 8.14×10-4 0.2962

 P(8) 39604.42 1.16×105 9.82×10-4 0.2710 38340.22 9.30×105 8.37×10-4 0.2960

 P(9) 39602.05 1.17×105 1.00×10-3 0.2712 38337.95 9.37×105 8.55×10-4 0.2958

P(10) 39599.59 1.18×105 1.02×10-3 0.2712 38335.61 9.42×105 8.70×10-4 0.2956

P(20) 39569.79 1.22×105 1.11×10-3 0.2727 38307.63 9.50×105 9.23×10-4 0.2911

P(30) 39530.47 1.23×105 1.14×10-3 0.2754 38271.31 9.24×105 9.14×10-4 0.2827

P(40) 39481.38 1.24×105 1.16×10-3 0.2794 38226.40 8.79×105 8.79×10-4 0.2704

P(70) 39271.01 1.27×105 1.22×10-3 0.2983 38035.65 6.59×105 6.73×10-4 0.2114

P(100) 38952.96 1.30×105 1.27×10-3 0.3262 37747.92 3.64×105 3.79×10-4 0.1252

P(150) 38110.58 1.10×105 1.13×10-3 0.3379 36980.23 2.68×103 2.92×10-6 0.0001

**Table S10. Rotational transitions of the R branch for the 1–0 and 1–1 bands of the A1Π1 – X1Σ+0+ system.**

 1–0 1–1

 *ṽ*/cm-1 *AJ'*→*J*″/s-1 *fJ'*→*J*″ FC factor *ṽ*/cm-1 *AJ'*→*J*″/s-1 *fJ'*→*J*″ FC factor

R(0) 39855.36 9.60×105 0.0027 0.1486 38577.70 2.56×106 0.0077 0.5439

 R(1) 39856.82 8.65×105 0.0014 0.1486 38579.17 2.30×106 0.0039 0.5437

 R(2) 39858.19 8.24×105 0.0011 0.1487 38580.57 2.19×106 0.0031 0.5435

 R(3) 39859.47 8.01×105 0.0010 0.1488 38581.89 2.13×106 0.0028 0.5433

 P(4) 39860.67 7.87×105 0.0009 0.1489 38583.13 2.09×106 0.0026 0.5430

 R(5) 39861.78 7.78×105 0.0009 0.1490 38584.30 2.06×106 0.0025 0.5427

 R(6) 39862.80 7.71×105 0.0008 0.1491 38585.39 2.04×106 0.0024 0.5424

 R(7) 39863.73 7.66×105 0.0008 0.1492 38586.41 2.03×106 0.0023 0.5420

 R(8) 39864.58 7.62×105 0.0008 0.1494 38587.34 2.01×106 0.0023 0.5416

 R(9) 39865.34 7.59×105 0.0008 0.1495 38588.21 2.00×106 0.0022 0.5412

R(10) 39866.01 7.57×105 0.0008 0.1497 38588.99 1.99×106 0.0022 0.5408

R(20) 39867.81 7.52×105 0.0007 0.1520 38592.62 1.93×106 0.0020 0.5345

R(30) 39860.59 7.60×105 0.0007 0.1555 38588.41 1.87×106 0.0019 0.5249

R(40) 39844.12 7.76×105 0.0008 0.1602 38576.11 1.81×106 0.0019 0.5119

R(70) 39735.19 8.53×105 0.0008 0.1828 38486.82 1.53×106 0.0016 0.4511

R(100) 39523.31 9.62×105 0.0009 0.2188 38305.27 1.13×106 0.0012 0.3525

R(149) 38865.21 1.11×106 0.0011 0.3022 37720.05 3.25×105 0.0003 0.1191