Supplemental Materials for:

Quantum effects in photosensitization: The case of singlet oxygen generation by thiothymines

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TABLE S1. Values of $FCWD$ integrated over different time intervals, for the three different thiothymines along select orientation directions and D values.

τ	2tThy (T_1^{ring}) Å to2X, D=2.6 Å	4tThy (T_1^{ring}) Å to56, D=3.0 Å	dtThy (T_1^{ring}) to4X, D=3.6 Å
30 fs	29.116	52.152	23.106
1 ps	6.595	51.365	32.371
2 ps	12.625	63.475	3.774
3 ps	3.678	50.379	30.902

TABLE S2. Value of FCWD with the use of different damping parameters for the T_1^{ring} structure of 4tThy along the to56 direction and D=3.0 Å, along with integration time, time taken for the function to get damped, and resulting photosensitization rate.

η (cm^{-1})	FCWD	k (s^{-1})	t–int[a] (fs)	t–damp[b] (fs)
0.5	37.670	5.18×10^6	200	55
0.1	37.670	5.18×10^6	200	120
0.05	34.765	4.79×10^6	500	180
0.01	29.562	4.07×10^6	500	380
0.005	26.240	3.61×10^6	2500	540
0.001	32.011	4.39×10^6	2500	1200
0.0005	48.801	6.71×10^6	3000	1750

[a]Integration time, [b]time after which the function gets damped.

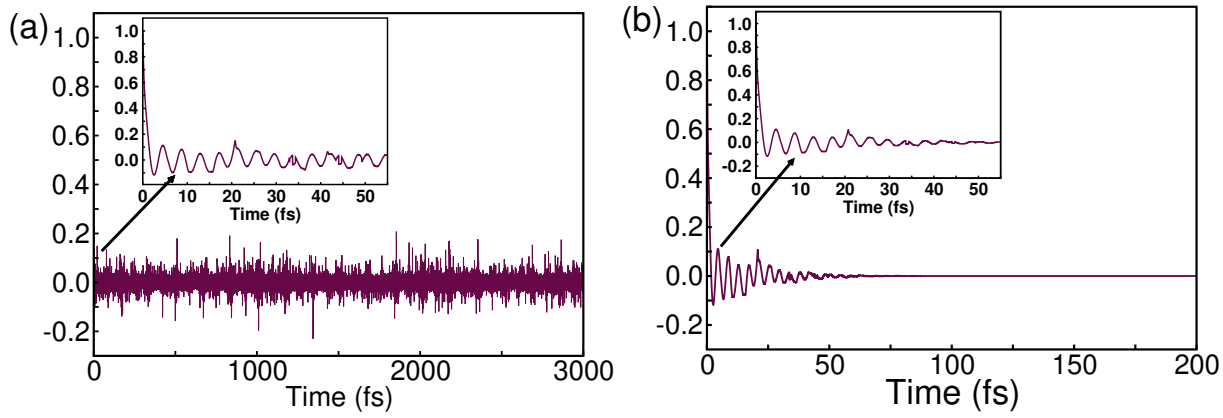

FIG. S1. The real parts of the FCWD(τ) function without any damping factor in (a) and with a Gaussian damping factor of 0.1 cm^{-1} in (b) for the T_1^{ring} structure of 4tThy along the to56 direction and D=3.0 Å.

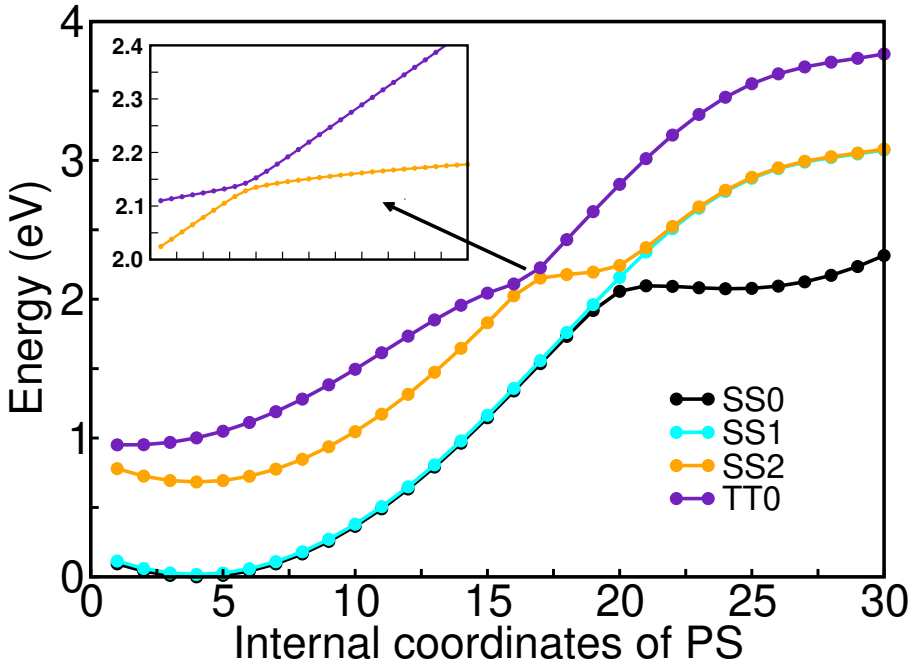

FIG. S2. Calculated adiabatic energies of states for the PS–O_2 composite system, along the internal coordinates of the PS which promote crossing. The PS considered here is the T_1^{ring} conformer of 4tThy, along the to4X approach direction, with a D value of 2.5 Å. The inset shows more densely calculated points close to the crossing between the TT0 and SS2 states. The diabatic coupling given as half of the energy gap at the crossing is 58.2 cm^{-1}. The diabatic coupling calculated in the D space at this D is 27.6 cm^{-1}.

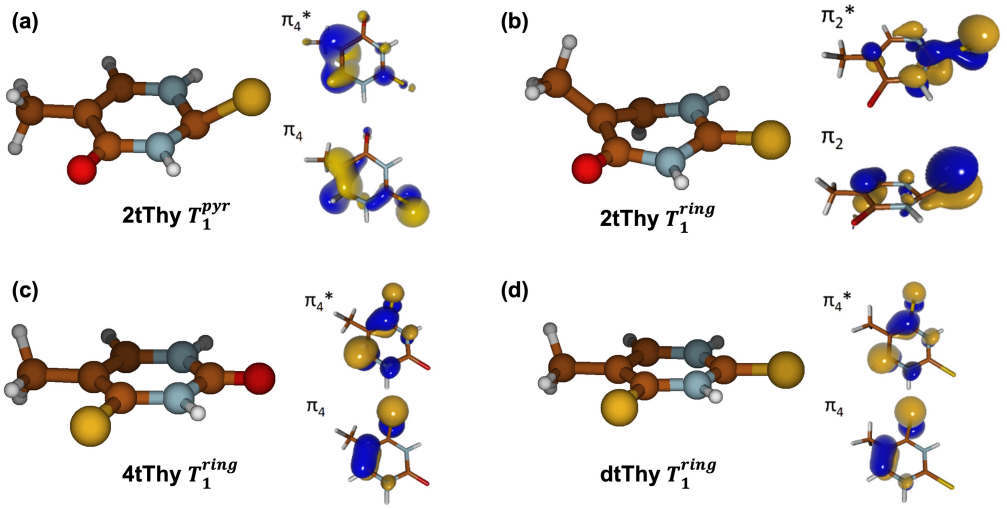

FIG. S3. T_1 minima of the thiothymines studied in this work. Brown, gray, blue, red and yellow atoms indicate C, H, N, O and S. The orbitals involved in the respective T_1 minima are shown alongside the structures.

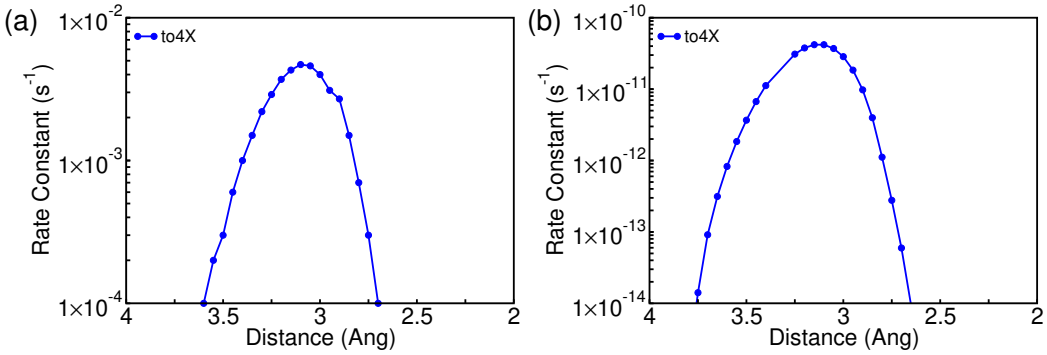

FIG. S4. Photosensitizing rate constants along the to4X direction as a function of D calculated using MT-FGR for T_1^{ring} minima of (a) 4tThy and (b) dtThy.

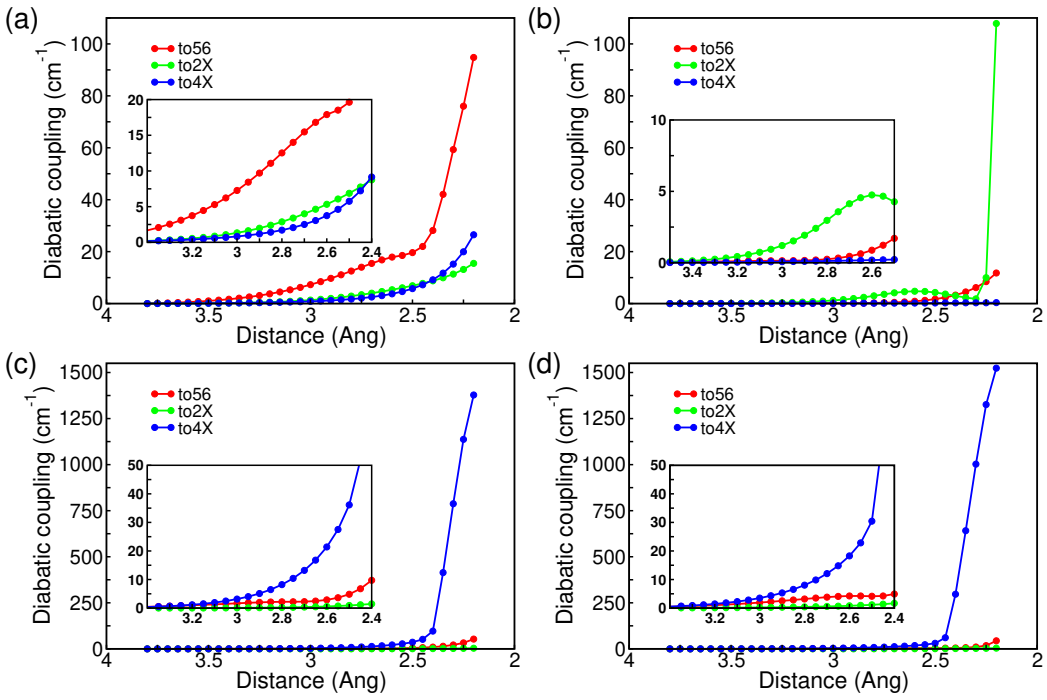

FIG. S5. Diabatic couplings plotted as a function of D for (a) T_1^{ring} and (b) T_1^{pyr} minima of 2tThy, and T_1^{ring} minimum of (c) 4tThy and (d) dtThy, for all 3 approach directions. Insets are shown for greater clarity.

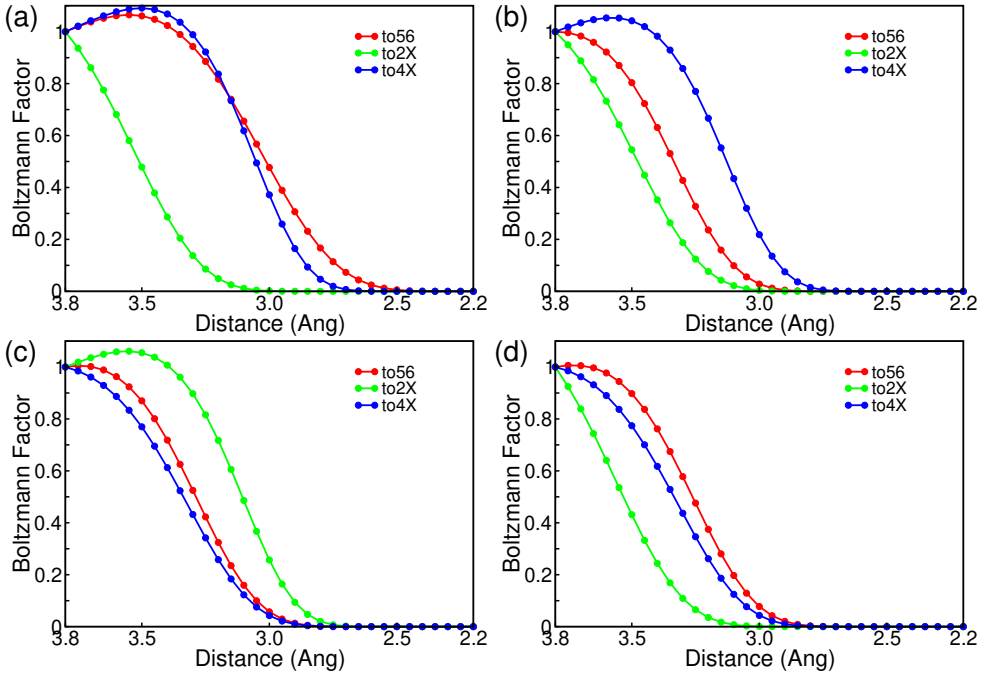

FIG. S6. Boltzmann factors plotted as a function of D for (a) T_1^{ring} and (b) T_1^{pyr} minima of 2tThy, and T_1^{ring} minimum of (c) 4tThy and (d) dtThy, for all 3 approach directions.

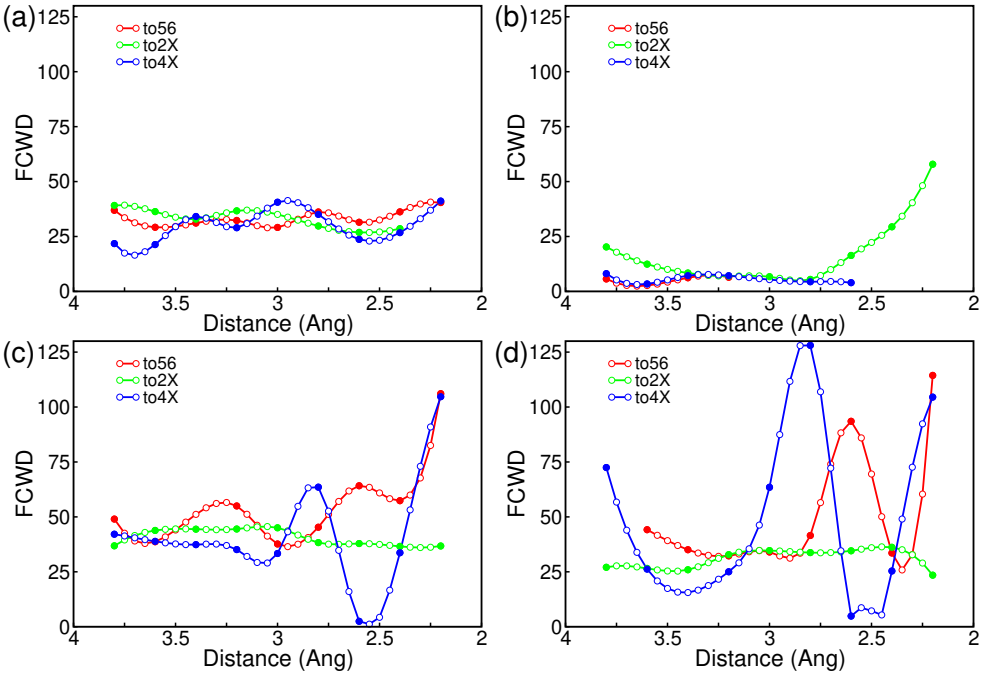

FIG. S7. *FCWD* values plotted as a function of D for (a) T_1^{ring} and (b) T_1^{pyr} minima of 2tThy, and T_1^{ring} minimum of (c) 4tThy and (d) dtThy, for all 3 approach directions. Filled circles indicate values where FCWD is calculated explicitly and unfilled circles indicate values where FCWD is interpolated.

Given below are geometries of the PS-O2 complexes for all
thiothymine studied in this work, given in internal coordinates

D=3.8 Angstrom for all structures given. The smallest D
considered in this study is 2.2 Angstrom

2tThy T1_ring to56

```
geometry={
 c
 n      1 nc2
 c      2 cn3          1 cnc3
 n      3 nc4          2 ncn4         1 dih4
 c      4 cn5          3 cnc5         2 dih5
 c      5 cc6          4 ccn6         3 dih6
 s      3 sc7          2 scn7         1 dih7
 o      5 oc8          4 ocn8         3 dih8
 c      6 cc9          5 ccc9         4 dih9
 h      9 hc10         6 hcc10        5 dih10
 h      9 hc11         6 hcc11        5 dih11
 h      9 hc12         6 hcc12        5 dih12
 h      4 hn13         3 hnc13        2 dih13
 h      2 hn14         3 hnc14        4 dih14
 h      1 hc15         2 hcn15        3 dih15
 o      6 oc16         5 occ16        4 dih16
 o      16 oo17         6 ooc17        1 dih17
}

nc2=        1.389068 ANG
cn3=        1.353852 ANG
cnc3=        125.114000 DEGREE
nc4=        1.363948 ANG
ncn4=        115.296000 DEGREE
dih4=        349.223000 DEGREE
cn5=        1.398182 ANG
cnc5=        125.974000 DEGREE
dih5=        346.666000 DEGREE
cc6=        1.441623 ANG
ccn6=        115.750000 DEGREE
dih6=        15.259000 DEGREE
sc7=        1.656716 ANG
scn7=        122.242000 DEGREE
dih7=        169.354000 DEGREE
oc8=        1.211626 ANG
ocn8=        119.562000 DEGREE
dih8=        194.513000 DEGREE
cc9=        1.490007 ANG
ccc9=        122.242000 DEGREE
dih9=        187.610000 DEGREE
hc10=        1.088545 ANG
hcc10=        110.600000 DEGREE
dih10=        116.129000 DEGREE
hc11=        1.080598 ANG
hcc11=        110.796000 DEGREE
dih11=        355.413000 DEGREE
hc12=        1.087650 ANG
hcc12=        110.526000 DEGREE
dih12=        234.636000 DEGREE
hn13=        0.996027 ANG
hnc13=        116.217000 DEGREE
dih13=        182.819000 DEGREE
hn14=        0.995308 ANG
hnc14=        114.507000 DEGREE
dih14=        181.704000 DEGREE
hc15=        1.074910 ANG
hcn15=        114.213000 DEGREE
dih15=        167.897000 DEGREE
oc16=        3.800000 ANG
occ16=        90.000000 DEGREE
dih16=        90.000000 DEGREE
oo17=        1.210000 ANG
```

```
ooc17=        95.000000 DEGREE
dih17=        0.000000 DEGREE

2tThy T1_ring to2X

geometry={
 c
 n      1 nc2
 c      2 cn3          1 cnc3
 n      3 nc4          2 ncn4         1 dih4
 c      4 cn5          3 cnc5         2 dih5
 c      5 cc6          4 ccn6         3 dih6
 s      3 sc7          2 scn7         1 dih7
 o      5 oc8          4 ocn8         3 dih8
 c      6 cc9          5 ccc9         4 dih9
 h      9 hc10         6 hcc10        5 dih10
 h      9 hc11         6 hcc11        5 dih11
 h      9 hc12         6 hcc12        5 dih12
 h      4 hn13         3 hnc13        2 dih13
 h      2 hn14         3 hnc14        4 dih14
 h      1 hc15         2 hcn15        3 dih15
 o      7 os16         3 osc16        2 dih16
 o      16 oo17         7 oos17        3 dih17
}

nc2=        1.389068 ANG
cn3=        1.353852 ANG
cnc3=        125.114000 DEGREE
nc4=        1.363948 ANG
ncn4=        115.296000 DEGREE
dih4=        349.223000 DEGREE
cn5=        1.398182 ANG
cnc5=        125.974000 DEGREE
dih5=        346.666000 DEGREE
cc6=        1.441623 ANG
ccn6=        115.750000 DEGREE
dih6=        15.259000 DEGREE
sc7=        1.656716 ANG
scn7=        122.242000 DEGREE
dih7=        169.354000 DEGREE
oc8=        1.211626 ANG
ocn8=        119.562000 DEGREE
dih8=        194.513000 DEGREE
cc9=        1.490007 ANG
ccc9=        122.242000 DEGREE
dih9=        187.610000 DEGREE
hc10=        1.088545 ANG
hcc10=        110.600000 DEGREE
dih10=        116.129000 DEGREE
hc11=        1.080598 ANG
hcc11=        110.796000 DEGREE
dih11=        355.413000 DEGREE
hc12=        1.087650 ANG
hcc12=        110.526000 DEGREE
dih12=        234.636000 DEGREE
hn13=        0.996027 ANG
hnc13=        116.217000 DEGREE
dih13=        182.819000 DEGREE
hn14=        0.995308 ANG
hnc14=        114.507000 DEGREE
dih14=        181.704000 DEGREE
hc15=        1.074910 ANG
hcn15=        114.213000 DEGREE
dih15=        167.897000 DEGREE
os16=        3.800000 ANG
osc16=        90.000000 DEGREE
dih16=        90.000000 DEGREE
oo17=        1.210000 ANG
oos17=        90.000000 DEGREE
dih17=        0.000000 DEGREE
```

2tThy T1_ring to4X

```
geometry={
 c
 n      1 nc2
 c      2 cn3          1 cnc3
 n      3 nc4          2 ncn4         1 dih4
 c      4 cn5          3 cnc5         2 dih5
 c      5 cc6          4 ccn6         3 dih6
 s      3 sc7          2 scn7         1 dih7
 o      5 oc8          4 ocn8         3 dih8
 c      6 cc9          5 ccc9         4 dih9
 h      9 hc10         6 hcc10        5 dih10
 h      9 hc11         6 hcc11        5 dih11
 h      9 hc12         6 hcc12        5 dih12
 h      4 hn13         3 hnc13        2 dih13
 h      2 hn14         3 hnc14        4 dih14
 h      1 hc15         2 hcn15        3 dih15
 o      8 oo16         5 ooc16        6 dih16
 o      16 oo17         8 ooo17        5 dih17
}

nc2=        1.389068 ANG
cn3=        1.353852 ANG
cnc3=        125.114000 DEGREE
nc4=        1.363948 ANG
ncn4=        115.296000 DEGREE
dih4=        349.223000 DEGREE
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cnc5=        125.974000 DEGREE
dih5=        346.666000 DEGREE
cc6=        1.441623 ANG
ccn6=        115.750000 DEGREE
dih6=        15.259000 DEGREE
sc7=        1.656716 ANG
scn7=        122.242000 DEGREE
dih7=        169.354000 DEGREE
oc8=        1.211626 ANG
ocn8=        119.562000 DEGREE
dih8=        194.513000 DEGREE
cc9=        1.490007 ANG
ccc9=        122.242000 DEGREE
dih9=        187.610000 DEGREE
hc10=        1.088545 ANG
hcc10=        110.600000 DEGREE
dih10=        116.129000 DEGREE
hc11=        1.080598 ANG
hcc11=        110.796000 DEGREE
dih11=        355.413000 DEGREE
hc12=        1.087650 ANG
hcc12=        110.526000 DEGREE
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hnc13=        116.217000 DEGREE
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hnc14=        114.507000 DEGREE
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hc15=        1.074910 ANG
hcn15=        114.213000 DEGREE
dih15=        167.897000 DEGREE
oo16=        3.800000 ANG
ooc16=        90.000000 DEGREE
dih16=        90.000000 DEGREE
oo17=        1.210000 ANG
ooo17=        90.000000 DEGREE
dih17=        0.000000 DEGREE
```

2tThy T1_pyr to56

```
geometry={
```

```
 c
 n      1 nc2
 c      2 cn3          1 cnc3
 n      3 nc4          2 ncn4         1 dih4
 c      4 cn5          3 cnc5         2 dih5
 c      5 cc6          4 ccn6         3 dih6
 s      3 sc7          2 scn7         1 dih7
 o      5 oc8          4 ocn8         3 dih8
 c      6 cc9          5 ccc9         4 dih9
 h      9 hc10         6 hcc10        5 dih10
 h      9 hc11         6 hcc11        5 dih11
 h      9 hc12         6 hcc12        5 dih12
 h      4 hn13         3 hnc13        2 dih13
 h      2 hn14         3 hnc14        4 dih14
 h      1 hc15         2 hcn15        3 dih15
 o      6 oc16         5 occ16        4 dih16
 o      16 oo17         6 ooc17        1 dih17
}

nc2=        1.377667 ANG
cn3=        1.388245 ANG
cnc3=        122.460000 DEGREE
nc4=        1.397746 ANG
ncn4=        113.037000 DEGREE
dih4=        344.825000 DEGREE
cn5=        1.379316 ANG
cnc5=        126.541000 DEGREE
dih5=        16.101000 DEGREE
cc6=        1.474617 ANG
ccn6=        115.383000 DEGREE
dih6=        350.993000 DEGREE
sc7=        1.818599 ANG
scn7=        111.801000 DEGREE
dih7=        211.706000 DEGREE
oc8=        1.206515 ANG
ocn8=        120.862000 DEGREE
dih8=        171.944000 DEGREE
cc9=        1.502361 ANG
ccc9=        118.181000 DEGREE
dih9=        181.315000 DEGREE
hc10=        1.084472 ANG
hcc10=        110.888000 DEGREE
dih10=        58.975000 DEGREE
hc11=        1.084469 ANG
hcc11=        110.864000 DEGREE
dih11=        300.036000 DEGREE
hc12=        1.084344 ANG
hcc12=        110.842000 DEGREE
dih12=        179.514000 DEGREE
hn13=        0.995137 ANG
hnc13=        117.350000 DEGREE
dih13=        185.247000 DEGREE
hn14=        0.992901 ANG
hnc14=        116.155000 DEGREE
dih14=        183.985000 DEGREE
hc15=        1.073720 ANG
hcn15=        114.980000 DEGREE
dih15=        187.604000 DEGREE
oc16=        3.800000 ANG
occ16=        90.000000 DEGREE
dih16=        90.000000 DEGREE
oo17=        1.210000 ANG
ooc17=        90.000000 DEGREE
dih17=        0.000000 DEGREE

2tThy T1_pyr to2X

geometry={
 c
 n      1 nc2
 c      2 cn3          1 cnc3
```

```
 n      3 nc4          2 ncn4         1 dih4
 c      4 cn5          3 cnc5         2 dih5
 c      5 cc6          4 ccn6         3 dih6
 s      3 sc7          2 scn7         1 dih7
 o      5 oc8          4 ocn8         3 dih8
 c      6 cc9          5 ccc9         4 dih9
 h      9 hc10         6 hcc10        5 dih10
 h      9 hc11         6 hcc11        5 dih11
 h      9 hc12         6 hcc12        5 dih12
 h      4 hn13         3 hnc13        2 dih13
 h      2 hn14         3 hnc14        4 dih14
 h      1 hc15         2 hcn15        3 dih15
 o      7 os16         3 osc16        2 dih16
 o      16 oo17         7 oos17        3 dih17
}

nc2=         1.377667 ANG
cn3=         1.388245 ANG
cnc3=         122.460000 DEGREE
nc4=         1.397746 ANG
ncn4=         113.037000 DEGREE
dih4=         344.825000 DEGREE
cn5=         1.379316 ANG
cnc5=         126.541000 DEGREE
dih5=         16.101000 DEGREE
cc6=         1.474617 ANG
ccn6=         115.383000 DEGREE
dih6=         350.993000 DEGREE
sc7=         1.818599 ANG
scn7=         111.801000 DEGREE
dih7=         211.706000 DEGREE
oc8=         1.206515 ANG
ocn8=         120.862000 DEGREE
dih8=         171.944000 DEGREE
cc9=         1.502361 ANG
ccc9=         118.181000 DEGREE
dih9=         181.315000 DEGREE
hc10=         1.084472 ANG
hcc10=         110.888000 DEGREE
dih10=         58.975000 DEGREE
hc11=         1.084469 ANG
hcc11=         110.864000 DEGREE
dih11=         300.036000 DEGREE
hc12=         1.084344 ANG
hcc12=         110.842000 DEGREE
dih12=         179.514000 DEGREE
hn13=         0.995137 ANG
hnc13=         117.350000 DEGREE
dih13=         185.247000 DEGREE
hn14=         0.992901 ANG
hnc14=         116.155000 DEGREE
dih14=         183.985000 DEGREE
hc15=         1.073720 ANG
hcn15=         114.980000 DEGREE
dih15=         187.604000 DEGREE
os16=         3.800000 ANG
osc16=         90.000000 DEGREE
dih16=         65.000000 DEGREE
oo17=         1.210000 ANG
oos17=         87.500000 DEGREE
dih17=         0.000000 DEGREE

2tThy T1_pyr to4X

geometry={
 c
 n      1 nc2
 c      2 cn3          1 cnc3
 n      3 nc4          2 ncn4         1 dih4
 c      4 cn5          3 cnc5         2 dih5
 c      5 cc6          4 ccn6         3 dih6
```

```
 s      3 sc7          2 scn7         1 dih7
 o      5 oc8          4 ocn8         3 dih8
 c      6 cc9          5 ccc9         4 dih9
 h      9 hc10         6 hcc10        5 dih10
 h      9 hc11         6 hcc11        5 dih11
 h      9 hc12         6 hcc12        5 dih12
 h      4 hn13         3 hnc13        2 dih13
 h      2 hn14         3 hnc14        4 dih14
 h      1 hc15         2 hcn15        3 dih15
 o      8 oo16         5 ooc16        6 dih16
 o      16 oo17         8 ooo17        5 dih17
}

nc2=        1.377667 ANG
cn3=        1.388245 ANG
cnc3=        122.460000 DEGREE
nc4=        1.397746 ANG
ncn4=        113.037000 DEGREE
dih4=        344.825000 DEGREE
cn5=        1.379316 ANG
cnc5=        126.541000 DEGREE
dih5=        16.101000 DEGREE
cc6=        1.474617 ANG
ccn6=        115.383000 DEGREE
dih6=        350.993000 DEGREE
sc7=        1.818599 ANG
scn7=        111.801000 DEGREE
dih7=        211.706000 DEGREE
oc8=        1.206515 ANG
ocn8=        120.862000 DEGREE
dih8=        171.944000 DEGREE
cc9=        1.502361 ANG
ccc9=        118.181000 DEGREE
dih9=        181.315000 DEGREE
hc10=        1.084472 ANG
hcc10=        110.888000 DEGREE
dih10=        58.975000 DEGREE
hc11=        1.084469 ANG
hcc11=        110.864000 DEGREE
dih11=        300.036000 DEGREE
hc12=        1.084344 ANG
hcc12=        110.842000 DEGREE
dih12=        179.514000 DEGREE
hn13=        0.995137 ANG
hnc13=        117.350000 DEGREE
dih13=        185.247000 DEGREE
hn14=        0.992901 ANG
hnc14=        116.155000 DEGREE
dih14=        183.985000 DEGREE
hc15=        1.073720 ANG
hcn15=        114.980000 DEGREE
dih15=        187.604000 DEGREE
oo16=        3.800000 ANG
ooc16=        90.000000 DEGREE
dih16=        90.000000 DEGREE
oo17=        1.210000 ANG
ooo17=        90.000000 DEGREE
dih17=        0.000000 DEGREE

4tThy T1_ring to56

geometry={
 c
 n      1 nc2
 c      2 cn3          1 cnc3
 n      3 nc4          2 ncn4         1 dih4
 c      4 cn5          3 cnc5         2 dih5
 c      5 cc6          4 ccn6         3 dih6
 o      3 oc7          2 ocn7         1 dih7
 s      5 sc8          4 scn8         3 dih8
 c      6 cc9          5 ccc9         4 dih9
```

```
 h      9 hc10         6 hcc10        5 dih10
 h      9 hc11         6 hcc11        5 dih11
 h      9 hc12         6 hcc12        5 dih12
 h      4 hn13         3 hnc13        2 dih13
 h      2 hn14         3 hnc14        4 dih14
 h      1 hc15         2 hcn15        3 dih15
 o      6 oc16         5 occ16        4 dih16
 o      16 oo17         6 ooc17        1 dih17
}

nc2=        1.389237 ANG
cn3=        1.370827 ANG
cnc3=        124.437000 DEGREE
nc4=        1.369467 ANG
ncn4=        114.189000 DEGREE
dih4=        359.583000 DEGREE
cn5=        1.403419 ANG
cnc5=        124.924000 DEGREE
dih5=        0.439000 DEGREE
cc6=        1.376884 ANG
ccn6=        119.453000 DEGREE
dih6=        359.657000 DEGREE
oc7=        1.202657 ANG
ocn7=        122.822000 DEGREE
dih7=        179.600000 DEGREE
sc8=        1.766416 ANG
scn8=        115.290000 DEGREE
dih8=        177.691000 DEGREE
cc9=        1.509355 ANG
ccc9=        123.861000 DEGREE
dih9=        178.285000 DEGREE
hc10=        1.080934 ANG
hcc10=        111.652000 DEGREE
dih10=        37.245000 DEGREE
hc11=        1.085441 ANG
hcc11=        111.093000 DEGREE
dih11=        276.808000 DEGREE
hc12=        1.083936 ANG
hcc12=        110.116000 DEGREE
dih12=        157.445000 DEGREE
hn13=        0.993278 ANG
hnc13=        115.635000 DEGREE
dih13=        178.824000 DEGREE
hn14=        0.993131 ANG
hnc14=        115.019000 DEGREE
dih14=        179.921000 DEGREE
hc15=        1.068959 ANG
hcn15=        116.837000 DEGREE
dih15=        179.087000 DEGREE
oc16=        3.800000 ANG
occ16=        90.000000 DEGREE
dih16=        90.000000 DEGREE
oo17=        1.210000 ANG
ooc17=        90.000000 DEGREE
dih17=        0.000000 DEGREE

4tThy T1_ring to2X

geometry={
 c
 n      1 nc2
 c      2 cn3          1 cnc3
 n      3 nc4          2 ncn4         1 dih4
 c      4 cn5          3 cnc5         2 dih5
 c      5 cc6          4 ccn6         3 dih6
 o      3 oc7          2 ocn7         1 dih7
 s      5 sc8          4 scn8         3 dih8
 c      6 cc9          5 ccc9         4 dih9
 h      9 hc10         6 hcc10        5 dih10
 h      9 hc11         6 hcc11        5 dih11
 h      9 hc12         6 hcc12        5 dih12
```

```
 h      4 hn13          3 hnc13         2 dih13
 h      2 hn14          3 hnc14         4 dih14
 h      1 hc15          2 hcn15         3 dih15
 o      7 oo16          3 ooc16         2 dih16
 o      16 oo17          7 ooo17         3 dih17
}

nc2=         1.389237 ANG
cn3=         1.370827 ANG
cnc3=         124.437000 DEGREE
nc4=         1.369467 ANG
ncn4=         114.189000 DEGREE
dih4=         359.583000 DEGREE
cn5=         1.403419 ANG
cnc5=         124.924000 DEGREE
dih5=         0.439000 DEGREE
cc6=         1.376884 ANG
ccn6=         119.453000 DEGREE
dih6=         359.657000 DEGREE
oc7=         1.202657 ANG
ocn7=         122.822000 DEGREE
dih7=         179.600000 DEGREE
sc8=         1.766416 ANG
scn8=         115.290000 DEGREE
dih8=         177.691000 DEGREE
cc9=         1.509355 ANG
ccc9=         123.861000 DEGREE
dih9=         178.285000 DEGREE
hc10=         1.080934 ANG
hcc10=         111.652000 DEGREE
dih10=         37.245000 DEGREE
hc11=         1.085441 ANG
hcc11=         111.093000 DEGREE
dih11=         276.808000 DEGREE
hc12=         1.083936 ANG
hcc12=         110.116000 DEGREE
dih12=         157.445000 DEGREE
hn13=         0.993278 ANG
hnc13=         115.635000 DEGREE
dih13=         178.824000 DEGREE
hn14=         0.993131 ANG
hnc14=         115.019000 DEGREE
dih14=         179.921000 DEGREE
hc15=         1.068959 ANG
hcn15=         116.837000 DEGREE
dih15=         179.087000 DEGREE
oo16=         3.800000 ANG
ooc16=         90.000000 DEGREE
dih16=         90.000000 DEGREE
oo17=         1.210000 ANG
ooo17=         90.000000 DEGREE
dih17=         0.000000 DEGREE

4tThy T1_ring to4X

geometry={
 c
 n      1 nc2
 c      2 cn3           1 cnc3
 n      3 nc4           2 ncn4          1 dih4
 c      4 cn5           3 cnc5          2 dih5
 c      5 cc6           4 ccn6          3 dih6
 o      3 oc7           2 ocn7          1 dih7
 s      5 sc8           4 scn8          3 dih8
 c      6 cc9           5 ccc9          4 dih9
 h      9 hc10          6 hcc10         5 dih10
 h      9 hc11          6 hcc11         5 dih11
 h      9 hc12          6 hcc12         5 dih12
 h      4 hn13          3 hnc13         2 dih13
 h      2 hn14          3 hnc14         4 dih14
 h      1 hc15          2 hcn15         3 dih15
```

```
 o      8 os16         5 osc16        6 dih16
 o      16 oo17         8 oos17        5 dih17
}

nc2=         1.389237 ANG
cn3=         1.370827 ANG
cnc3=         124.437000 DEGREE
nc4=         1.369467 ANG
ncn4=         114.189000 DEGREE
dih4=         359.583000 DEGREE
cn5=         1.403419 ANG
cnc5=         124.924000 DEGREE
dih5=         0.439000 DEGREE
cc6=         1.376884 ANG
ccn6=         119.453000 DEGREE
dih6=         359.657000 DEGREE
oc7=         1.202657 ANG
ocn7=         122.822000 DEGREE
dih7=         179.600000 DEGREE
sc8=         1.766416 ANG
scn8=         115.290000 DEGREE
dih8=         177.691000 DEGREE
cc9=         1.509355 ANG
ccc9=         123.861000 DEGREE
dih9=         178.285000 DEGREE
hc10=         1.080934 ANG
hcc10=         111.652000 DEGREE
dih10=         37.245000 DEGREE
hc11=         1.085441 ANG
hcc11=         111.093000 DEGREE
dih11=         276.808000 DEGREE
hc12=         1.083936 ANG
hcc12=         110.116000 DEGREE
dih12=         157.445000 DEGREE
hn13=         0.993278 ANG
hnc13=         115.635000 DEGREE
dih13=         178.824000 DEGREE
hn14=         0.993131 ANG
hnc14=         115.019000 DEGREE
dih14=         179.921000 DEGREE
hc15=         1.068959 ANG
hcn15=         116.837000 DEGREE
dih15=         179.087000 DEGREE
os16=         3.800000 ANG
osc16=         90.000000 DEGREE
dih16=         90.000000 DEGREE
oo17=         1.210000 ANG
oos17=         87.500000 DEGREE
dih17=         0.000000 DEGREE

dtThy T1_ring to56

geometry={
 c
 n      1 nc2
 c      2 cn3          1 cnc3
 n      3 nc4          2 ncn4         1 dih4
 c      4 cn5          3 cnc5         2 dih5
 c      5 cc6          4 ccn6         3 dih6
 s      3 sc7          2 scn7         1 dih7
 s      5 sc8          4 scn8         3 dih8
 c      6 cc9          5 ccc9         4 dih9
 h      9 hc10         6 hcc10        5 dih10
 h      9 hc11         6 hcc11        5 dih11
 h      9 hc12         6 hcc12        5 dih12
 h      4 hn13         3 hnc13        2 dih13
 h      2 hn14         3 hnc14        4 dih14
 h      1 hc15         2 hcn15        3 dih15
 o      6 oc16         5 occ16        4 dih16
 o      16 oo17         6 ooc17        1 dih17
}
```

```
nc2=        1.390965 ANG
cn3=        1.347412 ANG
cnc3=        124.705000 DEGREE
nc4=        1.345660 ANG
ncn4=        114.863000 DEGREE
dih4=        0.144000 DEGREE
cn5=        1.407899 ANG
cnc5=        125.122000 DEGREE
dih5=        0.156000 DEGREE
cc6=        1.376121 ANG
ccn6=        118.897000 DEGREE
dih6=        359.691000 DEGREE
sc7=        1.675227 ANG
scn7=        122.437000 DEGREE
dih7=        180.167000 DEGREE
sc8=        1.763966 ANG
scn8=        115.086000 DEGREE
dih8=        181.447000 DEGREE
cc9=        1.508233 ANG
ccc9=        124.012000 DEGREE
dih9=        182.013000 DEGREE
hc10=        1.085541 ANG
hcc10=        110.659000 DEGREE
dih10=        89.280000 DEGREE
hc11=        1.080268 ANG
hcc11=        111.674000 DEGREE
dih11=        328.936000 DEGREE
hc12=        1.083855 ANG
hcc12=        110.126000 DEGREE
dih12=        208.472000 DEGREE
hn13=        0.994691 ANG
hnc13=        116.052000 DEGREE
dih13=        180.488000 DEGREE
hn14=        0.994384 ANG
hnc14=        115.293000 DEGREE
dih14=        180.029000 DEGREE
hc15=        1.068495 ANG
hcn15=        116.792000 DEGREE
dih15=        180.420000 DEGREE
oc16=        3.800000 ANG
occ16=        90.000000 DEGREE
dih16=        90.000000 DEGREE
oo17=        1.210000 ANG
ooc17=        90.000000 DEGREE
dih17=        0.000000 DEGREE

dtThy T1_ring to2X

geometry={
 c
 n      1 nc2
 c      2 cn3          1 cnc3
 n      3 nc4          2 ncn4         1 dih4
 c      4 cn5          3 cnc5         2 dih5
 c      5 cc6          4 ccn6         3 dih6
 s      3 sc7          2 scn7         1 dih7
 s      5 sc8          4 scn8         3 dih8
 c      6 cc9          5 ccc9         4 dih9
 h      9 hc10         6 hcc10        5 dih10
 h      9 hc11         6 hcc11        5 dih11
 h      9 hc12         6 hcc12        5 dih12
 h      4 hn13         3 hnc13        2 dih13
 h      2 hn14         3 hnc14        4 dih14
 h      1 hc15         2 hcn15        3 dih15
 o      7 os16         3 osc16        2 dih16
 o      16 oo17         7 oos17        3 dih17
}

nc2=        1.390965 ANG
cn3=        1.347412 ANG
```

```
cnc3=        124.705000 DEGREE
nc4=        1.345660 ANG
ncn4=        114.863000 DEGREE
dih4=        0.144000 DEGREE
cn5=        1.407899 ANG
cnc5=        125.122000 DEGREE
dih5=        0.156000 DEGREE
cc6=        1.376121 ANG
ccn6=        118.897000 DEGREE
dih6=        359.691000 DEGREE
sc7=        1.675227 ANG
scn7=        122.437000 DEGREE
dih7=        180.167000 DEGREE
sc8=        1.763966 ANG
scn8=        115.086000 DEGREE
dih8=        181.447000 DEGREE
cc9=        1.508233 ANG
ccc9=        124.012000 DEGREE
dih9=        182.013000 DEGREE
hc10=        1.085541 ANG
hcc10=        110.659000 DEGREE
dih10=        89.280000 DEGREE
hc11=        1.080268 ANG
hcc11=        111.674000 DEGREE
dih11=        328.936000 DEGREE
hc12=        1.083855 ANG
hcc12=        110.126000 DEGREE
dih12=        208.472000 DEGREE
hn13=        0.994691 ANG
hnc13=        116.052000 DEGREE
dih13=        180.488000 DEGREE
hn14=        0.994384 ANG
hnc14=        115.293000 DEGREE
dih14=        180.029000 DEGREE
hc15=        1.068495 ANG
hcn15=        116.792000 DEGREE
dih15=        180.420000 DEGREE
os16=        3.800000 ANG
osc16=        90.000000 DEGREE
dih16=        90.000000 DEGREE
oo17=        1.210000 ANG
oos17=        90.000000 DEGREE
dih17=        0.000000 DEGREE

dtThy T1_ring to4X

geometry={
 c
 n      1 nc2
 c      2 cn3          1 cnc3
 n      3 nc4          2 ncn4         1 dih4
 c      4 cn5          3 cnc5         2 dih5
 c      5 cc6          4 ccn6         3 dih6
 s      3 sc7          2 scn7         1 dih7
 s      5 sc8          4 scn8         3 dih8
 c      6 cc9          5 ccc9         4 dih9
 h      9 hc10         6 hcc10        5 dih10
 h      9 hc11         6 hcc11        5 dih11
 h      9 hc12         6 hcc12        5 dih12
 h      4 hn13         3 hnc13        2 dih13
 h      2 hn14         3 hnc14        4 dih14
 h      1 hc15         2 hcn15        3 dih15
 o      8 os16         5 osc16        6 dih16
 o      16 oo17         8 oos17        5 dih17
}

nc2=        1.390965 ANG
cn3=        1.347412 ANG
cnc3=        124.705000 DEGREE
nc4=        1.345660 ANG
ncn4=        114.863000 DEGREE
```

```
dih4=        0.144000 DEGREE
cn5=        1.407899 ANG
cnc5=        125.122000 DEGREE
dih5=        0.156000 DEGREE
cc6=        1.376121 ANG
ccn6=        118.897000 DEGREE
dih6=        359.691000 DEGREE
sc7=        1.675227 ANG
scn7=        122.437000 DEGREE
dih7=        180.167000 DEGREE
sc8=        1.763966 ANG
scn8=        115.086000 DEGREE
dih8=        181.447000 DEGREE
cc9=        1.508233 ANG
ccc9=        124.012000 DEGREE
dih9=        182.013000 DEGREE
hc10=        1.085541 ANG
hcc10=        110.659000 DEGREE
dih10=        89.280000 DEGREE
hc11=        1.080268 ANG
hcc11=        111.674000 DEGREE
dih11=        328.936000 DEGREE
hc12=        1.083855 ANG
hcc12=        110.126000 DEGREE
dih12=        208.472000 DEGREE
hn13=        0.994691 ANG
hnc13=        116.052000 DEGREE
dih13=        180.488000 DEGREE
hn14=        0.994384 ANG
hnc14=        115.293000 DEGREE
dih14=        180.029000 DEGREE
hc15=        1.068495 ANG
hcn15=        116.792000 DEGREE
dih15=        180.420000 DEGREE
os16=        3.800000 ANG
osc16=        90.000000 DEGREE
dih16=        90.000000 DEGREE
oo17=        1.210000 ANG
oos17=        87.500000 DEGREE
dih17=        0.000000 DEGREE

Given below is a full run through of obtaining the rate for one case

Case chosen: 4tThy, along to56, D=3.0 Angstrom

1. Optimized geometry for PS-O2 on TT0 (reactant) state
in Cartesian coordinates

  17
 CASSCF/6-31G**  ENERGY=-923.72420547
 C          1.3872302805       -0.8294821734        0.6748727766
 N          0.9062516942       -0.1951180436        1.8230689956
 C         -0.0251373739        0.8021788148        1.8269819800
 N         -0.4127396630        1.2208199696        0.5890503818
 C          0.1029658625        0.7309129346       -0.6348016930
 C          1.0066686962       -0.2909340488       -0.6172047079
 O         -0.4648919027        1.2745989341        2.8386043311
 S         -0.5213910560        1.4992066562       -2.0750198925
 C          1.6422520836       -0.9217075855       -1.8266103672
 H          1.2667050271       -0.5093278942       -2.7503728350
 H          1.4555405626       -1.9910797662       -1.8275966000
 H          2.7185590224       -0.7784166750       -1.8003958069
 H         -1.0651035572        1.9690630091        0.5814004927
 H          1.1515723642       -0.5338965590        2.7238464211
 H          2.2568216480       -1.4419773770        0.7955338859
 O         -1.4093139067       -2.0691781715       -0.6468003560
 O         -1.0918795973       -2.5183923306        0.4309482689

2. Optimized geometry for PS-O2 on SS2 (product) state
in Cartesian coordinates
```

```
 17
MULTI001/6-31G**  ENERGY=-923.76385757
C          1.3521039098       -0.7578756321        0.5902462579
N          0.8686741377       -0.2470698355        1.7847703146
C         -0.0213969470        0.7795637294        1.8467485255
N         -0.3930408385        1.2687597287        0.6179958588
C          0.0273271563        0.8457232126       -0.6275318571
C          0.9760948527       -0.2733640308       -0.6099484131
O         -0.4497366372        1.2252071297        2.8705107399
S         -0.5299594195        1.5757270491       -1.9863636761
C          1.5221611727       -0.8333114839       -1.8954460958
H          2.0591871794       -0.0750255209       -2.4528469634
H          0.7251903045       -1.1996474061       -2.5309612386
H          2.2014293002       -1.6525206981       -1.6884664137
H         -1.0416016098        2.0243023801        0.6542125611
H          1.1509777695       -0.6275864586        2.6577458314
H          2.0440979714       -1.5707503706        0.6895871999
O         -1.2935078292       -2.2335828927       -0.6902334016
O         -0.9559456079       -2.6685532991        0.3872416526
```

3. Normal modes for PS-O2 on TT0 (reactant) state

Normal Modes

	1 A	2 A	3 A	4 A	5 A
Wavenumbers [cm-1]	101.98	107.89	123.77	192.00	219.17
Intensities [km/mol]	0.86	0.54	0.19	12.69	0.06
Intensities [relative]	0.08	0.05	0.02	1.12	0.01
CX1	0.05413	-0.01904	0.06365	0.11755	-0.00266
CY1	0.04558	-0.02007	0.05949	0.10715	-0.00678
CZ1	0.00191	0.00034	0.00725	-0.01433	-0.00738
NX2	-0.01174	-0.00825	0.12394	-0.07514	0.00292
NY2	-0.01154	-0.00649	0.11486	-0.07290	-0.00865
NZ2	0.00546	-0.00178	0.00298	-0.00043	-0.00381
CX3	0.01899	0.00116	0.00310	-0.01644	0.00524
CY3	0.01718	0.00112	0.00447	-0.02116	-0.00673
CZ3	0.00365	-0.00186	0.00256	-0.00327	0.00334
NX4	0.10313	-0.06145	-0.04074	-0.06722	0.00524
NY4	0.09499	-0.05693	-0.04072	-0.07773	0.00286
NZ4	0.00495	-0.00281	0.00147	-0.00775	0.00643
CX5	0.04911	-0.00785	-0.01165	-0.01416	-0.00116
CY5	0.04360	-0.00652	-0.01396	-0.02959	0.00547
CZ5	0.00317	-0.00049	0.00169	-0.01183	0.00286
CX6	0.04562	0.01610	0.00775	0.05968	-0.00670
CY6	0.04059	0.01635	0.00096	0.02344	0.00093
CZ6	0.00407	-0.00140	0.00409	-0.00290	-0.00457
OX7	-0.02245	0.05262	-0.05057	0.05533	0.00742
OY7	-0.02141	0.05042	-0.04418	0.05391	-0.01220
OZ7	0.00380	-0.00263	0.00215	-0.00597	0.00689
SX8	-0.03574	-0.00319	0.03443	-0.00731	-0.00701
SY8	-0.03509	0.00002	0.03425	0.03646	0.00384
SZ8	-0.00300	0.00228	0.00373	0.00607	0.00534
CX9	0.04396	0.04004	-0.04863	0.04260	-0.01627
CY9	0.04141	0.03636	-0.05521	-0.03641	0.00643
CZ9	0.00255	0.00156	0.00340	0.01090	-0.01171
HX10	0.10114	0.40039	-0.02424	-0.05667	-0.01497
HY10	0.09762	0.37923	-0.03121	-0.15515	0.01884
HZ10	0.00450	0.00827	0.00411	-0.00353	-0.00649
HX11	-0.01794	-0.36191	-0.14155	0.12773	-0.02634
HY11	0.05209	0.10543	-0.03896	-0.05000	0.00832
HZ11	-0.04376	-0.27572	0.01314	0.12827	-0.02234
HX12	0.05141	0.08724	-0.03676	0.03181	-0.01486
HY12	-0.02189	-0.37561	-0.14816	0.05533	-0.00370
HZ12	0.04592	0.27536	-0.00959	-0.08099	-0.01337
HX13	0.06976	-0.01260	-0.12064	0.05079	0.00543
HY13	0.06572	-0.01394	-0.11075	0.02488	0.00305
HZ13	0.00499	-0.00123	-0.00297	-0.00790	0.01207
HX14	-0.05560	0.03549	0.13638	-0.01440	0.01016
HY14	-0.04904	0.03214	0.12484	-0.03819	-0.00720
HZ14	0.00314	0.00072	0.00381	-0.00461	-0.00532
HX15	0.06436	-0.00303	0.06584	0.06844	0.00149

HY15	0.06200	0.00221	0.06067	0.04979	-0.00234
HZ15	0.00918	0.00233	-0.00375	0.01748	-0.01322
OX16	-0.06339	-0.00704	-0.04263	-0.02218	0.11542
OY16	-0.05945	-0.01118	-0.04173	-0.00958	-0.10940
OZ16	-0.01110	0.00113	-0.01633	0.00398	-0.08056
OX17	-0.09500	-0.01015	-0.05167	-0.04900	-0.09731
OY17	-0.07628	-0.01236	-0.03540	-0.01098	0.11841
OZ17	-0.00882	0.00173	-0.01172	0.01001	0.07686

	6 A	7 A	8 A	9 A	10 A
Wavenumbers [cm-1]	247.82	266.01	295.15	332.39	341.31
Intensities [km/mol]	4.25	18.56	38.29	4.14	41.04
Intensities [relative]	0.37	1.64	3.38	0.37	3.62
CX1	0.00444	0.03971	0.01707	-0.00781	-0.06822
CY1	-0.00778	0.02140	-0.07652	-0.01815	-0.07008
CZ1	0.00303	0.00473	0.03509	0.01022	-0.00093
NX2	-0.00032	-0.03323	-0.01669	0.00011	0.01433
NY2	0.00365	-0.02655	-0.00736	0.01248	0.00375
NZ2	-0.00357	0.00056	-0.00131	0.01127	-0.01402
CX3	-0.00284	-0.01237	-0.00735	-0.01948	-0.00537
CY3	0.00147	-0.00765	0.00336	0.00080	-0.01875
CZ3	-0.00005	0.02328	-0.03296	-0.00552	-0.00065
NX4	-0.01625	-0.03762	0.03832	-0.03490	-0.05652
NY4	-0.00192	0.01581	0.00002	-0.05774	-0.02606
NZ4	0.00229	0.03078	-0.03405	-0.01129	0.00301
CX5	-0.00732	-0.04679	0.01556	0.11114	0.08816
CY5	0.00590	0.00963	-0.04036	0.04775	0.12217
CZ5	0.00554	0.02942	-0.00339	0.02212	-0.00557
CX6	-0.00808	-0.02644	0.00043	0.09825	0.04135
CY6	0.01179	0.04479	-0.03462	0.03885	0.08774
CZ6	-0.00234	0.00575	-0.01164	0.00446	-0.00079
OX7	0.00810	0.03287	-0.03988	-0.03858	0.03207
OY7	0.00386	-0.01487	0.04251	0.04702	-0.03560
OZ7	0.00320	0.04560	-0.06625	-0.03607	0.02337
SX8	0.00681	0.07311	-0.01233	0.00898	-0.02850
SY8	-0.02180	-0.05870	0.02139	-0.03469	0.00734
SZ8	-0.00498	-0.03937	0.06988	0.04717	-0.03640
CX9	-0.04271	-0.08580	-0.01010	-0.06397	0.00643
CY9	0.00895	0.06992	-0.01154	0.03523	-0.05751
CZ9	-0.01661	-0.03516	-0.02341	-0.08583	0.06631
HX10	-0.06150	-0.11829	-0.01261	-0.20664	0.00331
HY10	0.01140	0.09199	0.01727	0.05456	-0.18279
HZ10	-0.00700	-0.00908	-0.00984	-0.01797	0.01086
HX11	-0.05418	-0.09834	-0.01664	-0.09592	-0.02759
HY11	0.01070	0.07151	-0.01078	0.04065	-0.05140
HZ11	-0.00961	-0.04638	-0.04655	-0.07309	0.23361
HX12	-0.03985	-0.08140	-0.00720	-0.05620	0.01256
HY12	-0.00375	0.05399	-0.02251	0.00802	-0.09481
HZ12	-0.04396	-0.07798	-0.02556	-0.26497	0.02884
HX13	-0.00189	0.00923	0.01498	0.11680	0.08249
HY13	0.01103	0.05822	-0.02137	0.07466	0.09576
HZ13	0.00452	0.04511	-0.05784	-0.02902	0.02366
HX14	0.01734	-0.02055	0.00398	-0.03707	0.01156
HY14	0.02431	-0.01836	0.05513	-0.01480	0.00899
HZ14	-0.00043	0.00042	0.01754	0.01123	-0.01038
HX15	0.10062	0.25154	0.45665	-0.17708	0.18086
HY15	0.12258	0.30948	0.52377	-0.24322	0.26037
HZ15	-0.00942	-0.02750	0.01219	0.06242	-0.04166
OX16	0.14193	-0.04244	-0.00843	-0.01273	-0.00719
OY16	0.11839	-0.02467	-0.00642	-0.01109	-0.01075
OZ16	0.02032	-0.00510	-0.00514	0.00092	0.00004
OX17	-0.10424	0.02760	0.01470	0.00383	0.00577
OY17	-0.10645	0.02717	0.01323	-0.00019	0.00119
OZ17	-0.00045	-0.00281	-0.00351	0.00122	-0.00010

	11 A	12 A	13 A	14 A	15 A
Wavenumbers [cm-1]	454.29	480.44	512.49	553.50	573.88
Intensities [km/mol]	2.36	39.94	31.36	65.92	27.48
Intensities [relative]	0.21	3.52	2.77	5.81	2.42
CX1	-0.01576	0.03219	-0.02759	0.00803	0.06087
CY1	0.02334	0.02473	0.01147	0.05081	0.02388

CZ1	-0.06949	-0.00704	0.00043	-0.04690	0.03079
NX2	-0.05170	0.03549	-0.02750	0.01118	-0.01788
NY2	0.03695	0.03453	0.04313	-0.05928	0.00831
NZ2	-0.10811	-0.02169	0.02136	0.02761	-0.01186
CX3	-0.04254	-0.00534	-0.03601	0.01850	-0.00431
CY3	0.04147	-0.00156	0.03359	-0.04826	0.01951
CZ3	-0.02833	-0.02606	0.08896	0.03700	-0.03661
NX4	-0.04414	-0.04404	0.00451	0.02278	-0.04352
NY4	0.06270	-0.00735	-0.02213	-0.04419	-0.00548
NZ4	-0.00809	-0.01272	0.03318	0.03624	-0.02741
CX5	0.00060	-0.00104	0.05785	0.04005	0.12667
CY5	0.01771	0.00242	-0.01644	0.10104	0.08520
CZ5	0.02613	0.00682	-0.00539	0.00342	0.00709
CX6	-0.00420	-0.06469	0.00591	-0.11543	-0.08281
CY6	0.00944	-0.05737	-0.07924	-0.01480	-0.11575
CZ6	-0.04924	0.01206	-0.06183	-0.04909	0.04084
OX7	0.02697	-0.00494	-0.02339	-0.05527	0.04550
OY7	-0.03029	-0.02848	0.01861	0.05459	-0.02290
OZ7	0.03551	-0.01614	0.11540	-0.04409	0.00246
SX8	0.03310	0.00115	-0.01245	0.01311	-0.00953
SY8	-0.04310	-0.00401	0.01279	-0.02095	0.00282
SZ8	0.08633	0.01780	-0.03438	0.00909	-0.00464
CX9	0.04211	0.00005	0.05706	-0.00046	-0.01994
CY9	-0.04615	0.00363	-0.04900	-0.00209	0.01676
CZ9	-0.00999	0.02736	-0.11751	0.00608	0.01426
HX10	0.09996	0.05607	0.04912	0.09426	-0.02144
HY10	-0.11024	0.04088	-0.00008	-0.03717	0.10436
HZ10	-0.06252	0.02207	-0.09467	-0.04855	0.05431
HX11	0.03966	0.04182	0.08978	0.05894	0.06257
HY11	-0.04585	-0.00337	-0.05355	-0.01276	0.00396
HZ11	0.06462	-0.04622	-0.19015	0.01577	-0.12663
HX12	0.04128	-0.00768	0.05127	-0.00931	-0.03262
HY12	-0.05088	0.04359	-0.01090	0.05185	0.10253
HZ12	0.05436	0.11590	-0.10880	0.14329	0.05723
HX13	-0.12186	0.60756	0.11290	0.05260	-0.30017
HY13	-0.00503	0.56168	0.07221	-0.01650	-0.23048
HZ13	-0.06767	0.00375	-0.03482	0.10788	-0.05939
HX14	0.08874	-0.18873	0.03456	0.42953	-0.23847
HY14	0.15042	-0.13434	0.02736	0.19236	-0.11265
HZ14	-0.10495	-0.02347	-0.00078	0.00719	0.00315
HX15	-0.04870	0.01109	0.06491	-0.01581	0.04004
HY15	-0.01194	-0.00504	0.14813	0.00857	0.00122
HZ15	-0.02858	-0.01551	0.05762	-0.12546	0.04848
OX16	-0.00086	0.00437	0.00088	-0.00287	-0.00145
OY16	-0.00114	0.00169	0.00095	0.00108	0.00026
OZ16	-0.00011	-0.00077	0.00111	-0.00005	0.00080
OX17	0.00008	0.00212	-0.00073	0.00071	-0.00075
OY17	0.00079	0.00044	-0.00033	0.00008	0.00056
OZ17	0.00075	-0.00205	-0.00037	0.00088	-0.00047

	16 A	17 A	18 A	19 A	20 A
Wavenumbers [cm-1]	581.90	721.11	824.33	847.34	938.11
Intensities [km/mol]	97.75	1.25	3.68	86.38	18.57
Intensities [relative]	8.62	0.11	0.32	7.62	1.64
CX1	0.02925	0.09455	-0.02319	-0.00202	0.11303
CY1	-0.02573	-0.10932	0.01787	-0.00782	-0.10059
CZ1	0.07414	-0.04851	-0.08132	-0.00756	0.01823
NX2	-0.05124	0.03043	-0.01666	-0.05096	0.02993
NY2	-0.00387	-0.03134	0.02280	-0.04168	-0.02821
NZ2	0.00585	-0.07872	-0.09757	-0.01017	0.02489
CX3	-0.03075	-0.01269	-0.03758	0.18460	-0.04319
CY3	-0.01122	0.00930	0.00005	0.17322	0.03964
CZ3	-0.03977	0.01757	0.03865	0.00602	0.03536
NX4	-0.01009	-0.05932	0.07249	-0.03930	-0.00651
NY4	0.03088	0.06717	-0.06874	-0.04907	0.00578
NZ4	-0.04048	0.07138	-0.01557	-0.00352	-0.06787
CX5	0.02245	-0.00008	0.06272	0.00171	-0.01285
CY5	-0.01768	-0.00564	-0.06974	-0.01036	0.02116
CZ5	-0.01587	0.11063	-0.01452	-0.00150	-0.10971
CX6	0.01485	0.02866	0.02650	0.00242	-0.02717
CY6	-0.02871	-0.03511	-0.02521	0.00017	0.02924

CZ6	0.04524	0.04910	0.02736	0.00141	−0.06435
OX7	0.03977	−0.05112	−0.01765	−0.06051	−0.02433
OY7	−0.05999	0.05614	0.03068	−0.04967	0.02869
OZ7	0.00888	−0.01304	0.05410	0.00664	0.08265
SX8	−0.01328	−0.01234	−0.00294	0.00003	0.00227
SY8	0.01620	0.01567	0.00388	0.00057	−0.00345
SZ8	−0.01743	−0.03767	−0.00790	−0.00091	0.01572
CX9	−0.01537	0.01575	−0.05610	−0.00498	−0.03502
CY9	0.02397	−0.01111	0.06009	0.00845	0.03394
CZ9	0.00178	−0.00001	0.11305	0.01089	0.01043
HX10	−0.06561	0.00417	−0.10916	−0.01493	0.09453
HY10	0.08117	0.00372	0.11900	0.00573	−0.10729
HZ10	0.04664	0.01097	0.16378	0.01384	−0.10348
HX11	0.00335	0.02685	−0.04934	−0.01380	−0.02486
HY11	0.02008	−0.01242	0.06118	0.01008	0.02905
HZ11	−0.05739	−0.02496	0.06156	0.02100	0.17581
HX12	−0.01527	0.01458	−0.05834	−0.00346	−0.03218
HY12	0.04723	0.00043	0.08018	0.00026	−0.00189
HZ12	−0.03980	−0.01698	0.06691	−0.00175	0.16607
HX13	0.11823	−0.06801	0.07954	0.02862	−0.00624
HY13	0.14485	0.06107	−0.06744	0.01027	0.00840
HZ13	−0.05823	0.08596	−0.11823	−0.01944	−0.16369
HX14	0.48951	0.08947	0.11470	0.05412	−0.04549
HY14	0.55516	0.00227	−0.01878	0.04523	−0.02875
HZ14	0.06597	−0.08125	−0.15218	−0.00720	0.05025
HX15	−0.03210	0.07324	0.00612	0.01106	0.03863
HY15	−0.09735	−0.13851	0.06371	0.00977	−0.21970
HZ15	0.11552	−0.02327	−0.07726	−0.00880	−0.00677
OX16	−0.00601	−0.00093	−0.00179	−0.00068	0.00017
OY16	0.00116	0.00019	0.00027	−0.00002	−0.00008
OZ16	−0.00041	0.00087	0.00022	−0.00003	−0.00091
OX17	−0.00017	−0.00150	−0.00177	−0.00017	0.00149
OY17	−0.00003	0.00017	−0.00079	0.00002	0.00055
OZ17	0.00300	0.00052	0.00158	0.00037	−0.00044

	21 A	22 A	23 A	24 A	25 A
Wavenumbers [cm−1]	1033.16	1126.97	1133.52	1243.14	1280.92
Intensities [km/mol]	17.66	1.16	0.55	41.55	110.61
Intensities [relative]	1.56	0.10	0.05	3.66	9.75
CX1	0.04203	−0.02877	−0.01081	−0.04784	−0.01067
CY1	−0.02714	0.03130	0.00066	0.05014	0.01118
CZ1	0.05471	−0.05403	−0.00952	0.06897	0.02913
NX2	−0.06786	0.01828	0.00413	0.03924	0.01694
NY2	0.07434	−0.02167	−0.00568	−0.04296	−0.01952
NZ2	−0.05565	0.08765	0.01555	−0.05237	−0.05137
CX3	0.01044	−0.01523	0.00137	0.02747	−0.01114
CY3	−0.01298	0.01436	0.00494	−0.02577	0.01156
CZ3	−0.02134	−0.01560	−0.00279	0.03231	0.00728
NX4	0.06744	−0.02789	−0.00835	−0.05328	0.04709
NY4	−0.07430	0.03353	0.00351	0.05640	−0.04831
NZ4	0.06706	−0.04337	−0.00806	0.00854	−0.07827
CX5	0.00230	0.07793	0.00800	0.02947	−0.04520
CY5	−0.00479	−0.09214	−0.01621	−0.02821	0.04728
CZ5	0.06318	0.11749	0.01724	−0.06997	0.04069
CX6	−0.02291	−0.00027	0.06814	0.03743	−0.04543
CY6	0.02104	−0.01899	0.05871	−0.04793	0.04166
CZ6	−0.04593	−0.01599	−0.00022	0.00392	0.17567
OX7	0.01168	0.01385	0.00156	−0.00918	−0.00807
OY7	−0.01163	−0.01437	−0.00307	0.00917	0.00848
OZ7	−0.02665	−0.00952	−0.00191	−0.01111	0.02810
SX8	−0.00508	−0.00693	−0.00018	−0.00014	−0.00050
SY8	0.00679	0.00830	0.00139	0.00003	0.00054
SZ8	−0.01689	−0.01228	−0.00115	0.00482	−0.00091
CX9	−0.03585	−0.02586	−0.09911	−0.03384	0.01562
CY9	0.03710	0.06007	−0.07499	0.04242	−0.01123
CZ9	−0.03373	−0.02711	−0.01044	−0.02413	−0.07986
HX10	0.17534	0.12778	0.23566	0.09120	0.14784
HY10	−0.18909	−0.19896	0.14302	−0.10355	−0.15048
HZ10	−0.21955	−0.20354	−0.04855	−0.13825	−0.20253
HX11	−0.00623	−0.07125	0.37528	0.00131	0.06882
HY11	0.02852	0.06605	−0.14964	0.03558	−0.02432

HZ11	0.22429	0.28468	−0.31657	0.17689	−0.03148
HX12	−0.03205	−0.01318	−0.16178	−0.02901	0.02666
HY12	−0.01929	−0.07123	0.37107	−0.02449	−0.07436
HZ12	0.21477	0.14713	0.43020	0.15364	−0.03926
HX13	0.07265	−0.02746	−0.01952	−0.06521	0.06002
HY13	−0.07649	0.03000	−0.00752	0.05577	−0.04812
HZ13	0.12027	−0.23688	−0.04225	0.09531	−0.22823
HX14	−0.17922	0.02136	0.00412	0.25767	0.11234
HY14	0.13577	0.00290	−0.00391	−0.29704	−0.11932
HZ14	−0.00634	0.09960	0.01708	−0.21391	−0.11936
HX15	−0.02490	−0.00602	−0.00113	−0.05689	−0.00133
HY15	−0.07763	0.03190	0.01154	0.11303	0.01373
HZ15	0.28035	−0.22770	−0.01230	0.42501	−0.05714
OX16	0.00019	0.00047	0.00011	−0.00006	0.00028
OY16	0.00054	0.00050	−0.00070	−0.00006	−0.00059
OZ16	−0.00129	−0.00041	0.00104	0.00018	0.00110
OX17	0.00132	0.00014	−0.00054	−0.00026	−0.00069
OY17	0.00002	−0.00031	0.00010	0.00000	0.00036
OZ17	0.00046	0.00082	−0.00082	−0.00011	−0.00099

	26 A	27 A	28 A	29 A	30 A
Wavenumbers [cm−1]	1339.31	1489.51	1548.64	1555.83	1599.85
Intensities [km/mol]	152.19	32.01	45.78	27.13	34.60
Intensities [relative]	13.42	2.82	4.04	2.39	3.05
CX1	0.00874	−0.00853	0.00481	−0.00759	0.01567
CY1	−0.00531	0.02089	−0.01910	0.01242	−0.00967
CZ1	0.00382	0.12562	−0.09269	0.03103	0.04870
NX2	0.01173	0.04405	0.00691	0.00327	−0.03187
NY2	−0.00868	−0.05548	−0.00161	−0.00533	0.03391
NZ2	0.00395	−0.03086	0.06994	−0.03775	−0.00431
CX3	0.02338	−0.09377	−0.07557	0.04145	0.02516
CY3	−0.02551	0.10282	0.08595	−0.04702	−0.02583
CZ3	0.03592	−0.07605	−0.07775	0.03414	0.00756
NX4	0.00541	0.02172	0.03370	−0.00939	−0.00693
NY4	−0.00255	−0.02550	−0.03557	0.01056	0.01041
NZ4	−0.07261	0.08328	−0.02978	−0.01018	−0.10092
CX5	−0.02978	0.02174	−0.04413	0.00287	0.04061
CY5	0.02543	−0.02663	0.04761	−0.00290	−0.04884
CZ5	0.12299	0.02047	0.02661	−0.00431	0.04428
CX6	−0.03188	−0.02945	0.03246	−0.00512	−0.03515
CY6	0.03245	0.04022	−0.04182	0.00676	0.04481
CZ6	−0.09934	−0.06408	0.02290	0.02114	−0.02523
OX7	0.00163	0.01096	0.01240	−0.01127	−0.00739
OY7	−0.00175	−0.01240	−0.01417	0.01250	0.00786
OZ7	−0.00279	−0.00970	0.01559	0.00559	0.02570
SX8	−0.00243	−0.00191	0.00135	−0.00055	−0.00181
SY8	0.00314	0.00242	−0.00146	0.00057	0.00206
SZ8	−0.00815	−0.00656	−0.00012	−0.00020	−0.00065
CX9	0.01930	0.01718	0.01416	0.05299	0.02480
CY9	−0.02261	−0.02174	−0.01072	−0.05301	−0.02574
CZ9	0.04318	0.00149	−0.03819	−0.09558	0.02322
HX10	−0.10630	−0.06351	−0.12237	−0.26855	0.07792
HY10	0.10615	0.07061	0.12761	0.26628	−0.13843
HZ10	0.15197	0.07588	0.08469	0.18595	−0.05785
HX11	−0.04106	−0.06892	−0.07583	−0.30188	−0.31473
HY11	−0.00961	−0.00451	0.01073	0.01887	0.03726
HZ11	−0.09505	−0.01491	0.20528	0.36884	−0.16062
HX12	0.01069	0.00182	−0.00774	−0.01509	−0.02310
HY12	0.04472	0.07276	0.07119	0.28870	0.30610
HZ12	−0.08792	−0.00568	0.19333	0.38420	−0.08845
HX13	0.01535	0.03484	0.03074	−0.00820	−0.02683
HY13	−0.00671	−0.02293	−0.03340	0.00927	0.00639
HZ13	−0.41016	−0.14365	0.36179	−0.12749	0.51257
HX14	0.09479	0.16606	0.18669	−0.13535	0.12548
HY14	−0.12165	−0.20150	−0.17617	0.13431	−0.17981
HZ14	−0.06162	−0.12567	−0.04135	0.05229	−0.13427
HX15	−0.04037	−0.00624	0.01010	−0.00428	0.01166
HY15	0.01792	−0.05011	0.05147	−0.00829	−0.06203
HZ15	0.49327	−0.23442	0.28504	−0.11633	−0.16410
OX16	0.00048	0.00091	0.00014	0.00007	0.00125
OY16	−0.00044	−0.00060	−0.00069	0.00019	−0.00101

OZ16	0.00110	0.00134	0.00171	−0.00056	0.00237
OX17	−0.00033	0.00003	−0.00090	0.00035	−0.00020
OY17	0.00044	0.00085	0.00061	−0.00020	0.00114
OZ17	−0.00126	−0.00173	−0.00136	0.00042	−0.00278

	31 A	32 A	33 A	34 A	35 A
Wavenumbers [cm−1]	1607.89	1617.29	1625.94	1628.99	1674.99
Intensities [km/mol]	65.01	7.45	55.51	11.41	89.12
Intensities [relative]	5.73	0.66	4.90	1.01	7.86
CX1	−0.01883	0.00133	0.01771	−0.01278	0.03301
CY1	0.01815	0.00009	−0.02648	0.01721	−0.03389
CZ1	−0.05574	0.00804	−0.04260	0.01913	−0.04971
NX2	0.06730	−0.00361	−0.04117	0.03364	−0.03561
NY2	−0.07209	0.00462	0.04807	−0.03950	0.04463
NZ2	−0.01595	−0.00090	0.04102	−0.02913	0.03473
CX3	−0.02365	0.00364	−0.00515	0.00278	0.00003
CY3	0.02559	−0.00432	0.00575	−0.00346	0.00105
CZ3	−0.04745	0.00278	0.03003	−0.02611	0.02011
NX4	0.00074	0.00009	−0.00385	0.00144	−0.01515
NY4	−0.00221	0.00093	0.00247	−0.00038	0.01557
NZ4	0.03423	−0.00840	0.06373	−0.03728	0.03012
CX5	0.04567	−0.00234	−0.00993	0.02110	0.08603
CY5	−0.04893	0.00198	0.01400	−0.02574	−0.09397
CZ5	−0.02962	0.00508	−0.04833	0.02514	−0.04650
CX6	−0.05224	−0.00736	0.01113	−0.02359	−0.11345
CY6	0.04972	−0.01327	−0.01341	0.02694	0.12055
CZ6	0.04118	−0.00564	0.03362	−0.01485	0.04866
OX7	−0.01186	−0.00045	0.02043	−0.01515	0.01287
OY7	0.01254	0.00052	−0.02190	0.01640	−0.01408
OZ7	0.02524	0.00107	−0.04797	0.03502	−0.02826
SX8	0.00029	−0.00013	0.00137	−0.00046	−0.00067
SY8	−0.00027	−0.00001	−0.00167	0.00058	0.00070
SZ8	0.00122	−0.00008	0.00233	−0.00125	0.00224
CX9	0.01930	−0.03837	0.01501	−0.00336	0.01680
CY9	−0.02257	−0.03714	−0.00811	0.01146	−0.02307
CZ9	0.01243	0.00031	0.00968	−0.00943	−0.03751
HX10	0.15551	0.50677	0.08450	−0.12886	−0.12285
HY10	−0.10813	0.47647	−0.14970	0.05385	0.16815
HZ10	−0.09370	0.00779	−0.09109	0.06562	0.10957
HX11	−0.27124	0.08889	−0.30203	0.20910	0.20190
HY11	0.03641	−0.04357	0.05245	−0.03008	−0.05840
HZ11	−0.11016	0.46231	−0.07966	−0.00065	0.05747
HX12	−0.02376	−0.03451	−0.03066	0.02879	0.04128
HY12	0.28556	0.13354	0.28960	−0.22649	−0.19685
HZ12	−0.15706	−0.46026	−0.02241	0.06462	0.02155
HX13	0.00203	0.00096	0.00501	−0.00523	−0.01815
HY13	−0.00024	0.00185	0.00309	−0.00093	0.01384
HZ13	0.01299	0.02520	−0.29752	0.21102	0.01019
HX14	−0.22481	0.00873	0.14205	−0.11524	0.12595
HY14	0.28216	−0.01576	−0.14550	0.14876	−0.17633
HZ14	0.20605	−0.01245	−0.08310	0.08521	−0.09555
HX15	−0.04471	0.00021	0.02582	−0.02442	0.00771
HY15	0.08382	−0.01021	−0.01370	0.01560	−0.03838
HZ15	0.38700	−0.03315	0.01248	0.05027	0.15245
OX16	−0.00409	0.00505	0.02702	0.03645	−0.00279
OY16	0.00569	−0.00697	−0.03873	−0.05185	0.00497
OZ16	−0.01329	0.01669	0.09308	0.12475	−0.01204
OX17	0.00380	−0.00490	−0.02764	−0.03693	0.00403
OY17	−0.00566	0.00700	0.03866	0.05185	−0.00483
OZ17	0.01362	−0.01676	−0.09290	−0.12451	0.01168

	36 A	37 A	38 A	39 A	40 A
Wavenumbers [cm−1]	1985.61	3191.24	3245.52	3320.22	3403.41
Intensities [km/mol]	1133.94	26.53	25.85	1.99	8.69
Intensities [relative]	100.00	2.34	2.28	0.18	0.77
CX1	−0.00240	0.00087	0.00009	0.00125	−0.06560
CY1	0.00493	−0.00004	−0.00001	−0.00071	0.04966
CZ1	0.00512	−0.00079	0.00023	−0.00009	−0.00899
NX2	0.02464	0.00028	0.00006	0.00007	0.00080
NY2	−0.02848	−0.00024	0.00016	−0.00024	−0.00183
NZ2	−0.03001	0.00033	0.00002	0.00006	−0.00106

CX3	-0.08430	-0.00015	-0.00000	-0.00014	0.00049
CY3	0.09053	0.00018	-0.00002	0.00016	-0.00092
CZ3	0.19252	-0.00057	0.00005	-0.00014	-0.00025
NX4	0.00765	-0.00013	-0.00004	0.00012	0.00004
NY4	-0.00726	0.00006	0.00004	-0.00023	-0.00004
NZ4	-0.04369	0.00038	-0.00002	0.00009	-0.00016
CX5	0.00040	0.00033	-0.00011	0.00016	0.00045
CY5	-0.00124	-0.00023	-0.00015	-0.00003	-0.00057
CZ5	0.00678	0.00025	-0.00006	-0.00012	0.00013
CX6	-0.00034	0.00061	-0.00051	-0.00029	-0.00046
CY6	0.00053	-0.00053	0.00003	0.00025	-0.00067
CZ6	-0.00082	-0.00047	-0.00010	0.00097	0.00134
OX7	0.04497	-0.00009	0.00001	-0.00000	-0.00012
OY7	-0.04834	0.00008	-0.00002	0.00002	0.00020
OZ7	-0.10354	0.00030	-0.00005	0.00009	0.00014
SX8	-0.00051	-0.00006	-0.00001	-0.00026	0.00012
SY8	0.00063	0.00010	-0.00000	0.00030	-0.00012
SZ8	-0.00055	-0.00010	0.00003	-0.00000	0.00009
CX9	0.00021	-0.03896	-0.06214	-0.03699	-0.00149
CY9	-0.00091	0.03243	-0.06218	0.04253	0.00204
CZ9	-0.00025	0.01936	-0.00386	-0.06505	-0.00106
HX10	-0.00079	-0.10869	0.00043	0.32298	0.00597
HY10	0.00155	0.11767	-0.02541	-0.35405	-0.00643
HZ10	0.00084	-0.24667	0.02932	0.77527	0.01110
HX11	-0.00190	-0.11980	0.11368	-0.04418	-0.00259
HY11	-0.00182	-0.61056	0.69233	-0.19892	-0.01403
HZ11	0.00045	0.00359	-0.00616	-0.00665	-0.00107
HX12	0.00112	0.68702	0.63234	0.17322	0.01447
HY12	0.00154	0.10282	0.07588	0.03294	0.00212
HZ12	0.00101	0.02199	0.02114	-0.00258	-0.00075
HX13	0.00109	-0.00121	0.00050	-0.00118	-0.00008
HY13	-0.00674	0.00104	-0.00049	0.00098	0.00003
HZ13	0.18107	0.00010	0.00014	-0.00065	-0.00022
HX14	-0.11337	-0.00159	-0.00044	0.00033	-0.00373
HY14	0.12769	-0.00185	-0.00084	0.00063	0.01013
HZ14	0.07104	-0.00118	-0.00018	-0.00034	-0.00311
HX15	-0.00480	-0.01328	-0.00003	-0.01651	0.76771
HY15	0.00357	0.00960	-0.00129	0.01206	-0.55506
HZ15	0.00842	0.00037	-0.00008	-0.00071	0.10976
OX16	0.00025	0.00014	-0.00003	0.00004	-0.00004
OY16	-0.00030	-0.00005	0.00004	-0.00007	-0.00001
OZ16	0.00064	0.00005	-0.00004	0.00016	0.00007
OX17	-0.00011	0.00008	0.00004	-0.00005	-0.00007
OY17	0.00030	0.00008	-0.00003	0.00007	-0.00002
OZ17	-0.00067	-0.00014	0.00005	-0.00016	0.00001

	41 A	42 A
Wavenumbers [cm-1]	3909.32	3917.65
Intensities [km/mol]	158.99	72.40
Intensities [relative]	14.02	6.39
CX1	-0.00068	-0.00011
CY1	0.00090	0.00044
CZ1	0.00195	0.00063
NX2	-0.01771	-0.00528
NY2	0.02350	0.00695
NZ2	-0.06172	-0.01739
CX3	0.00082	-0.00006
CY3	-0.00069	0.00003
CZ3	-0.00014	-0.00088
NX4	-0.01217	0.04548
NY4	0.01395	-0.05176
NZ4	0.00009	0.00105
CX5	0.00036	-0.00052
CY5	-0.00049	0.00042
CZ5	-0.00026	0.00191
CX6	-0.00012	-0.00050
CY6	0.00014	0.00060
CZ6	0.00012	0.00039
OX7	0.00006	0.00009
OY7	-0.00008	-0.00011
OZ7	-0.00014	-0.00017

SX8	0.00003	-0.00015
SY8	-0.00004	0.00019
SZ8	0.00000	-0.00019
CX9	-0.00005	0.00009
CY9	0.00033	-0.00054
CZ9	-0.00009	-0.00001
HX10	0.00008	-0.00027
HY10	-0.00023	0.00068
HZ10	0.00039	-0.00069
HX11	-0.00024	0.00017
HY11	-0.00125	0.00101
HZ11	0.00007	0.00008
HX12	0.00128	-0.00050
HY12	0.00030	-0.00023
HZ12	0.00013	0.00012
HX13	0.16825	-0.60831
HY13	-0.19266	0.69679
HZ13	0.00496	-0.01685
HX14	0.23697	0.06419
HY14	-0.32131	-0.08982
HZ14	0.83511	0.22969
HX15	0.00421	0.00099
HY15	-0.00474	-0.00136
HZ15	-0.00122	-0.00019
OX16	-0.00005	0.00005
OY16	0.00004	0.00000
OZ16	-0.00011	-0.00005
OX17	-0.00001	0.00007
OY17	-0.00005	0.00000
OZ17	0.00013	0.00000

Normal Modes of imaginary frequencies

	1
Wavenumbers [cm-1]	18.80
Intensities [km/mol]	6.55
Intensities [relative]	0.58
CX1	-0.03929
CY1	-0.06623
CZ1	-0.00368
NX2	0.05801
NY2	0.03186
NZ2	-0.01355
CX3	0.00672
CY3	-0.01726
CZ3	-0.01397
NX4	-0.04445
NY4	-0.05595
NZ4	-0.01159
CX5	-0.01159
CY5	-0.01655
CZ5	-0.00831
CX6	-0.00270
CY6	0.00632
CZ6	-0.02036
OX7	0.00837
OY7	-0.01822
OZ7	-0.01486
SX8	0.01807
SY8	-0.01116
SZ8	-0.00193
CX9	0.10527
CY9	0.11636
CZ9	-0.01831
HX10	0.01780
HY10	0.02689
HZ10	-0.02250
HX11	0.31736
HY11	0.07781
HZ11	0.00525

HX12	0.07952
HY12	0.32819
HZ12	−0.02450
HX13	−0.05130
HY13	−0.06016
HZ13	−0.00496
HX14	0.04080
HY14	0.02697
HZ14	−0.01051
HX15	0.04639
HY15	0.04523
HZ15	−0.03248
OX16	−0.05458
OY16	0.00916
OZ16	0.04338
OX17	−0.07410
OY17	0.00749
OZ17	0.05154

Normal Modes of low/zero frequencies

	1	2	3	4	5
Wavenumbers [cm-1]	0.00	0.00	0.00	0.00	0.00
Intensities [km/mol]	0.00	0.00	0.00	0.00	0.00
Intensities [relative]	0.00	0.00	0.00	0.00	0.00
CX1	0.00685	−0.00174	−0.00515	−0.03940	−0.02663
CY1	0.05200	0.00237	−0.05650	−0.05537	0.03455
CZ1	−0.01896	−0.05687	−0.04325	0.04225	0.04764
NX2	0.03533	0.00420	0.03882	−0.02940	−0.03409
NY2	0.07806	−0.01043	−0.06691	−0.02434	0.01938
NZ2	−0.02143	−0.04731	−0.01908	0.02930	0.05289
CX3	0.03958	0.01952	0.05431	0.00938	−0.03436
CY3	0.08203	0.00383	−0.05261	0.01198	0.01910
CZ3	−0.02137	−0.03286	0.02413	0.00668	0.06004
NX4	0.01348	0.03007	0.02391	0.04154	−0.02658
NY4	0.05771	0.03157	−0.02742	0.01381	0.03523
NZ4	−0.02143	−0.02678	0.04216	−0.00277	0.06306
CX5	−0.01610	0.02661	−0.02009	0.03814	−0.01867
CY5	0.02992	0.04517	−0.01638	−0.01939	0.05140
CZ5	−0.02276	−0.03369	0.01921	0.00909	0.05992
CX6	−0.01997	0.01083	−0.03532	−0.00188	−0.01853
CY6	0.02651	0.03096	−0.03059	−0.05439	0.05139
CZ6	−0.02168	−0.04866	−0.02356	0.03161	0.05228
OX7	0.06431	0.02343	0.09172	0.01483	−0.04091
OY7	0.10506	−0.00721	−0.06153	0.03994	0.00573
OZ7	−0.02138	−0.02601	0.04455	−0.00401	0.06343
SX8	−0.04529	0.04321	−0.05112	0.08650	−0.00969
SY8	0.00234	0.08011	0.01560	−0.01051	0.07013
SZ8	−0.02481	−0.02224	0.04972	−0.00714	0.06602
CX9	−0.04981	0.00515	−0.08106	−0.01096	−0.01068
CY9	−0.00148	0.04246	−0.02162	−0.09210	0.06740
CZ9	−0.02276	−0.05765	−0.05227	0.04651	0.04805
HX10	−0.06887	0.01456	−0.10220	0.01693	−0.00490
HY10	−0.01927	0.06449	−0.00149	−0.08738	0.07942
HZ10	−0.02295	−0.05164	−0.03469	0.03728	0.05107
HX11	−0.05429	−0.01129	−0.09757	−0.05259	−0.01041
HY11	−0.00072	0.04535	−0.01872	−0.08484	0.06737
HZ11	0.00385	−0.07709	−0.06331	0.05557	0.03284
HX12	−0.04862	0.00727	−0.07807	−0.00572	−0.01088
HY12	−0.00542	0.02545	−0.03862	−0.13374	0.06732
HZ12	−0.04998	−0.05155	−0.08210	0.05876	0.05678
HX13	0.01643	0.04161	0.03521	0.07078	−0.02671
HY13	0.06027	0.04173	−0.01724	0.03913	0.03517
HZ13	−0.02243	−0.01578	0.07320	−0.01914	0.06872
HX14	0.05418	−0.00401	0.06041	−0.05413	−0.03974
HY14	0.09591	−0.03005	−0.08467	−0.02424	0.00763
HZ14	−0.01985	−0.05246	−0.03165	0.03607	0.05001
HX15	0.00701	−0.01156	−0.01100	−0.06480	−0.02724
HY15	0.05090	−0.01312	−0.07178	−0.08794	0.03318
HZ15	−0.02568	−0.06476	−0.07865	0.05995	0.04514

OX16	-0.02805	-0.01642	-0.06362	-0.07076	-0.01791
OY16	0.03597	0.06864	0.00712	0.03937	0.05119
OZ16	0.06993	-0.08798	0.02078	0.01972	0.01359
OX17	-0.00568	-0.02691	-0.03845	-0.10205	-0.02466
OY17	0.05723	0.04479	-0.01450	0.03856	0.03714
OZ17	0.07220	-0.09483	0.00436	0.02860	0.00972

	6	7	8
Wavenumbers [cm-1]	0.00	34.26	42.47
Intensities [km/mol]	0.00	0.00	0.00
Intensities [relative]	0.00	0.00	0.00
CX1	0.07438	0.02790	0.06738
CY1	0.00546	0.02154	0.03319
CZ1	0.01620	-0.03962	0.00796
NX2	0.08046	-0.03192	0.03088
NY2	0.00228	-0.04345	0.00223
NZ2	0.02050	-0.02979	0.00925
CX3	0.07966	-0.03326	-0.00237
CY3	0.00151	-0.04412	-0.02840
CZ3	0.02827	-0.02283	0.00615
NX4	0.07222	0.01967	0.00441
NY4	0.00420	0.01142	-0.02796
NZ4	0.03152	-0.02004	0.00432
CX5	0.06559	0.02038	0.01231
CY5	0.00760	0.02038	-0.02342
CZ5	0.02737	-0.02476	0.00462
CX6	0.06653	0.02130	0.04527
CY6	0.00830	0.01605	0.00290
CZ6	0.01969	-0.02959	0.01011
OX7	0.08508	-0.07584	-0.03398
OY7	-0.00132	-0.09020	-0.05400
OZ7	0.03195	-0.01918	0.00468
SX8	0.05670	0.02262	-0.04550
SY8	0.01060	0.04214	-0.07026
SZ8	0.03282	-0.01851	0.00081
CX9	0.06010	-0.00855	0.02996
CY9	0.01176	-0.00614	-0.01797
CZ9	0.01451	-0.03479	0.01181
HX10	0.05447	0.06868	0.07506
HY10	0.01370	0.07625	0.02301
HZ10	0.01767	-0.02951	0.01163
HX11	0.06097	-0.13118	-0.03982
HY11	0.01161	0.01553	-0.00571
HZ11	0.01298	-0.08813	-0.01194
HX12	0.06014	0.00615	0.03814
HY12	0.01258	-0.13020	-0.08820
HZ12	0.00868	0.00560	0.03544
HX13	0.07156	-0.00140	-0.02990
HY13	0.00369	-0.00747	-0.05818
HZ13	0.03708	-0.01567	0.00085
HX14	0.08590	-0.06085	0.02743
HY14	0.00028	-0.08002	-0.00277
HZ14	0.01827	-0.03564	0.00834
HX15	0.07558	0.00968	0.06423
HY15	0.00588	-0.00123	0.03119
HZ15	0.00972	-0.03177	0.01558
OX16	0.06781	0.00906	-0.01733
OY16	0.00640	0.01873	0.12300
OZ16	0.02923	0.11515	-0.02572
OX17	0.07436	0.01821	-0.01146
OY17	0.00403	0.01729	0.12597
OZ17	0.02631	0.11083	-0.02674

4. Frequencies for PS-O2 on TT0 (reactant) state

Imaginary Vibration Nr	Wavenumber [1/cm]
1	18.80

Low Vibration Nr	Wavenumber [1/cm]

1	0.00
2	0.00
3	0.00
4	0.00
5	0.00
6	0.00
7	34.26
8	42.47

Vibration Nr	Wavenumber [1/cm]
1	101.98
2	107.89
3	123.77
4	192.00
5	219.17
6	247.82
7	266.01
8	295.15
9	332.39
10	341.31
11	454.29
12	480.44
13	512.49
14	553.50
15	573.88
16	581.90
17	721.11
18	824.33
19	847.34
20	938.11
21	1033.16
22	1126.97
23	1133.52
24	1243.14
25	1280.92
26	1339.31
27	1489.51
28	1548.64
29	1555.83
30	1599.85
31	1607.89
32	1617.29
33	1625.94
34	1628.99
35	1674.99
36	1985.61
37	3191.24
38	3245.52
39	3320.22
40	3403.41
41	3909.32
42	3917.65

5. Normal modes for PS-O2 on SS2 (product) state

Normal Modes

	1 A	2 A	3 A	4 A	5 A
Wavenumbers [cm-1]	109.67	124.24	142.70	198.30	272.79
Intensities [km/mol]	0.07	0.95	0.02	0.01	3.80
Intensities [relative]	0.01	0.09	0.00	0.00	0.35
CX1	-0.03961	-0.05618	0.03088	-0.00263	0.00604
CY1	-0.03644	-0.04798	0.02725	-0.00261	-0.00698
CZ1	-0.00742	-0.00131	0.00269	-0.00123	0.00226
NX2	-0.09276	-0.06344	0.05145	0.02840	0.00240
NY2	-0.08434	-0.05438	0.04508	0.02340	-0.00491
NZ2	-0.00892	-0.00147	0.00355	0.00020	-0.00244
CX3	0.00997	-0.01182	0.01137	0.00534	0.00402
CY3	0.00423	-0.00989	0.01077	0.00346	-0.00365
CZ3	-0.00340	0.00058	0.00137	-0.00067	-0.02821

NX4	0.07143	0.04476	0.12565	0.00005	0.02482
NY4	0.05938	0.03855	0.10893	−0.00062	−0.02784
NZ4	−0.00001	0.00274	0.00607	−0.00075	−0.03364
CX5	0.02107	0.00313	0.05038	−0.00559	0.01930
CY5	0.01819	0.00219	0.04382	−0.00494	−0.01788
CZ5	−0.00287	0.00104	0.00286	−0.00110	−0.03643
CX6	0.02676	−0.02672	0.02469	−0.01785	0.02788
CY6	0.02301	−0.02285	0.02181	−0.01513	−0.02705
CZ6	−0.00417	0.00007	0.00219	−0.00137	−0.01683
OX7	0.04020	−0.01462	−0.10557	−0.00949	−0.01885
OY7	0.02879	−0.01192	−0.09000	−0.00959	0.02540
OZ7	−0.00144	0.00033	−0.00369	−0.00122	−0.05088
SX8	−0.04404	−0.01798	−0.02613	−0.00845	−0.07045
SY8	−0.03531	−0.01623	−0.02207	−0.00669	0.07948
SZ8	−0.00510	−0.00024	−0.00125	−0.00102	0.04927
CX9	0.10910	−0.06306	−0.03351	0.01683	0.09364
CY9	0.09634	−0.05478	−0.02883	0.01327	−0.11306
CZ9	−0.00114	−0.00139	−0.00050	0.00082	0.04378
HX10	0.10889	−0.03632	−0.04912	0.49327	0.13387
HY10	0.14224	−0.08323	−0.05590	−0.10785	−0.15846
HZ10	0.06053	−0.01432	−0.05216	0.28809	0.01924
HX11	0.15586	−0.08623	−0.06530	−0.00289	0.13055
HY11	0.09421	−0.02530	−0.04343	0.51712	−0.16107
HZ11	−0.05877	0.01105	0.04788	−0.25924	0.02358
HX12	0.13094	−0.09665	−0.03436	−0.40333	0.07782
HY12	0.11413	−0.08297	−0.02925	−0.34126	−0.10058
HZ12	−0.00275	−0.00238	0.00061	−0.02309	0.14457
HX13	0.10008	0.06772	0.09662	−0.00818	0.02453
HY13	0.08383	0.05822	0.08406	−0.00769	−0.02806
HZ13	0.00258	0.00341	0.00465	−0.00075	−0.04351
HX14	−0.12170	−0.10028	−0.06121	0.00880	−0.00113
HY14	−0.11001	−0.08569	−0.05101	0.00656	0.00002
HZ14	−0.01079	−0.00322	−0.00183	−0.00079	0.00077
HX15	−0.05547	−0.09375	0.01131	−0.00455	0.00341
HY15	−0.05019	−0.07999	0.01051	−0.00433	−0.00773
HZ15	−0.00984	−0.00259	0.00216	−0.00175	0.01422
OX16	−0.03767	0.10397	−0.02431	−0.00348	−0.00025
OY16	−0.02628	0.08631	−0.02449	0.00203	−0.00037
OZ16	0.01751	−0.00106	−0.00474	0.00416	0.00017
OX17	−0.01123	0.10091	−0.02930	0.00270	−0.00008
OY17	−0.00623	0.09091	−0.02693	0.00155	−0.00032
OZ17	0.01745	0.00137	−0.00403	0.00209	0.00015

	6 A	7 A	8 A	9 A	10 A
Wavenumbers [cm-1]	323.04	350.49	391.68	465.64	539.52
Intensities [km/mol]	1.30	5.52	18.19	16.35	99.09
Intensities [relative]	0.12	0.50	1.66	1.49	9.05
CX1	0.07668	0.02717	0.11811	−0.01916	−0.02539
CY1	0.06403	−0.03851	0.10168	0.02238	−0.02363
CZ1	0.00460	0.02193	0.00364	−0.06023	−0.00001
NX2	−0.08731	0.00204	−0.06772	−0.05000	−0.03041
NY2	−0.07434	0.00283	−0.05780	0.06316	−0.02452
NZ2	−0.00228	0.01801	−0.00336	−0.08510	−0.00313
CX3	−0.02702	−0.00589	−0.01367	−0.05116	−0.01339
CY3	−0.02236	0.00987	−0.01160	0.05967	−0.01150
CZ3	−0.00043	−0.02069	−0.00061	0.00661	−0.00219
NX4	−0.02676	0.03235	0.05083	−0.04201	0.02226
NY4	−0.02396	−0.03473	0.04325	0.04865	0.01939
NZ4	−0.00092	−0.02383	0.00207	0.01549	−0.00029
CX5	0.05068	0.04556	−0.08512	0.01557	0.04307
CY5	0.04186	−0.05506	−0.07390	−0.01769	0.03581
CZ5	0.00309	0.01580	−0.00350	0.03586	0.00168
CX6	0.13110	0.03981	−0.08231	0.01743	−0.01900
CY6	0.11021	−0.05230	−0.07214	−0.01561	−0.01692
CZ6	0.00551	0.00468	−0.00409	−0.07433	0.00077
OX7	0.02184	−0.07005	0.00101	0.00760	−0.01408
OY7	0.02223	0.08391	0.00249	−0.01233	−0.01430
OZ7	0.00069	−0.07991	−0.00054	0.06786	−0.00118
SX8	−0.00840	0.00443	0.01618	0.02776	−0.00521
SY8	−0.00889	−0.00931	0.01320	−0.03709	−0.00379
SZ8	0.00049	0.07700	0.00262	0.07087	−0.00012

CX9	−0.05231	−0.04867	−0.00465	0.05295	0.00216
CY9	−0.04053	0.06360	−0.00571	−0.05601	0.00372
CZ9	−0.00697	−0.08656	−0.00052	−0.07776	0.00188
HX10	0.03161	−0.11526	0.00274	0.08079	−0.00203
HY10	−0.18427	0.13831	0.02827	−0.08359	0.03290
HZ10	−0.12118	−0.04858	0.05227	−0.08842	0.03708
HX11	−0.18936	−0.10995	0.03302	0.07702	0.03031
HY11	0.06303	0.13932	−0.00062	−0.08649	−0.00087
HZ11	0.10563	−0.05287	−0.05017	−0.09054	−0.03049
HX12	−0.19259	−0.02192	−0.00045	0.04274	0.02087
HY12	−0.15975	0.04512	−0.00230	−0.04883	0.01885
HZ12	−0.01819	−0.24796	−0.00078	−0.01118	0.00026
HX13	−0.03617	0.03281	0.13379	−0.04261	−0.05332
HY13	−0.03200	−0.03390	0.11428	0.05217	−0.04535
HZ13	−0.00208	−0.05798	0.00493	−0.07034	−0.00383
HX14	0.03042	−0.01343	0.06494	−0.03793	0.70604
HY14	0.02615	0.00968	0.05400	0.05198	0.60724
HZ14	0.00334	0.02639	0.00236	−0.09473	0.03370
HX15	0.07169	0.02336	0.31441	−0.02650	−0.07129
HY15	0.05980	−0.03863	0.26944	0.02429	−0.06271
HZ15	0.00541	0.05821	0.01133	0.00932	−0.00066
OX16	−0.01099	−0.00046	0.00037	0.00000	0.00039
OY16	−0.01151	−0.00007	0.00165	0.00010	0.00011
OZ16	−0.00166	−0.00007	−0.00057	0.00018	0.00008
OX17	−0.01073	0.00088	−0.00279	−0.00031	0.00096
OY17	−0.00757	0.00070	−0.00074	−0.00017	0.00103
OZ17	0.00015	−0.00021	−0.00045	0.00019	0.00048

	11 A	12 A	13 A	14 A	15 A
Wavenumbers [cm−1]	549.11	581.50	675.05	721.18	742.60
Intensities [km/mol]	8.49	13.18	0.80	82.75	2.27
Intensities [relative]	0.78	1.20	0.07	7.56	0.21
CX1	−0.02902	0.02640	0.05305	−0.01154	−0.10524
CY1	0.03151	−0.03476	0.04793	−0.01266	0.12021
CZ1	0.00331	0.09383	0.00185	−0.00038	0.00270
NX2	−0.00062	−0.04448	−0.01109	0.02763	−0.03078
NY2	−0.00226	0.05169	−0.00833	0.02283	0.03573
NZ2	0.07336	0.01125	−0.00052	0.00124	0.01782
CX3	−0.00434	−0.03569	−0.01717	−0.04784	0.00198
CY3	−0.00069	0.04374	−0.01395	−0.04164	−0.00263
CZ3	0.11784	−0.03210	−0.00055	−0.00153	−0.01134
NX4	0.05014	−0.01885	−0.04317	−0.04503	0.07952
NY4	−0.05927	0.02507	−0.03940	−0.03601	−0.08940
NZ4	0.03993	−0.05784	−0.00294	−0.00114	−0.06570
CX5	0.01297	0.03674	0.16784	0.00042	0.04591
CY5	−0.01423	−0.04467	0.14062	0.00179	−0.05390
CZ5	−0.03521	−0.04633	0.00663	0.00113	−0.06642
CX6	0.01986	0.06226	−0.10385	0.02091	−0.03596
CY6	−0.02337	−0.07596	−0.08882	0.01694	0.04840
CZ6	−0.05894	0.04901	−0.00455	0.00116	−0.02921
OX7	−0.04907	0.06451	0.01110	0.00243	0.03327
OY7	0.05206	−0.07797	0.00869	0.00321	−0.03932
OZ7	0.08961	0.06500	0.00146	−0.00008	0.01306
SX8	−0.01456	−0.02750	−0.01608	−0.00424	0.01210
SY8	0.02026	0.03431	−0.01342	−0.00318	−0.01607
SZ8	−0.05616	−0.02540	−0.00078	−0.00080	0.03609
CX9	0.03317	−0.00762	−0.01109	0.00369	−0.03121
CY9	−0.03192	0.00986	−0.00824	0.00204	0.03429
CZ9	−0.10724	−0.02335	0.00073	−0.00095	0.04680
HX10	0.02023	−0.07801	−0.02175	0.00509	−0.02500
HY10	−0.01573	0.08436	0.07093	−0.01016	0.02473
HZ10	−0.09830	0.00924	0.09759	−0.01614	0.04035
HX11	0.02131	−0.07377	0.06899	−0.00890	−0.02646
HY11	−0.01673	0.09111	−0.02369	0.00426	0.02730
HZ11	−0.10184	0.01197	−0.09040	0.01351	0.04537
HX12	0.03879	0.01833	0.03742	−0.00291	−0.03843
HY12	−0.03559	−0.01123	0.03203	−0.00353	0.03838
HZ12	−0.13732	−0.19282	0.00067	−0.00121	0.07715
HX13	0.04778	−0.01755	0.01501	0.70052	0.09178
HY13	−0.06040	0.03116	0.01051	0.60256	−0.07962
HZ13	0.02685	−0.14628	−0.00253	0.03167	−0.13632

HX14	0.06528	−0.12006	−0.12295	0.07674	−0.00184
HY14	−0.05939	0.12253	−0.10524	0.06470	0.00549
HZ14	0.02872	0.06636	−0.00655	0.00366	−0.00649
HX15	−0.03001	0.02072	0.04350	−0.02118	−0.10261
HY15	0.03142	−0.03024	0.03980	−0.02090	0.12412
HZ15	0.02341	0.18987	0.00235	−0.00039	−0.02661
OX16	0.00001	−0.00018	0.00071	−0.00016	0.00015
OY16	0.00021	−0.00010	0.00049	−0.00005	0.00013
OZ16	0.00025	−0.00010	0.00007	0.00010	0.00002
OX17	0.00007	0.00036	−0.00002	0.00005	−0.00040
OY17	−0.00010	0.00042	−0.00025	−0.00022	−0.00035
OZ17	0.00003	−0.00014	−0.00010	−0.00003	0.00007

	16 A	17 A	18 A	19 A	20 A
Wavenumbers [cm-1]	844.58	853.55	872.03	1021.97	1102.52
Intensities [km/mol]	4.10	67.73	52.58	8.00	2.09
Intensities [relative]	0.37	6.19	4.80	0.73	0.19
CX1	−0.05383	0.04657	−0.09143	−0.03215	0.05766
CY1	0.06364	0.03480	−0.07859	0.03578	−0.06826
CZ1	0.07489	−0.00199	−0.00348	0.02826	0.02370
NX2	−0.00100	−0.04952	−0.01106	−0.06397	−0.03538
NY2	−0.00951	−0.04216	−0.01027	0.07880	0.04080
NZ2	0.11783	−0.00751	−0.00023	−0.09511	0.00740
CX3	0.03715	0.16856	0.07796	0.03042	−0.00846
CY3	−0.02442	0.14772	0.06746	−0.03396	0.01047
CZ3	−0.05697	0.01009	0.00320	−0.02210	−0.01522
NX4	−0.03522	−0.04958	−0.02590	0.05219	0.04468
NY4	0.03587	−0.04617	−0.02125	−0.06634	−0.05209
NZ4	0.00217	−0.00228	−0.00076	0.11275	0.00326
CX5	−0.04245	−0.00974	0.02973	−0.01148	0.00022
CY5	0.04952	−0.01214	0.02512	0.00923	−0.00205
CZ5	0.01586	−0.00151	0.00179	0.07443	0.03005
CX6	−0.02178	−0.00554	0.00807	0.02528	−0.02731
CY6	0.02166	−0.00637	0.00665	−0.03013	0.03111
CZ6	−0.00201	−0.00048	0.00054	0.01762	−0.00136
OX7	0.04145	−0.05467	−0.02365	0.01198	0.00562
OY7	−0.04926	−0.04307	−0.02026	−0.01111	−0.00667
OZ7	−0.07651	0.00137	−0.00121	−0.05752	0.00404
SX8	0.01002	0.00022	−0.00258	−0.00688	−0.00261
SY8	−0.01282	0.00105	−0.00196	0.00973	0.00358
SZ8	0.01761	−0.00069	−0.00036	−0.02917	−0.00887
CX9	0.04036	−0.00355	0.00646	0.01517	−0.05389
CY9	−0.04060	0.00063	0.00517	−0.01813	0.06619
CZ9	−0.11568	0.00543	0.00003	0.00772	−0.06590
HX10	0.05614	−0.00261	0.00119	−0.05748	0.24516
HY10	−0.05480	0.01416	−0.04181	0.05041	−0.20003
HZ10	−0.12152	0.02402	−0.06682	0.03074	−0.13666
HX11	0.05531	0.00991	−0.04447	−0.04399	0.17241
HY11	−0.05858	0.00193	0.00345	0.06394	−0.26937
HZ11	−0.12573	−0.01136	0.06293	0.03444	−0.15346
HX12	0.03945	0.00906	−0.03549	0.03611	−0.13582
HY12	−0.03878	0.01119	−0.03014	−0.03505	0.13238
HZ12	−0.09245	0.00520	−0.00194	−0.12952	0.49067
HX13	−0.02903	0.12920	0.03907	0.05578	0.04746
HY13	0.03753	0.10715	0.03446	−0.07601	−0.05382
HZ13	0.10977	−0.00023	0.00172	0.26873	−0.01238
HX14	−0.04676	0.02340	0.02439	−0.07236	−0.14074
HY14	0.05371	0.01617	0.02166	0.08425	0.15760
HZ14	0.16228	−0.00587	0.00226	−0.09848	0.09405
HX15	−0.06802	−0.25742	0.59815	−0.04989	0.05418
HY15	0.04971	−0.22500	0.51080	0.04964	−0.06541
HZ15	0.05206	−0.01164	0.01997	0.22819	0.12916
OX16	0.00011	−0.00022	0.00033	0.00001	−0.00008
OY16	0.00019	−0.00030	0.00010	0.00007	−0.00000
OZ16	0.00013	−0.00010	0.00018	−0.00003	0.00001
OX17	0.00005	−0.00061	0.00101	−0.00004	0.00013
OY17	−0.00001	−0.00030	0.00090	−0.00006	0.00007
OZ17	−0.00000	0.00003	−0.00008	−0.00002	0.00003

	21 A	22 A	23 A	24 A	25 A
Wavenumbers [cm-1]	1145.21	1230.83	1287.65	1305.00	1370.32

Intensities [km/mol]	0.89	52.38	94.36	103.93	153.24
Intensities [relative]	0.08	4.78	8.62	9.49	13.99
CX1	−0.00700	0.06417	−0.00453	−0.00974	0.00153
CY1	−0.00685	−0.07278	0.00089	0.01170	0.00015
CZ1	−0.00072	−0.04506	0.08372	0.00864	−0.05369
NX2	−0.00448	−0.04312	0.02171	0.01598	−0.01752
NY2	−0.00285	0.04934	−0.02077	−0.01783	0.01829
NZ2	0.00026	0.02391	−0.09438	−0.01868	0.04519
CX3	0.00351	−0.00238	0.01765	−0.02872	0.03919
CY3	0.00267	0.00271	−0.02196	0.03406	−0.04782
CZ3	0.00021	−0.00407	0.03840	−0.01552	0.05000
NX4	−0.00058	0.05550	0.01730	0.02368	0.00205
NY4	−0.00111	−0.06263	−0.01641	−0.02666	0.00172
NZ4	−0.00046	−0.03858	−0.07836	−0.01608	−0.07961
CX5	−0.00632	−0.08208	−0.06055	0.03907	−0.04966
CY5	−0.00396	0.09846	0.07327	−0.05508	0.05122
CZ5	−0.00061	−0.03574	−0.04034	0.16072	0.13188
CX6	0.06734	−0.04888	−0.03534	−0.06071	0.03742
CY6	0.05884	0.05496	0.03557	0.06646	−0.03897
CZ6	0.00292	0.00805	0.09714	0.09053	−0.09250
OX7	−0.00065	−0.00149	−0.01512	0.00436	0.00737
OY7	−0.00070	0.00038	0.01609	−0.00496	−0.00775
OZ7	0.00010	0.02918	0.02675	−0.00308	−0.01459
SX8	0.00074	0.01104	0.00738	−0.01188	−0.00247
SY8	0.00037	−0.01415	−0.00965	0.01565	0.00337
SZ8	0.00030	0.02073	0.01829	−0.03017	−0.00922
CX9	−0.09508	0.04087	0.01236	0.03114	−0.00229
CY9	−0.08300	−0.04674	−0.01179	−0.03410	0.00113
CZ9	−0.00480	0.01540	−0.04640	−0.03807	0.03019
HX10	−0.03726	−0.10836	0.04162	−0.01103	−0.05469
HY10	0.25608	0.06365	−0.05020	−0.01406	0.06402
HZ10	0.49967	0.01710	−0.07570	−0.05310	0.07120
HX11	0.27229	−0.05238	0.04770	0.01876	−0.05974
HY11	−0.04138	0.11715	−0.04552	0.01091	0.06113
HZ11	−0.47923	0.03364	−0.07593	−0.04992	0.07284
HX12	0.20566	0.08020	0.01858	0.05075	−0.01315
HY12	0.16860	−0.08300	−0.01737	−0.05052	0.00954
HZ12	0.00281	−0.26428	−0.06197	−0.14668	0.07423
HX13	0.00575	0.05849	0.01721	0.02667	0.00216
HY13	0.00426	−0.06871	−0.01634	−0.01202	0.01544
HZ13	0.00013	0.03290	−0.08231	−0.39038	−0.39509
HX14	−0.01299	−0.21923	0.20189	0.00628	0.02137
HY14	−0.00852	0.24551	−0.22482	−0.00669	−0.02544
HZ14	0.00053	0.17091	−0.25133	−0.01062	0.01690
HX15	0.07993	0.07748	−0.02575	0.01210	−0.03150
HY15	0.06743	−0.08192	0.01703	−0.00303	0.02162
HZ15	0.00165	−0.17595	0.36250	−0.31688	0.37836
OX16	−0.00045	−0.00004	0.00010	−0.00000	−0.00012
OY16	−0.00029	−0.00019	−0.00002	0.00022	0.00004
OZ16	−0.00005	−0.00000	0.00013	−0.00031	−0.00012
OX17	−0.00011	0.00013	−0.00003	−0.00006	0.00011
OY17	−0.00017	0.00018	0.00002	−0.00021	−0.00001
OZ17	0.00017	−0.00005	−0.00016	0.00035	0.00010

	26 A	27 A	28 A	29 A	30 A
Wavenumbers [cm−1]	1498.55	1535.71	1562.45	1603.57	1604.42
Intensities [km/mol]	15.46	157.62	3.83	2.28	3.58
Intensities [relative]	1.41	14.39	0.35	0.21	0.33
CX1	0.03090	0.00476	−0.00083	−0.00053	−0.00065
CY1	−0.03553	−0.00658	0.00045	0.00089	0.00054
CZ1	−0.00478	0.01690	0.01197	0.00097	−0.00026
NX2	0.03245	0.03203	0.00752	0.00184	0.00158
NY2	−0.03796	−0.03909	−0.00797	−0.00206	−0.00168
NZ2	0.00360	0.03897	−0.01621	−0.00158	−0.00094
CX3	−0.01914	−0.11615	0.00299	−0.00062	−0.00040
CY3	0.02310	0.13995	−0.00324	0.00026	0.00019
CZ3	−0.02338	−0.10366	−0.00466	−0.00007	−0.00098
NX4	−0.01163	0.04843	0.00065	0.00039	0.00029
NY4	0.01069	−0.05743	−0.00018	−0.00036	−0.00011
NZ4	0.05778	0.02284	−0.01212	0.00404	−0.00041
CX5	0.05846	−0.05413	0.00464	−0.00068	0.00058

CY5	-0.06761	0.06143	-0.00535	0.00199	0.00076
CZ5	-0.02689	0.03544	-0.00263	-0.00187	0.00023
CX6	-0.09738	0.02524	-0.01373	-0.00673	-0.00955
CY6	0.11660	-0.02698	0.01497	-0.00615	-0.00779
CZ6	-0.06193	-0.05306	0.01967	-0.00134	-0.00039
OX7	-0.00034	0.01551	-0.00533	-0.00004	-0.00043
OY7	0.00059	-0.01852	0.00561	0.00014	0.00050
OZ7	-0.00372	0.01008	0.01155	-0.00058	0.00105
SX8	-0.00151	0.00264	-0.00005	0.00014	0.00001
SY8	0.00194	-0.00301	0.00002	-0.00019	-0.00003
SZ8	-0.00280	-0.00146	0.00065	0.00015	0.00001
CX9	0.02628	-0.00047	0.04750	-0.02602	-0.03204
CY9	-0.03148	-0.00045	-0.04768	-0.01926	-0.02728
CZ9	0.01990	0.01278	-0.11249	-0.00173	-0.00325
HX10	-0.15112	-0.03029	-0.05831	0.22805	0.28027
HY10	0.04946	0.03326	0.35925	-0.20324	-0.25983
HZ10	-0.04717	0.02877	0.35963	-0.02289	-0.03947
HX11	-0.01997	-0.02969	-0.36566	-0.16766	-0.22117
HY11	0.15770	0.03466	0.09227	0.22254	0.30860
HZ11	-0.03697	0.02812	0.34280	0.05098	0.05917
HX12	0.03219	-0.00623	-0.05816	0.32521	0.42223
HY12	-0.03854	0.00536	0.02721	0.27244	0.35636
HZ12	-0.06640	0.04156	0.47942	0.00389	0.02445
HX13	-0.01123	0.05207	0.00023	0.00001	-0.00018
HY13	0.01659	-0.06326	-0.00389	0.00040	-0.00066
HZ13	-0.06260	0.08648	0.07247	-0.02239	0.00276
HX14	-0.06572	0.23392	-0.03288	-0.00643	-0.00439
HY14	0.07266	-0.26408	0.03702	0.01020	0.00733
HZ14	0.08949	-0.12486	0.01629	0.00662	0.00512
HX15	-0.01044	0.00759	0.00304	0.00111	0.00205
HY15	-0.01103	-0.01132	-0.00237	0.00257	0.00365
HZ15	0.57474	0.05864	-0.03002	0.00232	0.00514
OX16	0.00015	0.00013	0.00050	0.03901	-0.02991
OY16	-0.00001	-0.00009	-0.00060	-0.05046	0.03877
OZ16	0.00015	0.00026	0.00151	0.12477	-0.09583
OX17	-0.00010	-0.00002	-0.00044	-0.03919	0.03010
OY17	0.00006	0.00021	0.00064	0.05032	-0.03861
OZ17	-0.00010	-0.00024	-0.00154	-0.12476	0.09582

	31 A	32 A	33 A	34 A	35 A
Wavenumbers [cm-1]	1613.91	1626.40	1643.01	1800.79	2000.34
Intensities [km/mol]	45.87	28.83	95.99	203.77	1095.07
Intensities [relative]	4.19	2.63	8.77	18.61	100.00
CX1	0.02872	-0.02317	-0.03204	0.02249	-0.00159
CY1	-0.03166	0.02463	0.03836	-0.03435	0.00181
CZ1	-0.04263	0.05446	-0.01740	0.18465	0.00379
NX2	-0.06167	0.03420	0.05720	-0.00982	0.02402
NY2	0.06904	-0.03750	-0.06497	0.01344	-0.02656
NZ2	0.05603	-0.04586	-0.03302	-0.03902	-0.02948
CX3	0.00987	0.00413	0.00089	0.02176	-0.08601
CY3	-0.01164	-0.00478	0.00142	-0.02595	0.09018
CZ3	0.01408	-0.00465	-0.04926	0.01695	0.19271
NX4	-0.00909	0.00484	0.00675	-0.00727	0.00644
NY4	0.01450	-0.00631	-0.00233	0.01013	-0.00558
NZ4	-0.07767	0.01341	-0.10961	-0.03252	-0.03728
CX5	0.04001	-0.02611	0.01025	0.00729	-0.00073
CY5	-0.04904	0.03116	-0.01678	-0.01072	0.00076
CZ5	0.03975	-0.00702	0.08638	0.03693	0.00068
CX6	-0.02513	0.03432	0.01060	-0.03006	0.00042
CY6	0.02713	-0.04021	-0.01156	0.04232	-0.00041
CZ6	0.02489	-0.01218	-0.00301	-0.16533	-0.00077
OX7	0.00933	-0.01019	-0.02564	-0.00559	0.04531
OY7	-0.01063	0.01115	0.02624	0.00620	-0.04719
OZ7	-0.00451	0.01350	0.07010	0.00544	-0.10766
SX8	-0.00391	0.00160	-0.00327	0.00008	0.00016
SY8	0.00483	-0.00200	0.00419	-0.00001	-0.00024
SZ8	-0.00456	0.00212	-0.00640	-0.00131	0.00092
CX9	0.01978	0.01768	-0.00807	-0.00431	0.00011
CY9	-0.02665	-0.02406	0.00921	0.00350	-0.00015
CZ9	0.00592	0.02128	0.00956	0.02517	-0.00025
HX10	-0.21578	-0.39083	0.05882	0.02350	0.00034

HY10	-0.00101	0.00967	-0.04030	0.01348	0.00281
HZ10	-0.19499	-0.34579	0.00998	0.06852	0.00345
HX11	0.02920	0.07224	0.03310	-0.02288	-0.00289
HY11	0.25359	0.41847	-0.07056	-0.02365	-0.00022
HZ11	-0.17354	-0.31896	0.00657	0.06647	0.00291
HX12	0.01021	-0.04058	0.00820	0.01406	0.00076
HY12	0.01678	0.03830	-0.00922	-0.00950	-0.00104
HZ12	0.16418	0.37466	-0.10118	-0.08860	0.00029
HX13	-0.01176	0.00538	0.00441	-0.00899	0.00509
HY13	-0.00911	0.00078	-0.03008	0.00581	-0.01474
HZ13	0.44319	-0.13569	0.50480	0.08728	0.17609
HX14	0.24564	-0.14971	-0.21065	0.03879	-0.10364
HY14	-0.27657	0.16938	0.23588	-0.04215	0.11701
HZ14	-0.19924	0.10533	0.19356	-0.08616	0.07935
HX15	0.03039	-0.01030	-0.05178	0.07197	-0.00129
HY15	-0.03424	0.01714	0.05373	-0.07168	0.00105
HZ15	-0.02300	-0.12920	0.14567	-0.27078	0.00784
OX16	0.00138	0.00053	0.00063	0.00001	-0.00000
OY16	-0.00187	-0.00061	-0.00077	0.00022	0.00003
OZ16	0.00447	0.00158	0.00203	-0.00020	-0.00002
OX17	-0.00144	-0.00050	-0.00069	0.00016	0.00002
OY17	0.00182	0.00060	0.00076	-0.00008	-0.00003
OZ17	-0.00447	-0.00154	-0.00201	0.00023	0.00003

	36 A	37 A	38 A	39 A	40 A
Wavenumbers [cm-1]	3202.30	3273.72	3278.93	3398.48	3870.15
Intensities [km/mol]	24.11	20.33	17.32	7.80	73.04
Intensities [relative]	2.20	1.86	1.58	0.71	6.67
CX1	-0.00078	-0.00127	0.00038	0.05413	0.00004
CY1	0.00084	0.00143	-0.00072	-0.06369	-0.00003
CZ1	0.00038	-0.00033	0.00018	0.01041	-0.00027
NX2	0.00016	-0.00011	0.00003	-0.00085	-0.00028
NY2	-0.00015	0.00010	-0.00009	0.00097	0.00030
NZ2	-0.00034	-0.00009	0.00002	0.00048	0.00028
CX3	-0.00027	0.00012	-0.00010	-0.00092	-0.00046
CY3	0.00031	-0.00017	0.00007	0.00106	0.00058
CZ3	0.00014	0.00024	-0.00010	0.00024	-0.00088
NX4	0.00012	-0.00008	-0.00001	0.00000	0.04629
NY4	-0.00015	0.00008	-0.00007	-0.00002	-0.05393
NZ4	0.00019	-0.00032	0.00015	0.00023	-0.00183
CX5	-0.00038	0.00006	0.00004	-0.00026	-0.00042
CY5	0.00047	-0.00005	0.00010	0.00032	0.00045
CZ5	-0.00053	0.00076	-0.00035	-0.00032	0.00064
CX6	-0.00030	0.00000	-0.00020	-0.00110	-0.00027
CY6	0.00023	-0.00018	-0.00008	0.00141	0.00031
CZ6	0.00156	0.00084	-0.00039	-0.00420	0.00032
OX7	0.00007	-0.00001	0.00002	0.00020	0.00010
OY7	-0.00007	0.00002	-0.00001	-0.00022	-0.00011
OZ7	-0.00011	-0.00005	0.00002	-0.00020	-0.00011
SX8	-0.00002	0.00004	0.00003	0.00001	0.00001
SY8	0.00001	-0.00000	0.00005	-0.00001	-0.00001
SZ8	0.00009	-0.00011	0.00005	0.00004	0.00002
CX9	0.02423	0.01407	-0.07969	0.00137	-0.00001
CY9	-0.02259	-0.07578	-0.02924	-0.00171	0.00001
CZ9	-0.03759	0.04386	-0.02498	0.00073	0.00001
HX10	-0.26641	0.33948	0.19515	0.00124	0.00017
HY10	-0.38792	0.46696	0.29851	0.00307	0.00000
HZ10	0.27181	-0.33735	-0.22416	-0.00080	-0.00012
HX11	0.38302	-0.08979	0.59266	-0.00294	-0.00001
HY11	0.16954	-0.05798	0.26816	-0.00046	-0.00016
HZ11	0.29137	-0.06252	0.47028	-0.00080	-0.00013
HX12	-0.39745	-0.41678	0.16459	-0.01610	-0.00043
HY12	0.48067	0.49456	-0.21665	0.01935	0.00052
HZ12	-0.13146	-0.13109	0.05442	-0.00390	-0.00005
HX13	0.00032	0.00029	-0.00017	-0.00004	-0.62496
HY13	-0.00035	-0.00040	0.00011	0.00003	0.72820
HZ13	-0.00067	0.00027	-0.00013	0.00022	0.03067
HX14	-0.00005	-0.00022	-0.00004	0.00630	-0.00241
HY14	0.00015	0.00019	-0.00016	-0.00757	0.00315
HZ14	-0.00149	-0.00058	0.00018	0.00291	-0.00578
HX15	0.00847	0.01332	-0.00526	-0.61422	0.00002

HY15	-0.00993	-0.01545	0.00664	0.72221	-0.00003
HZ15	0.00036	0.00078	-0.00030	-0.08707	0.00009
OX16	-0.00003	0.00002	-0.00006	0.00001	-0.00000
OY16	-0.00001	0.00000	-0.00001	0.00000	-0.00000
OZ16	0.00004	-0.00000	0.00005	-0.00001	0.00000
OX17	0.00001	0.00000	0.00002	-0.00002	0.00000
OY17	0.00001	0.00000	0.00000	0.00000	-0.00000
OZ17	-0.00001	-0.00001	0.00000	0.00000	-0.00000

	41 A
Wavenumbers [cm-1]	3911.03
Intensities [km/mol]	145.43
Intensities [relative]	13.28
CX1	-0.00063
CY1	0.00066
CZ1	0.00197
NX2	-0.02088
NY2	0.02793
NZ2	-0.06247
CX3	0.00078
CY3	-0.00087
CZ3	-0.00022
NX4	0.00053
NY4	-0.00064
NZ4	0.00050
CX5	-0.00013
CY5	0.00016
CZ5	-0.00024
CX6	0.00007
CY6	-0.00010
CZ6	0.00062
OX7	0.00004
OY7	-0.00004
OZ7	-0.00020
SX8	0.00002
SY8	-0.00003
SZ8	0.00005
CX9	0.00005
CY9	-0.00007
CZ9	-0.00004
HX10	-0.00019
HY10	-0.00016
HZ10	0.00031
HX11	0.00022
HY11	0.00015
HZ11	0.00034
HX12	-0.00055
HY12	0.00066
HZ12	-0.00012
HX13	-0.00405
HY13	0.00468
HZ13	0.00051
HX14	0.27973
HY14	-0.37511
HZ14	0.83776
HX15	0.00456
HY15	-0.00533
HZ15	-0.00103
OX16	0.00000
OY16	0.00000
OZ16	-0.00000
OX17	-0.00000
OY17	0.00000
OZ17	0.00000

Normal Modes of imaginary frequencies

	1	2
Wavenumbers [cm-1]	160.76	100.69
Intensities [km/mol]	0.02	0.09

Intensities [relative]	0.00	0.01
CX1	0.00325	0.00123
CY1	−0.00153	0.00060
CZ1	−0.00759	−0.00254
NX2	0.00938	0.00015
NY2	−0.00426	0.00001
NZ2	−0.00404	−0.00213
CX3	0.00724	0.00691
CY3	−0.00661	0.00575
CZ3	0.00266	−0.00140
NX4	0.00101	0.00295
NY4	−0.00386	0.00323
NZ4	0.00553	−0.00119
CX5	−0.00310	−0.00323
CY5	0.00085	−0.00097
CZ5	0.00258	−0.00169
CX6	−0.00230	0.00382
CY6	0.00131	0.00420
CZ6	−0.00483	−0.00200
OX7	0.01073	0.01435
OY7	−0.01006	0.01167
OZ7	0.00560	−0.00085
SX8	−0.00810	−0.01931
SY8	0.00563	−0.01327
SZ8	0.00713	−0.00158
CX9	−0.00339	0.00641
CY9	0.00897	0.00905
CZ9	−0.00868	−0.00289
HX10	−0.00080	0.00763
HY10	0.01178	0.01169
HZ10	−0.00246	0.00178
HX11	−0.00351	0.00824
HY11	0.01559	0.01158
HZ11	−0.01191	−0.00613
HX12	−0.00561	0.00637
HY12	0.00573	0.00856
HZ12	−0.01414	−0.00464
HX13	0.00084	0.00197
HY13	−0.00424	0.00236
HZ13	0.01054	−0.00056
HX14	0.01139	0.00599
HY14	−0.00828	0.00491
HZ14	−0.00645	−0.00188
HX15	0.00514	0.00366
HY15	−0.00066	0.00251
HZ15	−0.01283	−0.00273
OX16	0.09801	0.13766
OY16	−0.11800	0.10933
OZ16	−0.08315	0.01106
OX17	−0.10335	−0.12952
OY17	0.12040	−0.11385
OZ17	0.07622	0.00466

Normal Modes of low/zero frequencies

	1	2	3	4	5
Wavenumbers [cm-1]	0.00	0.00	0.00	0.00	0.00
Intensities [km/mol]	0.00	0.00	0.00	0.00	0.00
Intensities [relative]	0.00	0.00	0.00	0.00	0.00
CX1	0.07001	−0.00146	−0.01104	0.04028	−0.00937
CY1	0.04494	−0.01701	0.08265	0.00613	−0.01096
CZ1	−0.04391	−0.01961	0.04603	0.01538	0.02372
NX2	0.09457	0.01085	−0.03436	−0.00026	−0.01043
NY2	0.04608	−0.04517	0.07824	−0.01156	0.02200
NZ2	−0.03446	−0.00258	0.03848	0.00654	0.00919
CX3	0.08530	0.02803	−0.05257	−0.01935	0.02116
CY3	0.03702	−0.03233	0.06331	−0.02717	0.05108
CZ3	−0.01751	0.03138	0.02430	−0.00906	−0.01882
NX4	0.04934	0.03214	−0.04583	0.00513	0.05436
NY4	0.02669	0.01101	0.05308	−0.02372	0.04467

NZ4	-0.01075	0.04739	0.01819	-0.01509	-0.03141
CX5	0.02258	0.02111	-0.02338	0.04555	0.05893
CY5	0.02462	0.04176	0.05625	-0.00670	0.01296
CZ5	-0.01908	0.03322	0.02469	-0.00723	-0.01910
CX6	0.03482	0.00266	-0.00458	0.06408	0.02327
CY6	0.03471	0.02554	0.07243	0.00927	-0.01680
CZ6	-0.03702	-0.00373	0.03988	0.00920	0.01113
OX7	0.10626	0.03872	-0.07268	-0.05423	0.02050
OY7	0.03785	-0.05623	0.05929	-0.04257	0.07977
OZ7	-0.00910	0.04625	0.01764	-0.01695	-0.03159
SX8	-0.01918	0.02879	-0.01915	0.06941	0.10163
SY8	0.01164	0.09211	0.04245	-0.00537	0.01050
SZ8	-0.00892	0.05712	0.01554	-0.01631	-0.03793
CX9	0.00850	-0.01076	0.02068	0.10789	0.02409
CY9	0.03376	0.05542	0.07762	0.02875	-0.05309
CZ9	-0.04778	-0.02245	0.04835	0.01932	0.02728
HX10	-0.01347	-0.00003	0.01462	0.10988	0.05612
HY10	0.03651	0.06341	0.08497	0.04230	-0.07832
HZ10	-0.06520	-0.00123	0.05251	0.03967	0.02382
HX11	-0.00357	-0.01888	0.03470	0.13107	0.02166
HY11	0.02204	0.08784	0.06205	0.02026	-0.03727
HZ11	-0.02589	-0.03095	0.03975	-0.00485	0.02121
HX12	0.02233	-0.02364	0.03207	0.11628	-0.00482
HY12	0.04200	0.03792	0.08982	0.03864	-0.07152
HZ12	-0.06053	-0.04944	0.05928	0.03094	0.04919
HX13	0.04228	0.04476	-0.05912	-0.00867	0.07774
HY13	0.02004	0.02064	0.04217	-0.03503	0.06573
HZ13	0.00156	0.07236	0.00784	-0.02640	-0.05194
HX14	0.12046	0.00739	-0.03858	-0.01709	-0.03506
HY14	0.05362	-0.07627	0.08582	-0.01370	0.02598
HZ14	-0.03955	-0.01502	0.04315	0.01105	0.01889
HX15	0.08107	-0.01459	0.00156	0.05144	-0.03652
HY15	0.05276	-0.03146	0.09473	0.01709	-0.03138
HZ15	-0.05702	-0.04646	0.05709	0.02739	0.04571
OX16	0.05348	-0.03002	0.02972	0.09951	-0.03760
OY16	0.01036	0.06551	0.03360	-0.02863	0.05382
OZ16	0.03011	-0.05571	0.01832	-0.06692	0.00739
OX17	0.08507	-0.03372	0.02392	0.07815	-0.06690
OY17	0.01955	0.02731	0.04277	-0.03145	0.05907
OZ17	0.02392	-0.06997	0.02384	-0.06137	0.01869

	6	7	8
Wavenumbers [cm-1]	0.00	16.36	30.00
Intensities [km/mol]	0.00	0.00	0.00
Intensities [relative]	0.00	0.00	0.00
CX1	0.02708	0.05940	-0.02251
CY1	-0.02183	0.01657	-0.01408
CZ1	0.06604	-0.01100	-0.04124
NX2	0.03120	0.03654	-0.02795
NY2	-0.01701	-0.00615	-0.03142
NZ2	0.06564	-0.01050	-0.03597
CX3	0.03375	-0.01256	-0.02750
CY3	-0.01474	-0.04879	-0.03173
CZ3	0.06466	-0.00972	-0.02496
NX4	0.03188	-0.02575	-0.00714
NY4	-0.01766	-0.05671	-0.00090
NZ4	0.06406	-0.00896	-0.01885
CX5	0.02784	0.00219	0.00842
CY5	-0.02249	-0.02883	0.02574
CZ5	0.06433	-0.00901	-0.02258
CX6	0.02526	0.04497	-0.00843
CY6	-0.02466	0.00728	0.01114
CZ6	0.06546	-0.01021	-0.03539
OX7	0.03731	-0.04166	-0.04250
OY7	-0.01057	-0.07662	-0.05567
OZ7	0.06433	-0.00979	-0.02082
SX8	0.02621	-0.01585	0.04542
SY8	-0.02539	-0.04004	0.07186
SZ8	0.06345	-0.00751	-0.01300
CX9	0.02080	0.06569	-0.01141
CY9	-0.02990	0.02901	0.02303

CZ9	0.06585	−0.01078	−0.04170
HX10	0.02121	0.02926	−0.00216
HY10	−0.03288	0.05152	0.02419
HZ10	0.06219	−0.01509	−0.03102
HX11	0.01839	0.07924	−0.01505
HY11	−0.03000	−0.00849	0.04025
HZ11	0.06894	−0.00661	−0.04751
HX12	0.01939	0.10310	−0.02133
HY12	−0.03085	0.05993	0.01234
HZ12	0.06672	−0.01136	−0.05159
HX13	0.03374	−0.05856	−0.00081
HY13	−0.01603	−0.08492	0.00413
HZ13	0.06332	−0.00809	−0.01040
HX14	0.03245	0.04405	−0.04528
HY14	−0.01497	−0.00241	−0.05557
HZ14	0.06613	−0.01130	−0.04089
HX15	0.02542	0.09004	−0.03300
HY15	−0.02314	0.04247	−0.02410
HZ15	0.06685	−0.01209	−0.05035
OX16	0.02048	−0.04016	0.02405
OY16	−0.01960	0.11442	−0.03115
OZ16	0.07708	0.04340	0.11674
OX17	0.02211	−0.03383	0.01170
OY17	−0.01706	0.11241	−0.03954
OZ17	0.07760	0.04062	0.11724

6. Frequencies for PS–O2 on SS2 (product) state

Imaginary Vibration Nr	Wavenumber [1/cm]
1	160.76
2	100.69

Low Vibration Nr	Wavenumber [1/cm]
1	0.00
2	0.00
3	0.00
4	0.00
5	0.00
6	0.00
7	16.36
8	30.00

Vibration Nr	Wavenumber [1/cm]
1	109.67
2	124.24
3	142.70
4	198.30
5	272.79
6	323.04
7	350.49
8	391.68
9	465.64
10	539.52
11	549.11
12	581.50
13	675.05
14	721.18
15	742.60
16	844.58
17	853.55
18	872.03
19	1021.97
20	1102.52
21	1145.21
22	1230.83
23	1287.65
24	1305.00
25	1370.32

26	1498.55
27	1535.71
28	1562.45
29	1603.57
30	1604.42
31	1613.91
32	1626.40
33	1643.01
34	1800.79
35	2000.34
36	3202.30
37	3273.72
38	3278.93
39	3398.48
40	3870.15
41	3911.03

7. Displacement vector (after satisfyinging Eckart Conditions)

0.00388395
−0.439627
−0.0942146
−2.75172
0.440412
−0.63253
−0.27842
−0.225683
−0.203802
−0.0230315
0.241474
0.225711
−0.00591381
0.0507408
−0.201204
−0.153447
−0.198813
0.445159
−0.0144018
0.324341
−0.165751
−0.149265
−0.235925
0.273035
−0.147082
0.404209
−0.125863
−0.680695
0.0588924
0.0646134
0.126156
−0.141349
0.0771214
0.37645
−0.0317917
1.76075
−0.110988
0.211587
0.10535
−0.00815724
−0.00147231
−0.178195
0.140724
2.20556
−0.920967

8. Duschinsky rotation matrix (after satisfyinging Eckart Conditions)

Note that the determinant of the Duschinsky matrix is 0.991402

0.519454	−0.426969	0.650834	0.061326	−0.039179
0.128338	−0.185711	−0.421501	0.356382	0.021110

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-0.016576 0.090186  0.014808  -0.008996 -0.032767
-0.180401 0.082756  -0.028184 -0.023663 -0.198620
-0.052493 -0.056536 -0.109506 -0.049337 -0.812113
-0.028774 0.029558  0.026805  -0.002414 0.329939
-0.008569 -0.002463 0.047525  -0.087795 -0.207224
-0.026633 0.020443  0.054021  -0.069696 0.135064
0.001503  0.000376  -0.025611 -0.008589 0.004549
-0.041805 0.022073  0.099837  0.069331  0.037497
0.017832  -0.012057 -0.005214 0.020143  0.012933
-0.057988 -0.018208 -0.009623 0.019548  0.005372
-0.030138 -0.038782 -0.080120 0.026251  -0.029985
0.009453  -0.029733 -0.042230 -0.023457 -0.035906
-0.001884 -0.024110 -0.005152 0.003633  -0.011815
0.021550  -0.002795 0.000556  -0.012743 -0.049190
0.000027  -0.002612 0.005906  -0.000075 -0.011134
-0.049804 0.013770  0.026696  0.004403  -0.003143
-0.023371 0.042324  0.044298  0.004311  -0.004309
-0.036639 0.013367  0.014847  0.012823  -0.051173
-0.057362 0.017154  0.027232  -0.019985 0.077494
-0.038055 0.001405  0.009934  0.002886  -0.022289
-0.003793 0.008687  0.011501  0.042508  0.004341
0.009699  -0.012409 -0.010307 -0.010294 0.014392
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-0.008646 -0.012559 0.006106  -0.121353 -0.007209
-0.004634 -0.010120 0.016649  -0.298559 -0.005563
-0.010992 0.013399  0.009648  0.004076  -0.002678
-0.023088 0.001523  0.011275  0.028973  -0.015270
0.022370  -0.007491 -0.013114 0.016772  -0.052805
-0.015988 0.007370  0.007626  -0.006603 -0.012227
0.013335  -0.007223 -0.008528 0.002119  0.006747
0.014139  -0.006802 -0.011577 -0.038243 0.012797
0.000087  0.000180  -0.002237 -0.003038 0.002387
0.004071  -0.044937 0.022836  -0.778978 0.014828
0.018839  -0.005274 -0.014325 0.059930  -0.036851
0.033943  -0.002028 -0.031536 0.245531  0.020979
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-0.001132 -0.000140 0.001884  0.000537  0.001179
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-0.091116  0.069753  0.050176  -0.040962  0.003138
-0.035351  -0.047051  -0.002313  -0.017721  0.000161
0.027444  -0.062757  -0.035740  0.041313  0.005745
-0.144403  0.041070  0.008140  -0.075865  0.010311
-0.011521  -0.073846  0.001585  0.012356  0.001609
0.048657  -0.030556  0.009079  0.005205  -0.006476
0.015967  -0.147294  -0.064610  0.199068  -0.019357
0.080884  -0.094077  -0.031164  0.054731  0.009453
0.015374  0.012341  -0.011863  0.020380  -0.008296
-0.192532  0.274488  0.119881  -0.258919  -0.018701
-0.292609  0.063965  -0.029711  -0.032148  0.071321
-0.376760  -0.382886  -0.469818  0.417881  0.219168
0.586112  -0.278269  -0.038895  -0.003421  0.019197
-0.199524  -0.723852  0.440260  -0.406670  -0.039607
-0.125104  0.118906  0.695044  0.552834  -0.097931
0.141658  -0.034799  0.249834  0.173253  0.815387
0.053445  -0.224793  -0.036376  0.344943  -0.333110
```

```
-0.028292  0.066167  -0.014475 -0.203113 0.131301
-0.048375  0.012796   0.015077  0.057450  0.074541
-0.045434 -0.009930   0.078405  0.017355 -0.148345
-0.073935 -0.013831  -0.009750  0.056362 -0.192163
 0.001462  0.092226  -0.003680  0.017646  0.007199
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 0.324279 -0.113805   0.010784 -0.035978 -0.023299
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 0.000253  0.008030  -0.011125 -0.000241 -0.003966
-0.000204  0.000912  -0.001272  0.010613  0.007795
-0.072649 -0.000417   0.016912 -0.021254 -0.021192
 0.032454 -0.003889  -0.004900  0.000674  0.016449
 0.013242  0.001899  -0.005410  0.003019  0.007464


 0.004613  0.001244   0.043594 -0.001225 -0.004282
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-0.009840 -0.003349   0.037026 -0.007565 -0.012515
 0.007623 -0.004421  -0.078317  0.008594  0.003736
 0.001143 -0.000002   0.005199 -0.025768  0.013096
 0.011354  0.001599  -0.000519  0.006776 -0.020409
 0.021543  0.005639  -0.000210 -0.021545 -0.016388
 0.031434 -0.006624   0.012466 -0.007986 -0.005940
 0.005690  0.002443  -0.035258 -0.051576 -0.064604
 0.040600  0.005134  -0.010515  0.024591  0.025773
-0.015937  0.002603   0.013708  0.030248  0.039654
-0.040680 -0.005389   0.011470  0.013138  0.013106
-0.005591 -0.016621  -0.008213 -0.004833 -0.010358
-0.018054  0.019610   0.009359  0.038496  0.059335
-0.059161  0.015884  -0.009629 -0.005908 -0.009532
 0.024789 -0.034300  -0.002634 -0.034286 -0.021051
 0.022056 -0.044751  -0.000184 -0.006882 -0.008685
-0.122391 -0.020283  -0.013445 -0.028489 -0.028823
 0.005054  0.037552  -0.000672 -0.002979 -0.001464
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-0.095112 -0.041921  -0.000832  0.079615  0.111995
-0.077964 -0.012366  -0.005927  0.001732 -0.001927
 0.078479 -0.040764   0.023070  0.044811  0.058365
-0.261214  0.024635  -0.012898  0.042636  0.045033
 0.356065  0.068820  -0.051000 -0.024569 -0.047627
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-0.033394  0.679350   0.310716 -0.022318 -0.020980
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-0.101409 -0.010770   0.061549  0.137036 -0.013500
-0.038637  0.015898  -0.072876  0.646081 -0.138790
 0.153059 -0.053688   0.066841  0.490148 -0.648596
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-0.005798 -0.026743   0.002192  0.003271 -0.001961
-0.061607 -0.015829  -0.157353  0.096093  0.115421
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-0.002521  0.000275   0.039263 -0.003041 -0.005440


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 0.008023  0.026210  -0.035460 -0.007270  0.000943
-0.007760 -0.024468  -0.005511  0.009012  0.000949
-0.007767 -0.039079   0.029787 -0.044350 -0.006506
```

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-0.031719 -0.072711  0.000209   0.070422  0.000806
-0.023384 -0.015820 -0.004989 -0.004647  0.008848
0.018208   0.043595  -0.006377 -0.029917 -0.000461
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0.030861   0.076313   0.005275  -0.049866  0.000240
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0.057940   -0.021718  0.042809  -0.055961 -0.001001
0.023267   0.010051   0.027355  -0.131984 -0.007153
-0.009327 -0.004945  0.005449  -0.012026  0.014586
-0.076333  0.001657  -0.076091  0.207481   0.007335
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0.083020   -0.092820  0.100218  -0.067715 -0.009056
0.087415   0.174619  -0.005247 -0.088595 -0.004053
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0.003737   0.041558   0.055135  -0.007243  0.003319
0.007818   0.069504  -0.023043 -0.005333 -0.011947
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0.009944   0.009988  -0.033471  0.010505  -0.001397
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-0.002901 -0.060157  0.151807   0.006814   0.001959
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0.075232   -0.022623  0.043442   0.005257   0.007047
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0.000692 0.001839 -0.001405 0.000824 0.003803
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-0.005916 -0.002820 -0.001405 0.019604 -0.006769
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-0.008478 0.023451 -0.013462 0.004779 -0.000678
0.008174 -0.003379 0.000649 0.001788 -0.003534
-0.006963 0.000162 -0.000185 -0.000447 -0.000844
-0.001911 -0.007450 -0.003003 0.058695 -0.022046
-0.000069 0.002787 0.001883 0.001223 0.004464
-0.000643 0.002865 0.002405 -0.009715 0.005634
-0.000084 0.000519 0.000945 0.011371 -0.003732
0.961626 -0.000097 0.000119 -0.000240 -0.000185
0.272475 -0.000082 -0.000035 0.000857 -0.000443
0.000169 0.057659 0.066972 0.445990 0.201643
0.000164 -0.028839 -0.052212 0.329875 0.847179
0.000023 0.007976 0.004204 0.812735 -0.467884

9. The correlation function for this complex, with and without the damping factor is given in Figure S1

10. Diabatic coupling as a function of D (in au)
(as seen in Figure S5c (red curve))

3.80	0.000000000000000E+000
3.75	8.203380098048892E-008
3.70	1.969566802124054E-007
3.65	3.595989896334144E-007
3.60	5.785105253478750E-007
3.55	8.551926109514758E-007
3.50	1.188774288422392E-006
3.45	1.579096781928937E-006
3.40	2.028149223021284E-006
3.35	2.537981017733336E-006
3.30	3.109979878133577E-006
3.25	3.744116599587323E-006
3.20	4.438067341846056E-006
3.15	5.186284487536107E-006
3.10	5.978848088278649E-006
3.05	6.799747207765892E-006
3.00	7.625280474457299E-006
2.95	8.421009218229659E-006
2.90	9.138880366846559E-006
2.85	9.711908744107661E-006
2.80	1.004805761604361E-005
2.75	1.009729390888059E-005
2.70	1.029111762259797E-005
2.65	1.118573415114458E-005
2.60	1.310439024274072E-005
2.55	1.651212227350761E-005
2.50	2.208856453131599E-005
2.45	3.084967639790852E-005
2.40	4.435079141871678E-005
2.35	6.505772342933503E-005
2.30	9.712167442403280E-005
2.25	1.485787315244304E-004
2.20	2.420212264199706E-004

11. Boltzmann factor as a function of D
(as seen in Figure S6c (red curve))

3.80	1.00000000000000
3.75	1.00499276645464
3.70	1.00190918596945
3.65	0.988516287911033
3.60	0.962979210834943
3.55	0.923700303349582
3.50	0.869652513600425
3.45	0.800833561505537
3.40	0.718485281648624
3.35	0.625229918807414
3.30	0.524936652926016
3.25	0.422709685197629
3.20	0.324230868685155
3.15	0.234938303659945
3.10	0.15929377810805
3.05	9.992293503535825E-002
3.00	5.720267883523220E-002
2.95	2.941679828354223E-002
2.90	1.333271828731101E-002
2.85	5.210821145018842E-003
2.80	1.711855078904717E-003
2.75	4.589946823603000E-004
2.70	9.716814451182585E-005
2.65	1.564980005857877E-005
2.60	1.840571103480987E-006
2.55	1.512234023085287E-007
2.50	8.285243341204754E-009
2.45	2.886652258346095E-010
2.40	6.105621630922543E-012
2.35	7.520932937901166E-014
2.30	5.211604436370388E-016
2.25	1.971748227240822E-018
2.20	3.839128487437594E-021

12. Value of FCWD for this complex is 37.6702355
(numerical integration of the damped correlation
function performed using SIMPSONS method)

11. Photosensitization rate constant as a
function of D, along the to56 direction
(as seen in Figure 5c (red curve))

3.80	0
3.75	11901.6
3.70	62709.9
3.65	200266
3.60	515370
3.55	1.14197e+06
3.50	2.23711e+06
3.45	3.93084e+06
3.40	6.24946e+06
3.35	9.01462e+06
3.30	1.17765e+07
3.25	1.38525e+07
3.20	1.45134e+07
3.15	1.3373e+07
3.10	1.08727e+07
3.05	7.87917e+06
3.00	5.17979e+06
2.95	3.1441e+06
2.90	1.72853e+06
2.85	825054
2.80	323630
2.75	98913.4
2.70	24263.8
2.65	5001.69
2.60	838.441
2.55	108.145
2.50	10.1765
2.45	0.661892
2.40	0.0284819
2.35	0.000788571
2.30	1.37617e-05
2.25	1.48478e-07
2.20	9.86149e-10