

Supplementary Material

-NDI-FC.7-

FC factor greater than 0.7, 3 transitions of 1B3u, 2 transitions of 1B2u
energies in cm^{-1} , atom coordinates in Angstrom, charges in 10^{-10} esu

```
10                                     # number of atoms
  -2.240      3.535      0.180      1.0000 # O1
    0.000      3.515      0.190      1.0000 # N1
    2.270      3.495      0.080      1.0000 # O4
  -2.390      0.705      0.120      1.0000 # C3
    2.400      0.695      0.210      1.0000 # C10
  -2.400     -0.685      0.050      1.0000 # C4
    2.400     -0.705      0.200      1.0000 # C9
  -2.250     -3.495     -0.220      1.0000 # O2
    0.000     -3.505     -0.020      1.0000 # N2
    2.240     -3.515      0.150      1.0000 # O3
&TRANSITION 1->...
  2  28235      # 1B3u, 354.17 nm, trans. mom. -0.932 D, on x axis
    -0.9316     0.0000     0.0000     1.000 # Electr. mom., scale fac.
    0.0000     0.0000     0.0000           # Magnet. mom.
    0.00000000     0.00000000     0.00000000     -1.000 # x y z q
   -0.93163531     0.00000000     0.00000000     1.000 # x y z q
  2  28299      # 1B3u, 353.37 nm, trans. mom. 0.715 D, on x axis
    -0.7146     0.0000     0.0000     1.000 # Electr. mom., scale fac.
    0.0000     0.0000     0.0000           # Magnet. mom.
    0.00000000     0.00000000     0.00000000     -1.000 # x y z q
   -0.71455524     0.00000000     0.00000000     1.000 # x y z q
  2  27876      # 1B3u, 358.73 nm, trans. mom. 0.660 D, on x axis
    -0.6603     0.0000     0.0000     1.000 # Electr. mom., scale fac.
    0.0000     0.0000     0.0000           # Magnet. mom.
    0.00000000     0.00000000     0.00000000     -1.000 # x y z q
   -0.66028522     0.00000000     0.00000000     1.000 # x y z q
  2  27030      # 1B2u, 369.96 nm, trans. mom. 2.546 D, on y axis
    0.0000     2.5455     0.0000     1.000 # Electr. mom., scale fac.
    0.0000     0.0000     0.0000           # Magnet. mom.
    0.00000000     0.00000000     0.00000000     -1.000 # x y z q
    0.00000000     2.54546662     0.00000000     1.000 # x y z q
  2  25892      # 1B2u, 386.22 nm, trans. mom. 2.224 D, on y axis
    0.0000     2.2242     0.0000     1.000 # Electr. mom., scale fac.
    0.0000     0.0000     0.0000           # Magnet. mom.
    0.00000000     0.00000000     0.00000000     -1.000 # x y z q
    0.00000000     2.22419413     0.00000000     1.000 # x y z q
&TRANSITION 2->...
  0  0
    0.0000     0.0000     0.0000     1.000 # electr. mom., scale fac.
    0.0000     0.0000     0.0000           # magnet. mom.
  0  0
    0.0000     0.0000     0.0000     1.000 # electr. mom., scale fac.
    0.0000     0.0000     0.0000           # magnet. mom.
  0  0
    0.0000     0.0000     0.0000     1.000 # electr. mom., scale fac.
```

| | | | | | |
|--------------------|--------|--------|--------|-------|----------------------------|
| | 0.0000 | 0.0000 | 0.0000 | | # magnet. mom. |
| 0 | 0 | | | | |
| | 0.0000 | 0.0000 | 0.0000 | 1.000 | # electr. mom., scale fac. |
| | 0.0000 | 0.0000 | 0.0000 | | # magnet. mom. |
| &TRANSITION 3->... | | | | | |
| 0 | 0 | | | | |
| | 0.0000 | 0.0000 | 0.0000 | 1.000 | # electr. mom., scale fac. |
| | 0.0000 | 0.0000 | 0.0000 | | # magnet. mom. |
| 0 | 0 | | | | |
| | 0.0000 | 0.0000 | 0.0000 | 1.000 | # electr. mom., scale fac. |
| | 0.0000 | 0.0000 | 0.0000 | | # magnet. mom. |
| 0 | 0 | | | | |
| | 0.0000 | 0.0000 | 0.0000 | 1.000 | # electr. mom., scale fac. |
| | 0.0000 | 0.0000 | 0.0000 | | # magnet. mom. |
| &TRANSITION 4->... | | | | | |
| 0 | 0 | | | | |
| | 0.0000 | 0.0000 | 0.0000 | 1.000 | # electr. mom., scale fac. |
| | 0.0000 | 0.0000 | 0.0000 | | # magnet. mom. |
| 0 | 0 | | | | |
| | 0.0000 | 0.0000 | 0.0000 | 1.000 | # electr. mom., scale fac. |
| | 0.0000 | 0.0000 | 0.0000 | | # magnet. mom. |
| &TRANSITION 5->... | | | | | |
| 0 | 0 | | | | |
| | 0.0000 | 0.0000 | 0.0000 | 1.000 | # electr. mom., scale fac. |
| | 0.0000 | 0.0000 | 0.0000 | | # magnet. mom. |
| &PERMANENT MOMENTS | | | | | |
| 0 | 0 | | | | |
| | 0.0000 | 0.0000 | 0.0000 | 1.000 | # electr. mom., scale fac. |
| 0 | 0 | | | | |
| | 0.0000 | 0.0000 | 0.0000 | 1.000 | # electr. mom., scale fac. |
| 0 | 0 | | | | |
| | 0.0000 | 0.0000 | 0.0000 | 1.000 | # electr. mom., scale fac. |
| 0 | 0 | | | | |
| | 0.0000 | 0.0000 | 0.0000 | 1.000 | # electr. mom., scale fac. |
| 0 | 0 | | | | |
| | 0.0000 | 0.0000 | 0.0000 | 1.000 | # electr. mom., scale fac. |