Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics


# Integrated experimental and computational spectroscopy study on the protonation of the α-nitronyl nitroxide radical unit

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**Supporting information**

Table S1. Optimized geometry of (**I**).

| | | | |
|---|---|---|---|
| C | -2.693136 | -0.481061 | 0.334078 |
| C | -1.380357 | -0.918445 | 0.076148 |
| C | -1.166727 | -2.282840 | -0.195723 |
| C | -2.232535 | -3.171942 | -0.201194 |
| C | -3.526812 | -2.729233 | 0.050298 |
| C | -3.748880 | -1.381870 | 0.314345 |
| C | -0.262889 | 0.024111 | 0.090147 |
| N | 0.964557 | -0.189300 | -0.455758 |
| C | 1.805699 | 1.065675 | -0.452136 |
| C | 1.103872 | 1.881776 | 0.672914 |
| N | -0.274370 | 1.263345 | 0.650775 |
| O | 1.368714 | -1.227129 | -1.072750 |
| O | -1.237844 | 1.829002 | 1.261386 |
| C | 0.998546 | 3.381825 | 0.426387 |
| C | 1.661735 | 1.620849 | 2.079081 |
| C | 1.660924 | 1.675347 | -1.853511 |
| C | 3.263334 | 0.707128 | -0.190169 |
| H | -4.355201 | -3.428266 | 0.041155 |
| H | -4.752929 | -1.024139 | 0.509814 |
| H | -2.874974 | 0.557496 | 0.557459 |
| H | -0.170589 | -2.634425 | -0.409536 |
| H | -2.046471 | -4.219139 | -0.408685 |
| H | 2.647388 | 2.072099 | 2.195866 |
| H | 0.989783 | 2.067582 | 2.811377 |
| H | 1.740347 | 0.555149 | 2.295591 |
| H | 1.995991 | 3.824688 | 0.403046 |
| H | 0.492432 | 3.615139 | -0.507930 |
| H | 0.435702 | 3.844115 | 1.235010 |
| H | 1.998580 | 0.946411 | -2.589709 |
| H | 0.626438 | 1.933964 | -2.081033 |
| H | 2.272409 | 2.572638 | -1.951836 |
| H | 3.635227 | 0.083496 | -1.000854 |
| H | 3.866950 | 1.615685 | -0.148921 |
| H | 3.395931 | 0.158747 | 0.739996 |

Table S2. Optimized geometry of (**II**).

| | | | |
|---|---|---|---|
| N | -0.255573 | 1.285492 | 0.605158 |
| C | -0.289013 | 0.062491 | 0.075393 |
| N | 0.935013 | -0.146015 | -0.527519 |
| C | 1.801673 | 1.100758 | -0.499678 |
| C | 1.136481 | 1.869269 | 0.693406 |
| C | -1.382381 | -0.882844 | 0.084540 |
| C | -2.716667 | -0.430481 | 0.095954 |
| C | -3.756278 | -1.341837 | 0.086994 |
| C | -3.487833 | -2.710092 | 0.095317 |
| C | -2.172782 | -3.167083 | 0.096456 |
| C | -1.120281 | -2.267302 | 0.076648 |
| O | 1.233932 | -1.153433 | -1.212749 |
| C | 1.613167 | 1.776543 | -1.865400 |
| C | 3.259980 | 0.711931 | -0.294469 |
| C | 1.086929 | 3.384646 | 0.530487 |
| C | 1.705127 | 1.494832 | 2.067699 |
| O | -1.179994 | 1.625156 | 1.572086 |
| H | -4.305950 | -3.419421 | 0.098764 |
| H | -4.779249 | -0.988735 | 0.075385 |
| H | -2.938150 | 0.626325 | 0.084393 |
| H | -0.105407 | -2.633534 | 0.068261 |
| H | -1.966120 | -4.229311 | 0.106962 |
| H | 2.708543 | 1.903415 | 2.178381 |
| H | 1.083456 | 1.916438 | 2.855732 |
| H | 1.753892 | 0.415646 | 2.215201 |
| H | 2.100920 | 3.780236 | 0.467580 |
| H | 0.546684 | 3.696756 | -0.361373 |
| H | 0.625449 | 3.846716 | 1.404208 |
| H | 1.932181 | 1.090742 | -2.649376 |
| H | 0.576256 | 2.054726 | -2.056469 |
| H | 2.229404 | 2.672113 | -1.931545 |
| H | 3.609818 | 0.140569 | -1.152371 |
| H | 3.871900 | 1.611595 | -0.219959 |
| H | 3.414335 | 0.111878 | 0.599252 |
| H | -1.535474 | 2.493222 | 1.310727 |

Table S3. Optimized geometry of (**III**).

| | | | |
|---|---|---|---|
| C | -2.723410 | -0.465989 | 0.169281 |
| C | -1.398382 | -0.933532 | 0.076116 |
| C | -1.158907 | -2.317152 | -0.030030 |
| C | -2.223957 | -3.203340 | -0.032875 |
| C | -3.531509 | -2.733544 | 0.050105 |
| C | -3.775969 | -1.366696 | 0.146278 |
| C | -0.287828 | 0.003571 | 0.089367 |
| N | 0.926885 | -0.151977 | -0.520513 |
| C | 1.810059 | 1.099463 | -0.471116 |
| C | 1.137367 | 1.880386 | 0.691847 |
| N | -0.245358 | 1.219911 | 0.714192 |
| O | 1.280561 | -1.141047 | -1.136772 |
| O | -1.169405 | 1.727887 | 1.323496 |
| C | 0.973401 | 3.380835 | 0.483873 |
| C | 1.732747 | 1.590864 | 2.079968 |
| C | 1.644221 | 1.751284 | -1.854129 |
| C | 3.258498 | 0.682707 | -0.247998 |
| H | -4.358962 | -3.431756 | 0.039569 |
| H | -4.791833 | -0.998288 | 0.207659 |
| H | -2.934250 | 0.588830 | 0.252705 |
| H | -0.153446 | -2.701448 | -0.103712 |
| H | -2.030695 | -4.265935 | -0.103676 |
| H | 2.719602 | 2.045001 | 2.153989 |
| H | 1.097362 | 2.036335 | 2.844118 |
| H | 1.824584 | 0.524427 | 2.284593 |
| H | 1.960260 | 3.840195 | 0.420372 |
| H | 0.420074 | 3.625956 | -0.419761 |
| H | 0.455252 | 3.819654 | 1.333807 |
| H | 1.987083 | 1.058989 | -2.621754 |
| H | 0.611377 | 2.023755 | -2.070029 |
| H | 2.258890 | 2.648355 | -1.909009 |
| H | 3.615494 | 0.107893 | -1.099835 |
| H | 3.876424 | 1.577325 | -0.165725 |
| H | 3.394611 | 0.085560 | 0.650727 |

Table S4. Optimized geometry of (**IV**).

| | | | |
|---|---|---|---|
| N | -0.234053 | 1.288025 | 0.633555 |
| C | -0.217316 | 0.063092 | 0.090528 |
| N | 0.994778 | -0.153402 | -0.438327 |
| C | 1.802027 | 1.122539 | -0.503106 |
| C | 1.158440 | 1.868115 | 0.724268 |
| C | -1.327817 | -0.873931 | 0.077148 |
| C | -2.634993 | -0.411951 | -0.133013 |
| C | -3.688697 | -1.311386 | -0.158810 |
| C | -3.453631 | -2.667993 | 0.050779 |
| C | -2.158967 | -3.130370 | 0.273540 |
| C | -1.095069 | -2.242651 | 0.274044 |
| O | 1.093693 | -1.033445 | -1.511006 |
| C | 1.518164 | 1.802601 | -1.847807 |
| C | 3.287932 | 0.818733 | -0.362730 |
| C | 1.110826 | 3.385479 | 0.600704 |
| C | 1.762581 | 1.458286 | 2.072784 |
| O | -1.099832 | 1.521349 | 1.697004 |
| H | -4.281034 | -3.366277 | 0.040463 |
| H | -4.694643 | -0.955562 | -0.340206 |
| H | -2.822306 | 0.638475 | -0.312886 |
| H | -0.093746 | -2.606098 | 0.464001 |
| H | -1.979819 | -4.183969 | 0.444659 |
| H | 2.765427 | 1.871110 | 2.173524 |
| H | 1.155476 | 1.854852 | 2.884508 |
| H | 1.822645 | 0.376357 | 2.192394 |
| H | 2.122665 | 3.788056 | 0.541128 |
| H | 0.558845 | 3.717840 | -0.276173 |
| H | 0.649226 | 3.818174 | 1.489085 |
| H | 1.817939 | 1.146728 | -2.663107 |
| H | 0.463515 | 2.045353 | -1.979024 |
| H | 2.095213 | 2.722656 | -1.930151 |
| H | 3.648900 | 0.301243 | -1.252374 |
| H | 3.854078 | 1.747605 | -0.284692 |
| H | 3.510767 | 0.208498 | 0.510195 |
| H | -1.649280 | 2.276487 | 1.427661 |
| H | 1.741919 | -1.705314 | -1.240717 |

Table S5. Optimized geometry of (**V**).

| | | | |
|---|---|---|---|
| N | -0.232782 | 1.236794 | 0.659700 |
| C | -0.288308 | 0.002227 | 0.090108 |
| N | 0.945879 | -0.144114 | -0.464062 |
| C | 1.810668 | 1.098636 | -0.482613 |
| C | 1.136902 | 1.880681 | 0.703829 |
| C | -1.384501 | -0.922333 | 0.076655 |
| C | -2.719089 | -0.446338 | 0.075736 |
| C | -3.766475 | -1.346226 | 0.043154 |
| C | -3.515248 | -2.719054 | 0.049456 |
| C | -2.204762 | -3.198682 | 0.069459 |
| C | -1.140631 | -2.318065 | 0.063898 |
| O | 1.185615 | -1.212900 | -1.222755 |
| C | 1.606453 | 1.754490 | -1.862777 |
| C | 3.279396 | 0.738266 | -0.264204 |
| C | 1.030407 | 3.391400 | 0.500749 |
| C | 1.730807 | 1.554033 | 2.088540 |
| O | -1.256546 | 1.644058 | 1.408941 |
| H | -4.342982 | -3.417011 | 0.038819 |
| H | -4.784540 | -0.980679 | 0.015781 |
| H | -2.935765 | 0.611158 | 0.061063 |
| H | -0.135229 | -2.710456 | 0.088816 |
| H | -2.016735 | -4.264131 | 0.086307 |
| H | 2.722301 | 1.998306 | 2.165930 |
| H | 1.119390 | 1.991687 | 2.877577 |
| H | 1.807196 | 0.482726 | 2.271048 |
| H | 2.032599 | 3.805776 | 0.386367 |
| H | 0.443734 | 3.670721 | -0.371716 |
| H | 0.616410 | 3.879652 | 1.386175 |
| H | 1.945914 | 1.087397 | -2.655025 |
| H | 0.565559 | 2.011413 | -2.056177 |
| H | 2.211458 | 2.658312 | -1.921899 |
| H | 3.703165 | 0.258544 | -1.149652 |
| H | 3.853998 | 1.655602 | -0.131715 |
| H | 3.445129 | 0.103176 | 0.603309 |
| H | -1.102726 | 2.579819 | 1.657046 |
| H | 2.137195 | -1.215583 | -1.458024 |

Table S6. Calculated absorption spectrum and singlet excited states of (**I**).

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-------------------------------------------------------------------------------
                         ABSORPTION SPECTRUM
-------------------------------------------------------------------------------
State   Energy  Wavelength   fosc         T2         TX         TY         TZ
        (cm-1)    (nm)                 (au**2)     (au)       (au)       (au)
-------------------------------------------------------------------------------
   1   19552.0    511.5   0.005254078   0.08847   0.16911  -0.19842  -0.14317
   2   23249.3    430.1   0.000288441   0.00408  -0.00996   0.01281  -0.06181
   3   25672.1    389.5   0.000164456   0.00211  -0.03493  -0.02981  -0.00065
   4   28580.0    349.9   0.002705766   0.03117  -0.13488  -0.11389  -0.00175
   5   30167.6    331.5   0.120718153   1.31737  -0.61143   0.71533   0.65713
   6   28100.2    355.9   0.000285534   0.00335   0.04412   0.03740   0.00062
   7   33316.2    300.2   0.000592955   0.00586  -0.04928   0.05816   0.00700
   8   31153.1    321.0   0.000138002   0.00146  -0.02925  -0.02455  -0.00036
   9   36494.6    274.0   0.033815358   0.30504  -0.42183  -0.35647  -0.00555
  10   36373.7    274.9   0.070839274   0.64115   0.43315  -0.50648  -0.44386
  11   36810.1    271.7   0.024335703   0.21765   0.35625   0.30119   0.00475
  12   37947.8    263.5   0.001245467   0.01080   0.06103  -0.06999  -0.04670
  13   38541.3    259.5   0.189709341   1.62046  -0.97319  -0.82050  -0.01185
  14   39202.2    255.1   0.001900133   0.01596   0.09773   0.08003   0.00094
  15   39944.8    250.3   0.009672745   0.07972   0.17920  -0.21196  -0.05175

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TD-DFT/TDA EXCITED STATES
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the weight of the individual excitations are printed if larger than 0.01

STATE  1:  E=   0.089085 au      2.424 eV    19552.0 cm**-1
    62a ->  63a  :     0.530323 (c=  0.72823300)
    62a ->  65a  :     0.017191 (c= -0.13111526)
    61b ->  62b  :     0.437787 (c=  0.66165496)

STATE  2:  E=   0.105932 au      2.883 eV    23249.3 cm**-1
    58b ->  63b  :     0.030350 (c=  0.17421309)
    59b ->  62b  :     0.943085 (c= -0.97112541)

STATE  3:  E=   0.116971 au      3.183 eV    25672.1 cm**-1
    58b ->  62b  :     0.735440 (c=  0.85757770)
    59b ->  63b  :     0.065741 (c= -0.25639923)
    59b ->  66b  :     0.010178 (c= -0.10088474)
    60b ->  62b  :     0.171432 (c= -0.41404347)

STATE  4:  E=   0.130220 au      3.543 eV    28580.0 cm**-1
    60a ->  64a  :     0.021759 (c= -0.14750860)
    61a ->  63a  :     0.379144 (c=  0.61574682)
    57b ->  63b  :     0.016111 (c= -0.12692853)
    60b ->  64b  :     0.022155 (c= -0.14884455)
    61b ->  63b  :     0.526083 (c=  0.72531555)

STATE  5:  E=   0.137454 au      3.740 eV    30167.6 cm**-1
    62a ->  63a  :     0.401354 (c=  0.63352495)
    62a ->  65a  :     0.017590 (c=  0.13262792)
    57b ->  62b  :     0.064506 (c=  0.25397987)
    61b ->  62b  :     0.475338 (c= -0.68944764)

STATE  6:  E=   0.128034 au      3.484 eV    28100.2 cm**-1
    58b ->  62b  :     0.169867 (c=  0.41214970)
    60b ->  62b  :     0.823028 (c=  0.90720911)

STATE  7:  E=   0.151800 au      4.131 eV    33316.2 cm**-1
    60a ->  63a  :     0.641100 (c=  0.80068742)
    60b ->  63b  :     0.221063 (c=  0.47017345)
    61b ->  64b  :     0.086879 (c= -0.29475274)

STATE  8:  E=   0.141944 au      3.862 eV    31153.1 cm**-1
    62a ->  64a  :     0.975752 (c=  0.98780177)
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STATE  9:  E=   0.166281 au      4.525 eV    36494.6 cm**-1
    57a ->  63a  :     0.051445 (c=  0.22681445)
    60a ->  64a  :     0.352714 (c=  0.59389750)
    61a ->  65a  :     0.011830 (c= -0.10876722)
    62a ->  64a  :     0.021481 (c= -0.14656383)
    57b ->  63b  :     0.062808 (c=  0.25061496)
    58b ->  64b  :     0.018785 (c=  0.13705911)
    60b ->  64b  :     0.293213 (c=  0.54149184)
    61b ->  63b  :     0.133629 (c=  0.36555233)
    61b ->  66b  :     0.017361 (c=  0.13176230)

STATE 10:  E=   0.165731 au      4.510 eV    36373.7 cm**-1
    62a ->  63a  :     0.043029 (c= -0.20743549)
    62a ->  65a  :     0.038321 (c= -0.19575674)
    57b ->  62b  :     0.861010 (c=  0.92790607)
    61b ->  64b  :     0.010317 (c=  0.10157239)

STATE 11:  E=   0.167719 au      4.564 eV    36810.1 cm**-1
    59a ->  63a  :     0.844923 (c= -0.91919670)
    60a ->  64a  :     0.010620 (c=  0.10305565)
    61a ->  63a  :     0.066684 (c=  0.25823257)
    60b ->  64b  :     0.020496 (c=  0.14316283)
    61b ->  63b  :     0.020633 (c= -0.14364035)

STATE 12:  E=   0.172903 au      4.705 eV    37947.8 cm**-1
    61a ->  64a  :     0.055757 (c= -0.23612821)
    57b ->  64b  :     0.021358 (c=  0.14614289)
    60b ->  63b  :     0.217152 (c= -0.46599527)
    61b ->  64b  :     0.679698 (c= -0.82443802)

STATE 13:  E=   0.175607 au      4.779 eV    38541.3 cm**-1
    57a ->  63a  :     0.081492 (c=  0.28546863)
    59a ->  63a  :     0.106233 (c= -0.32593455)
    60a ->  64a  :     0.063939 (c= -0.25286176)
    61a ->  63a  :     0.258038 (c= -0.50797432)
    57b ->  63b  :     0.135546 (c=  0.36816596)
    59b ->  63b  :     0.016651 (c= -0.12903829)
    60b ->  64b  :     0.131035 (c= -0.36198803)
    61b ->  63b  :     0.148010 (c=  0.38472078)
    61b ->  66b  :     0.021625 (c=  0.14705568)

STATE 14:  E=   0.178618 au      4.860 eV    39202.2 cm**-1
    57a ->  63a  :     0.035534 (c=  0.18850503)
    59a ->  63a  :     0.011085 (c= -0.10528314)
    57b ->  63b  :     0.017198 (c=  0.13114014)
    58b ->  62b  :     0.066159 (c=  0.25721482)
    59b ->  63b  :     0.825074 (c=  0.90833572)

STATE 15:  E=   0.182002 au      4.953 eV    39944.8 cm**-1
    57a ->  64a  :     0.012403 (c=  0.11136725)
    58a ->  63a  :     0.339158 (c=  0.58237255)
    60a ->  63a  :     0.170238 (c= -0.41259859)
    61a ->  64a  :     0.223025 (c= -0.47225517)
    60b ->  63b  :     0.224051 (c=  0.47334066)
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Table S7. Calculated absorption spectrum and singlet excited states of (II).

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-------------------------------------------------------------------------------
                         ABSORPTION SPECTRUM
-------------------------------------------------------------------------------
State   Energy  Wavelength   fosc         T2         TX         TY         TZ
        (cm-1)    (nm)                 (au**2)     (au)       (au)       (au)
-------------------------------------------------------------------------------
   1   16736.5    597.5   0.000130562   0.00257   0.00509  -0.03624  -0.03506
   2   18220.0    548.8   0.045060725   0.81419   0.57971   0.67173   0.16403
   3   18232.4    548.5   0.014087498   0.25437   0.24021   0.44065   0.04999
   4   27375.0    365.3   0.031271392   0.37607   0.51186   0.32559  -0.08976
   5   29976.2    333.6   0.003555813   0.03905   0.19125  -0.03456   0.03579
   6   30586.5    326.9   0.020063738   0.21595   0.38775   0.24089  -0.08704
   7   33242.6    300.8   0.040286148   0.39897   0.34363  -0.27802  -0.45121
   8   34734.5    287.9   0.051616053   0.48921  -0.35554   0.39761   0.45245
   9   37131.9    269.3   0.014988713   0.13289   0.27433   0.23975   0.01252
  10   37257.0    268.4   0.026926178   0.23793   0.40026  -0.27286  -0.05711
  11   37018.2    270.1   0.009025284   0.08026   0.22543   0.14398  -0.09335
  12   38866.7    257.3   0.081108007   0.68701   0.72865   0.35022  -0.18283
  13   39340.8    254.2   0.014785769   0.12373   0.19232  -0.20665  -0.20985
  14   39845.5    251.0   0.051659767   0.42682  -0.39576  -0.50691  -0.11506
  15   40356.7    247.8   0.238661878   1.94690  -0.97122  -0.99161  -0.14265

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TD-DFT/TDA EXCITED STATES
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the weight of the individual excitations are printed if larger than 0.01

STATE  1:  E=   0.076257 au      2.075 eV    16736.5 cm**-1
    59b ->  62b  :     0.730401 (c= -0.85463530)
    59b ->  63b  :     0.039084 (c=  0.19769560)
    60b ->  62b  :     0.046098 (c=  0.21470489)
    61b ->  62b  :     0.151554 (c= -0.38929960)

STATE  2:  E=   0.083017 au      2.259 eV    18220.0 cm**-1
    60a ->  63a  :     0.046810 (c= -0.21635544)
    59b ->  62b  :     0.018502 (c=  0.13602048)
    60b ->  62b  :     0.434481 (c= -0.65915139)
    61b ->  62b  :     0.469909 (c= -0.68549876)

STATE  3:  E=   0.083073 au      2.261 eV    18232.4 cm**-1
    60a ->  63a  :     0.014910 (c= -0.12210453)
    59b ->  62b  :     0.168215 (c= -0.41014038)
    60b ->  62b  :     0.438167 (c= -0.66194164)
    61b ->  62b  :     0.347819 (c=  0.58976209)

STATE  4:  E=   0.124730 au      3.394 eV    27375.0 cm**-1
    62a ->  63a  :     0.650944 (c= -0.80681087)
    58b ->  62b  :     0.270524 (c=  0.52011925)
    60b ->  63b  :     0.019170 (c=  0.13845545)

STATE  5:  E=   0.136581 au      3.717 eV    29976.2 cm**-1
    60a ->  63a  :     0.010543 (c=  0.10267960)
    61a ->  63a  :     0.721088 (c=  0.84916923)
    61b ->  62b  :     0.019416 (c= -0.13934198)
    61b ->  63b  :     0.200460 (c=  0.44772808)
    61b ->  65b  :     0.010336 (c=  0.10166841)

STATE  6:  E=   0.139362 au      3.792 eV    30586.5 cm**-1
    60a ->  63a  :     0.404601 (c=  0.63608291)
    61a ->  63a  :     0.022817 (c= -0.15105200)
    61a ->  64a  :     0.033363 (c= -0.18265543)
    58b ->  62b  :     0.116804 (c= -0.34176618)
    60b ->  62b  :     0.039229 (c= -0.19806333)
    60b ->  63b  :     0.284559 (c=  0.53344076)
    60b ->  65b  :     0.010799 (c=  0.10391865)
    61b ->  64b  :     0.014904 (c= -0.12208196)
```

```
STATE  7:  E=   0.151464 au      4.122 eV    33242.6 cm**-1
    60a ->  63a  :     0.035324 (c= -0.18794565)
    62a ->  63a  :     0.108699 (c= -0.32969535)
    54b ->  62b  :     0.012736 (c=  0.11285245)
    56b ->  62b  :     0.016603 (c=  0.12885089)
    57b ->  62b  :     0.463663 (c=  0.68092826)
    58b ->  62b  :     0.291819 (c= -0.54020309)
    60b ->  63b  :     0.016729 (c= -0.12934245)

STATE  8:  E=   0.158262 au      4.307 eV    34734.5 cm**-1
    60a ->  63a  :     0.020914 (c=  0.14461732)
    62a ->  63a  :     0.136763 (c=  0.36981428)
    55b ->  62b  :     0.022487 (c= -0.14995518)
    57b ->  62b  :     0.495251 (c=  0.70374070)
    58b ->  62b  :     0.247727 (c=  0.49772170)
    60b ->  63b  :     0.031156 (c=  0.17651050)

STATE  9:  E=   0.169185 au      4.604 eV    37131.9 cm**-1
    60a ->  63a  :     0.080355 (c=  0.28347044)
    61a ->  64a  :     0.409508 (c=  0.63992826)
    60b ->  64b  :     0.051769 (c= -0.22752712)
    61b ->  64b  :     0.391744 (c=  0.62589458)

STATE 10:  E=   0.169755 au      4.619 eV    37257.0 cm**-1
    60a ->  64a  :     0.042931 (c=  0.20719771)
    61a ->  63a  :     0.158599 (c=  0.39824453)
    61a ->  65a  :     0.013769 (c=  0.11734071)
    62a ->  64a  :     0.029949 (c= -0.17305700)
    55b ->  62b  :     0.014559 (c=  0.12066178)
    56b ->  62b  :     0.062469 (c= -0.24993740)
    59b ->  63b  :     0.017353 (c= -0.13173210)
    60b ->  63b  :     0.048879 (c=  0.22108669)
    60b ->  64b  :     0.016484 (c= -0.12838809)
    61b ->  63b  :     0.547076 (c= -0.73964570)

STATE 11:  E=   0.168667 au      4.590 eV    37018.2 cm**-1
    59a ->  63a  :     0.012341 (c=  0.11109226)
    61a ->  63a  :     0.013465 (c= -0.11603767)
    56b ->  62b  :     0.835595 (c= -0.91410886)
    59b ->  63b  :     0.012975 (c= -0.11390597)
    60b ->  63b  :     0.018393 (c= -0.13561947)
    61b ->  63b  :     0.044660 (c=  0.21132883)

STATE 12:  E=   0.177090 au      4.819 eV    38866.7 cm**-1
    59a ->  63a  :     0.021168 (c=  0.14549247)
    60a ->  63a  :     0.025936 (c=  0.16104522)
    60a ->  65a  :     0.015871 (c=  0.12597916)
    62a ->  63a  :     0.022781 (c= -0.15093246)
    50b ->  62b  :     0.011498 (c= -0.10722879)
    53b ->  62b  :     0.019332 (c=  0.13904036)
    54b ->  62b  :     0.595831 (c= -0.77190062)
    55b ->  62b  :     0.129833 (c= -0.36032321)
    60b ->  63b  :     0.068468 (c= -0.26166447)
    61b ->  63b  :     0.016640 (c= -0.12899789)

STATE 13:  E=   0.179250 au      4.878 eV    39340.8 cm**-1
    59a ->  63a  :     0.199006 (c= -0.44610115)
    53b ->  62b  :     0.013517 (c=  0.11626406)
    54b ->  62b  :     0.065804 (c=  0.25652377)
    55b ->  62b  :     0.508877 (c= -0.71335633)
    56b ->  62b  :     0.016881 (c= -0.12992765)
    59b ->  62b  :     0.013780 (c=  0.11738948)
    59b ->  63b  :     0.091835 (c=  0.30304366)
    60b ->  63b  :     0.012103 (c=  0.11001554)

STATE 14:  E=   0.181549 au      4.940 eV    39845.5 cm**-1
    59a ->  63a  :     0.511809 (c=  0.71540799)
    60a ->  63a  :     0.053060 (c= -0.23034830)
    54b ->  62b  :     0.018728 (c=  0.13685186)
    55b ->  62b  :     0.194999 (c= -0.44158706)
    59b ->  63b  :     0.051131 (c= -0.22612250)
    60b ->  63b  :     0.095628 (c=  0.30923721)
```

```
STATE 15:  E=   0.183879 au      5.004 eV    40356.7 cm**-1
    59a ->  63a  :     0.109929 (c= -0.33155607)
    60a ->  63a  :     0.212361 (c= -0.46082673)
    61a ->  64a  :     0.023176 (c=  0.15223826)
    62a ->  65a  :     0.020333 (c=  0.14259259)
    54b ->  62b  :     0.212276 (c= -0.46073386)
    55b ->  62b  :     0.013531 (c=  0.11632213)
    59b ->  63b  :     0.028706 (c= -0.16942732)
    60b ->  63b  :     0.248223 (c=  0.49821985)
    61b ->  63b  :     0.053316 (c=  0.23090354)
```

Table S8. Calculated absorption spectrum and singlet excited states of (**III**).

```
-------------------------------------------------------------------------------
                         ABSORPTION SPECTRUM
-------------------------------------------------------------------------------
State   Energy  Wavelength   fosc         T2         TX         TY         TZ
        (cm-1)    (nm)                 (au**2)     (au)       (au)       (au)
-------------------------------------------------------------------------------
   1    8349.4   1197.7   0.000000000   0.00000   0.00000   0.00000   0.00000
   2   12154.0    822.8   0.000000000   0.00000  -0.00000   0.00000  -0.00000
   3   12019.0    832.0   0.000166085   0.00455   0.05155   0.04349   0.00061
   4   17745.7    563.5   0.000000000   0.00000  -0.00000  -0.00000   0.00000
   5   14892.9    671.5   0.014251363   0.31503  -0.28187   0.32918   0.35668
   6   21409.8    467.1   0.000000000   0.00000  -0.00000   0.00000  -0.00000
   7   21820.8    458.3   0.001028480   0.01552   0.02022  -0.02560   0.12022
   8   20628.7    484.8   0.000000000   0.00000  -0.00000  -0.00000  -0.00000
   9   25006.0    399.9   0.000358958   0.00473  -0.05256  -0.04430  -0.00060
  10   27783.3    359.9   0.000000000   0.00000   0.00000   0.00000  -0.00000
  11   30141.3    331.8   0.000000000   0.00000  -0.00000  -0.00000   0.00000
  12   31757.6    314.9   0.000000000   0.00000  -0.00000   0.00000  -0.00000
  13   34342.6    291.2   0.076482323   0.73317  -0.65431  -0.55225  -0.00792
  14   32904.1    303.9   0.016880412   0.16889   0.19531  -0.22745  -0.28109
  15   32692.4    305.9   0.000000000   0.00000   0.00000   0.00000  -0.00000

-------------------------
TD-DFT/TDA EXCITED STATES
-------------------------

the weight of the individual excitations are printed if larger than 0.01

STATE  1:  E=   0.038043 au      1.035 eV     8349.4 cm**-1
    58a ->  62a  :     0.048135 (c=  0.21939738)
    59a ->  62a  :     0.028361 (c= -0.16840665)
    61a ->  62a  :     0.419087 (c= -0.64736902)
    58b ->  62b  :     0.048135 (c= -0.21939738)
    59b ->  62b  :     0.028361 (c=  0.16840665)
    61b ->  62b  :     0.419087 (c=  0.64736902)

STATE  2:  E=   0.055378 au      1.507 eV    12154.0 cm**-1
    57a ->  62a  :     0.010209 (c=  0.10103757)
    60a ->  62a  :     0.487798 (c= -0.69842505)
    57b ->  62b  :     0.010209 (c= -0.10103757)
    60b ->  62b  :     0.487798 (c=  0.69842505)

STATE  3:  E=   0.054763 au      1.490 eV    12019.0 cm**-1
    60a ->  62a  :     0.498328 (c=  0.70592359)
    60b ->  62b  :     0.498328 (c=  0.70592359)

STATE  4:  E=   0.080855 au      2.200 eV    17745.7 cm**-1
    55a ->  62a  :     0.010866 (c=  0.10424022)
    58a ->  62a  :     0.145547 (c= -0.38150659)
    59a ->  62a  :     0.325664 (c= -0.57067007)
    55b ->  62b  :     0.010866 (c= -0.10424022)
    58b ->  62b  :     0.145547 (c=  0.38150659)
    59b ->  62b  :     0.325664 (c=  0.57067007)

STATE  5:  E=   0.067857 au      1.846 eV    14892.9 cm**-1
    58a ->  62a  :     0.047046 (c= -0.21690030)
    59a ->  62a  :     0.027645 (c=  0.16626893)
    61a ->  62a  :     0.416935 (c= -0.64570536)
    58b ->  62b  :     0.047046 (c= -0.21690030)
    59b ->  62b  :     0.027645 (c=  0.16626893)
    61b ->  62b  :     0.416935 (c= -0.64570536)

STATE  6:  E=   0.097550 au      2.654 eV    21409.8 cm**-1
    53a ->  62a  :     0.018958 (c=  0.13768919)
    57a ->  62a  :     0.440561 (c= -0.66374786)
    60a ->  62a  :     0.012001 (c= -0.10954876)
    53b ->  62b  :     0.018958 (c= -0.13768919)
    57b ->  62b  :     0.440561 (c=  0.66374786)
    60b ->  62b  :     0.012001 (c=  0.10954876)
```

```
STATE  7:  E=   0.099423 au      2.705 eV    21820.8 cm**-1
    58a ->  62a  :     0.151716 (c= -0.38950773)
    59a ->  62a  :     0.333193 (c= -0.57722865)
    58b ->  62b  :     0.151716 (c= -0.38950773)
    59b ->  62b  :     0.333193 (c= -0.57722865)

STATE  8:  E=   0.093991 au      2.558 eV    20628.7 cm**-1
    58a ->  62a  :     0.285407 (c= -0.53423505)
    59a ->  62a  :     0.116155 (c=  0.34081489)
    61a ->  62a  :     0.078960 (c= -0.28099860)
    58b ->  62b  :     0.285407 (c=  0.53423505)
    59b ->  62b  :     0.116155 (c= -0.34081489)
    61b ->  62b  :     0.078960 (c=  0.28099860)

STATE  9:  E=   0.113936 au      3.100 eV    25006.0 cm**-1
    57a ->  62a  :     0.473162 (c=  0.68786806)
    57b ->  62b  :     0.473162 (c=  0.68786805)

STATE 10:  E=   0.126590 au      3.445 eV    27783.3 cm**-1
    60a ->  64a  :     0.016573 (c= -0.12873659)
    61a ->  63a  :     0.455682 (c=  0.67504225)
    60b ->  64b  :     0.016573 (c=  0.12873659)
    61b ->  63b  :     0.455682 (c= -0.67504225)

STATE 11:  E=   0.137334 au      3.737 eV    30141.3 cm**-1
    60a ->  63a  :     0.477186 (c= -0.69078630)
    60a ->  65a  :     0.013794 (c=  0.11744587)
    60b ->  63b  :     0.477186 (c=  0.69078630)
    60b ->  65b  :     0.013794 (c= -0.11744587)

STATE 12:  E=   0.144698 au      3.937 eV    31757.6 cm**-1
    48a ->  62a  :     0.012967 (c=  0.11387198)
    56a ->  62a  :     0.436248 (c=  0.66049083)
    48b ->  62b  :     0.012967 (c= -0.11387198)
    56b ->  62b  :     0.436248 (c= -0.66049083)

STATE 13:  E=   0.156476 au      4.258 eV    34342.6 cm**-1
    53a ->  62a  :     0.019250 (c=  0.13874489)
    56a ->  62a  :     0.455036 (c=  0.67456382)
    61a ->  63a  :     0.011105 (c=  0.10537876)
    53b ->  62b  :     0.019250 (c=  0.13874372)
    56b ->  62b  :     0.455033 (c=  0.67456112)
    61b ->  63b  :     0.011109 (c=  0.10539879)

STATE 14:  E=   0.149922 au      4.080 eV    32904.1 cm**-1
    55a ->  62a  :     0.396151 (c=  0.62940499)
    58a ->  62a  :     0.031433 (c= -0.17729234)
    59a ->  62a  :     0.042109 (c=  0.20520541)
    55b ->  62b  :     0.396150 (c=  0.62940486)
    58b ->  62b  :     0.031433 (c= -0.17729288)
    59b ->  62b  :     0.042109 (c=  0.20520583)

STATE 15:  E=   0.148958 au      4.053 eV    32692.4 cm**-1
    55a ->  62a  :     0.479607 (c=  0.69253655)
    59a ->  62a  :     0.013639 (c=  0.11678414)
    55b ->  62b  :     0.479607 (c= -0.69253655)
    59b ->  62b  :     0.013639 (c= -0.11678414)
```

Table S9. Calculated absorption spectrum and singlet excited states of (**IV**).

```
-------------------------------------------------------------------------------
                         ABSORPTION SPECTRUM
-------------------------------------------------------------------------------
State   Energy  Wavelength   fosc         T2         TX         TY         TZ
        (cm-1)    (nm)                 (au**2)     (au)       (au)       (au)
-------------------------------------------------------------------------------
   1   27816.0    359.5   0.000000000   0.00000  -0.00000   0.00000   0.00000
   2   28758.2    347.7   0.000000000   0.00000   0.00000   0.00000   0.00000
   3   29598.7    337.9   0.000000000   0.00000  -0.00000   0.00000  -0.00000
   4   34524.1    289.7   0.014099178   0.13445   0.21815  -0.26099   0.13690
   5   36908.8    270.9   0.000000000   0.00000   0.00000   0.00000   0.00000
   6   37628.3    265.8   0.424740574   3.71607   1.47351   1.24279   0.01760
   7   38956.0    256.7   0.096415590   0.81480   0.43936  -0.51416  -0.59783
   8   41948.1    238.4   0.000000000   0.00000  -0.00000   0.00000   0.00000
   9   43859.9    228.0   0.000000000   0.00000  -0.00000  -0.00000  -0.00000
  10   45760.4    218.5   0.000000000   0.00000  -0.00000  -0.00000  -0.00000
  11   46357.2    215.7   0.000000000   0.00000  -0.00000   0.00000   0.00000
  12   46705.7    214.1   0.000025162   0.00018  -0.01071  -0.00791   0.00015
  13   47038.5    212.6   0.000000000   0.00000   0.00000  -0.00000   0.00000
  14   47461.8    210.7   0.003747715   0.02600  -0.10428   0.12276   0.00719
  15   48083.4    208.0   0.002029810   0.01390   0.06304  -0.07543   0.06507

-------------------------
TD-DFT/TDA EXCITED STATES
-------------------------

the weight of the individual excitations are printed if larger than 0.01

STATE  1:  E=   0.126739 au      3.449 eV    27816.0 cm**-1
    60a ->  63a  :     0.447127 (c= -0.66867585)
    60a ->  65a  :     0.019281 (c= -0.13885517)
    62a ->  63a  :     0.022638 (c=  0.15046025)
    60b ->  63b  :     0.447127 (c=  0.66867585)
    60b ->  65b  :     0.019281 (c=  0.13885517)
    62b ->  63b  :     0.022638 (c= -0.15046025)

STATE  2:  E=   0.131032 au      3.566 eV    28758.2 cm**-1
    61a ->  63a  :     0.444174 (c=  0.66646362)
    61a ->  65a  :     0.024072 (c= -0.15515018)
    62a ->  64a  :     0.022543 (c= -0.15014215)
    61b ->  63b  :     0.444174 (c= -0.66646362)
    61b ->  65b  :     0.024072 (c=  0.15515018)
    62b ->  64b  :     0.022543 (c=  0.15014215)

STATE  3:  E=   0.134861 au      3.670 eV    29598.7 cm**-1
    60a ->  63a  :     0.022569 (c= -0.15023140)
    62a ->  63a  :     0.455168 (c= -0.67466165)
    62a ->  65a  :     0.015810 (c=  0.12573710)
    60b ->  63b  :     0.022569 (c=  0.15023140)
    62b ->  63b  :     0.455168 (c=  0.67466165)
    62b ->  65b  :     0.015810 (c= -0.12573710)

STATE  4:  E=   0.157303 au      4.280 eV    34524.1 cm**-1
    61a ->  64a  :     0.034407 (c=  0.18548998)
    62a ->  63a  :     0.455987 (c=  0.67526841)
    61b ->  64b  :     0.034407 (c=  0.18548998)
    62b ->  63b  :     0.455987 (c=  0.67526841)

STATE  5:  E=   0.168169 au      4.576 eV    36908.8 cm**-1
    61a ->  63a  :     0.033330 (c=  0.18256421)
    62a ->  64a  :     0.438611 (c=  0.66227677)
    61b ->  63b  :     0.033330 (c= -0.18256421)
    62b ->  64b  :     0.438611 (c= -0.66227677)

STATE  6:  E=   0.171447 au      4.665 eV    37628.3 cm**-1
    61a ->  63a  :     0.462025 (c=  0.67972411)
    61a ->  65a  :     0.014667 (c=  0.12110873)
    61b ->  63b  :     0.462025 (c=  0.67972411)
    61b ->  65b  :     0.014667 (c=  0.12110873)
```

```
STATE  7:  E=   0.177497 au      4.830 eV    38956.0 cm**-1
    60a ->  63a  :     0.460241 (c=  0.67841065)
    60b ->  63b  :     0.460241 (c=  0.67841065)

STATE  8:  E=   0.191130 au      5.201 eV    41948.1 cm**-1
    61a ->  64a  :     0.471185 (c= -0.68642947)
    62a ->  65a  :     0.014939 (c= -0.12222596)
    61b ->  64b  :     0.471185 (c=  0.68642947)
    62b ->  65b  :     0.014939 (c=  0.12222596)

STATE  9:  E=   0.199840 au      5.438 eV    43859.9 cm**-1
    54a ->  63a  :     0.041900 (c=  0.20469492)
    55a ->  63a  :     0.028828 (c= -0.16978815)
    59a ->  63a  :     0.064462 (c=  0.25389446)
    61a ->  63a  :     0.010958 (c= -0.10468087)
    61a ->  65a  :     0.319482 (c= -0.56522720)
    54b ->  63b  :     0.041900 (c= -0.20469492)
    55b ->  63b  :     0.028828 (c=  0.16978815)
    59b ->  63b  :     0.064462 (c= -0.25389446)
    61b ->  63b  :     0.010958 (c=  0.10468087)
    61b ->  65b  :     0.319482 (c=  0.56522720)

STATE 10:  E=   0.208500 au      5.674 eV    45760.4 cm**-1
    59a ->  63a  :     0.413789 (c=  0.64326423)
    61a ->  65a  :     0.055707 (c=  0.23602308)
    59b ->  63b  :     0.413789 (c= -0.64326423)
    61b ->  65b  :     0.055707 (c= -0.23602308)

STATE 11:  E=   0.211219 au      5.748 eV    46357.2 cm**-1
    56a ->  63a  :     0.026424 (c= -0.16255492)
    58a ->  63a  :     0.371359 (c= -0.60939254)
    62a ->  65a  :     0.074912 (c=  0.27370126)
    56b ->  63b  :     0.026424 (c=  0.16255492)
    58b ->  63b  :     0.371359 (c=  0.60939254)
    62b ->  65b  :     0.074912 (c= -0.27370126)

STATE 12:  E=   0.212807 au      5.791 eV    46705.7 cm**-1
    59a ->  63a  :     0.484497 (c= -0.69605793)
    59b ->  63b  :     0.484497 (c= -0.69605793)

STATE 13:  E=   0.214323 au      5.832 eV    47038.5 cm**-1
    58a ->  63a  :     0.077902 (c= -0.27910976)
    61a ->  64a  :     0.014222 (c=  0.11925769)
    62a ->  65a  :     0.380538 (c= -0.61687792)
    58b ->  63b  :     0.077902 (c=  0.27910976)
    61b ->  64b  :     0.014222 (c= -0.11925769)
    62b ->  65b  :     0.380538 (c=  0.61687792)

STATE 14:  E=   0.216252 au      5.885 eV    47461.8 cm**-1
    58a ->  63a  :     0.249914 (c=  0.49991428)
    61a ->  64a  :     0.121134 (c=  0.34804312)
    62a ->  65a  :     0.108799 (c= -0.32984710)
    58b ->  63b  :     0.249914 (c=  0.49991428)
    61b ->  64b  :     0.121134 (c=  0.34804312)
    62b ->  65b  :     0.108799 (c= -0.32984710)

STATE 15:  E=   0.219084 au      5.962 eV    48083.4 cm**-1
    58a ->  63a  :     0.223913 (c=  0.47319408)
    61a ->  64a  :     0.112749 (c= -0.33578058)
    62a ->  65a  :     0.142447 (c=  0.37742120)
    58b ->  63b  :     0.223913 (c=  0.47319408)
    61b ->  64b  :     0.112749 (c= -0.33578058)
    62b ->  65b  :     0.142447 (c=  0.37742120)
```

Table S10. Calculated absorption spectrum and singlet excited states of (**V**).

```
-------------------------------------------------------------------------------
                         ABSORPTION SPECTRUM
-------------------------------------------------------------------------------
State   Energy  Wavelength   fosc         T2         TX         TY         TZ
        (cm-1)    (nm)                 (au**2)     (au)       (au)       (au)
-------------------------------------------------------------------------------
   1    5292.7   1889.4   0.000168802   0.01050   0.07892   0.06535   0.00018
   2    6870.1   1455.6   0.005846866   0.28018   0.26483  -0.30905  -0.33843
   3   24724.4    404.5   0.034410056   0.45818   0.32710  -0.38090  -0.45398
   4   24914.9    401.4   0.000899533   0.01189  -0.06973   0.08269  -0.01368
   5   25974.9    385.0   0.003845396   0.04874  -0.16858  -0.14252  -0.00221
   6   27636.3    361.8   0.001650097   0.01966   0.10717   0.09039   0.00123
   7   26853.7    372.4   0.005082055   0.06230   0.12249  -0.15746  -0.15002
   8   28200.5    354.6   0.028994709   0.33848  -0.44658  -0.37288  -0.00285
   9   28436.1    351.7   0.001864845   0.02159   0.11227   0.09478   0.00139
  10   31501.8    317.4   0.016599452   0.17347   0.26642  -0.31609   0.05079
  11   32341.1    309.2   0.000321866   0.00328  -0.03577   0.04276  -0.01296
  12   32993.4    303.1   0.001787482   0.01784  -0.10208  -0.08610  -0.00132
  13   34192.7    292.5   0.005320356   0.05123   0.04288  -0.04599  -0.21742
  14   35195.5    284.1   0.009998285   0.09352   0.11920  -0.13989  -0.24442
  15   35676.4    280.3   0.457747692   4.22397   1.57094   1.32504   0.01926

-------------------------
TD-DFT/TDA EXCITED STATES
-------------------------

the weight of the individual excitations are printed if larger than 0.01

STATE  1:  E=   0.024115 au      0.656 eV     5292.7 cm**-1
    61b ->  62b  :     0.999586 (c= -0.99979297)

STATE  2:  E=   0.031303 au      0.852 eV     6870.1 cm**-1
    60a ->  63a  :     0.016710 (c=  0.12926594)
    60b ->  62b  :     0.970804 (c=  0.98529411)

STATE  3:  E=   0.112653 au      3.065 eV    24724.4 cm**-1
    60a ->  63a  :     0.120577 (c=  0.34724184)
    59b ->  62b  :     0.840079 (c= -0.91655846)

STATE  4:  E=   0.113521 au      3.089 eV    24914.9 cm**-1
    62a ->  63a  :     0.728139 (c=  0.85331035)
    61b ->  63b  :     0.243570 (c=  0.49352820)
    61b ->  65b  :     0.011105 (c=  0.10538032)

STATE  5:  E=   0.118350 au      3.220 eV    25974.9 cm**-1
    61a ->  63a  :     0.524388 (c=  0.72414613)
    61a ->  65a  :     0.010655 (c= -0.10322287)
    60b ->  63b  :     0.415841 (c= -0.64485717)
    60b ->  65b  :     0.011717 (c= -0.10824494)

STATE  6:  E=   0.125920 au      3.426 eV    27636.3 cm**-1
    55b ->  62b  :     0.506969 (c=  0.71201750)
    56b ->  62b  :     0.320674 (c= -0.56628082)
    57b ->  62b  :     0.152867 (c= -0.39098150)

STATE  7:  E=   0.122354 au      3.329 eV    26853.7 cm**-1
    60a ->  63a  :     0.071097 (c=  0.26664009)
    58b ->  62b  :     0.862819 (c=  0.92888033)
    59b ->  62b  :     0.040501 (c=  0.20124789)

STATE  8:  E=   0.128491 au      3.496 eV    28200.5 cm**-1
    55b ->  62b  :     0.093307 (c=  0.30546265)
    56b ->  62b  :     0.589300 (c=  0.76765888)
    57b ->  62b  :     0.298041 (c= -0.54593125)

STATE  9:  E=   0.129564 au      3.526 eV    28436.1 cm**-1
    55b ->  62b  :     0.391807 (c= -0.62594522)
    56b ->  62b  :     0.070851 (c= -0.26617793)
    57b ->  62b  :     0.516761 (c= -0.71886072)
```

```
STATE 10:  E=   0.143533 au      3.906 eV    31501.8 cm**-1
    60a ->  63a  :     0.012224 (c=  0.11056100)
    61a ->  64a  :     0.016187 (c=  0.12722883)
    62a ->  63a  :     0.230193 (c= -0.47978424)
    62a ->  65a  :     0.016237 (c= -0.12742301)
    60b ->  64b  :     0.017921 (c=  0.13386942)
    61b ->  63b  :     0.690118 (c=  0.83073328)

STATE 11:  E=   0.147357 au      4.010 eV    32341.1 cm**-1
    51b ->  62b  :     0.033880 (c=  0.18406427)
    54b ->  62b  :     0.940272 (c=  0.96967602)

STATE 12:  E=   0.150329 au      4.091 eV    32993.4 cm**-1
    53b ->  62b  :     0.988127 (c=  0.99404598)

STATE 13:  E=   0.155793 au      4.239 eV    34192.7 cm**-1
    50b ->  62b  :     0.014815 (c=  0.12171861)
    51b ->  62b  :     0.137388 (c=  0.37065927)
    52b ->  62b  :     0.817567 (c=  0.90419433)

STATE 14:  E=   0.160362 au      4.364 eV    35195.5 cm**-1
    60a ->  63a  :     0.277292 (c= -0.52658555)
    47b ->  62b  :     0.011860 (c=  0.10890288)
    51b ->  62b  :     0.423754 (c=  0.65096379)
    52b ->  62b  :     0.112648 (c= -0.33563059)
    54b ->  62b  :     0.017658 (c= -0.13288299)
    58b ->  62b  :     0.072380 (c=  0.26903534)
    59b ->  62b  :     0.039913 (c= -0.19978128)

STATE 15:  E=   0.162554 au      4.423 eV    35676.4 cm**-1
    61a ->  63a  :     0.385054 (c= -0.62052685)
    61a ->  65a  :     0.020931 (c= -0.14467607)
    62a ->  64a  :     0.032747 (c=  0.18096187)
    60b ->  63b  :     0.358817 (c= -0.59901297)
    61b ->  64b  :     0.131724 (c=  0.36293798)
```

Figure S1. Molecular orbitals involved in the main transitions of (**II**), the labeling is according to Table 3 and the number in brackets indicate occupied (1) or empty (0) orbitals, respectively.

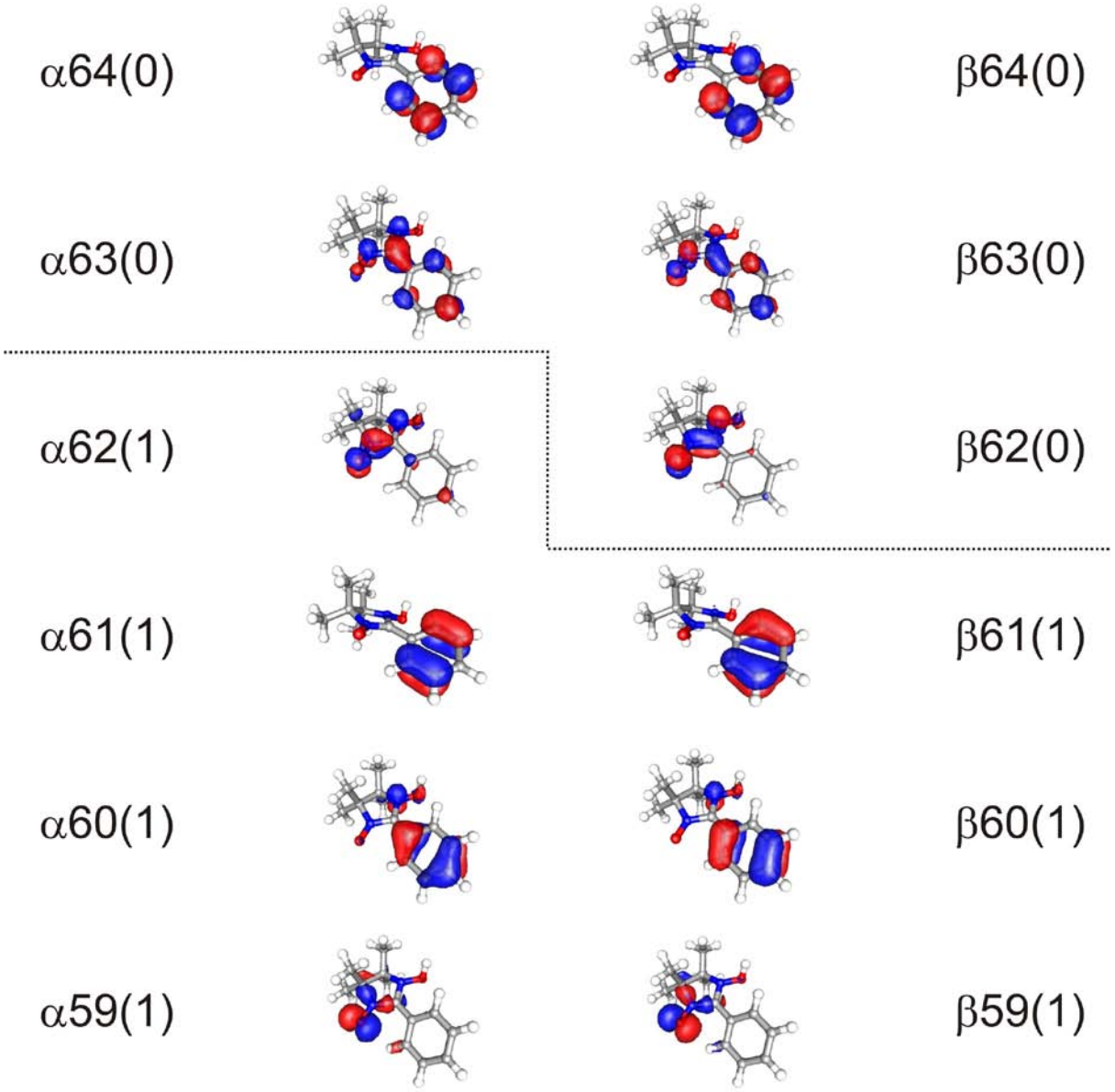

Figure S2. Molecular orbitals involved in the main transitions of (**V**), the labeling is according to Table 3 and the number in brackets indicate occupied (1) or empty (0) orbitals, respectively.