

# Molecular Structure, Matrix-Isolation IR Spectrum and UV-Induced Transformations of 2-Amino-5-(4-Methoxyphenyl)-1,3,4-Oxadiazole

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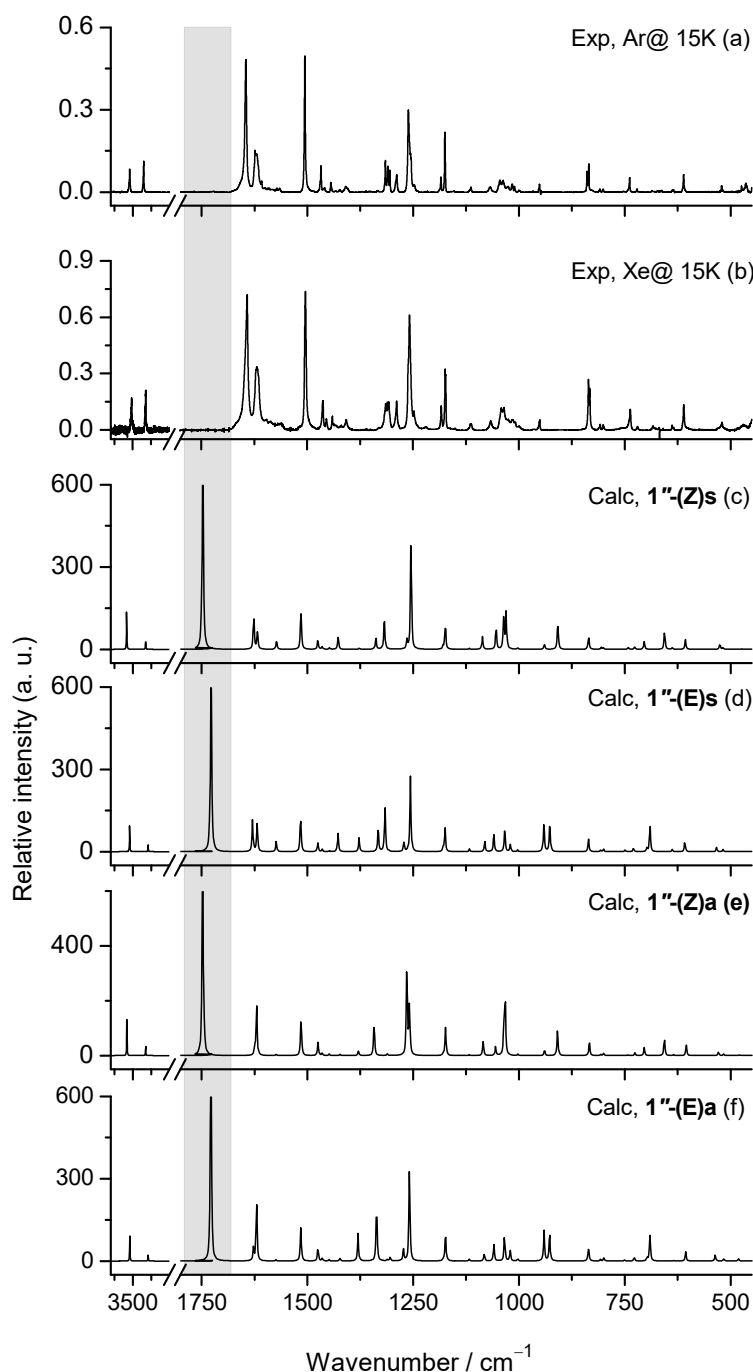
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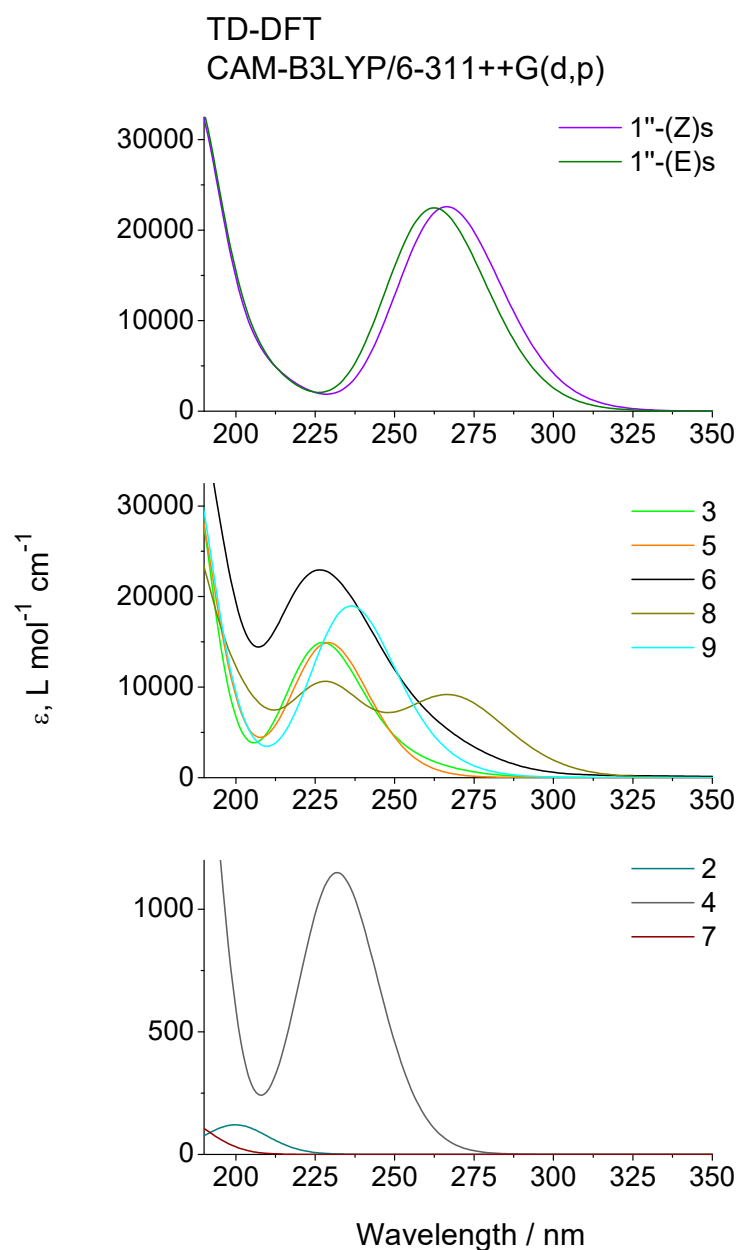
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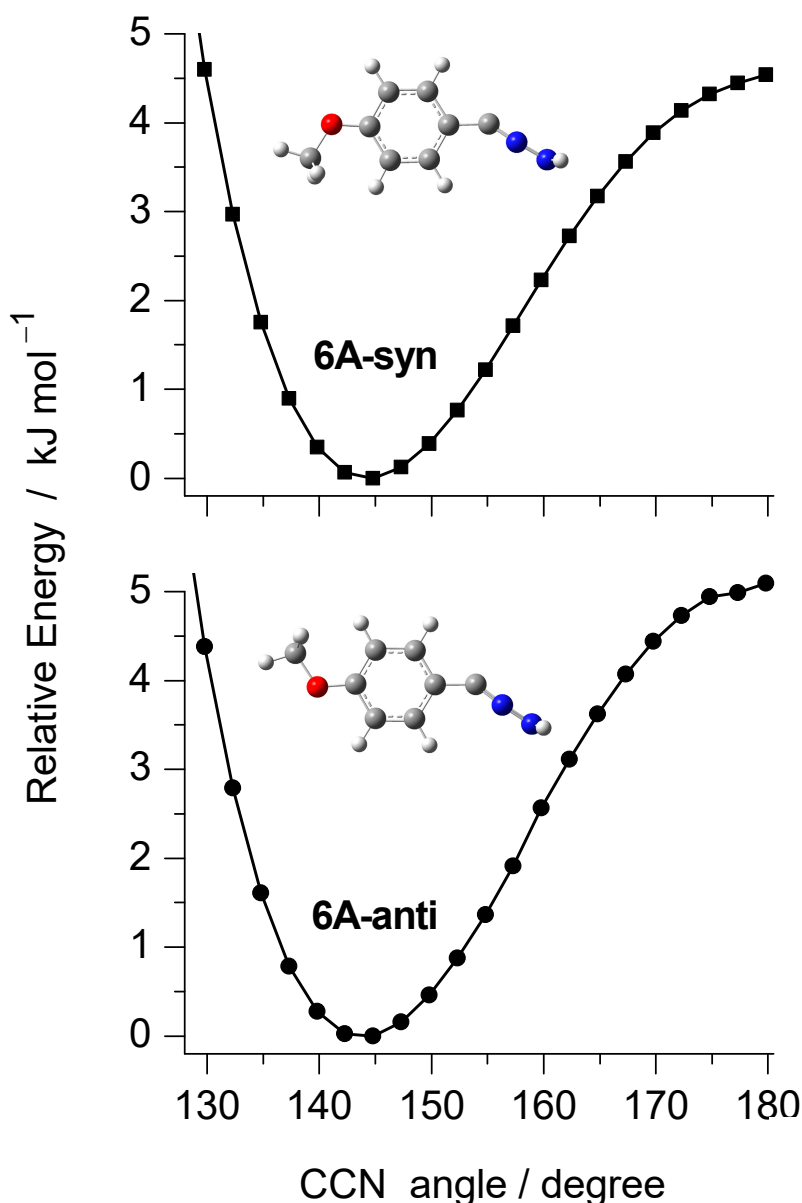


**Figure S1.** (a,b) Experimental IR spectra of 2-Amino-5-(4-methoxyphenyl)-1,3,4-oxadiazole **1** isolated in Ar and Xe matrices (15 K), compared with the (c-f) spectra calculated for the four isomeric forms adopted by tautomer 5-(4-methoxyphenyl)-1,3,4-oxadiazol-2(3H)-imine **1''**, simulated from the wavenumbers (scaled) and IR intensities extracted from the vibrational calculations carried out at the B3LYP/6-311++G(d,p) level of theory. The grey rectangle highlights the region where this tautomeric form exhibits its strongest absorption at 1745-1726  $\text{cm}^{-1}$ , assigned to the stretching vibration of the exocyclic C=N bond [ $\nu(\text{C}=\text{N})$ ], which is absent in the experimental spectrum.



**Figure S2.** TD-DFT UV absorption spectra simulated at the CAM-B3LYP/6-311++G(d,p) level for the species generated upon broadband UV irradiation ( $\lambda > 200$  nm) of matrix-isolated 2-amino-5-(4-methoxyphenyl)-1,3,4-oxadiazole **1**.

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**Figure S3.** B3LYP/6-311++G(d,p) relaxed potential energy scans as a function of the CCN angle for C-(4-methoxyphenyl)-nitrilimine **6**, considering both syn (top) and anti (bottom) orientations of the methoxy (OCH<sub>3</sub>) and nitrilimine (CNN) groups. The CCN angle was incrementally constrained in 2.5° steps, while all other geometrical parameters were fully optimized at each point. For both scans, only one minimum was identified, characterized by bent CCN fragment (CCN angle ~145°) and a non-planar geometry (CCNH dihedral ~ 99°), consistent with an allenic-type structure, labeled as **6A**. The propargylic isomer, characterized by a CCN angle of ~180° and planar geometry (CCNH dihedral ~ 180°), does not represent a minimum on the potential energy surface.

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2. Tables

**Table S1.** B3LYP/6-311++G(d,p) calculated vibrational frequencies ( $\nu/\text{cm}^{-1}$ ; scaled) and infrared intensities ( $A^{\text{th}}/\text{km mol}^{-1}$ ; unscaled) for species resulting from the UV-induced photochemistry of 2-Amino-5-(4-methoxyphenyl)-1,3,4-oxadiazole **1**.<sup>a</sup>

| 1''-(Z)s    |            | 1''-(Z)a    |            | 1''-(E)s    |            | 1''-(E)a    |            | 2           |            | 3           |             |
|-------------|------------|-------------|------------|-------------|------------|-------------|------------|-------------|------------|-------------|-------------|
| $\nu$       | I          | $\nu$       | I          | $\nu$       | I          | $\nu$       | I          | $\nu$       | I          | $\nu$       | I           |
| 3549        | 139        | 3548        | 135        | 3529        | 97         | 3528        | 93         | 3503        | 71         | 3081        | 5           |
| 3419        | 35         | 3419        | 36         | 3402        | 25         | 3402        | 25         | 3413        | 43         | 3068        | 2           |
| 3083        | 6          | 3081        | 7          | 3083        | 6          | 3081        | 7          | <b>2258</b> | <b>126</b> | 3063        | 6           |
| 3074        | 3          | 3076        | 2          | 3074        | 3          | 3077        | 1          | 1600        | 48         | 3049        | 7           |
| 3066        | 3          | 3063        | 0          | 3068        | 3          | 3063        | 0          | 1166        | 0          | 3010        | 20          |
| 3060        | 3          | 3062        | 5          | 3060        | 2          | 3062        | 4          | 1075        | 10         | 2941        | 37          |
| 3013        | 20         | 3013        | 20         | 3013        | 20         | 3013        | 20         | 535         | 117        | 2884        | 57          |
| 2947        | 34         | 2947        | 34         | 2948        | 33         | 2947        | 34         | 469         | 140        | <b>2268</b> | <b>1850</b> |
| 2888        | 59         | 2889        | 60         | 2889        | 59         | 2888        | 60         | 402         | 0          | 1621        | 8           |
| <b>1745</b> | <b>887</b> | <b>1746</b> | <b>897</b> | <b>1726</b> | <b>806</b> | <b>1726</b> | <b>813</b> |             |            | 1579        | 42          |
| 1625        | 115        | 1623        | 27         | 1628        | 115        | 1626        | 47         |             |            | 1529        | 189         |
| 1616        | 69         | 1618        | 186        | 1617        | 101        | 1618        | 203        |             |            | 1475        | 28          |
| 1571        | 33         | 1572        | 5          | 1572        | 40         | 1573        | 4          |             |            | 1463        | 10          |
| 1514        | 146        | 1513        | 140        | 1514        | 129        | 1514        | 121        |             |            | 1462        | 47          |
| 1474        | 35         | 1473        | 49         | 1474        | 32         | 1473        | 48         |             |            | 1442        | 35          |
| 1463        | 10         | 1464        | 10         | 1464        | 10         | 1464        | 10         |             |            | 1421        | 5           |
| 1446        | 5          | 1447        | 6          | 1446        | 3          | 1447        | 5          |             |            | 1305        | 25          |
| 1426        | 46         | 1421        | 5          | 1426        | 67         | 1421        | 10         |             |            | 1299        | 5           |
| 1376        | 4          | 1378        | 20         | 1377        | 52         | 1379        | 101        |             |            | 1247        | 307         |
| 1337        | 45         | 1341        | 117        | 1331        | 91         | 1335        | 203        |             |            | 1178        | 11          |
| 1317        | 124        | 1310        | 7          | 1315        | 163        | 1310        | 5          |             |            | 1168        | 34          |
| 1306        | 1          | 1304        | 1          | 1306        | 2          | 1303        | 14         |             |            | 1144        | 1           |
| 1264        | 32         | 1264        | 310        | 1271        | 33         | 1272        | 46         |             |            | 1123        | 29          |
| 1254        | 382        | 1258        | 178        | 1255        | 286        | 1258        | 327        |             |            | 1108        | 14          |
| 1178        | 11         | 1177        | 7          | 1178        | 13         | 1178        | 5          |             |            | 1037        | 69          |
| 1173        | 94         | 1172        | 102        | 1174        | 88         | 1172        | 106        |             |            | 1003        | 1           |
| 1144        | 1          | 1144        | 1          | 1144        | 1          | 1144        | 1          |             |            | 941         | 0           |
| 1116        | 3          | 1117        | 3          | 1116        | 11         | 1116        | 7          |             |            | 921         | 1           |
| 1085        | 46         | 1084        | 52         | 1080        | 40         | 1081        | 24         |             |            | 825         | 69          |
| 1053        | 76         | 1054        | 32         | 1058        | 68         | 1058        | 61         |             |            | 813         | 0           |
| 1035        | 123        | 1035        | 83         | 1033        | 85         | 1033        | 92         |             |            | 796         | 2           |
| 1029        | 132        | 1032        | 217        | 1019        | 25         | 1020        | 38         |             |            | 709         | 0           |
| 1002        | 4          | 1002        | 5          | 1002        | 6          | 1002        | 7          |             |            | 693         | 35          |
| 965         | 0          | 959         | 0          | 965         | 0          | 962         | 0          |             |            | 641         | 12          |

|     |     |     |     |     |     |     |     |  |  |     |    |
|-----|-----|-----|-----|-----|-----|-----|-----|--|--|-----|----|
| 939 | 19  | 942 | 1   | 940 | 94  | 943 | 3   |  |  | 614 | 31 |
| 935 | 1   | 939 | 20  | 939 | 14  | 940 | 112 |  |  | 558 | 27 |
| 908 | 101 | 908 | 100 | 926 | 112 | 927 | 107 |  |  | 511 | 10 |
| 835 | 50  | 833 | 53  | 835 | 50  | 835 | 51  |  |  | 508 | 5  |
| 805 | 8   | 806 | 4   | 807 | 6   | 807 | 5   |  |  | 420 | 0  |
| 800 | 5   | 799 | 9   | 800 | 10  | 799 | 11  |  |  | 383 | 6  |
| 741 | 6   | 742 | 2   | 749 | 7   | 750 | 4   |  |  | 374 | 1  |
| 726 | 10  | 725 | 10  | 729 | 13  | 727 | 13  |  |  | 364 | 0  |
| 704 | 28  | 703 | 29  | 697 | 13  | 697 | 12  |  |  | 234 | 1  |
| 681 | 0   | 681 | 0   | 690 | 92  | 690 | 94  |  |  | 221 | 7  |
| 655 | 61  | 656 | 60  | 667 | 1   | 667 | 0   |  |  | 159 | 3  |
| 637 | 6   | 634 | 3   | 637 | 8   | 634 | 1   |  |  | 87  | 3  |
| 606 | 37  | 604 | 38  | 608 | 36  | 606 | 34  |  |  | 76  | 1  |
| 525 | 18  | 528 | 13  | 533 | 16  | 536 | 24  |  |  | 42  | 0  |
| 518 | 6   | 516 | 6   | 517 | 9   | 515 | 9   |  |  |     |    |
| 473 | 2   | 479 | 3   | 475 | 1   | 481 | 9   |  |  |     |    |
| 418 | 4   | 414 | 1   | 417 | 1   | 413 | 0   |  |  |     |    |
| 393 | 36  | 394 | 40  | 386 | 14  | 382 | 18  |  |  |     |    |
| 379 | 3   | 360 | 10  | 378 | 14  | 365 | 3   |  |  |     |    |
| 318 | 61  | 319 | 62  | 310 | 74  | 312 | 72  |  |  |     |    |
| 272 | 1   | 299 | 1   | 274 | 0   | 299 | 6   |  |  |     |    |
| 237 | 5   | 233 | 2   | 242 | 9   | 242 | 9   |  |  |     |    |
| 235 | 2   | 221 | 1   | 237 | 1   | 222 | 2   |  |  |     |    |
| 184 | 3   | 186 | 4   | 205 | 10  | 206 | 8   |  |  |     |    |
| 109 | 14  | 106 | 17  | 150 | 17  | 151 | 16  |  |  |     |    |
| 99  | 0   | 100 | 1   | 102 | 1   | 101 | 0   |  |  |     |    |
| 67  | 11  | 73  | 10  | 98  | 2   | 98  | 1   |  |  |     |    |
| 50  | 9   | 55  | 6   | 56  | 3   | 59  | 4   |  |  |     |    |
| 45  | 1   | 39  | 1   | 48  | 3   | 40  | 0   |  |  |     |    |

Table S1. Continued.

| 4    |      | 5    |    | 6A   |    | 7    |     | 8    |    | 9    |    |
|------|------|------|----|------|----|------|-----|------|----|------|----|
| v    | I    | v    | I  | v    | I  | v    | I   | v    | I  | v    | I  |
| 3391 | 11   | 3084 | 4  | 3258 | 2  | 3542 | 170 | 3234 | 5  | 3429 | 69 |
| 3325 | 2    | 3075 | 2  | 3082 | 7  | 2246 | 783 | 3083 | 5  | 3080 | 6  |
| 2219 | 1001 | 3062 | 1  | 3069 | 3  | 1311 | 1   | 3072 | 2  | 3066 | 2  |
| 1645 | 18   | 3061 | 3  | 3060 | 4  | 749  | 200 | 3056 | 1  | 3061 | 7  |
| 1422 | 12   | 3016 | 17 | 3053 | 2  | 620  | 4   | 3054 | 2  | 3045 | 5  |
| 1303 | 2    | 2952 | 31 | 3014 | 19 | 557  | 97  | 3017 | 17 | 3009 | 21 |
| 1044 | 91   | 2892 | 50 | 2946 | 33 |      |     | 2954 | 31 | 2940 | 38 |

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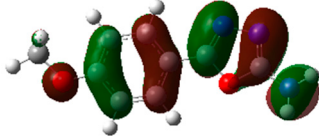
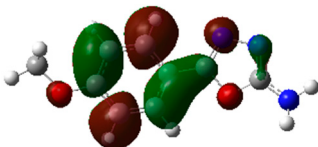
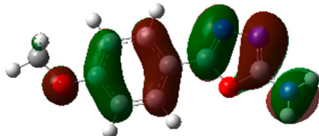
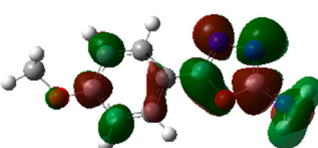
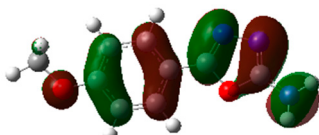
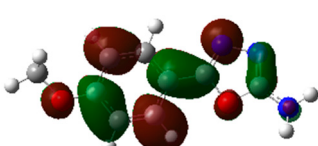
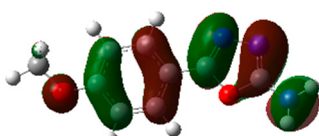
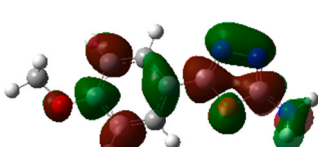
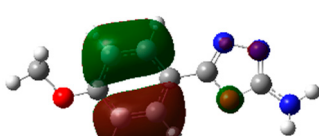
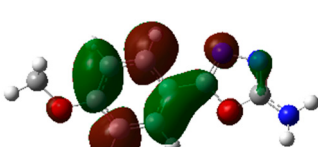
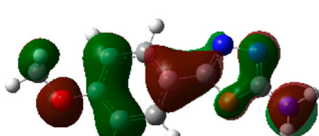
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| 847 | 5  | <b>2233</b> | <b>80</b>  | 2888 | 59  |  |  | 2893        | 51         | 2884        | 62          |
| 640 | 45 | <b>1615</b> | <b>144</b> | 2080 | 385 |  |  | <b>1776</b> | <b>169</b> | <b>2138</b> | <b>1395</b> |
| 581 | 30 | 1568        | 16         | 1612 | 134 |  |  | <b>1614</b> | <b>191</b> | 1618        | 14          |
| 203 | 15 | <b>1509</b> | <b>124</b> | 1565 | 49  |  |  | 1573        | 34         | 1579        | 43          |
| 44  | 59 | 1473        | 39         | 1510 | 54  |  |  | <b>1509</b> | <b>122</b> | <b>1512</b> | <b>226</b>  |
|     |    | 1464        | 10         | 1474 | 36  |  |  | 1473        | 36         | 1475        | 45          |
|     |    | 1446        | 10         | 1464 | 10  |  |  | 1464        | 10         | 1463        | 9           |
|     |    | 1420        | 4          | 1448 | 3   |  |  | 1446        | 10         | 1447        | 9           |
|     |    | 1308        | 52         | 1419 | 10  |  |  | 1426        | 24         | 1421        | 4           |
|     |    | 1304        | 18         | 1385 | 141 |  |  | 1332        | 8          | 1398        | 10          |
|     |    | <b>1259</b> | <b>258</b> | 1307 | 41  |  |  | 1316        | 43         | 1305        | 22          |
|     |    | 1201        | 0          | 1298 | 29  |  |  | 1302        | 6          | 1299        | 3           |
|     |    | 1178        | 4          | 1267 | 65  |  |  | <b>1260</b> | <b>306</b> | <b>1246</b> | <b>317</b>  |
|     |    | 1170        | 65         | 1253 | 599 |  |  | 1207        | 36         | 1178        | 11          |
|     |    | 1144        | 1          | 1179 | 11  |  |  | 1178        | 6          | 1167        | 37          |
|     |    | 1113        | 8          | 1171 | 110 |  |  | 1165        | 107        | 1144        | 1           |
|     |    | 1031        | 64         | 1144 | 1   |  |  | 1144        | 1          | 1121        | 13          |
|     |    | 1005        | 0          | 1109 | 16  |  |  | 1115        | 4          | 1107        | 13          |
|     |    | 959         | 0          | 1106 | 11  |  |  | 1067        | 30         | 1038        | 64          |
|     |    | 938         | 1          | 1035 | 67  |  |  | 1029        | 71         | 1003        | 1           |
|     |    | 834         | 58         | 1003 | 1   |  |  | 1002        | 2          | 943         | 0           |
|     |    | 815         | 3          | 958  | 0   |  |  | 986         | 35         | 924         | 1           |
|     |    | 805         | 6          | 938  | 1   |  |  | 963         | 1          | <b>887</b>  | <b>462</b>  |
|     |    | 722         | 0          | 832  | 59  |  |  | 939         | 1          | 828         | 69          |
|     |    | 682         | 19         | 812  | 5   |  |  | 833         | 55         | 818         | 1           |
|     |    | 646         | 1          | 804  | 4   |  |  | 812         | 5          | 797         | 2           |
|     |    | 559         | 0          | 717  | 2   |  |  | 807         | 7          | 715         | 1           |
|     |    | 557         | 23         | 686  | 10  |  |  | 713         | 1          | 715         | 19          |
|     |    | 493         | 5          | 637  | 16  |  |  | 687         | 6          | 640         | 15          |
|     |    | 476         | 1          | 603  | 67  |  |  | 634         | 3          | 616         | 43          |
|     |    | 411         | 0          | 556  | 73  |  |  | 571         | 24         | 570         | 48          |
|     |    | 378         | 1          | 501  | 13  |  |  | 543         | 40         | 508         | 25          |
|     |    | 275         | 0          | 490  | 1   |  |  | 482         | 2          | 506         | 2           |
|     |    | 253         | 4          | 418  | 2   |  |  | 475         | 2          | 433         | 62          |
|     |    | 213         | 0          | 370  | 16  |  |  | 468         | 8          | 421         | 1           |
|     |    | 141         | 4          | 367  | 3   |  |  | 411         | 0          | 381         | 1           |
|     |    | 123         | 9          | 352  | 9   |  |  | 317         | 0          | 378         | 4           |
|     |    | 72          | 0          | 312  | 38  |  |  | 270         | 2          | 341         | 27          |
|     |    |             |            | 229  | 5   |  |  | 249         | 5          | 233         | 3           |
|     |    |             |            | 222  | 10  |  |  | 212         | 1          | 222         | 5           |
|     |    |             |            | 159  | 13  |  |  | 123         | 2          | 153         | 9           |
|     |    |             |            | 94   | 5   |  |  | 120         | 9          | 92          | 1           |
|     |    |             |            | 72   | 4   |  |  | 88          | 3          | 85          | 3           |

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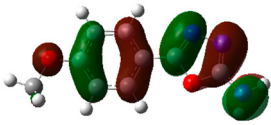
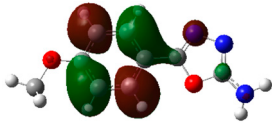
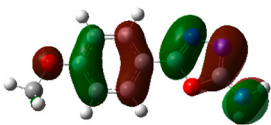
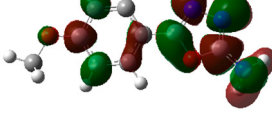
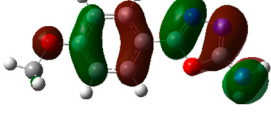
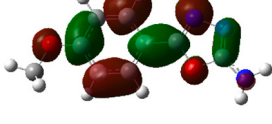
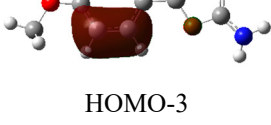
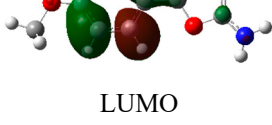
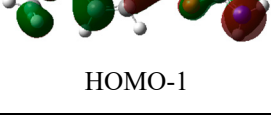
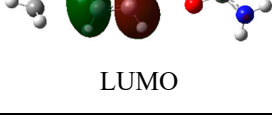
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|--|--|--|--|----|---|--|--|----|---|----|---|
|  |  |  |  | 44 | 2 |  |  | 68 | 1 | 40 | 3 |
|--|--|--|--|----|---|--|--|----|---|----|---|

<sup>a</sup> Calculated frequencies are scaled by 0.960 in the range of 4000 - 1800 cm<sup>-1</sup>, and 0.980 below 1800 cm<sup>-1</sup>. For the photoproducts exhibiting two conformers [**1''**(Z)s and **1''**(E)s, **3**, **6A**, **8** and **9**], only the most stable was considered.

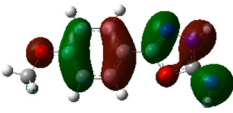
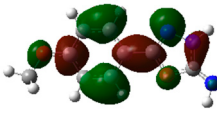
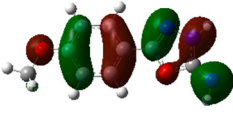
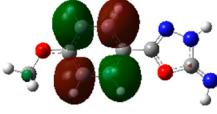
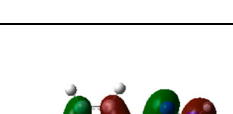
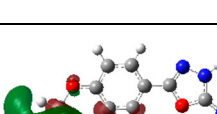
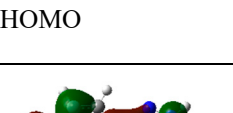
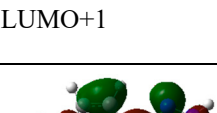
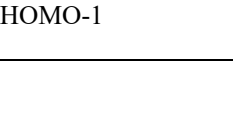
**Table S2.** Excitation energies ( $\lambda$ , in nm), oscillator strengths ( $f$ ), main orbital transitions (with corresponding amplitudes in parentheses) and isosurface representations of the orbitals involved for the six longest singlet states of conformer **1'-a** of 2-Amino-5-(4-methoxyphenyl)-1,3,4-oxadiazole **1**, obtained from TD-DFT calculations at the CAM-B3LYP/6-311++G(d,p) level of theory.

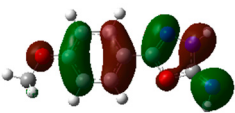
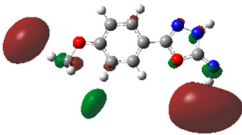
| State | $\lambda$ | $f$    | Major contribution     | Donor orbital                                                                                  | Acceptor orbital                                                                                |
|-------|-----------|--------|------------------------|------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------|
| S1    | 260.15    | 0.6037 | HOMO→<br>LUMO (0.67)   | <br>HOMO     | <br>LUMO     |
| S2    | 251.03    | 0.0562 | HOMO→<br>LUMO+3 (0.58) | <br>HOMO     | <br>LUMO+3   |
| S3    | 232.54    | 0.0043 | HOMO→<br>LUMO+1 (0.63) | <br>HOMO    | <br>LUMO+1  |
| S4    | 216.47    | 0.0028 | HOMO→<br>LUMO+2 (0.60) | <br>HOMO   | <br>LUMO+2 |
| S5    | 207.84    | 0.0029 | HOM-3→<br>LUMO (0.64)  | <br>HOMO-3 | <br>LUMO   |
| S6    | 202.40    | 0.0516 | HOMO-1→<br>LUMO (0.45) | <br>HOMO-1 | <br>LUMO   |

**Table S3.** Excitation energies ( $\lambda$ , in nm), oscillator strengths ( $f$ ), main orbital transitions (with corresponding amplitudes in parentheses) and isosurface representations of the orbitals involved for the six longest singlet states of conformer **1'-s** of 2-Amino-5-(4-methoxyphenyl)-1,3,4-oxadiazole **1**, obtained from TD-DFT calculations at the CAM-B3LYP/6-311++G(d,p) level of theory.

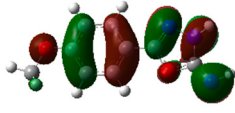
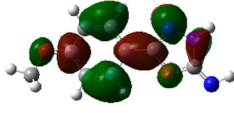
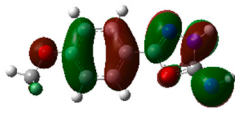
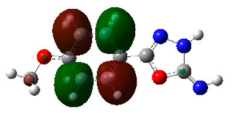
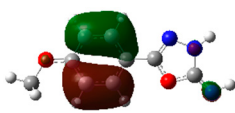
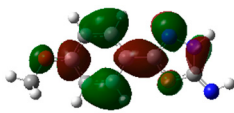
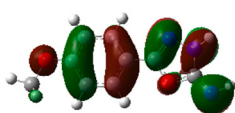
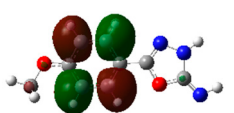
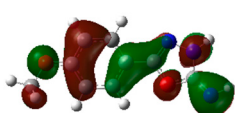
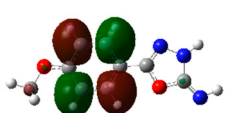
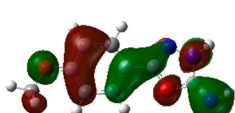
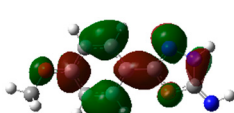
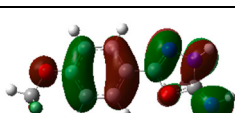
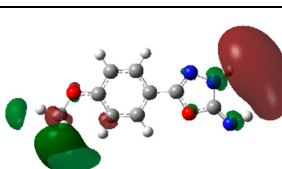
| State | $\lambda$ | $f$    | Major contribution                  | Donor orbital                                                                                  | Acceptor orbital                                                                                |
|-------|-----------|--------|-------------------------------------|------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------|
| S1    | 258.79    | 0.6334 | HOMO $\rightarrow$<br>LUMO (0.68)   | <br>HOMO     | <br>LUMO     |
| S2    | 250.63    | 0.0258 | HOMO $\rightarrow$<br>LUMO+3 (0.59) | <br>HOMO     | <br>LUMO+3   |
| S3    | 233.13    | 0.0046 | HOMO $\rightarrow$<br>LUMO+1 (0.61) | <br>HOMO    | <br>LUMO+1  |
| S4    | 217.43    | 0.0024 | HOMO $\rightarrow$<br>LUMO+2 (0.60) | <br>HOMO   | <br>LUMO+2 |
| S5    | 207.69    | 0.0041 | HOMO-3 $\rightarrow$<br>LUMO (0.63) | <br>HOMO-3 | <br>LUMO   |
| S6    | 202.12    | 0.1328 | HOMO-1 $\rightarrow$<br>LUMO (0.58) | <br>HOMO-1 | <br>LUMO   |

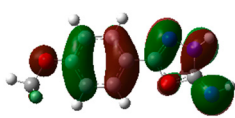
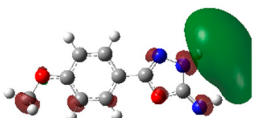
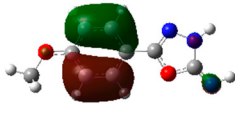
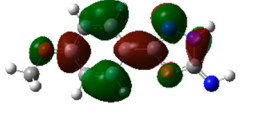
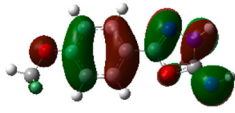
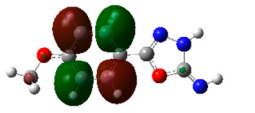
**Table S4.** Excitation energies ( $\lambda$ , in nm), oscillator strengths ( $f$ ), main orbital transitions (with corresponding amplitudes in parentheses) and isosurface representations of the orbitals involved for the six longest singlet states for the imino tautomer of 2-Amino-5-(4-methoxyphenyl)-1,3,4-oxadiazole **1'-(Z)s**, obtained from TD-DFT calculations at the CAM-B3LYP/6-311++G(d,p) level of theory.

| State | $\lambda$ | $f$    | Major contribution                       | Donor orbital                                                                                  | Acceptor orbital                                                                                |
|-------|-----------|--------|------------------------------------------|------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------|
| S1    | 266.64    | 0.5499 | HOMO→LUMO (0.64)                         | <br>HOMO     | <br>LUMO     |
| S2    | 251.75    | 0.0127 | HOMO→LUMO+2 (0.56)                       | <br>HOMO     | <br>LUMO+2   |
| S3    | 233.38    | 0.0017 | HOMO→LUMO+3 (0.5)                        | <br>HOMO    | <br>LUMO+3  |
| S4    | 215.84    | 0.0051 | HOMO→LUMO+1 (0.52)                       | <br>HOMO   | <br>LUMO+1 |
| S5    | 215.53    | 0.0422 | HOMO-1→LUMO (0.66)                       | <br>HOMO-1 | <br>LUMO   |
| S6    | 205.87    | 0.0009 | HOMO→LUMO+4 (0.51)<br>HOMO→LUMO+6 (0.37) | <br>HOMO   | <br>LUMO+4 |

|  |  |  |  |                                                                                            |                                                                                               |
|--|--|--|--|--------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------|
|  |  |  |  | <br>HOMO | <br>LUMO+6 |
|--|--|--|--|--------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------|

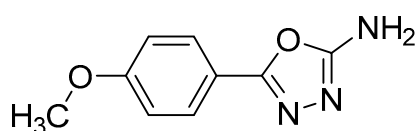
**Table S5.** Excitation energies ( $\lambda$ , in nm), oscillator strengths ( $f$ ), main orbital transitions (with corresponding amplitudes in parentheses) and isosurface representations of the orbitals involved for the six longest singlet states for the imino tautomer of 2-Amino-5-(4-methoxyphenyl)-1,3,4-oxadiazole **1'-(E)s**, obtained from TD-DFT calculations at the CAM-B3LYP/6-311++G(d,p) level of theory.

| State | $\lambda$ | $f$    | Major contribution                        | Donor orbital                                                                                  | Acceptor orbital                                                                                |
|-------|-----------|--------|-------------------------------------------|------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------|
| S1    | 262.70    | 0.5451 | HOMO→LUMO (0.69)                          | <br>HOMO     | <br>LUMO     |
| S2    | 250.06    | 0.0128 | HOMO→LUMO+3 (0.55)<br>HOMO-2→LUMO (0.33)  | <br>HOMO    | <br>LUMO+3  |
|       |           |        |                                           | <br>HOMO-2 | <br>LUMO   |
| S3    | 242.81    | 0.0012 | HOMO→LUMO+1 (0.50)<br>HOMO→LUMO+2 (-0.39) | <br>HOMO   | <br>LUMO+3 |
|       |           |        |                                           | <br>HOMO-1 | <br>LUMO+3 |
| S4    | 215.24    | 0.0372 | HOMO-1→LUMO (0.65)                        | <br>HOMO-1 | <br>LUMO   |
| S5    | 215.15    | 0.0067 | HOMO→LUMO+2 (0.42)<br>HOMO→LUMO+1 (0.36)  | <br>HOMO   | <br>LUMO+2 |

|    |        |        |                                           |                                                                                    |                                                                                     |
|----|--------|--------|-------------------------------------------|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|    |        |        |                                           |  | LUMO+2                                                                              |
|    |        |        |                                           | HOMO                                                                               |  |
|    |        |        |                                           |                                                                                    | LUMO+1                                                                              |
| S6 | 201.41 | 0.1042 | HOMO-2→LUMO (0.53)<br>HOMO→LUMO+3 (-0.40) |  |  |
|    |        |        |                                           | HOMO-2                                                                             | LUMO                                                                                |
|    |        |        |                                           |  |  |
|    |        |        |                                           | HOMO                                                                               | LUMO+3                                                                              |

### 3. Computational data

3.1. Cartesian coordinates of the optimized structures of the species investigated in this work. In cases where multiple conformers exist, only the lowest-energy conformer is reported.



1'-a

| B3LYP/6-311++G(d,p) |           |           |           | B3LYP/aug-cc-pVTZ |           |           |           |
|---------------------|-----------|-----------|-----------|-------------------|-----------|-----------|-----------|
| 8                   | 2.357304  | 0.730425  | -0.003232 | 8                 | 2.354044  | -0.729197 | 0.001432  |
| 6                   | 3.568070  | 0.119246  | -0.006632 | 6                 | 3.562354  | -0.118234 | 0.004344  |
| 7                   | 3.493875  | -1.172896 | 0.000516  | 7                 | 3.488254  | 1.171370  | 0.001013  |
| 7                   | 2.126261  | -1.469594 | 0.021084  | 7                 | 2.120938  | 1.466977  | -0.015535 |
| 6                   | 1.487783  | -0.347306 | 0.012083  | 6                 | 1.484808  | 0.346518  | -0.008921 |
| 6                   | 0.055384  | -0.098142 | 0.007209  | 6                 | 0.054949  | 0.097362  | -0.005159 |
| 6                   | -0.465389 | 1.206062  | 0.020933  | 6                 | -0.465426 | -1.203220 | -0.016398 |
| 6                   | -1.833483 | 1.419164  | 0.017289  | 6                 | -1.830113 | -1.416453 | -0.013733 |
| 6                   | -2.717150 | 0.332500  | 0.000712  | 6                 | -2.712510 | -0.333140 | -0.000742 |
| 6                   | -2.209071 | -0.972063 | -0.012296 | 6                 | -2.205095 | 0.968126  | 0.009711  |
| 6                   | -0.833903 | -1.178326 | -0.009344 | 6                 | -0.833678 | 1.173921  | 0.007806  |
| 8                   | -4.041720 | 0.644729  | -0.001192 | 8                 | -4.035448 | -0.643464 | 0.000518  |
| 6                   | -4.994872 | -0.411838 | -0.014103 | 6                 | -4.985508 | 0.412826  | 0.011241  |
| 7                   | 4.679690  | 0.912222  | 0.051521  | 7                 | 4.673168  | -0.908832 | -0.056222 |
| 1                   | 0.207435  | 2.054410  | 0.036455  | 1                 | 0.205175  | -2.050224 | -0.028905 |
| 1                   | -2.243733 | 2.421494  | 0.028447  | 1                 | -2.237067 | -2.417633 | -0.022803 |
| 1                   | -2.869713 | -1.828176 | -0.025077 | 1                 | -2.864689 | 1.821886  | 0.019644  |
| 1                   | -0.438057 | -2.186358 | -0.019729 | 1                 | -0.439911 | 2.180139  | 0.016137  |
| 1                   | -4.896070 | -1.026801 | -0.914722 | 1                 | -4.885468 | 1.028583  | 0.908155  |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| 1 | -5.970808 | 0.070235  | -0.011661 | 1 | -5.961220 | -0.064604 | 0.009222  |
| 1 | -4.900345 | -1.044690 | 0.874482  | 1 | -4.889010 | 1.043436  | -0.875668 |
| 1 | 5.539866  | 0.420879  | -0.143617 | 1 | 5.531156  | -0.420637 | 0.143445  |
| 1 | 4.603754  | 1.813868  | -0.396151 | 1 | 4.597057  | -1.812499 | 0.381488  |

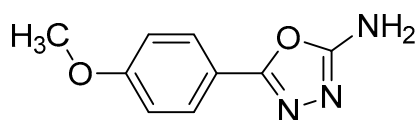
MP2/6-311++G(d,p)

|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | 2.351083  | -0.729406 | 0.104801  |
| 6 | 3.557501  | -0.116483 | 0.055656  |
| 7 | 3.485513  | 1.175463  | -0.118083 |
| 7 | 2.122117  | 1.461978  | -0.206954 |
| 6 | 1.488273  | 0.328001  | -0.063269 |
| 6 | 0.054532  | 0.083556  | -0.020185 |
| 6 | -0.467088 | -1.217372 | -0.149499 |
| 6 | -1.843057 | -1.423136 | -0.124945 |
| 6 | -2.723744 | -0.333437 | -0.022237 |
| 6 | -2.208141 | 0.967276  | 0.096520  |
| 6 | -0.824605 | 1.170069  | 0.087815  |
| 8 | -4.050015 | -0.645022 | -0.027072 |
| 6 | -4.961019 | 0.438123  | 0.104977  |
| 7 | 4.676910  | -0.914814 | 0.085284  |
| 1 | 0.205044  | -2.065320 | -0.244295 |
| 1 | -2.263276 | -2.420399 | -0.217547 |
| 1 | -2.862922 | 1.826734  | 0.183433  |
| 1 | -0.418242 | 2.173146  | 0.181931  |
| 1 | -4.815149 | 0.963095  | 1.055465  |
| 1 | -5.954260 | -0.008576 | 0.083610  |
| 1 | -4.859626 | 1.144524  | -0.726236 |
| 1 | 5.519059  | -0.368688 | 0.215010  |
| 1 | 4.613145  | -1.687060 | 0.736073  |

79

80

81



1'-s

B3LYP/6-311++G(d,p)

B3LYP/aug-cc-pVTZ

|   |           |           |           |   |          |           |           |
|---|-----------|-----------|-----------|---|----------|-----------|-----------|
| 8 | -2.250005 | -0.807533 | 0.003593  | 8 | 2.246454 | -0.806372 | -0.001642 |
| 6 | -3.523196 | -0.339816 | 0.004512  | 6 | 3.517420 | -0.339273 | -0.002628 |
| 7 | -3.598543 | 0.952151  | -0.003983 | 7 | 3.593240 | 0.950145  | 0.001740  |
| 7 | -2.274267 | 1.404625  | -0.022949 | 7 | 2.269362 | 1.402168  | 0.016992  |
| 6 | -1.510597 | 0.363560  | -0.011681 | 6 | 1.507702 | 0.362992  | 0.008666  |

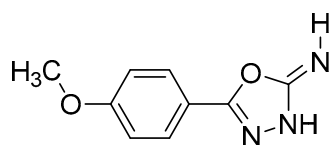
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|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| 6 | -0.059239 | 0.283735  | -0.004775 | 6 | 0.058824  | 0.283552  | 0.003228  |
| 6 | 0.608541  | -0.942931 | -0.019192 | 6 | -0.609003 | -0.939327 | 0.014875  |
| 6 | 2.001496  | -1.001760 | -0.013852 | 6 | -1.998345 | -0.997946 | 0.010832  |
| 6 | 2.744246  | 0.181601  | 0.005251  | 6 | -2.739667 | 0.182234  | -0.004165 |
| 6 | 2.079919  | 1.417911  | 0.019153  | 6 | -2.075810 | 1.415098  | -0.015233 |
| 6 | 0.699656  | 1.468483  | 0.014488  | 6 | -0.699016 | 1.464938  | -0.011844 |
| 8 | 4.103650  | 0.241104  | 0.011602  | 8 | -4.097133 | 0.240433  | -0.008944 |
| 6 | 4.842274  | -0.974503 | -0.003937 | 6 | -4.832920 | -0.974249 | 0.003407  |
| 7 | -4.536146 | -1.255560 | -0.054401 | 7 | 4.529321  | -1.253112 | 0.058551  |
| 1 | 0.040792  | -1.864985 | -0.036741 | 1 | -0.043744 | -1.860076 | 0.028969  |
| 1 | 2.488211  | -1.967352 | -0.026001 | 1 | -2.484401 | -1.961065 | 0.020583  |
| 1 | 2.672961  | 2.324163  | 0.033869  | 1 | -2.665497 | 2.320807  | -0.026684 |
| 1 | 0.186950  | 2.422250  | 0.025400  | 1 | -0.188074 | 2.416874  | -0.020500 |
| 1 | 5.891243  | -0.683901 | 0.003964  | 1 | -5.880773 | -0.688031 | -0.002624 |
| 1 | 4.633556  | -1.556081 | -0.908099 | 1 | -4.622010 | -1.557686 | 0.902847  |
| 1 | 4.627471  | -1.582707 | 0.881108  | 1 | -4.617482 | -1.578615 | -0.881041 |
| 1 | -5.447460 | -0.865335 | 0.137199  | 1 | 5.438252  | -0.866528 | -0.138459 |
| 1 | -4.358774 | -2.140818 | 0.397278  | 1 | 4.350591  | -2.140684 | -0.382217 |

MP2/6-311++G(d,p)

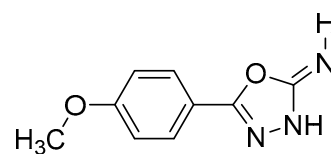
|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | 2.243272  | -0.805356 | -0.092165 |
| 6 | 3.513153  | -0.338478 | -0.035760 |
| 7 | 3.592619  | 0.953988  | 0.129664  |
| 7 | 2.271839  | 1.400142  | 0.202881  |
| 6 | 1.509755  | 0.347700  | 0.061451  |
| 6 | 0.057781  | 0.275775  | 0.006560  |
| 6 | -0.612754 | -0.949558 | 0.114197  |
| 6 | -2.011968 | -1.003211 | 0.072300  |
| 6 | -2.749559 | 0.184584  | -0.036694 |
| 6 | -2.076163 | 1.415730  | -0.135285 |
| 6 | -0.687938 | 1.465419  | -0.110404 |
| 8 | -4.109540 | 0.253737  | -0.072155 |
| 6 | -4.814342 | -0.973058 | 0.060935  |
| 7 | 4.530885  | -1.263464 | -0.050614 |
| 1 | -0.045713 | -1.870788 | 0.213483  |
| 1 | -2.502855 | -1.966288 | 0.153067  |
| 1 | -2.668227 | 2.321810  | -0.225945 |
| 1 | -0.165721 | 2.414460  | -0.189478 |
| 1 | -5.871131 | -0.711301 | 0.026126  |
| 1 | -4.587164 | -1.456910 | 1.017347  |
| 1 | -4.579728 | -1.656032 | -0.763113 |
| 1 | 5.432523  | -0.820605 | -0.174443 |
| 1 | 4.382971  | -2.025485 | -0.699809 |



**1''-(Z)s**

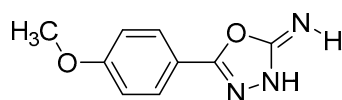
B3LYP/6-311++G(d,p)

|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | -2.235850 | -0.857224 | 0.017669  |
| 6 | -3.586268 | -0.508024 | 0.001158  |
| 7 | -3.557876 | 0.863004  | 0.017718  |
| 7 | -2.278362 | 1.368179  | -0.007620 |
| 6 | -1.523492 | 0.324391  | 0.003163  |
| 6 | -0.071244 | 0.272353  | 0.002863  |
| 6 | 0.604923  | -0.949779 | 0.003147  |
| 6 | 1.998035  | -0.997375 | 0.000930  |
| 6 | 2.731523  | 0.191889  | -0.001554 |
| 6 | 2.057636  | 1.424056  | -0.001558 |
| 6 | 0.677644  | 1.463690  | 0.000938  |
| 8 | 4.088971  | 0.262748  | -0.003641 |
| 6 | 4.839015  | -0.946975 | -0.003088 |
| 7 | -4.592116 | -1.272620 | -0.017825 |
| 1 | -4.354924 | 1.468955  | -0.069762 |
| 1 | 0.041679  | -1.874410 | 0.005152  |
| 1 | 2.492231  | -1.959146 | 0.001347  |
| 1 | 2.644211  | 2.334564  | -0.002859 |
| 1 | 0.161048  | 2.415557  | 0.001828  |
| 1 | 5.885064  | -0.646325 | -0.004858 |
| 1 | 4.631083  | -1.544337 | -0.896866 |
| 1 | 4.633448  | -1.542043 | 0.892762  |
| 1 | -4.326962 | -2.252302 | -0.020869 |

**1''-(Z)a**

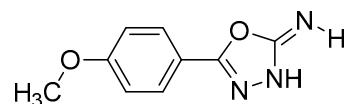
B3LYP/6-311++G(d,p)

|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | 2.348796  | 0.777827  | 0.022482  |
| 6 | 3.649138  | 0.273355  | 0.001932  |
| 7 | 3.460980  | -1.085259 | 0.020023  |
| 7 | 2.130733  | -1.437056 | -0.011384 |
| 6 | 1.503298  | -0.312128 | 0.003355  |
| 6 | 0.066911  | -0.087968 | 0.003419  |
| 6 | -0.460775 | 1.213497  | 0.000844  |
| 6 | -1.830036 | 1.417552  | -0.001767 |
| 6 | -2.706844 | 0.325227  | -0.001683 |
| 6 | -2.190763 | -0.977145 | 0.001365  |
| 6 | -0.814945 | -1.174463 | 0.004314  |
| 8 | -4.032152 | 0.628303  | -0.004080 |
| 6 | -4.980260 | -0.433464 | -0.004021 |
| 7 | 4.737267  | 0.915161  | -0.020042 |
| 1 | 4.180785  | -1.778546 | -0.087022 |
| 1 | 0.209076  | 2.063953  | 0.000896  |
| 1 | -2.246578 | 2.417253  | -0.003672 |
| 1 | -2.846555 | -1.837001 | 0.002425  |
| 1 | -0.416456 | -2.181639 | 0.007886  |
| 1 | -5.958328 | 0.044043  | -0.006519 |
| 1 | -4.881967 | -1.055005 | 0.892018  |
| 1 | -4.878811 | -1.057935 | -0.897670 |
| 1 | 4.588476  | 1.919144  | -0.022284 |

**1''-(E)s**

B3LYP/6-311++G(d,p)

|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | -2.223265 | -0.856226 | 0.045111  |
| 6 | -3.568911 | -0.529183 | 0.001332  |
| 7 | -3.562444 | 0.852578  | 0.041796  |
| 7 | -2.277893 | 1.368191  | -0.023772 |
| 6 | -1.523172 | 0.324685  | 0.007832  |

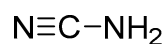
**1''-(E)a**

B3LYP/6-311++G(d,p)

|   |          |           |           |
|---|----------|-----------|-----------|
| 8 | 2.336663 | 0.779200  | 0.049576  |
| 6 | 3.634793 | 0.297000  | 0.003568  |
| 7 | 3.466751 | -1.074968 | 0.040265  |
| 7 | 2.130204 | -1.435873 | -0.029617 |
| 6 | 1.503180 | -0.311166 | 0.006918  |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| 6 | -0.070339 | 0.275045  | 0.008269  | 6 | 0.065900  | -0.089397 | 0.007501  |
| 6 | 0.603669  | -0.948360 | 0.004807  | 6 | -0.460264 | 1.212724  | -0.003389 |
| 6 | 1.996427  | -0.996623 | -0.000963 | 6 | -1.829351 | 1.416414  | -0.009613 |
| 6 | 2.730682  | 0.192435  | -0.003032 | 6 | -2.706069 | 0.323779  | -0.004663 |
| 6 | 2.058360  | 1.425481  | 0.001624  | 6 | -2.190818 | -0.978927 | 0.007663  |
| 6 | 0.678295  | 1.465998  | 0.008153  | 6 | -0.814944 | -1.176147 | 0.014802  |
| 8 | 4.088014  | 0.261904  | -0.008070 | 8 | -4.031190 | 0.626897  | -0.010957 |
| 6 | 4.836977  | -0.948739 | -0.010606 | 6 | -4.979669 | -0.434426 | -0.005540 |
| 7 | -4.462218 | -1.422751 | -0.035160 | 7 | 4.626595  | 1.079705  | -0.030743 |
| 1 | -4.333204 | 1.444753  | -0.217699 | 1 | 4.161722  | -1.750567 | -0.229550 |
| 1 | 0.038037  | -1.871547 | 0.006267  | 1 | 0.211234  | 2.061898  | -0.007258 |
| 1 | 2.489916  | -1.958720 | -0.003412 | 1 | -2.245961 | 2.416028  | -0.018008 |
| 1 | 2.646003  | 2.335284  | 0.001928  | 1 | -2.847026 | -1.838421 | 0.014112  |
| 1 | 0.162098  | 2.418104  | 0.014172  | 1 | -0.416132 | -2.183162 | 0.027254  |
| 1 | 5.883274  | -0.648960 | -0.013814 | 1 | -5.957539 | 0.043452  | -0.012739 |
| 1 | 4.626763  | -1.544544 | -0.904817 | 1 | -4.883098 | -1.050153 | 0.894700  |
| 1 | 4.632314  | -1.544812 | 0.884708  | 1 | 5.508640  | 0.575737  | -0.894937 |

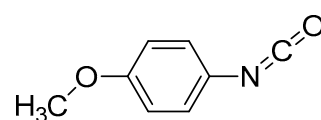
85



2

B3LYP/6-311++G(d,p)

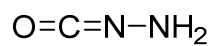
|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 1.378598  | 0.000001  | 0.012281  |
| 6 | 0.220906  | -0.000003 | -0.000774 |
| 7 | -1.117297 | 0.000000  | -0.076325 |
| 1 | -1.577266 | 0.847654  | 0.226476  |
| 1 | -1.577277 | -0.847645 | 0.226478  |
| 7 | 1.378598  | 0.000001  | 0.012281  |
| 6 | 0.220906  | -0.000003 | -0.000774 |



3

B3LYP/6-311++G(d,p)

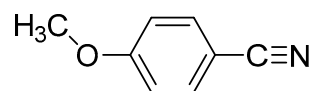
|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 2.420820  | 0.584738  | 0.000000  |
| 6 | 1.056402  | 0.270189  | 0.000000  |
| 6 | 0.128965  | 1.308713  | 0.000000  |
| 6 | -1.239899 | 1.040802  | 0.000000  |
| 6 | -1.690453 | -0.281343 | 0.000000  |
| 6 | -0.757655 | -1.327016 | 0.000000  |
| 6 | 0.600254  | -1.056523 | 0.000000  |
| 8 | -3.001641 | -0.655577 | 0.000000  |
| 6 | -3.998486 | 0.358127  | 0.000000  |
| 6 | 3.501068  | 0.058377  | 0.000000  |
| 8 | 4.603374  | -0.340233 | 0.000000  |
| 1 | 0.482960  | 2.332200  | 0.000000  |
| 1 | -1.935631 | 1.868677  | 0.000000  |
| 1 | -1.120892 | -2.347458 | 0.000000  |
| 1 | 1.313884  | -1.872637 | 0.000000  |
| 1 | -3.929149 | 0.986352  | -0.894641 |
| 1 | -3.929149 | 0.986352  | 0.894641  |
| 1 | -4.953397 | -0.164495 | 0.000000  |



4

B3LYP/6-311++G(d,p)

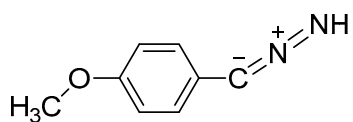
|   |           |           |           |
|---|-----------|-----------|-----------|
| 7 | 0.443215  | -0.444430 | -0.000012 |
| 6 | -0.701877 | -0.042301 | 0.000000  |
| 8 | -1.853851 | 0.155000  | 0.000004  |
| 7 | 1.654883  | 0.308145  | 0.000012  |
| 1 | 2.177682  | -0.016057 | -0.811155 |
| 1 | 2.177701  | -0.016143 | 0.811131  |



5

B3LYP/6-311++G(d,p)

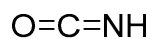
|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 2.965658  | -0.179731 | -0.000006 |
| 6 | 1.545432  | -0.026363 | 0.000000  |
| 6 | 0.711584  | -1.149771 | 0.000010  |
| 6 | -0.672387 | -1.007779 | 0.000015  |
| 6 | -1.238358 | 0.272476  | 0.000010  |
| 6 | -0.406686 | 1.402714  | 0.000000  |
| 6 | 0.967468  | 1.256320  | -0.000002 |
| 8 | -2.571103 | 0.523263  | 0.000020  |
| 6 | -3.480668 | -0.573741 | -0.000026 |
| 7 | 4.115485  | -0.302499 | -0.000010 |
| 1 | 1.149227  | -2.140544 | 0.000014  |
| 1 | -1.292965 | -1.893100 | 0.000024  |
| 1 | -0.865232 | 2.383711  | -0.000003 |
| 1 | 1.606399  | 2.130797  | -0.000009 |
| 1 | -3.357185 | -1.191388 | 0.895206  |
| 1 | -3.357158 | -1.191328 | -0.895297 |
| 1 | -4.474910 | -0.131507 | -0.000025 |



**6A**

B3LYP/6-311++G(d,p)

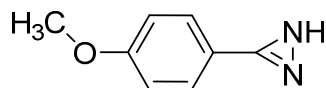
|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -2.408751 | -0.591787 | -0.032478 |
| 6 | -1.005248 | -0.283429 | -0.016394 |
| 6 | -0.547283 | 1.051891  | -0.017077 |
| 6 | 0.804682  | 1.334911  | -0.010158 |
| 6 | 1.744990  | 0.292170  | 0.000898  |
| 6 | 1.308458  | -1.036790 | 0.001499  |
| 6 | -0.056127 | -1.312177 | -0.010556 |
| 8 | 3.047637  | 0.675345  | 0.009333  |
| 6 | 4.059936  | -0.326245 | 0.017289  |
| 7 | -3.494952 | -0.117991 | 0.036719  |
| 7 | -4.673384 | 0.284527  | -0.107443 |
| 1 | -1.267178 | 1.861898  | -0.026147 |
| 1 | 1.164681  | 2.356587  | -0.012419 |
| 1 | 2.013748  | -1.856407 | 0.007727  |
| 1 | -0.396749 | -2.340494 | -0.015908 |
| 1 | 4.003619  | -0.955070 | -0.877090 |
| 1 | 3.992298  | -0.952458 | 0.912757  |
| 1 | 5.006396  | 0.210987  | 0.022488  |
| 1 | -5.123502 | 0.335187  | 0.810860  |



**7**

B3LYP/6-311++G(d,p)

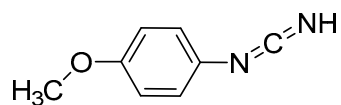
|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | -1.210331 | 0.013970  | -0.000005 |
| 6 | -0.044846 | 0.021688  | 0.000014  |
| 7 | 1.158142  | -0.122204 | -0.000004 |
| 1 | 1.844734  | 0.613537  | -0.000008 |
| 8 | -1.210331 | 0.013970  | -0.000005 |
| 6 | -0.044846 | 0.021688  | 0.000014  |
| 7 | 1.158142  | -0.122204 | -0.000004 |
| 1 | 1.844734  | 0.613537  | -0.000008 |



**8**

B3LYP/6-311++G(d,p)

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 0.871079  | 1.437251  | 0.020043  |
| 6 | -0.505955 | 1.352508  | 0.011938  |
| 6 | -1.138962 | 0.095493  | -0.007643 |
| 6 | -0.359307 | -1.063519 | -0.022255 |
| 6 | 1.030425  | -0.987651 | -0.016091 |
| 6 | 1.650802  | 0.266883  | 0.005998  |
| 1 | 1.377360  | 2.394452  | 0.035256  |
| 1 | -1.107539 | 2.254046  | 0.020734  |



**9**

B3LYP/6-311++G(d,p)

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -0.709990 | 1.310958  | -0.017421 |
| 6 | 0.635122  | 0.983404  | -0.026802 |
| 6 | 1.039417  | -0.360936 | -0.018847 |
| 6 | 0.067013  | -1.358112 | -0.003968 |
| 6 | -1.290020 | -1.035459 | 0.006869  |
| 6 | -1.685057 | 0.304256  | 0.000567  |
| 1 | -1.031995 | 2.345268  | -0.025241 |
| 1 | 1.380980  | 1.770520  | -0.045548 |

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|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| 1 | -0.847601 | -2.030980 | -0.049074 | 1 | 0.380772  | -2.394857 | -0.001714 |
| 1 | 1.612682  | -1.898476 | -0.031310 | 1 | -2.019645 | -1.833649 | 0.018636  |
| 8 | 2.992154  | 0.459453  | 0.014427  | 8 | -2.980382 | 0.732709  | 0.009469  |
| 6 | 3.854589  | -0.675242 | -0.004367 | 6 | -4.017497 | -0.239017 | 0.021868  |
| 1 | 4.866597  | -0.275512 | 0.004944  | 1 | -4.950465 | 0.322024  | 0.025388  |
| 1 | 3.702759  | -1.302985 | 0.879313  | 1 | -3.980227 | -0.874641 | -0.869517 |
| 1 | 3.706295  | -1.270410 | -0.910835 | 1 | -3.967887 | -0.865179 | 0.919370  |
| 6 | -2.574658 | -0.010036 | -0.015382 | 7 | 2.391506  | -0.750245 | -0.035120 |
| 7 | -3.644938 | 0.632194  | -0.045916 | 6 | 3.417455  | -0.100779 | 0.024447  |
| 7 | -3.560458 | -1.023626 | -0.067517 | 7 | 4.502398  | 0.460279  | -0.075874 |
| 1 | -3.778088 | -1.299854 | 0.896143  | 1 | 5.035536  | 0.672711  | 0.759544  |