**Supplemental data**

**Semiexperimental equilibrium molecular structures of the maleimide and phthalimide**

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**Table S1**. Optimized Cartesian coordinates of phthalimide, Å.

|  |  |  |  |
| --- | --- | --- | --- |
|  | MP2-AE/wCVTZ | MP2-FC/wCVTZ | MP2-FC/VQZ |
| At | x | y | x | y | x | y |
| C1  | –0.000003 | –0.000005 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| C2  | 0.000005 | 1.388022 | 0.000000 | 1.391000 | 0.000000 | 1.390711 |
| C3  | 1.408893 | 1.858798 | 1.411882 | 1.862719 | 1.411739 | 1.861218 |
| N4  | 2.172677 | 0.693986 | 2.176661 | 0.695562 | 2.176288 | 0.695355 |
| C5  | 1.408856 | –0.470806 | 1.411876 | –0.471590 | 1.411739 | –0.470507 |
| C6  | –1.175687 | 2.111995 | –1.178104 | 2.116548 | –1.177612 | 2.116226 |
| C7  | –2.367109 | 1.391644 | –2.371959 | 1.394543 | –2.370590 | 1.394095 |
| C8  | –2.367121 | –0.003592 | –2.371964 | –0.003557 | –2.370590 | –0.003384 |
| C9  | –1.175709 | –0.723959 | –1.178114 | –0.725571 | –1.177612 | –0.725515 |
| O10 | 1.835331 | 2.988902 | 1.839548 | 2.994407 | 1.840033 | 2.991678 |
| O11 | 1.835279 | –1.600921 | 1.839633 | –1.603244 | 1.840033 | –1.600967 |
| H12 | 3.179138 | 0.693960 | 3.184061 | 0.695578 | 3.183406 | 0.695355 |
| H13 | –1.162572 | 3.191644 | –1.165210 | 3.197471 | –1.165107 | 3.196719 |
| H14 | –3.309722 | 1.918401 | –3.315749 | 1.921836 | –3.314076 | 1.921018 |
| H15 | –3.309741 | –0.530334 | –3.315758 | –0.530844 | –3.314076 | –0.530306 |
| H16 | –1.162614 | –1.803608 | –1.165209 | –1.806494 | –1.165107 | –1.806007 |
|  | MP2-FC/VTZ | CCSD(T)-FC/VTZ | *r*e(BO) |
| At | x | y | x | y | x | y |
| C1  | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| C2  | 0.000000 | 1.392600 | 0.000000 | 1.394806 | 0.000000 | 1.389900 |
| C3  | 1.412812 | 1.864565 | 1.419300 | 1.868301 | 1.415261 | 1.860969 |
| N4  | 2.178190 | 0.696330 | 2.186459 | 0.697403 | 2.180483 | 0.694701 |
| C5  | 1.412816 | –0.471907 | 1.419300 | –0.473494 | 1.415058 | –0.471434 |
| C6  | –1.179576 | 2.118867 | –1.181522 | 2.123620 | –1.177181 | 2.116374 |
| C7  | –2.374862 | 1.396173 | –2.380591 | 1.398844 | –2.371648 | 1.393834 |
| C8  | –2.374862 | –0.003637 | –2.380591 | –0.004038 | –2.371648 | –0.003866 |
| C9  | –1.179577 | –0.726331 | –1.181522 | –0.728814 | –1.177181 | –0.726407 |
| O10 | 1.841316 | 2.997508 | 1.847716 | 2.999062 | 1.842379 | 2.987733 |
| O11 | 1.841363 | –1.604834 | 1.847716 | –1.604256 | 1.841865 | –1.598315 |
| H12 | 3.186180 | 0.696347 | 3.193646 | 0.697403 | 3.185983 | 0.694525 |
| H13 | –1.166819 | 3.199962 | –1.168922 | 3.205855 | –1.164546 | 3.196800 |
| H14 | –3.318895 | 1.923584 | –3.325603 | 1.927422 | –3.315005 | 1.921491 |
| H15 | –3.318896 | –0.531046 | –3.325603 | –0.532616 | –3.315005 | –0.531523 |
| H16 | –1.166778 | –1.807425 | –1.168922 | –1.811049 | –1.164591 | –1.806833 |

(*to be continued*)

**Table S1**. (*continued*).

|  |
| --- |
| *r*e(SE) |
| At | x | y |
| C1  | –0.220706 | 0.694381 |
| C2  | –0.220706 | –0.694381 |
| C3  | 1.193014 | –1.164961 |
| N4  | 1.961675 | 0.000000 |
| C5  | 1.193014 | 1.164961 |
| C6  | –1.396951 | –1.420278 |
| C7  | –2.590476 | –0.698307 |
| C8  | –2.590476 | 0.698307 |
| C9  | –1.396951 | 1.420278 |
| O10 | 1.619773 | –2.290827 |
| O11 | 1.619773 | 2.290827 |
| H12 | 2.967175 | 0.000000 |
| H13 | –1.384316 | –2.500704 |
| H14 | –3.533834 | –1.225963 |
| H15 | –3.533834 | 1.225963 |
| H16 | –1.384316 | 2.500704 |

**Table S2** . Optimized theoretical structural parameters for phthalimide (distances in Å, angles in degrees). a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Method | MP2(FC) | MP2(AE) | MP2 | MP2 |
| Basis set | wCVTZ | wCVTZ | VTZ | VQZ |
| C1–C2 | 1.3910 | 1.3880 | 1.3926 | 1.3907 |
| C2–C3 | 1.4886 | 1.4855 | 1.4895 | 1.4881 |
| C3–N4 | 1.3954 | 1.3929 | 1.3966 | 1.3942 |
| C6–C2 | 1.3836 | 1.3807 | 1.3852 | 1.3832 |
| C7–C6 | 1.3952 | 1.3923 | 1.3967 | 1.3945 |
| C8–C7 | 1.3981 | 1.3952 | 1.3998 | 1.3975 |
| C3–O10 | 1.2098 | 1.2079 | 1.2112 | 1.2089 |
| N4–H12 | 1.0074 | 1.0065 | 1.0079 | 1.0071 |
| C6–H13 | 1.0810 | 1.0797 | 1.0811 | 1.0806 |
| C7–H14 | 1.0811 | 1.0798 | 1.0813 | 1.0807 |
| C1–C2–C3 | 108.47 | 108.48 | 108.47 | 108.43 |
| N4–C3–C2 | 104.76 | 104.78 | 104.76 | 104.82 |
| C5–N4–C3 | 113.53 | 113.49 | 113.54 | 113.49 |
| C6–C2–C3 | 129.90 | 129.90 | 129.91 | 129.93 |
| C7–C6–C2 | 117.21 | 117.22 | 117.22 | 117.18 |
| C8–C7–C6 | 121.16 | 121.16 | 121.16 | 121.19 |
| C2–C3–O10 | 129.18 | 129.15 | 129.19 | 129.18 |
| C3–N4–H12 | 123.23 | 123.25 | 123.23 | 123.26 |
| C2–C6–H13 | 120.94 | 120.93 | 120.94 | 120.97 |
| C6–C7–H14 | 119.64 | 119.64 | 119.65 | 119.63 |

a For atom numbering see Figure 2.

**Table S3**. Optimized Cartesian coordinates of maleimide, Å.

|  |  |  |  |
| --- | --- | --- | --- |
|  | MP2-AE/wCVTZ | MP2-FC/wCVTZ | MP2-FC/VQZ |
| At | x | y | x | y | x | y |
| N1  | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| C2  | 0.000000 | 1.387392 | 0.000000 | 1.389903 | 0.000000 | 1.388512 |
| C3  | 1.439806 | 1.780346 | 1.442900 | 1.783414 | 1.441259 | 1.783906 |
| C4  | 2.187728 | 0.675662 | 2.192102 | 0.676178 | 2.190984 | 0.677594 |
| C5  | 1.288170 | –0.515241 | 1.290215 | –0.516890 | 1.289658 | –0.514536 |
| O6  | –0.970827 | 2.105321 | –0.972401 | 2.108844 | –0.972579 | 2.105867 |
| O7  | 1.594216 | –1.683257 | 1.595966 | –1.686914 | 1.595536 | –1.683701 |
| H8  | 1.751407 | 2.810312 | 1.755041 | 2.814566 | 1.751479 | 2.815036 |
| H9  | 3.259754 | 0.582477 | 3.265378 | 0.582457 | 3.263662 | 0.583625 |
| H10 | –0.832206 | –0.563442 | –0.833113 | –0.563719 | –0.832525 | –0.564185 |
|  | MP2-FC/VTZ | CCSD(T)-FC/VTZ | MP2-AE/AwCVQZ |
| At | x | y | x | y | x | y |
| N1  | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.0000000 | 0.0000000 |
| C2  | 0.000000 | 1.391121 | 0.000000 | 1.394553 | 0.0000000 | 1.3856297 |
| C3  | 1.443776 | 1.785083 | 1.450768 | 1.789895 | 1.4369693 | 1.7815820 |
| C4  | 2.194020 | 0.676231 | 2.201753 | 0.678776 | 2.1859757 | 0.6785465 |
| C5  | 1.291312 | –0.517426 | 1.293990 | –0.519970 | 1.2879359 | –0.5110683 |
| O6  | –0.973694 | 2.110849 | –0.972307 | 2.112652 | –0.9718929 | 2.1013745 |
| O7  | 1.597238 | –1.688962 | 1.597774 | –1.689911 | 1.5947493 | –1.6784293 |
| H8  | 1.756005 | 2.816299 | 1.760532 | 2.823465 | 1.7452330 | 2.8120483 |
| H9  | 3.267383 | 0.582499 | 3.276289 | 0.580828 | 3.2574873 | 0.5850044 |
| H10 | –0.833569 | –0.563988 | –0.833529 | –0.563366 | –0.8316911 | –0.5647524 |
|  | MP2-AE/wCVQZ | CCSD(T)-AE/wCVQZ | *r*e(BO) |
| At | x | y | x | y | x | y |
| N1  | 0.0000000 | 0.0000000 | 0.0000000 | 0.000000 | 0.000000 | 0.000000 |
| C2  | 0.0000000 | 1.3853376 | 0.0000000 | 1.3889509 | 0.000000 | 1.3892400 |
| C3  | 1.4373535 | 1.7799938 | 1.4450045 | 1.7849570 | 1.4446183 | 1.7865574 |
| C4  | 2.1854002 | 0.6770444 | 2.1937223 | 0.6794788 | 2.1942943 | 0.6809955 |
| C5  | 1.2870918 | –0.5124012 | 1.2897829 | –0.5154070 | 1.2906153 | –0.5140557 |
| O6  | –0.9704000 | 2.1012894 | –0.9688907 | 2.1031619 | -0.9703897 | 2.1032362 |
| O7  | 1.5933433 | –1.6787944 | 1.5934683 | –1.6801481 | 1.5948478 | –1.6797698 |
| H8  | 1.7469155 | 2.8097349 | 1.7524916 | 2.8171956 | 1.7508119 | 2.8195215 |
| H9  | 3.2566129 | 0.5837777 | 3.2663627 | 0.5819725 | 3.2672383 | 0.5832177 |
| H10 | –0.8314959 | –0.5639404 | –0.8316292 | –0.5632456 | -0.8318221 | –0.5640544 |

(*to be continued*)

**Table S3**. (*continued*).

|  |
| --- |
| *r*e(SE) |
| At | x | y |
| N1  | 0.000000 | 0.907766 |
| C2  | 1.145882 | 0.130778 |
| C3  | 0.673397 | –1.283535 |
| C4  | –0.673397 | –1.283535 |
| C5  | –1.145882 | 0.130778 |
| O6  | 2.283363 | 0.540450 |
| O7  | –2.283363 | 0.540450 |
| H8  | 1.356529 | –2.116675 |
| H9  | –1.356529 | –2.116675 |
| H10 | 0.000000 | 1.917206 |

**Table S4**. Optimized theoretical structural parameters for maleimide (distances in Å, angles in degrees). a

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Method | MP2(FC) | MP2(AE) | MP2(FC) | MP2(FC) | MP2(AE) | MP2(AE) | CCSD(T) |
| Basis set | wCVTZ | wCVTZ | VTZ | VQZ | wCVQZ | AwCVQZ | VTZ(FC) |
| N1–C2  | 1.3899 | 1.3874 | 1.3911 | 1.3885 | 1.3853 | 1.3856 | 1.3946 |
| C2–C3  | 1.4956 | 1.4925 | 1.4966 | 1.4945 | 1.4906 | 1.4905 | 1.5037 |
| C3–C4  | 1.3369 | 1.3341 | 1.3388 | 1.3364 | 1.3327 | 1.3333 | 1.3411 |
| N1–C5  | 1.3899 | 1.3874 | 1.3911 | 1.3885 | 1.3853 | 1.3856 | 1.3946 |
| C2–O6  | 1.2093 | 1.2074 | 1.2108 | 1.2085 | 1.2059 | 1.2070 | 1.2088 |
| C5–O7  | 1.2093 | 1.2074 | 1.2108 | 1.2085 | 1.2059 | 1.2070 | 1.2088 |
| C3–H8  | 1.0774 | 1.0761 | 1.0774 | 1.0768 | 1.0753 | 1.0756 | 1.0790 |
| N1–H10 | 1.0059 | 1.0050 | 1.0064 | 1.0057 | 1.0047 | 1.0053 | 1.0061 |
| N1–C2–C3  | 105.25 | 105.27 | 105.26 | 105.34 | 105.35 | 105.41 | 105.24 |
| N1–C5–C4  | 105.25 | 105.27 | 105.26 | 105.34 | 105.35 | 105.41 | 105.24 |
| C2–C3–C4  | 108.83 | 108.83 | 108.82 | 108.78 | 108.79 | 108.77 | 108.81 |
| C2–N1–C5  | 111.83 | 111.80 | 111.84 | 111.75 | 111.71 | 111.64 | 111.89 |
| N1–C2–O6  | 126.48 | 126.48 | 126.47 | 126.41 | 126.42 | 126.37 | 126.45 |
| C3–C2–O6  | 128.27 | 128.25 | 128.27 | 128.25 | 128.23 | 128.23 | 128.31 |
| C2–N1–H10 | 124.08 | 124.10 | 124.08 | 124.12 | 124.15 | 124.18 | 124.05 |
| C4–C5–O7  | 128.27 | 128.25 | 128.27 | 128.25 | 128.23 | 128.23 | 128.31 |
| C4–C3–H8  | 129.07 | 129.07 | 129.07 | 129.13 | 129.12 | 122.06 | 129.26 |
| C5–C4–H9  | 122.10 | 122.10 | 122.11 | 122.09 | 122.09 | 122.06 | 121.93 |

a For atom numbering see Figure 1.