Supporting Information

for

Dienophilic reactivity of 2-phosphaindolizines: a conceptual DFT investigation

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Cartesian coordinates of the geometries optimized (Table S1) at the B3LYP/6-31+G (d) level of theory
SUPPORTING INFORMATION

TABLE 1 Cartesian coordinates of the optimized geometries

1,3-Butadiene

|   | x       | y       | z       |
|---|---------|---------|---------|
| 6 | -1.549183489 | -0.492897259 | 0.077638860 |
| 6 | -0.728115488  | 0.553030384  | -0.104873515 |
| 6 | 0.728127071   | 0.553033406  | 0.104877238  |
| 6 | 1.549180213   | -0.492906623 | -0.077640900 |
| 1 | 1.160286392   | 1.505783795  | 0.413862811  |
| 1 | -1.160281995  | 1.505775381  | -0.413867354 |
| 1 | 1.185701601   | -1.452197280 | -0.439297815 |
| 1 | 2.615414737   | -0.414374326 | 0.116296987  |
| 1 | -1.185756365  | -1.452201275 | 0.439315654  |
| 1 | -2.615414219  | -0.414345753 | -0.116320379 |

6Aa

|   | x       | y       | z       |
|---|---------|---------|---------|
| 6 | 1.135408817 | 1.461803535 | 0.000000000 |
| 6 | 2.377218971 | 0.901224866 | 0.000000000 |
| 6 | 2.523395259 | -0.520771783 | 0.000000000 |
| 6 | 1.406181714 | -1.313579209 | 0.000000000 |
| 6 | 0.099907209 | -0.743634664 | 0.000000000 |
| 7 | 0.000000000 | 0.668016140  | 0.000000000 |
| 6 | -1.155359429 | -1.339702113 | 0.000000000 |
|   |        |        |        |        |
|---|--------|--------|--------|--------|
| 15| -2.466398535| -0.168064527| 0.000000000|   |
| 6 | -1.296961626| 1.113899673| 0.000000000|   |
| 1 | 3.246988557| 1.549530126| 0.000000000|   |
| 1 | 3.515293349| -0.962149905| 0.000000000|   |
| 1 | 1.482677709| -2.396756290| 0.000000000|   |
| 1 | 0.955433005| 2.530693343| 0.000000000|   |
| 1 | -1.280110865| -2.416253477| 0.000000000|   |
| 1 | -1.463049218| 2.184349305| 0.000000000|   |

**6Ab**

|   |        |        |        |        |
|---|--------|--------|--------|--------|
| 6 | 0.000000000| 0.629868440| 0.000000000|   |
| 7 | -1.166205425| 1.421176507| 0.000000000|   |
| 6 | -1.105857665| 2.801698877| 0.000000000|   |
| 6 | 0.095514903| 3.445969712| 0.000000000|   |
| 6 | 1.300266824| 2.686565074| 0.000000000|   |
| 6 | 1.248412740| 1.314877689| 0.000000000|   |
| 6 | -2.330070146| 0.682508331| 0.000000000|   |
| 15| -2.080236624| -1.021034918| 0.000000000|   |
| 6 | -0.326235752| -0.738148662| 0.000000000|   |
| 6 | 0.590203673| -1.882877720| 0.000000000|   |
| 8 | 0.228561831| -3.048813000| 0.000000000|   |
| 1 | 0.115510139| 4.530593177| 0.000000000|   |
|   | x1   | y1   | z1   | x2   | y2   | z2   |
|---|------|------|------|------|------|------|
| 1 | 2.259333155 | 3.195733173 | 0.000000000 |
| 1 | 2.147555495  | 0.714152284  | 0.000000000 |
| 1 | -2.064035910  | 3.308078757  | 0.000000000 |
| 1 | -3.266243517  | 1.227637009  | 0.000000000 |
| 8 | 1.910340685  | -1.539225606 | 0.000000000 |
| 6 | 2.835553505  | -2.640908603 | 0.000000000 |
| 1 | 3.826683971  | -2.184776462 | 0.000000000 |
| 1 | 2.695117668  | -3.258569855 | 0.891038950 |
| 1 | 2.695117668  | -3.258569855 | -0.891038950 |

**6Ac**

|   | x1   | y1   | z1   | x2   | y2   | z2   |
|---|------|------|------|------|------|------|
| 6 | 1.085017173 | -1.547463964 | 0.000000000 |
| 7 | 0.000000000 | -0.646005700 | 0.000000000 |
| 6 | -1.296496114 | -1.134074486 | 0.000000000 |
| 6 | -1.542122529 | -2.478777584 | 0.000000000 |
| 6 | -0.471172698 | -3.412700502 | 0.000000000 |
| 6 | 0.816776210  | -2.941892837 | 0.000000000 |
| 6 | 0.424327996  | 0.684390037  | 0.000000000 |
| 6 | -0.418401421 | 1.881739459  | 0.000000000 |
| 8 | 0.041926357  | 3.012416728  | 0.000000000 |
| 6 | 2.318106994  | -0.891873833 | 0.000000000 |
| 15| 2.174097295  | 0.839368490  | 0.000000000 |
|    |        |            |            |            |
|----|--------|------------|------------|------------|
| 1  | -2.574020694 | -2.813990225 | 0.000000000 |
| 1  | -0.673751310  | -4.479331322 | 0.000000000 |
| 1  | 1.668397947   | -3.615215270 | 0.000000000 |
| 1  | -2.074132379  | -0.387904263 | 0.000000000 |
| 1  | 3.251170586   | -1.443441703 | 0.000000000 |
| 8  | -1.764047719  | 1.655472126  | 0.000000000 |
| 6  | -2.588375045  | 2.837592308  | 0.000000000 |
| 1  | -3.615472482  | 2.470340546  | 0.000000000 |
| 1  | -2.391321783  | 3.438156161  | 0.891432139 |
| 1  | -2.391321783  | 3.438156161  | -0.891432139 |

6Ad

|    |        |            |            |            |
|----|--------|------------|------------|------------|
| 6  | -1.042284052 | 0.066797303 | 0.000000000 |
| 7  | 0.000000000  | 1.014881894 | 0.000000000 |
| 6  | -0.285818671  | 2.367806363 | 0.000000000 |
| 6  | -1.577558132  | 2.814802502 | 0.000000000 |
| 6  | -2.650196907  | 1.890152817 | 0.000000000 |
| 6  | -2.379515314  | 0.543702910 | 0.000000000 |
| 6  | 1.268254405   | 0.416393395 | 0.000000000 |
| 6  | 2.571875028   | 1.094501675 | 0.000000000 |
| 8  | 3.625612936   | 0.480456694 | 0.000000000 |
| 6  | -0.543353638  | -1.254581778 | 0.000000000 |
|   | x   | y   | z   |   |
|---|-----|-----|-----|---|
| 6 | -1.306337810 | -2.512639509 | 0.000000000 |   |
| 8 | -0.788539216  | -3.617216513  | 0.000000000 |   |
| 15| 1.209376711   | -1.324847351  | 0.000000000 |   |
| 1 | -1.756471018  | 3.884765328   | 0.000000000 |   |
| 1 | -3.677352808  | 2.242407034   | 0.000000000 |   |
| 1 | -3.169474673  | -0.194055084  | 0.000000000 |   |
| 1 | 0.570319552   | 3.022006918   | 0.000000000 |   |
| 8 | -2.658006441  | -2.351373314  | 0.000000000 |   |
| 8 | 2.534117194   | 2.456102042   | 0.000000000 |   |
| 6 | 3.819746150   | 3.109754639   | 0.000000000 |   |
| 1 | 3.597227345   | 4.177395574   | 0.000000000 |   |
| 1 | 4.386394065   | 2.830931856   | 0.891616002 |   |
| 1 | 4.386394065   | 2.830931856   | -0.891616002|   |
| 6 | -3.426306840  | -3.569414873  | 0.000000000 |   |
| 1 | -4.469597540  | -3.250934631  | 0.000000000 |   |
| 1 | -3.202295363  | -4.161157854  | -0.891269385|   |
| 1 | -3.202295363  | -4.161157854  | 0.891269385 |   |

**6Ba**

|   | x   | y   | z   |   |
|---|-----|-----|-----|---|
| 7 | 0.000000000 | 0.691286879 | 0.000000000 |   |
| 6 | 1.155512695  | 1.447786127  | 0.000000000 |   |
| 6 | 2.375636821  | 0.836144959  | 0.000000000 |   |
| 6 | 2.462840575 | -0.587955601 | 0.000000000 |
|---|-------------|--------------|--------------|
| 6 | 1.321059601 | -1.347264114 | 0.000000000 |
| 6 | 0.037925359 | -0.727924772 | 0.000000000 |
| 7 | -1.140226341 | -1.322729568 | 0.000000000 |
| 15 | -2.395963181 | -0.191371566 | 0.000000000 |
| 6 | -1.299613481 | 1.146186581  | 0.000000000 |
| 1  | 3.271633717  | 1.446626319  | 0.000000000 |
| 1  | 3.438484732  | -1.064928081 | 0.000000000 |
| 1  | 1.344438858  | -2.431511811 | 0.000000000 |
| 1  | 1.017971188  | 2.522988083  | 0.000000000 |
| 1  | -1.471665769 | 2.215658733  | 0.000000000 |

**6Bb**

| 6 | -1.497640561 | -1.129655105 | 0.000000000 |
| 7 | -0.132539212 | -0.765602865 | 0.000000000 |
| 6 | 0.863680221  | -1.722256851 | 0.000000000 |
| 6 | 0.533601335  | -3.050536530 | 0.000000000 |
| 6 | -0.826800933 | -3.457753727 | 0.000000000 |
| 6 | -1.821740390 | -2.511113706 | 0.000000000 |
| 6 | 0.000000000  | 0.622458402  | 0.000000000 |
| 15 | -1.585403936 | 1.356905184  | 0.000000000 |
| 7 | -2.362711286 | -0.120733612 | 0.000000000 |
|   | 1.333594990 | -3.783268613 | 0.000000000 |
|---|-------------|-------------|-------------|
| 1 | -1.075380887 | -4.514980088 | 0.000000000 |
| 1 | -2.874901675 | -2.768878251 | 0.000000000 |
| 1 | 1.874172235  | -1.33858917  | 0.000000000 |
| 6 | 1.304389676  | 1.281080847  | 0.000000000 |
| 8 | 1.156754399  | 2.626992680  | 0.000000000 |
| 8 | 2.400154185  | 0.733974565  | 0.000000000 |
| 6 | 2.371183964  | 3.397285770  | 0.000000000 |
| 1 | 2.047921018  | 4.43844976   | 0.000000000 |
| 1 | 2.963549157  | 3.176762497  | 0.892148179 |
| 1 | 2.963549157  | 3.176762497  | -0.892148179 |

6Ca

|   | 0.0000000000 | -0.636390025 | 0.000000000 |
|---|-------------|-------------|-------------|
| 6 | 1.138916368 | -1.408876761 | 0.000000000 |
| 6 | 2.369691001 | -0.814436780 | 0.000000000 |
| 6 | 2.476972560 | 0.606258297  | 0.000000000 |
| 6 | 1.341259164 | 1.377201740  | 0.000000000 |
| 6 | 0.055984072 | 0.766476806  | 0.000000000 |
| 6 | -1.235995893 | 1.294766847  | 0.000000000 |
| 15| -2.398118281 | -0.004986169 | 0.000000000 |
| 7 | -1.219615311 | -1.196731623 | 0.000000000 |
|   | x            | y            | z            |
|---|--------------|--------------|--------------|
| 1 | 3.256289095  | -1.439122331 | 0.000000000  |
| 1 | 3.457451768  | 1.072917599  | 0.000000000  |
| 1 | 1.392975080  | 2.461451479  | 0.000000000  |
| 1 | 0.957780790  | -2.476234998 | 0.000000000  |
| 1 | -1.436378949 | 2.359291457  | 0.000000000  |

**6Cb**

|   | x            | y            | z            |
|---|--------------|--------------|--------------|
| 6 | -0.015280176 | -0.783462523 | 0.000000000  |
| 7 | -1.335439252 | -1.239140227 | 0.000000000  |
| 6 | -1.647939066 | -2.576792641 | 0.000000000  |
| 6 | -0.647787858 | -3.509888407 | 0.000000000  |
| 6 | 0.710411810  | -3.091140205 | 0.000000000  |
| 6 | 1.022740583  | -1.751698103 | 0.000000000  |
| 7 | -2.310312266 | -0.304820754 | 0.000000000  |
| 15| -1.652699248 | 1.223933398  | 0.000000000  |
| 6 | 0.000000000  | 0.625405846  | 0.000000000  |
| 1 | -0.908176836 | -4.562843339 | 0.000000000  |
| 1 | 1.502593422  | -3.833922555 | 0.000000000  |
| 1 | 2.043944992  | -1.390859646 | 0.000000000  |
| 1 | -2.709181723 | -2.790263330 | 0.000000000  |
| 6 | 1.232203031  | 1.417755535  | 0.000000000  |
| 8 | 0.965079848  | 2.748228389  | 0.000000000  |
|   |       |       |             |             |             |
|---|-------|-------|------------|------------|------------|
|   | 8     | 2.370974462 | 0.973241804 | 0.000000000 |
|   | 6     | 2.106563790 | 3.622266795 | 0.000000000 |
|   | 1     | 1.694553369 | 4.631885995 | 0.000000000 |
|   | 1     | 2.716554485 | 3.45414728  | 0.891802494 |
|   | 1     | 2.716554485 | 3.45414728  | -0.891802494 |

**6D**

|   |       |       |             |             |             |
|---|-------|-------|------------|------------|------------|
|   | 7     | 0.000000000 | 0.661506117 | 0.000000000 |
|   | 6     | 1.156920455 | 1.398832231 | 0.000000000 |
|   | 6     | 2.364722683 | 0.754050248 | 0.000000000 |
|   | 6     | 2.416004737 | -0.66755306  | 0.000000000 |
|   | 6     | 1.256496531 | -1.406184551 | 0.000000000 |
|   | 6     | -0.002099445 | -0.748734990 | 0.000000000 |
|   | 7     | -1.221362549 | -1.27566225  | 0.000000000 |
|   | 15    | -2.330449497 | -0.026297918 | 0.000000000 |
|   | 7     | -1.225330092 | 1.222037059  | 0.000000000 |
|   | 1     | 3.275681552 | 1.342433917  | 0.000000000 |
|   | 1     | 3.380007254 | -1.167729487 | 0.000000000 |
|   | 1     | 1.257335759 | -2.490477079 | 0.000000000 |
|   | 1     | 1.018296648 | 2.472629163  | 0.000000000 |