**Theoretical study on the mechanism of stable phosphorus ylides derived from 2-aminothiophenol in the presence of different dialkyl acetyelenedicarboxylates**

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**Supplemental Materials**

**Figure S 1:** Potential energy diagram (including zero point energy) along the different reaction pathways (**I** and **II**) in the presence of DEAD. Relative energies are in kJ/mol.



**Figure S 2:** Optimized geometries of all structures (including transition states, intermediates and products) along the reaction paths **I** and **II** in the presence of DEAD.

**Figure S 3:** Potential energy diagram (kJ/mol) (including zero point energy) for ( and ) conversion.

**Figure S 4:** Potential energy diagram (including zero point energy) along the different reaction pathways (**I** and **II**) for the first step of reaction in the presence of DTAD.



**Figure S 5:** Optimized geometries of all structures participate in the first step of the reaction (including transition states and intermediates) along the reaction paths (**I** and **II**)in the presence of DTAD.

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| **Table S 1:** Natural charges from NBO analysis at B3LYP/6-311++G(d,p) level of theory |
| **1** | **2a** | **2b** | **2c** | **Ts1-M-I** | **Ts1-M-II** | **Ts1-E-I** | **Ts1-E-II** |
| **atom** | **charge** | **atom** | **charge** | **atom** | **charge** | **atom** | **charge** | **atom** | **charge** | **atom** | **charge** | **atom** | **charge** | **atom** | **charge** |
| P11 | 0.085 | C1 | -0.205 | C1 | -0.025 | C1 | 0.291 | P11 | 1.057 | P11 | 1.271 | P11 | 1.051 | P11 | 0.909 |
| C12 | -0.329 | O2 | -0.526 | O2 | -0.542 | O2 | -0.567 | O2 | -0.556 | O2 | -0.554 | O2 | -0.568 | O2 | -0.57 |
| C23 | -0.329 | C3 | 0.733 | C3 | 0.734 | C3 | 0.738 | C3 | 0.68 | C3 | 0.688 | C3 | 0.683 | C3 | 0.679 |
| C34 | -0.329 | O4 | -0.549 | O4 | -0.553 | O4 | -0.567 | O4 | -0.629 | O4 | -0.634 | O4 | -0.635 | O4 | -0.644 |
|  |  | C5 | -0.036 | C5 | -0.021 | C5 | -0.022 | C5 | -0.344 | C5 | -0.074 | C5 | -0.328 | C5 | -0.397 |
|  |  | C6 | -0.008 | C6 | -0.021 | C6 | -0.022 | C6 | 0.524 | C6 | -0.307 | C6 | 0.514 | C6 | 0.512 |
|  |  | C7 | 0.731 | C7 | 0.734 | C7 | 0.738 | C7 | 0.477 | C7 | 0.764 | C7 | 0.471 | C7 | 0.571 |
|  |  | O8 | -0.549 | O8 | -0.542 | O8 | -0.567 | O8 | -0.632 | O8 | -0.568 | O8 | -0.635 | O8 | -0.58 |
|  |  | O9 | -0.527 | O9 | -0.553 | O9 | -0.567 | O9 | -0.532 | O9 | -0.563 | O9 | -0.546 | O9 | -0.601 |
|  |  |  |  |  |  |  |  | **CT** | -0.316 | **CT** | -0.549 | **CT** | -0.316 | **CT** | -0.298 |
| **Ts1-T-I** | **Ts1-T-II** | **I1-M-I** | **I1-M-II** | **I1-E-I** | **I1-E-II** | **I1-T-I** | **I1-T-II** |
| **atom** | **charge** | **atom** | **charge** | **atom** | **charge** | **atom** | **charge** | **atom** | **charge** | **atom** | **charge** | **atom** | **charge** | **atom** | **charge** |
| P11 | 1.17 | P11 | 1.295 | P11 | 1.493 | P11 | 1.5 | P11 | 1.49 | P11 | 1.505 | P11 | 0.915 | P11 | 0.929 |
| O2 | -0.595 | O2 | -0.592 | O2 | -0.571 | O2 | -0.571 | O2 | -0.583 | O2 | -0.583 | O2 | -0.613 | O2 | -0.614 |
| C3 | 0.654 | C3 | 0.693 | C3 | 0.664 | C3 | 0.662 | C3 | 0.667 | C3 | 0.667 | C3 | 0.655 | C3 | 0.64 |
| O4 | -0.644 | O4 | -0.658 | O4 | -0.665 | O4 | -0.667 | O4 | -0.667 | O4 | -0.673 | O4 | -0.684 | O4 | -0.693 |
| C5 | -0.653 | C5 | -0.099 | C5 | -0.084 | C5 | -0.077 | C5 | -0.085 | C5 | -0.092 | C5 | -0.293 | C5 | -0.399 |
| C6 | 0.269 | C6 | -0.315 | C6 | -0.512 | C6 | -0.535 | C6 | -0.509 | C6 | -0.537 | C6 | 0.368 | C6 | 0.335 |
| C7 | 0.457 | C7 | 0.783 |  |  |  |  |  |  |  |  |  |  |  |  |
| O8 | -0.659 | O8 | -0.583 |  |  |  |  |  |  |  |  |  |  |  |  |
| O9 | -0.578 | O9 | -0.601 |  |  |  |  |  |  |  |  |  |  |  |  |