



## Supporting Information

for

### **Dienophilic reactivity of 2-phosphaindolizines: a conceptual DFT investigation**

Nosheen Beig, Aarti Peswani and Raj Kumar Bansal

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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**

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**

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

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**

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

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

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	1.333594990	-3.783268613	0.000000000
1	-1.075380887	-4.514980088	0.000000000
1	-2.874901675	-2.768878251	0.000000000
1	1.874172235	-1.338858917	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	4.438445976	0.000000000
1	2.963549157	3.176762497	0.892148179
1	2.963549157	3.176762497	-0.892148179

**6Ca**

7	0.000000000	-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



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**

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	3.454144728	0.891802494
1	2.716554485	3.454144728	-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	-0.667555306	0.000000000
6	1.256496531	-1.406184551	0.000000000
6	-0.002099445	-0.748734990	0.000000000
7	-1.221362549	-1.275662252	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