**Supporting Information File 1**

**Table S1**. Total energies (E), zero-point vibrational energies (ZPVE) and thermal corrections for Gibbs energies (TCGE) calculated for compounds **1-15**.a

|  |  |  |  |
| --- | --- | --- | --- |
| Compound | E (a.u) | ZPVE (a. u.) | TCGE (a.u.) |
| **1** (S0) | -609.9060587 | 0.176762 | 0.141739 |
| **1** (S1) | -609.8996567 |  |  |
| **2** | -611.0968762 | 0.199189 | 0.163241 |
| **3** | -611.0866456 | 0.199260 | 0.163686 |
| **4** | -612.3055856 | 0.222345 | 0.186106 |
| **5** | -611.090726 | 0.199031 | 0.163115 |
| **6** | -611.0904228 | 0.199084 | 0.163161 |
| **7** | -612.3213374 | 0.222925 | 0.186554 |
| **8** | -379.9757466 | 0.117380 | 0.087238 |
| **9** | -381.1757085 | 0.140157 | 0.109153 |
| **10** | -381.169404 | 0.139909 | 0.109333 |
| **11** | -382.3796935 | 0.163231 | 0.131183 |
| **12** | -233.5049978 | 0.121901 | 0.094336 |
| **13** | -234.7365585 | 0.145754 | 0.117773 |
| **14** | -232.330161 | 0.100194 | 0.075076 |

a Values computed at the B3LYP-D3BJ/6.311++G(d,p)%DefTZVPP(Ba) level.

**Table S2**. Total energies (E), zero-point vibrational energies (ZPVE) and thermal corrections for Gibbs energies (TCGE) calculated for compounds **15a-d, 16a-d, 17a-d**, **19** and **·Ba(ClO4)2**.a

|  |  |  |  |
| --- | --- | --- | --- |
| Compound | E (a.u) | ZPVE (a. u.) | TCGE (a.u.) |
| **15a** | -640.6658645 | 0.248434 | 0.208982 |
| **15b** | -794.6007494 | 0.309634 | 0.264037 |
| **15c** | -948.533772 | 0.371660 | 0.320205 |
| **15d** | -1102.443735 | 0.433721 | 0.378415 |
| **16a** | -615.5355929 | 0.245247 | 0.207758 |
| **16b** | -769.4247609 | 0.306950 | 0.262335 |
| **16c** | -923.3163967 | 0.368607 | 0.320017 |
| **16d** | -1077.208118 | 0.429505 | 0.373651 |
| **17a** | -873.050199 | 0.349293 | 0.295361 |
| **17b** | -1026.9762566 | 0.410893 | 0.353034 |
| **17c** | -1180.8999491 | 0.472725 | 0.411279 |
| **17d** | -1334.7818278 | 0.534993 | 0.470533 |
| **19** (S0) | -1971.2608099 | 0.661267 | 0.584192 |
| **19** (S1) | -1971.1557349 |  |  |
| **19·Ba(ClO4)2** (S0) | -3518.7683558 | 0.686340 | 0.591384 |
| **19·Ba(ClO4)2** (S1) | -3518.6550761 |  |  |

a Values computed at the B3LYP-D3BJ/6.311++G(d,p)%DefTZVPP(Ba) level.

**Table S3**. Total energies calculated for compounds **19** and **19·Ba(ClO4)2** at S0 and S1 states with different functionals.a

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Functional |  | S0 | | | | | | S1 | | | |
| **19** | | **Ba(ClO4)2** |  | **19** | | | | **Ba(ClO4)2** | |
| BHandH | -1957.14463621 | | -3498.81290051 | | |  | -1956.9999427 | | | -3498.6296551 | |
| BHandHLYP | -1969.94831606 | | -3516.90526237 | | |  | -1969.8128635 | | | -3516.7529069 | |
| B3LYP | -1971.2608099 | | -3518.76835587 | | |  | -1971.1557349 | | | -3518.6550761 | |
| CAM-B3LYP | -1970.15492224 | | -3517.34937615 | | |  | -1970.0276974 | | | -3517.2112303 | |
| M06 | -1969.78065911 | | -3516.87448682 | | |  | -1969.6462543 | | | -3516.7563090 | |
| M06-L | -1970.84848954 | | -3518.23281981 | | |  | -1969.6714904 | | | -3518.1215546 | |
| M06-2X | -1970.33142837 | | -3517.42930374 | | |  | -1970.2099690 | | | -3517.2858321 | |
| PBE | -1968.84831481 | | -3515.32524575 | | |  | -1968.7408013 | | | -3515.1955066 | |
| wB97XD | -1970.47373002 | | -3517.74326079 | | |  | -1970.3499872 | | | -3517.6037878 | |

a Values computed with the 6.311++G(d,p)&DefTZVPP(Ba) basis set.