Electronic Supplementary Material (ESI) for RSC Advances


# Computational Design and Selection of Optimal building blocks and linking topologies for construction of high-performance host materials

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## Supporting Information

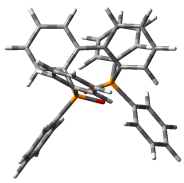
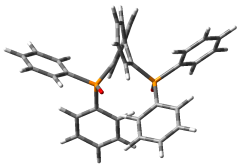
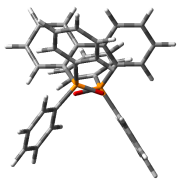
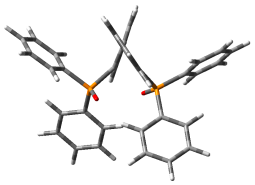
| | $T_1$ | | Cationic | |
|---|---|---|---|---|
| | Front view | Side view | Front view | Side view |
| o-PBP |  |  |  |  |

**Fig. S1.** Optimized geometries of of *o*-PBP in the lowest triplet ($T_1$) and cationic states using B3LYP/6-31G(d). They are found tortile probably due to the strong interaction of the two oxygen atoms in diphenyl phosphine oxide. The optimized geometry of *o*-PBP in $T_1$ state using HF/6-31G(d) seems the most reasonable after further trials using other DFT and ab initio methods (*e.g.* BLYP, BP86, B3P86, BPW91, B3PW91, X3LYP, HF and MP2).