

**Electronic Supplementary Information:**  
**Perturbative triples correction to Domain-based Local  
Pair Natural Orbital variant of Mukherjee's state specific  
coupled cluster method**

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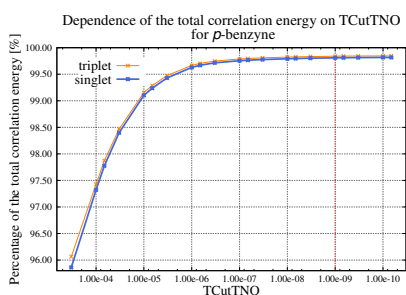
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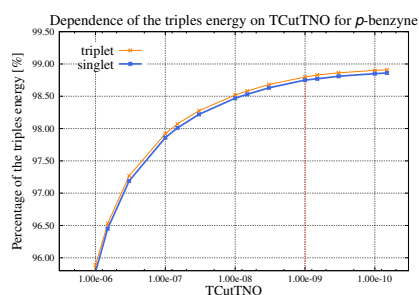
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# 1 Dependence of the total correlation energy and triples energy on different cut-offs for *p*-benzyne

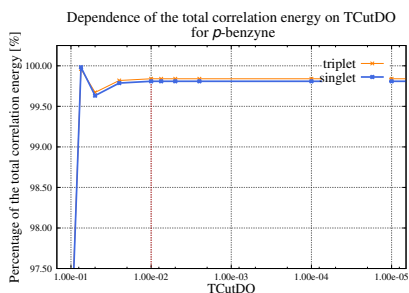


(a)

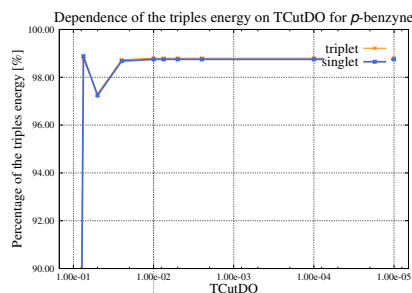


(b)

Figure S1: Percentage of the (a) total correlation and (b) triples energy recovered for *p*-benzyne by DLPNO-MkCCSD(T) as a function of *TCutTNO*. Red dashed line corresponds to default cut-off.

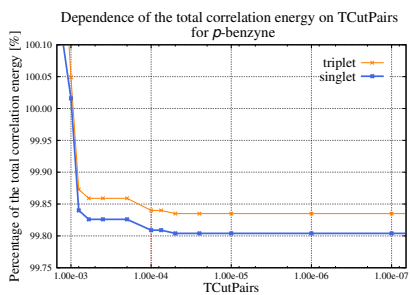


(a)

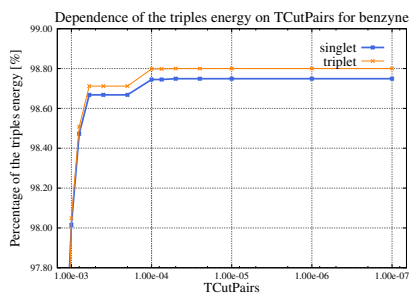


(b)

Figure S2: Percentage of the (a) total correlation and (b) triples energy recovered for *p*-benzyne by DLPNO-MkCCSD(T) as a function of *TCutDO*. Red dashed line corresponds to default cut-off.



(a)



(b)

Figure S3: Percentage of the (a) total correlation and (b) triples energy recovered for *p*-benzyne by DLPNO-MkCCSD(T) as a function of *TCutPairs*. Red dashed line corresponds to default cut-off.