Electronic Supplementary Information

A companion perturbation theory for state-specific multireference coupled cluster methods

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Content: Cartesian geometries of *m*-benzyne.

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Cartesian geometries of *m*-benzyne (bohr)

Singlet *m*-benzyne CASSCF(2,2)-Mk-MRPT2/cc-pVTZ (delocalized orbitals)

```
C   0.0000000000   0.0000000000   3.1195985811
C  -1.7693072723   0.0000000000   1.2715194943
C   1.7693072723   0.0000000000   1.2715194943
C  -2.1923862589   0.0000000000  -1.2867045880
C   2.1923862589   0.0000000000  -1.2867045880
C   0.0000000000   0.0000000000  -2.7706573707
H   0.0000000000   0.0000000000   5.1561026409
H  -4.0791288681   0.0000000000  -2.0643719130
H   4.0791288681   0.0000000000  -2.0643719130
H   0.0000000000   0.0000000000  -4.8205294077
```

Singlet *m*-benzyne CASSCF(2,2)-Mk-MRPT2/cc-pVTZ (pseudo second-order energy, see Summary for details)

```
C   0.0000000000    0.0000000000    3.0470373022
C  -1.8865017420    0.0000000000    1.2931693564
C   1.8865017420    0.0000000000    1.2931693564
C  -2.2046008719    0.0000000000   -1.2810831066
C   2.2046008719    0.0000000000   -1.2810831066
C   0.0000000000    0.0000000000   -2.7420677640
H   0.0000000000    0.0000000000    5.0812378793
H  -4.0730622789    0.0000000000   -2.1042204534
H   4.0730622789    0.0000000000   -2.1042204534
H   0.0000000000    0.0000000000   -4.7918348289
```

Singlet *m*-benzyne RHF-CCSD/cc-pVTZ

```
C   0.0000000000    0.0000000000    3.2821665466
C  -1.4773325610    0.0000000000    1.2058898704
C   1.4773325610    0.0000000000    1.2058898704
C  -2.2053008006    0.0000000000   -1.3021161025
C   2.2053008006    0.0000000000   -1.3021161025
C   0.0000000000    0.0000000000   -2.7947461161
H   0.0000000000    0.0000000000    5.3224020033
H  -4.1188181607    0.0000000000   -1.9958824107
H   4.1188181607    0.0000000000   -1.9958824107
H   0.0000000000    0.0000000000   -4.8427702250
```

Singlet *m*-benzyne RHF-CCSD(T)/cc-pVTZ

```
C    0.0000000000   0.0000000000   3.0206193239
C   -1.9446035084   0.0000000000   1.3066182076
C    1.9446035084   0.0000000000   1.3066182076
C   -2.2211840167   0.0000000000  -1.2835648143
C    2.2211840167   0.0000000000  -1.2835648143
C    0.0000000000   0.0000000000  -2.7315373917
H    0.0000000000   0.0000000000   5.0567659303
H   -4.0817850222   0.0000000000  -2.1318138780
H    4.0817850222   0.0000000000  -2.1318138780
H    0.0000000000   0.0000000000  -4.7841728240
```

Triplet *m*-benzyne ROHF-CCSD(T)/cc-pVTZ

```
C    0.0000000000   0.0000000000   2.7546494324
C   -2.2120212435   0.0000000000   1.3495051972
C    2.2120212435   0.0000000000   1.3495051972
C   -2.3174985136   0.0000000000  -1.2625570232
C    2.3174985136   0.0000000000  -1.2625570232
C    0.0000000000   0.0000000000  -2.5608968797
H    0.0000000000   0.0000000000   4.8020415863
H   -4.0876536255   0.0000000000  -2.2850633597
H    4.0876536255   0.0000000000  -2.2850633597
H    0.0000000000   0.0000000000  -4.6094473435
```