**Deposition Material**

**1) Table 2, extended by the quantities T, V and H**
**2) Multipole population coefficients**

The characteristics at the (3,-1) bond critical points and at the (3,+1) ring critical points. 1. line: experimental, 2. line: from B3LYP calculation.

| bond | lengths [Å] | $d_1$ [Å]*) | $\rho(\mathbf{r})$ [e/Å$^3$] | $-\nabla^2\rho(\mathbf{r})$ [$e$/Å$^5$] | T [a.u.] | V [a.u.] | H [a.u.] | $\epsilon$ |
|---|---|---|---|---|---|---|---|---|
| C(1)–F(1) | 1.306(1) | 0.478 | 2.22(4) | -27.6(3) | 0.259 | -0.805 | -0.546 | 0.40 |
| B3LYP | 1.312 | 0.440 | 2.01 | -2.7 | 0.363 | -0.753 | -0.391 | 0.17 |
| C(1)–F(2) | 1.310(1) | 0.484 | 2.21(5) | -27.3(3) | 0.258 | -0.799 | -0.541 | 0.40 |
| B3LYP | 1.311 | 0.440 | 2.01 | -2.8 | 0.362 | -0.753 | -0.391 | 0.17 |
| C(6)–F(7) | 1.310(1) | 0.484 | 2.21(5) | -27.3(3) | 0.258 | -0.799 | -0.541 | 0.40 |
| B3LYP | 1.311 | 0.440 | 2.01 | -2.8 | 0.362 | -0.753 | -0.391 | 0.17 |
| C(6)–F(8) | 1.304(1) | 0.476 | 2.23(4) | -27.6(3) | 0.263 | -0.816 | -0.549 | 0.40 |
| B3LYP | 1.312 | 0.440 | 2.01 | -2.7 | 0.363 | -0.753 | -0.391 | 0.17 |
| C(3)–F(3) | 1.347(1) | 0.546 | 2.11(5) | -20.9(2) | 0.269 | -0.755 | -0.486 | 0.09 |
| B3LYP | 1.347 | 0.457 | 1.87 | -7.1 | 0.289 | -0.652 | -0.363 | 0.15 |
| C(3)–F(4) | 1.344(1) | 0.543 | 2.11(4) | -21.2(2) | 0.267 | -0.754 | -0.487 | 0.06 |
| B3LYP | 1.347 | 0.457 | 1.87 | -7.1 | 0.289 | -0.652 | -0.363 | 0.15 |
| C(4)–F(5) | 1.345(1) | 0.544 | 2.11(4) | -21.1(2) | 0.268 | -0.754 | -0.487 | 0.09 |
| B3LYP | 1.347 | 0.457 | 1.87 | -7.1 | 0.289 | -0.652 | -0.363 | 0.15 |
| C(4)–F(6) | 1.345(1) | 0.543 | 2.11(5) | -21.0(2) | 0.268 | -0.755 | -0.486 | 0.06 |
| B3LYP | 1.347 | 0.457 | 1.87 | -7.1 | 0.289 | -0.652 | -0.363 | 0.15 |
| C(1)–C(2) | 1.325(1) | 0.738 | 2.40(4) | -26.7(2) | 0.328 | -0.933 | -0.605 | 0.51 |
| B3LYP | 1.326 | 0.734 | 2.39 | -26.9 | 0.323 | -0.925 | -0.602 | 0.51 |
| C(5)–C(6) | 1.323(1) | 0.586 | 2.41(4) | -27.0(2) | 0.329 | -0.939 | -0.610 | 0.51 |
| B3LYP | 1.326 | 0.592 | 2.39 | -26.9 | 0.323 | -0.925 | -0.602 | 0.51 |
| C(2)–C(5) | 1.458(1) | 0.730 | 1.85(2) | -15.79(9) | 0.223 | -0.610 | -0.387 | 0.34 |
| B3LYP | 1.461 | 0.731 | 1.83 | -16.4 | 0.213 | -0.596 | -0.383 | 0.14 |
| C(2)–C(3) | 1.509(1) | 0.741 | 1.63(3) | -13.8(1) | 0.175 | -0.490 | -0.317 | 0.24 |
| B3LYP | 1.515 | 0.746 | 1.76 | -15.4 | 0.199 | -0.558 | -0.359 | 0.03 |
| C(4)–C(5) | 1.508(1) | 0.771 | 1.64(3) | -13.9(1) | 0.176 | -0.495 | -0.320 | 0.24 |
| B3LYP | 1.515 | 0.771 | 1.76 | -15.4 | 0.199 | -0.558 | -0.359 | 0.03 |
| C(3)–C(4) | 1.574(1) | 0.788 | 1.65(2) | -13.06(7) | 0.185 | -0.504 | -0.319 | 0.13 |
| B3LYP | 1.580 | 0.791 | 1.66 | -13.8 | 0.182 | -0.507 | -0.325 | 0.05 |
| ring 1$^{xx)}$ | | | 0.41(1) | 10.8(3) | | | | |
| B3LYP | | | 0.59 | 9.4 | | | | |
| ring 2$^{xx)}$ | | | 0.02(1) | 0.40(1) | | | | |
| B3LYP | | | 0.03 | 0.6 | | | | |

*) $d_1$ is the distance from the bcp to the first atom given in the first column.

$^{xx)}$ ring 1 is the cyclobutane ring, ring 2 is the non closed ring region F(1)-C(1)-C(2)-C(5)-C(6)-F(8).