# Supramolecular assemblies of dimolybdenum transoids built by the $Mo_2$-enhanced perfluorophenyl-perfluorophenyl synthons

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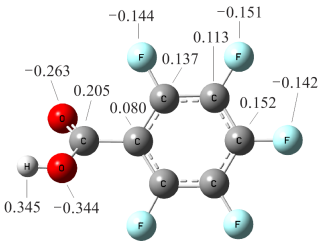
## Supporting information

**Table S1**. Selective bond lengths [Å], angles [°]

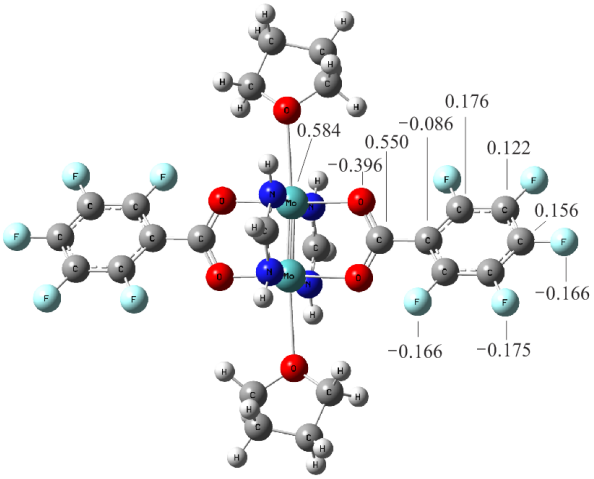
| | | |
|---|---|---|
| Mo(1)-Mo(1A) | 2.0895(4) | 2.1176(5) |
| Mo(1)-O(1) | 2.126(2) | 2.119(3) |
| Mo(1)-O(2) | | 2.117(3) |
| Mo(1)-O(2A) | 2.113 (2) | |
| Mo(1)-N(1) | 2.143(2) | 2.143(3) |
| Mo(1)-N(2) | 2.127(2) | 2.150(3) |
| | | |
| O(1)-Mo(1)-O(2) | | 176.83(9) |
| O(1)-Mo(1)-O(2A) | 176.03(7) | |
| O(1)-Mo(1)-N(1) | 92.76(7) | 90.88(11) |
| O(1)-Mo(1)-N(2) | 88.70(7) | 89.14(11) |
| Mo(1)A-Mo(1)-O(1) | 91.34(5) | 91.81(7) |
| Mo(1)A-Mo(1)-O(2) | | 91.31(7) |
| Mo(1)A-Mo(1)-O(2A) | 92.61(5) | |
| Mo(1)A-Mo(1)-N(1) | 92.79(6) | 91.84(7) |
| Mo(1)A-Mo(1)-N(2) | 92.66(6) | 93.03(7) |
| O(1)-C(7)-C(1)-C(6) | 43.977(3) | 28.093(5) |
| O(2) -C(7)-C(1)-C(6) | 44.300(3) | |
| O(2)A-C(7)-C(1)-C(6) | | 26.275(5) |

Calculated Mulliken charge distribution over a perfluorophenyl group for:

1. Pentafluorobenzoic acid




2. Model compound, *trans*-$Mo_2(NHCHNH)_2(O_2CC_6F_5)_2(THF)_{2ax}$




3.Model compound, *trans*-$Mo_2(NHCHNH)_2(O_2CC_6F_5)_2$