

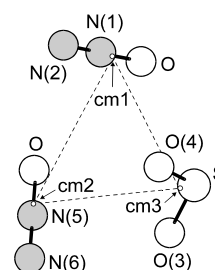
| | | | |
|------------|------------------------------------|---|---|
| 314 | N₄O₄S | Sulfur dioxide – dinitrogen monoxide (1/2) | C₁ |
| MW | | (weakly bound complex) | (large-amplitude motion) SO ₂ · 2N ₂ O |

| $r_0^a)$ | Å | $\theta_0^a)$ | deg |
|-----------|------------|------------------------------------|-------------|
| cm1...cm2 | 3.8558(23) | cm3...cm1...cm2 | 52.494(26) |
| cm1...cm3 | 3.5316(13) | N(1)–cm1...cm2 | 83.330(85) |
| | | N(5)–cm2...cm3 | 97.672(95) |
| | | S–cm3...cm1 | 90.75(14) |
| | | N(1)–cm1...cm2...cm3 ^{b)} | –129.99(10) |
| | | N(5)–cm2...cm3...cm1 ^{b)} | –151.19(21) |
| | | S–cm3...cm1...cm2 ^{b)} | 163.83(84) |
| | | O(3)–S–cm3...cm1 ^{b)} | –118.66(36) |

The configuration aligns the centers of mass of the three monomers in an approximate equilateral triangle. The monomers twist relative to this plane so that the two N₂O molecules are intermediate between T-shaped and crossed rather than the usual slipped-parallel planar. The SO₂ is oriented so that its oxygen atoms are straddling one N₂O, while its S atom is closest to the oxygen end of the other N₂O.

^{a)} cm1, cm2 and cm3 denote the centers of mass of N(2)=N(1)=O, N(6)=N(5)=O and O(3)=S=O(4), respectively.

^{b)} Dihedral angle.



Peebles, R.A., Kuczkowski, R.L.: J. Chem. Phys. **112** (2000) 8839.