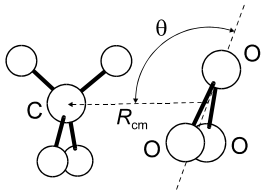
133 **CH_4O_3** **Methane – ozone (1/1)** **C_s**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)
$CH_4 \cdot O_3$

r_0	Å [a])	θ_0	deg
R [b])	3.57(2)	θ [c])	118.2(5)



An *a*-type pure-rotational and a *c*-type rotation-inversion electric-dipole spectrum is observed; the spectrum is complicated by the nearly free internal rotation of the CH_4 top and the inversion tunneling of the O_3. The transition state has a heavy-atom, C_{2v}-symmetry geometry. The tunneling splitting is determined to be 30 to 40 MHz, depending on the CH_4 internal-rotor state. Only two of the three methane internal-rotor states have been assigned. These two states of A and F symmetry have asymmetric-rotor energy-level structures, weakly perturbed by the ozone-inversion tunneling. The zero-point structure of the complex has a heavy-atom plane of symmetry with the two terminal O atoms equidistant above and below this plane.

[a]) Uncertainty was not estimated in the original paper.
[b]) The shortest O...C separation.
[c]) See figure for the definition.

Walker, A.R.H., Fraser, G.T., Suenram, R.D., Lovas, F.J.: J. Chem. Phys. **113** (2000) 2139.