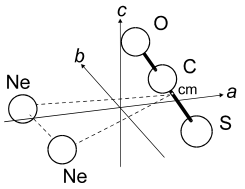
**158** **$CNe_2OS$** **Carbonyl sulfide – neon (1/2)** **$C_s$**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)
O=C=S · 2Ne

| $r_0$ | Å [a]) |
|---|---|
| $R_{cm}$ | 3.106(5) |
| Ne...Ne | 3.303(5) |
| Ne...C | 3.378(5) |

| $\theta_0$ | deg [a]) |
|---|---|
| Ne...C=O | 78.8(5) |
| $\varphi$ [b]) | 112.3(5) |




Force constants and wavenumbers for the intermolecular vibrational modes are derived as follows: $F_{55} = 0.6003$ N m$^{-1}$, $F_{66} = 0.832$ N m$^{-1}$, $F_{77} = 0.584\times10^{-20}$ N m, $F_{88} = 0.1866$ N m$^{-1}$, $F_{99} = 0.4931\times10^{-20}$ N m; $\nu_5 = 30.4$ cm$^{-1}$, $\nu_6 = 29.0$ cm$^{-1}$, $\nu_7 = 22.0$ cm$^{-1}$, $\nu_8 = 15.7$ cm$^{-1}$, $\nu_9 = 13.2$ cm$^{-1}$.

[a]) Uncertainties were not estimated in the original paper.
[b]) Angle between OCS and the plane made by the two Ne atoms and the center of mass of OCS, see figure.

Xu, Y., Jäger, W.: Phys. Chem. Chem. Phys. **2** (2000) 3549.