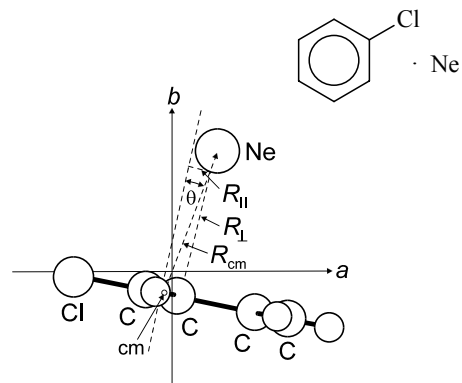


708
MW $\text{C}_6\text{H}_5\text{ClNe}$ **Chlorobenzene – neon (1/1)**
(weakly bound complex) C_s
(effective symmetry class)
(large-amplitude motion)

| r_0 | $\text{\AA}^{\text{a)}}$ | θ_0 | $\text{deg}^{\text{a)}}$ |
|---------------------------------------|--------------------------|----------------------|--------------------------|
| R_{cm} | 3.446(5) | $\theta^{\text{b)}}$ | 12.7(5) |
| R_{\parallel} | 0.755(3) | | |
| R_{\perp} | 3.362(3) | | |
| $\text{C}\cdots\text{Ne}^{\text{c)}}$ | 3.569(5) | | |

| Atom | $ a_s [\text{\AA}]$ | $ b_s [\text{\AA}]$ |
|------|----------------------|----------------------|
| Cl | 2.312 | 0.0 |
| Ne | 1.231 | 2.635 |

The structure has the usual stacked configuration with the neon above the aromatic ring. The neon is shifted from above the nominal ring center towards the substituted carbon atom.



^{a)} Uncertainties were not estimated in the original paper.

^{b)} See figure for the definition.

^{c)} Distance between Ne and the substituted carbon atom.

Oh, J.J., Park, I., Peebles, S.A., Kuczkowski, R.L.: J. Mol. Struct. **599** (2001) 15.