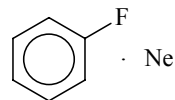
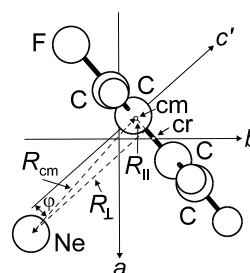


711
MW $\text{C}_6\text{H}_5\text{FNe}$ **Fluorobenzene – neon (1/1)**
(weakly bound complex) C_s
(effective symmetry class)
(large-amplitude motion)

r_0	\AA	θ_0	deg
R_{cm}	3.448(7)	φ^a	6.6(2)
R_{\perp}^b	3.422(1)		
R_{\parallel}^c	-0.39(1)		



Atom	a_0 [\AA]	b_0 [\AA]	c_0 [\AA]
F(1)	-2.087	-1.079	0.0
H(2)	-0.986	-0.091	-2.158
H(3)	0.849	1.554	-2.151
H(4)	1.778	2.387	0.0
H(5)	0.849	1.554	2.151
H(6)	-0.986	-0.091	2.158
C(1)	-1.079	-0.175	0.0
C(2)	-0.589	0.265	-1.218
C(3)	0.451	1.197	-1.209
C(4)	0.974	1.666	0.0
C(5)	0.451	1.197	1.209
C(6)	-0.589	0.265	1.218
cm ^d	-0.444	0.394	0.0
cr ^e	-0.053	0.745	0.0
Ne	2.136	-1.893	0.0



The neon atom sits nearly above the center of the fluorobenzene, shifted 0.13(1) \AA from the center of the ring toward the fluorinated carbon atom.

^a) See figure for the definition (c' is the principal axis of fluorobenzene).

^b) Distance between Ne and the ring plane.

^c) Minus sign indicates a shift from the center of mass of fluorobenzene toward the ring center.

^d) Center of mass of the fluorobenzene monomer.

^e) Center of the ring of the fluorobenzene monomer.

Wilson, R.J., Peebles, S.A., Antolínez, S., Sanz, M.E., Kuczkowski, R.L.: J. Phys. Chem. A **102** (1998) 10630.