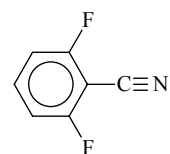
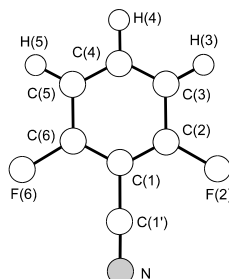


773  
MW $C_7H_3F_2N$ 

2,6-Difluorobenzonitrile

 $C_{2v}$ 

Atom	$a_0$ [ $\text{\AA}$ ] <sup>a)</sup>	$b_0$ [ $\text{\AA}$ ] <sup>a)</sup>
C(1)	-1.3883	0.0
C(2,6)	-0.6788	$\pm 1.1749$
C(3,5)	0.6987	$\pm 1.2102$
C(4)	1.3974	0.0
C(1')	-2.8434	0.0
F(2,6)	-1.3558	$\pm 2.3475$
H(3,5)	1.2407	$\pm 2.1490$
H(4)	2.4814	0.0
N	-4.0025	0.0



<sup>a)</sup> Estimated by referring to the data on related molecules and adjusted so as to reproduce the observed rotational constants. These coordinates lead to the following structural parameters: C(1)–C(2,6) = 1.3726, C(2,6)–C(3,5) = 1.3780, C(3,5)–C(4) = 1.3974, C(2)–C(1)–C(6) = 117.8, C(1)–C(2,6)–C(3,5) = 122.6, C(2,6)–C(3,5)–C(4) = 118.5, in  $\text{\AA}$  and degrees for bond lengths and angles, respectively.

Sharma, S.D., Doraiswamy, S.: J. Mol. Spectrosc. **180** (1996) 7.