

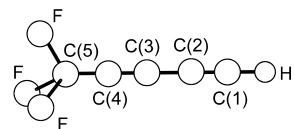
619  
MW

 $\text{C}_5\text{HF}_3$ 

5,5,5-Trifluoro-1,3-pentadiyne

 $\text{C}_{3v}$   
 $\text{F}_3\text{C}-\text{C}\equiv\text{C}-\text{C}\equiv\text{CH}$ 

$r_s$	$\text{\AA}$	$\theta_s$	deg
C(1)–H	1.0563(8)	F–C(5)–F	107.20(8)
C(1)≡C(2)	1.2075(6)		
C(2)–C(3)	1.3689(11)		
C(3)≡C(4)	1.2153(56)		
C(4)–C(5)	1.4455(57)		
C(5)–F	1.3413(21)		


 Kang, L., Novick, S.E.: J. Phys. Chem. A **106** (2002) 3749.