

CH (benzene) parameters

	r6	E ele	exp						
	1.20654	11.27671	11.2603						
	Exp		r sp3	E sp3					
C3+	64.4939	10	0.919153831	14.802532					
C2+	47.8878			14.61166867					
C+	24.38332			r3					
C	11.2603			0.84317					
total	148.02532								
			Emag (a0)	Emag (r3)					
			0.114411043	0.19086					
	Theory		r sp3	E sp3					
C3+	64.3921	10	0.91771	14.82575					
C2+	48.3125			14.63489					
C+	24.2762								
C	11.27671								
total	148.25751								
	Theory		r sp3	E sp3					
C3+	64.3921	9.5	0.85252	15.95955					
C2+	48.3125			15.76868					
C+	24.2762								
C	14.63488977								
total	151.6156898								