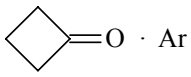
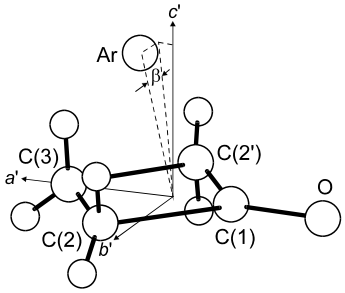
525 **C_4H_6ArO** **Cyclobutanone – argon (1/1)** **C_s**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)



r_0	Å [a])	θ_0	deg [a])
C(1)=O	1.206(18)	H–C(2)–H	110.1(5)
C(1)–C(2)	1.531(29)	H–C(3)–H	110.6
C(2)–C(3)	1.556(25)	C(1)–C(2)–H	112.3(20)
C(2)–H	1.104(32)	C(2)–C(3)–H	113.5(2)
C(3)–H	1.107	C(2')–C(1)–C(2)	93.1(9)
Ar...C(1)	3.614	C(1)–C(2)–C(3)	87.9(8)
Ar...O	4.061	C(2)–C(3)–C(2')	91.1(8)
Ar...H [C(2)]	3.444	C(3)...C(1)...Ar	76.9(15)
Ar...H [C(3)]	3.271	β [b]) [c])	8.9(1)
Ar...H [C(2')]	2.844	C(2')–C(1)–C(2)–H [d])	117.6
		C(1)–C(2)–C(3)–H [d])	116.3
		C(2)–C(3)...C(1)...Ar [d])	98.9

Atom	a_0' [Å] [e])	b_0' [Å] [e])	c_0' [Å] [e])
C(1)	–0.593	0.0	0.0
C(2,2')	0.460	±1.111	0.0
C(3)	1.549	0.0	0.0
O	–1.800	0.0	0.0
H [C(2)]	0.405	±1.741	±0.905
H [C(3)]	2.1791	0.0	±0.9100
Ar	0.2312	±0.5469 [c])	3.4762



The cyclobutanone ring was found to remain planar after complexation with argon.

[a]) Estimated standard errors. Parameters without uncertainty are dependent.
[b]) See figure for the definition.
[c]) Corresponding to the amplitude of a large-amplitude motion.
[d]) Dihedral angle.
[e]) In the principal axis system of the cyclobutanone monomer.

Munrow, M.R., Pringle, W.C., Novick, S.E.: J. Phys. Chem. A **103** (1999) 2256.