486 **C_4H_2** **1,3-Butadiyne** **$D_{\infty h}$**
IR Diacetylene H–C≡C–C≡C–H

r_0	Å [a])
C–H	1.0559(3)
C≡C	1.2089(2)
C–C	1.3737(3)

r_s	Å [a])
C–H	1.0559(1)
C≡C	1.2088(2)
C–C	1.3737(5)

r_m^{ρ}	Å [a])
C–H	1.0554(1)
C≡C	1.2092(1)
C–C	1.3726(1)

The r_0 structure was derived from the rotational constants B_0 of nine isotopomers, whereas the r_s structure was obtained from the average substitution coordinates.

[a]) Estimated standard errors.

Tay, R., Metha, G.F., Shanks, F., McNaughton, D.: Struct. Chem. **6** (1995) 47.

Replaces II/25C (**3**, 1500), IR