342 **C_3HP** **1-Phospha-1,3-butadiyne** **$C_{\infty v}$**
MW, *ab initio* calculations 2-Propynylidynephosphine HC≡C–C≡P

r_0	Å
H–C	1.05577(3)
C≡C	1.21393(5)
C–C	1.3658(2)
C≡P	1.5540(2)

r_s	Å
H–C	1.055763(4)
C≡C	1.213923(8)
C–C	1.3677(2)
C≡P	1.5515(3)

r_e [a])	Å
H–C	1.06174(4)
C≡C	1.21364(7)
C–C	1.3660(3)
C≡P	1.5523(2)

[a]) Derived by combining the observed ground-state rotational constants with the vibration-rotation coupling constants from CCSD(T)/cc-pVQZ calculations.

Bizzocchi, L., Degli Esposti, C., Botschwina, P.: Chem. Phys. Lett. **319** (2000) 411.
Replaces II/25C (**3**, 1045)