

324 C₂NPMW, *ab initio*
calculations**Phosphinidynesacetonitrile**

C-Cyanophosphaethyne

C_{∞v}

N≡C–C≡P

r_0	Å
N≡C	1.1631(8)
C–C	1.374(3)
C≡P	1.549(3)

r_s	Å
N≡C	1.162927(5)
C–C	1.3911(1)
C≡P	1.5258(2)

r_e^a	Å
N≡C	1.16406(8)
C–C	1.3759(3)
C≡P	1.5456(3)

^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.: J. Chem. Phys. **113** (2000) 1465.

Replaces [II/25B\(3, 978\)](#)