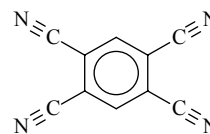


880 **C₁₀H₂N₄**
ED, *ab initio* and DFT
calculations

1,2,4,5-Benzenetetracarbonitrile
1,2,4,5-Tetracyanobenzene

D_{2h} assumed



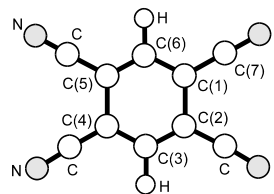
r_g	Å ^{a)}	θ_a	deg ^{a)}
C(2)–C(3)	1.403(4)	C(1)–C(6)–C(5)	118.0(4)
C(1)–C(2)	1.413(6)	C(2)–C(1)–C(7)	120.8(3)
C(1)–C(7)	1.429(3)	C(2)–C(1)–C(6) ^{b)}	121.0(3)
C–C (ring) ^{c)}	1.406(3)		
C≡N	1.161(2)		
C–H	1.050(16)		

The C–C≡N fragments were assumed to be linear.
The nozzle temperature was *ca.* 232 °C.

^{a)} Estimated total errors.

^{b)} Dependent parameter.

^{c)} Average value.



Schultz, G., Szabados, A., Tarczay, G., Zauer, K.: Struct. Chem. **10** (1999) 149.