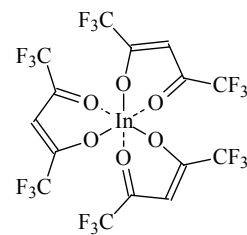


928 **C₁₅H₃F₁₈InO₆**
ED, *ab initio* and DFT
calculations

Tris(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato- κ O, κ O')indium

D₃ assumed

r_a	\AA^a	θ_a	deg a
In–O	2.125(5)	In–O–C	126.4(6)
O–C	1.251(5)	O–In–O	84.8(4)
C–C(ring)	1.392(6) ^{b)}	O–C–C(1,5)	114.1(5) ^{b)}
C–C(1,5)	1.527(4) ^{b)}	C–C–F	110.6(3)
C–F	1.338(2)	τ^c	41.1(12)
C–H	1.093(18) ^{b)}	D ₃ twist ^{d)}	48.4(4)



The local C_{3v} symmetry was assumed for the C–CF₃ groups.

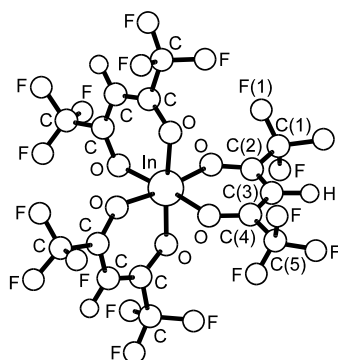
The nozzle temperature was 437 K.

^{a)} Estimated standard errors.

^{b)} Flexibly restrained with values from HF/6-31G* and BP86/6-31G* calculations.

^{c)} O–C–C–F(1) torsional angle from the *syn* position, positive value for the clockwise rotation of the CF₃ group.

^{d)} Twist angle of the rings about their C₂ axis relative to a starting position with all oxygen atoms coplanar, positive value for the clockwise rotation.



Brain, P.T., Bühl, M., Robertson, H.E., Jackson, A.D., Lickiss, P.D., MacKerracher, D., Rankin, D.W.H., Shah, D., Thiel, W.: J. Chem. Soc., Dalton Trans. (1998) 545.