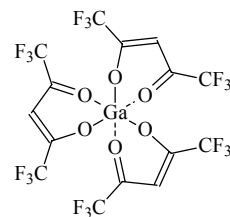
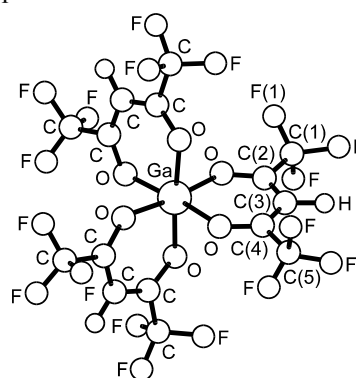


**927**      **C<sub>15</sub>H<sub>3</sub>F<sub>18</sub>GaO<sub>6</sub>**ED, *ab initio* and  
DFT calculations**Tris(1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-  
 $\kappa$ O, $\kappa$ O')gallium****D<sub>3</sub> assumed**

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
Ga–O	1.945(4)	Ga–O–C	127.8(6)
O–C	1.262(7)	O–Ga–O	90.3(5)
C–C(ring)	1.384(5) <sup>b)</sup>	O–C–C(1,5)	114.1(5)
C–C(1,5)	1.524(5) <sup>b)</sup>	C–C–F	111.2(2)
C–F	1.337(2)	$\tau^c$	38.5(11)
C–H	1.094(19) <sup>b)</sup>	D <sub>3</sub> twist <sup>d)</sup>	49.9(4)

Local C<sub>3v</sub> symmetry was assumed for the C–CF<sub>3</sub> groups.

The nozzle temperature was 428 K.

<sup>a)</sup> Estimated standard errors.<sup>b)</sup> Flexibly restrained with values from HF/6-31G\* and BP86/6-31G\* calculations.<sup>c)</sup> O–C–C–F(1) torsional angle from the *syn* position, positive value for the clockwise rotation of the CF<sub>3</sub> group.<sup>d)</sup> Twist angle of the rings about their C<sub>2</sub> 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.