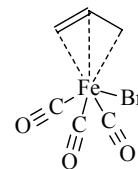
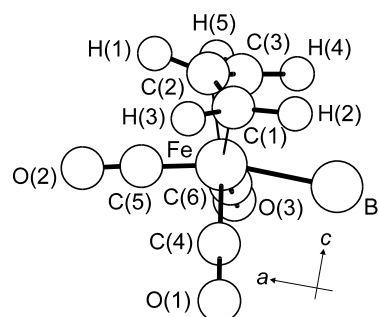


707
MW $\text{C}_6\text{H}_5\text{BrFeO}_3$ η^3 -Allylbromotricarbonyliron
Bromotricarbonyl[η^3 -2-propenyl]iron C_s

r_0	\AA	θ_0	deg
Fe–Br	2.472(9)	Br–Fe–C(5)	172.1(7)
Fe–C(1,3)	2.156(11)	C(1)–C(2)–C(3)	125.1(9)
Fe–C(2)	2.080(12)	C(4)–Fe–C(5)	104.9(5)
Fe–C(4,6)	1.817(7)	Br–Fe–C(4,6)	82.8(4)
Fe–C(5)	1.800(12)	C(3)–C(2)–Fe–Br ^{a)}	67.5(10)
C(2)–C(1,3)	1.396(11)		



Atom	a_0 [\AA]	b_0 [\AA]	c_0 [\AA]
Br	−1.9324	0.0	0.0833
Fe	0.5394	0.0	0.0551
C(1)	0.4756	−1.2383	1.8190
C(2)	1.0700	0.0	2.0661
C(3)	0.4756	1.2383	1.8190
H(1)	2.0588	0.0	2.4773
H(2)	−0.3979	−1.1945 ^{b)}	1.9426
H(3)	0.8958	−2.2290 ^{b)}	1.7735
H(4)	−0.3979	1.1945 ^{b)}	1.9426
H(5)	0.8958	2.2290 ^{b)}	1.7735
C(4)	0.3003	−1.4407	−1.0264
C(5)	2.3186	0.0	−0.2140
C(6)	0.3003	1.4407	−1.0264
O(1)	0.1514	−2.3466	−1.7106
O(2)	3.4463	0.0	−0.3855
O(3)	0.1514	2.3466	−1.7106



Two distinct structural isomers, *anti* and *syn*, were detected. Isomers with the central carbon atom C(2) farthest and closest to the Br atom are designated as *anti* (see figure) and *syn*, respectively. Both isomers are accidental near-prolate symmetric tops and have a dipole component along the *a* axis, but the *anti* isomer has a “*c*” dipole component, whereas a “*b*” dipole component is found for the *syn* isomer. The change in dipole assignments implies that there is a switch of inertial axes upon isomerization resulting from a subtle shift of the allyl center-of-mass coordinates, upon reorientation of the allyl ligand. Structural parameters were given only for *anti* in the original paper.

^{a)} Dihedral angle.

^{b)} Coordinates reported in the original paper are slightly modified to restore C_s symmetry.

Drouin, B.J., Dannemiller, J.J., Kukolich, S.G.: Inorg. Chem. **39** (2000) 827.