

54
MW

CFeO

Monocarbonyliron

 $\text{C}_{\infty\text{v}}$
 $\text{Fe}-\text{C}\equiv\text{O}$

r_s	$\text{\AA}^{\text{a})}$
Fe–C	1.7268(20)
C≡O	1.1598(20)

Atom	$z_s [\text{\AA}]$	
	$^{56}\text{Fe}^{12}\text{C}^{16}\text{O}$	$^{56}\text{Fe}^{13}\text{C}^{16}\text{O}$
Fe	–0.7973	–0.8081
C	0.9296	0.9187
O	2.0907	2.0773

Rotational transitions in the $\Omega = 0$ spin component of the $^3\Sigma^-$ ground electronic state were observed.

^{a)} Uncertainties were not estimated in the original paper.

Kasai, Y., Obi, K., Ohshima, Y., Endo, Y., Kawaguchi, K.: J. Chem. Phys. **103** (1995) 90.