Related literature. The structures of a large number of tris(cyclopentadienyl)uranium complexes of the series $[U(C_5H_5)_3]X$, where X is an anion or a monodentate Lewis base, have been previously reported (Burns, 1986, and references therein; Rogers & Rogers, 1991, and references therein; Spirlet, Rebizant, Apostolidis, Andreetti & Kanellakopulos, 1989; Spirlet, Rebizant, Apostolidis, Van den Bossche & Kanellakopulos, 1990; Rebizant, Spirlet, Apostolidis & Kanellakopulos, 1991). The structure analysis of the title complex was carried out in order to complete the series.

Tris(cyclopentadienyl)uranium thiocyanate is known to form adducts with Lewis bases such as CH_3CN and water but only the structure of the complex $[(C_5H_5)_3U(NCS)(NCCH_3)]$ has been previously reported (Aslan, Yunlu, Fischer, Bombieri & Benetollo, 1988).

References

ASLAN, H., YUNLU, K., FISCHER, R. D., BOMBIERI, G. & BENETOLLO, F. (1988). *J. Organomet. Chem.* **354**, 63–76.

BURNS, J. H. (1986). *The Chemistry of the Actinide Elements*, II, pp. 1458–1479. London: Chapman and Hall.

Enraf–Nonius (1986). *Structure Determination Package*. Version 18. Enraf–Nonius, Delft, The Netherlands.

JOHNSON, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

NORTH, A. C. T., PHILLIPS, D. C. & MATHEWS, F. S. (1968). *Acta Cryst.* A**24**, 351–356.

REBIZANT, J., SPIRLET, M. R., APOSTOLIDIS, C. & KANELLAKOPULOS, B. (1991). *Acta Cryst.* C**47**, 854–856.

ROGERS, R. D. & ROGERS, L. M. (1991). *Organomet. Chem.* **416**, 201–290.

SPIRLET, M. R., REBIZANT, J., APOSTOLIDIS, C., ANDREETTI, G. D. & KANELLAKOPULOS, B. (1989). *Acta Cryst.* C**45**, 739–741.

SPIRLET, M. R., REBIZANT, J., APOSTOLIDIS, C., VAN DEN BOSSCHE, G. & KANELLAKOPULOS, B. (1990). *Acta Cryst.* C**46**, 2318–2320.

Acta Cryst. (1993). C**49**, 931–932

Structure of 3-Ferrocenyl-2-butenoic Acid

BY ZHU YING

Instrumental Analysis and Research Center, Lanzhou University, Lanzhou 730000, *Gansu, People's Republic of China*

(*Received* 24 *June* 1991; *accepted* 23 *October* 1992)

Abstract. [1-(1-Carboxyisopropenyl)-η^5-cyclopentadienyl](η^5-cyclopentadienyl)iron, $[Fe(C_9H_9O_2)(C_5H_5)]$, $M_r = 270.11$, monoclinic, $P2_1/c$, $a = 11.813\ (4)$, $b = 8.353\ (5)$, $c = 12.297\ (4)$ Å, $\beta = 102.31\ (3)°$, $V = 1185.4$ Å^3, $Z = 4$, $D_x = 1.513$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 12.55$ cm^{-1}, $F(000) = 560$, $T = 293$ K, $R = 0.061$ for 1655 observed reflections. The molecular geometry shows the (*E*) stereochemical conformation. The Fe atom and the centroid of the Cp rings form an angle of 179.7 (3)°. The two cyclopentadienide rings are almost eclipsed, forming a 1.1° twist angle.

Experimental. An orange crystal synthesized by Professor Yin You-jin (Zhang, Yin, Zhou & Wang, 1990), of size 0.4 × 0.3 × 0.29 mm, was used for data collection on an Enraf–Nonius CAD-4 diffractometer with graphite-monochromated Mo $K\alpha$ radiation. Cell dimension were refined from 25 accurately centred reflections in the range $18 < 2\theta < 30°$. Intensities were measured using ω–2θ scans of width $(0.64 + 0.35\tan\theta)°$, for θ range 1 to 26° ($h = -14$ to 14, $k = 0$ to 10, $l = 0$ to 5). 2621 reflections were measured, of which 2387 were unique. 1655 observed reflections [$I \geq 3\sigma(I)$] were retained for structure determination. Three standard reflections, monitored every 3600 s, showed 0.5% variation in intensity; correction applied. $R_{int} = 0.052$. Lp corrections, as well as ψ semi-empirical absorption corrections (maximum and minimum transmission 1.000 and 0.874, respectively), were applied.

The structure was solved by Patterson methods and difference Fourier syntheses, with anisotropic full-matrix least-squares refinement (on *F*) for non-H atoms. All H atoms were found on a difference

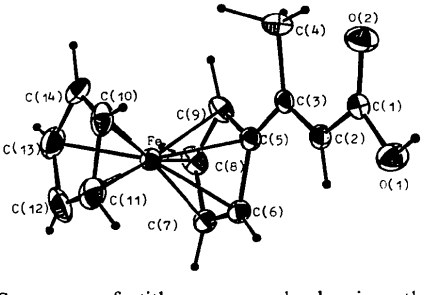

Fig. 1. Structure of title compound showing the atomic numbering.

0108-2701/93/050931-02$06.00

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$B_{eq} = (4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

	x	y	z	B_{eq}
Fe	0.69887 (7)	0.1619 (1)	0.42116 (7)	3.36 (2)
O(1)	1.0530 (4)	0.0840 (7)	0.1362 (4)	5.5 (1)
O(2)	0.9051 (4)	−0.0748 (7)	0.0664 (4)	5.4 (1)
C(1)	0.9598 (5)	0.0061 (8)	0.1443 (5)	4.0 (1)
C(2)	0.9295 (5)	0.0248 (8)	0.2527 (5)	3.7 (1)
C(3)	0.8402 (5)	−0.0390 (7)	0.2854 (5)	3.4 (1)
C(4)	0.7546 (6)	−0.1499 (9)	0.2141 (6)	4.9 (2)
C(5)	0.8178 (5)	−0.0025 (8)	0.3956 (5)	3.5 (1)
C(6)	0.8713 (5)	0.1210 (8)	0.4696 (5)	3.9 (1)
C(7)	0.8223 (6)	0.1193 (9)	0.5631 (5)	4.4 (2)
C(8)	0.7360 (7)	0.0021 (9)	0.5490 (5)	4.9 (2)
C(9)	0.7333 (6)	−0.0765 (8)	0.4471 (5)	4.3 (2)
C(10)	0.6220 (7)	0.2569 (9)	0.2708 (6)	5.5 (2)
C(11)	0.6785 (7)	0.3762 (9)	0.3394 (6)	5.6 (2)
C(12)	0.6272 (9)	0.380 (1)	0.4314 (7)	9.0 (2)
C(13)	0.5411 (7)	0.255 (1)	0.4234 (7)	6.7 (2)
C(14)	0.5393 (6)	0.182 (1)	0.3220 (6)	6.0 (2)

Table 2. *Selected bond distances* (Å), *bond angles* (°) *and torsion angles* (°)

O(1)—C(1)	1.302 (4)	O(2)—C(1)	1.236 (4)
C(1)—C(2)	1.460 (4)	C(3)—C(5)	1.467 (4)
C(2)—C(3)	1.319 (4)	C(3)—C(4)	1.507 (4)
Fe—C(Cp) (mean)	2.035 (4)	C—C(Cp)	1.408 (5)
O(1)—C(1)—O(2)	121.8 (3)	O(1)—C(1)—C(2)	113.2 (3)
O(2)—C(1)—C(2)	125.2 (4)	C(2)—C(3)—C(4)	123.5 (3)
C(1)—C(2)—C(3)	127.1 (3)	C(3)—C(5)—C(9)	126.8 (3)
C(2)—C(3)—C(5)	120.7 (3)	C(3)—C(5)—C(6)	126.6 (3)
C(4)—C(3)—C(5)	115.8 (3)		
C—C—C(Cp) (mean)	108.0 (4)		
C(1)—C(2)—C(3)—C(5)	−176.91	C(1)—C(2)—C(3)—C(4)	2.15
H(2)—C(2)—C(3)—C(5)	−176.83	H(2)—C(2)—C(3)—C(4)	4.11

Fourier map and refined with fixed isotropic thermal parameters ($B = 4.0$ Å^2), but were only included in the structure-factor calculations in the last cycle of refinement. $\sum w(F_o - F_c)^2$ was minimized, where $w = 1/\sigma^2(F_o)$ for all observed reflections. Final $R = 0.061$, $wR = 0.067$, $S = 4.551$, $(\Delta/\sigma)_{max} = 0.18$ for 154 variables. The largest peak in the final ΔF map was 0.969 e Å^{-3}. Atomic scattering factors were obtained from *International Tables for X-ray Crystallography* (1974, Vol. IV). All computations were performed on a PDP 11/44 computer, using the Enraf–Nonius *SDP* (Frenz, 1984).

The structure of the title compound is shown in Fig. 1. Positional parameters and equivalent values of the anisotropic temperature factors of non-H atoms are given in Table 1,* bond distances, selected bond angles and torsion angles are listed in Table 2.

Related literature. The structure of the butenoic acid group in the title compound is similar to that of crotonic acid $CH_3CH{=}CHCOOH$ (Shimizu, Kekka, Kashino & Haisa, 1974). The structure of the title compound shows the (*E*) stereochemical conformation, which is compared with (*Z*)-(1,2-diphenylenethenyl)ferrocence (Cardin Crawford, Watts & Hathaway, 1979).

The author is grateful to Professor Yin for supplying crystals.

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55657 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH0554]

References

CARDIN, C. J., CRAWFORD, W., WATTS, W. E. & HATHAWAY, B. J. (1979). *J. Chem. Soc. Dalton Trans.* pp. 970–973.

FRENZ, B. A. (1984). *Enraf–Nonius Structure Determination Package*. College Station, Texas, USA, and Enraf–Nonius, Delft, The Netherlands.

SHIMIZU, S., KEKKA, S., KASHINO, S. & HAISA, M. (1974). *Bull. Chem. Soc. Jpn*, **47**, 1627–1631.

ZHANG, C. R., YIN, Y.-J., ZHOU, Y. K. & WANG, L. F. (1990). *Chem. J. Chinese Univ.* **11**, 762–764.

Acta Cryst. (1993). C**49**, 932–934

3-Methoxyazetidinium Chloride

BY SØREN BENTZEN, PER HALFDAN NIELSEN, UFFE ANTHONI, CARSTEN CHRISTOPHERSEN AND MICHAEL GAJHEDE*

Chemical Institute, The HC Ørsted Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark

(*Received* 5 *February* 1992; *accepted* 2 *September* 1992)

Abstract. $C_4H_{10}NO^+.Cl^-$, $M_r = 123.58$, triclinic, $P\bar{1}$, $a = 4.9016$ (8), $b = 7.975$ (1), $c = 8.4134$ (7) Å, $\alpha = 100.40$ (1), $\beta = 102.417$ (1), $\gamma = 94.083$ (1)°, $V = 313.8$ (2) Å^3, $Z = 2$, $D_x = 1.308$ (2) g cm^{-3}, monochromatized Cu $K\alpha$, $\lambda = 1.5418$ Å, $\mu = 46.08$ cm^{-1}, $F(000) = 132$, $T = 122$ K, final $R = 0.0474$, for 1262

* Author to whom correspondence should be addressed.

0108-2701/93/050932-03$06.00