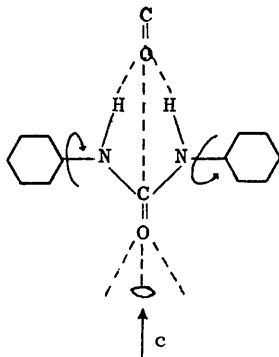


called the *c* direction. The data given in Table 1 were obtained from *hk0*, *hk1* and *hk2* Weissenberg photographs.

Density was measured by flotation. Except for the triclinic *p*-anisyl derivative, all the compounds are orthorhombic. The *m*-tolyl and *m*-chlorophenyl ureas are undoubtedly isomorphous. Their space group and the number of molecules per unit cell, two, require that each molecule have a twofold axis along the C=O bond coinciding with the *c* direction. Although no molecular symmetry is imposed on the other compounds by their space groups and cell dimensions, it is likely that the twofold molecular symmetry is at least approximately preserved. The length of *c* is about equal to or double that of urea. Thus it is likely that



the C=O bond is aligned with *c* and that two hydrogen bonds are formed between the two nitrogen atoms of one molecule and the oxygen of the next molecule, as is found for urea (Vaughan & Donohue, 1952).

Molecular chains would thus be formed along the *c* direction; since the disubstituted ureas have no more hydrogen bonds available, cleavage would be parallel to *c*.

The repeat distance along *b* of about 14 Å (or twice this value) for the *m*- and *p*-substituted compounds is approximately equal to the longest molecular dimension. The latter is not very sensitive to rotation of the phenyl ring around the N-C bond. The repeat of 10 Å along *a*, which is about twice the length of *c*, can accommodate two phenyl rings tilted 45° with respect to *a* and *c*.

The low crystal symmetry of the *p*-anisyl compound is unexpected. It may be due to interaction between the polar nitrogen and the ether oxygen atoms.

A three-dimensional structural analysis of the *m*-chlorophenyl compound is in progress. Further analysis of the other compounds is not contemplated.

The authors are greatly indebted to Professor B. N. Mandak of Sardar Patel University for the synthesis and crystallization of the compounds studied.

Reference

VAUGHAN, P. & DONOHUE, J. (1952). *Acta Cryst.* **5**, 530

Acta Cryst. (1968). **B24**, 1397

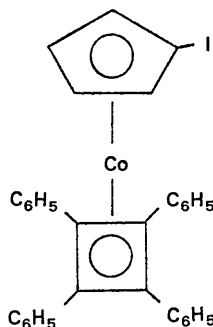
The lattice constants and space group of π -iodocyclopentadienyltetraphenylcyclobutadienylcobalt,

$(\pi\text{-C}_5\text{H}_4\text{I})\text{Co}[(\text{C}_6\text{H}_5)_4\text{C}_4]$. By AIMERY CARON, *Department of Chemistry, University of Massachusetts, Amherst, Mass. 01002, U.S.A.*

(Received 27 May 1968)

The compound crystallizes in space group *Pbcn* with $a=21.24$, $b=15.30$, $c=32.25$ Å with 16 molecules per unit cell.

The compound π -iodocyclopentadienyltetraphenylcyclobutadienylcobalt, $(\pi\text{-C}_5\text{H}_4\text{I})\text{Co}[(\text{C}_6\text{H}_5)_4\text{C}_4]$, was first synthesized by Rausch & Genetti (1967). These authors kindly supplied yellowish brown crystalline needles of this compound.



The following crystallographic data were obtained from rotation and Weissenberg photographs taken about the *b* (needle-axis) and *c* axes:

M.W. 606.4

System: orthorhombic

Lattice constants: $a=21.24 \pm 0.02$, $b=15.30 \pm 0.02$,

$c=32.25 \pm 0.02$ Å

$\lambda(\text{Cu } K\alpha)=1.5418$ Å

Systematic absences: $hk0$; $h+k=2n+1$

$h0l$; $l=2n+1$

$0kl$; $k=2n+1$

Space group: *Pbcn*, No. 60

Density: $D_m=1.54 \pm 1$ g.cm⁻³, $D_x=1.537$ g.cm⁻³
on the basis of $Z=16$.

Since the molecular symmetry would not be expected to be 2 or $\bar{1}$, the asymmetric unit should include two molecules in 8(*d*) general positions. Because of this complication no further work is contemplated on this structure.

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Reference

RAUSCH, M. D. & GENETTI, R. A. (1967). *J. Amer. Chem. Soc.* **89**, 5502.