culated by the computer program of Mueller, Heaton & Miller (1960), and the d spacings were obtained by the program of Mueller, Meyer & Simonsen (1962). The density, measured by the immersion method, is 12·44 g.cm^{-3}, and the X-ray density is 12·52 g.cm^{-3}. The observed and calculated d spacings and observed intensities are listed in Table 1. The observed intensities are in satisfactory agreement with the observed and calculated F^2 values reported by Bertaut, Lemaire & Schweizer (1965) for $HoCo_3$. The unit-cell constants of UCo_3 and of several isostructural rare-earth compounds are listed in Table 2. In this Table the Figure in parentheses is the least-squares standard error of the last significant digit. The rare-earth compounds received various heat treatments (see Table 2), but all X-ray patterns were equally well resolved.

The author acknowledges the assistance of R. A. Conner, Jr, and J. W. Downey in the experimental work, and thanks to Dr J. B. Darby, Jr for reviewing the manuscript.

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Crystallographic data on disubstituted symmetric ureas.

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(*Received* 5 *June* 1968)

The unit-cell dimensions and space groups of six disubstituted, symmetric ureas $(RHN)_2C=O$ have been established. The substituents R in this series were phenyl, p- and m-tolyl, m- and o-chlorophenyl and p-anisyl. Similar packing of the molecules in the unit cells is suggested by the data.

We report here the unit cells and space groups of six disubstituted symmetric ureas, $(RHN)_2C=O$, with R = phenyl, p- and m-tolyl, m and o-chlorophenyl and p-anisyl.

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Needle crystals were obtained for all the compounds by slow evaporation of their solutions in 96% ethanol. They all showed good cleavage along two directions parallel to the needle axis and no cleavage perpendicular to it. Preliminary unit-cell dimensions were derived by indexing rotation photographs around the needle axis which was

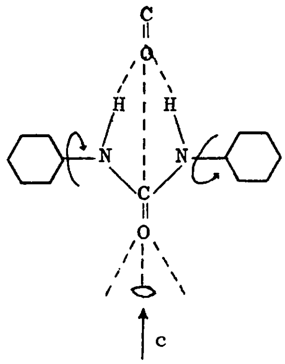
Table 1. *Crystal data for urea derivatives*

	Molecular weight	Axial lengths a	b	c	Measured density	Number of molecules	Space group	Crystal system	Remarks
Urea*	60·06	5·66 Å	5·66 Å	4·72 Å	1·33 g.cm^{-3}	2·02	$P\bar{4}2_1m$	Tetragonal	
Diphenylurea	212·25	10·51	11·73	9·07	1·23	3·90	$P2_1cn$	Orthorhombic	
Di-p-tolylurea	240·29	9·85	27·77	4·66	1·26	4·02	$Pn2_1a$	Orthorhombic	
Di-m-tolylurea	240·29	9·72	14·56	4·60	1·25	2·04	$P2_12_12$ ($P2_12_12_1$)	Orthorhombic	
Di-m-chlorophenylurea	281·14	9·72	14·36	4·55	1·47	2·00	$P2_12_12$ ($P2_12_12_1$)	Orthorhombic	
Di-o-chlorophenylurea	281·14	23·00	23·20	4·64	1·48	7·85	$Pban$	Orthorhombic	Poor crystals. $h=2n$, very weak for $h00$, $h0l$. $k=2n$, very weak for $0k0$, $0kl$
Di-p-anisylurea	272·29	($\gamma^*=81°$) 21·20 ($=d_{100}$)	13·38 ($=d_{010}$)	9·31	1·35	7·95	$P1$ or $P\bar{1}$	Triclinic	Odd layer lines on rotation about c axis very weak. $hk0$ with $h+k$ odd absent; h and k odd very weak.

* Vaughan & Donohue (1952).

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. Mankad of Sardar Patel University for the synthesis and crystallization of the compounds studied.

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The lattice constants and space group of π-iodocyclopentadienyltetraphenylcyclobutadienylcobalt, $(\pi\text{-}C_5H_4I)Co[(C_6H_5)_4C_4]$.

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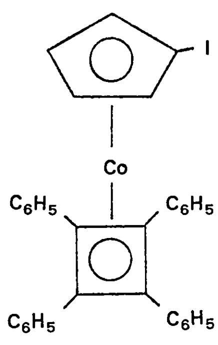
(*Received* 27 *May* 1968)

The compound crystallizes in space group *Pbcn* with $a=21{\cdot}24$, $b=15{\cdot}30$, $c=32{\cdot}25$ Å with 16 molecules per unit cell.

The compound π-iodocyclopentadienyltetraphenylcyclobutadienylcobalt, $(\pi\text{-}C_5H_4I)Co[(C_6H_5)_4C_4]$, 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: $a=21{\cdot}24\pm0{\cdot}02$, $b=15{\cdot}30\pm0{\cdot}02$,
$c=32{\cdot}25\pm0{\cdot}02$ Å
$\lambda(\text{Cu } K\alpha)=1{\cdot}5418$ Å

Systematic absences: $hk0$; $h+k=2n+1$
$h0l$; $l=2n+1$
$0kl$; $k=2n+1$

Space group: *Pbcn*, No. 60
Density: $D_m=1{\cdot}54\pm1$ g.cm^{-3}, $D_x=1{\cdot}537$ 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.

This study was supported by a grant from the Research Council at the University of Massachusetts.

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