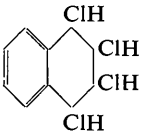
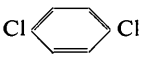
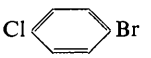
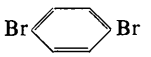
Table 1. *Molecular susceptibilities of naphthalene tetrachloride compared with those of some p-substituted benzene molecules (Lasheen, 1964) all in* 10^{-6} *e.m.u./g.*

Name and formula ($L \leftrightarrow$ and $M \updownarrow$ in each case)		K_L	K_M	K_N	ΔK
Naphthalene tetrachloride		−147·5	−145·0	−201·2	54·9
p-Dichlorobenzene		−78·8	−50·3	−120·2	55·9
p-Bromochlorobenzene		−87·6	−59·9	−129·0	55·2
p-Dibromobenzene		−97·1	−70·5	−136·7	52·9

The direction cosines calculated from the atomic coordinates given by Farag (1954) are:

Central ring

	a	*b*	*c*
L	0·1730	−0·0055	−0·9847
M	0·1000	−0·9949	0·0231
N	0·9789	0·1025	0·1768

First phenyl ring

	a	*b*	*c*
L	0·1374	0	−0·9837
M	0·5218	0·8498	0·0729
N	0·8416	−0·5269	0·1179

Second phenyl ring

	a	*b*	*c*
L	0·2085	−0·0072	0·9780
M	0·3073	0·9498	−0·0585
N	0·9311	−0·3128	−0·1875

Third phenyl ring

	a	*b*	*c*
L	0·1651	0·0754	0·9834
M	0·2994	−0·9538	0·0229
N	0·9400	0·2908	−0·1786

Thus the mean molecular susceptibilities and anisotropy for one benzene ring are:

$K_L = -33{\cdot}7$, $K_M = -32{\cdot}5$, $K_N = -85{\cdot}9$, $\Delta K = 52{\cdot}8$ (all in 10^{-6} e.m.u./g.).

Comparing the value of the molecular anisotropy with that of the benzene molecule $\Delta K = 59{\cdot}7$ given by Hoarau, Joussot-Dubien, Lemanceau, Lumbroso & Pacault (1956), it is evident that the replacement of one hydrogen atom by a phenyl ring decreases the molecular anisotropy. Considering three replacements in the central benzene ring and one in each phenyl ring, it follows that the decrease in anisotropy due to each substitution is equal to 4·6. This gives the molecular anisotropy of the central ring as $\Delta K = 45{\cdot}9$ and that of any of the three phenyl rings as $\Delta K = 55{\cdot}1$.

It should be noted that the 1,3,5-triphenylbenzene molecule is non-planar and thus some approximation is involved with the consequence that the conclusions drawn are less rigorous.

References

FARAG, M. S. (1954). *Acta Cryst.* **7**, 117.

HOARAU, J., JOUSSOT-DUBIEN, J., LEMANCEAU, B., LUMBROSO, N. & PACAULT, A. (1956). *Cah. Phys.* no. 74, 34.

KRISHNAN, K. S. & BANERJEE, S. (1934). *Phil. Trans.* A, **234**, 265.

LASHEEN, M. A. (1952). *Acta Cryst.* **5**, 593.

LASHEEN, M. A. (1956). *Proc. Math. Phys. Soc. Egypt*, **5**, no. 4, 23.

LASHEEN, M. A. (1964). *Phil. Trans.* A, **256**, 357.

LASHEEN, M. A. & HEDDEWI, S. (1966). To be published.

LONSDALE, K. (1937). *Z. Kristallogr.* **97**, 91.

LONSDALE, K. & KRISHNAN, K. S. (1936). *Proc. Roy. Soc.* A, **156**, 597.

Acta Cryst. (1966). **20**, 927

A table of the real part of the dispersion correction for X-ray scattering.

By LUIS R. SARAVIA and S. CATICHA-ELLIS, *Depto. de Física del Estado Sólido, Instituto de Física, Facultad de Ingeniería y Agrimensura, Montevideo, Uruguay*

(*Received* 30 *April* 1965 *and in revised form* 1 *September* 1965)

In a previous paper, one of us (Caticha-Ellis, 1962), described a method using the real part of the dispersion correction $\Delta f'$ in the X-ray atomic scattering factor for the solution of centrosymmetric crystal structures.

Until now, values of $\Delta f'$ have been available only for a few wavelengths. The table published by Dauben & Templeton (1955) includes the real and imaginary parts of the dispersion corrections for elements with $Z \geq 20$ for the wavelengths: Cr $K\alpha$, Cu $K\alpha$ and Mo $K\alpha$. A second table calculated by Templeton (1962), includes the effect of the diffraction angle θ, for the same three wavelengths, for elements with $Z \geq 5$. Cooper (1963) performed similar cal-

culations with wavelengths Co $K\alpha$ and Ag $K\alpha$. Cromer (1965) has recently published anomalous dispersion corrections for elements from $Z=10$ to $Z=98$ for Cr, Fe, Cu, Mo and Ag $K\alpha_1$ radiations.

The present table includes the value of $\Delta f'$ for elements between $Z=20$ (Ca) and $Z=83$ (Bi) for 32 different $K\alpha$ wavelengths, ranging from Ti $K\alpha$ (2·750 Å) to I $K\alpha$ (0·435 Å). The wavelengths of some elements which are not usable as target material have also been included.

The values of $\Delta f'$ listed in Table 1 were obtained by the method indicated by Parratt & Hempstead (1954), as were those previously published; they take into account the

Table 1. *Real part of the dispersion corrections for X-ray scattering*

Target		Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	Rb
λK_α(Å)		2,750	2,505	2,291	2,103	1,937	1,791	1,659	1,542	1,437	1,341	1,256	1,177	1,106	1,041	0,981	0,927
20	Ca	-1.4	-0.6	-0.1	0.0	0.2	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3
21	Sc	-3.7*	-1.6	-0.7	-0.2	0.0	0.1	0.2	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.3	0.3
22	Ti	-2.4	-4.0*	-1.7	-0.8	-0.3	0.0	0.1	0.2	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.4
23	V	-1.8	-2.3	-3.9*	-1.7	-0.8	-0.4	0.0	0.1	0.2	0.3	0.3	0.4	0.4	0.4	0.4	0.4
24	Cr	-1.5	-1.8	-2.3	-3.9*	-1.8	-0.9	-0.4	-0.1	0.1	0.2	0.3	0.3	0.4	0.4	0.4	0.4
25	Mn	-1.3	-1.5	-1.7	-2.2	-3.8	-1.9	-1.0	-0.5	-0.1	0.0	0.2	0.2	0.3	0.3	0.4	0.4
26	Fe	-1.1	-1.3	-1.5	-1.7	-2.2	-3.5	-2.0	-1.1	-0.6	-0.2	0.0	0.1	0.2	0.3	0.3	0.3
27	Co	-1.0	-1.1	-1.3	-1.5	-1.8	-2.2	-3.3	-2.2	-1.3	-0.6	-0.3	0.0	0.1	0.2	0.2	0.3
28	Ni	-0.9	-1.0	-1.2	-1.3	-1.5	-1.8	-2.2	-3.2	-2.4	-1.4	-0.7	-0.4	-0.1	0.0	0.1	0.2
29	Cu	-0.8	-0.9	-1.0	-1.2	-1.3	-1.5	-1.7	-2.2	-3.0	-2.6	-1.5	-0.8	-0.4	-0.1	0.0	0.1
30	Zn	-0.8	-0.8	-0.9	-1.1	-1.2	-1.3	-1.5	-1.7	-2.1	-3.0	-3.3	-1.5	-0.9	-0.5	-0.2	0.0
31	Ga	-0.7	-0.8	-0.8	-0.9	-1.1	-1.2	-1.3	-1.5	-1.7	-2.1	-2.8	-3.4*	-1.6	-1.0	-0.5	-0.2
32	Ge	-0.7	-0.7	-0.8	-0.9	-1.0	-1.1	-1.2	-1.3	-1.5	-1.7	-2.1	-2.8	-3.4*	-1.7	-1.1	-0.6
33	As	-0.6	-0.7	-0.7	-0.8	-0.9	-1.0	-1.1	-1.2	-1.3	-1.5	-1.7	-2.0	-2.7	-3.4*	-1.8	-1.1
34	Se	-0.6	-0.6	-0.6	-0.7	-0.8	-0.9	-0.9	-1.0	-1.2	-1.3	-1.5	-1.7	-2.0	-2.6	-3.6*	-1.8
35	Br	-0.6	-0.6	-0.6	-0.6	-0.7	-0.8	-0.9	-1.0	-1.1	-1.2	-1.3	-1.5	-1.7	-2.0	-2.5	-3.6*
36	Kr	-0.5	-0.5	-0.6	-0.6	-0.6	-0.7	-0.8	-0.8	-0.9	-1.0	-1.2	-1.3	-1.4	-1.6	-1.9	-2.5
37	Rb	-0.6	-0.5	-0.5	-0.6	-0.6	-0.6	-0.7	-0.8	-0.8	-0.9	-1.0	-1.2	-1.3	-1.4	-1.6	-1.9
38	Sr	-0.6	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.8	-0.8	-0.9	-1.0	-1.2	-1.3	-1.4	-1.6
39	Y	-0.7	-0.6	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.8	-0.8	-0.9	-1.0	-1.2	-1.3	-1.4
40	Zr	-0.9	-0.7	-0.6	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.8	-0.8	-0.9	-1.0	-1.2	-1.3
41	Nb	-1.0	-0.7	-0.6	-0.5	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.8	-0.8	-0.9	-1.0	-1.1
42	Mo	-1.2	-0.9	-0.7	-0.6	-0.5	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.8	-0.8	-0.9	-1.0
43	Tc	-1.5	-1.1	-0.8	-0.7	-0.6	-0.5	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.8	-0.8	-0.9
44	Ru	-1.7	-1.2	-0.9	-0.7	-0.6	-0.5	-0.5	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.8	-0.8
45	Rh	-2.2	-1.5	-1.1	-0.8	-0.6	-0.5	-0.5	-0.5	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.8
46	Pd	-2.6	-1.8	-1.3	-0.9	-0.7	-0.6	-0.5	-0.5	-0.5	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7
47	Ag	-3.2	-2.2	-1.5	-1.1	-0.8	-0.7	-0.5	-0.5	-0.5	-0.4	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6
48	Cd	-4.4	-2.7	-1.9	-1.3	-1.0	-0.8	-0.6	-0.5	-0.5	-0.5	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6
49	In	-5.6	-3.3	-2.3	-1.6	-1.1	-0.9	-0.7	-0.6	-0.5	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.5
50	Sn	-7.9*	-4.6	-2.8	-2.0	-1.4	-1.0	-0.8	-0.6	-0.5	-0.5	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5
51	Sb	-9.3	-5.8	-3.5	-2.4	-1.7	-1.2	-0.9	-0.7	-0.6	-0.5	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5
52	Te	-10.7	-7.7*	-4.7	-2.8	-2.1	-1.5	-1.1	-0.8	-0.7	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4	-0.5
53	I	-11.7*	-9.7*	-6.0	-3.8	-2.5	-1.8	-1.3	-1.0	-0.8	-0.6	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4
54	Xe	-9.3	-10.4	-8.1	-4.9	-3.0	-2.2	-1.6	-1.2	-0.9	-0.7	-0.6	-0.5	-0.4	-0.4	-0.4	-0.4
55	Cs	-7.9	-11.4*	-9.5*	-6.3	-4.0	-2.6	-1.9	-1.4	-1.0	-0.8	-0.7	-0.5	-0.5	-0.4	-0.4	-0.4
56	Ba	-7.0	-9.0	-10.2	-8.2*	-5.1	-3.2	-2.3	-1.7	-1.2	-0.9	-0.7	-0.6	-0.5	-0.5	-0.4	-0.4
57	La	-6.5	-7.7	-11.1*	-9.7*	-6.9*	-4.3	-2.7	-2.0	-1.5	-1.1	-0.9	-0.7	-0.6	-0.5	-0.5	-0.4
58	Ce	-5.9	-6.9	-8.8	-10.1	-8.2	-5.3	-3.4	-2.4	-1.8	-1.3	-1.0	-0.8	-0.6	-0.5	-0.4	-0.4
59	Pr	-5.6	-6.3	-7.6	-10.9*	-9.5*	-7.0*	-4.4	-2.8	-2.1	-1.6	-1.2	-0.9	-0.7	-0.6	-0.5	-0.4
60	Nd	-5.3	-6.0	-6.9	-8.9	-9.8	-8.3	-5.5	-3.6	-2.5	-1.8	-1.4	-1.1	-0.8	-0.7	-0.6	-0.5
61	Pm	-5.1	-5.6	-6.4	-7.7	-10.8*	-9.4*	-7.0*	-4.5	-3.0	-2.2	-1.6	-1.2	-1.0	-0.8	-0.6	-0.5
62	Sm	-5.0	-5.4	-6.0	-7.0	-8.9	-9.6	-8.4	-5.7	-3.8	-2.6	-1.9	-1.5	-1.1	-0.9	-0.7	-0.6
63	Eu	-4.8	-5.2	-5.7	-6.4	-7.7	-10.6*	-9.3	-7.4*	-4.8	-3.2	-2.3	-1.7	-1.3	-1.0	-0.8	-0.7
64	Gd	-4.7	-5.0	-5.4	-6.0	-7.0	-8.9	-9.4	-8.7*	-6.1	-4.0	-2.8	-2.0	-1.6	-1.2	-1.0	-0.8
65	Tb	-4.7	-4.9	-5.3	-5.8	-6.5	-7.8	-10.6*	-9.0	-7.6*	-5.0	-3.4	-2.5	-1.8	-1.5	-1.1	-0.9
66	Dy	-4.6	-4.8	-5.1	-5.5	-6.1	-7.0	-8.8	-10.0	-8.7*	-6.7*	-4.4	-3.0	-2.3	-1.7	-1.4	-1.1
67	Ho	-4.6	-4.8	-5.0	-5.3	-5.8	-6.6	-7.8	-10.5*	-8.8	-7.8*	-5.2	-3.6	-2.6	-2.0	-1.6	-1.2
68	Er	-4.7	-4.8	-4.9	-5.2	-5.6	-6.2	-7.2	-9.2	-9.1	-8.8*	-6.7*	-4.5	-3.1	-2.4	-1.8	-1.4
69	Tm	-4.7	-4.7	-4.9	-5.1	-5.4	-5.9	-6.7	-7.9	-10.4*	-8.6	-8.1	-5.5	-3.9	-2.8	-2.1	-1.7
70	Yb	-4.8	-4.7	-4.8	-5.0	-5.3	-5.7	-6.3	-7.2	-9.3	-8.9	-8.8*	-6.8*	-4.7	-3.3	-2.5	-1.9
71	Lu	-4.5	-4.4	-4.5	-4.6	-4.9	-5.3	-5.8	-6.6	-7.9	-9.8	-8.3	-8.2*	-5.7	-4.0	-2.8	-2.2
72	Hf	-4.6	-4.4	-4.4	-4.6	-4.8	-5.1	-5.6	-6.2	-7.1	-9.2	-8.6	-8.6	-7.2*	-4.9	-3.4	-2.6
73	Ta	-4.8	-4.5	-4.4	-4.5	-4.7	-4.9	-5.4	-5.9	-6.6	-7.9	-10.2	-8.1	-8.1*	-6.4*	-4.2	-3.1
74	W	-5.0	-4.6	-4.5	-4.5	-4.6	-4.9	-5.2	-5.6	-6.2	-7.1	-9.1	-8.6	-8.2	-7.5*	-5.2	-3.7
75	Re	-5.3	-4.8	-4.5	-4.5	-4.6	-4.8	-5.0	-5.4	-5.9	-6.6	-7.9	-10.0*	-8.0	-8.3*	-6.5*	-4.5
76	Os	-5.4	-4.9	-4.6	-4.5	-4.5	-4.7	-4.9	-5.2	-5.6	-6.2	-7.1	-9.1	-8.5	-8.0	-8.1	-5.6
77	Ir	-5.7	-5.1	-4.7	-4.5	-4.5	-4.6	-4.8	-5.1	-5.4	-5.9	-6.6	-7.8	-9.9*	-7.8	-8.2*	-7.0*
78	Pt	-6.0	-5.3	-4.8	-4.6	-4.5	-4.6	-4.7	-5.0	-5.3	-5.7	-6.2	-7.1	-9.0	-8.6	-7.7	-7.9*
79	Au	-6.3	-5.5	-5.0	-4.7	-4.5	-4.5	-4.7*	-4.8	-5.1	-5.5	-5.9	-6.7	-7.9	-9.9*	-7.8	-8.0
80	Hg	-6.8	-5.8	-5.2	-4.8	-4.6	-4.5	-4.6	-4.8	-5.0	-5.3	-5.7	-6.3	-7.1	-9.0	-8.6	-7.6
81	Tl	-7.2	-6.1	-5.4	-4.9	-4.6	-4.5	-4.6	-4.7	-4.9	-5.2	-5.5	-6.0	-6.6	-7.8	-9.8*	-7.7
82	Pb	-7.9	-6.5	-5.7	-5.1	-4.8	-4.6	-4.6	-4.7	-4.8	-5.1	-5.3	-5.7	-6.3	-7.1	-8.9	-9.0
83	Bi	-8.4	-6.7	-5.8	-5.3	-4.9	-4.6	-4.6	-4.6	-4.7	-4.9	-5.2	-5.6	-6.0	-6.7	-7.8	-9.7*

Table 1 (*cont.*)

Target		Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I
λK_α(Å)		0,877	0,831	0,788	0,748	0,710	0,674	0,644	0,614	0,587	0,561	0,536	0,514	0,492	0,472	0,453	0,435
20	Ca	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.1	0.1	0.1
21	Sc	0.3	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2
22	Ti	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2
23	V	0.4	0.4	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.2
24	Cr	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.2	0.2	0.2	0.2
25	Mn	0.4	0.4	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.2	0.2
26	Fe	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
27	Co	0.3	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.3	0.3	0.3
28	Ni	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.3	0.3
29	Cu	0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3
30	Zn	0.1	0.2	0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.3	0.3
31	Ga	0.0	0.0	0.2	0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4
32	Ge	-0.3	-0.1	0.0	0.1	0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4
33	As	-0.6	-0.4	-0.1	0.0	0.1	0.2	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4	0.4
34	Se	-1.2	-0.7	-0.4	-0.1	0.0	0.1	0.2	0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.4
35	Br	-1.9	-1.3	-0.8	-0.5	-0.2	0.0	0.1	0.2	0.2	0.3	0.3	0.3	0.4	0.4	0.4	0.4
36	Kr	-3.6	-2.1	-1.4	-0.8	-0.5	-0.2	0.0	0.0	0.1	0.2	0.3	0.3	0.3	0.3	0.4	0.4
37	Rb	-2.4	-3.6*	-2.3	-1.5	-0.9	-0.5	-0.3	-0.1	0.0	0.1	0.2	0.2	0.3	0.3	0.3	0.4
38	Sr	-1.9	-2.3	-3.4	-2.5	-1.5	-0.9	-0.6	-0.3	-0.1	0.0	0.1	0.2	0.2	0.3	0.3	0.3
39	Y	-1.6	-1.9	-2.3	-3.2	-3.0	-1.6	-1.1	-0.6	-0.4	-0.2	0.0	0.1	0.1	0.2	0.3	0.3
40	Zr	-1.4	-1.6	-1.8	-2.2	-3.1	-3.2*	-1.7*	-1.1	-0.7	-0.4	-0.2	0.0	0.0	0.1	0.2	0.2
41	Nb	-1.2	-1.4	-1.6	-1.8	-2.2	-3.0	-3.2*	-1.7*	-1.2	-0.7	-0.5	-0.3	0.0	0.0	0.1	0.2
42	Mo	-1.1	-1.2	-1.4	-1.6	-1.8	-2.2	-2.9	-3.2*	-1.8*	-1.3	-0.8	-0.5	-0.3	-0.1	0.0	0.1
43	Tc	-1.0	-1.1	-1.2	-1.4	-1.6	-1.8	-2.2	-2.8	-3.2*	-1.8*	-1.3	-0.9	-0.5	-0.3	-0.1	0.0
44	Ru	-0.9	-1.0	-1.1	-1.2	-1.4	-1.5	-1.8	-2.1	-2.7	-3.5*	-1.9	-1.4	-0.9	-0.6	-0.4	-0.2
45	Rh	-0.8	-0.9	-1.0	-1.1	-1.2	-1.4	-1.5	-1.8	-2.1	-2.6	-3.5*	-2.1*	-1.4	-1.0	-0.6	-0.4
46	Pd	-0.8	-0.8	-0.9	-1.0	-1.1	-1.2	-1.4	-1.5	-1.7	-2.0	-2.6	-3.5*	-2.2*	-1.5	-1.1	-0.7
47	Ag	-0.7	-0.8	-0.8	-0.9	-1.0	-1.1	-1.2	-1.4	-1.5	-1.7	-2.0	-2.5	-3.5*	-2.4*	-1.6	-1.1
48	Cd	-0.6	-0.7	-0.8	-0.8	-0.9	-1.0	-1.1	-1.2	-1.3	-1.5	-1.7	-2.0	-2.5	-3.5*	-2.9	-1.6
49	In	-0.6	-0.6	-0.7	-0.8	-0.8	-0.9	-1.0	-1.1	-1.2	-1.3	-1.5	-1.7	-2.0	-2.4	-3.4	-3.1
50	Sn	-0.5	-0.6	-0.6	-0.7	-0.8	-0.8	-0.9	-1.0	-1.1	-1.2	-1.3	-1.5	-1.7	-1.9	-2.4	-3.3
51	Sb	-0.5	-0.5	-0.6	-0.6	-0.7	-0.8	-0.8	-0.9	-1.0	-1.1	-1.2	-1.3	-1.5	-1.6	-1.9	-2.3
52	Te	-0.5	-0.5	-0.6	-0.6	-0.6	-0.7	-0.8	-0.8	-0.9	-1.0	-1.1	-1.2	-1.3	-1.5	-1.6	-1.9
53	I	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.7	-0.8	-0.8	-0.9	-1.0	-1.1	-1.2	-1.3	-1.5	-1.6
54	Xe	-0.4	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.7	-0.8	-0.8	-0.9	-1.0	-1.1	-1.2	-1.3	-1.4
55	Cs	-0.4	-0.4	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.7	-0.8	-0.8	-0.9	-1.0	-1.1	-1.2	-1.3
56	Ba	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.7	-0.8	-0.8	-0.9	-1.0	-1.1	-1.2
57	La	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.7	-0.8	-0.8	-0.9	-1.0	-1.1
58	Ce	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.7	-0.8	-0.8	-0.9	-1.0
59	Pr	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.7	-0.8	-0.8	-0.9
60	Nd	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.7	-0.8	-0.8
61	Pm	-0.5	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.6	-0.6	-0.7	-0.7	-0.8
62	Sm	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5	-0.6	-0.6	-0.6	-0.7	-0.7
63	Eu	-0.6	-0.5	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.6	-0.6	-0.6	-0.7
64	Gd	-0.6	-0.6	-0.5	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.6	-0.6	-0.6
65	Tb	-0.7	-0.6	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.5	-0.6	-0.6
66	Dy	-0.9	-0.7	-0.6	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.6	-0.6
67	Ho	-1.0	-0.8	-0.7	-0.6	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.6
68	Er	-1.2	-0.9	-0.8	-0.7	-0.6	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.5
69	Tm	-1.3	-1.1	-0.9	-0.7	-0.6	-0.6	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4	-0.5	-0.5	-0.5	-0.5
70	Yb	-1.5	-1.2	-1.0	-0.8	-0.7	-0.6	-0.5	-0.5	-0.5	-0.4	-0.4	-0.4	-0.	-0.5	-0.5	-0.5
71	Lu	-1.7	-1.4	-1.1	-0.9	-0.7	-0.6	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4	-0.5
72	Hf	-2.0	-1.6	-1.3	-1.1	-0.9	-0.7	-0.6	-0.5	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4
73	Ta	-2.4	-1.8	-1.5	-1.2	-1.0	-0.8	-0.7	-0.6	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4	-0.4	-0.4
74	W	-2.8	-2.2	-1.7	-1.4	-1.1	-0.9	-0.8	-0.7	-0.6	-0.5	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4
75	Re	-3.3	-2.6	-1.9	-1.6	-1.3	-1.1	-0.9	-0.7	-0.6	-0.6	-0.5	-0.5	-0.4	-0.4	-0.4	-0.4
76	Os	-4.0	-3.0	-2.3	-1.8	-1.5	-1.2	-1.0	-0.9	-0.7	-0.6	-0.6	-0.5	-0.5	-0.5	-0.4	-0.4
77	Ir	-4.8	-3.5	-2.7	-2.1	-1.7	-1.4	-1.2	-1.0	-0.8	-0.7	-0.6	-0.6	-0.5	-0.5	-0.5	-0.4
78	Pt	-6.3*	-4.3	-3.2	-2.5	-1.9	-1.6	-1.3	-1.1	-0.9	-0.8	-0.7	-0.6	-0.6	-0.5	-0.5	-0.5
79	Au	-7.4*	-5.2	-3.8	-3.0	-2.3	-1.8	-1.5	-1.3	-1.1	-0.9	-0.8	-0.7	-0.6	-0.6	-0.5	-0.5
80	Hg	-8.0*	-6.5*	-4.6	-3.4	-2.7	-2.1	-1.7	-1.4	-1.2	-1.0	-0.9	-0.8	-0.7	-0.6	-0.6	-0.5
81	Tl	-7.7	-7.9*	-5.8	-4.1	-3.1	-2.5	-2.0	-1.6	-1.4	-1.2	-1.0	-0.8	-0.7	-0.7	-0.6	-0.6
82	Pb	-7.5	-8.0*	-7.1*	-5.0	-3.7	-2.9	-2.3	-1.8	-1.5	-1.3	-1.1	-1.0	-0.8	-0.7	-0.7	-0.6
83	Bi	-7.6	-7.4	-7.7*	-6.3*	-4.4	-3.3	-2.7	-2.2	-1.7	-1.5	-1.3	-1.1	-0.9	-0.8	-0.7	-0.7

contributions of the *K*, *L*, *M* and *N* electrons. The absorption edges were taken directly from the tables of Cauchois & Hulubei (1947). In some cases, interpolations for the *M* and *N* electrons had to be made. The oscillator strengths for *K* and *L* electrons are those recently published by Cromer (1965); for *M* and *N* electrons global values of the oscillator strengths have been used which are simply obtained by adding up Cromer's values for each of these two shells. This approximation is justified since the elements included in the table have *M* and *N* absorption edges far from the incident wavelengths used. The values of $\Delta f'$ differ from those of Cromer not only for this reason but also

because different sets of incident and absorption edge wavelengths have been used. The differences amount to no more than some tenths of an electron except for wavelengths close to an absorption edge; these values are particularly uncertain and have been marked with an asterisk.

The dispersion corrections calculated in this paper are not regarded as being necessarily superior to those of Cromer (1965).

The variation of the absorption coefficient follows closely a λ^p relation, where λ is the wavelength. The exponents p depend on the electron shell and on the atomic number involved. They have been chosen according to the examples given by Parratt & Hempstead.

Neither damping effects nor variation with diffraction angle were taken into account in evaluating $\Delta f'$.

It is quite difficult to evaluate the total error in the final values of $\Delta f'$; they are given to one decimal place, but this should not be taken as an indication of their accuracy.

The present table is intended as an aid in the use of the two-wavelength method for solving centrosymmetric crystal structures. The use of this method requires a suitable selection of two wavelengths λ_1 and λ_2 so that, for the anomalous scatterers in the structure, the difference $\Delta f'(\lambda_1)-\Delta f'(\lambda_2)$ is as great as possible. For a given element, the maximum difference ranges between 20% or more to about 6·5% of the atomic number. Only the elements in the range $Z=38$ to $Z=48$ have a difference less than 10% for the wavelengths included in the present table. If necessary longer wavelengths can be used to remove this limitation.

Thanks are given to Dr S.C. Abrahams for helpful suggestions.

The calculations were carried out with a program for the IBM 1401 in FORTRAN language by one of us (L.R. S.). We are indebted to IBM del Uruguay S.A. for the use of their IBM 1401 computer. This research was supported by a grant from 'Fondo de Investigación Científica' of the Universidad de la Republica, Montevideo, Uruguay.

References

CATICHA-ELLIS, S. (1962). *Acta Cryst.* **15**, 863.

CAUCHOIS, Y. & HULUBEI, H. (1947). *Longueurs d'Onde des Émissions X et des Discontinuités d'Absorption X.* Paris: Hermann et Cie.

COOPER, M. J. (1963). *Acta Cryst.* **16**, 1067.

CROMER, D. T. (1965). *Acta Cryst.* **18**, 17.

DAUBEN, C. H. & TEMPLETON, D. H. (1955). *Acta Cryst.* **8**, 841.

PARRATT, L. G. & HEMPSTEAD, C. F. (1954). *Phys. Rev.* **94**, 1593.

TEMPLETON, D. H. (1962). *International Tables for X-Ray Crystallography*, Vol. III. Birmingham: Kynoch Press.

Acta Cryst. (1966). **20**, 930

Crystal data (I) for some cholestane derivatives.

By BARBARA HANER and DORITA A. NORTON, *Biophysics Department, Roswell Park Memorial Institute, Buffalo, New York, U.S.A.*

(*Received* 10 *September* 1965)

The lattice constants of seven cholestane derivatives given in Table 1 have been determined by procedures described in earlier papers (Haner & Norton, 1964; Ohrt, Haner & Norton, 1964). No further work is anticipated on these compounds at the present time.

This investigation was supported in part by Public Health Service Research Grant Number CA-06183 from the National Cancer Institute.

References

HANER, B. & NORTON, D. A. (1964). *Acta Cryst.* **17**, 1610.

OHRT, J. M., HANER, B. & NORTON, D. A. (1964). *Acta Cryst.* **17**, 1611.

Table 1. *Crystal data for some cholestane deriwatives*

	(1)	(2)	(3)	(4)	(5)	(6)	(7)
Formula	$C_{27}H_{48}$	$C_{27}H_{48}O \cdot 2H_2O$	$C_{27}H_{46}O$	$C_{27}H_{44}O$	$C_{27}H_{44}O$	$C_{27}H_{46}O_2$	$C_{27}H_{44}O_2 \cdot H_2O$
Mol. wt.	372·65	424·68	386·64	384·62	384·62	402·64	418·64
D_m (g.cm^{-3})	1·010	0·957	1·025	1·077	1·080	0·996	1·022
D_x (g.cm^{-3})	1·024	0·959	1·035	1·080	1·069	1·070	1·023
Space group	$P2_1$	P_1	$P2_1$	$P2_1$	$P2_12_12_1$	P_1	$P2_1$
Z	4	4	12	2	4	2	4
a (Å)*	19·509	11·235	34·120	14·625	11·236	10·716	23·245
b (Å)*	11·093	23·941	19·967	7·851	19·137	19·963	12·284
c (Å)*	11·479	11·118	11·036	10·672	11·110	6·138	9·663
α (°)	—	103·48	—	—	—	90·94	—
β (°)	103·40	89·82	98·33	105·13	—	107·33	100·02
γ (°)	—	96·22	—	—	—	94·22	—
Volume (Å^3)	2417	2941	7439	1183	2389	1250	2717
Solvent	Ethanol	Toluene	Methanol–acetone	Ethanol	Methanol–acetone	Unknown	Ethanol–acetone

(1) 5α-Cholestane
(2) 5α-Cholestan-3β-ol . $2H_2O$
(3) 5α-Cholestan-3-one
(4) 4-Cholesten-3-one
(5) 5-Cholesten-3-one
(6) 5α-Cholestan-3β-ol-6-one
(7) 5-Cholesten-3β-ol-7-one . H_2O

* Estimated standard deviation 0·04%.