Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

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X-ray study of monothiourea-cadmium sulphate dihydrate crystal.

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Work on the structure of monothiourea-cadmium sulphate dihydrate was started in connexion with an investigation of crystal structures of some of the metallic complexes of thiourea to study the sulphur bridging in coordination compounds.

The crystals of monothiourea-cadmium sulphate dihydrate are transparent rectangular plates. The *a* axis was chosen along the length, the *b* axis parallel to the width, and the *c* axis along the thickness of the plates. These crystals cleave perfectly and easily in a plane perpendicular to *b* axis.

Rotation and Weissenberg photographs were taken about *a* and *b* axes with unfiltered copper radiation. The unit cell was found to be orthorhombic, with edges $a=7.88$, $b=13.70$, and $c=16.15$ Å. These lattice parameters were measured from *a*- and *b*-axis zero layer Weissenberg photographs and refined by Taylor, Sinclair, Nelson & Riley's extrapolation method.

The conditions limiting the possible reflexions, as obtained from the zero and higher layer Weissenberg photographs taken about *a* and *b* axes, led to the space group *Pcab* (D_{2h}^{15}) without any ambiguity. The density calculated on the basis of eight molecules per unit cell agrees well with the measured value.

Experimental

A structure was derived by Patterson methods and refined by difference synthesis and least squares. *R* indices of 0.18 for the 0*kl* reflexions and 0.32 for the *h*0*l* reflexions were obtained. Three-dimensional work was started but was discontinued when the author learned that an essentially similar structure had been derived by Cavalca, Domiano, Fava Gasparri & Boldrini (1967).

The author wishes to express his gratitude to Dr E. M. Gopalakrishna and Dr B. V. R. Murty of the Physics Department, I. I. T., Madras, for their encouragement in this work. Because there was an overlap in the work, Prof. L. Cavalca was kind enough to send a preprint of his work on the same crystal for comparison; and, the author wishes to express his thanks to him for this gesture.

References

Cavalca, L., Domiano, P., Fava Gasparri, G. & Boldrini, P. (1967). *Acta Cryst.* **22**, 878.

Acta Cryst. (1967). **23**, 1096

Anomalous scattering corrections for X-rays. β-Radiations.

By A. C. Hazell, *Department of Inorganic Chemistry, University of Aarhus,* 8000 *Aarhus, Denmark*

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The real and imaginary components of the anomalous scattering corrections have been calculated for elements $Z=10$ (Ne) to $Z=98$ (Cf) for the following $K\beta_1$ radiations: Cr, Mn, Fe, Co, Ni, Cu, Zn, Mo, Rh, Pd, and Ag, by the method of Parratt & Hempstead, using the oscillator strengths calculated by Cromer.

Introduction

The total atomic scattering factor, *f*, is in general complex and given by

$$f=f_0+\Delta f'+i\Delta f'',$$

where f_0 is the Fourier transform of the electron distribution and $\Delta f'$ and $\Delta f''$ are the real and imaginary components of the anomalous scattering correction. The imaginary term is positive and corresponds to an advance in phase of the scattered radiation.

The use of anomalous scattering in the solution of the phase-problem is limited by the number of X-ray targets available. By using β radiations as well as α radiations the number of available wavelengths is increased. The lower intensity of the β radiations is compensated for in some cases by the larger values of $|\Delta f|$ which can be obtained; *e.g.* for Cu with Cu $K\beta$ radiation $\Delta f'=-4{\cdot}6$.

In the solution of centrosymmetric structures by the comparison of data collected with two wavelengths (Ramaseshan, Venkatesan & Mani, 1957; Catticha-Ellis, 1962; Hazell, 1964) it is possible (Hazell, 1966) to use the α and β radiations from the same target to obtain the two sets of data and to use the known ratio (calculated from the ratio *in vacuo* or determined experimentally) between the inten-

Table 1. *Anomalous dispersion terms* (*electron units*)

atom	Cr K beta		Mn K beta		Fe K beta		Co K beta		Ni K beta		Cu K beta		Zn K beta		Mo K beta		Rh K beta		Pd K beta		Ag K beta		atom
	Δf'	Δf"	Δf'	Δf"	Δf'	Δf"	Δf'	Δf"	Δf'	Δf"	Δf'	Δf"	Δf'	Δf"	Δf'	Δf"	Δf'	Δf"	Δf'	Δf"	Δf'	Δf"	
10 Ne	0.13	0.16	0.12	0.14	0.11	0.12	0.10	0.10	0.09	0.09	0.08	0.08	0.07	0.07	0.02	0.02	0.02	0.02	0.02	0.01	0.02	0.01	10 Ne
Na	0.17	0.23	0.16	0.20	0.14	0.17	0.13	0.15	0.12	0.13	0.10	0.12	0.09	0.10	0.03	0.03	0.03	0.02	0.03	0.02	0.02	0.02	Na
Mg	0.22	0.33	0.20	0.28	0.18	0.24	0.16	0.21	0.15	0.19	0.14	0.16	0.12	0.14	0.05	0.04	0.04	0.03	0.03	0.03	0.03	0.03	Mg
Al	0.26	0.45	0.24	0.38	0.22	0.33	0.20	0.29	0.18	0.25	0.17	0.22	0.15	0.20	0.06	0.06	0.05	0.04	0.04	0.04	0.04	0.04	Al
Si	0.31	0.60	0.29	0.51	0.26	0.44	0.24	0.39	0.22	0.34	0.21	0.30	0.19	0.26	0.07	0.08	0.06	0.06	0.06	0.06	0.05	0.05	Si
P	0.34	0.77	0.32	0.66	0.30	0.57	0.28	0.50	0.26	0.44	0.24	0.38	0.22	0.34	0.09	0.10	0.07	0.08	0.07	0.07	0.07	0.07	P
S	0.36	0.98	0.35	0.84	0.34	0.73	0.32	0.64	0.30	0.56	0.28	0.49	0.26	0.43	0.11	0.13	0.09	0.10	0.09	0.09	0.08	0.08	S
Cl	0.36	1.22	0.36	1.05	0.36	0.91	0.34	0.79	0.33	0.69	0.31	0.61	0.29	0.54	0.13	0.16	0.11	0.12	0.10	0.11	0.10	0.11	Cl
Ar	0.33	1.50	0.36	1.29	0.37	1.12	0.37	0.97	0.36	0.85	0.34	0.75	0.33	0.66	0.15	0.20	0.13	0.15	0.12	0.14	0.11	0.13	Ar
K	0.24	1.86	0.32	1.60	0.35	1.39	0.37	1.21	0.37	1.06	0.37	0.93	0.36	0.83	0.18	0.24	0.15	0.19	0.14	0.18	0.13	0.16	K
20 Ca	0.09	2.25	0.22	1.94	0.30	1.68	0.35	1.46	0.37	1.28	0.38	1.13	0.37	1.00	0.21	0.30	0.17	0.23	0.16	0.21	0.15	0.20	20 Ca
Sc	-0.20	2.71	0.06	2.33	0.20	2.02	0.29	1.76	0.34	1.54	0.37	1.36	0.38	1.20	0.23	0.36	0.20	0.28	0.19	0.26	0.18	0.24	Sc
Ti	-0.69	3.19	-0.24	2.75	0.02	2.38	0.18	2.07	0.27	1.82	0.33	1.60	0.36	1.42	0.26	0.42	0.22	0.33	0.21	0.30	0.20	0.28	Ti
V	-1.67	3.74	-0.74	3.22	-0.28	2.79	-0.01	2.43	0.15	2.13	0.25	1.88	0.31	1.66	0.28	0.49	0.24	0.38	0.23	0.35	0.22	0.33	V
Cr	-5.03	0.62	-1.72	3.74	-0.79	3.24	-0.32	2.83	-0.05	2.48	0.12	2.18	0.23	1.93	0.31	0.57	0.27	0.45	0.26	0.41	0.24	0.38	Cr
Mn	-2.32	0.72	-4.92	0.63	-1.77	3.76	-0.84	3.28	-0.36	2.87	-0.08	2.53	0.09	2.24	0.33	0.66	0.29	0.52	0.28	0.48	0.27	0.44	Mn
Fe	-1.78	0.82	-2.33	0.72	-4.84	0.64	-1.82	3.76	-0.88	3.30	-0.40	2.90	-0.12	2.57	0.35	0.76	0.31	0.59	0.30	0.55	0.29	0.51	Fe
Co	-1.49	0.93	-1.79	0.82	-2.34	0.72	-4.76	0.64	-1.87	3.76	-0.92	3.31	-0.44	2.93	0.36	0.87	0.33	0.68	0.32	0.62	0.31	0.58	Co
Ni	-1.31	1.04	-1.52	0.92	-1.82	0.81	-2.37	0.72	-4.73	0.64	-1.93	3.78	-0.97	3.34	0.37	0.99	0.35	0.77	0.34	0.71	0.33	0.66	Ni
Cu	-1.17	1.16	-1.33	1.02	-1.54	0.90	-1.84	0.80	-2.38	0.72	-4.64	0.64	-1.97	3.78	0.37	1.12	0.36	0.87	0.35	0.80	0.34	0.74	Cu
30 Zn	-1.07	1.30	-1.20	1.14	-1.35	1.01	-1.56	0.90	-1.86	0.81	-2.39	0.72	-4.54	0.65	0.37	1.26	0.37	0.99	0.36	0.91	0.36	0.84	30 Zn
Ga	-0.93	1.52	-1.04	1.34	-1.17	1.18	-1.33	1.05	-1.53	0.94	-1.82	0.84	-2.34	0.76	0.35	1.44	0.38	1.12	0.38	1.03	0.37	0.96	Ga
Ge	-0.89	1.62	-0.99	1.43	-1.09	1.26	-1.22	1.13	-1.37	1.01	-1.58	0.90	-1.87	0.81	0.32	1.60	0.37	1.24	0.37	1.15	0.37	1.06	Ge
As	-0.81	1.83	-0.89	1.61	-0.99	1.42	-1.09	1.26	-1.22	1.13	-1.37	1.01	-1.57	0.91	0.27	1.78	0.36	1.39	0.37	1.28	0.37	1.19	As
Se	-0.74	2.03	-0.81	1.79	-0.89	1.58	-0.99	1.41	-1.09	1.26	-1.22	1.13	-1.37	1.02	0.20	1.98	0.33	1.54	0.35	1.42	0.36	1.32	Se
Br	-0.69	2.26	-0.75	1.99	-0.82	1.76	-0.90	1.57	-1.00	1.40	-1.10	1.26	-1.23	1.13	0.10	2.21	0.29	1.72	0.32	1.59	0.35	1.47	Br
Kr	-0.63	2.53	-0.68	2.23	-0.75	1.97	-0.82	1.75	-0.90	1.56	-0.99	1.40	-1.10	1.26	-0.03	2.44	0.24	1.90	0.28	1.76	0.32	1.63	Kr
Rb	-0.60	2.82	-0.64	2.48	-0.69	2.19	-0.75	1.95	-0.82	1.74	-0.91	1.56	-1.00	1.41	-0.22	2.71	0.16	2.11	0.23	1.95	0.28	1.80	Rb
Sr	-0.56	3.11	-0.59	2.74	-0.63	2.42	-0.68	2.16	-0.75	1.93	-0.82	1.73	-0.90	1.55	-0.48	2.98	0.05	2.32	0.15	2.15	0.22	1.98	Sr
Y	-0.55	3.44	-0.56	3.02	-0.59	2.67	-0.63	2.38	-0.69	2.12	-0.75	1.90	-0.83	1.71	-0.86	3.29	-0.09	2.56	0.04	2.37	0.13	2.19	Y
40 Zr	-0.55	3.76	-0.54	3.31	-0.56	2.93	-0.60	2.60	-0.64	2.32	-0.70	2.08	-0.77	1.88	-1.46	3.62	-0.29	2.82	-0.12	2.60	0.02	2.41	40 Zr
Nb	-0.56	4.14	-0.52	3.64	-0.53	3.22	-0.55	2.86	-0.59	2.56	-0.63	2.29	-0.69	2.06	-2.65	3.95	-0.56	3.07	-0.31	2.84	-0.13	2.63	Nb
Mo	-0.60	4.50	-0.54	3.96	-0.52	3.50	-0.53	3.11	-0.56	2.78	-0.60	2.49	-0.65	2.24	-3.49	0.79	-0.96	3.36	-0.59	3.10	-0.34	2.87	Mo
Tc	-0.64	4.89	-0.55	4.30	-0.51	3.80	-0.51	3.38	-0.52	3.02	-0.55	2.71	-0.60	2.44	-2.36	0.86	-1.52	3.65	-0.95	3.37	-0.59	3.12	Tc
Ru	-0.73	5.29	-0.60	4.66	-0.53	4.12	-0.51	3.66	-0.51	3.27	-0.53	2.93	-0.56	2.64	-1.86	0.93	-2.82	3.97	-1.60	3.67	-1.01	3.39	Ru
Rh	-0.84	5.71	-0.67	5.02	-0.57	4.44	-0.52	3.95	-0.50	3.53	-0.51	3.16	-0.53	2.85	-1.60	1.00	-3.37	0.81	-2.89	3.99	-1.64	3.69	Rh
Pd	-0.98	6.15	-0.76	5.41	-0.62	4.78	-0.54	4.25	-0.51	3.80	-0.50	3.40	-0.51	3.06	-1.42	1.08	-2.31	0.87	-3.35	0.81	-2.95	4.00	Pd
Ag	-1.16	6.64	-0.87	5.84	-0.69	5.17	-0.58	4.59	-0.52	4.10	-0.50	3.68	-0.50	3.31	-1.28	1.16	-1.88	0.94	-2.31	0.87	-3.33	0.82	Ag
Cd	-1.39	7.20	-1.01	6.33	-0.77	5.60	-0.63	4.98	-0.54	4.44	-0.50	3.98	-0.49	3.59	-1.16	1.26	-1.62	1.01	-1.88	0.95	-2.31	0.89	Cd
In	-1.66	7.74	-1.18	6.81	-0.88	6.02	-0.65	5.35	-0.57	4.78	-0.51	4.29	-0.48	3.86	-1.05	1.35	-1.42	1.09	-1.61	1.02	-1.87	0.95	In
50 Sn	-2.01	8.37	-1.41	7.36	-1.03	6.51	-0.79	5.79	-0.63	5.17	-0.54	4.63	-0.48	4.17	-0.97	1.46	-1.28	1.18	-1.42	1.10	-1.61	1.03	50 Sn
Sb	-2.46	9.00	-1.70	7.91	-1.22	7.00	-0.91	6.22	-0.71	5.56	-0.58	4.98	-0.51	4.48	-0.89	1.57	-1.16	1.27	-1.28	1.18	-1.43	1.11	Sb
Te	-3.02	9.67	-2.05	8.50	-1.45	7.52	-1.06	6.68	-0.81	5.97	-0.64	5.35	-0.54	4.81	-0.83	1.69	-1.07	1.36	-1.17	1.27	-1.29	1.19	Te
I	-3.76	10.38	-2.50	9.13	-1.74	8.08	-1.25	7.18	-0.93	6.41	-0.72	5.74	-0.59	5.17	-0.77	1.81	-0.98	1.46	-1.07	1.36	-1.17	1.27	I
Xe	-4.65	11.11	-3.01	9.77	-2.06	8.64	-1.46	7.68	-1.07	6.86	-0.81	6.15	-0.64	5.53	-0.71	1.94	-0.91	1.56	-0.99	1.46	-1.08	1.36	Xe
Cs	-6.26	12.06	-3.76	10.61	-2.50	9.38	-1.74	8.34	-1.25	7.44	-0.92	6.67	-0.71	6.00	-0.64	2.10	-0.83	1.69	-0.90	1.58	-0.98	1.48	Cs
Ba	-9.14	10.45	-4.74	11.36	-3.06	10.04	-2.09	8.93	-1.48	7.97	-1.08	7.14	-0.81	6.42	-0.59	2.25	-0.76	1.81	-0.83	1.69	-0.90	1.58	Ba
La	-10.36	11.24	-6.34	12.20	-3.82	10.79	-2.55	9.59	-1.78	8.56	-1.28	7.67	-0.94	6.90	-0.54	2.41	-0.70	1.95	-0.76	1.82	-0.83	1.70	La
Ce	-10.35	8.82	-8.72	10.53	-4.84	11.49	-3.14	10.21	-2.17	9.11	-1.54	8.17	-1.12	7.35	-0.50	2.57	-0.65	2.07	-0.71	1.93	-0.77	1.81	Ce
Pr	-14.03	3.54	-10.34	11.16	-6.45	12.18	-3.91	10.82	-2.65	9.66	-1.86	8.66	-1.35	7.79	-0.48	2.72	-0.61	2.19	-0.66	2.05	-0.72	1.91	Pr
60 Nd	-9.35	3.79	-9.99	8.71	-8.62	10.47	-4.93	11.49	-3.23	10.26	-2.25	9.19	-1.62	8.27	-0.45	2.89	-0.57	2.33	-0.62	2.18	-0.67	2.03	60 Nd
Pm	-8.11	3.98	-12.42	9.13	-10.11	10.98	-6.21	12.03	-3.88	10.74	-2.66	9.62	-1.90	8.66	-0.43	3.03	-0.54	2.44	-0.59	2.28	-0.64	2.13	Pm
Sm	-7.23	4.27	-9.65	3.75	-9.60	8.58	-8.59	10.40	-5.04	11.46	-3.34	10.27	-2.35	9.24	-0.41	3.23	-0.51	2.60	-0.55	2.43	-0.59	2.27	Sm
Eu	-6.69	4.51	-8.21	3.95	-11.74	9.05	-11.23	10.98	-6.62	12.08	-4.09	10.83	-2.82	9.74	-0.40	3.40	-0.48	2.74	-0.52	2.56	-0.56	2.39	Eu
Gd	-6.27	4.77	-7.39	4.18	-10.12	3.69	-9.40	8.46	-8.42	10.30	-5.09	11.41	-3.41	10.26	-0.40	3.59	-0.46	2.89	-0.49	2.70	-0.53	2.52	Gd
Tb	-5.95	5.04	-6.83	4.42	-8.43	3.90	-10.82	8.92	-11.43	10.88	-6.76	12.04	-4.18	10.83	-0.40	3.79	-0.44	3.05	-0.47	2.85	-0.50	2.66	Tb
Dy	-5.67	5.34	-6.38	4.69	-7.52	4.13	-10.58	3.66	-9.17	8.38	-8.36	10.28	-5.23	11.42	-0.40	3.99	-0.43	3.22	-0.45	3.00	-0.48	2.81	Dy
Ho	-5.47	5.55	-6.07	4.87	-6.97	4.29	-8.68	3.80	-10.20	8.75	-11.9	7.8	-6.92	11.97	-0.42	4.18	-0.42	3.37	-0.44	3.15	-0.47	2.94	Ho
Er	-5.30	5.86	-5.81	5.14	-6.54	4.53	-7.73	4.01	-11.48	3.57	-9.00	8.25	-8.37	10.21	-0.44	4.41	-0.42	3.56	-0.43	3.32	-0.45	3.10	Er
Tm	-5.15	6.19	-5.58	5.42	-6.18	4.78	-7.10	4.24	-8.92	3.78	-9.80	8.68	-10.19	7.79	-0.48	4.64	-0.43	3.74	-0.43	3.49	-0.45	3.26	Tm
70 Yb	-5.04	6.45	-5.41	5.65	-5.92	4.99	-6.66	4.42	-7.90	3.94	-13.03	3.52	-8.80	8.14	-0.52	4.86	-0.44	3.92	-0.44	3.66	-0.44	3.42	70 Yb
Lu	-4.92	6.75	-5.24	5.92	-5.68	5.22	-6.29	4.63	-7.23	4.12	-9.21	3.68	-9.40	8.51	-0.57	5.09	-0.45	4.10	-0.45	3.83	-0.45	3.58	Lu
Hf	-4.82	7.15	-5.09	6.27	-5.46	5.53	-5.98	4.90	-6.73	4.37	-8.02	3.90	-14.78	8.98	-0.62	5.36	-0.47	4.32	-0.45	4.03	-0.44	3.77	Hf
Ta	-4.75	7.53	-4.97	6.60	-5.29	5.82	-5.73	5.16	-6.35	4.60	-7.32	4.11	-9.44	3.69	-0.69	5.62	-0.49	4.53	-0.46	4.23	-0.45	3.95	Ta
W	-4.68	7.97	-4.86	6.99	-5.13	6.17	-5.51	5.46	-6.03	4.87	-6.79	4.35	-8.13	3.90	-0.77	5.90	-0.53	4.76	-0.49	4.44	-0.47	4.15	W
Re	-4.62	8.46	-4.75	7.42	-4.98	6.54	-5.30	5.80	-5.75	5.16	-6.37	4.61	-7.35	4.14	-0.86	6.20	-0.56	4.99	-0.51	4.66	-0.48	4.35	Re
Os	-4.61	8.89	-4.69	7.79	-4.88	6.87	-5.15	6.09	-5.54	5.42	-6.06	4.85	-6.83	4.35	-0.98	6.49	-0.61	5.23	-0.55	4.88	-0.50	4.56	Os
Ir	-4.59	9.37	-4.63	8.21	-4.77	7.24	-5.01	6.42	-5.33	5.72	-5.78	5.11	-6.41	4.59	-1.10	6.79	-0.67	5.47	-0.55	5.11	-0.53	4.77	Ir
Pt	-4.62	9.82	-4.61	8.61	-4.71	7.60	-4.91	6.73	-5.19	6.00	-5.57	5.36	-6.10	4.81	-1.27	7.11	-0.75	5.73	-0.65	5.35	-0.59	5.00	Pt
Au	-4.65	10.45	-4.58	9.17	-4.63	8.08	-4.79	7.16	-5.03	6.38	-5.36	5.70	-5.81	5.12	-1.43	7.47	-0.82	6.02	-0.71	5.62	-0.62	5.25	Au
80 Hg	-4.69	11.08	-4.56	9.72	-4.57	8.57	-4.69	7.59	-4.89	6.76	-5.17	6.05	-5.56	5.43	-1.63	7.84	-0.91	6.32	-0.78	5.90	-0.68	5.51	80 Hg
Tl	-4.78	11.63	-4.59	10.20	-4.55	8.99	-4.62	7.97	-4.78	7.10	-5.02	6.34	-5.36	5.69	-1.87	8.19	-1.02	6.60	-0.86	6.16	-0.74	5.75	Tl
Pb	-4.90	12.31	-4.64	10.80	-4.55	9.52	-4.58	8.44	-4.70	7.51	-4.91	6.72	-5.19	6.03	-2.16	8.60	-1.16	6.93	-0.97	6.47	-0.83	6.04	Pb
Bi	-5.04	13.01	-4.70	11.41	-4.55	10.06	-4.53	8.92	-4.61	7.94	-4.78	7.10	-5.03	6.37	-2.49	9.01	-1.31	7.26	-1.09	6.77	-0.92	6.33	Bi
Po	-5.17	13.68	-4.75	12.00	-4.54	10.58	-4.48	9.38	-4.53	8.35	-4.66	7.47	-4.88	6.70	-2.86	9.40	-1.47	7.57	-1.21	7.06	-1.02	6.60	Po
At	-5.41	14.44	-4.88	12.66	-4.60	11.17	-4.49	9.90	-4.50	8.81	-4.60	7.88	-4.78	7.07	-3.36	9.85	-1.68	7.93	-1.38	7.40	-1.15	6.92	At
Rn	-5.66	15.22	-5.02	13.35	-4.66	11.77	-4.49	10.43	-4.45	9.29	-4.51	8.31	-4.66	7.45	-3.96	10.28	-1.91	8.28	-1.56	7.73	-1.29	7.22	Rn
Fr	-5.98	16.07	-5.21	14.09	-4.76	12.43	-4.53	11.01	-4.44	9.81	-4.46	8.77	-4.57	7.87	-4.80	10.78	-2.19	8.68	-1.77	8.10	-1.45	7.57	Fr
Ra	-6.41	17.02	-5.46	14.92	-4.90	13.16	-4.59	11.66	-4.45	10.39	-4.43	9.29	-4.50	8.33	-6.16	11.28	-2.53	9.09	-2.03	8.48	-1.65	7.92	Ra
Ac	-6.87	17.99	-5.74	15.78	-5.06	13.91	-4.67	12.33	-4.47	10.98	-4.40	9.82	-4.43	8.81	-7.72	9.59	-2.93	9.50	-2.32	8.87	-1.88	8.29	Ac
90 Th	-7.47	18.78	-6.10	16.47	-5.28	14.53	-4.80	12.88	-4.54	11.46	-4.42	10.25	-4.41	9.20	-8.86	7.05	-3.43	9.90	-2.69	9.24	-2.16	8.64	90 Th
Pa	-8.07	19.67	-6.45	17.25	-5.50	15.21	-4.93	13.48	-4.60	12.00	-4.43	10.73	-4.39	9.63	-6.93	7.34	-4.06	10.34	-3.13	9.65	-2.48	9.02	Pa
U	-9.02	20.55	-7.00	18.02	-5.84	15.89	-5.15	14.09	-4.74	12.54	-4.51	11.21	-4.42	10.06	-6.66	7.64	-4.94	10.79	-3.68	10.07	-2.88	9.41	U
Np	-10.00	21.46	-7.48	18.82	-6.13	16.60	-5.32	14.71	-4.83	13.10	-4.55	11.71	-4.42	10.51	-6.56	7.95	-6.50	11.23	-4.40	10.48	-3.35	9.80	Np
Pu	-11.94	22.32	-8.16	19.57	-6.54	17.26	-5.59	15.30	-5.00	13.62	-4.66	12.18	-4.48	10.93	-6.77	8.26	-7.67	9.53	-5.48	10.94	-3.98	10.22	Pu
Am	-12.45	21.23	-9.01	20.42	-7.01	18.01	-5.88	15.96	-5.18	14.21	-4.76	12.71	-4.52	11.40	-7.17	8.57	-7.69	6.87	-10.3	9.2	-4.80	10.61	Am
Cm	-15.24	22.22	-10.28	21.38	-7.62	18.86	-6.25	16.71	-5.42	14.88	-4.91	13.31	-4.61	11.94	-7.99	8.93	-6.60	7.16	-8.91	9.67	-6.23	11.09	Cm
Bk	-13.43	20.30	-12.32	20.29	-8.33	19.63	-6.66	17.40	-5.68	15.49	-5.08	13.85	-4.71	12.43	-10.03	9.28	-6.25	7.44	-6.95	6.93	-7.53	9.39	Bk
Cf	-13.55	21.10	-12.50	21.12	-9.29	20.43	-7.19	18.11	-6.02	16.12	-5.30	14.41	-4.86	12.93	-9.56	4.41	-6.19	7.72	-6.34	7.20	-7.84	6.72	Cf

Table 2. *Interpolated values (Rydbergs) for the absorption edges not listed by Sandström or by Cromer*

The values for potassium were obtained by linear interpolation, the others by four-point interpolation.

	$1s\frac{1}{2}$	$2s\frac{1}{2}$	$2p\frac{1}{2}$	$2p\frac{3}{2}$	$3s\frac{1}{2}$	$3p\frac{1}{2}$	$3p\frac{3}{2}$	$3d\frac{3}{2}$	$3d\frac{5}{2}$	$4s\frac{1}{2}$	$4p\frac{1}{2}$	$4p\frac{3}{2}$	$4d\frac{3}{2}$	$4d\frac{5}{2}$	$4f\frac{5}{2}$	$4f\frac{7}{2}$
K	—	—	—	—	—	1·5	1·5									
Kr	1055	141	127	123	21	16	16	6·9	6·7							
Ra	7676	—	—	—	—	329	—	—	—	—	—	—	—	44	22	21

sities of the α and β radiations to obtain the scale factor between the two sets of data.

The anomalous scattering corrections have therefore been calculated for elements $Z=10$ (Ne) to $Z=98$ (Cf) for the $K\beta_1$ radiations of Cr, Mn, Fe, Co, Ni, Cu, Zn, Mo, Rh, Pd, and Ag.

Calculations

The values of $\Delta f'$ and $\Delta f''$ were calculated by the method of Parratt & Hempstead (1954) and are listed in Table 1; values are printed to only one decimal place if the wavelengths of the incident radiation and one of the absorption edges differ by less than 0·1 %; this is not intended as an absolute measure of the accuracy but to indicate which values are most likely to be in error. The oscillator strengths used were those calculated by Cromer (1965); the frequencies of the absorption edges were those of Sandström (1957) or the eigenvalues calculated by Cromer (1965) where Sandström (1957) gave no values. These two sources gave values for all but a few edges for which the frequencies were obtained by interpolation (Table 2). The wavelengths of the β_1 incident radiations are those listed in *International Tables for X-ray Crystallography* (1962).

For elements Ne to and including Cl four edges were considered; Ar to Ni, seven edges; Cu to Xe, nine edges; Cs to Lu, fourteen edges; Hf to Cf, sixteen edges. For all elements the values of n used were: 11/4 for the $1s\frac{1}{2}$ edge, 7/3 for the $2s\frac{1}{2}$ edge, and 5/2 for the remaining edges. These are the values of n used by Dauben & Templeton (1955) and by Cromer (1965) in their calculations of anomalous scattering corrections for α radiations. Neither damping effects nor the change of Δf with $\sin(\theta/\lambda)$ have been considered.

The calculations were carried out with a program written in GIER-Algol on the Aarhus University GIER computer. The program was checked by calculating some values for α radiations and comparing them with those of Cromer (1965).

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The rigid-body motion of molecules referred to triclinic coordinates.

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The rigid body analysis of the anisotropic temperature parameters, including the translation–libration correlation term introduced by Schomaker & Trueblood, is presented in triclinic coordinates. It is shown that the equations relating U^{ij} to **T**, **S** and **ω** have the same form as in orthogonal coordinates provided that reduced covariant coordinates defined by $x_i g^{-\frac{1}{2}}$ are used.

The analysis of the anisotropic thermal vibrations in molecular crystals in terms of rigid-body motions of the molecules was first suggested by Cruickshank (1956). In the original work the librations were taken to be about the mass-centre of the molecule as origin, but this procedure was criticized by Pawley (1963) who found improved agreement in the case of azulene by moving the origin 0·53 Å from the mass centre. A survey of the whole problem by Schomaker & Trueblood (1966) showed that the choice of origin is in fact arbitrary provided that correlations between translations and librations are properly taken into account. In order, however, to ensure that results published by different workers should be directly comparable, they suggested a procedure for specifying a unique coordinate system, a procedure that involves reducing the complex 20-parameter rigid-body motion to three principal mean-square translations and three screw motions about and along non-intersecting orthogonal axes. The object of the present note is to suggest that compatibility between different workers can more easily be achieved by referring everything to the crystal axes. A secondary object is to show how the use of the full notation of tensor algebra helps materially to avoid such errors as have been pointed out by Scheringer (1966).

When a rigid body is rotated through a small angle **λ** and simultaneously undergoes a translation **t**, a point of