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Dispersion corrections for X-ray scattering of atoms for Ag $K\alpha$ and Co $K\alpha$ radiations.

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Dispersion corrections for X-ray scattering of atoms for Cr $K\alpha$, Cu $K\alpha$ and Mo $K\alpha$ radiations have been tabulated by Dauben & Templeton (1955) for $\sin\theta/\lambda=0$ and in *International Tables for X-ray Crystallography* (1962) for various values of $\sin\theta/\lambda$. Although these are the most commonly used radiations, it is desirable that dispersion corrections for other conventional radiations should be readily available. Corrections for several elements for Ag $K\alpha$ and Co $K\alpha$ radiations were required for work in progress in this laboratory and the calculation of these was therefore extended to cover elements with atomic numbers up to 92 and for suitable ranges of $\sin\theta/\lambda$. These corrections are listed in Tables 1 and 2; values for $\sin\theta/\lambda=0{\cdot}6$ Å^{-1} for Co $K\alpha$ radiation have been included to permit the estimation of values for $\sin\theta/\lambda$ between 0·4 and 0·56 Å^{-1} ($=1/\lambda$).

The corrections for $\sin\theta/\lambda$ have been calculated by the methods of Parratt & Hempstead (1954) for the

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Table 1. *Dispersion corrections for* Ag $K\alpha$ *radiation*
($\lambda=0{\cdot}5609$ Å)

	$\Delta f'$				$\Delta f''$			
	$\sin\theta/\lambda$ (Å^{-1})				$\sin\theta/\lambda$ (Å^{-1})			
Atom	0	0·6	1·0	1·3	0	0·6	1·0	1·3
6 C	0·00	0·00	0·00	0·00				
7 N	0·01	0·01	0·01	0·01				
8 O	0·01	0·01	0·01	0·01				
9 F	0·02	0·02	0·01	0·01				
10 Ne	0·02	0·02	0·02	0·02				
11 Na	0·03	0·03	0·03	0·02				
12 Mg	0·04	0·04	0·03	0·03				
13 Al	0·05	0·05	0·04	0·04	0·0	0·0	0·0	0·0
14 Si	0·06	0·06	0·05	0·05	0·1	0·1	0·0	0·0
15 P	0·08	0·07	0·06	0·06	0·1	0·1	0·1	0·1
16 S	0·09	0·09	0·08	0·07	0·1	0·1	0·1	0·1
17 Cl	0·11	0·10	0·09	0·08	0·1	0·1	0·1	0·1
18 A	0·13	0·12	0·11	0·10	0·1	0·1	0·1	0·1
19 K	0·16	0·14	0·13	0·12	0·2	0·2	0·1	0·1
20 Ca	0·18	0·17	0·15	0·14	0·2	0·2	0·2	0·2
21 Sc	0·21	0·19	0·17	0·16	0·3	0·2	0·2	0·2
22 Ti	0·23	0·21	0·19	0·18	0·3	0·3	0·3	0·2
23 V	0·26	0·23	0·21	0·20	0·4	0·3	0·3	0·3
24 Cr	0·29	0·26	0·24	0·22	0·4	0·4	0·4	0·4
25 Mn	0·31	0·28	0·26	0·24	0·5	0·5	0·5	0·4
26 Fe	0·34	0·30	0·28	0·26	0·6	0·6	0·5	0·5
27 Co	0·36	0·32	0·30	0·28	0·7	0·7	0·6	0·6
28 Ni	0·38	0·34	0·31	0·29	0·8	0·8	0·7	0·7
29 Cu	0·39	0·35	0·32	0·30	0·9	0·9	0·8	0·8
30 Zn	0·40	0·36	0·33	0·31	1·0	0·9	0·9	0·9
31 Ga	0·40	0·36	0·33	0·30	1·1	1·1	1·1	1·0
32 Ge	0·39	0·35	0·32	0·29	1·3	1·2	1·2	1·1
33 As	0·38	0·33	0·30	0·27	1·4	1·4	1·4	1·3
34 Se	0·34	0·30	0·26	0·23	1·6	1·6	1·5	1·4
35 Br	0·29	0·25	0·21	0·18	1·7	1·7	1·7	1·6
36 Kr	0·22	0·18	0·14	0·11	2·0	1·9	1·9	1·8
37 Rb	0·12	0·08	0·04	0·02	2·2	2·1	2·1	2·0
38 Sr	−0·01	−0·05	−0·09	−0·12	2·4	2·3	2·3	2·2
39 Y	−0·18	−0·22	−0·26	−0·28	2·6	2·5	2·5	2·4
40 Zr	−0·40	−0·44	−0·48	−0·51	2·9	2·9	2·8	2·7
41 Nb	−0·69	−0·73	−0·78	−0·81	3·2	3·1	3·1	3·0
42 Mo	−1·24	−1·28	−1·32	−1·34	3·6	3·5	3·5	3·3
43 Tc	−1·77	−1·82	−1·85	−1·87	3·9	3·9	3·8	3·6
44 Ru	*	*	*	*	3·1	3·0	2·9	2·8
45 Rh	−2·57	−2·62	−2·65	−2·67	0·7	0·7	0·6	0·5
46 Pd	−1·98	−2·03	−2·06	−2·10	0·8	0·7	0·6	0·5
47 Ag	−1·64	−1·69	−1·73	−1·77	0·8	0·8	0·7	0·6
48 Cd	−1·45	−1·49	−1·54	−1·58	0·9	0·8	0·8	0·7
49 In	−1·29	−1·35	−1·39	−1·44	1·0	0·9	0·8	0·7
50 Sn	−1·21	−1·26	−1·32	−1·37	1·1	1·0	0·9	0·8
51 Sb	−1·06	−1·12	−1·17	−1·23	1·2	1·1	1·0	0·9
52 Te	−0·97	−1·03	−1·08	−1·14	1·3	1·2	1·1	1·0
53 I	−0·89	−0·95	−1·01	−1·07	1·4	1·3	1·2	1·1
54 Xe	−0·83	−0·89	−0·95	−1·01	1·5	1·4	1·3	1·2
55 Cs	−0·77	−0·83	−0·89	−0·96	1·6	1·6	1·4	1·3
56 Ba	−0·70	−0·76	−0·83	−0·90	1·8	1·7	1·5	1·4
57 La	−0·63	−0·70	−0·77	−0·84	1·9	1·8	1·7	1·5
58 Ce	−0·58	−0·65	−0·72	−0·80	2·1	2·0	1·9	1·7
59 Pr	−0·54	−0·61	−0·69	−0·76	2·2	2·1	1·9	1·8
60 Nd	−0·50	−0·57	−0·65	−0·74	2·3	2·2	2·1	1·9
61 Pm	−0·46	−0·53	−0·62	−0·71	2·5	2·4	2·2	2·0
62 Sm	−0·44	−0·52	−0·60	−0·69	2·6	2·5	2·4	2·2
63 Eu	−0·42	−0·50	−0·58	−0·67	2·8	2·7	2·5	2·3
64 Gd	−0·41	−0·49	−0·57	−0·66	2·9	2·8	2·7	2·5
65 Tb	−0·38	−0·46	−0·55	−0·64	3·1	3·0	2·9	2·7
66 Dy	−0·35	−0·44	−0·54	−0·63	3·3	3·2	3·1	2·8
67 Ho	−0·34	−0·44	−0·54	−0·63	3·6	3·4	3·3	3·1
68 Er	−0·32	−0·43	−0·53	−0·63	3·7	3·6	3·4	3·2
69 Tm	−0·31	−0·42	−0·52	−0·62	4·0	3·8	3·7	3·4
70 Yb	−0·30	−0·41	−0·52	−0·62	4·2	4·1	3·9	3·6
71 Lu	−0·31	−0·42	−0·53	−0·64	4·4	4·3	4·1	3·8
72 Hf	−0·32	−0·43	−0·56	−0·66	4·7	4·6	4·4	4·1
73 Ta	−0·32	−0·44	−0·58	−0·67	5·0	4·8	4·6	4·3
74 W	−0·35	−0·47	−0·61	−0·71	5·3	5·1	4·9	4·6
75 Re	−0·39	−0·51	−0·65	−0·76	5·6	5·4	5·2	4·9
76 Os	−0·45	−0·56	−0·71	−0·81	5·9	5·7	5·5	5·2
77 Ir	−0·50	−0·62	−0·76	−0·87	6·2	6·0	5·8	5·5
78 Pt	−0·55	−0·67	−0·81	−0·94	6·6	6·4	6·1	5·8
79 Au	−0·68	−0·80	−0·95	−1·06	6·9	6·7	6·4	6·1
80 Hg	−0·90	−1·01	−1·16	−1·28	7·3	7·1	6·8	6·5
81 Tl	−1·03	−1·14	−1·29	−1·42	7·7	7·4	7·2	6·8
82 Pb	−1·16	−1·28	−1·43	−1·55	8·1	7·8	7·5	7·2
83 Bi	−1·32	−1·44	−1·58	−1·71	8·5	8·3	8·0	7·6
84 Po	−1·54	−1·65	−1·80	−1·92	9·0	8·7	8·4	8·1
85 At	−1·74	−1·85	−2·00	−2·12	9·4	9·1	8·7	8·4
86 Rn	−1·94	−2·05	−2·23	−2·32	9·8	9·6	9·3	8·8
87 Fr	−2·23	−2·34	−2·50	−2·60	10·3	10·0	9·7	9·3
88 Ra	−2·49	−2·60	−2·76	−2·85	10·8	10·5	10·2	9·7
89 Ac	−3·00	−3·10	−3·26	−3·34	11·3	11·0	10·6	10·2
90 Th	−3·57	−3·67	−3·81	−3·87	11·8	11·5	11·1	10·6
91 Pa	−4·03	−4·12	−4·26	−4·32	12·4	12·0	11·7	11·2
92 U	−4·65	−4·73	−4·87	−4·92	13·0	12·6	12·2	11·7

Table 2. *Dispersion corrections for* Co $K\alpha$ *radiation*
($\lambda = 1{\cdot}790$ Å)

	$\Delta f'$			$\Delta f''$				$\Delta f'$			$\Delta f''$		
	sin θ/λ (Å^{-1})			sin θ/λ (Å^{-1})				sin θ/λ (Å^{-1})			sin θ/λ (Å^{-1})		
Atom	0	0·4	0·6	0	0·4	0·6	Atom	0	0·4	0·6	0	0·4	0·6
3 Li	0·00	0·00	0·00				48 Cd	−0·99	−1·06	−1·13	6·5	6·2	6·0
4 Be	0·01	0·01	0·01				49 In	−1·16	−1·23	−1·28	6·9	6·6	6·4
5 B	0·01	0·01	0·01				50 Sn	−1·33	−1·39	−1·45	7·5	7·2	6·9
6 C	0·03	0·03	0·02				51 Sb	−1·57	−1·63	−1·69	8·1	7·8	7·5
7 N	0·04	0·04	0·04	0·0	0·0	0·0	52 Te	−1·89	−1·96	−2·00	8·6	8·3	7·9
8 O	0·06	0·06	0·06	0·1	0·0	0·0	53 I	−2·27	−2·33	−2·37	9·2	8·8	8·5
9 F	0·08	0·08	0·07	0·1	0·1	0·1	54 Xe	−2·76	−2·81	−2·85	10·0	9·6	9·2
10 Ne	0·10	0·10	0·09	0·1	0·1	0·1	55 Cs	−3·37	−3·43	−3·45	10·6	10·3	9·9
11 Na	0·15	0·14	0·13	0·2	0·2	0·2	56 Ba	−4·01	−4·07	−4·08	11·3	10·9	10·6
12 Mg	0·19	0·17	0·17	0·2	0·2	0·2	57 La	−5·03	−5·07	−5·07	12·0	11·6	11·2
13 Al	0·22	0·21	0·20	0·3	0·3	0·3	58 Ce	−6·07	−6·10	−6·11	12·7	12·3	11·8
14 Si	0·26	0·25	0·24	0·4	0·4	0·4	59 Pr	*	*	*	13·3	12·9	12·4
15 P	0·30	0·29	0·27	0·6	0·6	0·5	60 Nd	−9·43	−9·43	−9·38	13·5	13·1	12·7
16 S	0·33	0·31	0·30	0·7	0·7	0·7	61 Pm	*	*	*	13·1	12·6	12·1
17 Cl	0·37	0·34	0·32	0·9	0·9	0·9	62 Sm	−10·73	−10·75	−10·70	14·1	13·5	12·9
18 A	0·38	0·34	0·32	1·1	1·1	1·1	63 Eu	*	*	*	4·0	3·6	3·3
19 K	0·36	0·32	0·30	1·3	1·3	1·3	64 Gd	−9·41	−9·49	−9·47	4·3	3·9	3·5
20 Ca	0·30	0·25	0·23	1·7	1·7	1·6	65 Tb	−8·12	−8·23	−8·23	4·6	4·1	3·7
21 Sc	0·17	0·12	0·10	2·0	2·0	1·9	66 Dy	−7·19	−7·30	−7·33	4·9	4·5	4·0
22 Ti	−0·06	−0·10	−0·12	2·4	2·4	2·3	67 Ho	−6·68	−6·80	−6·87	5·2	4·8	4·3
23 V	−0·36	−0·41	−0·43	2·8	2·8	2·7	68 Er	−6·19	−6·32	−6·39	5·5	5·0	4·6
24 Cr	−0·87	−0·91	−0·94	3·4	3·3	3·2	69 Tm	−5·78	−5·90	−5·99	5·8	5·3	4·8
25 Mn	−1·92	−1·95	−1·96	4·0	3·9	3·8	70 Yb	−5·47	−5·60	−5·73	6·2	5·8	5·3
26 Fe	−3·50	−3·51	−3·52	0·5	0·5	0·4	71 Lu	−5·22	−5·34	−5·48	6·5	6·1	5·5
27 Co	−2·17	−2·20	−2·24	0·6	0·6	0·5	72 Hf	−4·96	−5·09	−5·21	6·9	6·4	6·0
28 Ni	−1·70	−1·73	−1·77	0·7	0·7	0·6	73 Ta	−4·74	−4·87	−5·00	7·3	6·8	6·3
29 Cu	−1·43	−1·47	−1·51	0·8	0·8	0·7	74 W	−4·59	−4·73	−4·86	7·8	7·3	6·7
30 Zn	−1·23	−1·30	−1·33	0·9	0·9	0·8	75 Re	−4·46	−4·58	−4·73	8·3	7·8	7·1
31 Ga	−1·08	−1·15	−1·19	1·1	1·0	0·9	76 Os	−4·39	−4·51	−4·64	8·7	8·2	7·6
32 Ge	−0·96	−1·03	−1·07	1·2	1·1	1·0	77 Ir	−4·30	−4·42	−4·56	9·3	8·7	8·1
33 As	−0·86	−0·93	−0·97	1·4	1·3	1·2	78 Pt	−4·24	−4·36	−4·50	9·8	9·1	8·5
34 Se	−0·77	−0·84	−0·89	1·6	1·5	1·4	79 Au	−4·13	−4·25	−4·39	10·3	9·7	8·9
35 Br	−0·70	−0·77	−0·83	1·8	1·7	1·6	80 Hg	−4·08	−4·21	−4·33	10·9	10·2	9·6
36 Kr	−0·64	−0·71	−0·77	2·1	1·9	1·8	81 Tl	−4·10	−4·23	−4·35	11·5	10·8	10·1
37 Rb	−0·59	−0·66	−0·72	2·3	2·1	2·0	82 Pb	−4·19	−4·31	−4·43	12·1	11·4	10·7
38 Sr	−0·55	−0·62	−0·68	2·5	2·4	2·2	83 Bi	−4·23	−4·35	−4·46	12·8	12·0	11·2
39 Y	−0·52	−0·58	−0·64	2·8	2·7	2·5	84 Po	−4·39	−4·49	−4·61	13·4	12·7	11·7
40 Zr	−0·51	−0·58	−0·64	3·2	3·0	2·8	85 At	−4·57	−4·66	−4·77	14·1	13·4	12·4
41 Nb	−0·51	−0·58	−0·63	3·4	3·2	3·0	86 Rn	−4·81	−4·90	−5·00	14·7	13·9	12·9
42 Mo	−0·53	−0·60	−0·66	3·8	3·6	3·4	87 Fr	−5·05	−5·13	−5·22	15·4	14·5	13·6
43 Tc	−0·54	−0·61	−0·68	4·2	4·0	3·8	88 Ra	−5·30	−5·36	−5·45	16·1	15·2	14·2
44 Ru	−0·60	−0·67	−0·73	4·6	4·3	4·1	89 Ac	−5·55	−5·61	−5·68	16·9	16·0	14·9
45 Rh	−0·66	−0·73	−0·79	5·0	4·7	4·5	90 Th	−5·86	−5·91	−5·97	17·6	16·7	15·5
46 Pd	−0·74	−0·81	−0·87	5·4	5·2	4·9	91 Pa	−6·28	−6·32	−6·36	18·3	17·2	16·1
47 Ag	−0·85	−0·93	−0·98	5·9	5·6	5·4	92 U	−6·61	−6·64	−6·66	19·1	18·0	16·8

contributions of the K, L, M and N electrons with the L shell subdivided into L_{I}, L_{II}, and L_{III} shells. The oscillator strengths for the K and L shells have been estimated by fitting smooth curves to the data tabulated by Compton & Allison (1935) and James (1958), together with those of Eisenlohr & Müller (1954), and the oscillator strengths for the M and N shells are based on the values given by Parratt & Hempstead in their examples. The exponents p have also been chosen according to their examples and the values of $Re[J_q - 1]$ determined by interpolation between their tabulated values. Damping effects have been neglected. The corrections for other values of sin θ/λ have been derived in the same way as those given in the *International Tables*, using the data of Veenendaal, MacGillavry, Stam, Potters & Römgens (1959).

The uncertainties associated with the parameters involved in these calculations are such that the reliability of the tabulated corrections is difficult to estimate and the fact that values of $\Delta f'$ have been given to two decimal places should not be taken as any indication of their accuracy. Values close to absorption edges are particularly uncertain, and in some cases have not been calculated (indicated by asterisks in the tables).

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The space group and unit cell dimensions of the tris(*p*-halophenyl)amines.

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The C–N–C bond angle in triphenylamine is of theoretical interest. Efforts to determine the structure of solid triphenylamine by X-ray diffraction studies terminated with the discovery that there are either two or four molecules in the asymmetric unit (Howells, 1950; Iveronova & Rojtburd, 1952; Howells, Lovell, Rogers & Wilson, 1954). Since it seemed possible the tris(*p*-halophenyl)amines might have unit cells with fewer molecules in the asymmetric unit, a preliminary investigation of these compounds was carried out.

The space group and unit-cell dimensions were determined from oscillation, Weissenberg, and precession photographs using Cu $K\alpha$ ($\lambda = 1{\cdot}5418$ Å) and Mo $K\alpha$ ($\lambda = 0{\cdot}7107$ Å) radiation. The fluoro, chloro, and bromo compounds are monoclinic. The iodo compound belongs to the trigonal crystal system. For the monoclinic compounds the extinctions observed were: $0k0$ with k odd and $h0l$ with h odd. For the trigonal compound there were no extinctions for the rhombohedral setting.

The densities of the fluoro and chloro compounds were measured by flotation in aqueous potassium iodide, and those of the bromo and iodo compounds in solutions of bromoform and cyclohexane. A comparison of the cell dimensions and an approximate comparison of intensities indicate that the chloro and bromo compounds are isomorphous. The fluoro compound may be isomorphous with these, but the evidence is not as conclusive.

About the time the work reported here was finished, we discovered we had overlooked the electron diffraction work of Sasaki, Kimura & Kubo (1959) on gaseous triphenylamine, in which they found a bond angle of $116 \pm 2°$. Therefore, the primary question has been answered. The trend, if any, in the C–N–C angle with changing halogen substituents would also be an interesting question, but we plan no further work on these compounds.

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Table 1. *Crystal data of tris(p-halophenyl)amines*

	$N(C_6H_4F)_3$	$N(C_6H_4Cl)_3$	$N(C_6H_4Br)_3$	$N(C_6H_4I)_3$ hexagonal	$N(C_6H_4I)_3$ rhombohedral
a	$10{\cdot}27 \pm 0{\cdot}01$ Å	$11{\cdot}25 \pm 0{\cdot}02$ Å	$11{\cdot}48 \pm 0{\cdot}01$ Å	$44{\cdot}52 \pm 0{\cdot}11$ Å	$25{\cdot}93 \pm 0{\cdot}06$ Å
b	$17{\cdot}51 \pm 0{\cdot}02$ Å	$16{\cdot}67 \pm 0{\cdot}02$ Å	$16{\cdot}74 \pm 0{\cdot}02$ Å	—	—
c	$8{\cdot}53 \pm 0{\cdot}02$ Å	$9{\cdot}21 \pm 0{\cdot}01$ Å	$9{\cdot}41 \pm 0{\cdot}01$ Å	$10{\cdot}19 \pm 0{\cdot}04$ Å	—
β	$104{\cdot}6 \pm 0{\cdot}1°$	$107{\cdot}2 \pm 0{\cdot}1°$	$107{\cdot}5 \pm 0{\cdot}1°$	—	—
α	—	—	—	—	$118° 19' \pm 30'$
U	1485 Å^3	1650 Å^3	1725 Å^3	17490 Å^3	5830 Å^3
D_m	$1{\cdot}35 \pm 0{\cdot}01$ g.cm^{-3}	$1{\cdot}41 \pm 0{\cdot}01$ g.cm^{-3}	$1{\cdot}84 \pm 0{\cdot}02$ g.cm^{-3}	$2{\cdot}14 \pm 0{\cdot}01$ g.cm^{-3}	
Z	4	4	4	36	12
D_c	$1{\cdot}352 \pm 0{\cdot}002$ g.cm^{-3}	$1{\cdot}416 \pm 0{\cdot}002$ g.cm^{-3}	$1{\cdot}867 \pm 0{\cdot}003$ g.cm^{-3}	$2{\cdot}139 \pm 0{\cdot}006$ g.cm^{-3}	
S.G.	$P2_1/a$	$P2_1/a$	$P2_1/a$	$R3$ or $R\bar{3}$	