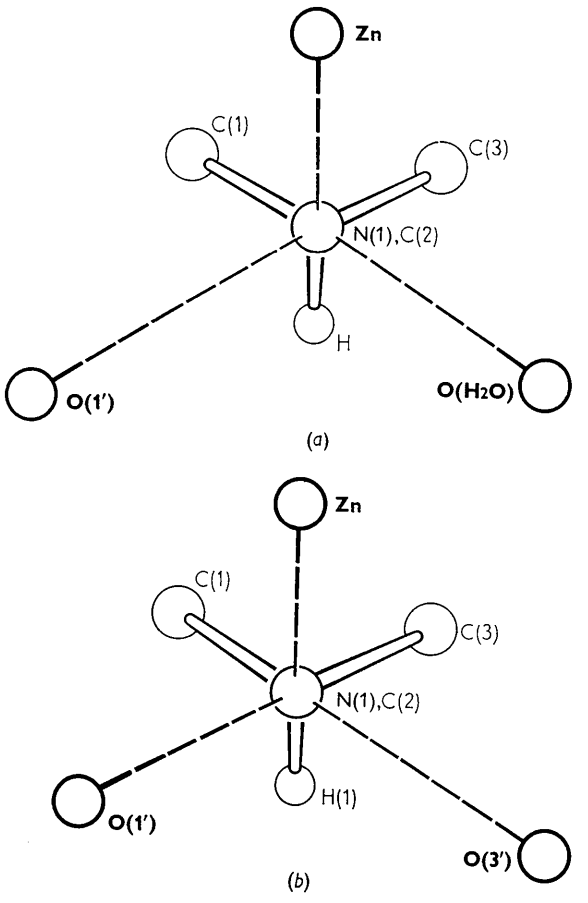

Fig. 3. View down N(1)–C(2) in histidino–zinc complexes: (*a*) in the dihydrate, (*b*) in the pentahydrate.

are shown. We feel it unnecessary to make the same detailed comparison among the various sets of bond angles as is done above for the bond distances.

There is an interesting point regarding the conformation of the histidino groups in the three compounds which has not been mentioned previously. DL&R pointed out that in histidine hydrochloride the disposition of the three proposed hydrogen bonds formed by the $-NH_3^+$ groups was satisfactory in terms of the angles C(2)–N(1)–H and H–N(1)–H, but they did not discuss the positions of these hydrogen atoms relative to the ligands of C(2). A view down the N(1)–C(2) bond is shown in Fig. 2, where it is seen that the conformation is the expected staggered one. Examination of the two histidino–zinc complexes shows that although in them the $-NH_2$ groups form, in addition to the N · · · Zn bond, two hydrogen bonds, one to an oxygen atom of a different histidino group and one to a water molecule, the conformation in each still closely approaches being exactly staggered, as shown in Fig. 3. We interpret these results to mean that preservation of the staggered conformation should be included in models proposed for larger molecules or complexes of which the histidino group is a part, unless stronger structural restrictions can be found which force relaxation of this condition.

This work was supported by a grant from the U.S. Army Research Office (Durham).

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The Fourier transform of the regular tetrahedron.

By RICHARD H. STANFORD, Jr., *Gates and Crellin Laboratories of Chemistry,* California Institute of Technology, Pasadena, California, U.S.A.*

(*Received* 13 *April* 1964)

As a part of the work on the crystalline structure of proteins, an investigation on trypsin has been initiated in these laboratories (Kay, 1963). Both the PtI_6^{2-} and the HgI_4^{2-} ions have been used to prepare isomorphous heavy-atom derivatives of diisopropylphosphoryltrypsin by diffusion of the ions from solution into the crystals.

The effect of orientation of an octahedral ion such as PtI_6^{2-} on its Fourier transform has been examined (Stanford, 1962), and it seems advisable now to perform a similar investigation for a regular tetrahedron, such as the iodine atoms in HgI_4^{2-}.

The transform of four atoms, each with atomic scattering factor f and located at $(b/2, b/2, b/2)$, $(-b/2, -b/2, b/2)$, $(-b/2, b/2, -b/2)$, and $(b/2, -b/2, -b/2)$, is given by:

$$F = A + iB ,$$

where

$$A = 4f \cos 2\pi h \cos 2\pi k \cos 2\pi l$$

and

$$B = 4f \sin 2\pi h \sin 2\pi k \sin 2\pi l .$$

The averaging of the function F is carried out on the

* Contribution No. 3106 from the Gates and Crellin Laboratories of Chemistry. These studies were aided by Contract Nonr–220(38) (Nr. 304–110) between the Office of Naval Research, Department of the Navy and the California Institute of Technology.

surface of a sphere in reciprocal space, which imposes the condition that

$$h^2+k^2+l^2=(b\sin\theta/\lambda)^2=p^2$$

where h, k, and l are not necessarily integers.

By changing to spherical polar coordinates, the expression for the average value of the transform becomes:

$$\bar{F}=(2f/\pi)\int_0^{\pi}\int_0^{\pi}\{\cos(2\pi p\sin\theta\cos\varphi)\cos(2\pi p\sin\theta\sin\varphi)\times\cos(2\pi p\cos\theta)+i\sin(2\pi p\sin\theta\cos\varphi)\times\sin(2\pi p\sin\theta\sin\varphi)\sin(2\pi p\cos\theta)\}\sin\theta\,d\theta\,d\varphi\,.$$

Evaluation of this integral leads to:

$$\bar{F}=4f\,(\sin(2\sqrt{(3)}\pi p))/(2\sqrt{(3)}\pi p)\,.$$

If $c=a\sin\theta/\lambda$, where $a/2$ is the radius of the tetrahedron and $b=a/\sqrt{3}$, then $c=\sqrt{(3)}b\,(\sin\theta)/\lambda=\sqrt{(3)}p$.

Therefore

$$\bar{F}=4f\,\frac{\sin(2\pi c)}{(2\pi c)}\,.$$

This is the transform of a spherical shell multiplied by $4f$. The function $|\bar{F}|/f$ is shown in curve C, Fig. 1 and selected values are listed in column 4, Table 1.

The expression for the mean-square value of F is:

$$\overline{|F|^2}=(32f^2/\pi)\int_0^{\pi/2}\int_0^{\pi/2}\{1-\sin^2(2\pi p\sin\theta\cos\varphi)-\sin^2(2\pi p\sin\theta\sin\varphi)-\sin^2(2\pi p\cos\theta)+\sin^2(2\pi p\sin\theta\cos\varphi)\sin^2(2\pi p\sin\theta\sin\varphi)+\sin^2(2\pi p\sin\theta\cos\varphi)\sin^2(2\pi p\cos\theta)+\sin^2(2\pi p\sin\theta\sin\varphi)\sin^2(2\pi p\cos\theta)\}\sin\theta\,d\theta\,d\varphi$$

or

$$\overline{|F|^2}=4f^2\left\{1+3\,\frac{\sin(4\sqrt{(2)}\pi p)}{4\sqrt{(2)}\pi p}\right\}.$$

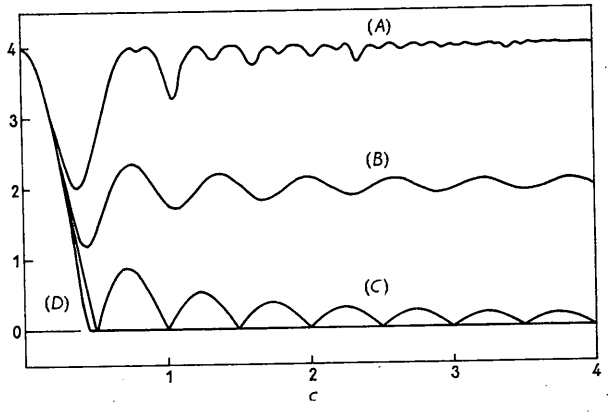

Fig. 1. A plot of the data contained in Table 1 showing the values from special cases of the Fourier transform of a tetrahedron: Curve A, $|F|_{max}/f$; Curve B, $(\overline{|F|^2})^{\frac{1}{2}}/f$; Curve C, $|\bar{F}|/f$; Curve D, $|F|_{min}/f$.

Table 1. *Selected values of* $(\overline{|F|^2})^{\frac{1}{2}}$, $|F|/f$ and $|F|_{min}/f$

(1) c	(2) $\frac{\lvert F\rvert_{max}}{f}$	(3) $\frac{\sqrt{\overline{\lvert F\rvert^2}}}{f}$	(4) $\frac{\lvert\bar{F}\rvert}{f}$	(5) $\frac{\lvert F\rvert_{min}}{f}$
0.00	4.00	4.000	4.000	4.00
0.05	3.94	3.955	3.955	3.93
0.10	3.74	3.742	3.742	3.74
0.15	3.44	3.434	3.434	3.42
0.20	3.06	3.030	3.027	2.99
0.25	2.65	2.559	2.546	2.47
0.30	2.27	2.061	2.018	1.86
0.35	2.03	1.596	1.472	1.19
0.40	2.03	1.265	0.955	0.48
0.45	2.26	1.189	0.437	0.01
0.50	2.64	1.366	0.000	0.01
0.55	3.06	1.652	0.358	0.00
0.60	3.44	1.937	0.624	0.00
0.65	3.74	2.163	0.792	0.00
0.70	3.93	2.304	0.868	0.00
0.75	4.00	2.354	0.849	0.00
0.80	3.93	2.318	0.757	0.00
0.85	3.99	2.211	0.606	0.00
0.90	3.97	2.061	0.416	0.00
0.95	3.81	1.900	0.207	0.00
1.00	3.54	1.770	0.000	0.00
1.05	3.25	1.707	0.187	0.00
1.10	3.60	1.727	0.340	0.00
1.15	3.86	1.815	0.448	0.00
1.20	3.98	1.938	0.505	0.00
1.25	3.98	2.059	0.509	0.00
1.30	3.85	2.151	0.466	0.00
1.35	3.81	2.198	0.382	0.00
1.40	3.97	2.194	0.267	0.00
1.45	4.00	2.144	0.136	0.00
1.50	4.00	2.060	0.000	0.00
1.55	3.93	1.963	0.127	0.00
1.60	3.74	1.877	0.234	0.00
1.65	3.82	1.826	0.312	0.00
1.70	3.97	1.822	0.356	0.00
1.75	3.99	1.866	0.364	0.00
1.80	3.88	1.939	0.336	0.00
1.85	3.96	2.021	0.278	0.00
1.90	4.00	2.090	0.197	0.00
1.95	4.00	2.133	0.101	0.00
2.00	3.89	2.141	0.000	0.00
2.05	3.87	2.113	0.096	0.00
2.10	3.99	2.059	0.178	0.00
2.15	3.98	1.991	0.240	0.00
2.20	3.93	1.926	0.275	0.00
2.25	4.00	1.881	0.283	0.00
2.30	3.95	1.869	0.265	0.00
2.35	3.75	1.891	0.219	0.00
2.40	3.94	1.940	0.156	0.00
2.45	4.00	2.001	0.080	0.00
2.50	3.93	2.057	0.000	0.00
2.55	4.00	2.096	0.077	0.00
2.60	4.00	2.109	0.144	0.00
2.65	3.93	2.095	0.194	0.00
2.70	3.95	2.058	0.224	0.00
2.75	4.00	2.006	0.231	0.00
2.80	3.96	1.954	0.216	0.00
2.85	4.00	1.914	0.181	0.00
2.90	3.98	1.897	0.129	0.00
2.95	3.93	1.907	0.067	0.00
3.00	4.00	1.941	0.000	0.00
3.05	3.95	1.988	0.065	0.00
3.10	4.00	2.036	0.121	0.00
3.15	3.98	2.072	0.164	0.00
3.20	3.96	2.088	0.189	0.00
3.25	4.00	2.083	0.196	0.00
3.30	3.98	2.056	0.185	0.00
3.35	3.98	2.016	0.154	0.00
3.40	3.89	1.972	0.110	0.00
3.45	3.99	1.936	0.057	0.00
3.50	3.96	1.917	0.000	0.00
3.55	4.00	1.920	0.055	0.00
3.60	3.98	1.943	0.104	0.00
3.65	3.99	1.980	0.141	0.00
3.70	3.98	2.021	0.164	0.00
3.75	4.00	2.054	0.170	0.00
3.80	3.98	2.073	0.159	0.00
3.85	3.99	2.073	0.134	0.00
3.90	3.98	2.054	0.096	0.00
3.95	4.00	2.023	0.050	0.00
4.00	3.97	1.986	0.000	0.00

The substitution for p which was used above gives the root mean-square value of the transform as:

$$(\overline{|F|^2})^{\frac{1}{2}}=2f\left\{1+3\,\frac{\sin(4\sqrt{(6)}\pi c/3)}{(4\sqrt{(6)}\pi c/3)}\right\}^{\frac{1}{2}}.$$

The function $(\overline{|F|^2})^{\frac{1}{2}}/f$ is shown in curve B, Fig. 1 and selected values are listed in column 3, Table 1. These values are close to the value 2 predicted by Wilson's (1942) theory for the r.m.s. scattering amplitude of four equal, randomly-distributed atoms.

As in the case of the octahedron, the absolute maximum and absolute minimum values of the function $|F|$ were obtained by evaluating $|F|$ at many closely-spaced values of h and k. The resulting functions $|F|_{max}/f$ and $|F|_{min}/f$ are shown in curves A and D, Fig. 1; selected values are listed in columns 2 and 5, Table 1.

All the calculations for $|\bar{F}|/f$, $(\overline{|F|^2})^{\frac{1}{2}}/f$, $|F|_{max}/f$, and $|F|_{min}/f$ were done on an IBM 7090 computer. The absolute error in $|\bar{F}|/f$ and $(\overline{|F|^2})^{\frac{1}{2}}/f$ is less than 0·001; the absolute error in $|F|_{max}/f$ and $|F|_{min}/f$ is less than 0·01.

The radius of the HgI_4^{2-} tetrahedron, the Hg–I distance, is 2·76 Å (Pauling, 1960). From Fig. 1 it may be clearly seen that for values of c less than about 0·35 the orientation of the tetrahedron has little effect on its Fourier transform. This value of c corresponds to a minimum spacing of approximately 8 Å.

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