ation of the coordinates, $\sigma(r)$, and the general temperature coefficient, B, calculated from the relationship

$$R=\frac{\int_0^{S_{\max}} 4\pi s^2 R(\sigma,s) f(s) \exp(-Bs^2/4)ds}{\int_0^{S_{\max}} 4\pi s^2 f(s) \exp(-Bs^2/4)ds}$$

where the integrals are taken over the range of $s=2\sin\theta/\lambda$ limited by the sphere of reflection of Cu $K\alpha$ radiation and $f(s)$ is the scattering factor for carbon atoms of the type proposed by Vand, Eiland & Pepinsky (1957).

Using the expression $\delta\sigma=\frac{|\Delta r_N|^2}{2N\sigma}$ given by Stanley (1964) and the values of σ and $dR/d\sigma$ from the tables corresponding to the observed values of R a comparison can be made between the theoretical reduction in R as the refinement progresses and that observed in practice. The example used is that of a problem with six atoms in the asymmetric unit (space group $P2_1/c$) whose structure has been determined and refined by Dr G. Germain (private communication). Table 3 gives the details of the progress in refinement in one typical cycle. The agreement, for a six-atom problem, is reasonably good.

Table 3. *Progress of refinement in a typical cycle*

Initial value of $R=24{\cdot}705\,\%$

Atom No.	$\lvert\Delta r_N\rvert$	R	ΔR obs.	ΔR calc.
1	0·10 Å	24·007 %	0·698 %	0·686 %
2	0·15	22·109	1·898	1·711
3	0·05	21·973	0·136	0·191
4	0·16	18·013	3·960	2·311
5	0·07	17·895	0·118	0·462
6	0·05	17·692	0·203	0·232

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The Fourier transform of the coiled-coil model for *a*-keratin. A correction.

By R. D. B. FRASER, T. P. MACRAE and A. MILLER. *Division of Protein Chemistry, C.S.I.R.O., Wool Research Laboratories, Parkville N. 2, Victoria, Australia*

(*Received* 29 *December* 1964)

In a recent communication (Fraser, MacRae & Miller, 1964) atomic coordinates were given for the asymmetric unit of the coiled-coil model for α-keratin. An error has since been discovered in a computer routine used to list these coordinates, and Table 2 in the original communication should be replaced by the following. The routine was not used in the Fourier-transform calculations.

References

FRASER, R. D. B., MACRAE, T. P. & MILLER, A. (1964). *Acta Cryst.* **17**, 813.

Table 2

(*a*) Atomic coordinates of asymmetric unit in a coiled-coil with $r_0=5{\cdot}2$ Å (Oz = major helix axis).

	x	y	z		x	y	z
β–C(1)	8·400	0·000	0·000	C(4)	6·487	0·182	4·180
α–C(1)	7·350	0·887	−0·697	O(4)	6·466	0·683	3·040
N(1)	6·242	1·151	0·233	β–C(5)	7·541	0·990	6·338
C(1)	5·090	1·658	−0·155	α–C(5)	6·282	1·040	5·456
O(1)	4·804	1·974	−1·315	N(5)	5·135	0·511	6·202
β–C(2)	4·636	2·845	2·016	C(5)	3·992	0·191	5·633
α–C(2)	4·082	1·843	0·998	O(5)	3·742	0·301	4·437
N(2)	3·855	0·547	1·636	β–C(6)	2·583	0·753	7·621
C(2)	3·634	−0·563	0·966	α–C(6)	2·939	−0·342	6·618
O(2)	3·577	−0·647	−0·256	N(6)	3·487	−1·509	7·305
β–C(3)	2·169	−1·591	2·712	C(6)	4·114	−2·488	6·691
α–C(3)	3·424	−1·795	1·864	O(6)	4·302	−2·547	5·473
N(3)	4·598	−1·960	2·721	β–C(7)	3·383	−4·259	8·317
C(3)	5·835	−1·893	2·275	α–C(7)	4·595	−3·602	7·647
O(3)	6·149	−1·693	1·089	N(7)	5·469	−3·009	8·666
β–C(4)	6·748	−3·509	3·996	C(7)	6·438	−2·164	8·376
α–C(4)	6·892	−2·101	3·392	O(7)	6·727	−1·778	7·225
N(4)	6·679	−1·095	4·444				

(*b*) Bond lengths and angles in a coiled-coil compared with values in an undistorted α-helix.

Bond	Maximum	Undistorted	Minimum	Angle	Maximum	Undistorted	Minimum
βC–αC	1·541	1·535	1·527	βC–αC–N	110·57	109·91	109·31
αC–N	1·471	1·465	1·461	αC–N–C*	123·65	123·16	122·71
N–C*	1·318	1·317	1·315	N–C*–O*	125·27	125·00	124·66
C–O	1·248	1·237	1·226	O–C–αC	122·44	121·79	121·08
C–αC	1·555	1·546	1·537	C–αC–βC	110·27	109·75	109·21
N · · · O†	2·864	2·841	2·812	N–C*–αC*	113·71	113·21	112·70
				C–αC–N	108·94	108·86	108·74
				C*–N · · · O†	116·00	115·44	114·88

† Hydrogen-bonded atoms. * Indicates next residue.