SHORT COMMUNICATION

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X-ray powder diagrams predicted for certain even-*n* alkanes.

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From the known crystal structure of an *n*-alkane it is possible to predict the structures of all those *n*-alkanes isostructural with it. These predictions are matched against published X-ray powder data for $n=10$, 12, 14 and 16. The overall agreement is good but some discrepancies, notably some predicted moderately strong reflexions not apparently observed, are not readily explained.

Norman & Mathisen (1972), hereinafter N & M, have published a note on the X-ray powder diagrams and derived cell dimensions for the triclinic *n*-alkanes having $n=10$, 12, 14 and 16.

It has been shown (Nyburg & Potworowski, 1973) that knowing the structure of any one 'key' *n*-alkane (in this case $n=18$: Nyburg & Lüth, 1972), the unit-cell dimensions and crystal structures of all other members of an isostructural series can be predicted. The unit cells predicted in the original paper are related to those used by N & M by $\mathbf{a},\mathbf{b},\mathbf{c} \rightarrow \mathbf{a}, -\mathbf{b}, -\mathbf{a}+\mathbf{c}$. Only the latter type of cell is referred to here.

N & M give the *d* spacings and their indexing of the powder lines but not, unfortunately, the relative intensities. This makes it difficult to know, in one important respect, to what extent our predictions are correct.

In the original paper (Nyburg & Potworowski, 1973) it was assumed that the triclinic parameters *a*, *b* and γ remained the same throughout the isostructural series. For the purpose of this note we have taken advantage of the known values of these parameters for $n=6$ (Norman & Mathisen, 1961), 8 (Mathisen, Norman & Pedersen, 1967), and 18, and used a smoothed interpolation for *n* values in between. The parameters obtained fit those assigned by N & M quite well except *a* and *b* for $n=10$ which have been changed accordingly. Of the remaining triclinic parameters, *c* and β were taken to be exactly as predicted in the earlier paper. The values of α given by N & M do not vary smoothly

Table 1. *Cell parameters* (Å *and* °) *listed by N & M and those used in this paper*

Dashes indicate that N & M values were used.

	N & M						This paper					
n	*a*	*b*	*c*	α	β	γ	*a*	*b*	*c*	α	β	γ
10	4·20	4·75	13·57	93·4	81·8	105·6	4·25	4·81	13·59	93·8	81·7	–
12	4·28	4·81	16·12	93·3	79·9	106·6	–	–	16·07	92·9	80·2	–
14	4·29	4·82	18·58	93·1	78·8	107·0	–	–	18·57	92·4	79·1	–
16	4·29	4·81	20·87	91·9	80·5	106·9	–	–	21·09	92·2	78·2	–

Table 2. *Summary of discrepancies between N & M spacings and indices, and those predicted*

n	Spacings (Å) of lines recorded by N & M with their indices, but not predicted (▲ in Fig. 1)	Lines (and intensities) predicted but not observed by N & M (▼ in Fig. 1)	Differences in ascribed indices (△ in Fig. 1) N & M	This paper
10	3·833, $01\bar{2}$	013 (*vw*), 105 (*vw*)	$01\bar{1}$	011
			$10\bar{2}$ or $10\bar{3}$	$10\bar{1}$
			$01\bar{4}$	110
			$1\bar{1}\bar{4}$	$1\bar{1}5$
12	3·085, $1\bar{1}\bar{2}$	101, (*w*), 106 (*vw*), 110 (*ms*)	$01\bar{1}$	011
		012 (*w*)	$01\bar{3}$	013
			016	$01\bar{6}$
14	none	(012+101) (*w*), 013 (*vw*)		
		$10\bar{2}$ (*vw*), 014 (*w*), $10\bar{3}$ (*vw*)	$01\bar{1}$	011
		006 (*vw*), 110 (*ms*)		
16	3·577, $10\bar{2}$	001 (*s*)*, 003 (*w*), 004 (*vw*)	$01\bar{1}$	011
			$01\bar{2}$	101
			102	100
		$01\bar{1}$ (*w*), 012 (*ms*), $10\bar{2}$ (*w*)	$01\bar{3}$	$10\bar{1}$
			006	$1\bar{1}\bar{1}$

* Possibly obscured by beam-stop.

with n so we have taken our predicted values slightly modified to fit exactly the known values for $n=6$, 8 and 18. The two sets of parameters are given in Table 1.

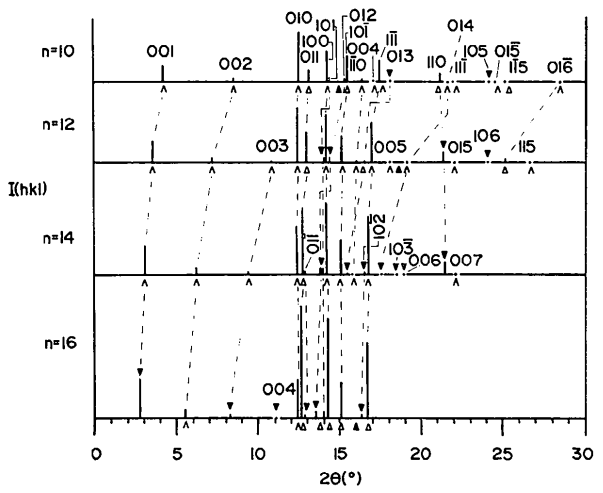

Fig. 1. Indices, 2θ values and relative intensities predicted and observed by N & M for powder diagrams of the n-alkanes ($n=10$, 12, 14, 16). See Table 2.
- ∧ Indices and measured 2θ agreeing with those of N & M.
- ▲ Lines recorded by N & M but not predicted.
- ▼ Lines predicted but not observed by N & M.
- △ Observed and predicted positions agreeing but with indices different from those assigned by N & M.

It will be seen from Fig. 1 that the agreement between observed and predicted positions of the powder lines is on the whole very good for all four alkanes; where both the position and N & M's indexing agree with our predictions we have indicated this by ∧. The discrepancies are of three kinds and are set out in Table 2. The most serious discrepancies concern the moderately strong reflexions (one each for $n=12$, 14 and 16) which were not observed by N & M. We do not know the reason for this. It should be noted from Table 2 that for $n=16$ there is virtually no agreement in the indexing. This is due to the differences in c and β parameters (Table 1). We agree with the γ parameter assigned by N & M but are uncertain how this value was obtained by them since no $hk0$ or hkl indices were assigned.

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