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X-ray powder diffraction studies of *n*-alkanes: a re-examination of the unit-cell parameters of $C_{24}H_{50}$ and $C_{26}H_{54}$.

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Abstract

Further analysis of the synchrotron X-ray powder diffraction patterns for *n*-tetracosane ($C_{24}H_{50}$) and *n*-hexacosane ($C_{26}H_{54}$) has yielded unit cells in addition to those proposed by Gerson, Roberts & Sherwood [*Acta Cryst.* (1991), B**47**, 280–284]. The new unit cells are very similar to those predicted by Nyburg & Potworowski [*Acta Cryst.* (1973), B**29**, 347–352] being triclinic and conforming to the series observed for $C_{18}H_{38}$, $C_{20}H_{42}$ and $C_{22}H_{46}$ [Gerson, Roberts & Sherwood (1991). *Acta Cryst.* B**47**, 280–284].

Discussion

Ab intio indexing (using the program *ITO*, Visser, 1969) of the synchrotron radiation powder diffraction patterns of $C_{24}H_{50}$ and $C_{26}H_{54}$ seemed to indicate bilayer $Z = 2$ pseudomonoclinic unit cells (Gerson, Roberts & Sherwood, 1991). From these unit cells a polytypic form of the triclinic $Z = 1$ type structure ($C_{18}H_{38}$, Nyburg & Lüth, 1972), was proposed. These unit cells did not agree with those predicted by Nyburg & Potworowski (1973). A single-crystal X-ray diffraction study (Gerson & Nyburg, 1992) has since shown $C_{24}H_{50}$ to be isostructural to the shorter even *n*-alkanes ($C_{20}H_{42}$, Nyburg & Gerson, 1992; $C_{18}H_{38}$, Nyburg & Lüth, 1972) as predicted. This result led us to re-examine our previous analysis of the powder data recorded for $C_{24}H_{50}$ and for $C_{26}H_{54}$.

The unit cells predicted by Nyburg & Potworowski (1973) for $C_{24}H_{50}$ and $C_{26}H_{54}$ were refined, using the program *ITO* (Visser, 1969), against the reflection positions observed (Gerson, Roberts & Sherwood, 1991). The resulting unit cells were then further refined against the indexed reflections using *REFCEL* (Daresbury Laboratory Powder Diffraction Library).

The newly refined $Z = 1$ unit cells (Table 1) were found to predict the reflection positions at least as well as the polytypic unit cells previously proposed (Gerson, Roberts & Sherwood, 1991). The proposed $Z = 2$ pseudomonoclinic unit cells for $C_{24}H_{50}$ and $C_{26}H_{54}$ are most probably the result of incorrect indexing. Both compounds almost certainly have the same triclinic $Z = 1$ lattice as observed for the shorter even *n*-alkanes ($C_{18}H_{38}$ to $C_{22}H_{46}$, Gerson, Roberts & Sherwood, 1991).

Table 1. *Measured and predicted* (*Nyburg & Potworowski,* 1973) *unit cells of* $C_{24}H_{50}$ *and* $C_{26}H_{54}$ *with e.s.d.'s below in parentheses*

(*a*) Figure of merit.* (*b*) Number of peak positions used as data in *ITO*.

	a (Å)	*b* (Å)	*c* (Å)	*α* (°)	*β* (°)	*γ* (°)	*V* (Å³)	*Z*	(*a*)	(*b*)
$C_{24}H_{50}$	4.277	4.817	32.544	86.29	68.86	72.74	597	1	47	40
	(0.001	0.001	0.005	0.02	0.03	0.03)				
$C_{24}H_{50}$†	4.285	4.82	32.50	86.43	68.71	72.70	596	1		
$C_{26}H_{54}$	4.269	4.803	34.883	86.92	69.94	73.10	642	1	45	40
	(0.001	0.001	0.005	0.05	0.05	0.03)				
$C_{26}H_{54}$†	4.285	4.82	35.04	86.73	68.92	72.70	644	1		

* See Gerson, Roberts & Sherwood (1991).
† Predicted.

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