été reportées: leur valeur absolue est inférieure à 2 × 10^{-2}.

Nous avons considéré l'interaction d'une molécule (x,y,z) avec ses voisines les plus proches et les énergies d'interactions correspondantes sont rassemblées dans le Tableau 5. Les valeurs ainsi calculées sont du même ordre de grandeur que celles obtenues dans l'étude de composés similaires. Cependant, l'énergie d'interaction avec la molécule 2 est très forte. Cette énergie est essentiellement due aux forces de van der Waals et traduit le fait que ces deux molécules se trouvent à une faible distance l'une de l'autre et la plupart de leurs atomes sont en interaction (voir Fig. 3). Ces molécules se déduisant l'une de l'autre par une translation d'une période dans la direction Ox, les interactions entre deux molécules voisines se répètent identiquement et l'on peut parler d'un empilement moléculaire uniforme dans cette direction. Etant donné l'ordre de grandeur de cette énergie par rapport aux autres énergies d'interaction, on peut penser que cette direction demeurera privilégiée lors du passage à la phase smectique.

Tableau 5. *Energie d'interaction entre une molécule A (x, y, z) et toutes ses voisines*

Molécule B*	Energie (kJ mol^{-1})	Molécule B*	Energie (kJ mol^{-1})
2	−130,5	7	−32,9
3	−48,90	8	−8,67
4	−55,10	9	−1,59
5	−6,83	10	−1,42
6	−40,6		

* Les correspondances sont les suivantes: (2) $1 + x, y, z$; (3) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (4) $-2 - x, 1 - y, -z$; (5) $4 + x, \frac{3}{2} - y, \frac{1}{2} + z$; (6) $-x, \frac{1}{2} + y, \frac{1}{2} - z$; (7) $-3 - x, 1 - y, -z$; (8) $3 + x, \frac{3}{2} - y, \frac{1}{2} + z$; (9) $-4 - x, 2 - y, -z$; (10) $2 + x, \frac{3}{2} - y, -\frac{1}{2} + z$.

Conclusion

A la différence de la plupart des composés smectogènes et plus particulièrement des composés DHP1, DHP2 et DHP3, les molécules de DHP5 adoptent une conformation non linéaire de type 'banane'. L'arrangement des molécules dans le cristal est de type imbriqué et ne préfigure pas l'arrangement d'une phase smectique. Toutefois, le calcul énergétique montre que les interactions moléculaires sont nettement prépondérantes suivant la direction Ox.

Aussi nous semble-t-il raisonnable de supposer que le type d'empilement observé pourrait subsister à l'état smectique.

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The Crystal and Molecular Structure of *N*-Mesitylbenzophenoneimine [*N*-(Diphenylmethylene)mesitylamine]

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Abstract

$C_{22}H_{21}N$ is monoclinic, space group $P2_1/c$, with $a = 11{\cdot}074\,(6)$, $b = 16{\cdot}92\,(1)$, $c = 9{\cdot}699\,(4)$ Å, $\beta = 107{\cdot}23\,(4)°$, $Z = 4$. Refinement of 2622 counter intensities led to a final R_F of 0·056 ($R_{wF} = 0{\cdot}067$). Appreciable departures from planarity are found, the mesityl and *Z*-phenyl groups making dihedral angles of 75·5 (3) and 61·9 (3)°, respectively, with the plane through the bonds of the central C atom, and the *E*-phenyl group being approximately coplanar with a dihedral angle of 15·3 (3)°.

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Introduction

P and As analogs of *N*-mesitylbenzophenoneimine [Mes—N=C(Ph)$_2$] appear to be thermally stable, whereas attempts to prepare the corresponding analogs of *N*-phenylbenzophenoneimine yielded polymeric material only (Klebach, Lourens & Bickelhaupt, 1978; Klebach, van Dongen & Bickelhaupt, 1979). The stability of the mesityl relative to the phenyl compounds indicated that steric hindrance to polymerization rather than a conjugative effect is responsible. As suitable crystals of the P and As analogs were not available it was considered desirable to obtain the molecular conformation of the title compound.

Experimental

A sample was kindly provided by Professor Dr F. Bickelhaupt and Dr Th. C. Klebach, Vrije Universiteit van Amsterdam. The yellow transparent block-shaped crystals are stable at room temperature. Space group, cell dimensions and intensities were obtained from measurements on an Enraf–Nonius CAD-4 diffractometer with Zr-filtered Mo $K\alpha$ radiation ($\lambda = 0{\cdot}7107$ Å) at room temperature.

Crystal data

$C_{22}H_{21}N$, $M_r = 299{\cdot}40$, monoclinic, $P2_1/c$; $a = 11{\cdot}074$ (6), $b = 16{\cdot}92$ (1), $c = 9{\cdot}699$ (4) Å, $\beta = 107{\cdot}23$ (4)°, $V = 1735{\cdot}8$ Å^3, $D_c = 1{\cdot}146$, $D_o = 1{\cdot}13$ Mg m^{-3}, $F(000) = 640$, μ(Mo $K\alpha$) = 0·077 mm^{-1}.

A tetartosphere of the reciprocal lattice was measured up to $\theta = 27{\cdot}5°$ in an $\omega/2\theta$ scan mode with a variable scan angle of $\Delta\omega = (0{\cdot}80 + 0{\cdot}35 \tan\theta)°$. 3965 independent reflexions were scanned, 2622 of which had $I \geq 2{\cdot}5\sigma(I)$ and were used in the subsequent structure determination. No correction for absorption was applied. The density was determined by flotation in a mixture of KCl and H_2O. Stability of the crystal was monitored every half hour of X-ray exposure time; there was no indication of decay.

Determination of the structure

In an E map based on the most probable phase set for 250 E values (*MULTAN* 77, Main, Lessinger, Woolfson, Germain & Declercq, 1977), the N and C atoms were located. After anisotropic block-diagonal least-squares refinement the H atoms were indicated by a difference synthesis (their temperature factors were fixed at $B = 5$ Å^2). The positional parameters for all atoms and the anisotropic parameters of the non-hydrogen atoms were varied during block-diagonal refinement. This resulted in an R_F of 0·057. A final full-matrix refinement converged to $R_F = 0{\cdot}056$ and $R_{wF} = 0{\cdot}067$.

The refinement was considered to be complete when the shifts were within the e.s.d.'s. Unit weights were applied. In the final difference map no significant density was observed (the highest peak was 0·2 e Å^{-3}).

The scattering factors for C and N were from Cromer & Mann (1968), for H from Stewart, Davidson & Simpson (1965). The final positional parameters are presented in Table 1.* Most calculations were carried

Table 1. *Final fractional coordinates* (×10^4; *for* H × 10^3)

Numbers in parentheses here and in other tables indicate e.s.d.'s in the least significant digits.

	x	y	z
N	6841 (2)	5081 (1)	9731 (2)
C(1)	7454 (2)	4699 (1)	9033 (3)
C(2)	8016 (2)	5052 (1)	7955 (2)
C(3)	7692 (2)	4784 (2)	6546 (3)
C(4)	8248 (3)	5093 (2)	5570 (3)
C(5)	9157 (3)	5660 (2)	6000 (3)
C(6)	9489 (3)	5932 (2)	7383 (3)
C(7)	8925 (3)	5632 (2)	8361 (3)
C(8)	7685 (2)	3840 (1)	9366 (3)
C(9)	7019 (3)	3439 (2)	10156 (3)
C(10)	7302 (3)	2668 (2)	10549 (4)
C(11)	8239 (3)	2282 (2)	10179 (4)
C(12)	8897 (3)	2660 (2)	9393 (3)
C(13)	8611 (3)	3436 (2)	8980 (3)
C(14)	6568 (2)	5902 (2)	9458 (3)
C(15)	5627 (2)	6147 (2)	8250 (3)
C(16)	5380 (3)	6951 (2)	8071 (3)
C(17)	6016 (3)	7502 (2)	9065 (3)
C(18)	6904 (3)	7233 (2)	10277 (3)
C(19)	7206 (3)	6438 (2)	10522 (3)
C(20)	4846 (3)	5569 (2)	7197 (3)
C(21)	5699 (4)	8361 (2)	8850 (4)
C(22)	8157 (3)	6159 (2)	11864 (3)
H(3)	706 (2)	442 (1)	630 (3)
H(4)	796 (2)	489 (1)	455 (3)
H(5)	950 (2)	582 (1)	530 (3)
H(6)	1014 (2)	627 (1)	775 (3)
H(7)	916 (2)	580 (1)	938 (2)
H(9)	630 (2)	369 (1)	1036 (3)
H(10)	682 (2)	247 (1)	1105 (3)
H(11)	849 (2)	*182 (1)*	*1049 (2)*
H(12)	952 (2)	244 (1)	919 (3)
H(13)	906 (2)	369 (1)	847 (2)
H(16)	472 (2)	711 (1)	719 (2)
H(18)	733 (2)	755 (1)	1097 (3)
H(201)	450 (2)	519 (1)	770 (3)
H(202)	408 (2)	582 (1)	663 (3)
H(203)	529 (2)	540 (1)	647 (3)
H(211)	512 (2)	852 (1)	935 (3)
H(212)	636 (2)	868 (1)	932 (3)
H(213)	567 (2)	843 (1)	807 (3)
H(221)	777 (2)	581 (1)	1242 (2)
H(222)	853 (2)	656 (1)	1242 (3)
H(223)	886 (2)	589 (1)	1163 (3)

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34563 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond distances* (Å)

N–C(1)	1·268 (4)	C(1)–C(2)	1·491 (4)
N–C(14)	1·430 (3)	C(1)–C(8)	1·495 (3)
C(2)–C(3)	1·382 (3)	C(8)–C(9)	1·388 (4)
C(3)–C(4)	1·376 (4)	C(9)–C(10)	1·369 (4)
C(4)–C(5)	1·364 (4)	C(10)–C(11)	1·361 (5)
C(5)–C(6)	1·362 (4)	C(11)–C(12)	1·361 (5)
C(6)–C(7)	1·378 (4)	C(12)–C(13)	1·382 (4)
C(7)–C(2)	1·378 (4)	C(13)–C(8)	1·373 (4)
C(14)–C(15)	1·381 (3)	C(15)–C(20)	1·492 (4)
C(15)–C(16)	1·389 (4)	C(17)–C(21)	1·495 (4)
C(16)–C(17)	1·375 (4)	C(19)–C(22)	1·488 (4)
C(17)–C(18)	1·368 (4)		
C(18)–C(19)	1·389 (4)		
C(19)–C(14)	1·399 (4)		
C(3)–H(3)	0·91 (2)	C(9)–H(9)	0·97 (3)
C(4)–H(4)	1·01 (2)	C(10)–H(10)	0·89 (3)
C(5)–H(5)	0·91 (3)	C(11)–H(11)	0·85 (2)
C(6)–H(6)	0·91 (2)	C(12)–H(12)	0·86 (3)
C(7)–H(7)	0·99 (2)	C(13)–H(13)	0·91 (3)
C(16)–H(16)	0·98 (2)	C(20)–H(201)	0·95 (3)
C(18)–H(18)	0·88 (2)	C(20)–H(202)	0·96 (2)
		C(20)–H(203)	1·02 (3)
C(21)–H(211)	0·95 (3)	C(22)–H(221)	0·98 (3)
C(21)–H(212)	0·91 (2)	C(22)–H(222)	0·89 (2)
C(21)–H(213)	0·76 (3)	C(22)–H(223)	0·99 (3)

Table 3. *Bond angles* (°)

C(1)–N–C(14)	120·8 (2)	C(1)–C(2)–C(3)	121·5 (2)
		C(1)–C(2)–C(7)	120·4 (2)
C(2)–C(1)–C(8)	117·4 (2)	C(3)–C(2)–C(7)	118·0 (2)
C(2)–C(1)–N	124·9 (2)		
C(8)–C(1)–N	117·6 (2)	C(2)–C(3)–C(4)	121·2 (2)
		C(3)–C(4)–C(5)	119·8 (2)
C(1)–C(8)–C(9)	120·6 (2)	C(4)–C(5)–C(6)	119·9 (3)
C(1)–C(8)–C(13)	121·3 (2)	C(5)–C(6)–C(7)	120·6 (3)
C(9)–C(8)–C(13)	118·0 (2)	C(2)–C(7)–C(6)	120·5 (2)
C(8)–C(9)–C(10)	120·3 (3)	C(15)–C(14)–N	120·9 (2)
C(9)–C(10)–C(11)	120·9 (3)	C(19)–C(14)–N	117·5 (2)
C(10)–C(11)–C(12)	119·9 (3)	C(15)–C(14)–C(19)	121·4 (2)
C(11)–C(12)–C(13)	119·6 (3)		
C(8)–C(13)–C(12)	121·3 (3)	C(14)–C(15)–C(16)	118·1 (2)
		C(14)–C(15)–C(20)	121·5 (2)
C(15)–C(16)–C(17)	122·4 (2)	C(16)–C(15)–C(20)	120·3 (2)
C(16)–C(17)–C(18)	117·7 (3)	C(14)–C(19)–C(18)	117·3 (2)
C(16)–C(17)–C(21)	120·7 (2)	C(14)–C(19)–C(22)	120·7 (3)
C(18)–C(17)–C(21)	121·5 (3)	C(18)–C(19)–C(22)	122·0 (3)
C(17)–C(18)–C(19)	123·1 (3)		
C(2)–C(3)–H(3)	116 (2)	C(8)–C(9)–H(9)	120 (1)
C(4)–C(3)–H(3)	123 (2)	C(10)–C(9)–H(9)	119 (1)
C(3)–C(4)–H(4)	118 (1)	C(9)–C(10)–H(10)	112 (2)
C(5)–C(4)–H(4)	122 (1)	C(11)–C(10)–H(10)	127 (2)
C(4)–C(5)–H(5)	115 (1)	C(10)–C(11)–H(11)	123 (2)
C(6)–C(5)–H(5)	125 (1)	C(12)–C(11)–H(11)	117 (2)
C(5)–C(6)–H(6)	123 (2)	C(11)–C(12)–H(12)	121 (2)
C(7)–C(6)–H(6)	116 (2)	C(13)–C(12)–H(12)	119 (2)
C(6)–C(7)–H(7)	123 (1)	C(12)–C(13)–H(13)	119 (2)
C(2)–C(7)–H(7)	117 (1)	C(8)–C(13)–H(13)	119 (2)
C(15)–C(16)–H(16)	116 (1)	C(17)–C(18)–H(18)	123 (2)
C(17)–C(16)–H(16)	122 (1)	C(19)–C(18)–H(18)	114 (1)
C(15)–C(20)–H(201)	109 (1)	C(17)–C(21)–H(211)	111 (1)
C(15)–C(20)–H(202)	110 (1)	C(17)–C(21)–H(212)	113 (2)
C(15)–C(20)–H(203)	111 (1)	C(17)–C(21)–H(213)	103 (2)
H(201)–C(20)–H(202)	99 (2)	H(211)–C(21)–H(212)	98 (2)
H(201)–C(20)–H(203)	121 (2)	H(211)–C(21)–H(213)	129 (2)
H(202)–C(20)–H(203)	105 (2)	H(212)–C(21)–H(213)	101 (2)
C(19)–C(22)–H(221)	111 (1)		
C(19)–C(22)–H(222)	112 (1)		
C(19)–C(22)–H(223)	111 (1)		
H(221)–C(22)–H(222)	109 (2)		
H(221)–C(22)–H(223)	111 (2)		
H(222)–C(22)–H(223)	104 (2)		

out with local adapted versions of the XRAY system (Stewart, 1976).

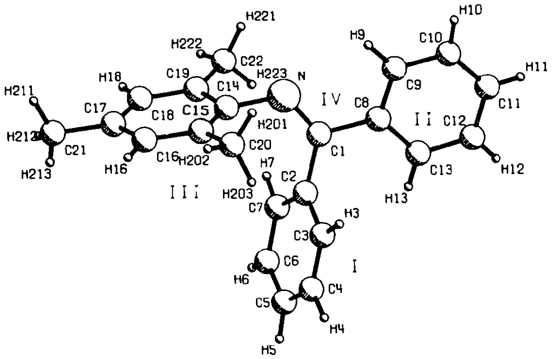

Fig. 1. Perspective view of the *N*-mesitylbenzophenoneimine molecule showing the atom numbering. Planar parts of the molecule are indicated by Roman numerals.

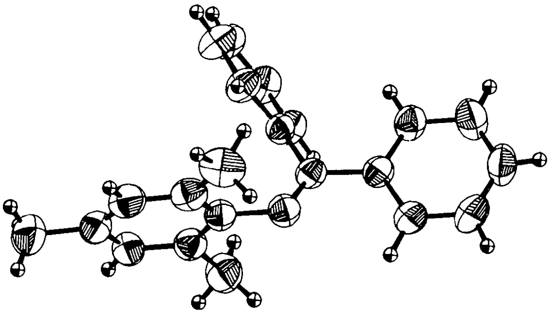

Fig. 2. The 50% probability ellipsoids for the *N*-mesitylbenzophenoneimine molecule. H atoms are represented as arbitrarily small spheres.

Discussion

Fig. 1 (*PLUTO* 78; W. D. S. Motherwell) gives the atom numbering. The thermal vibrational ellipsoids are shown in Fig. 2 (*ORTEP*; Johnson, 1965). Bond lengths and angles are given in Tables 2 and 3. They all lie within the expected range. Table 4 lists the distances of the non-hydrogen atoms from the four least-squares planes of interest. The phenyl groups are planar within the limits of precision; however, rather large distortions from planarity of the ring C atoms of the mesityl group are found. The *para*-methyl C atom is coplanar with the plane through the ring, whereas the *ortho*-methyl C atoms show significant departures, probably induced

Table 4. *Least-squares planes*

(i) Distances of the non-hydrogen atoms from the planes (I,II,III,IV) (Å)[a,b]

	I	II	III	IV
C(1)	−0·067	0·121	0·983	−0·013*
C(2)	−0·001*	−1·136	2·330	0·007*
C(3)	−0·005*	−1·358	2·948	−1·004
C(4)	0·008*	−1·572	4·210	−0·956
C(5)	−0·006*	−0·557	4·884	0·121
C(6)	−0·000*	0·655	4·291	1·127
C(7)	0·003*	0·871	3·021	1·077
C(8)	−1·276	0·007*	0·840	−0·002*
C(9)	−1·309	−0·001*	−0·415	−0·254
C(10)	−2·454	−0·005*	−0·535	−0·144
C(11)	−3·579	0·005*	0·567	0·216
C(12)	−3·567	0·002*	1·808	0·457
C(13)	−2·413	−0·008*	1·940	0·336
C(14)	1·988	0·594	0·022*	−0·009*
C(15)	3·034	−0·530	−0·015*	−1·183
C(16)	4·181	−0·351	−0·002*	−1·152
C(17)	4·317	0·895	0·013*	−0·009
C(18)	3·281	1·983	−0·007*	1·120
C(19)	2·102	1·880	−0·010*	1·164
C(20)	2·975	−1·900	−0·135	−2·471
C(21)	5·583	1·044	−0·008	−0·026
C(22)	1·001	3·079	−0·062	2·397
N	0·797	0·481	−0·033	0·017*

The equations of the planes are:

I: $-7{\cdot}316x + 11{\cdot}894y - 0{\cdot}543z + 0{\cdot}287 = 0$
II: $4{\cdot}835x + 5{\cdot}169y + 6{\cdot}585z - 11{\cdot}861 = 0$
III: $9{\cdot}686x + 1{\cdot}588y - 6{\cdot}917z - 0{\cdot}735 = 0$
IV: $7{\cdot}267x + 3{\cdot}688y + 4{\cdot}808z - 11{\cdot}506 = 0$

(ii) Angles (°) between planes[c]

	I	II	III
IV	61·9	15·3	75·5
III	67·3	89·5	
II	72·8		

[a] Atoms defining a plane are indicated with an asterisk.
[b] E.s.d.'s are of the order of 0·005 Å.
[c] E.s.d.'s are of the order of 0·3°.

Table 5. *Selected torsion angles*(°)

C(2)—C(1)—N—C(14)	3·9 (3)
C(8)—C(1)—N—C(14)	−179·1 (2)
C(3)—C(2)—C(1)—C(8)	60·9 (3)
C(3)—C(2)—C(1)—N	−122·1 (3)
C(9)—C(8)—C(1)—C(2)	−168·7 (2)
C(9)—C(8)—C(1)—N	14·2 (3)
C(15)—C(14)—N—C(1)	76·3 (3)
C(14)—C(15)—C(20)—H(201)	52 (2)
C(14)—C(15)—C(20)—H(202)	160 (2)
C(14)—C(15)—C(20)—H(203)	−84 (1)
C(16)—C(17)—C(21)—H(211)	96 (1)
C(16)—C(17)—C(21)—H(212)	−155 (2)
C(16)—C(17)—C(21)—H(213)	−47 (2)
C(14)—C(19)—C(22)—H(221)	−62 (2)
C(14)—C(19)—C(22)—H(222)	176 (2)
C(14)—C(19)—C(22)—H(223)	61 (2)

by cooperative interactions between the mesityl and phenyl groups. This repulsion is also reflected in the enlargement of the Ph(I)—C(1)—N angle (124·9°), the Ph(II)—C(1)—N angle being 117·6°. Unique positions for the methyl H atoms are found and it appears that in all three methyl groups one C—H bond is more or less coplanar with the ring (Table 5). Overall molecular planarity is prohibited by steric overcrowding; the dihedral angles between the planar parts of the molecule are given in Table 4.

The structure consists of monomeric molecules held together by van der Waals forces. There are no abnormally short intermolecular contacts.

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