Tables 1 to 3 give the atomic coordinates of compounds (1) to (3) respectively, and Table 4 lists some geometric data.* Views of the compounds are given in Figs. 1 to 3, and views of the projection of each compound along the *a* axis are presented in Figs. 4, 5 and 6.

Related literature. In complexes with metal ions, glycine and other amino acids may coordinate as their anions or as zwitterionic acids, depending on conditions. In the former case the amino group may take direct part in the coordination (Low, Hirshfeld & Richards, 1959; Stosick, 1945; Dejehet & Debuyst, 1978); in the zwitterion form, the protonated amine N atom is prevented from doing so, and coordination is *via* the carboxylate oxygen atoms alone, to give either mono-dentate or bidentate bonding (Dejehet, Debuyst, Ledieu, Declercq, Germain & Van Meerssche, 1978; Glowiak & Kozlowski, 1980; Ardon, Bino, Cohen & Felthouse, 1984, and references therein). In some cases,

mixtures of the two types of complex are formed (Herzog & Kalies, 1967).

We thank SERC for a research grant towards crystallographic equipment, and the University of Newcastle upon Tyne for the award of a Ridley Fellowship to OML.

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* Lists of structure factors, anisotropic thermal parameters and additional bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43638 (27 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Structure of an Antisickling Agent, N-Phenylacetyl-L-phenylalanine

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Abstract. $C_{17}H_{17}NO_3$, $M_r = 283 \cdot 3$, orthorhombic, $P2_12_12_1$, $a = 8 \cdot 400\,(1)$, $b = 5 \cdot 423\,(1)$, $c = 32 \cdot 548\,(3)$ Å, $V = 1482 \cdot 7\,(1)$ Å^3, $Z = 4$, $D_x = 1 \cdot 270$ g cm^{-3}, $\lambda(\text{Cu}K\alpha) = 1 \cdot 5418$ Å, $\mu = 6 \cdot 25$ cm^{-1}, $F(000) = 600$, $T = 263$ K, $R = 0 \cdot 048$ for 1199 unique observed reflections. The molecule has adopted a compact and amphipathic conformation. Peptide torsion angles: L-Phe: $\varphi = 76 \cdot 8\,(4)$, $\omega = 171 \cdot 5\,(4)$, $\chi^1 = -61 \cdot 2\,(5)$, $\chi^{2 \cdot 1} = -72 \cdot 6\,(5)$; phenyl: $\chi^1 = -72 \cdot 9\,(5)$, $\chi^{2 \cdot 1} = 96 \cdot 1\,(5)°$. Intramolecular edge-to-face interaction between phenyl rings: phenyl-(L-Phe)···phenyl(phenylacetyl) centroid separation =

$5 \cdot 05\,(1)$ Å and interplanar angle $= 70 \cdot 1\,(5)°$. Inter-molecular hydrogen bond: OH(L-Phe)···O(phenyl-acetyl') $= 2 \cdot 678\,(6)$ Å. Intermolecular edge-to-face interaction between phenyl rings: phenyl(L-Phe)··· phenyl(phenylacetyl') centroid separation $= 4 \cdot 85\,(1)$ Å and interplanar angle $= 70 \cdot 1\,(5)°$.

Experimental. Rectangular crystal, $0 \cdot 2 \times 0 \cdot 3 \times 0 \cdot 6$ mm, Nicolet *P*3 diffractometer, Ni-filtered radiation, ω-scan method, $(\sin\theta)/\lambda < 0 \cdot 58$ Å^{-1}, lattice parameters from the 2θ values of nine reflections with

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters*

$$U_{eq} = \tfrac{1}{3}(U_{11} + U_{22} + U_{33}).$$

	x	y	z	$U_{eq}(\text{Å}^2)$
F1N	−0·4223 (5)	0·3834 (8)	0·43177 (10)	0·058
F1CA	−0·5939 (5)	0·4211 (9)	0·43576 (12)	0·052
F1CB	−0·6840 (6)	0·2045 (9)	0·41701 (12)	0·061
F1CG	−0·6480 (5)	0·1791 (8)	0·37170 (12)	0·052
F1CD1	−0·5483 (6)	−0·0042 (9)	0·35693 (12)	0·058
F1CE1	−0·5123 (6)	−0·0209 (9)	0·31576 (13)	0·065
F1CZ	−0·5761 (6)	0·1441 (10)	0·28857 (14)	0·070
F1CE2	−0·6738 (6)	0·3293 (10)	0·30264 (13)	0·068
F1CD2	−0·7099 (6)	0·3470 (9)	0·34396 (14)	0·063
F1C	−0·6407 (6)	0·4631 (9)	0·48062 (13)	0·063
F1O	−0·5651 (5)	0·4093 (8)	0·50956 (9)	0·102
F1OH	−0·7798 (4)	0·5753 (8)	0·48266 (9)	0·078
A1C1	−0·1500 (5)	0·5212 (12)	0·42328 (13)	0·072
A1C2	−0·3216 (6)	0·5741 (11)	0·43381 (12)	0·056
A1C2O	−0·3689 (4)	0·7847 (6)	0·44196 (9)	0·063
P1C1	−0·1216 (5)	0·5869 (9)	0·37882 (13)	0·057
P1C2	−0·1825 (6)	0·4411 (10)	0·34780 (13)	0·064
P1C3	−0·1570 (6)	0·4983 (12)	0·30701 (15)	0·077
P1C4	−0·0699 (7)	0·7011 (12)	0·29664 (18)	0·083
P1C5	−0·0100 (7)	0·8481 (11)	0·32633 (19)	0·086
P1C6	−0·0359 (6)	0·7935 (10)	0·36784 (18)	0·075

33·02 < 2θ < 44·53°, no absorption corrections, $h = 0$ to 10, $k = 0$ to 10, $l = 0$ to 40, reflections 0,0,16, 020 and 400 as intensity standards, intensity variation <2%. 1487 unique reflections measured, 288 excluded during refinement [$F_o < 3\sigma(F_o)$]. Structure solved by the direct method (*MULTAN*78, Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), first E map revealed the positions of all non-H atoms; least-squares refinement using *SHELX*76 (Sheldrick, 1976), F magnitudes; isotropic and then anisotropic temperature factors gave $R = 0·048$, $S = 0·71$ with unit weights, including H atoms at positions calculated or located by difference synthesis. 193 parameters varied: x, y, z, U_{ij} for all non-H atoms, and a U for all H atoms of the two phenyl rings, x, y, z and a U for the carboxyl terminal H atom located by difference synthesis, and a U for all other H atoms of the atomic backbone connecting the two phenyl rings. In final cycle $(\Delta/\sigma)_{max} = 0·028$. Final difference synthesis $(\Delta\rho)_{max} = 0·28$ e Å⁻³ and $(\Delta\rho)_{min} = −0·13$ e Å⁻³. Scattering factors from *International Tables for X-ray Crystallography* (1974). Table 1* gives the atom parameters. Fig. 1 shows the molecule; Fig. 2 the packing in the unit cell. The numbering scheme is shown in Fig. 1 (*a*).

Related literature. The compound was synthesized according to Votano, Altman, Wilchek, Gorecki & Rich (1984). Single-crystal studies of chemically and

functionally related compounds were reported by Burley & Wang (1987), Wang & Burley (1987) and Fujii, Burley & Wang (1987), and a mechanism of antisickling action was proposed by Burley, Wang, Votano & Rich (1986). The intra- and intermolecular edge-to-face interactions between phenyl rings are enthalpically favorable (Burley & Petsko, 1986).
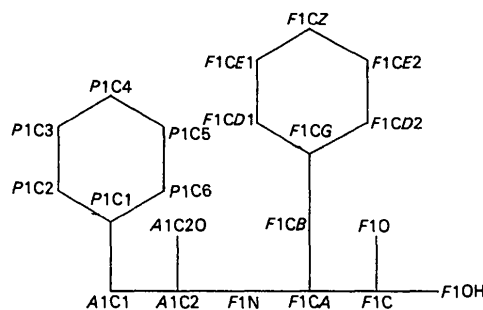
(*a*)
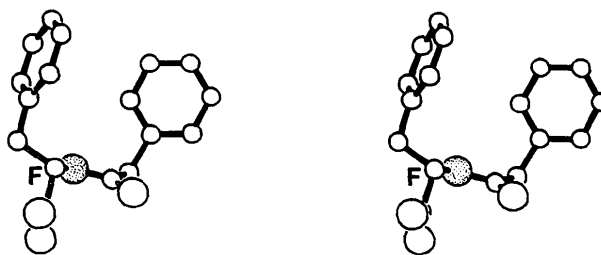
(*b*)

Fig. 1. (*a*) N-Phenylacetyl-L-phenylalanine, showing the numbering scheme. (*b*) Ball-and-stick stereodrawing of the molecular structure. The small open circles represent C atoms and the α-C is labeled with an *F*. Large open circles represent O atoms, and large shaded circles represent N atoms.
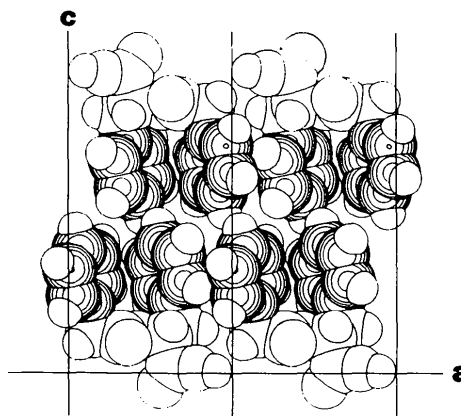

Fig. 2. *b*-Axis-projection van der Waals drawing of the crystal structure.

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Structure of Dibenzo-54-crown-18*

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Abstract. $C_{44}H_{72}O_{18}$, $M_r = 889 \cdot 05$, monoclinic, $P2_1/c$, $a = 27 \cdot 441$ (2), $b = 8 \cdot 9808$ (4), $c = 9 \cdot 3493$ (4) Å, $\beta = 90 \cdot 296$ (4)°, $V = 2304 \cdot 0$ (4) Å^3, $Z = 2$, $D_x = 1 \cdot 28$ g cm^{-3}, $\lambda(Cu\,K\alpha) = 1 \cdot 5418$ Å, $\mu = 7 \cdot 8$ cm^{-1}, $F(000) = 960$, $T = 161$ K, final $R = 4 \cdot 1\%$ for 2228 observed reflections. The molecule has a centre of symmetry. It consists of two benzo moieties connected by two parallel, helical polyether bridges, with the torsion angle sequence ag^-g^+ $(ag^-a)_7$. Shortest non-bonded contacts are $3 \cdot 5$ Å for non-H atoms.

Experimental. Dibenzo-54-crown-18† was formed as a by-product during the synthesis of benzo-27-crown-9† (Talma, van Vossen, Sudhölter, van Eerden & Reinhoudt, 1986) and obtained as colorless crystals after chromatography, m.p. 351–353 K. 80 MHz ^{1}H NMR (CDCl$_3$, Me$_4$Si as an internal standard): δ 6·90 (s, 8 H, ArH), 4·16 (m, 8 H, ArOCH_2), 3·84 (m, 8 H, ArOCH$_2$CH_2), 3·7–3·6 (m, 48 H, OCH$_2$); 50 MHz ^{13}C NMR (CDCl$_3$, Me$_4$Si): δ 148·96 (s, Ar-1,

Ar-2), 121·56 (d, Ar-4, Ar-5), 114·83 (d, Ar-3, Ar-6), 70·82, 70·54, 69·78, 68·92 (t, CH$_2$). Mass spectrum: m/e 888·472 (M$^+$; calcd 888·472). Elemental analysis for $C_{44}H_{72}O_{18}$, found: C 59·24, H 8·31%, calculated: C 59·44, H 8·16%. D_m not determined.

Intensities measured at 161 K on a Philips PW 1100 diffractometer (Cu $K\alpha$ radiation, graphite monochromator); crystal dimensions 0·10 × 0·40 × 0·40 mm. Lattice parameters determined by least squares from 25 reflections ($6 \cdot 5 < \theta < 20°$). A total of 3430 unique reflections up to $\theta = 60°$ ($-30 \leq h \leq 30$, $0 \leq k \leq 10$, $0 \leq l \leq 10$) measured in the $\theta/2\theta$ scan mode [scan speed 0·05° s^{-1}, scan width $(1 \cdot 1 + 0 \cdot 2\tan\theta)°$]; 2228 reflections considered observed $[F_o^2 > 3\sigma(F_o^2)]$. The intensity variation of three standard reflections, measured every hour, was less than 1%.

Structure solved with *MULTAN* (Germain, Main & Woolfson, 1971) and refined by full-matrix least squares. After convergence of the isotropic refinement an empirical absorption correction ($\mu = 7 \cdot 8$ cm^{-1}; correction factors 0·67–1·70) using the *DIFABS* procedure (Walker & Stuart, 1983) was applied, upon which R_{int} (F) of 153 pairs of symmetry-related reflections was reduced from 12·2 to 2·0%. Refinement was continued with anisotropic thermal parameters for the non-H atoms. H atoms located on

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* IUPAC name: 6,7,9,10,12,13,15,16,18,19,21,22,24,25,27,28,-35,36,38,39,41,42,44,45,47,48,50,51,53,54,56,57-dotriacontahydro-dibenzo[*b,c*][1,4,7,10,13,16,19,22,25,28,31,34,37,40,43,46,49,52]-octadecaoxacyclotetrapentacontin.

† Trivial nomenclature following Pedersen (1967).