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Evidence for Conserved Molecular Structures in *N*-Acyl 1,1'-Bis(tetrahydroisoquinoline) Derivatives

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X-ray crystallographic data

X-ray determination: Reflexion data were measured with an Enraf-Nonius CAD-4 diffractometer in $\theta/2\theta$ scan mode using graphite monochromatised copper radiation (λ 1.54184Å) for **4** and molybdenum radiation (λ 0.71073Å) for **5**. Data were corrected for absorption using the analytical method of De Meuleunaer and Tompa.[1] Reflexions with $I > 3\sigma(I)$ were considered observed. The structures were determined by direct phasing and Fourier methods. Hydrogen atoms were included in calculated positions and were assigned thermal parameters equal to those of the atom to which they were bonded. Positional and anisotropic thermal parameters for the non-hydrogen atoms were refined using full matrix least squares. Positional disorder was present in both structures, with the acyl group containing Cl2 having two orientations with occupancies *ca* 0.7 and 0.3 in each case. In **5** the two orientations were related by a rotation of *ca* 180° about the N2-C22 bond.

Reflexion weights used were $1/\sigma^2(F_o)$, with $\sigma(F_o)$ being derived from $\sigma(I_o)=[\sigma^2 (I_o) + (0.04I_o)^2]^{1/2}$. The weighted residual is defined as $R_w= (\Sigma w\Delta^2/\Sigma wF_o^2)^{1/2}$ Atomic scattering factors and anomalous dispersion parameters were from International Tables for X-ray Crystallography.[2] Structure solutions were by SIR92[3] and refinements used RAELS[4]

ORTEP-II[5] running on a Macintosh IIcx was used for the structural diagrams, and a DEC Alpha-AXP workstation was used for calculation.

References

1. De Meuleunaer, J., Tompa, H. *Acta Cryst*., 1965, **19**, 1014.
2. Ibers, J. A., Hamilton, W. C. (Eds) 'International Tables for X-Ray Crystallography', **4**, Kynoch Press, Birmingham, 1974.
3. Altomare, A., Burla, M.C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Polidori, G., *J. Appl. Cryst*., 1994, **27**, 435.
4. Rae, A.D., RAELS. A comprehensive Constrained Least Squares Refinement Program, University of New South Wales, 1989.
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X-ray crystallographic data for rac-*2,2'-di(chloroethanoyl)-6,6',7,7'-tetramethoxy-1,1',2,2',3,3',4,4'-octahydro-1,1'-bisisoquinoline* **4**

Formula $C_{26}H_{30}N_2O_6Cl_2$, M = 536, monoclinic, space group C 2/c, a = 28.389(9), b = 14.968(3), c = 13.176(4)Å, β = 11.95(1)°, V = 5193(3)Å^3, D_{calc} = 1.37 cm^{-3}, Z = 8, μ(Cu-Kα) = 26.42 cm^{-1}. Crystal size 0.25 x 0.24 x 0.12 mm, θ_{max} = 70°. The number of reflexions was 3664 considered observed out of 4925 unique data. Final residuals R, R_w were 0.048, 0.065. Atomic coordinates, bond lengths and angles, and thermal parameters are shown below.

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X-ray crystallographic data for rac-*2,2'-di(chlorocarbonyl)-6,6',7,7'-tetramethoxy-1,1',2,2',3,3',4,4'-octahydro-1,1'-bisisoquinoline* **5**

Formula $C_{24}H_{26}N_2O_6Cl_2$, M = 512, orthorhombic, space group P n a 2_1, a = 20.984(4), b = 9.664(3), c = 12.424(3)Å, β = 90°, V = 2363(1)$Å^3$, D_{calc} = 1.43 cm^{-3}, Z = 4, μ(Cu-Kα) = 3.15 cm^{-1}. Crystal size 0.23 x 0.18 x 0.14 mm, θ_{max} = 25°. The number of reflexions was 1619 considered observed out of 2173 unique data. Final residuals R, R_w were 0.046, 0.057. Atomic coordinates, bond lengths and angles, and thermal parameters are shown below.

ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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O3 0.049(2) 0.050(2) 0.043(2) 0.002(2) 0.003(2) 0.016(2) O
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C7 0.033(3) 0.050(4) 0.046(3) 0.004(3) -0.002(3) -0.003(3) C
C8 0.033(3) 0.081(5) 0.074(5) 0.005(3) 0.003(3) 0.018(4) C
C9 0.043(3) 0.074(5) 0.086(5) 0.018(3) 0.017(4) 0.006(4) C
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C22 0.081(6) 0.087(6) 0.065(6) -0.044(5) 0.027(5) -0.033(5) C
C21' 0.075(6) 0.066(6) 0.087(6) 0.013(5) 0.022(5) 0.029(5) C
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C20 0.83150(9) 0.80058(15) 0.87558(18) 0.0399(5) Uani C  ?
C21 0.7888(1) 0.7900(2) 0.9167(2) 0.0466(6) Uani C  ?
C22 0.7387(1) 0.8187(2) 0.8304(2) 0.0504(6) Uani C  ?
C23 0.68861(5) 0.79347(28) 0.62999(15) 0.057(2) Uani C  0.70
C24 0.6442(1) 0.8435(2) 0.6413(5) 0.066(2) Uani C  0.70
C23' 0.6844(1) 0.7896(6) 0.6400(3) 0.023(1) Uani C  0.30
C24' 0.6458(2) 0.8422(3) 0.6714(8) 0.067(2) Uani C  0.30
C25 0.9360(1) 0.8088(3) 0.6417(3) 0.090(1) Uani C  ?
C26 0.9776(1) 0.9000(3) 1.0649(3) 0.103(2) Uani C  ?
HC1 0.7872 0.6253 0.8104 0.035 Uani H  ?
HC3 0.8732 0.5910 0.8271 0.041 Uani H  ?
HC6 0.8058 0.4837 0.4597 0.048 Uani H  ?
H1C8 0.7222 0.5345 0.4440 0.046 Uani H  ?
H2C8 0.7307 0.6375 0.4880 0.046 Uani H  ?
H1C9 0.6950 0.4904 0.5780 0.044 Uani H  ?
H2C9 0.6665 0.5859 0.5360 0.044 Uani H  ?
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H2C11 0.6485 0.4818 0.6898 0.058 Uani H  ?
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H2C13 0.9455 0.3842 0.6745 0.092 Uani H  ?
H3C13 0.8964 0.3315 0.5884 0.092 Uani H  ?
HC14 0.7664 0.7406 0.6230 0.035 Uani H  ?
HC16 0.8518 0.7703 0.6466 0.040 Uani H  ?
HC19 0.8864 0.8520 1.0181 0.045 Uani H  ?
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H2C21 0.7865 0.7259 0.9356 0.047 Uani H  ?
H1C22 0.7383 0.8853 0.8248 0.050 Uani H  ?
H2C22 0.7106 0.7987 0.8535 0.050 Uani H  ?
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H2C24 0.6256 0.8761 0.5714 0.066 Uani H  0.70
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O1 0.056(1) 0.057(1) 0.0384(9) -0.0123(8) 0.0214(8) -0.0041(8) O
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O3 0.075(1) 0.069(1) 0.066(1) 0.017(1) 0.046(1) -0.001(1) O
O4 0.056(2) 0.052(3) 0.048(2) 0.019(2) 0.008(2) -0.001(1) O
O4' 0.039(3) 0.049(4) 0.054(4) 0.026(2) 0.006(3) -0.016(3) O
O5 0.0372(9) 0.109(2) 0.053(1) -0.004(1) 0.0181(8) -0.009(1) O
O6 0.043(1) 0.116(2) 0.057(1) -0.017(1) 0.0092(9) -0.020(1) O
N1 0.042(1) 0.036(1) 0.0322(9) -0.0041(8) 0.0126(8) -0.0034(7) N
N2 0.044(1) 0.036(1) 0.043(1) -0.0005(8) 0.0203(9) -0.0059(8) N
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C2 0.045(1) 0.031(1) 0.034(1) -0.0004(9) 0.0169(9) -0.0006(9) C
C3 0.048(1) 0.037(1) 0.039(1) 0.002(1) 0.017(1) -0.0001(9) C
C4 0.049(1) 0.043(1) 0.048(1) 0.004(1) 0.022(1) 0.003(1) C
C5 0.061(2) 0.048(1) 0.047(1) 0.002(1) 0.032(1) -0.004(1) C
C6 0.062(2) 0.049(1) 0.040(1) -0.004(1) 0.025(1) -0.009(1) C
C7 0.051(1) 0.037(1) 0.036(1) -0.003(1) 0.017(1) -0.0041(9) C
C8 0.052(1) 0.052(2) 0.032(1) -0.001(1) 0.012(1) -0.007(1) C
C9 0.046(1) 0.045(1) 0.034(1) -0.004(1) 0.008(1) -0.008(1) C
C10 0.048(1) 0.034(1) 0.041(1) -0.005(1) 0.017(1)  0.000(1) C
C11 0.054(2) 0.067(2) 0.062(2) -0.018(1) 0.031(1) -0.014(1) C
C12 0.049(2) 0.120(3) 0.060(2) 0.015(2) 0.009(1) -0.012(2) C
C13 0.130(3) 0.067(2) 0.104(3) 0.025(2) 0.073(3) -0.005(2) C
C14 0.040(1) 0.035(1) 0.031(1) 0.0006(9) 0.0150(9) -0.0018(9) C
C15 0.041(1) 0.032(1) 0.034(1) -0.0016(9) 0.0138(9) -0.0009(9) C
C16 0.041(1) 0.043(1) 0.036(1) 0.002(1) 0.014(1) 0.000(1) C
C17 0.038(1) 0.054(1) 0.044(1) 0.004(1) 0.014(1) 0.002(1) C
C18 0.039(1) 0.054(1) 0.043(1) -0.001(1) 0.006(1) -0.004(1) C
C19 0.049(1) 0.048(1) 0.035(1) -0.004(1) 0.010(1) -0.004(1) C
C20 0.048(1) 0.036(1) 0.036(1) -0.004(1) 0.017(1) -0.0017(9) C
C21 0.058(1) 0.049(1) 0.039(1) -0.012(1) 0.025(1) -0.010(1) C
C22 0.055(2) 0.052(2) 0.052(2) -0.007(1) 0.029(1) -0.019(1) C
C23 0.056(3) 0.049(3) 0.065(4) 0.009(3) 0.021(3) 0.006(3) C
C24 0.064(3) 0.063(3) 0.068(3) 0.006(2) 0.021(2) -0.007(2) C
C23' 0.022(3) 0.018(3) 0.034(4) -0.006(3) 0.013(3) -0.009(3) C
C24' 0.037(5) 0.079(5) 0.090(6) 0.013(4) 0.030(4) -0.050(4) C
C25 0.045(2) 0.180(4) 0.052(2) -0.008(2) 0.024(1) -0.005(2) C
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# MOLECULAR GEOMETRY

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; Altomare, A., Burla, M.C., Camalli, M., Cascarano, G., Giacovazzo,
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Guagliardi, A., Polidori, G., J. Appl. Cryst., 1994, 27, 435.

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Program, University of New South Wales, 1989.
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 4     1/2+x,1/2-y,z

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O5 0.0245(2) 0.5383(5) 0.6579(4) 0.069(1) Uani O  ?
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C9 0.2424(3) 0.2503(7) 0.2742(6) 0.068(2) Uani C  ?
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C12 0.0759(3) -0.0262(7) 0.6636(6) 0.064(2) Uani C  ?
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C21 0.1344(3) 0.7628(10) 0.1974(6) 0.076(3) Uani C  0.69
C22 0.2450(2) 0.7042(8) 0.2551(8) 0.078(3) Uani C  0.69
C21' 0.1231(6) 0.7330(19) 0.1926(6) 0.076(3) Uani C  0.31
C22' 0.2362(4) 0.7183(14) 0.2338(12) 0.078(3) Uani C  0.31
C23 0.0667(4) 0.4306(8) 0.7034(6) 0.081(2) Uani C  ?
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HC15 0.1221 0.4778 0.5295 0.044 Uani H  ?
HC18 -0.0138 0.8590 0.3996 0.047 Uani H  ?
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H2C21' 0.0972 0.6507 0.1616 0.076 Uani H  0.31
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O4' 0.129(3) 0.068(2) 0.150(3) -0.057(2) 0.089(3) -0.023(2) O
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N2' 0.047(3) 0.040(3) 0.061(3) -0.016(2) 0.019(3) -0.009(3) N
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C15 C16 C17 C18   -1.9(8)  1_555  1_555  1_555  1_555 no
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