Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 2-Chloro-1,2-diphenylethanone (desyl chloride)

**Richard Betz,* Cedric McCleland and Eric Hosten**

Nelson Mandela Metropolitan University, Summerstrand Campus, Department of Chemistry, University Way, Summerstrand, PO Box 77000, Port Elizabeth 6031, South Africa
Correspondence e-mail: richard.betz@webmail.co.za

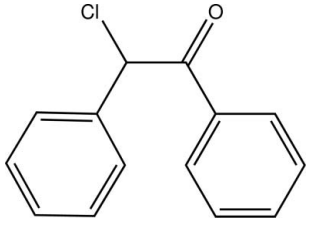
Received 5 April 2011; accepted 18 April 2011

Key indicators: single-crystal X-ray study; $T$ = 200 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.037; $wR$ factor = 0.104; data-to-parameter ratio = 19.4.

The title compound, $C_{14}H_{11}ClO$, is a racemic derivative of benzoin. Its carbonyl group adopts a nearly eclipsed conformation with the Cl substituent characterized by a dihedral angle of 17.5 (2)°. The closest intermolecular $\pi$–$\pi$ contact is 4.258 (1) Å.

## Related literature

For the crystal structure of benzoin, see: Haisa *et al.* (1980); Sole *et al.* (1998). For the crystal structure of 2-phenylacetophenone, see: Rieker *et al.* (1993). For the crystal structure of 2-chloroacetophenone, see: Grossert *et al.* (1984). Structures containing similar angles were retrieved from the Cambridge Structural Database (Allen, 2002).




## Experimental

### Crystal data

$C_{14}H_{11}ClO$
$M_r$ = 230.68
Monoclinic, $P2_1/c$
$a$ = 12.6233 (11) Å
$b$ = 5.8227 (5) Å
$c$ = 15.6745 (14) Å
$\beta$ = 97.317 (3)°
$V$ = 1142.72 (17) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.31 mm$^{-1}$
$T$ = 200 K
0.53 × 0.29 × 0.16 mm

### Data collection

Bruker APEXII CCD diffractometer
9777 measured reflections
2816 independent reflections
2366 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.104
$S$ = 1.07
2816 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT* (Bruker, 2010); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

The authors thank Mr Neil van der Vyver for helpful discussions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LD2009).

## References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bruker (2010). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Grossert, J. S., Dubey, P. K., Gill, G. H., Cameron, T. S. & Gardner, P. A. (1984). *Can. J. Chem.* **62**, 798–807.
Haisa, M., Kashino, S. & Morimoto, M. (1980). *Acta Cryst.* B**36**, 2832–2834.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Rieker, T. P., Haltiwanger, C., Eidman, K., Walba, D. W., Clark, N. A. & Larson, A. C. (1993). *Acta Cryst.* C**49**, 406–408.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sole, S., Gornitzka, H., Guerret, O. & Bertrand, G. (1998). *J. Am. Chem. Soc.* **120**, 9100–9101.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

# supplementary materials

*Acta Cryst.* (2011). E**67**, o1199 [ **doi:10.1107/S1600536811014541** ]

# 2-Chloro-1,2-diphenylethanone (desyl chloride)

**R. Betz, C. McCleland and E. Hosten**

## Comment

The title compound was studied as a reference structure for a series of transition-metal complexes employing it as a ligand.

Bond lengths and angles are usual. The torsion angle O=C—C—Cl is 17.5 (2) °. A statistics of values for the similar angles reported in the CSD (Allen, 2002) shows that this eclipsed conformation is the most preferable for α-cloroketones (Fig. 1 and Fig. 2). However, possibly due to steric hindrances from the bulky phenyl group next to the Cl substituent, the dihedral value is somewhat distorted in comparison to the molecular structure of 2-chloroacetophenone (Grossert *et al.* (1984)), where the respective angle was found at 2.4 °.

Unlike the crystal structure of 2-chloroacetophenone, which is dominated by strong C–H···O and C–H···Cl contacts, the crystal structure of the title compound does not show any intermolecular contacts whose range falls short of the sum of van-der-Waals radii. The closest π···π-contact was measured at 4.258 (1) Å.

## Experimental

The compound was synthesized by reacting benzoin with thionyl chloride. Crystals suitable for X-ray diffraction were obtained upon recrystallization from ethanol.

## Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.99 Å for the methylene group and C—H 0.95 Å for aromatic carbon atoms) and were included in the refinement in the riding model approximation, with $U$(H) set to 1.2$U_{eq}$(C).

## Figures

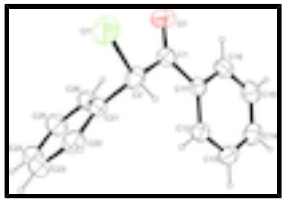


Fig. 1. The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids drawn at 50% probability level.

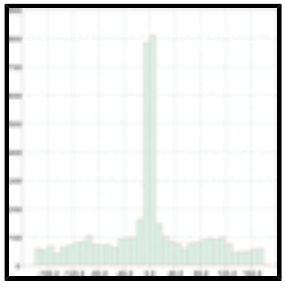


Fig. 2. Statistical distribution of O=C—C—Cl dihedral angles (data based on CSD search including all deposited crystal structures up to November 2010).

## 2-Chloro-1,2-diphenylethanone

*Crystal data*

| | |
|---|---|
| $C_{14}H_{11}ClO$ | $F(000) = 480$ |
| $M_r = 230.68$ | $D_x = 1.341$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 5815 reflections |
| $a = 12.6233$ (11) Å | $\theta = 2.6$–$28.3°$ |
| $b = 5.8227$ (5) Å | $\mu = 0.31$ mm$^{-1}$ |
| $c = 15.6745$ (14) Å | $T = 200$ K |
| $\beta = 97.317$ (3)° | Rod, colourless |
| $V = 1142.72$ (17) Å$^3$ | 0.53 × 0.29 × 0.16 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 2366 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int} = 0.024$ |
| graphite | $\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$ |
| φ and ω scans | $h = -16\rightarrow16$ |
| 9777 measured reflections | $k = -7\rightarrow6$ |
| 2816 independent reflections | $l = -20\rightarrow20$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.037$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.104$ | H-atom parameters constrained |
| $S = 1.07$ | $w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 0.3595P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 2816 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 145 parameters | $\Delta\rho_{max} = 0.36$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.42$ e Å$^{-3}$ |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.36760 (3) | 0.54577 (9) | 0.02422 (2) | 0.05873 (16) |
| O1 | 0.19610 (9) | 0.8528 (2) | 0.05035 (8) | 0.0585 (3) |
| C1 | 0.17721 (11) | 0.6644 (2) | 0.07711 (8) | 0.0369 (3) |
| C2 | 0.26188 (10) | 0.4753 (2) | 0.08663 (8) | 0.0361 (3) |

| | | | | |
|---|---|---|---|---|
| H2 | 0.2277 | 0.3291 | 0.0637 | 0.043* |
| C11 | 0.07080 (10) | 0.6085 (2) | 0.10402 (7) | 0.0318 (3) |
| C12 | 0.04806 (11) | 0.4010 (2) | 0.14191 (9) | 0.0369 (3) |
| H12 | 0.1014 | 0.2853 | 0.1511 | 0.044* |
| C13 | −0.05239 (11) | 0.3628 (3) | 0.16633 (10) | 0.0436 (3) |
| H13 | −0.0673 | 0.2221 | 0.1931 | 0.052* |
| C14 | −0.13073 (11) | 0.5290 (3) | 0.15188 (10) | 0.0454 (3) |
| H14 | −0.1996 | 0.5017 | 0.1682 | 0.054* |
| C15 | −0.10909 (12) | 0.7350 (3) | 0.11366 (10) | 0.0456 (3) |
| H15 | −0.1632 | 0.8486 | 0.1032 | 0.055* |
| C16 | −0.00869 (11) | 0.7752 (2) | 0.09067 (8) | 0.0395 (3) |
| H16 | 0.0063 | 0.9181 | 0.0655 | 0.047* |
| C21 | 0.30932 (9) | 0.4355 (2) | 0.17883 (8) | 0.0313 (3) |
| C22 | 0.36130 (11) | 0.2294 (2) | 0.20111 (10) | 0.0411 (3) |
| H22 | 0.3639 | 0.1128 | 0.1590 | 0.049* |
| C23 | 0.40932 (12) | 0.1938 (3) | 0.28445 (11) | 0.0485 (4) |
| H23 | 0.4461 | 0.0542 | 0.2991 | 0.058* |
| C24 | 0.40391 (12) | 0.3604 (3) | 0.34634 (10) | 0.0483 (4) |
| H24 | 0.4364 | 0.3348 | 0.4036 | 0.058* |
| C25 | 0.35139 (12) | 0.5639 (3) | 0.32497 (9) | 0.0451 (3) |
| H25 | 0.3470 | 0.6780 | 0.3677 | 0.054* |
| C26 | 0.30485 (11) | 0.6021 (2) | 0.24116 (8) | 0.0372 (3) |
| H26 | 0.2697 | 0.7436 | 0.2265 | 0.045* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0447 (2) | 0.0974 (4) | 0.0365 (2) | −0.0071 (2) | 0.01475 (15) | −0.00083 (19) |
| O1 | 0.0538 (6) | 0.0513 (7) | 0.0703 (8) | −0.0085 (5) | 0.0077 (6) | 0.0241 (6) |
| C1 | 0.0385 (6) | 0.0400 (7) | 0.0312 (6) | −0.0051 (5) | 0.0003 (5) | 0.0047 (5) |
| C2 | 0.0319 (6) | 0.0449 (7) | 0.0321 (6) | −0.0058 (5) | 0.0068 (5) | −0.0049 (5) |
| C11 | 0.0332 (6) | 0.0338 (6) | 0.0271 (5) | −0.0019 (5) | −0.0011 (4) | 0.0001 (5) |
| C12 | 0.0344 (6) | 0.0325 (6) | 0.0429 (7) | −0.0001 (5) | 0.0020 (5) | 0.0033 (5) |
| C13 | 0.0412 (7) | 0.0392 (7) | 0.0508 (8) | −0.0069 (6) | 0.0075 (6) | 0.0037 (6) |
| C14 | 0.0335 (7) | 0.0558 (9) | 0.0472 (8) | −0.0025 (6) | 0.0066 (6) | −0.0046 (7) |
| C15 | 0.0403 (7) | 0.0479 (8) | 0.0474 (8) | 0.0116 (6) | 0.0010 (6) | −0.0026 (6) |
| C16 | 0.0459 (7) | 0.0355 (7) | 0.0358 (7) | 0.0032 (6) | 0.0003 (5) | 0.0031 (5) |
| C21 | 0.0268 (5) | 0.0337 (6) | 0.0339 (6) | −0.0021 (5) | 0.0063 (4) | −0.0003 (5) |
| C22 | 0.0364 (7) | 0.0336 (7) | 0.0539 (8) | 0.0008 (5) | 0.0081 (6) | −0.0030 (6) |
| C23 | 0.0386 (7) | 0.0413 (8) | 0.0646 (10) | 0.0038 (6) | 0.0026 (6) | 0.0153 (7) |
| C24 | 0.0422 (7) | 0.0584 (9) | 0.0423 (7) | −0.0050 (7) | −0.0018 (6) | 0.0155 (7) |
| C25 | 0.0503 (8) | 0.0510 (9) | 0.0335 (7) | −0.0008 (7) | 0.0029 (6) | −0.0026 (6) |
| C26 | 0.0413 (7) | 0.0348 (7) | 0.0351 (6) | 0.0041 (5) | 0.0031 (5) | −0.0002 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cl1—C2 | 1.7997 (13) | C15—C16 | 1.381 (2) |
| O1—C1 | 1.2092 (18) | C15—H15 | 0.9500 |
| C1—C11 | 1.4941 (18) | C16—H16 | 0.9500 |

| | | | |
|---|---|---|---|
| C1—C2 | 1.529 (2) | C21—C26 | 1.3829 (18) |
| C2—C21 | 1.5100 (18) | C21—C22 | 1.3910 (18) |
| C2—H2 | 1.0000 | C22—C23 | 1.384 (2) |
| C11—C12 | 1.3921 (18) | C22—H22 | 0.9500 |
| C11—C16 | 1.3929 (18) | C23—C24 | 1.379 (2) |
| C12—C13 | 1.3883 (19) | C23—H23 | 0.9500 |
| C12—H12 | 0.9500 | C24—C25 | 1.378 (2) |
| C13—C14 | 1.381 (2) | C24—H24 | 0.9500 |
| C13—H13 | 0.9500 | C25—C26 | 1.3871 (19) |
| C14—C15 | 1.384 (2) | C25—H25 | 0.9500 |
| C14—H14 | 0.9500 | C26—H26 | 0.9500 |
| O1—C1—C11 | 121.31 (13) | C14—C15—H15 | 120.1 |
| O1—C1—C2 | 121.41 (13) | C15—C16—C11 | 120.67 (13) |
| C11—C1—C2 | 117.27 (11) | C15—C16—H16 | 119.7 |
| C21—C2—C1 | 113.02 (10) | C11—C16—H16 | 119.7 |
| C21—C2—Cl1 | 108.91 (9) | C26—C21—C22 | 119.22 (12) |
| C1—C2—Cl1 | 109.90 (10) | C26—C21—C2 | 121.45 (12) |
| C21—C2—H2 | 108.3 | C22—C21—C2 | 119.30 (12) |
| C1—C2—H2 | 108.3 | C23—C22—C21 | 120.13 (13) |
| Cl1—C2—H2 | 108.3 | C23—C22—H22 | 119.9 |
| C12—C11—C16 | 119.03 (12) | C21—C22—H22 | 119.9 |
| C12—C11—C1 | 123.44 (12) | C24—C23—C22 | 120.25 (14) |
| C16—C11—C1 | 117.52 (12) | C24—C23—H23 | 119.9 |
| C13—C12—C11 | 120.11 (13) | C22—C23—H23 | 119.9 |
| C13—C12—H12 | 119.9 | C25—C24—C23 | 119.92 (14) |
| C11—C12—H12 | 119.9 | C25—C24—H24 | 120.0 |
| C14—C13—C12 | 120.18 (14) | C23—C24—H24 | 120.0 |
| C14—C13—H13 | 119.9 | C24—C25—C26 | 120.06 (14) |
| C12—C13—H13 | 119.9 | C24—C25—H25 | 120.0 |
| C13—C14—C15 | 120.10 (13) | C26—C25—H25 | 120.0 |
| C13—C14—H14 | 120.0 | C21—C26—C25 | 120.40 (13) |
| C15—C14—H14 | 120.0 | C21—C26—H26 | 119.8 |
| C16—C15—C14 | 119.89 (13) | C25—C26—H26 | 119.8 |
| C16—C15—H15 | 120.1 | | |
| O1—C1—C2—C21 | 104.41 (15) | C12—C11—C16—C15 | −0.8 (2) |
| C11—C1—C2—C21 | −74.29 (14) | C1—C11—C16—C15 | 179.73 (12) |
| O1—C1—C2—Cl1 | −17.47 (17) | C1—C2—C21—C26 | −21.38 (17) |
| C11—C1—C2—Cl1 | 163.83 (9) | Cl1—C2—C21—C26 | 101.06 (13) |
| O1—C1—C11—C12 | −174.40 (14) | C1—C2—C21—C22 | 160.45 (11) |
| C2—C1—C11—C12 | 4.30 (18) | Cl1—C2—C21—C22 | −77.11 (13) |
| O1—C1—C11—C16 | 5.09 (19) | C26—C21—C22—C23 | −1.02 (19) |
| C2—C1—C11—C16 | −176.21 (11) | C2—C21—C22—C23 | 177.18 (12) |
| C16—C11—C12—C13 | −0.4 (2) | C21—C22—C23—C24 | 1.4 (2) |
| C1—C11—C12—C13 | 179.07 (12) | C22—C23—C24—C25 | −0.6 (2) |
| C11—C12—C13—C14 | 1.1 (2) | C23—C24—C25—C26 | −0.6 (2) |
| C12—C13—C14—C15 | −0.6 (2) | C22—C21—C26—C25 | −0.2 (2) |
| C13—C14—C15—C16 | −0.6 (2) | C2—C21—C26—C25 | −178.35 (13) |
| C14—C15—C16—C11 | 1.3 (2) | C24—C25—C26—C21 | 1.0 (2) |

**Fig. 1**

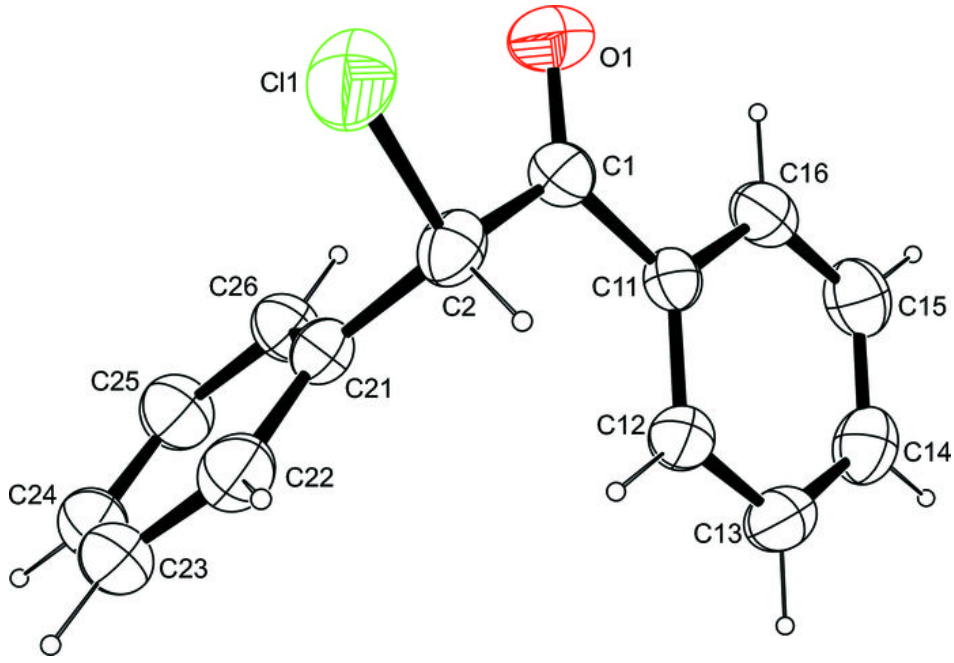
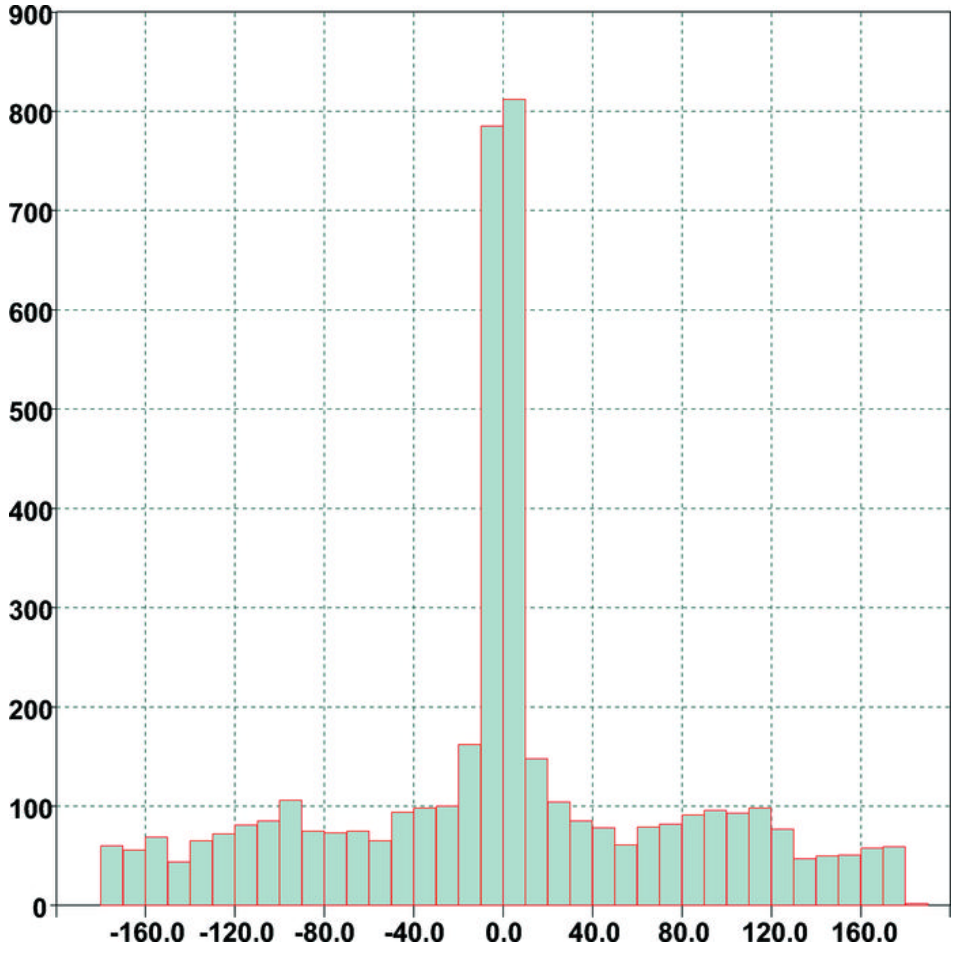


**Fig. 2**


900
800
700
600
500
400
300
200
100
0
-160.0
-120.0
-80.0
-40.0
0.0
40.0
80.0
120.0
160.0