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# 3,3′-(*m*-Phenylenedioxy)diphthalonitrile

**Wei Lv,[a] Kang Wang,[b] Daopeng Zhang,[a] Jianzhuang Jiang[a]* and Xiaomei Zhang[a]***

[a]Department of Chemistry, Shandong University, Jinan 250100, People's Republic of China, and [b]Department of Chemistry, University of Science and Technology Beijing, Beijing 100083, People's Republic of China
Correspondence e-mail: jianzhuang@ustb.edu.cn, zhangxiaomei@sdu.edu.cn

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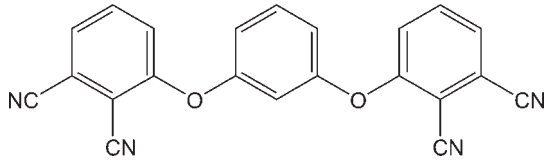
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.039; $wR$ factor = 0.111; data-to-parameter ratio = 15.7.

In the title compound, $C_{22}H_{10}N_4O_2$, the dihedral angles between the mean planes of the central benzene ring and the pendant rings are 79.20 (6) and 80.29 (6)°. The dihedral angle between the pendant rings is 10.27 (7)°.

## Related literature

For background to 'semi-rigid' molecules as ligands, see: Wang *et al.* (2005, 2009). For related structures, see: Huang *et al.* (2005); Zhang & Lu (2007).




## Experimental

### *Crystal data*

$C_{22}H_{10}N_4O_2$
$M_r$ = 362.34
Monoclinic, $C2/c$
$a$ = 15.668 (3) Å
$b$ = 12.722 (3) Å
$c$ = 19.004 (5) Å
$\beta$ = 109.911 (6)°
$V$ = 3561.7 (14) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 298 K
0.20 × 0.15 × 0.10 mm

### *Data collection*

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Siemens, 1996)
$T_{min}$ = 0.982, $T_{max}$ = 0.991
10307 measured reflections
3992 independent reflections
3145 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.111
$S$ = 1.03
3992 reflections
254 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5363).

## References

Huang, X., Zhao, F., Wang, R.-J., Zhang, F. & Tung, C.-H. (2005). *Acta Cryst.* E**61**, o4384–o4386.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SMART*, *SAINT* and *SADABS*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Wang, X., Qin, C., Wang, E., Li, Y., Su, Z., Xu, L. & Carlucci, L. (2005). *Angew. Chem. Int. Ed.* **44**, 5824–5827
Wang, H., Zhang, D., Sun, D., Chen, Y., Zhang, L., Tian, L., Jiang, J. & Ni, Z.-H. (2009). *Cryst. Growth Des*. pp. 5273–5282
Zhang, X.-M. & Lu, J.-T. (2007). *Acta Cryst.* E**63**, o3861.

# supplementary materials

*Acta Cryst.* (2010). E**66**, o1011 [ **doi:10.1107/S1600536810011578** ]

# 3,3'-(*m*-Phenylenedioxy)diphthalonitrile

**W. Lv, K. Wang, D. Zhang, J. Jiang and X. Zhang**

## Comment

In the past few years, the semirigidity of molecules have been extensively employed for search of novel functional compounds. For example,a new family of multidentate O-donor ligands with a semirigid V-shaped molecular framework have been used to construct metal-organic coordination frameworks (Wang *et al.*, 2009; Wang *et al.*, 2005), in which some showed interesting properties. Here, we present the structure of a new semirigid organic ligand.

The crystal structure of the title compound is given in Fig. 1. As can be found, all the bond lengths and angles are normal and correspond to those observed in related compound (Huang *et al.*, 2005; Zhang *et al.*, 2007). The aromatic rings (C3—C8 and C15—C20) in sides of the molecule are in the same direction of the aromatic rings(C9—C14) with a cis configuration. The three dihedral angles in the title compound are 79.81Å for C3—C8 and C9—C14, 80.83Å for C15—C20 and C9—C14,and 10.54 Å for C3—C8 and C15—C20, respectively.

## Experimental

Resorcinol (0.53 g, 5 mmol) and anhydrous $K_2CO_3$ was added to the solution of 2,3-dicyanophenyl nitrate (1.73 g, 10 mmol) in DMSO (25 ml). A kind of brown solution was generated after the solution was stirred for 48 hours at room temperature. The brown solution was added to 200 ml water, and was stirred for 30 min at room temperature. The precipitate formed was filtered, and washed by water. Yellow rods of (I) were obtained by solvent evaporation of the solution of the title compound in acetonitrile. Yield: 1.65 g, 91.2% Anal. for: $C_{22}H_{10}N_4O_2$ Calc. C, 72.92; H, 2.76; N, 15.47; Found: C, 72.85; H, 2.88; N, 15.44.

## Refinement

All H atoms were placed in geometrically idealized positions and treated as riding on their parent atoms with C($sp_2$ hybrid)-H distances of 0.93Å ($U_{iso}$(H)=1.2$U_{eq}$(C)).

## Figures

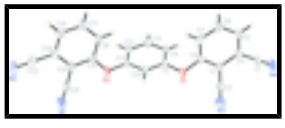


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at 30% probability level.

## 3,3'-(*m*-Phenylenedioxy)diphthalonitrile

*Crystal data*

$C_{22}H_{10}N_4O_2$ $F(000) = 1488$

| | |
|---|---|
| $M_r$ = 362.34 | $D_x$ = 1.351 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation, λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 4716 reflections |
| *a* = 15.668 (3) Å | θ = 2.6–27.4° |
| *b* = 12.722 (3) Å | μ = 0.09 mm$^{-1}$ |
| *c* = 19.004 (5) Å | *T* = 298 K |
| β = 109.911 (6)° | Rod, yellow |
| *V* = 3561.7 (14) Å$^3$ | 0.20 × 0.15 × 0.10 mm |
| *Z* = 8 | |

*Data collection*

| | |
|---|---|
| Bruker SMART 1000 CCD diffractometer | 3992 independent reflections |
| Radiation source: fine-focus sealed tube | 3145 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int}$ = 0.034 |
| ω scans | $\theta_{max}$ = 27.6°, $\theta_{min}$ = 2.1° |
| Absorption correction: multi-scan (SADABS; Siemens, 1996) | *h* = −14→20 |
| $T_{min}$ = 0.982, $T_{max}$ = 0.991 | *k* = −15→15 |
| 10307 measured reflections | *l* = −24→23 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.039 | H-atom parameters constrained |
| $wR(F^2)$ = 0.111 | $w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 1.0114P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| *S* = 1.03 | $(\Delta/\sigma)_{max} < 0.001$ |
| 3992 reflections | $\Delta\rho_{max}$ = 0.20 e Å$^{-3}$ |
| 254 parameters | $\Delta\rho_{min}$ = −0.16 e Å$^{-3}$ |
| 0 restraints | Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.0032 (4) |

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor wR and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-

factors(gt) etc. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C2 | 0.24878 (8) | 0.23670 (11) | 0.58469 (7) | 0.0496 (3) |
| O1 | 0.41988 (6) | 0.16069 (8) | 0.64684 (5) | 0.0597 (3) |
| O2 | 0.73624 (5) | 0.20407 (7) | 0.70914 (6) | 0.0582 (3) |
| C9 | 0.49526 (7) | 0.15184 (9) | 0.62398 (7) | 0.0425 (3) |
| C10 | 0.57791 (7) | 0.17608 (9) | 0.67719 (7) | 0.0437 (3) |
| H10 | 0.5826 | 0.1926 | 0.7260 | 0.052* |
| C20 | 0.88271 (8) | 0.16165 (10) | 0.78616 (7) | 0.0438 (3) |
| C11 | 0.65301 (7) | 0.17492 (9) | 0.65542 (7) | 0.0459 (3) |
| C14 | 0.48704 (8) | 0.12738 (10) | 0.55183 (7) | 0.0474 (3) |
| H14 | 0.4308 | 0.1110 | 0.5168 | 0.057* |
| C3 | 0.26451 (7) | 0.12567 (10) | 0.58820 (6) | 0.0420 (3) |
| C4 | 0.19286 (7) | 0.05388 (10) | 0.56020 (6) | 0.0443 (3) |
| C15 | 0.79734 (7) | 0.12689 (9) | 0.74065 (7) | 0.0448 (3) |
| C12 | 0.64815 (9) | 0.15132 (11) | 0.58405 (8) | 0.0554 (3) |
| H12 | 0.7000 | 0.1512 | 0.5707 | 0.067* |
| N3 | 0.23572 (10) | 0.32515 (11) | 0.58276 (8) | 0.0727 (4) |
| C21 | 0.90124 (8) | 0.27171 (11) | 0.79679 (8) | 0.0535 (3) |
| C8 | 0.35196 (8) | 0.08751 (11) | 0.61986 (7) | 0.0466 (3) |
| C16 | 0.77924 (9) | 0.02090 (10) | 0.73059 (8) | 0.0558 (3) |
| H16 | 0.7222 | −0.0022 | 0.7005 | 0.067* |
| C5 | 0.20892 (9) | −0.05263 (11) | 0.56674 (8) | 0.0528 (3) |
| H5 | 0.1612 | −0.1000 | 0.5485 | 0.063* |
| C19 | 0.95031 (8) | 0.08725 (11) | 0.82021 (7) | 0.0499 (3) |
| C13 | 0.56427 (9) | 0.12762 (11) | 0.53235 (8) | 0.0543 (3) |
| H13 | 0.5597 | 0.1115 | 0.4835 | 0.065* |
| N2 | 1.11044 (8) | 0.15377 (13) | 0.89675 (8) | 0.0774 (4) |
| C1 | 0.10262 (8) | 0.09249 (11) | 0.52163 (8) | 0.0524 (3) |
| C6 | 0.29672 (9) | −0.08846 (11) | 0.60074 (8) | 0.0585 (3) |
| H6 | 0.3077 | −0.1604 | 0.6061 | 0.070* |
| C18 | 0.93170 (10) | −0.01859 (12) | 0.80996 (8) | 0.0630 (4) |
| H18 | 0.9762 | −0.0681 | 0.8328 | 0.076* |
| C17 | 0.84594 (11) | −0.05017 (12) | 0.76525 (9) | 0.0661 (4) |
| H17 | 0.8332 | −0.1216 | 0.7585 | 0.079* |
| C22 | 1.03960 (9) | 0.12385 (12) | 0.86413 (8) | 0.0577 (4) |
| N4 | 0.03136 (8) | 0.12171 (11) | 0.48961 (8) | 0.0725 (4) |
| C7 | 0.36803 (9) | −0.01905 (12) | 0.62679 (8) | 0.0564 (3) |
| H7 | 0.4269 | −0.0441 | 0.6490 | 0.068* |
| N1 | 0.91780 (9) | 0.35902 (11) | 0.80612 (9) | 0.0809 (4) |

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

| $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0399 (6) | 0.0575 (8) | 0.0501 (7) | −0.0042 (6) | 0.0137 (5) | −0.0057 (6) |
| O1 | 0.0322 (4) | 0.0797 (7) | 0.0681 (6) | −0.0119 (4) | 0.0181 (4) | −0.0269 (5) |
| O2 | 0.0293 (4) | 0.0448 (5) | 0.0869 (7) | −0.0052 (3) | 0.0020 (4) | −0.0088 (4) |
| C9 | 0.0287 (5) | 0.0456 (6) | 0.0512 (7) | −0.0002 (4) | 0.0111 (5) | −0.0022 (5) |
| C10 | 0.0347 (6) | 0.0455 (6) | 0.0463 (6) | −0.0043 (5) | 0.0080 (5) | −0.0018 (5) |
| C20 | 0.0333 (6) | 0.0515 (7) | 0.0468 (6) | −0.0069 (5) | 0.0137 (5) | −0.0004 (5) |
| C11 | 0.0286 (5) | 0.0389 (6) | 0.0635 (8) | −0.0048 (4) | 0.0071 (5) | −0.0023 (5) |
| C14 | 0.0357 (6) | 0.0514 (7) | 0.0482 (7) | −0.0012 (5) | 0.0056 (5) | −0.0031 (5) |
| C3 | 0.0334 (5) | 0.0526 (7) | 0.0406 (6) | −0.0027 (5) | 0.0134 (5) | −0.0007 (5) |
| C4 | 0.0323 (6) | 0.0554 (7) | 0.0442 (6) | −0.0035 (5) | 0.0117 (5) | 0.0026 (5) |
| C15 | 0.0326 (5) | 0.0463 (7) | 0.0540 (7) | −0.0043 (5) | 0.0129 (5) | −0.0004 (5) |
| C12 | 0.0422 (7) | 0.0545 (7) | 0.0764 (9) | −0.0084 (6) | 0.0290 (6) | −0.0085 (7) |
| N3 | 0.0745 (9) | 0.0599 (8) | 0.0802 (9) | 0.0003 (7) | 0.0219 (7) | −0.0093 (6) |
| C21 | 0.0306 (6) | 0.0589 (8) | 0.0642 (8) | −0.0086 (5) | 0.0076 (5) | −0.0030 (6) |
| C8 | 0.0313 (5) | 0.0621 (8) | 0.0462 (6) | −0.0049 (5) | 0.0128 (5) | −0.0072 (5) |
| C16 | 0.0443 (7) | 0.0484 (7) | 0.0661 (8) | −0.0098 (6) | 0.0077 (6) | 0.0010 (6) |
| C5 | 0.0432 (7) | 0.0544 (8) | 0.0602 (8) | −0.0089 (6) | 0.0168 (6) | 0.0020 (6) |
| C19 | 0.0383 (6) | 0.0640 (8) | 0.0453 (6) | −0.0011 (6) | 0.0116 (5) | 0.0054 (6) |
| C13 | 0.0537 (7) | 0.0589 (8) | 0.0534 (7) | −0.0065 (6) | 0.0223 (6) | −0.0070 (6) |
| N2 | 0.0416 (7) | 0.1071 (11) | 0.0731 (8) | −0.0068 (7) | 0.0059 (6) | 0.0123 (8) |
| C1 | 0.0369 (6) | 0.0569 (8) | 0.0581 (7) | −0.0078 (6) | 0.0094 (6) | 0.0031 (6) |
| C6 | 0.0523 (8) | 0.0527 (8) | 0.0718 (9) | 0.0046 (6) | 0.0229 (7) | 0.0087 (7) |
| C18 | 0.0578 (8) | 0.0600 (9) | 0.0630 (8) | 0.0099 (7) | 0.0098 (7) | 0.0136 (7) |
| C17 | 0.0674 (9) | 0.0459 (7) | 0.0737 (9) | −0.0043 (6) | 0.0093 (8) | 0.0075 (7) |
| C22 | 0.0395 (7) | 0.0768 (10) | 0.0532 (7) | 0.0029 (6) | 0.0111 (6) | 0.0111 (7) |
| N4 | 0.0399 (6) | 0.0705 (8) | 0.0914 (10) | −0.0021 (6) | 0.0018 (6) | 0.0083 (7) |
| C7 | 0.0360 (6) | 0.0694 (9) | 0.0617 (8) | 0.0092 (6) | 0.0140 (6) | 0.0056 (7) |
| N1 | 0.0538 (7) | 0.0594 (8) | 0.1145 (12) | −0.0151 (6) | 0.0094 (8) | −0.0088 (8) |

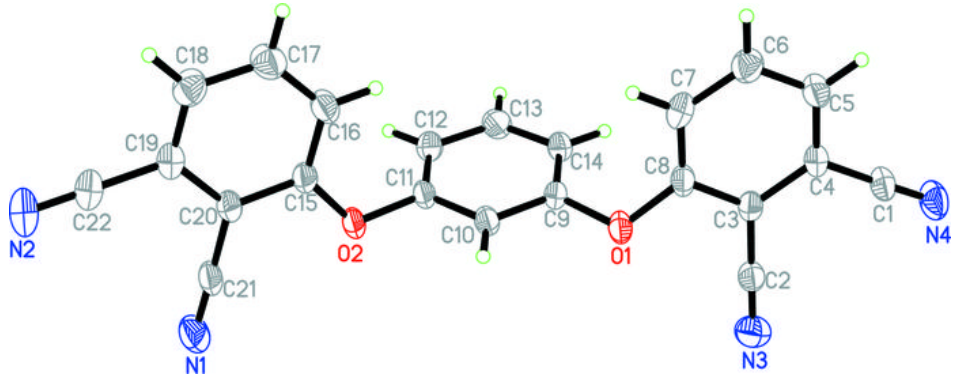
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C2—N3 | 1.1421 (19) | C15—C16 | 1.3777 (18) |
| C2—C3 | 1.4315 (19) | C12—C13 | 1.3798 (19) |
| O1—C8 | 1.3750 (15) | C12—H12 | 0.9300 |
| O1—C9 | 1.3949 (14) | C21—N1 | 1.1406 (19) |
| O2—C15 | 1.3596 (15) | C8—C7 | 1.377 (2) |
| O2—C11 | 1.4048 (14) | C16—C17 | 1.369 (2) |
| C9—C14 | 1.3686 (17) | C16—H16 | 0.9300 |
| C9—C10 | 1.3795 (16) | C5—C6 | 1.3828 (19) |
| C10—C11 | 1.3740 (16) | C5—H5 | 0.9300 |
| C10—H10 | 0.9300 | C19—C18 | 1.377 (2) |
| C20—C15 | 1.3946 (16) | C19—C22 | 1.4406 (18) |
| C20—C19 | 1.4035 (18) | C13—H13 | 0.9300 |
| C20—C21 | 1.4303 (19) | N2—C22 | 1.1369 (18) |
| C11—C12 | 1.3657 (19) | C1—N4 | 1.1368 (16) |
| C14—C13 | 1.3808 (18) | C6—C7 | 1.377 (2) |
| C14—H14 | 0.9300 | C6—H6 | 0.9300 |
| C3—C8 | 1.3834 (16) | C18—C17 | 1.382 (2) |
| C3—C4 | 1.4038 (16) | C18—H18 | 0.9300 |

| | | | |
|---|---|---|---|
| C4—C5 | 1.3761 (19) | C17—H17 | 0.9300 |
| C4—C1 | 1.4393 (17) | C7—H7 | 0.9300 |
| N3—C2—C3 | 178.96 (15) | N1—C21—C20 | 178.61 (16) |
| C8—O1—C9 | 117.33 (9) | O1—C8—C7 | 122.54 (11) |
| C15—O2—C11 | 118.00 (9) | O1—C8—C3 | 116.79 (12) |
| C14—C9—C10 | 121.99 (11) | C7—C8—C3 | 120.59 (11) |
| C14—C9—O1 | 121.98 (10) | C17—C16—C15 | 119.49 (12) |
| C10—C9—O1 | 115.89 (11) | C17—C16—H16 | 120.3 |
| C11—C10—C9 | 117.60 (11) | C15—C16—H16 | 120.3 |
| C11—C10—H10 | 121.2 | C4—C5—C6 | 119.28 (12) |
| C9—C10—H10 | 121.2 | C4—C5—H5 | 120.4 |
| C15—C20—C19 | 119.07 (12) | C6—C5—H5 | 120.4 |
| C15—C20—C21 | 120.25 (11) | C18—C19—C20 | 120.26 (12) |
| C19—C20—C21 | 120.67 (11) | C18—C19—C22 | 121.00 (13) |
| C12—C11—C10 | 122.52 (11) | C20—C19—C22 | 118.73 (13) |
| C12—C11—O2 | 120.25 (11) | C12—C13—C14 | 121.25 (12) |
| C10—C11—O2 | 117.16 (11) | C12—C13—H13 | 119.4 |
| C9—C14—C13 | 118.43 (11) | C14—C13—H13 | 119.4 |
| C9—C14—H14 | 120.8 | N4—C1—C4 | 178.29 (16) |
| C13—C14—H14 | 120.8 | C7—C6—C5 | 120.85 (13) |
| C8—C3—C4 | 118.83 (12) | C7—C6—H6 | 119.6 |
| C8—C3—C2 | 119.73 (11) | C5—C6—H6 | 119.6 |
| C4—C3—C2 | 121.43 (10) | C19—C18—C17 | 119.06 (13) |
| C5—C4—C3 | 120.56 (11) | C19—C18—H18 | 120.5 |
| C5—C4—C1 | 119.98 (11) | C17—C18—H18 | 120.5 |
| C3—C4—C1 | 119.41 (12) | C16—C17—C18 | 121.77 (14) |
| O2—C15—C16 | 124.39 (11) | C16—C17—H17 | 119.1 |
| O2—C15—C20 | 115.27 (10) | C18—C17—H17 | 119.1 |
| C16—C15—C20 | 120.34 (11) | N2—C22—C19 | 177.82 (15) |
| C11—C12—C13 | 118.21 (12) | C8—C7—C6 | 119.83 (12) |
| C11—C12—H12 | 120.9 | C8—C7—H7 | 120.1 |
| C13—C12—H12 | 120.9 | C6—C7—H7 | 120.1 |
| C8—O1—C9—C14 | 41.14 (17) | C9—O1—C8—C3 | −129.48 (12) |
| C8—O1—C9—C10 | −143.02 (12) | C4—C3—C8—O1 | −179.70 (10) |
| C14—C9—C10—C11 | −0.04 (18) | C2—C3—C8—O1 | 0.21 (16) |
| O1—C9—C10—C11 | −175.87 (11) | C4—C3—C8—C7 | −2.83 (18) |
| C9—C10—C11—C12 | 0.24 (18) | C2—C3—C8—C7 | 177.08 (12) |
| C9—C10—C11—O2 | 177.36 (10) | O2—C15—C16—C17 | −179.83 (13) |
| C15—O2—C11—C12 | −77.49 (16) | C20—C15—C16—C17 | −0.4 (2) |
| C15—O2—C11—C10 | 105.33 (13) | C3—C4—C5—C6 | −0.51 (19) |
| C10—C9—C14—C13 | −0.24 (19) | C1—C4—C5—C6 | 176.87 (12) |
| O1—C9—C14—C13 | 175.35 (12) | C15—C20—C19—C18 | −1.39 (19) |
| C8—C3—C4—C5 | 2.48 (17) | C21—C20—C19—C18 | 179.66 (13) |
| C2—C3—C4—C5 | −177.43 (11) | C15—C20—C19—C22 | 176.97 (12) |
| C8—C3—C4—C1 | −174.92 (11) | C21—C20—C19—C22 | −1.98 (18) |
| C2—C3—C4—C1 | 5.17 (17) | C11—C12—C13—C14 | −0.1 (2) |
| C11—O2—C15—C16 | −8.46 (19) | C9—C14—C13—C12 | 0.3 (2) |
| C11—O2—C15—C20 | 172.12 (11) | C4—C5—C6—C7 | −1.1 (2) |

| | | | |
|---|---|---|---|
| C19—C20—C15—O2 | −179.22 (11) | C20—C19—C18—C17 | 0.6 (2) |
| C21—C20—C15—O2 | −0.27 (17) | C22—C19—C18—C17 | −177.77 (14) |
| C19—C20—C15—C16 | 1.32 (19) | C15—C16—C17—C18 | −0.4 (2) |
| C21—C20—C15—C16 | −179.72 (13) | C19—C18—C17—C16 | 0.4 (2) |
| C10—C11—C12—C13 | −0.2 (2) | O1—C8—C7—C6 | 177.91 (12) |
| O2—C11—C12—C13 | −177.18 (11) | C3—C8—C7—C6 | 1.2 (2) |
| C9—O1—C8—C7 | 53.72 (17) | C5—C6—C7—C8 | 0.8 (2) |

**Fig. 1**


C18
C17
C16
C19
C12
C13
C14
C11
C15
C20
C22
N2
O2
C10
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O1
C8
C7
C6
C5
C4
C1
N4
C3
C2
N3
C21
N1