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## Structure Reports

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**(Z)-3-(9-Anthryl)-1-(4-chlorophenyl)-2-(4-nitro-1*H*-imidazol-1-yl)prop-2-en-1-one**

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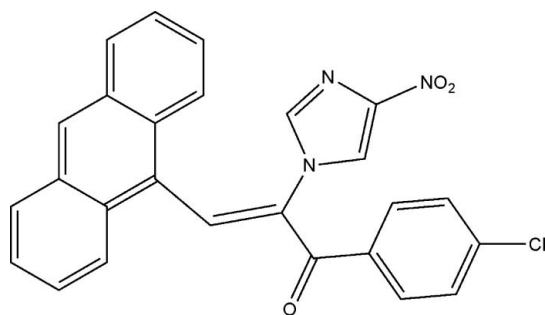
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Key indicators: single-crystal X-ray study;  $T = 292$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.044;  $wR$  factor = 0.113; data-to-parameter ratio = 13.6.

In the title compound,  $\text{C}_{26}\text{H}_{16}\text{ClN}_3\text{O}_3$ , the dihedral angle between the anthracene mean plane and imidazole ring is  $64.75(2)^\circ$ . In the crystal,  $\pi$ - $\pi$  interactions between anthracene fragments lead to the formation of stacks of molecules propagating in  $[100]$ . The short distance between the carbonyl groups of symmetry-related molecules [ $\text{C}\cdots\text{O} = 2.985(2)$  Å] indicates the existence of dipole-dipole interactions. The crystal packing also exhibits short intermolecular contacts between the nitro groups and Cl atoms [ $\text{Cl}\cdots\text{O} = 3.181(2)$  Å].

## Related literature

For general background, see: Corrêa *et al.* (2001); Daskiewicz *et al.* (2005); Sivakumar *et al.* (2009); Vogel *et al.* (2008). The synthesis was described by Erhardt *et al.* (1985).



## Experimental

## Crystal data

 $\text{C}_{26}\text{H}_{16}\text{ClN}_3\text{O}_3$   
 $M_r = 453.87$ 

 Triclinic,  $P\bar{1}$   
 $a = 8.0511(9)$  Å

 $b = 11.0406(12)$  Å  
 $c = 12.9274(14)$  Å  
 $\alpha = 76.065(2)^\circ$   
 $\beta = 85.974(2)^\circ$   
 $\gamma = 71.258(2)^\circ$   
 $V = 1056.1(2)$  Å<sup>3</sup>
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.22$  mm<sup>-1</sup>  
 $T = 292$  K  
 $0.16 \times 0.12 \times 0.10$  mm

## Data collection

 Bruker SMART APEX CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1997)  
 $T_{\min} = 0.956$ ,  $T_{\max} = 0.979$ 

 6168 measured reflections  
 4070 independent reflections  
 3354 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.014$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.113$   
 $S = 1.04$   
 4070 reflections

 299 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.56$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.50$  e Å<sup>-3</sup>

Table 1

Selected interatomic distances (Å).

$\text{C17}\cdots\text{O1}^{\text{i}}$	2.985 (2)	$\text{Cg1}\cdots\text{Cg2}^{\text{iii}}$	3.746 (7)
$\text{Cl1}\cdots\text{O3}^{\text{ii}}$	3.181 (3)	$\text{Cg2}\cdots\text{Cg2}^{\text{iv}}$	3.863 (8)

Symmetry codes: (i)  $-x + 1, -y + 2, -z$ ; (ii)  $x + 1, y + 1, z$ ; (iii)  $-x + 1, -y + 2, -z + 1$ ; (iv)  $-x, -y + 2, -z + 1$ . Cg1 and Cg2 are the centroids of atoms C1/C2/C14/C7-C9 and C2-C7, respectively.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: PLATON.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2548).

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**supplementary materials**

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**(Z)-3-(9-Anthryl)-1-(4-chlorophenyl)-2-(4-nitro-1H-imidazol-1-yl)prop-2-en-1-one**

**G. Wang, Y. Lu, C. Zhou and Y. Zhang**

**Comment**

Chalcones or 1,3-diaryl-2-propen-1-ones are natural or synthetic compounds belonging to the flavonoid family (Corrêa *et al.*, 2001). They exhibit different kinds of biological activities, such as antimicrobial, anticancer, antiviral, ant-malarial, anti-inflammatory activities (Daskiewicz *et al.*, 2005; Vogel *et al.*, 2008; Sivakumar *et al.*, 2009). Hence, chalcones are considered as a class of important therapeutic potentials. The title compound, (I), is part of our effort in order to contribute this research, and we report its crystal structure here.

In (I) (Fig. 1), the dihedral angle between the anthracene and imidazole rings is  $64.75(2)^\circ$  and the nitroimidazole is slightly twisted away from the 4-chlorophenyl ring with a dihedral angle of  $11.55(2)^\circ$ . In the crystal, the  $\pi$ - $\pi$  interactions between the anthracene fragments (Table 1) lead to formation of stacks of the molecules propagated in direction [100]. The short distance between the carbonyl groups [C17 $\cdots$ O1(1-x, 2-y, -z) 2.985(2) Å] (Table 1) reveals an existence of dipole-dipole interactions. The crystal packing also exhibits short intermolecular contacts between the nitro groups and chlorine atoms [Cl $\cdots$ O 3.181(2) Å] (Table 1).

**Experimental**

Compound (I) was synthesized according to the procedure of Erhardt *et al.* (1985). A crystal of (I) suitable for X-ray analysis was grown from a mixture solution of chloroform and acetone by slow evaporation at room temperature.

**Refinement**

All the hydrogen atoms were placed at their geometrical positions with C—H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

**Figures**

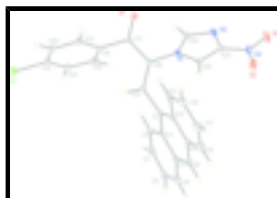


Fig. 1. The molecular structure of (I) showing the atomic numbering and 30% probability displacement ellipsoids.

**(Z)-3-(9-Anthryl)-1-(4-chlorophenyl)-2-(4-nitro-1H-imidazol-1-yl)prop-2-en-1-one**

*Crystal data*

C<sub>26</sub>H<sub>16</sub>ClN<sub>3</sub>O<sub>3</sub>  
 $M_r = 453.87$

$Z = 2$   
 $F_{000} = 468$

# supplementary materials

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Triclinic, <i>P</i> $\bar{1}$	$D_x = 1.427 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 8.0511 (9) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 11.0406 (12) \text{ \AA}$	Cell parameters from 2837 reflections
$c = 12.9274 (14) \text{ \AA}$	$\theta = 1.4\text{--}25.3^\circ$
$\alpha = 76.065 (2)^\circ$	$\mu = 0.22 \text{ mm}^{-1}$
$\beta = 85.974 (2)^\circ$	$T = 292 \text{ K}$
$\gamma = 71.258 (2)^\circ$	Block, orange
$V = 1056.1 (2) \text{ \AA}^3$	$0.16 \times 0.12 \times 0.10 \text{ mm}$

## Data collection

Bruker SMART APEX CCD area-detector diffractometer	4070 independent reflections
Radiation source: fine focus sealed Siemens Mo tube	3354 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.014$
$T = 292 \text{ K}$	$\theta_{\text{max}} = 26.0^\circ$
$0.3^\circ$ wide $\omega$ exposures scans	$\theta_{\text{min}} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1997)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.956$ , $T_{\text{max}} = 0.979$	$k = -13 \rightarrow 10$
6168 measured reflections	$l = -15 \rightarrow 15$

## Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 0.4068P]$
$wR(F^2) = 0.113$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{\text{max}} = 0.001$
4070 reflections	$\Delta\rho_{\text{max}} = 0.56 \text{ e \AA}^{-3}$
299 parameters	$\Delta\rho_{\text{min}} = -0.50 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.138 (5)

## Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.4503 (2)	0.91044 (16)	0.38505 (12)	0.0381 (4)
C2	0.3150 (2)	0.99845 (18)	0.43057 (13)	0.0427 (4)
C3	0.2324 (3)	1.13103 (19)	0.37653 (16)	0.0532 (5)
H3	0.2673	1.1618	0.3078	0.064*
C4	0.1039 (3)	1.2135 (2)	0.4233 (2)	0.0690 (6)
H4	0.0521	1.2999	0.3863	0.083*
C5	0.0482 (3)	1.1702 (3)	0.5267 (2)	0.0758 (7)
H5	-0.0389	1.2284	0.5581	0.091*
C6	0.1195 (3)	1.0455 (3)	0.58072 (18)	0.0671 (6)
H6	0.0806	1.0181	0.6491	0.080*
C7	0.2544 (2)	0.9537 (2)	0.53486 (14)	0.0507 (5)
C8	0.3284 (3)	0.8240 (2)	0.58804 (14)	0.0570 (5)
H8	0.2870	0.7948	0.6553	0.068*
C9	0.4618 (3)	0.7360 (2)	0.54475 (14)	0.0528 (5)
C10	0.5404 (4)	0.6035 (2)	0.60138 (18)	0.0751 (7)
H10	0.4981	0.5739	0.6682	0.090*
C11	0.6738 (4)	0.5211 (2)	0.5604 (2)	0.0864 (8)
H11	0.7210	0.4345	0.5983	0.104*
C12	0.7438 (4)	0.5643 (2)	0.45999 (19)	0.0730 (7)
H12	0.8385	0.5065	0.4332	0.088*
C13	0.6736 (3)	0.68926 (18)	0.40237 (15)	0.0516 (5)
H13	0.7218	0.7164	0.3368	0.062*
C14	0.5276 (2)	0.77936 (17)	0.44076 (13)	0.0428 (4)
C15	0.5225 (2)	0.96316 (15)	0.28220 (12)	0.0370 (4)
H15	0.5605	1.0348	0.2804	0.044*
C16	0.5410 (2)	0.92308 (15)	0.19171 (12)	0.0351 (4)
C17	0.6425 (2)	0.97302 (15)	0.10011 (12)	0.0364 (4)
C18	0.6982 (2)	1.08892 (16)	0.10310 (12)	0.0372 (4)
C19	0.5813 (2)	1.21059 (17)	0.10958 (14)	0.0442 (4)
H19	0.4615	1.2227	0.1122	0.053*
C20	0.6414 (3)	1.31410 (18)	0.11219 (15)	0.0503 (5)
H20	0.5631	1.3961	0.1153	0.060*
C21	0.8197 (3)	1.29305 (19)	0.11011 (15)	0.0532 (5)
C22	0.9379 (3)	1.1743 (2)	0.10195 (16)	0.0563 (5)
H22	1.0576	1.1626	0.0995	0.068*
C23	0.8762 (2)	1.07254 (18)	0.09746 (15)	0.0474 (4)
H23	0.9550	0.9922	0.0906	0.057*
C24	0.5604 (3)	0.70649 (17)	0.15237 (15)	0.0488 (4)
H24	0.6791	0.6812	0.1360	0.059*
C25	0.2993 (3)	0.70981 (18)	0.17933 (14)	0.0480 (4)

## supplementary materials

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C26	0.3024 (2)	0.82478 (17)	0.19785 (13)	0.0425 (4)
H26	0.2098	0.8902	0.2183	0.051*
Cl1	0.90255 (10)	1.41713 (6)	0.11994 (6)	0.0886 (3)
N1	0.47212 (18)	0.82266 (13)	0.17975 (10)	0.0378 (3)
N2	0.4588 (2)	0.63534 (15)	0.15188 (13)	0.0554 (4)
N3	0.1473 (3)	0.6670 (2)	0.18554 (14)	0.0685 (5)
O1	0.68863 (17)	0.91581 (12)	0.02841 (10)	0.0486 (3)
O2	0.0083 (3)	0.7406 (2)	0.21193 (17)	0.0925 (6)
O3	0.1648 (3)	0.5612 (2)	0.16539 (18)	0.1061 (7)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0429 (9)	0.0474 (9)	0.0326 (8)	-0.0239 (7)	-0.0008 (7)	-0.0116 (7)
C2	0.0408 (9)	0.0578 (11)	0.0399 (9)	-0.0234 (8)	0.0005 (7)	-0.0200 (8)
C3	0.0511 (11)	0.0579 (12)	0.0554 (11)	-0.0168 (9)	-0.0008 (9)	-0.0223 (9)
C4	0.0561 (13)	0.0703 (14)	0.0842 (16)	-0.0094 (11)	-0.0040 (11)	-0.0377 (13)
C5	0.0495 (13)	0.108 (2)	0.0832 (17)	-0.0176 (13)	0.0071 (11)	-0.0576 (16)
C6	0.0482 (12)	0.119 (2)	0.0535 (12)	-0.0369 (13)	0.0112 (9)	-0.0440 (13)
C7	0.0441 (10)	0.0823 (14)	0.0407 (9)	-0.0335 (10)	0.0028 (8)	-0.0241 (10)
C8	0.0605 (12)	0.0901 (16)	0.0345 (9)	-0.0445 (12)	0.0046 (8)	-0.0135 (10)
C9	0.0681 (13)	0.0633 (12)	0.0366 (9)	-0.0377 (10)	-0.0063 (8)	-0.0040 (8)
C10	0.113 (2)	0.0690 (15)	0.0459 (12)	-0.0430 (15)	-0.0093 (12)	0.0035 (11)
C11	0.137 (3)	0.0527 (13)	0.0578 (14)	-0.0232 (15)	-0.0204 (15)	0.0063 (11)
C12	0.0934 (18)	0.0528 (12)	0.0627 (14)	-0.0081 (12)	-0.0162 (12)	-0.0099 (10)
C13	0.0619 (12)	0.0490 (10)	0.0441 (10)	-0.0177 (9)	-0.0071 (9)	-0.0085 (8)
C14	0.0505 (10)	0.0486 (10)	0.0365 (9)	-0.0249 (8)	-0.0043 (7)	-0.0089 (7)
C15	0.0408 (9)	0.0366 (8)	0.0385 (8)	-0.0177 (7)	-0.0019 (7)	-0.0091 (7)
C16	0.0384 (9)	0.0322 (8)	0.0376 (8)	-0.0142 (6)	-0.0030 (6)	-0.0083 (6)
C17	0.0361 (8)	0.0373 (8)	0.0358 (8)	-0.0104 (7)	-0.0018 (6)	-0.0092 (7)
C18	0.0439 (9)	0.0390 (8)	0.0318 (8)	-0.0178 (7)	0.0038 (6)	-0.0080 (6)
C19	0.0456 (10)	0.0416 (9)	0.0458 (9)	-0.0154 (8)	0.0034 (7)	-0.0092 (7)
C20	0.0647 (12)	0.0386 (9)	0.0493 (10)	-0.0194 (8)	0.0072 (9)	-0.0107 (8)
C21	0.0713 (13)	0.0516 (11)	0.0508 (11)	-0.0378 (10)	0.0146 (9)	-0.0169 (9)
C22	0.0508 (11)	0.0676 (13)	0.0648 (12)	-0.0333 (10)	0.0149 (9)	-0.0256 (10)
C23	0.0452 (10)	0.0499 (10)	0.0526 (10)	-0.0186 (8)	0.0091 (8)	-0.0195 (8)
C24	0.0616 (12)	0.0385 (9)	0.0507 (10)	-0.0185 (8)	0.0026 (8)	-0.0152 (8)
C25	0.0647 (12)	0.0497 (10)	0.0391 (9)	-0.0343 (9)	-0.0065 (8)	-0.0038 (8)
C26	0.0461 (10)	0.0467 (9)	0.0402 (9)	-0.0221 (8)	-0.0022 (7)	-0.0089 (7)
Cl1	0.1041 (5)	0.0745 (4)	0.1183 (6)	-0.0626 (4)	0.0236 (4)	-0.0392 (4)
N1	0.0449 (8)	0.0364 (7)	0.0372 (7)	-0.0181 (6)	-0.0005 (6)	-0.0107 (6)
N2	0.0803 (12)	0.0435 (9)	0.0524 (9)	-0.0313 (8)	-0.0009 (8)	-0.0133 (7)
N3	0.0902 (15)	0.0785 (13)	0.0566 (10)	-0.0601 (12)	-0.0108 (10)	-0.0030 (9)
O1	0.0552 (8)	0.0524 (7)	0.0465 (7)	-0.0217 (6)	0.0111 (6)	-0.0232 (6)
O2	0.0715 (12)	0.1073 (15)	0.1141 (15)	-0.0560 (11)	0.0001 (11)	-0.0155 (12)
O3	0.1425 (18)	0.1018 (14)	0.1193 (16)	-0.0927 (14)	-0.0026 (13)	-0.0342 (12)

Geometric parameters (Å, °)

C1—C2	1.408 (2)	C15—H15	0.9300
C1—C14	1.408 (2)	C16—N1	1.4318 (19)
C1—C15	1.477 (2)	C16—C17	1.488 (2)
C2—C3	1.421 (3)	C17—O1	1.2162 (19)
C2—C7	1.429 (2)	C17—C18	1.495 (2)
C3—C4	1.355 (3)	C18—C23	1.384 (2)
C3—H3	0.9300	C18—C19	1.389 (2)
C4—C5	1.402 (4)	C19—C20	1.384 (2)
C4—H4	0.9300	C19—H19	0.9300
C5—C6	1.341 (4)	C20—C21	1.378 (3)
C5—H5	0.9300	C20—H20	0.9300
C6—C7	1.432 (3)	C21—C22	1.374 (3)
C6—H6	0.9300	C21—C11	1.7382 (18)
C7—C8	1.384 (3)	C22—C23	1.380 (3)
C8—C9	1.385 (3)	C22—H22	0.9300
C8—H8	0.9300	C23—H23	0.9300
C9—C10	1.425 (3)	C24—N2	1.305 (2)
C9—C14	1.439 (2)	C24—N1	1.369 (2)
C10—C11	1.336 (4)	C24—H24	0.9300
C10—H10	0.9300	C25—C26	1.355 (2)
C11—C12	1.415 (4)	C25—N2	1.360 (3)
C11—H11	0.9300	C25—N3	1.437 (3)
C12—C13	1.357 (3)	C26—N1	1.364 (2)
C12—H12	0.9300	C26—H26	0.9300
C13—C14	1.422 (3)	N3—O3	1.219 (3)
C13—H13	0.9300	N3—O2	1.235 (3)
C15—C16	1.330 (2)		
C17...O1 <sup>i</sup>	2.985 (2)	Cg1...Cg2 <sup>iii</sup>	3.746 (7)
C11...O3 <sup>ii</sup>	3.181 (3)	Cg2...Cg2 <sup>iv</sup>	3.863 (8)
C2—C1—C14	121.15 (15)	C16—C15—H15	115.3
C2—C1—C15	117.97 (15)	C1—C15—H15	115.3
C14—C1—C15	120.54 (15)	C15—C16—N1	121.23 (14)
C1—C2—C3	122.84 (16)	C15—C16—C17	122.54 (14)
C1—C2—C7	119.41 (17)	N1—C16—C17	116.12 (13)
C3—C2—C7	117.74 (17)	O1—C17—C16	120.77 (14)
C4—C3—C2	121.3 (2)	O1—C17—C18	120.97 (14)
C4—C3—H3	119.4	C16—C17—C18	118.09 (13)
C2—C3—H3	119.4	C23—C18—C19	119.23 (15)
C3—C4—C5	120.8 (2)	C23—C18—C17	117.30 (15)
C3—C4—H4	119.6	C19—C18—C17	123.47 (15)
C5—C4—H4	119.6	C20—C19—C18	120.67 (17)
C6—C5—C4	120.4 (2)	C20—C19—H19	119.7
C6—C5—H5	119.8	C18—C19—H19	119.7
C4—C5—H5	119.8	C21—C20—C19	118.55 (17)
C5—C6—C7	121.2 (2)	C21—C20—H20	120.7

## supplementary materials

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C5—C6—H6	119.4	C19—C20—H20	120.7
C7—C6—H6	119.4	C22—C21—C20	121.89 (17)
C8—C7—C2	119.04 (17)	C22—C21—C11	117.65 (16)
C8—C7—C6	122.40 (19)	C20—C21—C11	120.45 (15)
C2—C7—C6	118.6 (2)	C21—C22—C23	118.98 (18)
C7—C8—C9	122.41 (17)	C21—C22—H22	120.5
C7—C8—H8	118.8	C23—C22—H22	120.5
C9—C8—H8	118.8	C22—C23—C18	120.63 (17)
C8—C9—C10	121.97 (19)	C22—C23—H23	119.7
C8—C9—C14	119.60 (18)	C18—C23—H23	119.7
C10—C9—C14	118.4 (2)	N2—C24—N1	112.21 (18)
C11—C10—C9	121.4 (2)	N2—C24—H24	123.9
C11—C10—H10	119.3	N1—C24—H24	123.9
C9—C10—H10	119.3	C26—C25—N2	112.81 (16)
C10—C11—C12	120.6 (2)	C26—C25—N3	125.7 (2)
C10—C11—H11	119.7	N2—C25—N3	121.48 (18)
C12—C11—H11	119.7	C25—C26—N1	104.26 (16)
C13—C12—C11	120.5 (2)	C25—C26—H26	127.9
C13—C12—H12	119.7	N1—C26—H26	127.9
C11—C12—H12	119.7	C26—N1—C24	106.95 (14)
C12—C13—C14	121.0 (2)	C26—N1—C16	125.02 (14)
C12—C13—H13	119.5	C24—N1—C16	128.00 (15)
C14—C13—H13	119.5	C24—N2—C25	103.77 (15)
C1—C14—C13	123.55 (16)	O3—N3—O2	124.9 (2)
C1—C14—C9	118.36 (17)	O3—N3—C25	118.1 (2)
C13—C14—C9	118.00 (17)	O2—N3—C25	116.95 (19)
C16—C15—C1	129.36 (14)		
C14—C1—C2—C3	-179.34 (15)	C1—C15—C16—C17	-169.86 (16)
C15—C1—C2—C3	7.3 (2)	C15—C16—C17—O1	164.24 (16)
C14—C1—C2—C7	-0.4 (2)	N1—C16—C17—O1	-12.1 (2)
C15—C1—C2—C7	-173.69 (14)	C15—C16—C17—C18	-11.0 (2)
C1—C2—C3—C4	-179.21 (18)	N1—C16—C17—C18	172.64 (13)
C7—C2—C3—C4	1.8 (3)	O1—C17—C18—C23	-54.0 (2)
C2—C3—C4—C5	-0.1 (3)	C16—C17—C18—C23	121.27 (17)
C3—C4—C5—C6	-1.0 (3)	O1—C17—C18—C19	125.09 (18)
C4—C5—C6—C7	0.4 (3)	C16—C17—C18—C19	-59.7 (2)
C1—C2—C7—C8	-1.1 (2)	C23—C18—C19—C20	-1.1 (3)
C3—C2—C7—C8	177.93 (16)	C17—C18—C19—C20	179.92 (15)
C1—C2—C7—C6	178.61 (15)	C18—C19—C20—C21	-1.1 (3)
C3—C2—C7—C6	-2.3 (2)	C19—C20—C21—C22	2.2 (3)
C5—C6—C7—C8	-178.96 (19)	C19—C20—C21—C11	-176.77 (14)
C5—C6—C7—C2	1.3 (3)	C20—C21—C22—C23	-1.1 (3)
C2—C7—C8—C9	1.3 (3)	C11—C21—C22—C23	177.95 (15)
C6—C7—C8—C9	-178.43 (17)	C21—C22—C23—C18	-1.2 (3)
C7—C8—C9—C10	178.23 (19)	C19—C18—C23—C22	2.2 (3)
C7—C8—C9—C14	0.0 (3)	C17—C18—C23—C22	-178.67 (16)
C8—C9—C10—C11	-177.3 (2)	N2—C25—C26—N1	0.8 (2)
C14—C9—C10—C11	0.9 (3)	N3—C25—C26—N1	-178.49 (16)
C9—C10—C11—C12	1.5 (4)	C25—C26—N1—C24	-0.45 (18)



C10—C11—C12—C13	-1.7 (4)	C25—C26—N1—C16	-178.48 (14)
C11—C12—C13—C14	-0.6 (3)	N2—C24—N1—C26	0.0 (2)
C2—C1—C14—C13	-174.85 (16)	N2—C24—N1—C16	177.96 (15)
C15—C1—C14—C13	-1.7 (2)	C15—C16—N1—C26	53.9 (2)
C2—C1—C14—C9	1.6 (2)	C17—C16—N1—C26	-129.70 (16)
C15—C1—C14—C9	174.79 (14)	C15—C16—N1—C24	-123.73 (19)
C12—C13—C14—C1	179.44 (18)	C17—C16—N1—C24	52.7 (2)
C12—C13—C14—C9	3.0 (3)	N1—C24—N2—C25	0.4 (2)
C8—C9—C14—C1	-1.5 (2)	C26—C25—N2—C24	-0.8 (2)
C10—C9—C14—C1	-179.75 (17)	N3—C25—N2—C24	178.53 (16)
C8—C9—C14—C13	175.20 (17)	C26—C25—N3—O3	179.18 (19)
C10—C9—C14—C13	-3.1 (3)	N2—C25—N3—O3	0.0 (3)
C2—C1—C15—C16	-126.63 (19)	C26—C25—N3—O2	-1.4 (3)
C14—C1—C15—C16	60.0 (2)	N2—C25—N3—O2	179.44 (19)
C1—C15—C16—N1	6.3 (3)		

Symmetry codes: (i)  $-x+1, -y+2, -z$ ; (ii)  $x+1, y+1, z$ ; (iii)  $-x+1, -y+2, -z+1$ ; (iv)  $-x, -y+2, -z+1$ .

Fig. 1

