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## Structure Reports

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# 4-Phenyl-9,12,15-trioxa-1,5,6,18-tetra-azatetracyclo[16.6.1.0<sup>2,6</sup>.0<sup>19,24</sup>]pentaconta-2,4,19,21,23-pentaen-25-one

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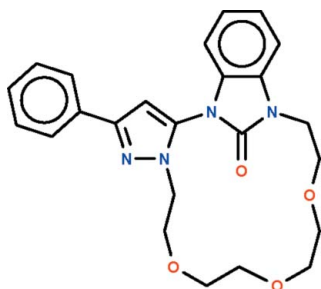
Received 14 September 2009; accepted 14 September 2009

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.055;  $wR$  factor = 0.176; data-to-parameter ratio = 15.8.

The title compound,  $\text{C}_{24}\text{H}_{26}\text{N}_4\text{O}_4$ , is a diaza-crown ether encompassing linked phenylpyrazolyl and benzimidazole units that contribute five atoms to the 16-atom ring. The two planar phenylpyrazolyl and benzimidazole units are aligned at an angle of  $66.4(1)^\circ$ . The carbonyl O atom of the benzimidazole unit is directed away from the middle of the ring.

## Related literature

For the selective recognition of sodium and potassium cyanide by diaza-crown ethers, see: Liu *et al.* (2005).



## Experimental

### Crystal data

$\text{C}_{24}\text{H}_{26}\text{N}_4\text{O}_4$	$V = 2262.6(3) \text{ \AA}^3$
$M_r = 434.49$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 13.348(1) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 15.785(1) \text{ \AA}$	$T = 293 \text{ K}$
$c = 11.007(1) \text{ \AA}$	$0.30 \times 0.30 \times 0.20 \text{ mm}$
$\beta = 102.681(1)^\circ$	

### Data collection

Nonius KappaCCD diffractometer	4559 independent reflections
Absorption correction: none	3705 reflections with $I > 2\sigma(I)$
4728 measured reflections	$R_{\text{int}} = 0.038$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$	289 parameters
$wR(F^2) = 0.176$	H-atom parameters constrained
$S = 1.16$	$\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$
4559 reflections	$\Delta\rho_{\text{min}} = -0.30 \text{ e \AA}^{-3}$

Data collection: *KappaCCD Server Software* (Nonius, 1998); cell refinement: *KappaCCD Server Software*; data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the Laboratoire de Cristalochimie de la Faculté des Sciences, Université Paul Cézanne Aix-Marseille III, for the diffraction measurements. The Université Mohammed V-Agdal and the University of Malaya are thanked for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2541).

## References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.  
 Liu, H., Shao, X.-B., Jia, M.-X., Jiang, X.-K., Li, Z.-T. & Chen, G.-J. (2005). *Tetrahedron*, **61**, 8095–8100.  
 Nonius (1998). *KappaCCD Server Software*. Nonius BV, Delft, The Netherlands.  
 Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Westrip, S. P. (2009). *publCIF*. In preparation.

## supporting information

*Acta Cryst.* (2009). E65, o2493 [doi:10.1107/S1600536809037131]

## 4-Phenyl-9,12,15-trioxa-1,5,6,18-tetraazatetracyclo- [16.6.1.0<sup>2,6</sup>.0<sup>19,24</sup>]pentaconta-2,4,19,21,23-pentaen-25-one

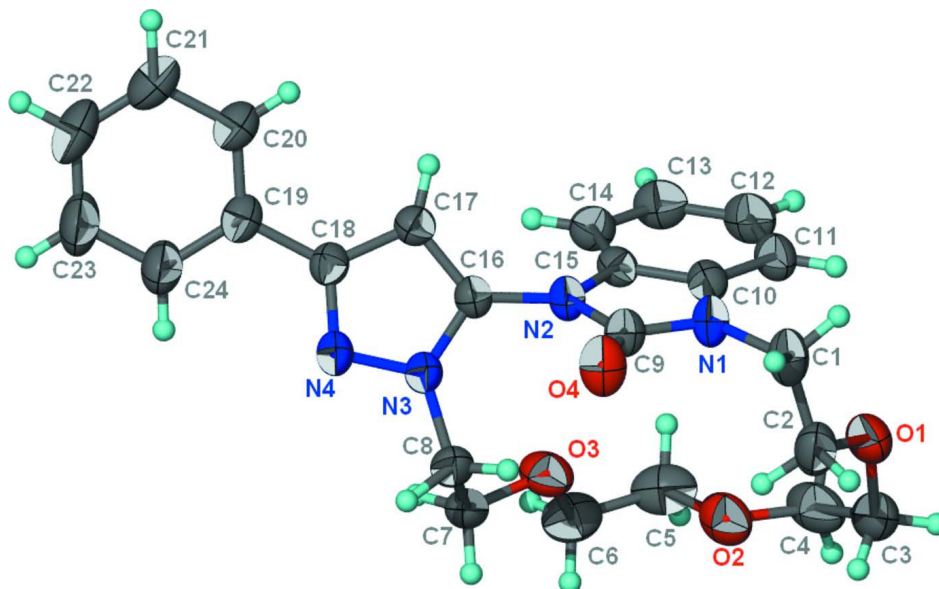
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### S1. Experimental

1-(3-Phenylpyrazolyl)benzimidazol-2-one (1 g, 4.5 mmol), dichlorotetraethyleneglycol (0.31 ml, 5.0 mmol), potassium carbonate (0.7 g, 5.0 mmol) and a catalytic quantity of tetra-*n*-butylammonium bromide were stirred in *N,N*-dimethylformamide (60 ml) in an oil bath heated to 353–363 K for 24 h. The insoluble salts were filtered off and the solvent removed in vacuum. The residue was separated by chromatography on silica gel with a hexane:ethyl acetate (7:3) solvent system. Evaporation of the solvent gave the compound as colorless crystals in 25% yield; m.p. 402–404 K.

### S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 to 0.97 Å) and were included in the refinement in the riding model approximation, with  $U(\text{H})$  set to  $1.2U(\text{C})$ .



**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of  $\text{C}_{24}\text{H}_{26}\text{N}_4\text{O}_4$  at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

4-Phenyl-9,12,15-trioxa-1,5,6,18-tetraazatetracyclo[16.6.1.0<sup>2,6</sup>.0<sup>19,24</sup>]pentaconta-2,4,19,21,23-pentaen-25-one

Crystal data

C<sub>24</sub>H<sub>26</sub>N<sub>4</sub>O<sub>4</sub>

*M<sub>r</sub>* = 434.49

Monoclinic, *P*2<sub>1</sub>/*c*

Hall symbol: -*P* 2ybc

*a* = 13.348 (1) Å

*b* = 15.785 (1) Å

*c* = 11.007 (1) Å

β = 102.681 (1)°

*V* = 2262.6 (3) Å<sup>3</sup>

*Z* = 4

*F*(000) = 920

*D<sub>x</sub>* = 1.276 Mg m<sup>-3</sup>

Mo *Kα* radiation, λ = 0.71073 Å

Cell parameters from 4728 reflections

θ = 1.3–26.4°

μ = 0.09 mm<sup>-1</sup>

*T* = 293 K

Prism, colorless

0.30 × 0.30 × 0.20 mm

Data collection

Nonius KappaCCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ scans

4728 measured reflections

4559 independent reflections

3705 reflections with *I* > 2σ(*I*)

*R*<sub>int</sub> = 0.038

θ<sub>max</sub> = 26.4°, θ<sub>min</sub> = 1.6°

*h* = -16→16

*k* = 0→19

*l* = 0→13

Refinement

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.055

*wR*(*F*<sup>2</sup>) = 0.176

*S* = 1.16

4559 reflections

289 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0966*P*)<sup>2</sup> + 0.3451*P*]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

(Δ/σ)<sub>max</sub> < 0.001

Δρ<sub>max</sub> = 0.34 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.30 e Å<sup>-3</sup>

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>iso</sub> */ <i>U</i> <sub>eq</sub>
O1	0.87698 (11)	0.57891 (11)	0.53630 (16)	0.0794 (5)
O2	0.74157 (12)	0.43571 (10)	0.44390 (16)	0.0745 (4)
O3	0.53984 (12)	0.47052 (9)	0.31375 (15)	0.0699 (4)
O4	0.54645 (11)	0.71208 (10)	0.41785 (13)	0.0682 (4)
N1	0.70082 (11)	0.67744 (10)	0.36647 (14)	0.0524 (4)
N2	0.55695 (10)	0.65098 (9)	0.22803 (13)	0.0449 (3)
N3	0.38396 (11)	0.60439 (10)	0.22449 (13)	0.0499 (4)
N4	0.28762 (10)	0.61095 (10)	0.15421 (14)	0.0520 (4)
C1	0.76670 (16)	0.69810 (14)	0.4862 (2)	0.0661 (5)
H1A	0.7322	0.7392	0.5282	0.079*
H1B	0.8293	0.7240	0.4728	0.079*
C2	0.79396 (16)	0.62171 (18)	0.5685 (2)	0.0753 (6)
H2A	0.8125	0.6392	0.6550	0.090*
H2B	0.7352	0.5841	0.5583	0.090*

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C3	0.88970 (18)	0.4930 (2)	0.5761 (3)	0.0900 (8)
H3A	0.8534	0.4834	0.6422	0.108*
H3B	0.9620	0.4816	0.6091	0.108*
C4	0.84994 (19)	0.43449 (18)	0.4718 (3)	0.0905 (9)
H4A	0.8749	0.4516	0.3991	0.109*
H4B	0.8743	0.3775	0.4943	0.109*
C5	0.6978 (2)	0.39909 (15)	0.3267 (2)	0.0809 (7)
H5A	0.7286	0.3441	0.3198	0.097*
H5B	0.7112	0.4350	0.2605	0.097*
C6	0.5855 (2)	0.38942 (13)	0.3138 (2)	0.0767 (6)
H6A	0.5561	0.3602	0.2367	0.092*
H6B	0.5720	0.3560	0.3824	0.092*
C7	0.43698 (16)	0.46653 (14)	0.32369 (19)	0.0647 (5)
H7A	0.4311	0.4322	0.3949	0.078*
H7B	0.3954	0.4409	0.2494	0.078*
C8	0.40064 (15)	0.55449 (14)	0.33892 (17)	0.0605 (5)
H8A	0.3369	0.5517	0.3673	0.073*
H8B	0.4509	0.5831	0.4027	0.073*
C9	0.59594 (13)	0.68361 (11)	0.34668 (17)	0.0499 (4)
C10	0.72822 (13)	0.64095 (10)	0.26302 (17)	0.0471 (4)
C11	0.82330 (14)	0.62168 (12)	0.2396 (2)	0.0590 (5)
H11	0.8837	0.6329	0.2978	0.071*
C12	0.82438 (17)	0.58505 (14)	0.1261 (2)	0.0685 (6)
H12	0.8871	0.5717	0.1074	0.082*
C13	0.73509 (17)	0.56767 (14)	0.0395 (2)	0.0652 (5)
H13	0.7389	0.5424	-0.0356	0.078*
C14	0.63960 (15)	0.58741 (12)	0.06293 (17)	0.0547 (4)
H14	0.5792	0.5761	0.0047	0.066*
C15	0.63804 (12)	0.62421 (10)	0.17555 (16)	0.0441 (4)
C16	0.45233 (12)	0.64657 (10)	0.17250 (15)	0.0438 (4)
C17	0.39923 (13)	0.68079 (10)	0.06243 (16)	0.0461 (4)
H17	0.4253	0.7126	0.0053	0.055*
C18	0.29661 (13)	0.65690 (10)	0.05540 (15)	0.0460 (4)
C19	0.20534 (13)	0.67861 (11)	-0.04115 (16)	0.0508 (4)
C20	0.20897 (16)	0.74172 (13)	-0.12711 (18)	0.0602 (5)
H20	0.2698	0.7715	-0.1231	0.072*
C21	0.12347 (19)	0.76134 (16)	-0.2191 (2)	0.0749 (6)
H21	0.1273	0.8037	-0.2766	0.090*
C22	0.0333 (2)	0.71854 (18)	-0.2258 (2)	0.0863 (8)
H22	-0.0239	0.7314	-0.2882	0.104*
C23	0.02757 (19)	0.65628 (19)	-0.1396 (3)	0.0910 (8)
H23	-0.0339	0.6277	-0.1434	0.109*
C24	0.11280 (16)	0.63617 (15)	-0.0476 (2)	0.0723 (6)
H24	0.1083	0.5942	0.0102	0.087*

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*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0499 (8)	0.0938 (11)	0.0948 (11)	-0.0035 (7)	0.0166 (7)	0.0240 (9)
O2	0.0620 (9)	0.0817 (10)	0.0879 (11)	0.0055 (7)	0.0339 (8)	0.0023 (8)
O3	0.0719 (10)	0.0537 (8)	0.0884 (11)	0.0005 (6)	0.0270 (8)	0.0132 (7)
O4	0.0574 (8)	0.0837 (10)	0.0644 (8)	0.0036 (7)	0.0153 (6)	-0.0271 (7)
N1	0.0391 (8)	0.0581 (9)	0.0564 (9)	-0.0015 (6)	0.0025 (6)	-0.0121 (7)
N2	0.0364 (7)	0.0515 (8)	0.0457 (7)	-0.0022 (5)	0.0066 (5)	-0.0064 (6)
N3	0.0381 (7)	0.0627 (9)	0.0476 (8)	-0.0022 (6)	0.0067 (6)	0.0078 (6)
N4	0.0375 (7)	0.0633 (9)	0.0525 (8)	-0.0039 (6)	0.0037 (6)	0.0032 (7)
C1	0.0534 (11)	0.0746 (13)	0.0643 (12)	-0.0117 (9)	-0.0002 (9)	-0.0193 (10)
C2	0.0507 (11)	0.1098 (18)	0.0612 (12)	-0.0070 (11)	0.0032 (9)	0.0040 (12)
C3	0.0520 (12)	0.110 (2)	0.106 (2)	0.0051 (13)	0.0119 (12)	0.0449 (17)
C4	0.0650 (14)	0.0863 (17)	0.133 (2)	0.0198 (12)	0.0494 (15)	0.0357 (17)
C5	0.105 (2)	0.0658 (13)	0.0814 (16)	0.0234 (12)	0.0423 (14)	0.0053 (12)
C6	0.1036 (19)	0.0526 (11)	0.0731 (14)	0.0036 (11)	0.0177 (13)	-0.0005 (10)
C7	0.0582 (12)	0.0722 (13)	0.0589 (11)	-0.0143 (9)	0.0027 (9)	0.0201 (10)
C8	0.0509 (10)	0.0840 (14)	0.0463 (9)	-0.0043 (9)	0.0101 (8)	0.0145 (9)
C9	0.0461 (9)	0.0509 (9)	0.0516 (9)	0.0000 (7)	0.0082 (7)	-0.0095 (8)
C10	0.0423 (9)	0.0435 (8)	0.0556 (10)	-0.0006 (6)	0.0107 (7)	0.0002 (7)
C11	0.0424 (9)	0.0630 (11)	0.0724 (12)	0.0028 (8)	0.0143 (8)	0.0057 (9)
C12	0.0590 (12)	0.0738 (13)	0.0806 (14)	0.0150 (10)	0.0328 (11)	0.0071 (11)
C13	0.0731 (13)	0.0671 (12)	0.0615 (11)	0.0087 (10)	0.0280 (10)	-0.0040 (10)
C14	0.0588 (11)	0.0551 (10)	0.0507 (9)	-0.0019 (8)	0.0133 (8)	-0.0033 (8)
C15	0.0431 (9)	0.0399 (8)	0.0509 (9)	-0.0011 (6)	0.0140 (7)	-0.0008 (7)
C16	0.0385 (8)	0.0468 (8)	0.0457 (8)	-0.0022 (6)	0.0083 (6)	-0.0028 (7)
C17	0.0469 (9)	0.0439 (8)	0.0473 (9)	-0.0019 (7)	0.0099 (7)	0.0013 (7)
C18	0.0443 (9)	0.0443 (8)	0.0469 (9)	-0.0001 (6)	0.0046 (7)	-0.0029 (7)
C19	0.0495 (10)	0.0497 (9)	0.0496 (9)	0.0060 (7)	0.0030 (7)	-0.0080 (8)
C20	0.0595 (11)	0.0609 (11)	0.0555 (10)	0.0093 (9)	0.0029 (8)	0.0008 (9)
C21	0.0790 (15)	0.0770 (14)	0.0611 (12)	0.0232 (12)	-0.0009 (10)	0.0070 (10)
C22	0.0712 (15)	0.0955 (17)	0.0761 (15)	0.0222 (13)	-0.0190 (12)	-0.0039 (13)
C23	0.0541 (13)	0.1033 (19)	0.0994 (19)	-0.0065 (12)	-0.0181 (12)	0.0013 (16)
C24	0.0528 (11)	0.0753 (14)	0.0789 (14)	-0.0048 (10)	-0.0071 (10)	0.0058 (11)

*Geometric parameters (Å, °)*

O1—C2	1.408 (3)	C6—H6B	0.9700
O1—C3	1.424 (3)	C7—C8	1.492 (3)
O2—C4	1.411 (3)	C7—H7A	0.9700
O2—C5	1.418 (3)	C7—H7B	0.9700
O3—C7	1.402 (2)	C8—H8A	0.9700
O3—C6	1.418 (3)	C8—H8B	0.9700
O4—C9	1.216 (2)	C10—C11	1.383 (2)
N1—C9	1.372 (2)	C10—C15	1.392 (2)
N1—C10	1.395 (2)	C11—C12	1.380 (3)
N1—C1	1.452 (2)	C11—H11	0.9300

N2—C9	1.394 (2)	C12—C13	1.380 (3)
N2—C16	1.398 (2)	C12—H12	0.9300
N2—C15	1.399 (2)	C13—C14	1.390 (3)
N3—N4	1.3513 (19)	C13—H13	0.9300
N3—C16	1.354 (2)	C14—C15	1.373 (3)
N3—C8	1.460 (2)	C14—H14	0.9300
N4—C18	1.334 (2)	C16—C17	1.373 (2)
C1—C2	1.504 (3)	C17—C18	1.406 (2)
C1—H1A	0.9700	C17—H17	0.9300
C1—H1B	0.9700	C18—C19	1.471 (2)
C2—H2A	0.9700	C19—C20	1.382 (3)
C2—H2B	0.9700	C19—C24	1.393 (3)
C3—C4	1.478 (4)	C20—C21	1.385 (3)
C3—H3A	0.9700	C20—H20	0.9300
C3—H3B	0.9700	C21—C22	1.368 (4)
C4—H4A	0.9700	C21—H21	0.9300
C4—H4B	0.9700	C22—C23	1.380 (4)
C5—C6	1.482 (4)	C22—H22	0.9300
C5—H5A	0.9700	C23—C24	1.384 (3)
C5—H5B	0.9700	C23—H23	0.9300
C6—H6A	0.9700	C24—H24	0.9300
C2—O1—C3	115.28 (18)	N3—C8—C7	113.37 (17)
C4—O2—C5	113.0 (2)	N3—C8—H8A	108.9
C7—O3—C6	112.79 (17)	C7—C8—H8A	108.9
C9—N1—C10	109.93 (14)	N3—C8—H8B	108.9
C9—N1—C1	121.44 (16)	C7—C8—H8B	108.9
C10—N1—C1	128.23 (16)	H8A—C8—H8B	107.7
C9—N2—C16	124.04 (14)	O4—C9—N1	127.12 (17)
C9—N2—C15	109.56 (13)	O4—C9—N2	126.59 (16)
C16—N2—C15	126.40 (14)	N1—C9—N2	106.29 (14)
N4—N3—C16	111.43 (13)	C11—C10—C15	121.28 (17)
N4—N3—C8	118.73 (14)	C11—C10—N1	131.19 (17)
C16—N3—C8	129.83 (15)	C15—C10—N1	107.53 (14)
C18—N4—N3	105.29 (13)	C12—C11—C10	116.95 (19)
N1—C1—C2	112.63 (18)	C12—C11—H11	121.5
N1—C1—H1A	109.1	C10—C11—H11	121.5
C2—C1—H1A	109.1	C11—C12—C13	121.98 (18)
N1—C1—H1B	109.1	C11—C12—H12	119.0
C2—C1—H1B	109.1	C13—C12—H12	119.0
H1A—C1—H1B	107.8	C12—C13—C14	121.01 (19)
O1—C2—C1	109.45 (19)	C12—C13—H13	119.5
O1—C2—H2A	109.8	C14—C13—H13	119.5
C1—C2—H2A	109.8	C15—C14—C13	117.28 (18)
O1—C2—H2B	109.8	C15—C14—H14	121.4
C1—C2—H2B	109.8	C13—C14—H14	121.4
H2A—C2—H2B	108.2	C14—C15—C10	121.50 (16)
O1—C3—C4	110.9 (2)	C14—C15—N2	131.82 (16)

O1—C3—H3A	109.4	C10—C15—N2	106.68 (14)
C4—C3—H3A	109.4	N3—C16—C17	107.53 (14)
O1—C3—H3B	109.4	N3—C16—N2	122.76 (15)
C4—C3—H3B	109.5	C17—C16—N2	129.72 (15)
H3A—C3—H3B	108.0	C16—C17—C18	104.54 (15)
O2—C4—C3	109.7 (2)	C16—C17—H17	127.7
O2—C4—H4A	109.7	C18—C17—H17	127.7
C3—C4—H4A	109.7	N4—C18—C17	111.20 (15)
O2—C4—H4B	109.7	N4—C18—C19	120.47 (16)
C3—C4—H4B	109.7	C17—C18—C19	128.30 (17)
H4A—C4—H4B	108.2	C20—C19—C24	118.42 (18)
O2—C5—C6	109.61 (18)	C20—C19—C18	120.97 (17)
O2—C5—H5A	109.7	C24—C19—C18	120.61 (18)
C6—C5—H5A	109.7	C19—C20—C21	121.0 (2)
O2—C5—H5B	109.7	C19—C20—H20	119.5
C6—C5—H5B	109.7	C21—C20—H20	119.5
H5A—C5—H5B	108.2	C22—C21—C20	120.2 (2)
O3—C6—C5	109.42 (19)	C22—C21—H21	119.9
O3—C6—H6A	109.8	C20—C21—H21	119.9
C5—C6—H6A	109.8	C21—C22—C23	119.7 (2)
O3—C6—H6B	109.8	C21—C22—H22	120.1
C5—C6—H6B	109.8	C23—C22—H22	120.1
H6A—C6—H6B	108.2	C22—C23—C24	120.4 (2)
O3—C7—C8	108.36 (16)	C22—C23—H23	119.8
O3—C7—H7A	110.0	C24—C23—H23	119.8
C8—C7—H7A	110.0	C23—C24—C19	120.3 (2)
O3—C7—H7B	110.0	C23—C24—H24	119.9
C8—C7—H7B	110.0	C19—C24—H24	119.9
H7A—C7—H7B	108.4		
C16—N3—N4—C18	1.09 (19)	C11—C10—C15—C14	0.5 (3)
C8—N3—N4—C18	-177.89 (16)	N1—C10—C15—C14	-179.58 (16)
C9—N1—C1—C2	94.0 (2)	C11—C10—C15—N2	179.97 (16)
C10—N1—C1—C2	-78.1 (3)	N1—C10—C15—N2	-0.06 (18)
C3—O1—C2—C1	-160.4 (2)	C9—N2—C15—C14	179.20 (18)
N1—C1—C2—O1	82.7 (2)	C16—N2—C15—C14	-0.8 (3)
C2—O1—C3—C4	101.9 (2)	C9—N2—C15—C10	-0.24 (18)
C5—O2—C4—C3	164.8 (2)	C16—N2—C15—C10	179.74 (15)
O1—C3—C4—O2	-73.7 (2)	N4—N3—C16—C17	-1.25 (19)
C4—O2—C5—C6	170.39 (18)	C8—N3—C16—C17	177.59 (18)
C7—O3—C6—C5	-169.59 (19)	N4—N3—C16—N2	178.75 (15)
O2—C5—C6—O3	64.1 (2)	C8—N3—C16—N2	-2.4 (3)
C6—O3—C7—C8	172.95 (17)	C9—N2—C16—N3	-58.0 (2)
N4—N3—C8—C7	97.73 (19)	C15—N2—C16—N3	122.04 (19)
C16—N3—C8—C7	-81.0 (2)	C9—N2—C16—C17	122.0 (2)
O3—C7—C8—N3	73.3 (2)	C15—N2—C16—C17	-58.0 (3)
C10—N1—C9—O4	179.75 (19)	N3—C16—C17—C18	0.86 (18)
C1—N1—C9—O4	6.3 (3)	N2—C16—C17—C18	-179.14 (16)

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C10—N1—C9—N2	-0.49 (19)	N3—N4—C18—C17	-0.51 (19)
C1—N1—C9—N2	-173.91 (16)	N3—N4—C18—C19	-178.65 (15)
C16—N2—C9—O4	0.2 (3)	C16—C17—C18—N4	-0.21 (19)
C15—N2—C9—O4	-179.79 (19)	C16—C17—C18—C19	177.74 (16)
C16—N2—C9—N1	-179.53 (15)	N4—C18—C19—C20	164.40 (17)
C15—N2—C9—N1	0.45 (19)	C17—C18—C19—C20	-13.4 (3)
C9—N1—C10—C11	-179.68 (18)	N4—C18—C19—C24	-15.2 (3)
C1—N1—C10—C11	-6.8 (3)	C17—C18—C19—C24	166.97 (19)
C9—N1—C10—C15	0.4 (2)	C24—C19—C20—C21	-1.3 (3)
C1—N1—C10—C15	173.20 (18)	C18—C19—C20—C21	179.05 (18)
C15—C10—C11—C12	-0.2 (3)	C19—C20—C21—C22	0.4 (3)
N1—C10—C11—C12	179.87 (19)	C20—C21—C22—C23	0.7 (4)
C10—C11—C12—C13	-0.4 (3)	C21—C22—C23—C24	-0.9 (4)
C11—C12—C13—C14	0.7 (3)	C22—C23—C24—C19	0.0 (4)
C12—C13—C14—C15	-0.4 (3)	C20—C19—C24—C23	1.1 (3)
C13—C14—C15—C10	-0.2 (3)	C18—C19—C24—C23	-179.2 (2)
C13—C14—C15—N2	-179.54 (18)		

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