Acta Cryst. (1997). C**53**, IUC9700032 [**doi:10.1107/S0108270197099241**]

7-(4-Nitrophenyl)-7-azabicyclo[4.1.0]heptane

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Abstract

The aziridine N atom is in a pyramidal coordination and the cyclohexane ring adopts a half-chair conformation.

Comment

The title compound (I) belongs to the aziridine family. The aziridines exhibit a radiomimetic type of toxicity which has led to extensive programmes for their synthesis and testing for pharmacological activity. Some of these substances have reached advanced stages of evaluation as cancer chemotheraputic agents (Fanda, 1964). Further, because of their high reactivity, they are useful intermediates in synthesizing several natural products such as mitomycin, crinine and reframidine (Kametani & Honda, 1986).

Scheme I

Fig. 1 shows a thermal ellipsoid plot of the two molecules in the asymmetric unit with atom-numbering scheme. One of the molecules exhibits disorder in its cyclohexane ring. Both show normal bond lengths and angles, except for those involving the disordered C10A and C10B. In both molecules, the nitro group is coplanar with the attached benzene ring and N2 is in a pyramidal coordination. The cyclohexane rings adopt a half-chair conformation except for the minor conformer of the disordered molecule, which adopts a distorted sofa conformation. The aziridine planes in the two molecules make dihedral angles of 51.2 (1)°, 50.7 (1)° and 74.3 (1)°, 74.2 (1)°, respectively with the benzene and the best plane through the cyclohexane ring. The benzene rings of the two molecules in the asymmetric unit make an angle of 64.69 (6)° between them.

Experimental

trans-2-amino-*N*-(4-nitrophenyl)-cyclohexanol (0.5 g m, 2.11 mmol) in 30 ml of benzene was stirred with 1.5 equivalent of *p*-toluenesulfonyl chloride, 0.2 equivalent of tetra-n-butylammonium hydrogen sulfate and 5 ml of 50% NaOH solution at room temperature. After completion of the reaction, the organic layer was separated and washed well with water, dried over anhydrous $MgSO_4$, and the solvent removed under vaccum; chromatographic purification of the residue furnished 0.480 g m of pale yellow crystalline solid (Sriraghavan, 1997). Single crystals were obtained by slow evaporation of the compound in chloroform.

Refinement

The structure was solved by direct methods and refined by full-matrix least-squares techniques. In one of two molecules in the asymmetric unit the atom C10 showed disorder with implausible C—C lengths. The occupancies of the disordered positions C10A and C10B were initially refined and then fixed at 0.75 for C10A and 0.25 for C10B. The disordered atoms were refined anisotropically but with the C9A—C10A distance restrained. Though most of the H atoms were located from

the difference Fourier map due to the low ratio of observed reflections to parameters they were not refined but instead were allowed to ride on those atoms to which they are attached.

Programs used: data collection, cell refinement and data reduction *XSCANS* (Siemens, 1994); structure solution and molecular graphics *SHELXTL*PC (Sheldrick, 1990); structure refinement *SHELXL93* (Sheldrick, 1993); geometrical calculations *PARST* (Nardelli, 1983).

Computing details

7-(4-Nitrophenyl)-7-azabicyclo[4.1.0]heptane

Crystal data

$C_{12}H_{14}N_2O_2$	$V = 2241.3\ (4)$ Å^3
$M_r = 218.25$	$Z = 8$
Monoclinic, $P2_1/c$	Mo $K\alpha$
$a = 10.7990\ (16)$ Å	$\mu = 0.09$ mm^{-1}
$b = 12.6741\ (12)$ Å	$T = 293\ (2)$ K
$c = 16.3797\ (13)$ Å	0.62 × 0.46 × 0.26 mm
$\beta = 91.303\ (10)^o$	

Data collection

Siemens P4 diffractometer	$R_{int} = 0.029$
Absorption correction: none	3 standard reflections
6502 measured reflections	every 97 reflections
5157 independent reflections	intensity decay: <3%
2057 reflections with $I > 2\sigma(I)$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$	1 restraint
$wR(F^2) = 0.126$	H-atom parameters constrained
$S = 0.82$	$\Delta\rho_{max} = 0.25$ e Å^{-3}
5157 reflections	$\Delta\rho_{min} = -0.15$ e Å^{-3}
299 parameters	

Table 1
Selected geometric parameters (Å, °)

C9—C10	1.467 (3)	C9A—C10A	1.466 (5)
C9A—C10B	1.430 (13)		
C4—N2—C7	119.8 (2)	C4A—N2A—C7A	121.2 (2)
C4—N2—C12	121.1 (2)	C4A—N2A—C12A	119.3 (2)
C7—N2—C12	60.91 (13)	C7A—N2A—C12A	61.05 (12)

C12—C7—C8—C9	−11.8 (3)	C12A—C7A—C8A—C9A	18.0 (3)
C7—C8—C9—C10	40.3 (3)	C7A—C8A—C9A—C10A	−48.5 (4)
C8—C9—C10—C11	−59.7 (3)	C8A—C9A—C10A—C11A	64.1 (4)
C9—C10—C11—C12	47.0 (3)	C9A—C10B—C11A—C12A	19.8 (14)
C8—C7—C12—C11	1.9 (3)	C8A—C7A—C12A—C11A	−1.0 (3)
C10—C11—C12—C7	−18.7 (3)	C10A—C11A—C12A—C7A	13.2 (3)

Acknowledgements

The authors would like to thank the Malaysian Government and Universiti Sains Malaysia for research grant R&D No. 190–9609-2801. KC thanks the Universiti Sains Malaysia for a Visiting Post Doctoral Fellowship.

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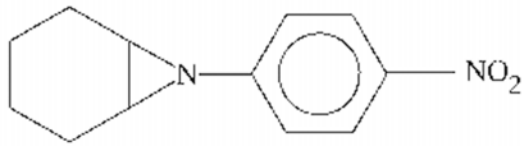
CIF access

Scheme 1



supplementary materials

7-(4-Nitrophenyl)-7-azabicyclo[4.1.0]heptane

Crystal data

$C_{12}H_{14}N_2O_2$	F_{000} = 928
M_r = 218.25	D_x = 1.293 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 33 reflections
a = 10.7990 (16) Å	θ = 5.4–12.5º
b = 12.6741 (12) Å	μ = 0.09 mm^{-1}
c = 16.3797 (13) Å	T = 293 (2) K
β = 91.303 (10)º	Rectangular slab, light yellow
V = 2241.3 (4) Å^3	0.62 × 0.46 × 0.26 mm
Z = 8	

Data collection

Siemens P4 diffractometer	R_{int} = 0.029
Radiation source: fine-focus sealed tube	θ_{max} = 27.5º
Monochromator: graphite	θ_{min} = 1.9º
T = 293(2) K	h = −1→14
ω/2θ scans	k = −1→16
Absorption correction: none	l = −21→21
6502 measured reflections	3 standard reflections
5157 independent reflections	every 97 reflections
2057 reflections with $I > 2\sigma(I)$	intensity decay: <3%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.126	Calculated $w = 1/[\sigma^2(F_o^2) + (0.0512P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$?
S = 0.82	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
5157 reflections	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
299 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
1 restraint	Extinction coefficient: 0.0092 (6)
Primary atom site location: structure-invariant direct methods	

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 on F^2 for ALL reflections. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating observed *R*-factor *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}	Occ. (<1)
N1	0.3799 (3)	1.1505 (2)	−0.06879 (14)	0.0789 (7)	
N2	0.36593 (15)	0.71052 (13)	−0.10967 (10)	0.0465 (4)	
O1	0.4703 (2)	1.1974 (2)	−0.09334 (14)	0.1088 (8)	
O2	0.2937 (2)	1.1937 (2)	−0.03526 (14)	0.1059 (7)	
C1	0.3757 (2)	1.0359 (2)	−0.07962 (13)	0.0562 (6)	
C2	0.4734 (2)	0.9862 (2)	−0.11599 (13)	0.0625 (7)	
H2	0.5402 (2)	1.0250 (2)	−0.13453 (13)	0.075*	
C3	0.4705 (2)	0.8781 (2)	−0.12451 (13)	0.0573 (6)	
H3	0.5361 (2)	0.8437 (2)	−0.14909 (13)	0.069*	
C4	0.3710 (2)	0.8197 (2)	−0.09683 (12)	0.0461 (5)	
C5	0.2734 (2)	0.8723 (2)	−0.06100 (12)	0.0529 (6)	
H5	0.2059 (2)	0.8340 (2)	−0.04289 (12)	0.063*	
C6	0.2751 (2)	0.9806 (2)	−0.05186 (13)	0.0597 (6)	
H6	0.2098 (2)	1.0155 (2)	−0.02750 (13)	0.072*	
C7	0.4738 (2)	0.6449 (2)	−0.08879 (13)	0.0541 (6)	
H7A	0.5436 (2)	0.6813 (2)	−0.06188 (13)	0.065*	
C8	0.5073 (2)	0.5604 (2)	−0.14985 (15)	0.0652 (7)	
H8A	0.4974 (2)	0.5889 (2)	−0.20457 (15)	0.078*	
H8B	0.5939 (2)	0.5418 (2)	−0.14163 (15)	0.078*	
C9	0.4299 (2)	0.4621 (2)	−0.1433 (2)	0.0802 (8)	
H9A	0.4369 (2)	0.4220 (2)	−0.1934 (2)	0.096*	
H9B	0.4635 (2)	0.4191 (2)	−0.0991 (2)	0.096*	
C10	0.2984 (2)	0.4817 (2)	−0.1287 (2)	0.0801 (8)	
H10A	0.2554 (2)	0.4146 (2)	−0.1264 (2)	0.096*	
H10B	0.2633 (2)	0.5212 (2)	−0.1744 (2)	0.096*	
C11	0.2762 (2)	0.5422 (2)	−0.05051 (13)	0.0589 (6)	
H11A	0.1905 (2)	0.5651 (2)	−0.05012 (13)	0.071*	
H11B	0.2898 (2)	0.4954 (2)	−0.00431 (13)	0.071*	
C12	0.3590 (2)	0.6368 (2)	−0.04077 (13)	0.0516 (6)	
H12A	0.3626 (2)	0.6686 (2)	0.01376 (13)	0.062*	
N1A	0.1384 (2)	0.8942 (2)	0.12864 (13)	0.0654 (6)	
N2A	0.13620 (15)	0.45321 (13)	0.16219 (10)	0.0471 (4)	
O1A	0.2219 (2)	0.94442 (14)	0.16219 (12)	0.0928 (6)	

O2A	0.0556 (2)	0.93510 (14)	0.08693 (12)	0.0861 (6)	
C1A	0.1375 (2)	0.7789 (2)	0.13876 (13)	0.0525 (6)	
C2A	0.2266 (2)	0.7322 (2)	0.18784 (14)	0.0582 (6)	
H2A	0.2870 (2)	0.7728 (2)	0.21431 (14)	0.070*	
C3A	0.2250 (2)	0.6241 (2)	0.19714 (13)	0.0541 (6)	
H3A	0.2848 (2)	0.5914 (2)	0.23009 (13)	0.065*	
C4A	0.1342 (2)	0.5634 (2)	0.15750 (12)	0.0449 (5)	
C5A	0.0464 (2)	0.6140 (2)	0.10784 (12)	0.0509 (6)	
H5A	−0.0134 (2)	0.5740 (2)	0.08028 (12)	0.061*	
C6A	0.0462 (2)	0.7217 (2)	0.09865 (13)	0.0543 (6)	
H6A	−0.0138 (2)	0.7551 (2)	0.06629 (13)	0.065*	
C7A	0.1373 (2)	0.3989 (2)	0.24111 (13)	0.0543 (6)	
H7B	0.1332 (2)	0.4443 (2)	0.28944 (13)	0.065*	
C8A	0.2165 (2)	0.3025 (2)	0.2499 (2)	0.0708 (7)	
H8C	0.2004 (2)	0.2693 (2)	0.3019 (2)	0.085*	
H8D	0.3029 (2)	0.3234 (2)	0.2502 (2)	0.085*	
C9A	0.1941 (3)	0.2239 (2)	0.1828 (2)	0.0944 (9)	
H9C	0.2289 (3)	0.2504 (2)	0.1327 (2)	0.113*	
H9D	0.2358 (3)	0.1584 (2)	0.1967 (2)	0.113*	
C10A	0.0616 (4)	0.2034 (4)	0.1693 (3)	0.0643 (12)	0.75
H10C	0.0269 (4)	0.1787 (4)	0.2200 (3)	0.077*	0.75
H10D	0.0519 (4)	0.1473 (4)	0.1294 (3)	0.077*	0.75
C10B	0.0906 (15)	0.2165 (15)	0.1270 (7)	0.096 (6)	0.25
H10E	0.0545 (15)	0.1467 (15)	0.1319 (7)	0.115*	0.25
H10F	0.1204 (15)	0.2234 (15)	0.0719 (7)	0.115*	0.25
C11A	−0.0115 (2)	0.2988 (2)	0.13970 (14)	0.0637 (7)	
H11C	0.0036 (2)	0.3103 (2)	0.08223 (14)	0.076*	
H11D	−0.0993 (2)	0.2854 (2)	0.14559 (14)	0.076*	
C12A	0.0242 (2)	0.3967 (2)	0.18719 (12)	0.0515 (6)	
H12B	−0.0447 (2)	0.4411 (2)	0.20449 (12)	0.062*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.115 (2)	0.049 (2)	0.072 (2)	−0.013 (2)	−0.029 (2)	0.0020 (12)
N2	0.0508 (10)	0.0400 (10)	0.0487 (10)	0.0018 (9)	0.0005 (8)	−0.0016 (8)
O1	0.136 (2)	0.0547 (12)	0.135 (2)	−0.0330 (13)	−0.016 (2)	0.0082 (12)
O2	0.153 (2)	0.0559 (13)	0.109 (2)	0.0118 (14)	0.0017 (15)	−0.0150 (11)
C1	0.078 (2)	0.0377 (13)	0.0521 (14)	−0.0064 (13)	−0.0172 (13)	0.0016 (11)
C2	0.066 (2)	0.056 (2)	0.064 (2)	−0.0127 (14)	−0.0086 (13)	0.0160 (13)
C3	0.0529 (14)	0.054 (2)	0.065 (2)	−0.0009 (12)	0.0041 (12)	0.0046 (12)
C4	0.0525 (13)	0.0427 (13)	0.0430 (12)	−0.0027 (11)	−0.0035 (10)	0.0017 (10)
C5	0.0569 (14)	0.0468 (14)	0.0551 (14)	−0.0071 (12)	0.0059 (11)	−0.0025 (11)
C6	0.073 (2)	0.0491 (15)	0.0572 (15)	0.0041 (13)	−0.0023 (12)	−0.0033 (12)
C7	0.0494 (13)	0.0482 (14)	0.0643 (15)	0.0022 (11)	−0.0056 (11)	−0.0043 (11)
C8	0.0592 (14)	0.060 (2)	0.077 (2)	0.0068 (13)	0.0087 (13)	−0.0080 (13)
C9	0.091 (2)	0.060 (2)	0.090 (2)	0.000 (2)	0.018 (2)	−0.0176 (15)
C10	0.073 (2)	0.066 (2)	0.102 (2)	−0.0074 (15)	0.002 (2)	−0.027 (2)

C11	0.0648 (14)	0.0464 (13)	0.0656 (15)	−0.0015 (12)	0.0042 (12)	0.0073 (12)
C12	0.0624 (14)	0.0466 (13)	0.0457 (13)	0.0025 (12)	−0.0021 (11)	−0.0013 (10)
N1A	0.084 (2)	0.0479 (14)	0.0647 (14)	−0.0041 (12)	0.0233 (12)	−0.0055 (11)
N2A	0.0513 (11)	0.0429 (11)	0.0473 (10)	−0.0025 (9)	0.0041 (8)	0.0008 (8)
O1A	0.120 (2)	0.0564 (12)	0.1019 (14)	−0.0225 (12)	0.0064 (13)	−0.0131 (10)
O2A	0.1031 (15)	0.0541 (12)	0.1013 (15)	0.0113 (11)	0.0075 (12)	0.0114 (10)
C1A	0.0643 (15)	0.0407 (13)	0.0532 (14)	−0.0001 (12)	0.0169 (12)	−0.0007 (11)
C2A	0.0577 (14)	0.0524 (15)	0.065 (2)	−0.0081 (12)	0.0070 (12)	−0.0118 (12)
C3A	0.0507 (13)	0.0514 (14)	0.0600 (14)	0.0005 (12)	−0.0032 (11)	−0.0058 (12)
C4A	0.0477 (12)	0.0449 (13)	0.0426 (12)	0.0002 (11)	0.0091 (10)	−0.0048 (10)
C5A	0.0537 (13)	0.0466 (14)	0.0523 (13)	−0.0056 (11)	0.0004 (11)	−0.0040 (11)
C6A	0.0611 (14)	0.0519 (15)	0.0503 (13)	0.0027 (13)	0.0064 (11)	0.0006 (11)
C7A	0.0585 (14)	0.0566 (15)	0.0478 (13)	−0.0066 (12)	0.0013 (11)	0.0017 (11)
C8A	0.0599 (15)	0.067 (2)	0.085 (2)	−0.0030 (14)	−0.0029 (13)	0.0259 (15)
C9A	0.086 (2)	0.069 (2)	0.128 (3)	0.022 (2)	0.001 (2)	−0.009 (2)
C10A	0.077 (3)	0.044 (2)	0.072 (3)	−0.008 (2)	0.009 (3)	−0.008 (3)
C10B	0.137 (15)	0.088 (11)	0.061 (9)	0.044 (11)	−0.027 (10)	−0.016 (10)
C11A	0.071 (2)	0.0519 (14)	0.068 (2)	−0.0102 (13)	−0.0090 (13)	−0.0019 (12)
C12A	0.0462 (12)	0.0505 (14)	0.0579 (14)	−0.0026 (11)	0.0043 (11)	−0.0020 (11)

Geometric parameters (Å, °)

N1—O1	1.219 (3)	N1A—O2A	1.227 (2)
N1—O2	1.221 (3)	N1A—C1A	1.472 (3)
N1—C1	1.464 (3)	N2A—C4A	1.399 (3)
N2—C4	1.400 (3)	N2A—C7A	1.464 (3)
N2—C7	1.465 (2)	N2A—C12A	1.472 (2)
N2—C12	1.468 (3)	C1A—C2A	1.374 (3)
C1—C2	1.375 (3)	C1A—C6A	1.378 (3)
C1—C6	1.379 (3)	C2A—C3A	1.379 (3)
C2—C3	1.378 (3)	C3A—C4A	1.394 (3)
C3—C4	1.389 (3)	C4A—C5A	1.391 (3)
C4—C5	1.389 (3)	C5A—C6A	1.373 (3)
C5—C6	1.381 (3)	C7A—C12A	1.492 (3)
C7—C12	1.487 (3)	C7A—C8A	1.496 (3)
C7—C8	1.515 (3)	C8A—C9A	1.499 (3)
C8—C9	1.505 (3)	C9A—C10B	1.430 (13)
C9—C10	1.467 (3)	C9A—C10A	1.466 (5)
C10—C11	1.517 (3)	C10A—C11A	1.518 (6)
C11—C12	1.502 (3)	C10B—C11A	1.54 (2)
N1A—O1A	1.223 (2)	C11A—C12A	1.509 (3)
O1—N1—O2	123.6 (2)	O2A—N1A—C1A	118.4 (2)
O1—N1—C1	117.8 (3)	C4A—N2A—C7A	121.2 (2)
O2—N1—C1	118.6 (3)	C4A—N2A—C12A	119.3 (2)
C4—N2—C7	119.8 (2)	C7A—N2A—C12A	61.05 (12)
C4—N2—C12	121.1 (2)	C2A—C1A—C6A	122.4 (2)
C7—N2—C12	60.91 (13)	C2A—C1A—N1A	119.2 (2)
C2—C1—C6	121.9 (2)	C6A—C1A—N1A	118.4 (2)
C2—C1—N1	119.0 (2)	C1A—C2A—C3A	118.8 (2)

C6—C1—N1	119.1 (2)	C2A—C3A—C4A	120.5 (2)
C1—C2—C3	118.9 (2)	C5A—C4A—C3A	118.7 (2)
C2—C3—C4	120.8 (2)	C5A—C4A—N2A	120.1 (2)
C5—C4—C3	118.8 (2)	C3A—C4A—N2A	121.0 (2)
C5—C4—N2	120.7 (2)	C6A—C5A—C4A	121.4 (2)
C3—C4—N2	120.4 (2)	C5A—C6A—C1A	118.1 (2)
C6—C5—C4	121.0 (2)	N2A—C7A—C12A	59.74 (13)
C1—C6—C5	118.6 (2)	N2A—C7A—C8A	117.5 (2)
N2—C7—C12	59.64 (13)	C12A—C7A—C8A	120.0 (2)
N2—C7—C8	116.6 (2)	C7A—C8A—C9A	113.0 (2)
C12—C7—C8	121.0 (2)	C10B—C9A—C8A	128.6 (7)
C9—C8—C7	113.4 (2)	C10A—C9A—C8A	111.7 (3)
C10—C9—C8	114.4 (2)	C9A—C10A—C11A	113.9 (3)
C9—C10—C11	113.3 (2)	C9A—C10B—C11A	114.9 (10)
C12—C11—C10	112.8 (2)	C12A—C11A—C10A	111.4 (2)
N2—C12—C7	59.44 (13)	C12A—C11A—C10B	116.9 (6)
N2—C12—C11	117.9 (2)	N2A—C12A—C7A	59.21 (12)
C7—C12—C11	120.0 (2)	N2A—C12A—C11A	117.3 (2)
O1A—N1A—O2A	123.4 (2)	C7A—C12A—C11A	121.1 (2)
O1A—N1A—C1A	118.2 (2)		
O1—N1—C1—C2	0.5 (3)	N1A—C1A—C2A—C3A	179.9 (2)
O2—N1—C1—C2	−178.8 (2)	C1A—C2A—C3A—C4A	−0.1 (3)
O1—N1—C1—C6	179.5 (2)	C2A—C3A—C4A—C5A	0.7 (3)
O2—N1—C1—C6	0.1 (3)	C2A—C3A—C4A—N2A	175.8 (2)
C6—C1—C2—C3	−0.3 (3)	C7A—N2A—C4A—C5A	−128.9 (2)
N1—C1—C2—C3	178.6 (2)	C12A—N2A—C4A—C5A	−56.9 (3)
C1—C2—C3—C4	−0.1 (3)	C7A—N2A—C4A—C3A	56.0 (3)
C2—C3—C4—C5	0.6 (3)	C12A—N2A—C4A—C3A	128.0 (2)
C2—C3—C4—N2	176.6 (2)	C3A—C4A—C5A—C6A	−1.3 (3)
C7—N2—C4—C5	−134.9 (2)	N2A—C4A—C5A—C6A	−176.5 (2)
C12—N2—C4—C5	−62.9 (3)	C4A—C5A—C6A—C1A	1.4 (3)
C7—N2—C4—C3	49.2 (3)	C2A—C1A—C6A—C5A	−0.8 (3)
C12—N2—C4—C3	121.2 (2)	N1A—C1A—C6A—C5A	179.5 (2)
C3—C4—C5—C6	−0.8 (3)	C4A—N2A—C7A—C12A	108.6 (2)
N2—C4—C5—C6	−176.7 (2)	C12A—N2A—C7A—C12A	0.0
C2—C1—C6—C5	0.1 (3)	C4A—N2A—C7A—C8A	−141.0 (2)
N1—C1—C6—C5	−178.8 (2)	C12A—N2A—C7A—C8A	110.4 (2)
C4—C5—C6—C1	0.4 (3)	N2A—C7A—C8A—C9A	−51.1 (3)
C4—N2—C7—C12	111.2 (2)	C12A—C7A—C8A—C9A	18.0 (3)
C12—N2—C7—C12	0.0	C7A—C8A—C9A—C10B	−17.5 (10)
C4—N2—C7—C8	−136.8 (2)	C7A—C8A—C9A—C10A	−48.5 (4)
C12—N2—C7—C8	112.0 (2)	C10B—C9A—C10A—C11A	−65.4 (16)
N2—C7—C8—C9	−80.8 (3)	C8A—C9A—C10A—C11A	64.1 (4)
C12—C7—C8—C9	−11.8 (3)	C10A—C9A—C10B—C11A	65.0 (13)
C7—C8—C9—C10	40.3 (3)	C8A—C9A—C10B—C11A	−1.6 (17)
C8—C9—C10—C11	−59.7 (3)	C9A—C10A—C11A—C12A	−44.3 (4)
C9—C10—C11—C12	47.0 (3)	C9A—C10A—C11A—C10B	62.7 (13)
C4—N2—C12—C7	−109.2 (2)	C9A—C10B—C11A—C12A	19.8 (14)
C7—N2—C12—C7	0.0	C9A—C10B—C11A—C10A	−66.7 (10)

C4—N2—C12—C11	140.6 (2)	C4A—N2A—C12A—C7A	−111.6 (2)
C7—N2—C12—C11	−110.2 (2)	C7A—N2A—C12A—C7A	0.0
N2—C7—C12—N2	0.0	C4A—N2A—C12A—C11A	136.7 (2)
C8—C7—C12—N2	−104.7 (2)	C7A—N2A—C12A—C11A	−111.7 (2)
N2—C7—C12—C11	106.6 (2)	N2A—C7A—C12A—N2A	0.0
C8—C7—C12—C11	1.9 (3)	C8A—C7A—C12A—N2A	−106.3 (2)
C10—C11—C12—N2	50.3 (3)	N2A—C7A—C12A—C11A	105.3 (2)
C10—C11—C12—C7	−18.7 (3)	C8A—C7A—C12A—C11A	−1.0 (3)
O1A—N1A—C1A—C2A	2.6 (3)	C10A—C11A—C12A—N2A	82.0 (3)
O2A—N1A—C1A—C2A	−177.5 (2)	C10B—C11A—C12A—N2A	49.9 (7)
O1A—N1A—C1A—C6A	−177.7 (2)	C10A—C11A—C12A—C7A	13.2 (3)
O2A—N1A—C1A—C6A	2.2 (3)	C10B—C11A—C12A—C7A	−19.0 (7)
C6A—C1A—C2A—C3A	0.2 (3)		