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# (*E*)-1,2-Bis(1-allylbenzimidazol-2-yl)-ethene

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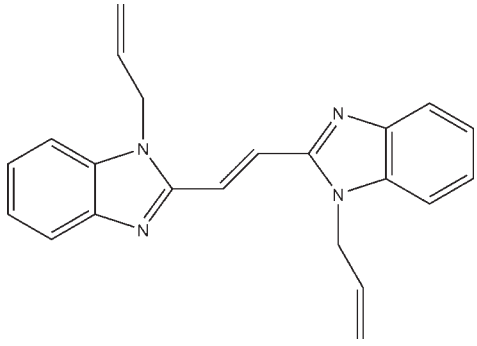
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.058; $wR$ factor = 0.149; data-to-parameter ratio = 16.5.

In the title compound, $C_{22}H_{20}N_4$, the two benzimidazole ring systems are nearly coplanar [dihedral angle = 4.70 (5)°]. Two terminal C atoms of one allyl group are disordered over two sites of equal occupancy. The crystal structure is stabilized by $\pi$–$\pi$ stacking interactions, the centroid–centroid distance between nearly parallel [dihedral angle = 19.82 (4)°] benzene and imidazole rings being 3.7885 (15) Å.

## Related literature

For the properties of bis(imidazole) compounds, see: Knapp *et al.* (1990); Stibrany (2001); Stibrany *et al.* (2002).



## Experimental

### *Crystal data*

$C_{22}H_{20}N_4$
$M_r$ = 340.42
Monoclinic, $P2_1/n$
$a$ = 11.008 (2) Å
$b$ = 13.884 (3) Å
$c$ = 12.540 (3) Å
$\beta$ = 106.98 (3)°
$V$ = 1833.2 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 293 K
0.30 × 0.25 × 0.22 mm

### *Data collection*

Rigaku SCXmini diffractometer
18577 measured reflections
4190 independent reflections
2460 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.061

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.149
$S$ = 1.03
4190 reflections
254 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2721).

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# supporting information

*Acta Cryst.* (2010). E**66**, o764 [doi:10.1107/S1600536810007890]

## (*E*)-1,2-Bis(1-allylbenzimidazol-2-yl)ethene

**Li-Zhuang Chen**

### S1. Comment

Recently, much attention has been devoted to compounds containing bis(imidazoles) due to their interesting properties, such as electron self-exchange (Knapp *et al.*, 1990), catalysts (Stibrany, 2001), and proton sponges (Stibrany *et al.*, 2002). In our laboratory a compound containing bis(imidazoles) has been synthesized, its crystal structure is reported herein.

In the title compound, $C_{22}H_{20}N_4$, the benzimidazole moieties are essentially planar; two allyl groups are not on the planar. The atoms C20 and C21 of terminal olefin show disorder. The crystal structure is stabilized by $\pi$-$\pi$ stacking between benzimidazolium units [the centroid-to-centroid distances between stacking benzene rings and imidazole are 3.7885 (15) Å.

### S2. Experimental

Under $N_2$ atmosphere, NaH (60 mmol, 1.44 g) was added to a mixture of (*E*)-1,2-bis(benzimidazol-2-yl)ethene (10 mmol, 2.6 g ) dimethylformamide (30 ml). After a reaction time of 20 min, the appropriate allyl bromide (20 mmol, 2.4 g) was added dropwise. After an additional 30 min, the product was precipitated with water, collected by filtration and recrystallized to give products in 70% yield. Crystals of title compound (0.3 g) were obtained by slow evaporation of an ethanol/water mixture (1:1 v/v, 10 ml).

### S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93-0.98 Å, and refined with a riding model, $U_{iso}$(H) = 1.2$U_{eq}$(C). The atoms of C20 and C21 are disordered over two sites with 0.5 occupancy for each component.

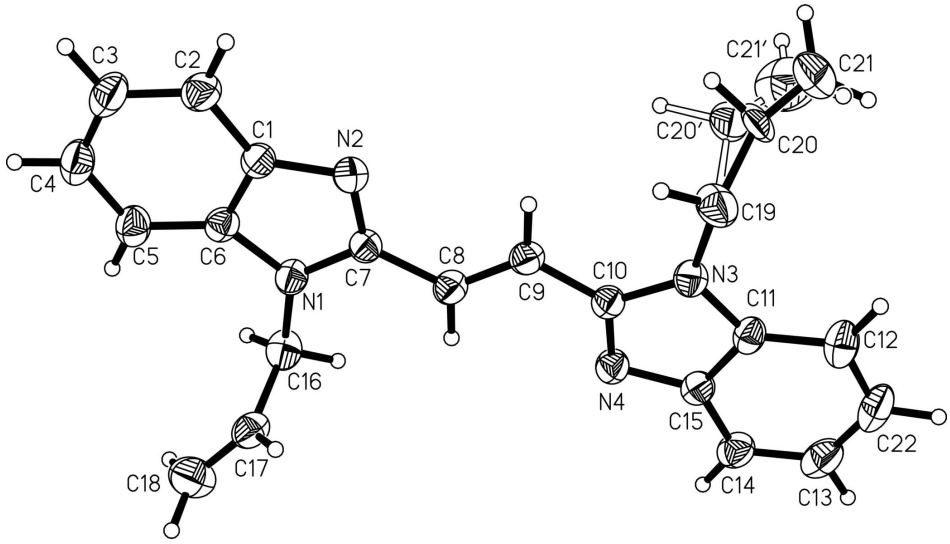


**Figure 1**

The molecular structure of the title compound with atom labels. Displacement ellipsoids were drawn at the 30% probability level. One disordered component is omitted for clarity.

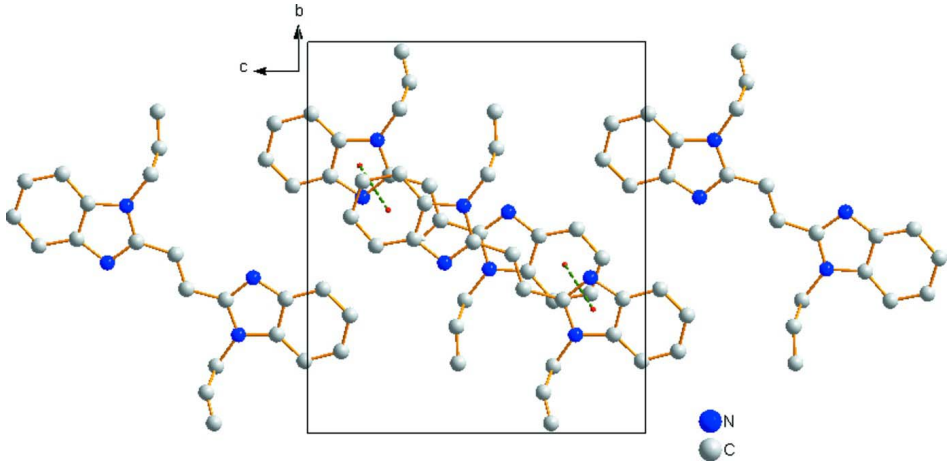


**Figure 2**

The unit cell packing diagram showing $\pi$-$\pi$ stacking between benzene and imidazole rings. H atoms have been omitted for clarity.

### (*E*)-1,2-Bis(1-allylbenzimidazol-2-yl)ethene

*Crystal data*

$C_{22}H_{20}N_4$
$M_r = 340.42$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 11.008$ (2) Å
$b = 13.884$ (3) Å
$c = 12.540$ (3) Å
$\beta = 106.98$ (3)°
$V = 1833.2$ (6) Å$^3$
$Z = 4$

$F(000) = 720$
$D_x = 1.233$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2460 reflections
$\theta = 3.3$–27.5°
$\mu = 0.08$ mm$^{-1}$
$T = 293$ K
Block, yellow
0.30 × 0.25 × 0.22 mm

*Data collection*

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm$^{-1}$
$\omega$ scans
18577 measured reflections
4190 independent reflections
2460 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -14 \rightarrow 14$
$k = -17 \rightarrow 17$
$l = -16 \rightarrow 15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.149$
$S = 1.03$
4190 reflections
254 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
$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2 + 0.2641P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.008$
$\Delta\rho_{max} = 0.15$ e Å$^{-3}$
$\Delta\rho_{min} = -0.17$ e Å$^{-3}$

*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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1 | 0.70227 (17) | 0.49610 (14) | 0.68558 (15) | 0.0475 (5) | |
| C2 | 0.7143 (2) | 0.47856 (16) | 0.79793 (16) | 0.0606 (6) | |
| H2A | 0.6965 | 0.4160 | 0.8224 | 0.073* | |
| C3 | 0.7536 (2) | 0.5530 (2) | 0.87212 (18) | 0.0695 (6) | |
| H3A | 0.7624 | 0.5425 | 0.9497 | 0.083* | |
| C4 | 0.7819 (2) | 0.64336 (18) | 0.83744 (18) | 0.0667 (6) | |
| H4A | 0.8079 | 0.6938 | 0.8917 | 0.080* | |
| C5 | 0.77246 (18) | 0.66223 (16) | 0.72750 (18) | 0.0607 (6) | |
| H5A | 0.7930 | 0.7243 | 0.7036 | 0.073* | |
| C6 | 0.73172 (17) | 0.58701 (14) | 0.65273 (15) | 0.0476 (5) | |
| C7 | 0.66687 (17) | 0.48863 (13) | 0.50843 (15) | 0.0463 (5) | |
| C8 | 0.63061 (18) | 0.45683 (15) | 0.39313 (16) | 0.0512 (5) | |
| H8A | 0.6325 | 0.5030 | 0.3366 | 0.061* | |
| C9 | 0.59503 (17) | 0.36809 (14) | 0.36025 (15) | 0.0497 (5) | |
| H9A | 0.5926 | 0.3208 | 0.4154 | 0.060* | |
| C10 | 0.55903 (17) | 0.34044 (14) | 0.24347 (15) | 0.0455 (4) | |
| C11 | 0.48500 (17) | 0.25237 (14) | 0.09206 (15) | 0.0485 (5) | |

| | | | | | |
|---|---|---|---|---|---|
| C12 | 0.4338 (2) | 0.18326 (17) | 0.01055 (19) | 0.0671 (6) | |
| H12A | 0.4073 | 0.1210 | 0.0286 | 0.081* | |
| C13 | 0.4604 (2) | 0.3003 (2) | −0.12454 (19) | 0.0736 (7) | |
| H13A | 0.4532 | 0.3147 | −0.2010 | 0.088* | |
| C14 | 0.5093 (2) | 0.36810 (17) | −0.04472 (16) | 0.0617 (6) | |
| H14A | 0.5331 | 0.4308 | −0.0640 | 0.074* | |
| C15 | 0.52313 (17) | 0.34327 (14) | 0.06632 (15) | 0.0487 (5) | |
| C16 | 0.7238 (2) | 0.66083 (15) | 0.46662 (17) | 0.0606 (6) | |
| H16A | 0.7323 | 0.6351 | 0.3981 | 0.073* | |
| H16B | 0.7996 | 0.6964 | 0.5020 | 0.073* | |
| C17 | 0.6124 (2) | 0.72847 (16) | 0.44099 (16) | 0.0595 (6) | |
| H17A | 0.5285 | 0.7013 | 0.4194 | 0.071* | |
| C18 | 0.6240 (3) | 0.82080 (18) | 0.4455 (2) | 0.0858 (8) | |
| H18A | 0.7070 | 0.8494 | 0.4669 | 0.103* | |
| H18B | 0.5499 | 0.8610 | 0.4285 | 0.103* | |
| C19 | 0.4846 (2) | 0.17117 (16) | 0.27155 (19) | 0.0695 (6) | |
| H19A | 0.4136 | 0.1329 | 0.2282 | 0.083* | |
| H19B | 0.4661 | 0.1938 | 0.3383 | 0.083* | |
| C20 | 0.6135 (9) | 0.1094 (6) | 0.3030 (5) | 0.0653 (18) | 0.625 (16) |
| H20A | 0.6899 | 0.1385 | 0.3413 | 0.078* | 0.625 (16) |
| C21 | 0.6122 (10) | 0.0200 (6) | 0.2758 (5) | 0.102 (3) | 0.625 (16) |
| H21A | 0.5361 | −0.0094 | 0.2375 | 0.122* | 0.625 (16) |
| H21B | 0.6874 | −0.0151 | 0.2945 | 0.122* | 0.625 (16) |
| C20′ | 0.5505 (16) | 0.0869 (8) | 0.2990 (8) | 0.070 (3) | 0.375 (16) |
| H20B | 0.5114 | 0.0332 | 0.3242 | 0.084* | 0.375 (16) |
| C21′ | 0.6665 (16) | 0.0799 (17) | 0.2913 (11) | 0.107 (6) | 0.375 (16) |
| H21C | 0.7040 | 0.1323 | 0.2672 | 0.129* | 0.375 (16) |
| H21D | 0.7113 | 0.0225 | 0.3099 | 0.129* | 0.375 (16) |
| C22 | 0.4227 (2) | 0.2096 (2) | −0.09844 (19) | 0.0763 (7) | |
| H22A | 0.3871 | 0.1647 | −0.1575 | 0.092* | |
| N1 | 0.70924 (15) | 0.58089 (11) | 0.53845 (13) | 0.0495 (4) | |
| N2 | 0.66254 (15) | 0.43508 (11) | 0.59442 (13) | 0.0508 (4) | |
| N3 | 0.50861 (14) | 0.25146 (11) | 0.20645 (13) | 0.0492 (4) | |
| N4 | 0.56959 (15) | 0.39678 (12) | 0.16199 (13) | 0.0519 (4) | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0431 (10) | 0.0553 (12) | 0.0437 (11) | 0.0080 (9) | 0.0123 (8) | −0.0019 (9) |
| C2 | 0.0664 (14) | 0.0683 (14) | 0.0493 (13) | 0.0101 (11) | 0.0202 (10) | 0.0043 (11) |
| C3 | 0.0678 (15) | 0.0964 (18) | 0.0427 (12) | 0.0113 (13) | 0.0139 (11) | −0.0080 (13) |
| C4 | 0.0583 (13) | 0.0808 (17) | 0.0566 (14) | −0.0005 (12) | 0.0097 (10) | −0.0224 (12) |
| C5 | 0.0548 (13) | 0.0643 (13) | 0.0594 (14) | −0.0063 (11) | 0.0113 (10) | −0.0127 (11) |
| C6 | 0.0397 (10) | 0.0556 (12) | 0.0455 (11) | 0.0020 (9) | 0.0092 (8) | −0.0026 (9) |
| C7 | 0.0444 (10) | 0.0472 (11) | 0.0463 (11) | 0.0044 (9) | 0.0115 (8) | −0.0026 (9) |
| C8 | 0.0558 (12) | 0.0531 (12) | 0.0433 (11) | 0.0033 (9) | 0.0123 (9) | −0.0003 (9) |
| C9 | 0.0508 (11) | 0.0540 (12) | 0.0436 (11) | 0.0039 (9) | 0.0124 (9) | 0.0024 (9) |
| C10 | 0.0440 (10) | 0.0477 (11) | 0.0443 (11) | 0.0011 (9) | 0.0121 (8) | −0.0009 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C11 | 0.0403 (10) | 0.0591 (12) | 0.0456 (11) | −0.0010 (9) | 0.0117 (8) | −0.0089 (9) |
| C12 | 0.0574 (13) | 0.0779 (16) | 0.0658 (15) | −0.0151 (12) | 0.0176 (11) | −0.0201 (12) |
| C13 | 0.0684 (15) | 0.104 (2) | 0.0456 (13) | 0.0098 (14) | 0.0120 (11) | −0.0023 (13) |
| C14 | 0.0674 (14) | 0.0716 (14) | 0.0464 (13) | 0.0084 (11) | 0.0169 (10) | 0.0015 (11) |
| C15 | 0.0464 (11) | 0.0558 (12) | 0.0446 (11) | 0.0046 (9) | 0.0143 (8) | −0.0021 (9) |
| C16 | 0.0659 (13) | 0.0631 (13) | 0.0562 (13) | −0.0127 (11) | 0.0233 (10) | −0.0037 (11) |
| C17 | 0.0653 (13) | 0.0626 (14) | 0.0462 (12) | −0.0072 (11) | 0.0095 (10) | 0.0053 (10) |
| C18 | 0.0754 (17) | 0.0703 (17) | 0.103 (2) | 0.0004 (13) | 0.0121 (14) | 0.0072 (15) |
| C19 | 0.0989 (18) | 0.0522 (13) | 0.0654 (15) | −0.0098 (13) | 0.0364 (13) | −0.0003 (11) |
| C20 | 0.077 (5) | 0.063 (4) | 0.061 (3) | −0.016 (3) | 0.028 (3) | 0.015 (2) |
| C21 | 0.116 (6) | 0.075 (5) | 0.112 (4) | 0.016 (4) | 0.031 (4) | −0.003 (3) |
| C20′ | 0.080 (8) | 0.054 (6) | 0.083 (5) | −0.005 (5) | 0.037 (5) | 0.015 (4) |
| C21′ | 0.095 (10) | 0.144 (17) | 0.097 (7) | 0.021 (9) | 0.053 (7) | 0.004 (9) |
| C22 | 0.0629 (15) | 0.105 (2) | 0.0547 (15) | −0.0058 (14) | 0.0068 (11) | −0.0297 (14) |
| N1 | 0.0527 (9) | 0.0499 (9) | 0.0451 (10) | −0.0033 (8) | 0.0127 (7) | −0.0031 (8) |
| N2 | 0.0559 (10) | 0.0492 (9) | 0.0473 (10) | 0.0033 (8) | 0.0149 (8) | −0.0004 (8) |
| N3 | 0.0505 (9) | 0.0498 (9) | 0.0485 (10) | −0.0029 (8) | 0.0163 (7) | −0.0027 (7) |
| N4 | 0.0586 (10) | 0.0524 (10) | 0.0451 (10) | −0.0021 (8) | 0.0155 (8) | −0.0013 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N2 | 1.387 (2) | C13—C22 | 1.395 (3) |
| C1—C6 | 1.395 (3) | C13—H13A | 0.9600 |
| C1—C2 | 1.398 (3) | C14—C15 | 1.399 (3) |
| C2—C3 | 1.373 (3) | C14—H14A | 0.9599 |
| C2—H2A | 0.9600 | C15—N4 | 1.377 (2) |
| C3—C4 | 1.392 (3) | C16—N1 | 1.467 (2) |
| C3—H3A | 0.9601 | C16—C17 | 1.503 (3) |
| C4—C5 | 1.377 (3) | C16—H16A | 0.9599 |
| C4—H4A | 0.9601 | C16—H16B | 0.9600 |
| C5—C6 | 1.388 (3) | C17—C18 | 1.288 (3) |
| C5—H5A | 0.9600 | C17—H17A | 0.9601 |
| C6—N1 | 1.384 (2) | C18—H18A | 0.9598 |
| C7—N2 | 1.322 (2) | C18—H18B | 0.9600 |
| C7—N1 | 1.378 (2) | C19—C20′ | 1.367 (10) |
| C7—C8 | 1.452 (3) | C19—N3 | 1.451 (2) |
| C8—C9 | 1.322 (3) | C19—C20 | 1.605 (8) |
| C8—H8A | 0.9601 | C19—H19A | 0.9700 |
| C9—C10 | 1.453 (3) | C19—H19B | 0.9700 |
| C9—H9A | 0.9598 | C20—C21 | 1.286 (14) |
| C10—N4 | 1.319 (2) | C20—H20A | 0.9300 |
| C10—N3 | 1.378 (2) | C21—H21A | 0.9300 |
| C11—N3 | 1.381 (2) | C21—H21B | 0.9300 |
| C11—C12 | 1.395 (3) | C20′—C21′ | 1.31 (3) |
| C11—C15 | 1.397 (3) | C20′—H20B | 0.9601 |
| C12—C22 | 1.385 (3) | C21′—H21C | 0.9300 |
| C12—H12A | 0.9600 | C21′—H21D | 0.9300 |
| C13—C14 | 1.365 (3) | C22—H22A | 0.9602 |

| | | | |
|---|---|---|---|
| N2—C1—C6 | 110.73 (16) | C17—C16—H16A | 109.1 |
| N2—C1—C2 | 129.69 (19) | N1—C16—H16B | 109.9 |
| C6—C1—C2 | 119.58 (19) | C17—C16—H16B | 108.8 |
| C3—C2—C1 | 118.0 (2) | H16A—C16—H16B | 107.9 |
| C3—C2—H2A | 121.1 | C18—C17—C16 | 123.2 (2) |
| C1—C2—H2A | 120.8 | C18—C17—H17A | 118.6 |
| C2—C3—C4 | 121.4 (2) | C16—C17—H17A | 118.2 |
| C2—C3—H3A | 119.3 | C17—C18—H18A | 119.9 |
| C4—C3—H3A | 119.2 | C17—C18—H18B | 120.1 |
| C5—C4—C3 | 121.7 (2) | H18A—C18—H18B | 120.0 |
| C5—C4—H4A | 119.4 | C20′—C19—N3 | 129.0 (7) |
| C3—C4—H4A | 118.9 | C20′—C19—C20 | 27.7 (5) |
| C4—C5—C6 | 116.6 (2) | N3—C19—C20 | 104.8 (3) |
| C4—C5—H5A | 121.8 | C20′—C19—H19A | 87.3 |
| C6—C5—H5A | 121.6 | N3—C19—H19A | 110.8 |
| N1—C6—C5 | 132.12 (19) | C20—C19—H19A | 110.8 |
| N1—C6—C1 | 105.28 (16) | C20′—C19—H19B | 106.9 |
| C5—C6—C1 | 122.59 (19) | N3—C19—H19B | 110.8 |
| N2—C7—N1 | 112.96 (16) | C20—C19—H19B | 110.8 |
| N2—C7—C8 | 125.19 (18) | H19A—C19—H19B | 108.9 |
| N1—C7—C8 | 121.85 (17) | C21—C20—C19 | 120.7 (10) |
| C9—C8—C7 | 124.36 (19) | C21—C20—H20A | 119.7 |
| C9—C8—H8A | 117.4 | C19—C20—H20A | 119.7 |
| C7—C8—H8A | 118.2 | C20—C21—H21A | 120.0 |
| C8—C9—C10 | 121.97 (18) | C20—C21—H21B | 120.0 |
| C8—C9—H9A | 118.8 | H21A—C21—H21B | 120.0 |
| C10—C9—H9A | 119.3 | C20—C21—H20B | 73.3 |
| N4—C10—N3 | 112.87 (16) | H21A—C21—H20B | 65.1 |
| N4—C10—C9 | 124.38 (17) | H21B—C21—H20B | 135.0 |
| N3—C10—C9 | 122.75 (17) | C21′—C20′—C19 | 120.1 (19) |
| N3—C11—C12 | 131.9 (2) | C21′—C20′—H20B | 120.5 |
| N3—C11—C15 | 105.67 (16) | C19—C20′—H20B | 119.5 |
| C12—C11—C15 | 122.43 (19) | C20′—C21′—H21C | 120.0 |
| C22—C12—C11 | 116.2 (2) | C20′—C21′—H21D | 120.0 |
| C22—C12—H12A | 121.7 | H21C—C21′—H21D | 120.0 |
| C11—C12—H12A | 122.1 | C12—C22—C13 | 121.5 (2) |
| C14—C13—C22 | 122.1 (2) | C12—C22—H22A | 119.3 |
| C14—C13—H13A | 119.2 | C13—C22—H22A | 119.2 |
| C22—C13—H13A | 118.7 | C7—N1—C6 | 106.49 (15) |
| C13—C14—C15 | 117.7 (2) | C7—N1—C16 | 128.65 (16) |
| C13—C14—H14A | 121.3 | C6—N1—C16 | 124.80 (15) |
| C15—C14—H14A | 121.0 | C7—N2—C1 | 104.53 (16) |
| N4—C15—C11 | 110.26 (16) | C10—N3—C11 | 106.07 (15) |
| N4—C15—C14 | 129.74 (19) | C10—N3—C19 | 128.38 (17) |
| C11—C15—C14 | 119.99 (18) | C11—N3—C19 | 125.55 (17) |
| N1—C16—C17 | 112.04 (17) | C10—N4—C15 | 105.12 (16) |
| N1—C16—H16A | 108.9 | | |