# Supporting Information

# for

# Bromine–lithium exchange: An efficient tool in the modular construction of biaryl ligands

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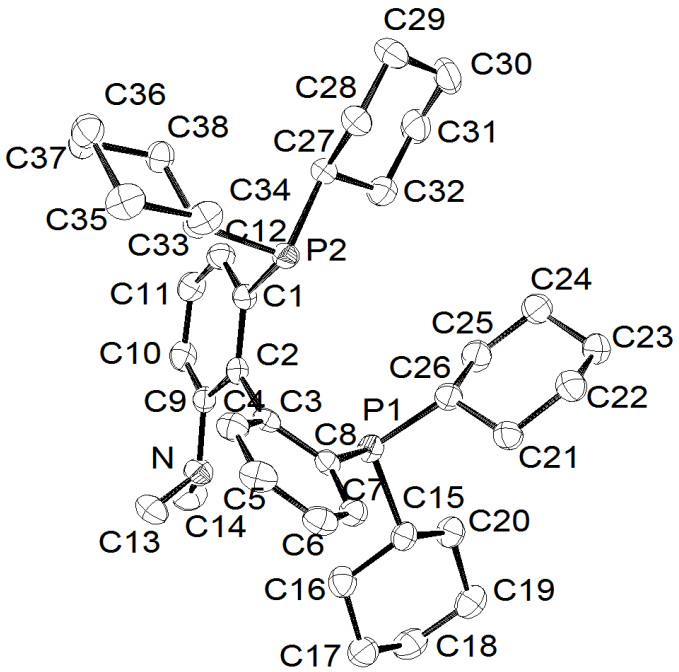
## Crystal structure data for 6c.
## CCDC 827190




*Crystal data*

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|---|---|
| $C_{38}H_{57}NP_2$ | |
| $M_r$ = 589.79 | $D_x$ = 1.126 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Melting point: ? K |
| Hall symbol: -P 2ybc | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| $a$ = 17.2800 (3) Å | Cell parameters from 9078 reflections |
| $b$ = 10.9970 (2) Å | θ = 1.0–29.1° |
| $c$ = 21.6860 (4) Å | μ = 0.15 mm$^{-1}$ |
| β = 122.3851 (8)° | $T$ = 173 K |
| $V$ = 3480.01 (11) Å$^3$ | Prism, colorless |
| $Z$ = 4 | 0.18 × 0.14 × 0.14 mm |
| $F$(000) = 1288 | |

*Data collection*

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|---|---|
| KappaCCD diffractometer | 5525 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int}$ = 0.048 |

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|---|---|
| graphite | $\theta_{max}$ = 29.2°, $\theta_{min}$ = 1.4° |
| Detector resolution: ? pixels $mm^{-1}$ | $h$ = −23→23 |
| π scans | $k$ = −15→13 |
| 15417 measured reflections | $l$ = −29→29 |
| 9362 independent reflections | |

*Refinement*

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|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.050 | H-atom parameters constrained |
| $wR(F^2)$ = 0.134 | $w = 1/[\sigma^2(F_o^2) + (0.0629P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.00 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 9362 reflections | $\Delta\rho_{max}$ = 0.29 e $Å^{-3}$ |
| 370 paramet rs | $\Delta\rho_{min}$ = −0.36 e $Å^{-3}$ |
| 0 restraints | Extinction correction: none |
| | |
| Primary atom site location: structure-invariant direct methods | |

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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| P1 | 0.91843 (3) | 0.14246 (4) | 0.65350 (2) | 0.02714 (12) |
| P2 | 0.60987 (3) | 0.16517 (4) | 0.46461 (2) | 0.02599 (12) |

| | | | | |
|---|---|---|---|---|
| N | 0.93937 (9) | 0.24522 (14) | 0.51579 (8) | 0.0307 (4) |
| C1 | 0.70170 (10) | 0.26860 (16) | 0.47772 (9) | 0.0245 (4) |
| C2 | 0.78540 (10) | 0.21866 (16) | 0.49289 (8) | 0.0236 (4) |
| C3 | 0.80320 (10) | 0.08453 (16) | 0.50451 (9) | 0.0239 (4) |
| C4 | 0.75907 (11) | 0.00450 (18) | 0.44538 (9) | 0.0306 (4) |
| H4 | 0.7165 | 0.0360 | 0.3982 | 0.037* |
| C5 | 0.77563 (11) | −0.11862 (18) | 0.45367 (10) | 0.0343 (4) |
| H5 | 0.7443 | −0.1712 | 0.4127 | 0.041* |
| C6 | 0.83822 (11) | −0.16567 (16) | 0.52203 (10) | 0.0317 (4) |
| H6 | 0.8505 | −0.2505 | 0.5282 | 0.038* |
| C7 | 0.88271 (11) | −0.08784 (16) | 0.58137 (9) | 0.0287 (4) |
| H7 | 0.9259 | −0.1205 | 0.6281 | 0.034* |
| C8 | 0.86593 (10) | 0.03763 (16) | 0.57454 (9) | 0.0236 (4) |
| C9 | 0.85503 (10) | 0.29652 (17) | 0.49934 (9) | 0.0254 (4) |
| C10 | 0.84011 (11) | 0.42097 (18) | 0.49296 (9) | 0.0316 (4) |
| H10 | 0.8866 | 0.4735 | 0.4976 | 0.038* |
| C11 | 0.75913 (11) | 0.47039 (17) | 0.48001 (9) | 0.0322 (4) |
| H11 | 0.7508 | 0.5561 | 0.4767 | 0.039* |
| C12 | 0.69042 (11) | 0.39491 (17) | 0.47189 (9) | 0.0300 (4) |
| H12 | 0.6345 | 0.4293 | 0.4622 | 0.036* |
| C13 | 0.93793 (12) | 0.16859 (19) | 0.46058 (11) | 0.0403 (5) |
| H13A | 0.8849 | 0.1140 | 0.4398 | 0.060* |
| H13B | 0.9944 | 0.1204 | 0.4829 | 0.060* |
| H13C | 0.9335 | 0.2197 | 0.4218 | 0.060* |
| C14 | 1.01711 (12) | 0.32833 (19) | 0.54717 (11) | 0.0420 (5) |
| H14A | 1.0104 | 0.3838 | 0.5092 | 0.063* |
| H14B | 1.0740 | 0.2817 | 0.5670 | 0.063* |

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|---|---|---|---|---|
| H14C | 1.0192 | 0.3754 | 0.5864 | 0.063* |
| C15 | 1.03232 (10) | 0.07045 (16) | 0.71507 (9) | 0.0288 (4) |
| H15 | 1.0242 | −0.0184 | 0.7197 | 0.035* |
| C16 | 1.08980 (11) | 0.08864 (19) | 0.68093 (10) | 0.0353 (4) |
| H16A | 1.0606 | 0.0440 | 0.6340 | 0.042* |
| H16B | 1.0902 | 0.1761 | 0.6703 | 0.042* |
| C17 | 1.18859 (12) | 0.04483 (19) | 0.73010 (11) | 0.0415 (5) |
| H17A | 1.1890 | −0.0446 | 0.7355 | 0.050* |
| H17B | 1.2233 | 0.0645 | 0.7070 | 0.050* |
| C18 | 1.23517 (12) | 0.1037 (2) | 0.80495 (11) | 0.0453 (5) |
| H18A | 1.2420 | 0.1920 | 0.8003 | 0.054* |
| H18B | 1.2972 | 0.0686 | 0.8366 | 0.054* |
| C19 | 1.17981 (12) | 0.0837 (2) | 0.83986 (10) | 0.0438 (5) |
| H19A | 1.2098 | 0.1266 | 0.8873 | 0.053* |
| H19B | 1.1787 | −0.0042 | 0.8493 | 0.053* |
| C20 | 1.08147 (12) | 0.12988 (18) | 0.79088 (10) | 0.0353 (4) |
| H20A | 1.0824 | 0.2192 | 0.7854 | 0.042* |
| H20B | 1.0470 | 0.1124 | 0.8144 | 0.042* |
| C21 | 0.86550 (11) | −0.02207 (17) | 0.72991 (10) | 0.0331 (4) |
| H21A | 0.9303 | −0.  260 | 0.7709 | 0.040* |
| H21B | 0.8554 | −0.0873 | 0.6949 | 0.040* |
| C22 | 0.80336 (12) | −0.04428 (18) | 0.75915 (10) | 0.0372 (5) |
| H22A | 0.7391 | −0.0514 | 0.7176 | 0.045* |
| H22B | 0.8207 | −0.1220 | 0.7864 | 0.045* |
| C23 | 0.81042 (12) | 0.05770 (19) | 0.80896 (10) | 0.0384 (5) |
| H23A | 0.8735 | 0.0608 | 0.8526 | 0.046* |
| H23B | 0.7678 | 0.0419 | 0.8254 | 0.046* |

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|---|---|---|---|---|
| C24 | 0.78699 (13) | 0.17862 (19) | 0.76925 (10) | 0.0394 (5) |
| H24A | 0.7937 | 0.2444 | 0.8029 | 0.047* |
| H24B | 0.7224 | 0.1774 | 0.7278 | 0.047* |
| C25 | 0.84945 (13) | 0.20475 (19) | 0.74069 (10) | 0.0382 (5) |
| H25A | 0.9131 | 0.2163 | 0.7826 | 0.046* |
| H25B | 0.8296 | 0.2812 | 0.7122 | 0.046* |
| C26 | 0.84759 (11) | 0.10080 (17) | 0.69212 (9) | 0.0286 (4) |
| H26 | 0.7829 | 0.0971 | 0.6493 | 0.034* |
| C27 | 0.54513 (11) | 0.26195 (17) | 0.49228 (9) | 0.0288 (4) |
| H27 | 0.5271 | 0.3394 | 0.4637 | 0.035* |
| C28 | 0.45866 (12) | 0.19574 (19) | 0.47743 (10) | 0.0370 (5) |
| H28A | 0.4181 | 0.1799 | 0.4244 | 0.044* |
| H28B | 0.4761 | 0.1164 | 0.5030 | 0.044* |
| C29 | 0.40661 (13) | 0.2705 (2) | 0.50328 (12) | 0.0458 (5) |
| H29A | 0.3837 | 0.3462 | 0.4742 | 0.055* |
| H29B | 0.3531 | 0.2235 | 0.4952 | 0.055* |
| C30 | 0.46771 (15) | 0.3025 (2) | 0.58376 (12) | 0.0496 (6) |
| H30A | 0.4336 | 0.3561 | 0.5978 | 0.060* |
| H30B | 0.4839 | 0.2273 | 0.6132 | 0.060* |
| C31 | 0.55485 (14) | 0.3663 (2) | 0.60044 (10) | 0.0448 (5) |
| H31A | 0.5951 | 0.3794 | 0.6538 | 0.054* |
| H31B | 0.5392 | 0.4468 | 0.5763 | 0.054* |
| C32 | 0.60619 (12) | 0.2915 (2) | 0.57394 (10) | 0.0388 (5) |
| H32A | 0.6279 | 0.2148 | 0.6021 | 0.047* |
| H32B | 0.6605 | 0.3376 | 0.5830 | 0.047* |
| C33 | 0.53870 (11) | 0.16834 (16) | 0.36168 (9) | 0.0266 (4) |
| H33 | 0.5839 | 0.1666 | 0.3463 | 0.032* |

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| C34 | 0.48207 (11) | 0.05179 (17) | 0.33029 (10) | 0.0345 (4) |
| H34A | 0.5227 | −0.0198 | 0.3519 | 0.041* |
| H34B | 0.4353 | 0.0479 | 0.3434 | 0.041* |
| C35 | 0.43479 (12) | 0.04816 (18) | 0.24727 (10) | 0.0387 (5) |
| H35A | 0.4817 | 0.0417 | 0.2345 | 0.046* |
| H35B | 0.3952 | −0.0248 | 0.2280 | 0.046* |
| C36 | 0.37714 (12) | 0.16064 (18) | 0.21178 (10) | 0.0357 (4) |
| H36A | 0.3261 | 0.1625 | 0.2201 | 0.043* |
| H36B | 0.3504 | 0.1572 | 0.1584 | 0.043* |
| C37 | 0.43393 (11) | 0.27612 (18) | 0.24251 (10) | 0.0345 (4) |
| H37A | 0.3938 | 0.3480 | 0.2201 | 0.041* |
| H37B | 0.4812 | 0.2783 | 0.2300 | 0.041* |
| C38 | 0.48031 (11) | 0.28176 (17) | 0.32547 (9) | 0.0303 (4) |
| H38A | 0.4330 | 0.2883 | 0.3378 | 0.036* |
| H38B | 0.5196 | 0.3550 | 0.3445 | 0.036* |

Atomic displacement parameters (Å$^2$)

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| P1 | 0.0310 (2) | 0.0232 (3) | 0.0256 (2) | −0.00075 (19) | 0.0141 (2) | −0.0011 (2) |
| P2 | 0.0234 (2) | 0.0271 (3) | 0.0287 (3) | 0.00086 (18) | 0.01474 (19) | 0.0025 (2) |
| N | 0.0244 (7) | 0.0334 (9) | 0.0354 (9) | −0.0037 (7) | 0.0166 (7) | 0.0008 (7) |
| C1 | 0.0247 (8) | 0.0266 (10) | 0.0225 (9) | 0.0005 (7) | 0.0129 (7) | −0.0003 (7) |
| C2 | 0.0262 (8) | 0.0260 (10) | 0.0189 (8) | −0.0015 (7) | 0.0122 (7) | 0.0003 (7) |
| C3 | 0.0202 (7) | 0.0262 (10) | 0.0298 (9) | −0.0018 (7) | 0.0164 (7) | −0.0024 (8) |

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|---|---|---|---|---|---|---|
| C4 | 0.0256 (8) | 0.0327 (11) | 0.0312 (10) | −0.0015 (8) | 0.0136 (8) | −0. 055 (8) |
| C5 | 0.0299 (9) | 0.0314 (11) | 0.0393 (11) | −0.0057 (8) | 0.0169 (8) | −0.0140 (9) |
| C6 | 0.0324 (9) | 0.0236 (10) | 0.0436 (11) | −0.0018 (8) | 0.0233 (9) | −0.0049 (9) |
| C7 | 0.0305 (8) | 0.0245 (10) | 0.0331 (10) | 0.0016 (8) | 0.0184 (8) | 0.0025 (8) |
| C8 | 0.0241 (8) | 0.0241 (10) | 0.0270 (9) | −0.0013 (7) | 0.0166 (7) | −0.0007 (8) |
| C9 | 0.0239 (8) | 0.0301 (10) | 0.0218 (9) | −0.0005 (7) | 0.0121 (7) | 0.0026 (8) |
| C10 | 0.0299 (9) | 0.0318 (11) | 0.0323 (10) | −0.0077 (8) | 0.0161 (8) | 0.0017 (8) |
| C11 | 0.0359 (9) | 0.0249 (10) | 0.0325 (10) | −0.0017 (8) | 0.0163 (8) | 0.0012 (8) |
| C12 | 0.0305 (9) | 0.0283 (11) | 0.0310 (10) | 0.0035 (8) | 0.0164 (8) | 0.0000 (8) |
| C13 | 0.0360 (10) | 0.0483 (14) | 0.0475 (12) | 0.0019 (9) | 0.0296 (9) | 0.0007 (10) |
| C14 | 0.0281 (9) | 0.0401 (13) | 0.0544 (13) | −0.0055 (8) | 0.0198 (9) | 0.0066 (10) |
| C15 | 0.0314 (9) | 0.0251 (10) | 0.0284 (9) | −0.0019 (8) | 0.0150 (8) | 0.0011 (8) |
| C16 | 0.0332 (9) | 0.0400 (12) | 0.0328 (10) | −0.0034 (9) | 0.0176 (8) | 0.0010 (9) |
| C17 | 0.0358 (10) | 0.0430 (13) | 0.0490 (12) | 0.0034 (9) | 0.0249 (10) | 0.0102 (10) |
| C18 | 0.0304 (9) | 0.0463 (14) | 0.0463 (12) | 0.0010 (9) | 0.0119 (9) | 0.0056 (11) |
| C19 | 0.0378 (10) | 0.0469 (14) | 0.0335 (11) | 0.0010 (10) | 0.0103 (9) | 0.0040 (10) |
| C20 | 0.0340 (9) | 0.0384 (12) | 0.0283 (10) | −0.0020 (8) | 0.0131 (8) | −0.0021 (9) |

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|---|---|---|---|---|---|---|
| C21 | 0.0366 (9) | 0.0295 (11) | 0.0383 (11) | 0.0034 (8) | 0.0234 (9) | 0.0016 (9) |
| C22 | 0.0375 (10) | 0.0370 (12) | 0.0414 (11) | 0.0005 (9) | 0.0242 (9) | 0.0030 (9) |
| C23 | 0.0372 (10) | 0.0495 (14) | 0.0303 (10) | 0.0060 (9) | 0.0192 (9) | 0.0051 (10) |
| C24 | 0.0462 (11) | 0.0422 (13) | 0.0320 (11) | 0.0101 (9) | 0.0224 (9) | −0.0014 (9) |
| C25 | 0.0520 (11) | 0.0299 (11) | 0.0363 (11) | 0.0064 (9) | 0.0260 (10) | −0.0010 (9) |
| C26 | 0.0330 (9) | 0.0253 (10) | 0.0285 (9) | 0.0026 (8) | 0.0171 (8) | −0.0010 (8) |
| C27 | 0.0279 (8) | 0.0335 (11) | 0.0288 (10) | 0.0056 (8) | 0.0177 (8) | 0.0052 (8) |
| C28 | 0.0327 (9) | 0.0441 (13) | 0.0401 (11) | 0.0023 (9) | 0.0233 (9) | 0.0064 (10) |
| C29 | 0.0407 (10) | 0.0558 (15) | 0.0563 (13) | 0.0082 (10) | 0.0360 (10) | 0.0081 (11) |
| C30 | 0.0692 (14) | 0.0507 (15) | 0.0550 (14) | 0.0177 (11) | 0.0506 (12) | 0.0151 (11) |
| C31 | 0.0563 (12) | 0.0491 (14) | 0.0350 (11) | 0.0111 (10) | 0.0285 (10) | 0.0027 (10) |
| C32 | 0.0375 (10) | 0.0477 (13) | 0.0305 (10) | 0.0105 (9) | 0.0177 (9) | 0.0033 (9) |
| C33 | 0.0255 (8) | 0.0252 (10) | 0.0306 (9) | −0.0002 (7) | 0.0160 (7) | 0.0013 (8) |
| C34 | 0.0332 (9) | 0.0264 (11) | 0.0368 (11) | −0.0012 (8) | 0.0141 (8) | −0.0011 (9) |
| C35 | 0.0371 (10) | 0.0313 (12) | 0.0387 (11) | −0.0027 (9) | 0.0143 (9) | −0.0079 (9) |
| C36 | 0.0324 (9) | 0.0414 (12) | 0.0299 (10) | −0.0019 (9) | 0.0144 (8) | −0.0012 (9) |
| C37 | 0.0364 (10) | 0.0366 (12) | 0.0278 (10) | −0.0019 (8) | 0.0153 (8) | 0.0022 (9) |

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|---|---|---|---|---|---|---|
| C38 | 0.0347 (9) | 0.0264 (10) | 0.0298 (10) | −0.0003 (8) | 0.0173 (8) | 0.0023 (8) |

Geometric parameters (Å, °)

| | | | |
|---|---|---|---|
| P1—C8 | 1.8494 (17) | C21—C26 | 1.524 (3) |
| P1—C15 | 1.8622 (17) | C21—C22 | 1.531 (2) |
| P1—C26 | 1.8731 (16) | C21—H21A | 0.9900 |
| P2—C1 | 1.8465 (16) | C21—H21B | 0.9900 |
| P2—C27 | 1.8610 (17) | C22—C23 | 1.516 (3) |
| P2—C33 | 1.8856 (17) | C22—H22A | 0.9900 |
| N—C9 | 1.419 (2) | C22—H22B | 0.9900 |
| N—C13 | 1.453 (2) | C23—C24 | 1.517 (3) |
| N—C14 | 1.457 (2) | C23—H23A | 0.9900 |
| C1—C12 | 1.399 (2) | C23—H23B | 0.9900 |
| C1—C2 | 1.411 (2) | C24—C25 | 1.532 (3) |
| C2—C9 | 1.421 (2) | C24—H24A | 0.9900 |
| C2—C3 | 1.500 (2) | C24—H24B | 0.9900 |
| C3—C4 | 1.398 (2) | C25—C26 | 1.543 (3) |
| C3—C8 | 1.408 (2) | C25—H25A | 0.9900 |
| C4—C5 | 1.376 (3) | C25—H25B | 0.9900 |
| C4—H4 | 0.9500 | C26—H26 | 1.0000 |
| C5—C6 | 1.385 (3) | C27—C28 | 1.533 (2) |
| C5—H5 | 0.9500 | C27—C32 | 1.534 (2) |
| C6—C7 | 1.386 (2) | C27—H27 | 1.0000 |
| C6—H6 | 0.9500 | C28—C29 | 1.530 (3) |
| C7—C8 | 1.401 (2) | C28—H28A | 0.9900 |
| C7—H7 | 0.9500 | C28—H28B | 0.9900 |

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|---|---|---|---|
| C9—C10 | 1.386 (3) | C29—C30 | 1.520 (3) |
| C10—C11 | 1.382 (2) | C29—H29A | 0.9900 |
| C10—H10 | 0.9500 | C29—H29B | 0.9900 |
| C11—C12 | 1.380 (2) | C30—C31 | 1.518 (3) |
| C11—H11 | 0.9500 | C30—H30A | 0.9900 |
| C12—H12 | 0.9500 | C30—H30B | 0.9900 |
| C13—H13A | 0.9800 | C31—C32 | 1.529 (3) |
| C13—H13B | 0.9800 | C31—H31A | 0.9900 |
| C13—H13C | 0.9800 | C31—H31B | 0.9900 |
| C14—H14A | 0.9800 | C32—H32A | 0.9900 |
| C14—H14B | 0.9800 | C32—H32B | 0.9900 |
| C14—H14C | 0.9800 | C33—C38 | 1.530 (2) |
| C15—C20 | 1.535 (2) | C33—C34 | 1.533 (2) |
| C15—C16 | 1.537 (2) | C33—H33 | 1.0000 |
| C15—H15 | 1.0000 | C34—C35 | 1.528 (3) |
| C16—C17 | 1.528 (2) | C34—H34A | 0.9900 |
| C16—H16A | 0.9900 | C34—H34B | 0.9900 |
| C16—H16B | 0.9900 | C35—C36 | 1.514 (3) |
| C17—C18 | 1.517 (3) | C35—H35A | 0.9900 |
| C17—H17A | 0.9900 | C35—H35B | 0.9900 |
| C17—H17B | 0.9900 | C36—C37 | 1.523 (3) |
| C18—C19 | 1.521 (3) | C36—H36A | 0.9900 |
| C18—H18A | 0.9900 | C36—H36B | 0.9900 |
| C18—H18B | 0.9900 | C37—C38 | 1.529 (2) |
| C19—C20 | 1.530 (2) | C37—H37A | 0.9900 |
| C19—H19A | 0.9900 | C37—H37B | 0.9900 |
| C19—H19B | 0.9900 | C38—H38A | 0.9900 |

| | | | |
|---|---|---|---|
| C20—H20A | 0.9900 | C38—H38B | 0.9900 |
| C20—H20B | 0.9900 | | |
| C8—P1—C15 | 101.82 (7) | C21—C22—H22A | 109.3 |
| C8—P1—C26 | 98.49 (7) | C23—C22—H22B | 109.3 |
| C15—P1—C26 | 105.56 (7) | C21—C22—H22B | 109.3 |
| C1—P2—C27 | 102.33 (8) | H22A—C22—H22B | 107.9 |
| C1—P2—C33 | 97.63 (7) | C22—C23—C24 | 110.42 (15) |
| C27—P2—C33 | 104.34 (7) | C22—C23—H23A | 109.6 |
| C9—N—C13 | 117.47 (14) | C24—C23—H23A | 109.6 |
| C9—N—C14 | 115.72 (15) | C22—C23—H23B | 109.6 |
| C13—N—C14 | 110.67 (14) | C24—C23—H23B | 109.6 |
| C12—C1—C2 | 118.90 (14) | H23A—C23—H23B | 108.1 |
| C12—C1—P2 | 122.08 (11) | C23—C24—C25 | 111.25 (15) |
| C2—C1—P2 | 119.02 (13) | C23—C24—H24A | 109.4 |
| C1—C2—C9 | 119.75 (16) | C25—C24—H24A | 109.4 |
| C1—C2—C3 | 120.93 (13) | C23—C24—H24B | 109.4 |
| C9—C2—C3 | 119.29 (13) | C25—C24—H24B | 109.4 |
| C4—C3—C8 | 119.04 (16) | H24A—C24—H24B | 108.0 |
| C4—C3—C2 | 120.19 (15) | C24—C25—C26 | 112.04 (16) |
| C8—C3—C2 | 120.75 (15) | C24—C25—H25A | 109.2 |
| C5—C4—C3 | 121.79 (16) | C26—C25—H25A | 109.2 |
| C5—C4—H4 | 119.1 | C24—C25—H25B | 109.2 |
| C3—C4—H4 | 119.1 | C26—C25—H25B | 109.2 |
| C4—C5—C6 | 119.75 (17) | H25A—C25—H25B | 107.9 |
| C4—C5—H5 | 120.1 | C21—C26—C25 | 111.47 (14) |
| C6—C5—H5 | 120.1 | C21—C26—P1 | 117.66 (11) |
| C5—C6—C7 | 119.35 (17) | C25—C26—P1 | 110.14 (12) |

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| C5—C6—H6 | 120.3 | C21—C26—H26 | 105.5 |
| C7—C6—H6 | 120.3 | C25—C26—H26 | 105.5 |
| C6—C7—C8 | 121.97 (16) | P1—C26—H26 | 105.5 |
| C6—C7—H7 | 119.0 | C28—C27—C32 | 109.49 (14) |
| C8—C7—H7 | 119.0 | C28—C27—P2 | 110.31 (13) |
| C7—C8—C3 | 118.08 (15) | C32—C27—P2 | 109.45 (11) |
| C7—C8—P1 | 123.01 (13) | C28—C27—H27 | 109.2 |
| C3—C8—P1 | 118.86 (13) | C32—C27—H27 | 109.2 |
| C10—C9—N | 121.94 (14) | P2—C27—H27 | 109.2 |
| C10—C9—C2 | 118.86 (14) | C29—C28—C27 | 111.46 (16) |
| N—C9—C2 | 119.12 (16) | C29—C28—H28A | 109.3 |
| C11—C10—C9 | 121.50 (15) | C27—C28—H28A | 109.3 |
| C11—C10—H10 | 119.2 | C29—C28—H28B | 109.3 |
| C9—C10—H10 | 119.2 | C27—C28—H28B | 109.3 |
| C12—C11—C10 | 119.82 (17) | H28A—C28—H28B | 108.0 |
| C12—C11—H11 | 120.1 | C30—C29—C28 | 111.23 (16) |
| C10—C11—H11 | 120.1 | C30—C29—H29A | 109.4 |
| C11—C12—C1 | 121.12 (15) | C28—C29—H29A | 109.4 |
| C11—C12—H12 | 119.4 | C30—C29—H29B | 109.4 |
| C1—C12—H12 | 119.4 | C28—C29—H29B | 109.4 |
| N—C13—H13A | 109.5 | H29A—C29—H29B | 108.0 |
| N—C13—H13B | 109.5 | C31—C30—C29 | 111.75 (15) |
| H13A—C13—H13B | 109.5 | C31—C30—H30A | 109.3 |
| N—C13—H13C | 109.5 | C29—C30—H30A | 109.3 |
| H13A—C13—H13C | 109.5 | C31—C30—H30B | 109.3 |
| H13B—C13—H13C | 109.5 | C29—C30—H30B | 109.3 |
| N—C14—H14A | 109.5 | H30A—C30—H30B | 107.9 |

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| N—C14—H14B | 109.5 | C30—C31—C32 | 111.32 (18) |
| H14A—C14—H14B | 109.5 | C30—C31—H31A | 109.4 |
| N—C14—H14C | 109.5 | C32—C31—H31A | 109.4 |
| H14A—C14—H14C | 109.5 | C30—C31—H31B | 109.4 |
| H14B—C14—H14C | 109.5 | C32—C31—H31B | 109.4 |
| C20—C15—C16 | 109.32 (14) | H31A—C31—H31B | 108.0 |
| C20—C15—P1 | 110.67 (12) | C31—C32—C27 | 111.65 (14) |
| C16—C15—P1 | 107.86 (11) | C31—C32—H32A | 109.3 |
| C20—C15—H15 | 109.7 | C27—C32—H32A | 109.3 |
| C16—C15—H15 | 109.7 | C31—C32—H32B | 109.3 |
| P1—C15—H15 | 109.7 | C27—C32—H32B | 109.3 |
| C17—C16—C15 | 113.06 (14) | H32A—C32—H32B | 108.0 |
| C17—C16—H16A | 109.0 | C38—C33—C34 | 111.41 (14) |
| C15—C16—H16A | 109.0 | C38—C33—P2 | 117.08 (12) |
| C17—C16—H16B | 109.0 | C34—C33—P2 | 111.51 (12) |
| C15—C16—H16B | 109.0 | C38—C33—H33 | 105.2 |
| H16A—C16—H16B | 107.8 | C34—C33—H33 | 105.2 |
| C18—C17—C16 | 111.50 (15) | P2—C33—H33 | 105.2 |
| C18—C17—H17A | 109.3 | C35—C34—C33 | 110.88 (15) |
| C16—C17—H17A | 109.3 | C35—C34—H34A | 109.5 |
| C18—C17—H17B | 109.3 | C33—C34—H34A | 109.5 |
| C16—C17—H17B | 109.3 | C35—C34—H34B | 109.5 |
| H17A—C17—H17B | 108.0 | C33—C34—H34B | 109.5 |
| C17—C18—C19 | 110.87 (15) | H34A—C34—H34B | 108.1 |
| C17—C18—H18A | 109.5 | C36—C35—C34 | 111.63 (16) |
| C19—C18—H18A | 109.5 | C36—C35—H35A | 109.3 |
| C17—C18—H18B | 109.5 | C34—C35—H35A | 109.3 |

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| C19—C18—H18B | 109.5 | C36—C35—H35B | 109.3 |
| H18A—C18—H18B | 108.1 | C34—C35—H35B | 109.3 |
| C18—C19—C20 | 111.55 (15) | H35A—C35—H35B | 108.0 |
| C18—C19—H19A | 109.3 | C35—C36—C37 | 111.37 (14) |
| C20—C19—H19A | 109.3 | C35—C36—H36A | 109.4 |
| C18—C19—H19B | 109.3 | C37—C36—H36A | 109.4 |
| C20—C19—H19B | 109.3 | C35—C36—H36B | 109.4 |
| H19A—C19—H19B | 108.0 | C37—C36—H36B | 109.4 |
| C19—C20—C15 | 111.95 (15) | H36A—C36—H36B | 108.0 |
| C19—C20—H20A | 109.2 | C36—C37—C38 | 110.95 (15) |
| C15—C20—H20A | 109.2 | C36—C37—H37A | 109.4 |
| C19—C20—H20B | 109.2 | C38—C37—H37A | 109.4 |
| C15—C20—H20B | 109.2 | C36—C37—H37B | 109.4 |
| H20A—C20—H20B | 107.9 | C38—C37—H37B | 109.4 |
| C26—C21—C22 | 112.25 (14) | H37A—C37—H37B | 108.0 |
| C26—C21—H21A | 109.2 | C37—C38—C33 | 110.89 (15) |
| C22—C21—H21A | 109.2 | C37—C38—H38A | 109.5 |
| C26—C21—H21B | 109.2 | C33—C38—H38A | 109.5 |
| C22—C21—H21B | 109.2 | C37—C38—H38B | 109.5 |
| H21A—C21—H21B | 107.9 | C33—C38—H38B | 109.5 |
| C23—C22—C21 | 111.75 (15) | H38A—C38—H38B | 108.0 |
| C23—C22—H22A | 109.3 | | |
| C27—P2—C1—C12 | −28. 1 (16) | C20—C15—C16—C17 | 53.7 (2) |
| C33—P2—C1—C12 | 78.55 (15) | P1—C15—C16—C17 | 174.15 (14) |
| C27—P2—C1—C2 | 153.08 (13) | C15—C16—C17—C18 | −54.8 (2) |
| C33—P2—C1—C2 | −100.37 (13) | C16—C17—C18—C19 | 54.6 (2) |
| C12—C1—C2—C9 | −2.2 (2) | C17—C18—C19—C20 | −55.9 (2) |

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| P2—C1—C2—C9 | 176.71 (12) | C18—C19—C20—C15 | 56.7 (2) |
| C12—C1—C2—C3 | 175.97 (15) | C16—C15—C20—C19 | −54.4 (2) |
| P2—C1—C2—C3 | −5.1 (2) | P1—C15—C20—C19 | −173.02 (12) |
| C1—C2—C3—C4 | 73.16 (19) | C26—C21—C22—C23 | −54.6 (2) |
| C9—C2—C3—C4 | −108.63 (17) | C21—C22—C23—C24 | 57.24 (19) |
| C1—C2—C3—C8 | −108. 3 (17) | C22—C23—C24—C25 | −57.4 (2) |
| C9—C2—C3—C8 | 69.88 (19) | C23—C24—C25—C26 | 54.9 (2) |
| C8—C3—C4—C5 | −0.4 (2) | C22—C21—C26—C25 | 51.2 (2) |
| C2—C3—C4—C5 | 178.16 (15) | C22—C21—C26—P1 | 179.75 (12) |
| C3—C4—C5—C6 | −0.6 (3) | C24—C25—C26—C21 | −51.5 (2) |
| C4—C5—C6—C7 | 0.6 (2) | C24—C25—C26—P1 | 176.00 (12) |
| C5—C6—C7—C8 | 0.4 (2) | C8—P1—C26—C21 | 72.34 (14) |
| C6—C7—C8—C3 | −1.4 (2) | C15—P1—C26—C21 | −32.52 (15) |
| C6—C7—C8—P1 | 175.90 (12) | C8—P1—C26—C25 | −158.44 (12) |
| C4—C3—C8—C7 | 1.4 (2) | C15—P1—C26—C25 | 96.70 (13) |
| C2—C3—C8—C7 | −177.17 (13) | C1—P2—C27—C28 | 174.01 (12) |
| C4—C3—C8—P1 | −176.06 (11) | C33—P2—C27—C28 | 72.70 (13) |
| C2—C3—C8—P1 | 5.42 (18) | C1—P2—C27—C32 | −65.46 (14) |
| C15—P1—C8—C7 | 33.38 (14) | C33—P2—C27—C32 | −166.77 (12) |
| C26—P1—C8—C7 | −74.57 (14) | C32—C27—C28—C29 | 56.6 (2) |
| C15—P1—C8—C3 | −149.34 (11) | P2—C27—C28—C29 | 177.08 (12) |
| C26—P1—C8—C3 | 102.71 (12) | C27—C28—C29—C30 | −56.2 (2) |
| C13—N—C9—C10 | −115.67 (19) | C28—C29—C30—C31 | 54.6 (2) |
| C14—N—C9—C10 | 18.1 (2) | C29—C30—C31—C32 | −54.3 (2) |
| C13—N—C9—C2 | 67.6 (2) | C30—C31—C32—C27 | 55.7 (2) |
| C14—N—C9—C2 | −158.57 (15) | C28—C27—C32—C31 | −56.4 (2) |
| C1—C2—C9—C10 | 2.2 (2) | P2—C27—C32—C31 | −177.40 (14) |

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| C3—C2—C9—C10 | −176.07 (14) | C1—P2—C33—C38 | −76.41 (13) |
| C1—C2—C9—N | 178.97 (14) | C27—P2—C33—C38 | 28.46 (14) |
| C3—C2—C9—N | 0.7 (2) | C1—P2—C33—C34 | 153.64 (12) |
| N—C9—C10—C11 | −177.19 (16) | C27—P2—C33—C34 | −101 49 (12) |
| C2—C9—C10—C11 | −0.5 (3) | C38—C33—C34—C35 | 54.68 (18) |
| C9—C10—C11—C12 | −1.1 (3) | P2—C33—C34—C35 | −172.46 (11) |
| C10—C11—C12—C1 | 1.1 (3) | C33—C34—C35—C36 | −54.95 (19) |
| C2—C1—C12—C11 | 0.6 (2) | C34—C35—C36—C37 | 56.0 (2) |
| P2—C1—C12—C11 | −178.29 (13) | C35—C36—C37—C38 | −56.29 (1 ) |
| C8—P1—C15—C20 | −169.54 (12) | C36—C37—C38—C33 | 55.88 (18) |
| C26—P1—C15—C20 | −67.14 (13) | C34—C33—C38—C37 | −55.37 (18) |
| C8—P1—C15—C16 | 70.91 (13) | P2—C33—C38—C37 | 174.62 (11) |
| C26—P1—C15—C16 | 173.31 (12) | | |

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

(type here to add refinement details)

## Computing details

Data collection: Collect (Nonius B.V., 1998); cell refinement: *DENZO* (Nonius B.V., 1998); data reduction: *DENZO* (Nonius B.V., 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* 98 (Spek, 1998); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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