Electronic Supplementary Information for Dalton Transactions


13-07-2010 08:12:16

# Crystal and Molecular Structure of CP881.

C52H66N4P2V2

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**Abstract.** "IUPAC-name", $C_{52}H_{66}N_4P_2V_2$, $M_r$ = 910.95, triclinic, *P*-1, *a* = 12.182(2), *b* = 14.323(3), *c* = 14.344(3) Å, α = 79.989(3)°, β = 83.952(3)°, γ = 88.051(3)°, *V* = 2450.6(8) Å$^3$, *Z* = 2, $D_x$ = 1.234 gcm$^{-3}$, *F*(000) = 964, $\mu$ = 4.85 cm$^{-1}$, λ(MoK$\overline{\alpha}$) = 0.71073 Å, T = 100(1) K, 16314 reflections measured, *GooF* = 0.903, *wR*($F^2$) = 0.1761 for 7680 unique reflections and 551 parameters, 360 restraints and *R*(*F*) = 0.0776 for 3226 reflections obeying $F_o \geq 4.0\ \sigma(F_o)$ criterion of observability.

The asymmetric unit consists of one molecule of the title compound, which is a di-nuclear V-complex coupled by N2.

## Experimental

### X-ray diffraction: Crystal and Molecular Structure.

Crystals were obtained by recrystallisation from pentane.

Although an X-ray structure determination was thwarted by persistent weak scattering power of the crystals, ultimately there was found a crystal ('more or less') fit to the X-ray experiment.

A red colored needle-shaped crystal with the dimensions of 0.30 x 0.065 x 0.035 mm was mounted on top of a glass fiber, by using inert-atmosphere handling techniques, and aligned on a *Bruker*[1] *SMART APEX CCD* diffractometer (Platform with full three-circle goniometer). The diffractometer was equipped with a 4K *CCD* detector set 60.0 mm from the crystal. The crystal was cooled to 100(1) K using the *Bruker KRYOFLEX* low-temperature device. Intensity measurements were performed using graphite monochromated Mo-K$\overline{\alpha}$ radiation from a sealed ceramic diffraction tube (*SIEMENS*). Generator settings were 50 KV/ 40 mA. *SMART* was used for preliminary determination of the unit cell constants and data collection control. The intensities of reflections of a hemisphere were collected by a combination of 3 sets of exposures (frames). Each set had a different ϕ angle for the crystal and each exposure covered a range of 0.3° in ω. A total of 1800 frames were collected with an exposure time of 30.0 seconds per frame. The overall data collection time was 18.3 h. Data integration and global cell refinement was performed with the program *SAINT*. The final unit cell was obtained from the *xyz* centroids of 2436 reflections after integration. Intensity data were corrected for Lorentz and polarization effects, scale variation, for decay and absorption: a multi-scan absorption correction was applied, based on the intensities of symmetry-related reflections measured at different angular settings (*SADABS*)[2], and reduced to $F_o^2$. The program suite *SHELXTL* was used for space group determination (*XPREP*).[1]

The unit cell[3] was identified as triclinic; space group *P*-1. Reduced cell calculations did not indicate any higher metric lattice symmetry[4] and examination of the final atomic coordinates of the structure did not yield obvious extra crystallographic or metric symmetry elements.[5,6]

The structure was solved by Patterson methods and extension of the model was accomplished by direct methods applied to difference structure factors using the program *DIRDIF*.[7] The positional and anisotropic displacement parameters for the non-hydrogen atoms were refined.

Some atoms showed unrealistic displacement parameters when allowed to vary anisotropically, suggesting dynamic disorder (dynamic means that the smeared electron density is due to fluctuations of the atomic positions within each unit cell). This is in line with the weak scattering power of the crystals investigated. To improve the parameters chemical more reasonable, ultimately restrain instructions (*DELU, SIMU*)[10] were applied in the refinement.

Hydrogen atoms were constrained to idealized geometries and allowed to ride on their carrier atoms with an isotropic displacement parameter related to the equivalent displacement parameter of their carrier atoms.

Final refinement on $F^2$ carried out by full-matrix least-squares techniques converged at $wR(F^2)$ = 0.1761 for 7680 reflections and $R(F)$ = 0.0776 for 3226 reflections with $F_o \geq 4.0\ \sigma(F_o)$ and 551 parameters and 360 restraints. The final difference Fourier map was essentially featureless: no significant peaks (0.5(1) e/Å$^3$) having chemical meaning above the general background were observed.

The positional and anisotropic displacement parameters for the non-hydrogen atoms and isotropic displacement parameters for hydrogen atoms were refined on $F^2$ with full-matrix least-squares procedures minimizing the function $Q = \sum_h[w(|(F_o^2) - k(F_c^2)|)^2]$, where $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, $P = [\max(F_o^2,0) + 2F_c^2] / 3$, $F_0$ and $F_c$ are the observed and calculated structure factor amplitudes, respectively; ultimately the suggested $a$ (=0.0593) and $b$ (= 0.0) were used in the final refinement.

Crystal data and numerical details on data collection and refinement are given in Table 1. Final fractional atomic coordinates, equivalent displacement parameters and anisotropic displacement parameters for the non-hydrogen atoms are given in Table 2. Molecular geometry data are collected in Table 3. Tables of atom positions, displacement parameters, comprehensive distances and angles and tables of $(F_o^2)$, $(F_c^2)$ and $\sigma(F_o^2)$ are given as supplementary material[*3] for this paper. Neutral atom scattering factors and anomalous dispersion corrections were taken from *International Tables for Crystallography.*[9]

All refinement calculations and graphics were performed on a Pentium-III / Debian-Linux computer at the University of Groningen with the program packages *SHELXL*[10] (least-square

[*3] Supplementary crystallographic data for this paper are available from the IUCr electronic archives (Reference: CCDCxxxxxxx). These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk).

refinements), a locally modified version of the program *PLUTO*[11] (preparation of illustrations) and *PLATON*[12] package (checking the final results for missed symmetry with the *MISSYM* option, solvent accessible voids with the *SOLV* option, calculation of geometric data and the *ORTEP*[12] illustrations).

**Results and discussion.**

The labeling scheme and the molecular geometry of the title compound are illustrated in the *PLUTO*[11] drawing of Fig. 1. The arrangement of molecules in the unit cell is shown in Fig. 2. Each asymmetric unit contains one formula unit, consisting of a di-nuclear V-complex, which are connected by a $N_2$. The triclinic unit cell contains two moieties of the title compound separated by normal van der Waals distances[13] (Fig. 2).

No classic hydrogen bonds, no missed symmetry (*MISSYM*), but potential solvent-accessible area (voids of 48.0 $Å^3$ / unit cell) were detected by procedures implemented in *PLATON.*[14,15]

**Legends to the Figures.**

Fig. 1. Perspective *PLUTO*[11] drawing showing the configuration of the title compound with the adopted labeling scheme for the non-hydrogen atoms.

Fig. 2. Projections of the crystal structure down the unit cell axes and a view of an unit cell with minimal overlap.

Fig. 3. Perspective *ORTEP*[12] drawing of the title compound with the atom-labeling scheme of the non-hydrogen atoms. All atoms are represented by their displacement ellipsoids drawn at the 50% probability level; hydrogen atoms have been omitted to improve clarity.

**References.**

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**Table 1.**

**a. Crystal data and details of the structure determination**.

| | |
|---|---|
| Moiety_Formula | $C_{52}H_{66}N_4P_2V_2$ |
| Formula_Weight, g.mol$^{-1}$ | 910.95 |
| Crystal system | triclinic |
| Space group, no.[16] | *P*-1, 2 |
| *a*, Å | 12.182(2) |
| *b*, Å | 14.323(3) |
| *c*, Å | 14.344(3) |
| $\alpha$, deg | 79.989(3) |
| $\beta$, deg | 83.952(3) |
| $\gamma$, deg | 88.051(3) |
| *V,* Å$^3$ | 2450.6(8) |
| Θ range unit cell: min.-max., deg; reflections | 2.39 - 23.24 ; 2436 |
| Formula_*Z* | 2 |
| SpaceGroup_*Z* | 2 |
| *Z*' (= Formula_Z / SpaceGroup_*Z)* | 1 |
| $\rho_{calc}$, g.cm$^{-3}$ | 1.234 |
| *F*(000), electrons | 964 |
| μ(Mo K$\bar{\alpha}$), cm$^{-1}$ | 4.85 |
| Color, habit | red, needle |
| Approx. crystal dimension, mm | 0.30 x 0.065 x 0.035 |

**b. Data collection.**

| | |
|---|---|
| λ( Mo K$\bar{\alpha}$), Å | 0.71073 |
| Monochromator | Graphite |
| Measurement device type | *CCD* area-detector diffractometer |
| Detector Area resolution (pixels / mm) | 4096 x 4096 / 62 x 62 (binned 512) |
| Temperature, K | 100(1) |
| Measurement method | φ- and ω-scans |
| θ range; min. max., deg | 2.20, 24.11 |
| Index ranges | h: -13→13; k: -16→16; l: -16→16 |
| Min.- Max. absorption transmission factor | 0.8203 – 0.9832 |
| X-ray exposure time, h | 18.3 |
| Total data | 16314 |
| Unique data | 7680 |
| Data with criterion: ($F_o \geq 4.0\ \sigma\ (F_o)$) | 3226 |
| $R_{int} = \sum [\lvert F_o^2 - F_o^2\ (\text{mean})\rvert] / \sum [F_o^2]$ | 0.1608 |
| $R_{sig} = \sum \sigma(F_o^2) / \sum [F_o^2]$ | 0.2944 |

**c. Refinement.**

| | |
|---|---|
| Number of reflections | 7680 |
| Number of refined parameters | 551 |
| Number of restraints | 360 |
| Final agreement factors: | |
| $wR(F^2) = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$ | 0.1761 |
| Weighting scheme: *a, b* | 0.0593, 0.0 |
| $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ | |
| And $P = [\max(F_o^2,0) + 2F_c^2] / 3$ | |
| $R(F) = \sum (\|\|F_o\| - \|F_c\|\|) / \sum \|F_o\|$ | 0.0776 |
| For $F_o > 4.0\ \sigma\ (F_o)$ | |
| $GooF = S = [\sum [w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$ | 0.903 |
| n = number of reflections | |
| p = number of parameters refined | |
| Residual electron density in final | |
| Difference Fourier map, e/Å$^3$ | -0.5, 0.5(1) |
| Max. (shift/σ) final cycle | <0.001 |
| Average (shift/σ) final cycle | 0.000 |

**Table 2. Final fractional atomic coordinates and equivalent isotropic displacement parameters with s.u.'s in parentheses.**
**Atoms of the Asymmetric Unit.**

**Non-Hydrogen parameters**

| *Atom* | *x* | *y* | *z* | $U_{eq}$ (Å$^2$)* |
|---|---|---|---|---|
| V1 | 0.08697(11) | 0.14280(8) | 0.27552(9) | 0.0148(5) |
| V2 | 0.35067(11) | -0.10726(8) | 0.32715(9) | 0.0131(5) |
| P1 | -0.00697(18) | 0.03373(14) | 0.20503(15) | 0.0203(8) |
| P2 | 0.46664(18) | -0.00728(14) | 0.21105(15) | 0.0190(8) |
| N1 | -0.1972(6) | 0.4585(4) | 0.2060(5) | 0.035(3) |
| N2 | 0.1869(5) | 0.0513(4) | 0.2927(4) | 0.016(2) |
| N3 | 0.2497(5) | -0.0161(4) | 0.3055(4) | 0.010(2) |
| N4 | 0.6416(6) | -0.4292(5) | 0.4409(5) | 0.035(3) |
| C1 | 0.0718(6) | 0.2473(5) | 0.3820(5) | 0.016(2) |
| C2 | 0.0688(6) | 0.1539(5) | 0.4314(5) | 0.020(2) |
| C3 | -0.0241(7) | 0.1094(5) | 0.4134(5) | 0.023(3) |
| C4 | -0.0832(6) | 0.1780(5) | 0.3519(5) | 0.020(2) |
| C5 | -0.0243(6) | 0.2626(5) | 0.3338(5) | 0.015(2) |
| C6 | -0.0553(6) | 0.3547(5) | 0.2760(6) | 0.027(2) |
| C7 | -0.1691(7) | 0.3607(5) | 0.2503(6) | 0.032(3) |
| C8 | -0.3152(8) | 0.4706(7) | 0.1996(8) | 0.063(4) |
| C9 | -0.1373(9) | 0.4891(6) | 0.1131(6) | 0.057(4) |
| C10 | 0.2526(7) | 0.4023(5) | 0.1162(5) | 0.026(3) |
| C11 | 0.3260(7) | 0.4734(5) | 0.1145(6) | 0.027(3) |
| C12 | 0.3985(7) | 0.4696(5) | 0.1810(5) | 0.025(3) |
| C13 | 0.3987(7) | 0.3926(5) | 0.2543(6) | 0.026(2) |
| C14 | 0.3255(6) | 0.3209(5) | 0.2584(5) | 0.019(2) |
| C15 | 0.2527(6) | 0.3224(5) | 0.1876(5) | 0.019(2) |
| C16 | 0.1743(6) | 0.2471(5) | 0.1933(5) | 0.019(2) |
| C17 | 0.1142(6) | 0.2141(5) | 0.1378(5) | 0.018(2) |
| C18 | 0.0985(6) | 0.2332(5) | 0.0356(5) | 0.0170(19) |
| C19 | 0.1771(7) | 0.2162(5) | -0.0331(5) | 0.020(2) |
| C20 | 0.1625(7) | 0.2381(5) | -0.1280(6) | 0.027(2) |
| C21 | 0.0634(7) | 0.2772(5) | -0.1575(6) | 0.027(3) |
| C22 | -0.0190(7) | 0.2954(5) | -0.0875(5) | 0.027(2) |
| C23 | -0.0033(7) | 0.2726(5) | 0.0069(5) | 0.024(2) |
| C24 | -0.1255(6) | 0.0690(5) | 0.1394(5) | 0.024(3) |
| C25 | -0.0602(7) | -0.0678(5) | 0.2891(5) | 0.030(3) |
| C26 | 0.0817(6) | -0.0230(5) | 0.1222(5) | 0.026(3) |
| C27 | 0.3553(7) | -0.2096(5) | 0.4668(5) | 0.021(2) |
| C28 | 0.3228(7) | -0.1192(5) | 0.4868(5) | 0.025(2) |
| C29 | 0.4111(7) | -0.0595(5) | 0.4542(5) | 0.024(3) |
| C30 | 0.4983(7) | -0.1109(5) | 0.4149(5) | 0.020(2) |
| C31 | 0.4653(7) | -0.2051(5) | 0.4235(5) | 0.021(2) |
| C32 | 0.5321(7) | -0.2853(5) | 0.3903(5) | 0.026(3) |
| C33 | 0.5823(7) | -0.3511(5) | 0.4700(5) | 0.030(3) |
| C34 | 0.6725(8) | -0.4970(6) | 0.5234(7) | 0.062(4) |
| C35 | 0.7398(8) | -0.3990(7) | 0.3784(7) | 0.058(4) |
| C36 | 0.1134(6) | -0.2860(5) | 0.3966(5) | 0.015(2) |

| | | | | |
|---|---|---|---|---|
| C37 | 0.0398(7) | -0.3585(5) | 0.4259(5) | 0.023(2) |
| C38 | 0.0455(7) | -0.4357(5) | 0.3805(5) | 0.025(3) |
| C39 | 0.1249(6) | -0.4410(5) | 0.3063(5) | 0.020(3) |
| C40 | 0.1992(6) | -0.3704(5) | 0.2776(5) | 0.018(2) |
| C41 | 0.1952(6) | -0.2899(5) | 0.3222(5) | 0.0115(19) |
| C42 | 0.2778(6) | -0.2159(5) | 0.2925(5) | 0.015(2) |
| C43 | 0.3518(6) | -0.1901(5) | 0.2229(5) | 0.013(2) |
| C44 | 0.3899(6) | -0.2210(4) | 0.1327(5) | 0.0128(19) |
| C45 | 0.4933(7) | -0.2656(5) | 0.1202(5) | 0.019(2) |
| C46 | 0.5282(7) | -0.3001(5) | 0.0375(5) | 0.024(2) |
| C47 | 0.4596(7) | -0.2920(5) | -0.0350(5) | 0.022(3) |
| C48 | 0.3570(7) | -0.2490(5) | -0.0230(5) | 0.026(2) |
| C49 | 0.3232(6) | -0.2133(5) | 0.0602(5) | 0.018(2) |
| C50 | 0.5998(6) | -0.0477(5) | 0.1618(5) | 0.024(3) |
| C51 | 0.4012(6) | 0.0415(5) | 0.1064(5) | 0.022(3) |
| C52 | 0.5037(7) | 0.1001(5) | 0.2511(5) | 0.030(3) |

**Hydrogen parameters:**

| | | | | |
|---|---|---|---|---|
| H1 | 0.12787(-) | 0.29196(-) | 0.38102(-) | 0.01940(-) |
| H2 | 0.12250(-) | 0.12531(-) | 0.47137(-) | 0.02409(-) |
| H3 | -0.04460(-) | 0.04559(-) | 0.43721(-) | 0.02752(-) |
| H4 | -0.15063(-) | 0.16799(-) | 0.32764(-) | 0.02442(-) |
| H6 | -0.04462(-) | 0.40607(-) | 0.31206(-) | 0.03241(-) |
| H6' | -0.00438(-) | 0.36592(-) | 0.21679(-) | 0.03241(-) |
| H7 | -0.22058(-) | 0.34095(-) | 0.30805(-) | 0.03832(-) |
| H7' | -0.17758(-) | 0.31687(-) | 0.20528(-) | 0.03832(-) |
| H8 | -0.33157(-) | 0.53654(-) | 0.17219(-) | 0.09417(-) |
| H8' | -0.35468(-) | 0.45520(-) | 0.26334(-) | 0.09417(-) |
| H8" | -0.33891(-) | 0.42833(-) | 0.15896(-) | 0.09417(-) |
| H9 | -0.16523(-) | 0.45597(-) | 0.06635(-) | 0.08497(-) |
| H9' | -0.05850(-) | 0.47433(-) | 0.11642(-) | 0.08497(-) |
| H9" | -0.14773(-) | 0.55763(-) | 0.09392(-) | 0.08497(-) |
| H10 | 0.20218(-) | 0.40736(-) | 0.06929(-) | 0.03070(-) |
| H11 | 0.32617(-) | 0.52704(-) | 0.06519(-) | 0.03178(-) |
| H12 | 0.44884(-) | 0.51961(-) | 0.17716(-) | 0.02946(-) |
| H13 | 0.44889(-) | 0.38954(-) | 0.30118(-) | 0.03068(-) |
| H14 | 0.32367(-) | 0.26909(-) | 0.30988(-) | 0.02332(-) |
| H19 | 0.24517(-) | 0.18794(-) | -0.01519(-) | 0.02349(-) |
| H20 | 0.22087(-) | 0.22646(-) | -0.17408(-) | 0.03257(-) |
| H21 | 0.05220(-) | 0.29092(-) | -0.22304(-) | 0.03240(-) |
| H22 | -0.08677(-) | 0.32409(-) | -0.10558(-) | 0.03247(-) |
| H23 | -0.06134(-) | 0.28323(-) | 0.05366(-) | 0.02843(-) |
| H24 | -0.10412(-) | 0.11899(-) | 0.08527(-) | 0.03525(-) |
| H24' | -0.18458(-) | 0.09285(-) | 0.18135(-) | 0.03525(-) |
| H24" | -0.15172(-) | 0.01416(-) | 0.11618(-) | 0.03525(-) |
| H25 | -0.09146(-) | -0.11242(-) | 0.25485(-) | 0.04460(-) |
| H25' | -0.11781(-) | -0.04672(-) | 0.33427(-) | 0.04460(-) |
| H25" | -0.00018(-) | -0.09917(-) | 0.32378(-) | 0.04460(-) |
| H26 | 0.14346(-) | -0.05477(-) | 0.15420(-) | 0.03897(-) |
| H26' | 0.11028(-) | 0.02482(-) | 0.06847(-) | 0.03897(-) |
| H26" | 0.03965(-) | -0.06977(-) | 0.09900(-) | 0.03897(-) |
| H27 | 0.31073(-) | -0.26437(-) | 0.48021(-) | 0.02560(-) |
| H28 | 0.25355(-) | -0.10229(-) | 0.51682(-) | 0.02923(-) |
| H29 | 0.41217(-) | 0.00603(-) | 0.45802(-) | 0.02855(-) |
| H30 | 0.56788(-) | -0.08629(-) | 0.38712(-) | 0.02315(-) |
| H32 | 0.59209(-) | -0.25880(-) | 0.34192(-) | 0.03149(-) |
| H32' | 0.48420(-) | -0.32257(-) | 0.35928(-) | 0.03149(-) |
| H33 | 0.63250(-) | -0.31422(-) | 0.49906(-) | 0.03617(-) |
| H33' | 0.52240(-) | -0.37512(-) | 0.51965(-) | 0.03617(-) |
| H34 | 0.71446(-) | -0.46442(-) | 0.56253(-) | 0.09321(-) |
| H34' | 0.71812(-) | -0.54816(-) | 0.50146(-) | 0.09321(-) |
| H34" | 0.60571(-) | -0.52366(-) | 0.56137(-) | 0.09321(-) |
| H35 | 0.71857(-) | -0.35875(-) | 0.32036(-) | 0.08730(-) |
| H35' | 0.78102(-) | -0.45472(-) | 0.36173(-) | 0.08730(-) |
| H35" | 0.78632(-) | -0.36301(-) | 0.41076(-) | 0.08730(-) |
| H36 | 0.10827(-) | -0.23245(-) | 0.42779(-) | 0.01873(-) |
| H37 | -0.01503(-) | -0.35520(-) | 0.47752(-) | 0.02796(-) |
| H38 | -0.00578(-) | -0.48556(-) | 0.40046(-) | 0.02942(-) |
| H39 | 0.12809(-) | -0.49430(-) | 0.27479(-) | 0.02401(-) |
| H40 | 0.25451(-) | -0.37542(-) | 0.22671(-) | 0.02112(-) |

| | | | | |
|---|---|---|---|---|
| H45 | 0.54050(-) | -0.27239(-) | 0.16968(-) | 0.02254(-) |
| H46 | 0.59904(-) | -0.32932(-) | 0.03033(-) | 0.02836(-) |
| H47 | 0.48279(-) | -0.31564(-) | -0.09199(-) | 0.02677(-) |
| H48 | 0.30900(-) | -0.24369(-) | -0.07177(-) | 0.03149(-) |
| H49 | 0.25281(-) | -0.18320(-) | 0.06672(-) | 0.02123(-) |
| H50 | 0.58981(-) | -0.10431(-) | 0.13396(-) | 0.03576(-) |
| H50' | 0.64879(-) | -0.06319(-) | 0.21247(-) | 0.03576(-) |
| H50" | 0.63245(-) | 0.00249(-) | 0.11245(-) | 0.03576(-) |
| H51 | 0.44850(-) | 0.08982(-) | 0.06635(-) | 0.03213(-) |
| H51' | 0.32994(-) | 0.07033(-) | 0.12499(-) | 0.03213(-) |
| H51" | 0.38939(-) | -0.00913(-) | 0.07063(-) | 0.03213(-) |
| H52 | 0.55135(-) | 0.13858(-) | 0.20052(-) | 0.04542(-) |
| H52' | 0.54320(-) | 0.08311(-) | 0.30790(-) | 0.04542(-) |
| H52" | 0.43663(-) | 0.13644(-) | 0.26638(-) | 0.04542(-) |

*) $U_{eq} = 1/3 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a_i}.\mathbf{a_j}$ [17]

## Anisotropic (displacement) parameters (Å$^2$)

| | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| V1 | 0.0184(9) | 0.0106(8) | 0.0150(8) | -0.0025(6) | 0.0002(7) | 0.0013(7) |
| V2 | 0.0155(9) | 0.0077(7) | 0.0170(8) | -0.0034(6) | -0.0039(7) | 0.0004(6) |
| P1 | 0.0244(14) | 0.0150(12) | 0.0213(13) | -0.0013(10) | -0.0033(11) | -0.0049(10) |
| P2 | 0.0212(14) | 0.0146(12) | 0.0204(13) | -0.0016(10) | -0.0003(11) | -0.0032(10) |
| N1 | 0.037(5) | 0.022(5) | 0.048(5) | -0.006(4) | -0.014(4) | 0.013(4) |
| N2 | 0.026(4) | 0.007(3) | 0.015(4) | 0.002(3) | -0.005(3) | -0.004(3) |
| N3 | 0.013(4) | 0.007(3) | 0.011(4) | -0.003(3) | 0.003(3) | -0.005(3) |
| N4 | 0.044(5) | 0.028(4) | 0.027(4) | 0.002(4) | 0.003(4) | 0.023(4) |
| C1 | 0.018(4) | 0.021(4) | 0.013(4) | -0.013(3) | 0.002(3) | 0.000(3) |
| C2 | 0.023(4) | 0.021(4) | 0.016(4) | -0.004(3) | 0.002(3) | 0.005(3) |
| C3 | 0.037(5) | 0.010(4) | 0.021(4) | -0.002(3) | 0.002(4) | -0.003(3) |
| C4 | 0.020(4) | 0.018(4) | 0.023(4) | -0.007(3) | 0.001(3) | 0.005(3) |
| C5 | 0.020(4) | 0.013(3) | 0.013(4) | -0.007(3) | 0.003(3) | 0.003(3) |
| C6 | 0.025(4) | 0.021(4) | 0.034(4) | -0.006(3) | 0.001(4) | -0.001(4) |
| C7 | 0.039(5) | 0.020(4) | 0.038(5) | 0.002(4) | -0.021(4) | 0.006(4) |
| C8 | 0.038(7) | 0.050(7) | 0.102(9) | -0.006(6) | -0.033(7) | 0.013(6) |
| C9 | 0.096(9) | 0.040(6) | 0.037(7) | -0.004(5) | -0.028(7) | 0.007(6) |
| C10 | 0.035(5) | 0.020(4) | 0.022(4) | -0.002(3) | -0.003(4) | -0.003(3) |
| C11 | 0.033(5) | 0.017(4) | 0.028(4) | -0.005(3) | 0.007(4) | 0.001(3) |
| C12 | 0.031(5) | 0.013(4) | 0.031(4) | -0.015(3) | 0.009(4) | 0.000(3) |
| C13 | 0.027(4) | 0.022(4) | 0.030(4) | -0.010(3) | -0.002(4) | -0.002(3) |
| C14 | 0.026(4) | 0.017(4) | 0.016(4) | -0.005(3) | -0.002(3) | 0.000(3) |
| C15 | 0.024(4) | 0.013(3) | 0.021(4) | -0.006(3) | 0.003(3) | 0.003(3) |
| C16 | 0.022(4) | 0.014(4) | 0.020(4) | -0.007(3) | -0.001(3) | 0.009(3) |
| C17 | 0.017(4) | 0.012(4) | 0.024(4) | -0.004(3) | -0.004(3) | 0.007(3) |
| C18 | 0.021(4) | 0.011(3) | 0.019(3) | -0.001(3) | -0.006(3) | 0.002(3) |
| C19 | 0.027(4) | 0.009(4) | 0.022(4) | 0.000(3) | -0.003(3) | 0.005(3) |
| C20 | 0.036(4) | 0.021(4) | 0.025(4) | -0.004(3) | -0.009(4) | -0.002(4) |
| C21 | 0.040(5) | 0.022(4) | 0.020(4) | 0.001(3) | -0.018(3) | -0.002(4) |
| C22 | 0.033(4) | 0.027(4) | 0.024(4) | -0.002(4) | -0.017(3) | -0.007(4) |
| C23 | 0.026(4) | 0.023(4) | 0.021(4) | 0.004(3) | -0.009(3) | 0.003(3) |
| C24 | 0.017(5) | 0.026(5) | 0.030(5) | -0.011(4) | -0.003(4) | 0.003(4) |
| C25 | 0.036(6) | 0.028(5) | 0.023(5) | 0.000(4) | 0.007(4) | -0.018(4) |
| C26 | 0.041(6) | 0.025(5) | 0.018(5) | -0.016(4) | -0.007(4) | -0.013(4) |
| C27 | 0.028(4) | 0.021(4) | 0.014(4) | 0.001(3) | -0.008(3) | 0.005(3) |
| C28 | 0.029(4) | 0.030(4) | 0.014(4) | -0.005(3) | 0.003(3) | 0.001(3) |
| C29 | 0.029(5) | 0.021(4) | 0.021(4) | -0.004(3) | 0.000(4) | 0.001(3) |
| C30 | 0.023(4) | 0.022(4) | 0.014(4) | -0.003(3) | -0.004(3) | 0.002(3) |
| C31 | 0.026(4) | 0.018(3) | 0.019(4) | -0.002(3) | -0.003(3) | 0.004(3) |
| C32 | 0.029(5) | 0.022(4) | 0.025(4) | 0.006(3) | -0.009(4) | 0.012(3) |
| C33 | 0.040(5) | 0.021(4) | 0.028(5) | 0.002(4) | -0.011(4) | 0.006(4) |
| C34 | 0.067(8) | 0.049(7) | 0.070(8) | -0.006(6) | -0.024(7) | 0.043(6) |
| C35 | 0.039(7) | 0.056(7) | 0.074(8) | -0.004(6) | 0.001(6) | 0.020(6) |
| C36 | 0.025(4) | 0.011(4) | 0.010(4) | -0.001(3) | -0.001(3) | -0.003(3) |
| C37 | 0.030(4) | 0.022(4) | 0.016(4) | -0.003(3) | 0.006(3) | -0.005(3) |
| C38 | 0.032(5) | 0.018(4) | 0.023(4) | -0.004(3) | 0.005(3) | -0.012(4) |
| C39 | 0.034(5) | 0.009(4) | 0.018(4) | -0.005(3) | -0.002(3) | -0.006(3) |
| C40 | 0.020(4) | 0.019(4) | 0.015(4) | -0.004(3) | -0.005(3) | -0.003(3) |
| C41 | 0.011(4) | 0.009(3) | 0.013(3) | 0.005(3) | -0.005(3) | -0.001(3) |
| C42 | 0.013(4) | 0.014(4) | 0.016(4) | 0.002(3) | -0.006(3) | -0.003(3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C43 | 0.015(4) | 0.010(4) | 0.014(4) | 0.000(3) | -0.009(3) | -0.003(3) |
| C44 | 0.021(4) | 0.001(3) | 0.015(3) | 0.001(3) | 0.002(3) | -0.003(3) |
| C45 | 0.028(4) | 0.008(4) | 0.021(4) | -0.004(3) | 0.001(3) | -0.005(3) |
| C46 | 0.034(4) | 0.011(4) | 0.027(4) | -0.007(3) | 0.004(3) | -0.004(3) |
| C47 | 0.039(5) | 0.011(4) | 0.015(4) | -0.004(3) | 0.006(3) | -0.003(3) |
| C48 | 0.037(4) | 0.022(4) | 0.020(4) | -0.005(3) | 0.000(4) | -0.006(4) |
| C49 | 0.026(4) | 0.009(4) | 0.018(4) | -0.004(3) | 0.002(3) | -0.005(3) |
| C50 | 0.017(5) | 0.029(5) | 0.023(5) | -0.006(4) | 0.015(4) | -0.004(4) |
| C51 | 0.022(5) | 0.017(4) | 0.024(5) | 0.002(4) | -0.004(4) | -0.004(4) |
| C52 | 0.048(6) | 0.013(5) | 0.032(5) | -0.003(4) | -0.011(5) | -0.009(4) |

Thermal vibration amplitudes ($Å^2$)

$$F(\mathbf{h}) = F_o(\mathbf{h}) \exp\left(-2\pi^2 \sum_{i=1}^{3}\sum_{j=1}^{3} h_i h_j a_i^* a_j^* U_{ij}\right)$$

or

$$F(\mathbf{h}) = F_o(\mathbf{h}) \exp\left(-8\pi^2 U_{iso} (\sin(\theta)/\lambda)^2\right)$$

**Table 3. Selected data on the geometry.**

**Standard deviations in the last decimal place are given in parentheses.**

**Interatomic Distances (Å)**

| | | | | | |
|---|---|---|---|---|---|
| V1 | -P1 | 2.385(2) | C10 | -C11 | 1.373(11) |
| V1 | -N2 | 1.761(6) | C10 | -C15 | 1.397(10) |
| V1 | -C1 | 2.307(7) | C11 | -C12 | 1.360(12) |
| V1 | -C2 | 2.256(7) | C12 | -C13 | 1.385(11) |
| V1 | -C3 | 2.263(8) | C13 | -C14 | 1.372(11) |
| V1 | -C4 | 2.323(7) | C14 | -C15 | 1.414(10) |
| V1 | -C5 | 2.363(7) | C15 | -C16 | 1.451(10) |
| V1 | -C16 | 1.996(7) | C16 | -C17 | 1.292(10) |
| V1 | -C17 | 2.059(7) | C17 | -C18 | 1.475(10) |
| V2 | -P2 | 2.373(3) | C18 | -C19 | 1.348(11) |
| V2 | -N3 | 1.773(6) | C18 | -C23 | 1.416(11) |
| V2 | -C27 | 2.272(7) | C19 | -C20 | 1.372(11) |
| V2 | -C28 | 2.257(7) | C20 | -C21 | 1.389(12) |
| V2 | -C29 | 2.254(8) | C21 | -C22 | 1.395(11) |
| V2 | -C30 | 2.296(8) | C22 | -C23 | 1.369(10) |
| V2 | -C31 | 2.329(8) | C27 | -C28 | 1.409(10) |
| V2 | -C42 | 1.978(7) | C27 | -C31 | 1.415(12) |
| V2 | -C43 | 2.063(7) | C28 | -C29 | 1.387(11) |
| P1 | -C24 | 1.816(8) | C29 | -C30 | 1.398(11) |
| P1 | -C25 | 1.811(8) | C30 | -C31 | 1.402(10) |
| P1 | -C26 | 1.801(7) | C31 | -C32 | 1.501(11) |
| P2 | -C50 | 1.817(8) | C32 | -C33 | 1.518(11) |
| P2 | -C51 | 1.796(7) | C36 | -C37 | 1.375(11) |
| P2 | -C52 | 1.819(8) | C36 | -C41 | 1.389(10) |
| N1 | -C7 | 1.479(10) | C37 | -C38 | 1.374(10) |
| N1 | -C8 | 1.453(12) | C38 | -C39 | 1.371(10) |
| N1 | -C9 | 1.454(11) | C39 | -C40 | 1.36(1) |
| N2 | -N3 | 1.212(8) | C40 | -C41 | 1.41(1) |
| N4 | -C33 | 1.411(10) | C41 | -C42 | 1.464(10) |
| N4 | -C34 | 1.468(12) | C42 | -C43 | 1.285(10) |
| N4 | -C35 | 1.448(12) | C43 | -C44 | 1.464(10) |
| C1 | -C2 | 1.401(10) | C44 | -C45 | 1.402(11) |
| C1 | -C5 | 1.413(10) | C44 | -C49 | 1.373(10) |
| C2 | -C3 | 1.386(11) | C45 | -C46 | 1.384(10) |
| C3 | -C4 | 1.431(10) | C46 | -C47 | 1.389(11) |
| C4 | -C5 | 1.40(1) | C47 | -C48 | 1.382(12) |
| C5 | -C6 | 1.491(11) | C48 | -C49 | 1.396(10) |
| C6 | -C7 | 1.468(11) | | | |

## Bond Angles (deg.)

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| P1 | -V1 | -N2 | 84.6(2) | N3 | -V2 | -C42 | 101.4(3) |
| P1 | -V1 | -C1 | 146.0(2) | N3 | -V2 | -C43 | 108.1(3) |
| P1 | -V1 | -C2 | 125.6(2) | C27 | -V2 | -C28 | 36.3(3) |
| P1 | -V1 | -C3 | 91.7(2) | C27 | -V2 | -C29 | 59.6(3) |
| P1 | -V1 | -C4 | 87.21(19) | C27 | -V2 | -C30 | 59.4(3) |
| P1 | -V1 | -C5 | 115.83(19) | C27 | -V2 | -C31 | 35.8(3) |
| P1 | -V1 | -C16 | 120.1(2) | C27 | -V2 | -C42 | 81.4(3) |
| P1 | -V1 | -C17 | 83.9(2) | C27 | -V2 | -C43 | 106.1(3) |
| N2 | -V1 | -C1 | 116.8(3) | C28 | -V2 | -C29 | 35.8(3) |
| N2 | -V1 | -C2 | 91.9(3) | C28 | -V2 | -C30 | 59.9(3) |
| N2 | -V1 | -C3 | 100.8(3) | C28 | -V2 | -C31 | 60.0(3) |
| N2 | -V1 | -C4 | 136.0(3) | C28 | -V2 | -C42 | 107.6(3) |
| N2 | -V1 | -C5 | 150.1(3) | C28 | -V2 | -C43 | 140.3(3) |
| N2 | -V1 | -C16 | 102.0(3) | C29 | -V2 | -C30 | 35.8(3) |
| N2 | -V1 | -C17 | 108.4(3) | C29 | -V2 | -C31 | 59.3(3) |
| C1 | -V1 | -C2 | 35.7(3) | C29 | -V2 | -C42 | 140.6(3) |
| C1 | -V1 | -C3 | 59.9(3) | C29 | -V2 | -C43 | 155.3(3) |
| C1 | -V1 | -C4 | 58.9(3) | C30 | -V2 | -C31 | 35.3(3) |
| C1 | -V1 | -C5 | 35.2(3) | C30 | -V2 | -C42 | 127.8(3) |
| C1 | -V1 | -C16 | 82.9(3) | C30 | -V2 | -C43 | 120.4(3) |
| C1 | -V1 | -C17 | 110.9(3) | C31 | -V2 | -C42 | 92.9(3) |
| C2 | -V1 | -C3 | 35.7(3) | C31 | -V2 | -C43 | 96.9(3) |
| C2 | -V1 | -C4 | 59.2(3) | C42 | -V2 | -C43 | 37.0(3) |
| C2 | -V1 | -C5 | 58.7(3) | V1 | -P1 | -C24 | 122.2(3) |
| C2 | -V1 | -C16 | 113.8(3) | V1 | -P1 | -C25 | 113.7(3) |
| C2 | -V1 | -C17 | 146.4(3) | V1 | -P1 | -C26 | 113.4(3) |
| C3 | -V1 | -C4 | 36.3(3) | C24 | -P1 | -C25 | 101.4(4) |
| C3 | -V1 | -C5 | 59.3(3) | C24 | -P1 | -C26 | 102.2(3) |
| C3 | -V1 | -C16 | 142.2(3) | C25 | -P1 | -C26 | 101.3(3) |
| C3 | -V1 | -C17 | 149.9(3) | V2 | -P2 | -C50 | 122.1(3) |
| C4 | -V1 | -C5 | 34.8(3) | V2 | -P2 | -C51 | 113.6(3) |
| C4 | -V1 | -C16 | 119.3(3) | V2 | -P2 | -C52 | 113.0(3) |
| C4 | -V1 | -C17 | 113.6(3) | C50 | -P2 | -C51 | 102.7(3) |
| C5 | -V1 | -C16 | 86.9(3) | C50 | -P2 | -C52 | 101.7(4) |
| C5 | -V1 | -C17 | 96.0(3) | C51 | -P2 | -C52 | 101.1(3) |
| C16 | -V1 | -C17 | 37.1(3) | C7 | -N1 | -C8 | 111.3(7) |
| P2 | -V2 | -N3 | 85.0(2) | C7 | -N1 | -C9 | 113.8(7) |
| P2 | -V2 | -C27 | 141.4(2) | C8 | -N1 | -C9 | 109.9(8) |
| P2 | -V2 | -C28 | 131.4(2) | V1 | -N2 | -N3 | 175.4(6) |
| P2 | -V2 | -C29 | 95.9(2) | V2 | -N3 | -N2 | 174.5(5) |
| P2 | -V2 | -C30 | 83.1(2) | C33 | -N4 | -C34 | 110.9(7) |
| P2 | -V2 | -C31 | 107.1(2) | C33 | -N4 | -C35 | 111.3(7) |
| P2 | -V2 | -C42 | 120.2(2) | C34 | -N4 | -C35 | 109.5(7) |
| P2 | -V2 | -C43 | 84.1(2) | V1 | -C1 | -C2 | 70.2(4) |
| N3 | -V2 | -C27 | 124.3(3) | V1 | -C1 | -C5 | 74.5(4) |
| N3 | -V2 | -C28 | 94.0(3) | C2 | -C1 | -C5 | 107.2(6) |
| N3 | -V2 | -C29 | 96.6(3) | V1 | -C2 | -C1 | 74.1(4) |
| N3 | -V2 | -C30 | 128.3(3) | V1 | -C2 | -C3 | 72.4(4) |
| N3 | -V2 | -C31 | 153.4(3) | C1 | -C2 | -C3 | 109.9(6) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| V1 | -C3 | -C2 | 71.9(4) | V2 | -C28 | -C27 | 72.5(4) |
| V1 | -C3 | -C4 | 74.1(4) | V2 | -C28 | -C29 | 72.0(4) |
| C2 | -C3 | -C4 | 106.8(6) | C27 | -C28 | -C29 | 107.0(7) |
| V1 | -C4 | -C3 | 69.6(4) | V2 | -C29 | -C28 | 72.2(4) |
| V1 | -C4 | -C5 | 74.2(4) | V2 | -C29 | -C30 | 73.7(4) |
| C3 | -C4 | -C5 | 108.0(6) | C28 | -C29 | -C30 | 109.3(7) |
| V1 | -C5 | -C1 | 70.3(4) | V2 | -C30 | -C29 | 70.5(5) |
| V1 | -C5 | -C4 | 71.1(4) | V2 | -C30 | -C31 | 73.7(5) |
| V1 | -C5 | -C6 | 125.2(5) | C29 | -C30 | -C31 | 108.2(7) |
| C1 | -C5 | -C4 | 108.1(6) | V2 | -C31 | -C27 | 69.9(4) |
| C1 | -C5 | -C6 | 124.4(7) | V2 | -C31 | -C30 | 71.1(4) |
| C4 | -C5 | -C6 | 127.6(7) | V2 | -C31 | -C32 | 122.6(5) |
| C5 | -C6 | -C7 | 114.8(6) | C27 | -C31 | -C30 | 106.8(7) |
| N1 | -C7 | -C6 | 110.8(6) | C27 | -C31 | -C32 | 126.4(7) |
| C11 | -C10 | -C15 | 119.4(7) | C30 | -C31 | -C32 | 126.8(7) |
| C10 | -C11 | -C12 | 122.3(7) | C31 | -C32 | -C33 | 113.4(6) |
| C11 | -C12 | -C13 | 119.8(7) | N4 | -C33 | -C32 | 114.2(6) |
| C12 | -C13 | -C14 | 119.2(8) | C37 | -C36 | -C41 | 121.0(7) |
| C13 | -C14 | -C15 | 121.4(7) | C36 | -C37 | -C38 | 120.0(7) |
| C10 | -C15 | -C14 | 117.8(7) | C37 | -C38 | -C39 | 120.2(7) |
| C10 | -C15 | -C16 | 121.0(7) | C38 | -C39 | -C40 | 120.4(7) |
| C14 | -C15 | -C16 | 121.0(6) | C39 | -C40 | -C41 | 120.9(7) |
| V1 | -C16 | -C15 | 147.4(5) | C36 | -C41 | -C40 | 117.5(7) |
| V1 | -C16 | -C17 | 74.1(5) | C36 | -C41 | -C42 | 122.2(7) |
| C15 | -C16 | -C17 | 138.4(7) | C40 | -C41 | -C42 | 120.3(6) |
| V1 | -C17 | -C16 | 68.8(4) | V2 | -C42 | -C41 | 146.2(5) |
| V1 | -C17 | -C18 | 154.6(6) | V2 | -C42 | -C43 | 75.1(5) |
| C16 | -C17 | -C18 | 136.6(7) | C41 | -C42 | -C43 | 138.6(7) |
| C17 | -C18 | -C19 | 123.3(7) | V2 | -C43 | -C42 | 67.9(4) |
| C17 | -C18 | -C23 | 119.1(6) | V2 | -C43 | -C44 | 155.8(5) |
| C19 | -C18 | -C23 | 117.6(7) | C42 | -C43 | -C44 | 136.3(7) |
| C18 | -C19 | -C20 | 122.4(8) | C43 | -C44 | -C45 | 120.7(6) |
| C19 | -C20 | -C21 | 120.8(8) | C43 | -C44 | -C49 | 121.4(7) |
| C20 | -C21 | -C22 | 117.6(8) | C45 | -C44 | -C49 | 117.7(6) |
| C21 | -C22 | -C23 | 120.8(8) | C44 | -C45 | -C46 | 121.6(7) |
| C18 | -C23 | -C22 | 120.7(7) | C45 | -C46 | -C47 | 120.0(8) |
| V2 | -C27 | -C28 | 71.3(4) | C46 | -C47 | -C48 | 118.9(7) |
| V2 | -C27 | -C31 | 74.3(4) | C47 | -C48 | -C49 | 120.6(7) |
| C28 | -C27 | -C31 | 108.6(7) | C44 | -C49 | -C48 | 121.2(7) |

## Torsion Angles (deg.)

| | | | | |
|---|---|---|---|---|
| N2 | -V1 | -P1 | -C24 | -169.4(3) |
| N2 | -V1 | -P1 | -C25 | 68.6(4) |
| N2 | -V1 | -P1 | -C26 | -46.4(3) |
| C1 | -V1 | -P1 | -C24 | 58.6(5) |
| C1 | -V1 | -P1 | -C25 | -63.5(5) |
| C1 | -V1 | -P1 | -C26 | -178.5(4) |
| C2 | -V1 | -P1 | -C24 | 102.2(4) |
| C2 | -V1 | -P1 | -C25 | -19.9(4) |
| C2 | -V1 | -P1 | -C26 | -134.9(3) |
| C3 | -V1 | -P1 | -C24 | 90.0(4) |
| C3 | -V1 | -P1 | -C25 | -32.1(4) |

| | | | | |
|---|---|---|---|---|
| C3 | -V1 | -P1 | -C26 | -147.1(3) |
| C4 | -V1 | -P1 | -C24 | 53.9(3) |
| C4 | -V1 | -P1 | -C25 | -68.1(3) |
| C4 | -V1 | -P1 | -C26 | 176.9(3) |
| C5 | -V1 | -P1 | -C24 | 33.5(4) |
| C5 | -V1 | -P1 | -C25 | -88.5(4) |
| C5 | -V1 | -P1 | -C26 | 156.5(3) |
| C16 | -V1 | -P1 | -C24 | -68.6(4) |
| C16 | -V1 | -P1 | -C25 | 169.3(4) |
| C16 | -V1 | -P1 | -C26 | 54.3(4) |
| C17 | -V1 | -P1 | -C24 | -60.2(4) |
| C17 | -V1 | -P1 | -C25 | 177.8(4) |
| C17 | -V1 | -P1 | -C26 | 62.8(3) |
| P1 | -V1 | -C1 | -C2 | 73.8(5) |
| P1 | -V1 | -C1 | -C5 | -41.4(6) |
| N2 | -V1 | -C1 | -C2 | -50.3(5) |
| N2 | -V1 | -C1 | -C5 | -165.5(4) |
| C2 | -V1 | -C1 | -C5 | -115.2(6) |
| C3 | -V1 | -C1 | -C2 | 36.8(4) |
| C3 | -V1 | -C1 | -C5 | -78.4(5) |
| C4 | -V1 | -C1 | -C2 | 79.2(5) |
| C4 | -V1 | -C1 | -C5 | -36.0(4) |
| C5 | -V1 | -C1 | -C2 | 115.2(6) |
| C16 | -V1 | -C1 | -C2 | -150.2(5) |
| C16 | -V1 | -C1 | -C5 | 94.6(4) |
| C17 | -V1 | -C1 | -C2 | -175.1(4) |
| C17 | -V1 | -C1 | -C5 | 69.7(5) |
| P1 | -V1 | -C2 | -C1 | -138.7(4) |
| P1 | -V1 | -C2 | -C3 | -21.2(5) |
| N2 | -V1 | -C2 | -C1 | 136.6(5) |
| N2 | -V1 | -C2 | -C3 | -105.9(5) |
| C1 | -V1 | -C2 | -C3 | 117.5(6) |
| C3 | -V1 | -C2 | -C1 | -117.5(6) |
| C4 | -V1 | -C2 | -C1 | -78.5(5) |
| C4 | -V1 | -C2 | -C3 | 39.0(4) |
| C5 | -V1 | -C2 | -C1 | -37.7(4) |
| C5 | -V1 | -C2 | -C3 | 79.8(5) |
| C16 | -V1 | -C2 | -C1 | 32.6(5) |
| C16 | -V1 | -C2 | -C3 | 150.1(4) |
| C17 | -V1 | -C2 | -C1 | 8.3(7) |
| C17 | -V1 | -C2 | -C3 | 125.8(6) |
| P1 | -V1 | -C3 | -C2 | 162.9(4) |
| P1 | -V1 | -C3 | -C4 | -82.9(4) |
| N2 | -V1 | -C3 | -C2 | 78.1(5) |
| N2 | -V1 | -C3 | -C4 | -167.8(4) |
| C1 | -V1 | -C3 | -C2 | -36.8(4) |
| C1 | -V1 | -C3 | -C4 | 77.4(4) |
| C2 | -V1 | -C3 | -C4 | 114.2(6) |
| C4 | -V1 | -C3 | -C2 | -114.2(6) |
| C5 | -V1 | -C3 | -C2 | -77.8(5) |
| C5 | -V1 | -C3 | -C4 | 36.3(4) |
| C16 | -V1 | -C3 | -C2 | -48.1(7) |
| C16 | -V1 | -C3 | -C4 | 66.1(6) |

| | | | | |
|---|---|---|---|---|
| C17 | -V1 | -C3 | -C2 | -116.4(6) |
| C17 | -V1 | -C3 | -C4 | -2.3(8) |
| P1 | -V1 | -C4 | -C3 | 96.7(4) |
| P1 | -V1 | -C4 | -C5 | -146.6(4) |
| N2 | -V1 | -C4 | -C3 | 17.4(6) |
| N2 | -V1 | -C4 | -C5 | 134.1(5) |
| C1 | -V1 | -C4 | -C3 | -80.3(5) |
| C1 | -V1 | -C4 | -C5 | 36.4(4) |
| C2 | -V1 | -C4 | -C3 | -38.4(4) |
| C2 | -V1 | -C4 | -C5 | 78.3(4) |
| C3 | -V1 | -C4 | -C5 | 116.7(6) |
| C5 | -V1 | -C4 | -C3 | -116.7(6) |
| C16 | -V1 | -C4 | -C3 | -140.1(4) |
| C16 | -V1 | -C4 | -C5 | -23.4(5) |
| C17 | -V1 | -C4 | -C3 | 178.8(4) |
| C17 | -V1 | -C4 | -C5 | -64.6(5) |
| P1 | -V1 | -C5 | -C1 | 155.8(4) |
| P1 | -V1 | -C5 | -C4 | 37.6(4) |
| P1 | -V1 | -C5 | -C6 | -85.5(6) |
| N2 | -V1 | -C5 | -C1 | 26.7(7) |
| N2 | -V1 | -C5 | -C4 | -91.5(6) |
| N2 | -V1 | -C5 | -C6 | 145.4(6) |
| C1 | -V1 | -C5 | -C4 | -118.1(6) |
| C1 | -V1 | -C5 | -C6 | 118.7(8) |
| C2 | -V1 | -C5 | -C1 | 38.2(4) |
| C2 | -V1 | -C5 | -C4 | -79.9(5) |
| C2 | -V1 | -C5 | -C6 | 156.9(7) |
| C3 | -V1 | -C5 | -C1 | 80.2(5) |
| C3 | -V1 | -C5 | -C4 | -38.0(4) |
| C3 | -V1 | -C5 | -C6 | -161.1(7) |
| C4 | -V1 | -C5 | -C1 | 118.1(6) |
| C4 | -V1 | -C5 | -C6 | -123.1(8) |
| C16 | -V1 | -C5 | -C1 | -82.1(4) |
| C16 | -V1 | -C5 | -C4 | 159.7(5) |
| C16 | -V1 | -C5 | -C6 | 36.6(6) |
| C17 | -V1 | -C5 | -C1 | -118.2(4) |
| C17 | -V1 | -C5 | -C4 | 123.7(4) |
| C17 | -V1 | -C5 | -C6 | 0.5(6) |
| P1 | -V1 | -C16 | -C15 | -169.7(9) |
| P1 | -V1 | -C16 | -C17 | 14.1(5) |
| N2 | -V1 | -C16 | -C15 | -79.(1) |
| N2 | -V1 | -C16 | -C17 | 104.7(5) |
| C1 | -V1 | -C16 | -C15 | 37.(1) |
| C1 | -V1 | -C16 | -C17 | -139.3(5) |
| C2 | -V1 | -C16 | -C15 | 18.5(11) |
| C2 | -V1 | -C16 | -C17 | -157.8(4) |
| C3 | -V1 | -C16 | -C15 | 46.9(13) |
| C3 | -V1 | -C16 | -C17 | -129.4(5) |
| C4 | -V1 | -C16 | -C15 | 85.2(11) |
| C4 | -V1 | -C16 | -C17 | -91.1(5) |
| C5 | -V1 | -C16 | -C15 | 72.1(10) |
| C5 | -V1 | -C16 | -C17 | -104.2(5) |
| C17 | -V1 | -C16 | -C15 | 176.3(13) |

| | | | | |
|---|---|---|---|---|
| P1 | -V1 | -C17 | -C16 | -167.8(5) |
| P1 | -V1 | -C17 | -C18 | 9.9(12) |
| N2 | -V1 | -C17 | -C16 | -85.6(5) |
| N2 | -V1 | -C17 | -C18 | 92.1(13) |
| C1 | -V1 | -C17 | -C16 | 43.9(5) |
| C1 | -V1 | -C17 | -C18 | -138.4(12) |
| C2 | -V1 | -C17 | -C16 | 38.7(7) |
| C2 | -V1 | -C17 | -C18 | -143.6(11) |
| C3 | -V1 | -C17 | -C16 | 109.4(6) |
| C3 | -V1 | -C17 | -C18 | -72.9(14) |
| C4 | -V1 | -C17 | -C16 | 108.0(5) |
| C4 | -V1 | -C17 | -C18 | -74.3(13) |
| C5 | -V1 | -C17 | -C16 | 76.8(5) |
| C5 | -V1 | -C17 | -C18 | -105.5(13) |
| C16 | -V1 | -C17 | -C18 | 177.7(15) |
| N3 | -V2 | -P2 | -C50 | -169.7(3) |
| N3 | -V2 | -P2 | -C51 | -45.8(3) |
| N3 | -V2 | -P2 | -C52 | 68.6(4) |
| C27 | -V2 | -P2 | -C50 | 47.6(4) |
| C27 | -V2 | -P2 | -C51 | 171.4(4) |
| C27 | -V2 | -P2 | -C52 | -74.2(4) |
| C28 | -V2 | -P2 | -C50 | 99.4(4) |
| C28 | -V2 | -P2 | -C51 | -136.8(4) |
| C28 | -V2 | -P2 | -C52 | -22.4(4) |
| C29 | -V2 | -P2 | -C50 | 94.2(4) |
| C29 | -V2 | -P2 | -C51 | -142.0(3) |
| C29 | -V2 | -P2 | -C52 | -27.5(4) |
| C30 | -V2 | -P2 | -C50 | 60.7(3) |
| C30 | -V2 | -P2 | -C51 | -175.4(3) |
| C30 | -V2 | -P2 | -C52 | -61.0(3) |
| C31 | -V2 | -P2 | -C50 | 34.6(4) |
| C31 | -V2 | -P2 | -C51 | 158.4(3) |
| C31 | -V2 | -P2 | -C52 | -87.1(4) |
| C42 | -V2 | -P2 | -C50 | -69.3(4) |
| C42 | -V2 | -P2 | -C51 | 54.5(4) |
| C42 | -V2 | -P2 | -C52 | 169.0(4) |
| C43 | -V2 | -P2 | -C50 | -60.9(4) |
| C43 | -V2 | -P2 | -C51 | 62.9(3) |
| C43 | -V2 | -P2 | -C52 | 177.4(4) |
| P2 | -V2 | -C27 | -C28 | 94.9(5) |
| P2 | -V2 | -C27 | -C31 | -21.6(6) |
| N3 | -V2 | -C27 | -C28 | -38.2(6) |
| N3 | -V2 | -C27 | -C31 | -154.7(4) |
| C28 | -V2 | -C27 | -C31 | -116.5(7) |
| C29 | -V2 | -C27 | -C28 | 37.9(5) |
| C29 | -V2 | -C27 | -C31 | -78.6(5) |
| C30 | -V2 | -C27 | -C28 | 79.7(5) |
| C30 | -V2 | -C27 | -C31 | -36.8(4) |
| C31 | -V2 | -C27 | -C28 | 116.5(7) |
| C42 | -V2 | -C27 | -C28 | -136.3(5) |
| C42 | -V2 | -C27 | -C31 | 107.3(5) |
| C43 | -V2 | -C27 | -C28 | -164.1(5) |
| C43 | -V2 | -C27 | -C31 | 79.4(5) |

| | | | | |
|---|---|---|---|---|
| P2 | -V2 | -C28 | -C27 | -124.0(4) |
| P2 | -V2 | -C28 | -C29 | -8.8(6) |
| N3 | -V2 | -C28 | -C27 | 149.2(5) |
| N3 | -V2 | -C28 | -C29 | -95.7(5) |
| C27 | -V2 | -C28 | -C29 | 115.2(7) |
| C29 | -V2 | -C28 | -C27 | -115.2(7) |
| C30 | -V2 | -C28 | -C27 | -78.2(5) |
| C30 | -V2 | -C28 | -C29 | 37.0(4) |
| C31 | -V2 | -C28 | -C27 | -37.2(5) |
| C31 | -V2 | -C28 | -C29 | 78.0(5) |
| C42 | -V2 | -C28 | -C27 | 45.8(6) |
| C42 | -V2 | -C28 | -C29 | 161.0(5) |
| C43 | -V2 | -C28 | -C27 | 24.3(7) |
| C43 | -V2 | -C28 | -C29 | 139.5(5) |
| P2 | -V2 | -C29 | -C28 | 173.4(4) |
| P2 | -V2 | -C29 | -C30 | -69.5(4) |
| N3 | -V2 | -C29 | -C28 | 87.8(5) |
| N3 | -V2 | -C29 | -C30 | -155.1(4) |
| C27 | -V2 | -C29 | -C28 | -38.4(5) |
| C27 | -V2 | -C29 | -C30 | 78.7(5) |
| C28 | -V2 | -C29 | -C30 | 117.1(6) |
| C30 | -V2 | -C29 | -C28 | -117.1(6) |
| C31 | -V2 | -C29 | -C28 | -80.2(5) |
| C31 | -V2 | -C29 | -C30 | 36.9(4) |
| C42 | -V2 | -C29 | -C28 | -29.3(7) |
| C42 | -V2 | -C29 | -C30 | 87.8(6) |
| C43 | -V2 | -C29 | -C28 | -97.8(8) |
| C43 | -V2 | -C29 | -C30 | 19.3(9) |
| P2 | -V2 | -C30 | -C29 | 110.2(4) |
| P2 | -V2 | -C30 | -C31 | -133.1(4) |
| N3 | -V2 | -C30 | -C29 | 32.2(6) |
| N3 | -V2 | -C30 | -C31 | 148.8(4) |
| C27 | -V2 | -C30 | -C29 | -79.3(5) |
| C27 | -V2 | -C30 | -C31 | 37.4(4) |
| C28 | -V2 | -C30 | -C29 | -37.1(4) |
| C28 | -V2 | -C30 | -C31 | 79.6(5) |
| C29 | -V2 | -C30 | -C31 | 116.7(6) |
| C31 | -V2 | -C30 | -C29 | -116.7(6) |
| C42 | -V2 | -C30 | -C29 | -126.6(5) |
| C42 | -V2 | -C30 | -C31 | -9.9(6) |
| C43 | -V2 | -C30 | -C29 | -170.8(4) |
| C43 | -V2 | -C30 | -C31 | -54.1(5) |
| P2 | -V2 | -C31 | -C27 | 166.1(4) |
| P2 | -V2 | -C31 | -C30 | 49.3(4) |
| P2 | -V2 | -C31 | -C32 | -72.8(6) |
| N3 | -V2 | -C31 | -C27 | 51.9(8) |
| N3 | -V2 | -C31 | -C30 | -64.9(8) |
| N3 | -V2 | -C31 | -C32 | 173.0(6) |
| C27 | -V2 | -C31 | -C30 | -116.8(6) |
| C27 | -V2 | -C31 | -C32 | 121.0(8) |
| C28 | -V2 | -C31 | -C27 | 37.7(4) |
| C28 | -V2 | -C31 | -C30 | -79.2(5) |

| | | | | |
|---|---|---|---|---|
| C28 | -V2 | -C31 | -C32 | 158.7(7) |
| C29 | -V2 | -C31 | -C27 | 79.4(5) |
| C29 | -V2 | -C31 | -C30 | -37.4(4) |
| C29 | -V2 | -C31 | -C32 | -159.5(7) |
| C30 | -V2 | -C31 | -C27 | 116.8(6) |
| C30 | -V2 | -C31 | -C32 | -122.1(8) |
| C42 | -V2 | -C31 | -C27 | -71.0(5) |
| C42 | -V2 | -C31 | -C30 | 172.2(5) |
| C42 | -V2 | -C31 | -C32 | 50.1(6) |
| C43 | -V2 | -C31 | -C27 | -107.9(4) |
| C43 | -V2 | -C31 | -C30 | 135.3(5) |
| C43 | -V2 | -C31 | -C32 | 13.1(7) |
| P2 | -V2 | -C42 | -C41 | -169.5(9) |
| P2 | -V2 | -C42 | -C43 | 14.0(5) |
| N3 | -V2 | -C42 | -C41 | -78.6(10) |
| N3 | -V2 | -C42 | -C43 | 104.9(5) |
| C27 | -V2 | -C42 | -C41 | 44.8(10) |
| C27 | -V2 | -C42 | -C43 | -131.7(5) |
| C28 | -V2 | -C42 | -C41 | 19.4(11) |
| C28 | -V2 | -C42 | -C43 | -157.1(5) |
| C29 | -V2 | -C42 | -C41 | 36.9(12) |
| C29 | -V2 | -C42 | -C43 | -139.6(5) |
| C30 | -V2 | -C42 | -C41 | 84.5(10) |
| C30 | -V2 | -C42 | -C43 | -92.0(5) |
| C31 | -V2 | -C42 | -C41 | 78.8(10) |
| C31 | -V2 | -C42 | -C43 | -97.7(5) |
| C43 | -V2 | -C42 | -C41 | 176.5(13) |
| P2 | -V2 | -C43 | -C42 | -167.9(5) |
| P2 | -V2 | -C43 | -C44 | 12.4(13) |
| N3 | -V2 | -C43 | -C42 | -85.1(5) |
| N3 | -V2 | -C43 | -C44 | 95.2(13) |
| C27 | -V2 | -C43 | -C42 | 50.2(5) |
| C27 | -V2 | -C43 | -C44 | -129.6(13) |
| C28 | -V2 | -C43 | -C42 | 35.5(7) |
| C28 | -V2 | -C43 | -C44 | -144.2(12) |
| C29 | -V2 | -C43 | -C42 | 100.8(8) |
| C29 | -V2 | -C43 | -C44 | -79.0(15) |
| C30 | -V2 | -C43 | -C42 | 113.7(5) |
| C30 | -V2 | -C43 | -C44 | -66.1(14) |
| C31 | -V2 | -C43 | -C42 | 85.6(5) |
| C31 | -V2 | -C43 | -C44 | -94.2(13) |
| C42 | -V2 | -C43 | -C44 | -179.8(16) |
| C8 | -N1 | -C7 | -C6 | -167.3(7) |
| C9 | -N1 | -C7 | -C6 | 67.9(9) |
| C34 | -N4 | -C33 | -C32 | -171.1(7) |
| C35 | -N4 | -C33 | -C32 | 66.7(9) |
| V1 | -C1 | -C2 | -C3 | -64.1(5) |
| C5 | -C1 | -C2 | -V1 | 65.9(5) |
| C5 | -C1 | -C2 | -C3 | 1.8(8) |
| V1 | -C1 | -C5 | -C4 | 61.3(5) |
| V1 | -C1 | -C5 | -C6 | -119.7(7) |
| C2 | -C1 | -C5 | -V1 | -63.0(5) |
| C2 | -C1 | -C5 | -C4 | -1.7(8) |

| | | | | |
|---|---|---|---|---|
| C2 | -C1 | -C5 | -C6 | 177.3(7) |
| V1 | -C2 | -C3 | -C4 | -66.4(5) |
| C1 | -C2 | -C3 | -V1 | 65.2(5) |
| C1 | -C2 | -C3 | -C4 | -1.3(8) |
| V1 | -C3 | -C4 | -C5 | -64.7(5) |
| C2 | -C3 | -C4 | -V1 | 64.9(5) |
| C2 | -C3 | -C4 | -C5 | 0.2(8) |
| V1 | -C4 | -C5 | -C1 | -60.8(5) |
| V1 | -C4 | -C5 | -C6 | 120.3(8) |
| C3 | -C4 | -C5 | -V1 | 61.7(5) |
| C3 | -C4 | -C5 | -C1 | 0.9(8) |
| C3 | -C4 | -C5 | -C6 | -178.0(7) |
| V1 | -C5 | -C6 | -C7 | 104.1(7) |
| C1 | -C5 | -C6 | -C7 | -166.9(7) |
| C4 | -C5 | -C6 | -C7 | 11.8(11) |
| C5 | -C6 | -C7 | -N1 | 171.5(6) |
| C15 | -C10 | -C11 | -C12 | -0.9(12) |
| C11 | -C10 | -C15 | -C14 | 3.2(11) |
| C11 | -C10 | -C15 | -C16 | 178.2(7) |
| C10 | -C11 | -C12 | -C13 | -0.9(12) |
| C11 | -C12 | -C13 | -C14 | 0.2(12) |
| C12 | -C13 | -C14 | -C15 | 2.3(12) |
| C13 | -C14 | -C15 | -C10 | -4.0(11) |
| C13 | -C14 | -C15 | -C16 | -179.0(7) |
| C10 | -C15 | -C16 | -V1 | -151.7(8) |
| C10 | -C15 | -C16 | -C17 | 22.9(14) |
| C14 | -C15 | -C16 | -V1 | 23.2(14) |
| C14 | -C15 | -C16 | -C17 | -162.2(9) |
| V1 | -C16 | -C17 | -C18 | -178.6(10) |
| C15 | -C16 | -C17 | -V1 | -177.0(11) |
| C15 | -C16 | -C17 | -C18 | 4.4(17) |
| V1 | -C17 | -C18 | -C19 | -110.2(13) |
| V1 | -C17 | -C18 | -C23 | 70.7(15) |
| C16 | -C17 | -C18 | -C19 | 66.7(13) |
| C16 | -C17 | -C18 | -C23 | -112.4(10) |
| C17 | -C18 | -C19 | -C20 | -177.2(7) |
| C23 | -C18 | -C19 | -C20 | 1.9(11) |
| C17 | -C18 | -C23 | -C22 | 176.9(7) |
| C19 | -C18 | -C23 | -C22 | -2.2(11) |
| C18 | -C19 | -C20 | -C21 | -1.6(12) |
| C19 | -C20 | -C21 | -C22 | 1.6(11) |
| C20 | -C21 | -C22 | -C23 | -2.0(11) |
| C21 | -C22 | -C23 | -C18 | 2.3(11) |
| V2 | -C27 | -C28 | -C29 | -64.2(5) |
| C31 | -C27 | -C28 | -V2 | 65.4(5) |
| C31 | -C27 | -C28 | -C29 | 1.3(8) |
| V2 | -C27 | -C31 | -C30 | 61.9(5) |
| V2 | -C27 | -C31 | -C32 | -116.3(7) |
| C28 | -C27 | -C31 | -V2 | -63.5(5) |
| C28 | -C27 | -C31 | -C30 | -1.6(8) |
| C28 | -C27 | -C31 | -C32 | -179.8(7) |
| V2 | -C28 | -C29 | -C30 | -64.9(5) |
| C27 | -C28 | -C29 | -V2 | 64.5(5) |

| | | | | |
|---|---|---|---|---|
| C27 | -C28 | -C29 | -C30 | -0.4(9) |
| V2 | -C29 | -C30 | -C31 | -64.5(5) |
| C28 | -C29 | -C30 | -V2 | 63.9(5) |
| C28 | -C29 | -C30 | -C31 | -0.6(9) |
| V2 | -C30 | -C31 | -C27 | -61.1(5) |
| V2 | -C30 | -C31 | -C32 | 117.0(7) |
| C29 | -C30 | -C31 | -V2 | 62.5(5) |
| C29 | -C30 | -C31 | -C27 | 1.4(8) |
| C29 | -C30 | -C31 | -C32 | 179.5(7) |
| V2 | -C31 | -C32 | -C33 | -168.5(5) |
| C27 | -C31 | -C32 | -C33 | -80.5(10) |
| C30 | -C31 | -C32 | -C33 | 101.7(9) |
| C31 | -C32 | -C33 | -N4 | 177.5(7) |
| C41 | -C36 | -C37 | -C38 | -1.0(12) |
| C37 | -C36 | -C41 | -C40 | 0.5(11) |
| C37 | -C36 | -C41 | -C42 | -177.1(7) |
| C36 | -C37 | -C38 | -C39 | 0.4(12) |
| C37 | -C38 | -C39 | -C40 | 0.6(12) |
| C38 | -C39 | -C40 | -C41 | -1.0(11) |
| C39 | -C40 | -C41 | -C36 | 0.5(11) |
| C39 | -C40 | -C41 | -C42 | 178.1(7) |
| C36 | -C41 | -C42 | -V2 | 17.1(14) |
| C36 | -C41 | -C42 | -C43 | -168.0(9) |
| C40 | -C41 | -C42 | -V2 | -160.4(8) |
| C40 | -C41 | -C42 | -C43 | 14.5(14) |
| V2 | -C42 | -C43 | -C44 | 179.9(9) |
| C41 | -C42 | -C43 | -V2 | -177.1(11) |
| C41 | -C42 | -C43 | -C44 | 2.8(17) |
| V2 | -C43 | -C44 | -C45 | 70.0(15) |
| V2 | -C43 | -C44 | -C49 | -114.5(13) |
| C42 | -C43 | -C44 | -C45 | -109.7(10) |
| C42 | -C43 | -C44 | -C49 | 65.9(12) |
| C43 | -C44 | -C45 | -C46 | 176.3(7) |
| C49 | -C44 | -C45 | -C46 | 0.6(10) |
| C43 | -C44 | -C49 | -C48 | -175.4(7) |
| C45 | -C44 | -C49 | -C48 | 0.3(10) |
| C44 | -C45 | -C46 | -C47 | -0.8(11) |
| C45 | -C46 | -C47 | -C48 | 0.2(11) |
| C46 | -C47 | -C48 | -C49 | 0.7(11) |

The sign of the torsion angle is positive if when looking from atom-2
to atom-3 a clockwise motion of atom-1 would superimpose it on atom-4.

File : cp881.doc
Number_of_Characters : 161972
Number_of_Words: 29166
Number_of_Lines : 2902
Number_of_Pages : 26
Date_and_Time : 13-07-2010 08:12:16
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File_Names :

| | |
|---|---|
| CP881.doc | Experimental Document (Microsoft® Word 2002 (1.0.2627.2625) |
| CP881.spf | Standard Crystallographic Parameter File |
| CP881.res | Input file for next cycle to *SHELXL* (version : 97.2) |
| CP881.lxl | Output file from *SHELXL* (version : 97.2) |
| CP881.lst | Output file from *PLATON* (version : 140603) |

Plot files :

| | |
|---|---|
| CP881.h1x | HPGL file(s) by *PLUTO* (version : 160503) |
| CP881.h2x | HPGL file(s) different cell projections by *PLUTO* |
| CP881.h3x | HPGL file(s) Ortep plot (by *PLATON* or *ORTEP*32) |
| CP881.hx | extra / special HPGL file(s) |