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# *N*,*N*′-Dibenzyl-*N*,*N*′-dimethyl-*N*″-(methylsulfonyl)phosphoric triamide

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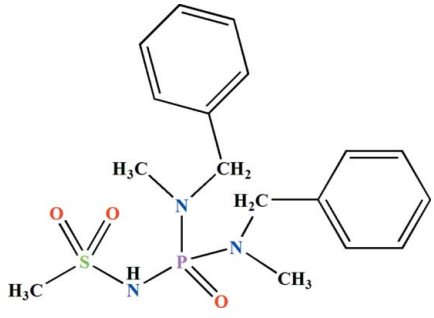
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.032; $wR$ factor = 0.094; data-to-parameter ratio = 18.4.

In the title compound, $C_{17}H_{24}N_3O_3PS$, the P and the S atoms are each in a distorted tetrahedral environment and the N atoms display $sp^2$ character. The phosphoryl group and the NH unit are *anti* with respect to one another. The dihedral angle between the mean planes of the benzene rings is 31.08 (8)°. The crystal packing is stabilized by N—H···O hydrogen bonds, forming an extended chain parallel to the *b* axis.

## Related literature

For phosphoramidates having a $P(O)[N(CH_3)(CH_2C_6H_5)]_2$ moiety, see: Pourayoubi *et al.* (2010); Gholivand *et al.* (2005). For bond lengths in a sulfonamide compound, see: Ibrahim *et al.* (2011) and references cited therein.



## Experimental

### Crystal data

$C_{17}H_{24}N_3O_3PS$ $M_r$ = 381.42
Orthorhombic, $P2_12_12_1$
$a$ = 8.5343 (4) Å
$b$ = 10.1800 (5) Å
$c$ = 22.0455 (10) Å
$V$ = 1915.29 (16) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.27 mm$^{-1}$
$T$ = 296 K
0.47 × 0.38 × 0.30 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min}$ = 0.700, $T_{max}$ = 0.746
65627 measured reflections
4155 independent reflections
3937 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.060

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.094
$S$ = 1.08
4155 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$
Absolute structure: Flack (1983), 1769 Friedel pairs
Flack parameter: 0.02 (7)

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H···O1$^{i}$ | 0.86 | 1.91 | 2.7152 (19) | 155 |

Symmetry code: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *enCIFer* (Allen *et al.*, 2004).

Support of this investigation by Ferdowsi University of Mashhad is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2084).

## References

Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.
Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Gholivand, K., Pourayoubi, M., Shariatinia, Z. & Mostaanzadeh, H. (2005). *Polyhedron*, **24**, 655–662.
Ibrahim, S., Tahir, M. N., Iqbal, N., Shahwar, D. & Raza, M. A. (2011). *Acta Cryst.* E**67**, o298.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Pourayoubi, M., Tarahhomi, A., Rheingold, A. L. & Golen, J. A. (2010). *Acta Cryst.* E**66**, o2524.
Sheldrick, G. M. (2004). *SADABS*. Uinversity of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

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## *N*,*N*′-Dibenzyl-*N*,*N*′-dimethyl-*N*′′-(methylsulfonyl)phosphoric triamide

**Mehrdad Pourayoubi, Sepideh Sadeghi Seraji, Giuseppe Bruno and Hadi Amiri Rudbari**

### S1. Comment

Structure determination of the title compound, $CH_3S(O)_2NHP(O)[N(CH_3)(CH_2C_6H_5)]_2$ (Fig. 1), was performed as a part of a project in our laboratory on the synthesis of new phosphoramidate compounds having a $P(O)[N(CH_3)(CH_2C_6H_5)]_2$ moiety (Pourayoubi *et al.*, 2010).

The P═O and P—N bond lengths are comparable to those in similar phosphoramidates of the formula $XP(O)[N(CH_3)(CH_2C_6H_5)]_2$ [where $X$ = Cl, $C_6H_5C(O)NH$, $CCl_3C(O)NH$] (Gholivand *et al.*, 2005). The P—N1 and P—N2 bonds (with bond lengths of 1.6326 (17) Å and 1.6285 (18) Å) are shorter than the P—N3 bond (1.6714 (15) Å). The S═O bond lengths of 1.4317 (16) Å & 1.4287 (18) Å are standard for sulfonamide compounds (Ibrahim *et al.*, 2011).

Each of the phosphorus and sulfur atoms has a distorted tetrahedral configuration. The surrounding bond angles are in the range of 104.84 (9)° to 117.02 (9)° around the P atom and 104.79 (12)° to 118.53 (12)° for the S atom. The average of surrounding angles around the tertiary nitrogen atom N2 (which is about 120°) shows that it is bonded in an essentially planar geometry; whereas, the environment of N1 is slightly deviated from planarity (average of bond angles is 118.3°). Furthermore, the S—N3—P angle is 125.05 (9)°. The dihedral angle between the mean planes of the benzene rings is 31.08 (8)°.

The phosphoryl group and the NH unit adopt the *anti* orientations with respect to each other. Crystal packing is stabilized by N—H···O hydrogen bonds, forming an extended chain parallel to the *b* axis (Fig. 2).

### S2. Experimental

$CH_3S(O)_2NHP(O)Cl_2$ was synthesized from the reaction between phosphorus pentachloride (16.7 mmol) and methanesulfonamide (16.7 mmol) in dry $CCl_4$ at 353 K (3 h) and then treated with formic acid 85% (16.7 mmol) at ice bath temperature.

To a solution of $CH_3S(O)_2NHP(O)Cl_2$ (2.35 mmol) in dry chloroform (30 ml), a solution of *N*-methylbenzylamine (9.40 mmol) in the same solvent (10 ml) was added at ice bath temperature. After 4 h stirring, the solvent was removed and the product was washed with distilled water and recrystallized from $CH_3CN/CHCl_3$ at room temperature.

### S3. Refinement

H atoms were placed in calculated positions and included in the refinement in a riding-model approximation with CH = 0.93, $CH_2$ = 0.97, $CH_3$ = 0.96 Å or N—H = 0.86 Å with $U_{iso}$(H) parameters equal to 1.5$U_{eq}$(C) for methyl H atoms and 1.2$U_{eq}$(C,N) for other H atoms.

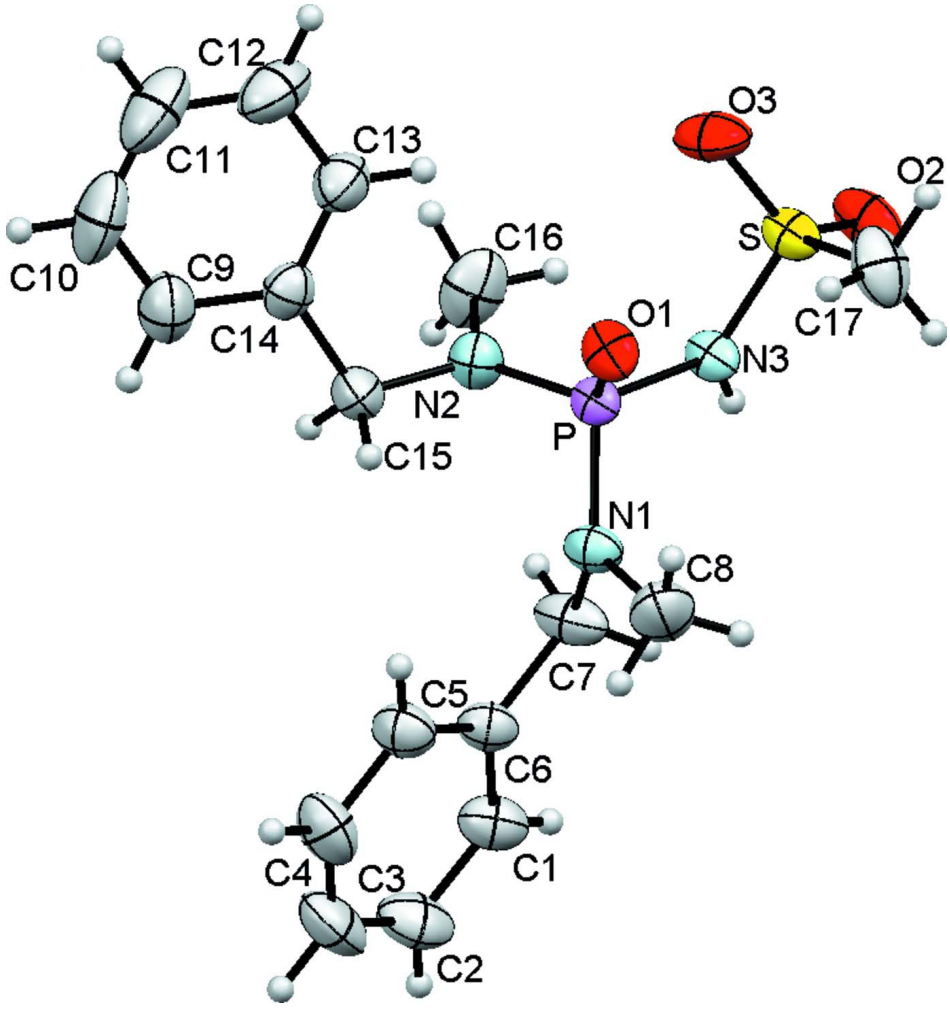


**Figure 1**

An *ORTEP*-style plot of title compound with labeling. Ellipsoids are given at the 50% probability level.

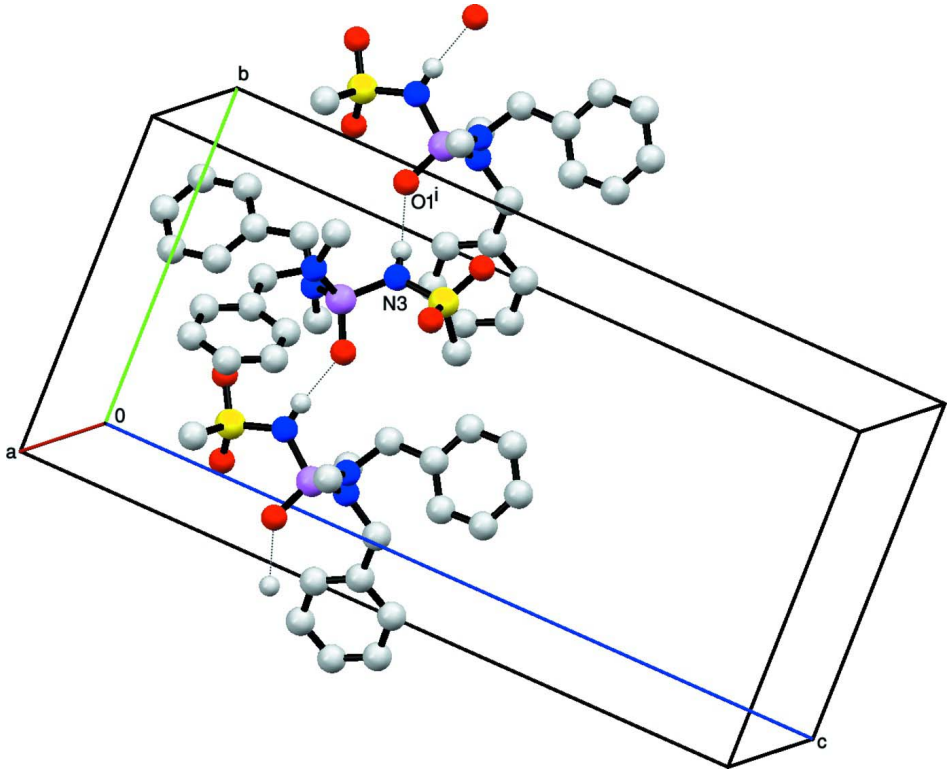


**Figure 2**

Partial packing view showing the formation of the chain through N—H···O hydrogen bonds which are shown as dotted lines. H atoms not involved in hydrogen bondings have been omitted for the sake of clarity. [Symmetry code: (i) -*x*, *y* + 1/2, -*z* + 1/2]

### *N*,*N*′-Dibenzyl-*N*,*N*′-dimethyl- *N*′′-(methylsulfonyl)phosphoric triamide

*Crystal data*

$C_{17}H_{24}N_3O_3PS$
$M_r$ = 381.42
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a$ = 8.5343 (4) Å
$b$ = 10.1800 (5) Å
$c$ = 22.0455 (10) Å
$V$ = 1915.29 (16) Å$^3$
$Z$ = 4
$F(000)$ = 808
$D_x$ = 1.323 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9705 reflections
$\theta$ = 2.6–29.5°
$\mu$ = 0.27 mm$^{-1}$
$T$ = 296 K
Irregular, colourless
0.47 × 0.38 × 0.30 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min}$ = 0.700, $T_{max}$ = 0.746
65627 measured reflections
4155 independent reflections
3937 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.060
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 2.2°
$h$ = −10→10
$k$ = −13→13
$l$ = −28→28

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.094$
$S = 1.08$
4155 reflections
226 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
$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2 + 0.4498P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.22$ e Å$^{-3}$
Absolute structure: Flack (1983), **1769 Friedel pairs**
Absolute structure parameter: 0.02 (7)

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s 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 $F^2 > 2\sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S | −0.14987 (6) | 0.66473 (5) | 0.33606 (2) | 0.03622 (13) |
| P | 0.01450 (6) | 0.58351 (4) | 0.22593 (2) | 0.02755 (11) |
| O2 | −0.1835 (2) | 0.78944 (16) | 0.36311 (8) | 0.0531 (5) |
| O3 | −0.2779 (2) | 0.58363 (18) | 0.31763 (9) | 0.0548 (4) |
| O1 | 0.0074 (2) | 0.45080 (12) | 0.25313 (7) | 0.0376 (3) |
| N2 | −0.1005 (2) | 0.61222 (17) | 0.16850 (8) | 0.0374 (4) |
| N1 | 0.19197 (19) | 0.61606 (16) | 0.20271 (8) | 0.0357 (4) |
| C16 | −0.2309 (3) | 0.7047 (3) | 0.16690 (14) | 0.0598 (7) |
| H16A | −0.2367 | 0.7506 | 0.2049 | 0.090* |
| H16B | −0.3268 | 0.6577 | 0.1601 | 0.090* |
| H16C | −0.2149 | 0.7666 | 0.1346 | 0.090* |
| C11 | −0.4106 (4) | 0.2282 (3) | 0.07992 (17) | 0.0756 (10) |
| H11 | −0.4817 | 0.1609 | 0.0724 | 0.091* |
| C10 | −0.3104 (4) | 0.2678 (3) | 0.03513 (15) | 0.0733 (9) |
| H10 | −0.3123 | 0.2269 | −0.0026 | 0.088* |
| C9 | −0.2056 (3) | 0.3697 (3) | 0.04626 (12) | 0.0551 (6) |
| H9 | −0.1402 | 0.3989 | 0.0154 | 0.066* |
| C14 | −0.1979 (2) | 0.4282 (2) | 0.10302 (9) | 0.0377 (4) |
| C15 | −0.0776 (3) | 0.5341 (2) | 0.11360 (10) | 0.0420 (5) |
| H15A | 0.0251 | 0.4935 | 0.1155 | 0.050* |
| H15B | −0.0780 | 0.5928 | 0.0789 | 0.050* |
| C7 | 0.2255 (3) | 0.7384 (2) | 0.17023 (13) | 0.0479 (6) |
| H7A | 0.2714 | 0.8007 | 0.1984 | 0.058* |

| | | | | |
|---|---|---|---|---|
| H7B | 0.1277 | 0.7753 | 0.1558 | 0.058* |
| C6 | 0.3355 (2) | 0.7211 (2) | 0.11683 (10) | 0.0370 (4) |
| C1 | 0.4198 (3) | 0.8292 (2) | 0.09625 (11) | 0.0451 (5) |
| H1 | 0.4106 | 0.9094 | 0.1161 | 0.054* |
| C2 | 0.5174 (3) | 0.8180 (3) | 0.04622 (12) | 0.0553 (6) |
| H2 | 0.5729 | 0.8907 | 0.0324 | 0.066* |
| C3 | 0.5322 (3) | 0.6990 (3) | 0.01694 (11) | 0.0621 (7) |
| H3 | 0.5980 | 0.6912 | −0.0165 | 0.074* |
| N3 | −0.0373 (2) | 0.69410 (14) | 0.27825 (7) | 0.0313 (3) |
| H | −0.0016 | 0.7726 | 0.2742 | 0.038* |
| C17 | −0.0341 (4) | 0.5731 (3) | 0.38565 (11) | 0.0583 (7) |
| H17A | 0.0536 | 0.6251 | 0.3986 | 0.087* |
| H17B | 0.0031 | 0.4958 | 0.3653 | 0.087* |
| H17C | −0.0952 | 0.5480 | 0.4203 | 0.087* |
| C8 | 0.3248 (3) | 0.5572 (3) | 0.23501 (12) | 0.0588 (7) |
| H8A | 0.2915 | 0.4778 | 0.2546 | 0.088* |
| H8B | 0.3631 | 0.6179 | 0.2649 | 0.088* |
| H8C | 0.4069 | 0.5375 | 0.2067 | 0.088* |
| C5 | 0.3510 (3) | 0.6022 (2) | 0.08697 (10) | 0.0448 (5) |
| H5 | 0.2952 | 0.5292 | 0.1002 | 0.054* |
| C4 | 0.4499 (3) | 0.5922 (3) | 0.03725 (11) | 0.0578 (6) |
| H4 | 0.4604 | 0.5120 | 0.0175 | 0.069* |
| C13 | −0.2991 (3) | 0.3855 (2) | 0.14752 (11) | 0.0478 (5) |
| H13 | −0.2951 | 0.4233 | 0.1859 | 0.057* |
| C12 | −0.4069 (3) | 0.2868 (3) | 0.13576 (15) | 0.0633 (8) |
| H12 | −0.4766 | 0.2604 | 0.1658 | 0.076* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S | 0.0438 (3) | 0.0249 (2) | 0.0400 (2) | −0.0002 (2) | 0.0118 (2) | 0.00027 (19) |
| P | 0.0334 (2) | 0.01673 (19) | 0.0325 (2) | −0.00014 (17) | 0.00382 (18) | −0.00090 (16) |
| O2 | 0.0683 (12) | 0.0342 (8) | 0.0568 (9) | 0.0053 (8) | 0.0255 (9) | −0.0081 (7) |
| O3 | 0.0429 (8) | 0.0435 (9) | 0.0780 (12) | −0.0137 (8) | 0.0150 (8) | −0.0002 (8) |
| O1 | 0.0544 (8) | 0.0169 (6) | 0.0414 (7) | −0.0007 (6) | 0.0042 (7) | −0.0001 (5) |
| N2 | 0.0398 (9) | 0.0332 (9) | 0.0393 (8) | 0.0046 (7) | −0.0017 (7) | −0.0013 (7) |
| N1 | 0.0336 (8) | 0.0301 (8) | 0.0433 (9) | 0.0012 (7) | 0.0082 (7) | −0.0015 (7) |
| C16 | 0.0598 (15) | 0.0479 (13) | 0.0715 (17) | 0.0193 (12) | −0.0217 (14) | −0.0054 (13) |
| C11 | 0.083 (2) | 0.0558 (17) | 0.088 (2) | −0.0198 (16) | −0.0378 (19) | 0.0022 (16) |
| C10 | 0.092 (2) | 0.0602 (17) | 0.0673 (18) | 0.0035 (17) | −0.0323 (18) | −0.0242 (15) |
| C9 | 0.0606 (15) | 0.0588 (15) | 0.0460 (12) | 0.0044 (12) | −0.0048 (11) | −0.0095 (11) |
| C14 | 0.0360 (10) | 0.0378 (10) | 0.0394 (10) | 0.0035 (9) | −0.0055 (8) | −0.0014 (8) |
| C15 | 0.0426 (11) | 0.0498 (12) | 0.0335 (10) | −0.0064 (10) | 0.0038 (9) | −0.0025 (9) |
| C7 | 0.0481 (12) | 0.0276 (10) | 0.0681 (15) | −0.0014 (9) | 0.0255 (12) | −0.0040 (10) |
| C6 | 0.0321 (10) | 0.0344 (10) | 0.0445 (11) | 0.0045 (8) | 0.0053 (9) | 0.0037 (8) |
| C1 | 0.0411 (11) | 0.0380 (11) | 0.0562 (13) | 0.0045 (10) | 0.0081 (10) | 0.0102 (10) |
| C2 | 0.0521 (13) | 0.0568 (14) | 0.0572 (14) | 0.0027 (12) | 0.0138 (12) | 0.0231 (12) |
| C3 | 0.0648 (17) | 0.0809 (19) | 0.0404 (12) | 0.0116 (15) | 0.0189 (12) | 0.0099 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N3 | 0.0405 (8) | 0.0157 (6) | 0.0376 (8) | −0.0018 (6) | 0.0083 (7) | −0.0012 (6) |
| C17 | 0.090 (2) | 0.0473 (13) | 0.0379 (11) | 0.0056 (14) | −0.0010 (12) | 0.0081 (10) |
| C8 | 0.0402 (12) | 0.0805 (19) | 0.0558 (14) | 0.0078 (13) | −0.0026 (11) | −0.0025 (13) |
| C5 | 0.0418 (11) | 0.0420 (12) | 0.0505 (12) | 0.0027 (10) | 0.0077 (10) | −0.0021 (9) |
| C4 | 0.0680 (16) | 0.0596 (16) | 0.0456 (12) | 0.0113 (13) | 0.0119 (11) | −0.0092 (12) |
| C13 | 0.0491 (12) | 0.0486 (13) | 0.0456 (12) | −0.0100 (10) | −0.0059 (9) | 0.0022 (10) |
| C12 | 0.0523 (15) | 0.0623 (17) | 0.0751 (18) | −0.0195 (13) | −0.0145 (13) | 0.0149 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S—O3 | 1.4287 (18) | C15—H15B | 0.9700 |
| S—O2 | 1.4317 (16) | C7—C6 | 1.516 (3) |
| S—N3 | 1.6236 (16) | C7—H7A | 0.9700 |
| S—C17 | 1.744 (3) | C7—H7B | 0.9700 |
| P—O1 | 1.4794 (13) | C6—C5 | 1.384 (3) |
| P—N2 | 1.6285 (18) | C6—C1 | 1.390 (3) |
| P—N1 | 1.6326 (17) | C1—C2 | 1.387 (3) |
| P—N3 | 1.6714 (15) | C1—H1 | 0.9300 |
| N2—C16 | 1.458 (3) | C2—C3 | 1.378 (4) |
| N2—C15 | 1.461 (3) | C2—H2 | 0.9300 |
| N1—C7 | 1.465 (3) | C3—C4 | 1.369 (4) |
| N1—C8 | 1.467 (3) | C3—H3 | 0.9300 |
| C16—H16A | 0.9600 | N3—H | 0.8600 |
| C16—H16B | 0.9600 | C17—H17A | 0.9600 |
| C16—H16C | 0.9600 | C17—H17B | 0.9600 |
| C11—C12 | 1.368 (5) | C17—H17C | 0.9600 |
| C11—C10 | 1.367 (5) | C8—H8A | 0.9600 |
| C11—H11 | 0.9300 | C8—H8B | 0.9600 |
| C10—C9 | 1.392 (4) | C8—H8C | 0.9600 |
| C10—H10 | 0.9300 | C5—C4 | 1.387 (3) |
| C9—C14 | 1.387 (3) | C5—H5 | 0.9300 |
| C9—H9 | 0.9300 | C4—H4 | 0.9300 |
| C14—C13 | 1.378 (3) | C13—C12 | 1.387 (4) |
| C14—C15 | 1.507 (3) | C13—H13 | 0.9300 |
| C15—H15A | 0.9700 | C12—H12 | 0.9300 |
| | | | |
| O3—S—O2 | 118.53 (12) | C6—C7—H7A | 108.8 |
| O3—S—N3 | 109.61 (10) | N1—C7—H7B | 108.8 |
| O2—S—N3 | 106.39 (9) | C6—C7—H7B | 108.8 |
| O3—S—C17 | 107.61 (13) | H7A—C7—H7B | 107.7 |
| O2—S—C17 | 109.08 (12) | C5—C6—C1 | 119.2 (2) |
| N3—S—C17 | 104.79 (12) | C5—C6—C7 | 121.98 (19) |
| O1—P—N2 | 117.02 (9) | C1—C6—C7 | 118.82 (19) |
| O1—P—N1 | 110.51 (9) | C2—C1—C6 | 120.3 (2) |
| N2—P—N1 | 106.20 (9) | C2—C1—H1 | 119.8 |
| O1—P—N3 | 108.94 (8) | C6—C1—H1 | 119.8 |
| N2—P—N3 | 104.84 (9) | C3—C2—C1 | 120.0 (2) |
| N1—P—N3 | 108.98 (8) | C3—C2—H2 | 120.0 |

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| C16—N2—C15 | 115.69 (19) | C1—C2—H2 | 120.0 |
| C16—N2—P | 126.49 (17) | C4—C3—C2 | 119.8 (2) |
| C15—N2—P | 117.76 (15) | C4—C3—H3 | 120.1 |
| C7—N1—C8 | 115.7 (2) | C2—C3—H3 | 120.1 |
| C7—N1—P | 120.48 (14) | S—N3—P | 125.05 (9) |
| C8—N1—P | 118.83 (16) | S—N3—H | 117.5 |
| N2—C16—H16A | 109.5 | P—N3—H | 117.5 |
| N2—C16—H16B | 109.5 | S—C17—H17A | 109.5 |
| H16A—C16—H16B | 109.5 | S—C17—H17B | 109.5 |
| N2—C16—H16C | 109.5 | H17A—C17—H17B | 109.5 |
| H16A—C16—H16C | 109.5 | S—C17—H17C | 109.5 |
| H16B—C16—H16C | 109.5 | H17A—C17—H17C | 109.5 |
| C12—C11—C10 | 120.5 (3) | H17B—C17—H17C | 109.5 |
| C12—C11—H11 | 119.8 | N1—C8—H8A | 109.5 |
| C10—C11—H11 | 119.8 | N1—C8—H8B | 109.5 |
| C11—C10—C9 | 119.6 (3) | H8A—C8—H8B | 109.5 |
| C11—C10—H10 | 120.2 | N1—C8—H8C | 109.5 |
| C9—C10—H10 | 120.2 | H8A—C8—H8C | 109.5 |
| C14—C9—C10 | 120.6 (3) | H8B—C8—H8C | 109.5 |
| C14—C9—H9 | 119.7 | C6—C5—C4 | 119.9 (2) |
| C10—C9—H9 | 119.7 | C6—C5—H5 | 120.1 |
| C13—C14—C9 | 118.5 (2) | C4—C5—H5 | 120.1 |
| C13—C14—C15 | 122.87 (19) | C3—C4—C5 | 120.8 (2) |
| C9—C14—C15 | 118.6 (2) | C3—C4—H4 | 119.6 |
| N2—C15—C14 | 115.23 (18) | C5—C4—H4 | 119.6 |
| N2—C15—H15A | 108.5 | C14—C13—C12 | 120.8 (2) |
| C14—C15—H15A | 108.5 | C14—C13—H13 | 119.6 |
| N2—C15—H15B | 108.5 | C12—C13—H13 | 119.6 |
| C14—C15—H15B | 108.5 | C11—C12—C13 | 119.9 (3) |
| H15A—C15—H15B | 107.5 | C11—C12—H12 | 120.0 |
| N1—C7—C6 | 113.73 (16) | C13—C12—H12 | 120.0 |
| N1—C7—H7A | 108.8 | | |

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| O1—P—N2—C16 | 114.6 (2) | P—N1—C7—C6 | −138.44 (18) |
| N1—P—N2—C16 | −121.5 (2) | N1—C7—C6—C5 | 24.7 (3) |
| N3—P—N2—C16 | −6.2 (2) | N1—C7—C6—C1 | −157.2 (2) |
| O1—P—N2—C15 | −62.24 (18) | C5—C6—C1—C2 | 0.3 (3) |
| N1—P—N2—C15 | 61.66 (17) | C7—C6—C1—C2 | −177.8 (2) |
| N3—P—N2—C15 | 176.96 (15) | C6—C1—C2—C3 | −0.5 (4) |
| O1—P—N1—C7 | 175.63 (16) | C1—C2—C3—C4 | 0.3 (4) |
| N2—P—N1—C7 | 47.76 (19) | O3—S—N3—P | −41.70 (16) |
| N3—P—N1—C7 | −64.70 (18) | O2—S—N3—P | −170.99 (13) |
| O1—P—N1—C8 | −30.5 (2) | C17—S—N3—P | 73.54 (16) |
| N2—P—N1—C8 | −158.39 (18) | O1—P—N3—S | −25.84 (16) |
| N3—P—N1—C8 | 89.15 (19) | N2—P—N3—S | 100.16 (13) |
| C12—C11—C10—C9 | −0.9 (5) | N1—P—N3—S | −146.48 (13) |
| C11—C10—C9—C14 | 2.4 (5) | C1—C6—C5—C4 | 0.1 (4) |
| C10—C9—C14—C13 | −1.7 (4) | C7—C6—C5—C4 | 178.2 (2) |

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| C10—C9—C14—C15 | 177.4 (2) | C2—C3—C4—C5 | 0.2 (4) |
| C16—N2—C15—C14 | −72.4 (3) | C6—C5—C4—C3 | −0.4 (4) |
| P—N2—C15—C14 | 104.8 (2) | C9—C14—C13—C12 | −0.3 (4) |
| C13—C14—C15—N2 | −15.1 (3) | C15—C14—C13—C12 | −179.4 (2) |
| C9—C14—C15—N2 | 165.9 (2) | C10—C11—C12—C13 | −1.2 (5) |
| C8—N1—C7—C6 | 66.9 (3) | C14—C13—C12—C11 | 1.8 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H···O1$^{i}$ | 0.86 | 1.91 | 2.7152 (19) | 155 |

Symmetry code: (i) −*x*, *y*+1/2, −*z*+1/2.