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3,5-Bis[(dimethylamino)methyl]-1-nitro-4-(trimethylsilyl)benzene

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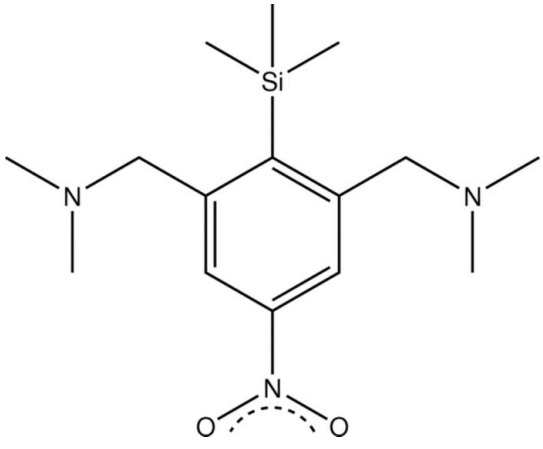
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.004 Å; R factor = 0.054; wR factor = 0.148; data-to-parameter ratio = 16.8.

The title compound, $C_{15}H_{27}N_3O_2Si$, which is an NCN {NCN = 2,6-bis[(dimethylamino)methyl]phenyl} pincer ligand, nitro-substituted in the *para* position, features intramolecular C—H···N and intermolecular C—H···O hydrogen-bond contacts producing dimeric units. The Si atoms are essentially tetrahedral with normal bond lengths and angles. The nitro groups are in the planes of the corresponding benzene rings and the amino groups are mutually *trans*. Despite the presence of four independent molecules in the asymmetric unit, all of which have essentially the same geometry, there is no pseudo-translational symmetry present.

Related literature

The synthesis of the title compound, (I), is described by Slagt *et al.* (2004). For related structures, see: Delugeard & Messager (1975); Steenwinkel *et al.* (1997). For related literature, see: Altomare *et al.* (1999); Mackay (1984).



Experimental

Crystal data

$C_{15}H_{27}N_3O_2Si$
M_r = 309.49
Triclinic, $P\overline{1}$
a = 14.2353 (2) Å
b = 16.1402 (2) Å
c = 17.1387 (3) Å
α = 75.0826 (7)°
β = 73.6940 (8)°
γ = 73.5679 (9)°
V = 3556.63 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 150 (2) K
0.38 × 0.20 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
37090 measured reflections
13201 independent reflections
9550 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.148
S = 1.04
13201 reflections
785 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C101—H10A···O24	0.99	2.66	3.411 (3)	133
C102—H10C···O23	0.99	2.70	3.452 (3)	133
C103—H10E···O22	0.99	2.63	3.402 (3)	135
C104—H10G···O21	0.99	2.59	3.390 (3)	138
C51—H51···N21	0.95	2.39	2.753 (3)	102
C52—H52···N22	0.95	2.41	2.754 (3)	101
C53—H53···N23	0.95	2.43	2.764 (3)	101
C54—H54···N24	0.95	2.42	2.755 (4)	101

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: manual editing of *SHELXL97* (Sheldrick, 1997) output.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2379).

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supplementary materials

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3,5-Bis[(dimethylamino)methyl]-1-nitro-4-(trimethylsilyl)benzene

L. S. von Chrzanowski, M. Lutz, A. L. Spek, M. Q. Slagt and G. van Koten

Comment

Organometallic transition metal complexes based on the NCN pincer ligand (NCN = 2,6-bis[(dimethylamino)methyl]phenyl) are found in numerous applications, e.g. in catalysis. Variations of the para substituent of the NCN pincer ligand have drawn interest for several reasons. The electronic properties can be fine-tuned by choosing the appropriate substituent and result in a variation of the catalytic, spectroscopic and diagnostic properties. Therefore we report here the structure of the title compound, (I), which is a nitro functionilized NCN pincer ligand in the para position. The asymmetric unit of (I) consist of four independent $C_{15}H_{27}N_3O_2Si$ molecules (Fig. 1). All four molecules have essentially the same geometry as can be seen in Fig. 2 in a quaternion fit (Mackay, 1984).

The coordination geometries of the Si atoms are slightly distorted tetrahedral, with the largest deviation for the angles C13X-SiX-C15X (X = 1, 2, 3 and 4) of 7° from the ideal value of 109°. The Si distances to the methyl groups vary between 1.864 (3) and 1.887 (3) Å, while the Si—C distances to the aromatic ring are longer [1.916 (2) - 1.922 (2) Å]. Similar geometric parameters were found in $[(Me_3Si)_2\{C_6(CH_2NMe_2)_4\}]$ reported by Steenwinkel *et al.* (1997). The deviation of the Si atom of the $SiMe_3$ group with respect to the plane of the aromatic ring varies between 0.264 (1) and 0.288 (1) Å.

The nitro groups are coplanar with the phenyl ring with torsion angles between -1.3 (3) and 5.5 (3) °. The N—O distances range of the nitro group is 1.216 (3) to 1.234 (3) Å, the O—N—O angles vary between 123.1 (2) to 123.7 (2)° and the C—N—O angles lay between 117.7 (2) and 118.9 (2)°. These geometric parameters agree well with those found in *m*-nitro-*N*,*N*-dimethylaniline (Delugeard & Messager, 1975). The N atoms of the nitro group are in the plane of the aromatic ring, with a deviation of 0.057 (3) to 0.073 (2) Å.

The torsion angles C9X—N1X—C7X—C2X (-179.8 (2) - -177.6 (2)°) and C12X—N2X—C10X—C6X (158.5 (3) - 165.9 (2)°) of the $N(CH_3)_2$ groups result in a non crystallographic C_S symmetry, with N atoms mutually trans. The N atoms of the $N(CH_3)_2$ groups show the largest difference with respect to the plane of the aromatic ring, N1X with 1.388 (3) to 1.469 (2) and N2X with 0.712 (2) to 0.816 (2) Å.

The molecules have acute intramolecular C—H···N contacts with H···N distances between 2.39 and 2.43 Å. The geometry of the involved N2X atoms are tetrahedral, the C—N—C angles vary between 110.0 (2) and 111.4 (2)°. The free electron pairs of the N atoms are pointing in the direction of the H atoms and therefore we assume the presence of C—H···N hydrogen bonds. Intermolecular C—H···O contacts occur between H10Y (Y = A, C, E and G) and O2X with a range of 2.63 and 2.70Å and connect two molecules into dimeric structures (Fig. 2), respectively (Table 1).

Despite the presence of four independent molecules there is no pseudo- translational symmetry present. The corresponding $<|E^2-1|>$ value of 0.985 is close to the expected value of 0.968 for a centrosymmetric structure (SHELXS-97, Sheldrick, 1997). An additional test on pseudo-translational symmetry as implemented in the program SIR-97 (Altomare *et al.*, 1999) also did not give an indication for pseudo-translational symmetry. The analyses of the normal probability distribution of equivalent bond distances shows that all distances are distributed normally, except three outliers. These outliers belong to

the substituents of N24. The corresponding C atoms (C104, C114 and C124) also show rather high anisotropic displacement parameters, which are the reason for the anomalous C—N bonds.

Experimental

Compound(I) was prepared according to a literature procedure by Slagt *et al.* (2004). Yellow crystals for data collection were obtained by recrystallization from petroleum ether (bp. 333 - 353 K).

Refinement

All the hydrogen atoms were introduced in geometrically idealized positions (C—H = 0.95-0.99 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C). C114 and C124 were restrained to approximate to isotropic behavior. The highest difference peak is 0.88Å from H11L and the deepest difference hole is 0.96Å from N24.

Figures

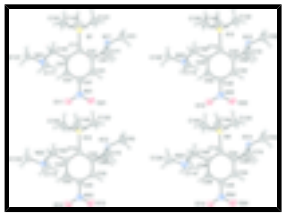

Fig. 1. : Displacement ellipsoid plot and atomic numbering scheme of the four independent molecules of (I). Molecules are shown independently using the same orientation. Ellipsoids are drawn at the 50% probability level (arbitrary spheres for the H atoms).

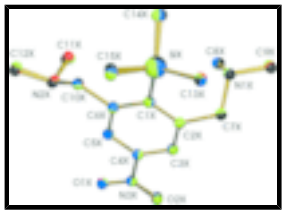

Fig. 2. : Quaternion fit of the four independent molecules of (I). Black atoms represent molecule 1 (X = 1), blue atoms molecule 2 (X = 2), green atoms molecule 3 (X = 3) and red atoms molecule 4 (X = 4).

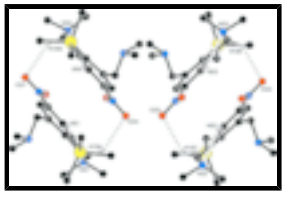

Fig. 3. : Hydrogen bond interactions in (I), viewed along the crystallographic [10$\bar{1}$] direction. A non crystallographic twofold axis can be seen vertically. The C—H···O and C—H···N contacts are shown with dashed lines.

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Crystal data

$C_{15}H_{27}N_3O_2Si$	$Z = 8$
$M_r = 309.49$	$F_{000} = 1344$
Triclinic, $P\bar{1}$	$D_x = 1.156$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 14.2353$ (2) Å	Cell parameters from 71004 reflections
$b = 16.1402$ (2) Å	$\theta = 1.0$–27.5º

c = 17.1387 (3) Å	μ = 0.14 mm^{-1}
α = 75.0826 (7)º	T = 150 (2) K
β = 73.6940 (8)º	Plate, yellow
γ = 73.5679 (9)º	0.38 × 0.20 × 0.10 mm
V = 3556.63 (9) Å^3	

Data collection

Nonius KappaCCD diffractometer	9550 reflections with $I > 2\sigma(I)$
Radiation source: rotating anode	R_{int} = 0.042
Monochromator: graphite	θ_{max} = 25.5º
T = 150(2) K	θ_{min} = 1.5º
φ and ω scans	h = −15→17
Absorption correction: none	k = −17→19
37090 measured reflections	l = −20→20
13201 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.054	$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2 + 1.78P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.148	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.04	$\Delta\rho_{max}$ = 1.23 e Å^{-3}
13201 reflections	$\Delta\rho_{min}$ = −0.49 e Å^{-3}
785 parameters	Extinction correction: none
12 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Si1	0.19786 (5)	0.34606 (5)	0.51366 (4)	0.03571 (18)
O11	0.08556 (16)	0.14027 (14)	0.91934 (12)	0.0540 (5)
O21	0.21565 (15)	0.04222 (12)	0.87465 (12)	0.0489 (5)
N11	0.27173 (14)	0.13914 (14)	0.50287 (13)	0.0343 (5)
N21	−0.07639 (15)	0.37310 (13)	0.73811 (12)	0.0332 (5)
N31	0.15340 (18)	0.11250 (14)	0.86384 (14)	0.0388 (5)
C11	0.17791 (17)	0.26834 (16)	0.61963 (15)	0.0307 (5)
C21	0.24341 (17)	0.18426 (16)	0.63599 (15)	0.0319 (5)
C31	0.23543 (18)	0.13435 (16)	0.71567 (15)	0.0332 (6)
H31	0.2810	0.0791	0.7262	0.040*
C41	0.16114 (18)	0.16533 (16)	0.77939 (15)	0.0318 (6)
C51	0.09055 (18)	0.24305 (15)	0.76585 (15)	0.0311 (5)
H51	0.0376	0.2615	0.8102	0.037*
C61	0.09812 (17)	0.29399 (15)	0.68619 (15)	0.0294 (5)
C71	0.31902 (18)	0.14127 (18)	0.56785 (16)	0.0378 (6)
H71A	0.3727	0.1743	0.5432	0.045*
H71B	0.3504	0.0804	0.5918	0.045*
C81	0.18901 (19)	0.09441 (17)	0.53594 (17)	0.0394 (6)
H81A	0.1598	0.0939	0.4907	0.059*
H81B	0.1375	0.1255	0.5766	0.059*
H81C	0.2141	0.0337	0.5627	0.059*
C91	0.3470 (2)	0.0949 (2)	0.43974 (19)	0.0515 (7)
H91A	0.3739	0.0340	0.4649	0.077*
H91B	0.4018	0.1259	0.4166	0.077*
H91C	0.3158	0.0951	0.3955	0.077*
C101	0.01617 (18)	0.37804 (16)	0.67543 (15)	0.0337 (6)
H10A	0.0408	0.4284	0.6784	0.040*
H10B	0.0020	0.3889	0.6199	0.040*
C111	−0.1303 (2)	0.31734 (18)	0.72233 (18)	0.0454 (7)
H11A	−0.1910	0.3138	0.7665	0.068*
H11B	−0.0871	0.2582	0.7210	0.068*
H11C	−0.1492	0.3423	0.6689	0.068*
C121	−0.1409 (2)	0.46004 (18)	0.74324 (18)	0.0501 (7)
H12A	−0.1638	0.4856	0.6915	0.075*
H12B	−0.1032	0.4979	0.7520	0.075*
H12C	−0.1991	0.4553	0.7897	0.075*
C131	0.3315 (2)	0.3301 (2)	0.45396 (18)	0.0516 (8)
H13A	0.3499	0.2769	0.4305	0.077*
H13B	0.3755	0.3239	0.4910	0.077*
H13C	0.3392	0.3812	0.4091	0.077*
C141	0.1148 (2)	0.33701 (19)	0.45041 (17)	0.0445 (7)
H14A	0.1260	0.3768	0.3965	0.067*
H14B	0.0443	0.3532	0.4795	0.067*
H14C	0.1304	0.2763	0.4421	0.067*
C151	0.1683 (2)	0.46361 (18)	0.52766 (18)	0.0508 (7)

H15A	0.1961	0.5002	0.4758	0.076*
H15B	0.1982	0.4662	0.5717	0.076*
H15C	0.0953	0.4855	0.5428	0.076*
Si2	−0.05642 (5)	0.80583 (4)	0.77250 (4)	0.03175 (17)
O22	0.39778 (13)	0.91426 (12)	0.68916 (13)	0.0487 (5)
O12	0.41794 (14)	0.86254 (15)	0.57979 (13)	0.0551 (5)
N12	−0.05073 (15)	0.98467 (13)	0.82475 (12)	0.0334 (5)
N22	0.14627 (15)	0.81032 (13)	0.50733 (12)	0.0331 (5)
N32	0.36744 (16)	0.88291 (14)	0.64502 (15)	0.0384 (5)
C12	0.06978 (17)	0.84025 (15)	0.72870 (14)	0.0283 (5)
C22	0.10688 (18)	0.88324 (15)	0.77254 (15)	0.0305 (5)
C32	0.20409 (18)	0.89615 (15)	0.74547 (15)	0.0331 (6)
H32	0.2293	0.9229	0.7762	0.040*
C42	0.26385 (17)	0.86969 (15)	0.67344 (16)	0.0315 (5)
C52	0.22868 (17)	0.83465 (15)	0.62492 (15)	0.0300 (5)
H52	0.2700	0.8201	0.5740	0.036*
C62	0.13120 (17)	0.82098 (14)	0.65202 (15)	0.0282 (5)
C72	0.04166 (19)	0.92473 (17)	0.84474 (15)	0.0357 (6)
H72A	0.0240	0.8779	0.8926	0.043*
H72B	0.0799	0.9577	0.8609	0.043*
C82	−0.02987 (19)	1.05283 (16)	0.75183 (17)	0.0385 (6)
H82A	0.0102	1.0877	0.7621	0.058*
H82B	−0.0934	1.0913	0.7404	0.058*
H82C	0.0076	1.0253	0.7041	0.058*
C92	−0.1088 (2)	1.0258 (2)	0.89534 (18)	0.0492 (7)
H92A	−0.1722	1.0636	0.8829	0.074*
H92B	−0.0702	1.0613	0.9063	0.074*
H92C	−0.1232	0.9800	0.9442	0.074*
C102	0.09651 (17)	0.78482 (16)	0.59340 (14)	0.0309 (5)
H10C	0.1106	0.7198	0.6089	0.037*
H10D	0.0230	0.8069	0.5997	0.037*
C112	0.1096 (2)	0.90263 (18)	0.47511 (18)	0.0483 (7)
H11D	0.0382	0.9136	0.4752	0.072*
H11E	0.1477	0.9184	0.4183	0.072*
H11F	0.1180	0.9384	0.5100	0.072*
C122	0.1355 (2)	0.7562 (2)	0.45584 (17)	0.0469 (7)
H12D	0.1763	0.7700	0.3998	0.070*
H12E	0.0648	0.7683	0.4536	0.070*
H12F	0.1582	0.6939	0.4795	0.070*
C132	−0.0967 (2)	0.78689 (18)	0.88807 (16)	0.0456 (7)
H13D	−0.1519	0.7563	0.9065	0.068*
H13E	−0.1195	0.8436	0.9061	0.068*
H13F	−0.0399	0.7509	0.9122	0.068*
C142	−0.15694 (19)	0.88781 (18)	0.72455 (17)	0.0425 (7)
H14D	−0.1676	0.9447	0.7400	0.064*
H14E	−0.2196	0.8672	0.7444	0.064*
H14F	−0.1363	0.8944	0.6641	0.064*
C152	−0.0437 (2)	0.69426 (18)	0.75079 (18)	0.0459 (7)
H15D	−0.1002	0.6693	0.7862	0.069*

H15E	0.0195	0.6553	0.7623	0.069*
H15F	−0.0439	0.7000	0.6925	0.069*
Si3	0.29048 (5)	0.70281 (5)	0.98179 (4)	0.03332 (17)
O13	0.41790 (15)	0.64199 (14)	0.58179 (12)	0.0546 (5)
O23	0.28075 (15)	0.59530 (13)	0.62388 (11)	0.0467 (5)
N13	0.22553 (15)	0.51868 (13)	0.99528 (12)	0.0340 (5)
N23	0.57115 (15)	0.70262 (14)	0.76667 (13)	0.0377 (5)
N33	0.34566 (17)	0.62428 (14)	0.63587 (13)	0.0368 (5)
C13	0.31410 (17)	0.66755 (15)	0.87812 (14)	0.0283 (5)
C23	0.25061 (17)	0.62266 (15)	0.86245 (15)	0.0303 (5)
C33	0.26030 (18)	0.60985 (15)	0.78295 (15)	0.0324 (6)
H33	0.2153	0.5825	0.7724	0.039*
C43	0.33587 (18)	0.63730 (15)	0.71989 (14)	0.0303 (5)
C53	0.40531 (18)	0.67382 (15)	0.73310 (15)	0.0302 (5)
H53	0.4593	0.6887	0.6892	0.036*
C63	0.39484 (17)	0.68850 (15)	0.81224 (14)	0.0278 (5)
C73	0.17633 (18)	0.57911 (17)	0.93075 (15)	0.0351 (6)
H73A	0.1219	0.6248	0.9557	0.042*
H73B	0.1457	0.5461	0.9071	0.042*
C83	0.3087 (2)	0.45113 (17)	0.96122 (17)	0.0409 (6)
H83A	0.2832	0.4168	0.9356	0.061*
H83B	0.3396	0.4120	1.0058	0.061*
H83C	0.3589	0.4793	0.9194	0.061*
C93	0.1520 (2)	0.47654 (19)	1.05929 (17)	0.0475 (7)
H93A	0.1844	0.4380	1.1033	0.071*
H93B	0.1257	0.4416	1.0349	0.071*
H93C	0.0967	0.5218	1.0825	0.071*
C103	0.47548 (17)	0.72712 (16)	0.82299 (15)	0.0316 (5)
H10E	0.4531	0.7921	0.8133	0.038*
H10F	0.4841	0.7064	0.8807	0.038*
C113	0.6176 (2)	0.6108 (2)	0.7890 (2)	0.0577 (8)
H11G	0.5715	0.5749	0.7908	0.087*
H11H	0.6330	0.5994	0.8435	0.087*
H11I	0.6798	0.5957	0.7477	0.087*
C123	0.6386 (2)	0.7573 (2)	0.7638 (2)	0.0598 (9)
H12G	0.6570	0.7439	0.8174	0.090*
H12H	0.6047	0.8195	0.7517	0.090*
H12I	0.6994	0.7451	0.7203	0.090*
C133	0.1578 (2)	0.71583 (19)	1.04220 (17)	0.0451 (7)
H13G	0.1481	0.7474	1.0867	0.068*
H13H	0.1430	0.6576	1.0663	0.068*
H13I	0.1125	0.7493	1.0054	0.068*
C143	0.3769 (2)	0.62534 (19)	1.04663 (17)	0.0470 (7)
H14G	0.3601	0.5675	1.0630	0.070*
H14H	0.3694	0.6482	1.0963	0.070*
H14I	0.4465	0.6196	1.0146	0.070*
C153	0.3102 (2)	0.81781 (19)	0.96185 (19)	0.0515 (7)
H15G	0.2843	0.8409	1.0133	0.077*
H15H	0.2744	0.8558	0.9197	0.077*

H15I	0.3821	0.8165	0.9422	0.077*
Si4	0.55029 (5)	0.15980 (5)	0.72471 (4)	0.03316 (17)
O14	0.08172 (14)	0.36777 (13)	0.91013 (13)	0.0543 (5)
O24	0.10430 (13)	0.46304 (12)	0.79620 (13)	0.0485 (5)
N14	0.55441 (15)	0.36854 (13)	0.66671 (12)	0.0326 (5)
N24	0.3467 (2)	0.1327 (2)	0.98601 (16)	0.0700 (8)
N34	0.13342 (15)	0.39411 (14)	0.84303 (15)	0.0379 (5)
C14	0.42679 (17)	0.23832 (15)	0.76472 (15)	0.0293 (5)
C24	0.39319 (17)	0.32353 (16)	0.71871 (14)	0.0300 (5)
C34	0.29717 (18)	0.37357 (16)	0.74374 (15)	0.0330 (6)
H34	0.2743	0.4291	0.7110	0.040*
C44	0.23527 (17)	0.34188 (15)	0.81653 (15)	0.0310 (5)
C54	0.26766 (17)	0.26353 (16)	0.86741 (15)	0.0312 (5)
H54	0.2255	0.2448	0.9191	0.037*
C64	0.36321 (16)	0.21212 (15)	0.84199 (15)	0.0280 (5)
C74	0.46169 (18)	0.36776 (17)	0.64528 (15)	0.0348 (6)
H74A	0.4789	0.3361	0.5990	0.042*
H74B	0.4262	0.4290	0.6266	0.042*
C84	0.5334 (2)	0.41329 (18)	0.73570 (16)	0.0398 (6)
H84A	0.5968	0.4130	0.7478	0.060*
H84B	0.4927	0.3827	0.7847	0.060*
H84C	0.4965	0.4742	0.7209	0.060*
C94	0.6186 (2)	0.4121 (2)	0.59433 (17)	0.0471 (7)
H94A	0.5835	0.4732	0.5779	0.071*
H94B	0.6340	0.3811	0.5484	0.071*
H94C	0.6812	0.4110	0.6083	0.071*
C104	0.39355 (18)	0.12733 (17)	0.90208 (16)	0.0369 (6)
H10G	0.3757	0.0789	0.8880	0.044*
H10H	0.4674	0.1129	0.8955	0.044*
C114	0.3908 (4)	0.1798 (3)	1.0148 (3)	0.0974 (13)
H11J	0.4618	0.1506	1.0119	0.146*
H11K	0.3568	0.1836	1.0725	0.146*
H11L	0.3856	0.2393	0.9809	0.146*
C124	0.3456 (3)	0.0442 (3)	1.0387 (2)	0.0873 (12)
H12J	0.4145	0.0123	1.0421	0.131*
H12K	0.3163	0.0114	1.0145	0.131*
H12L	0.3052	0.0503	1.0945	0.131*
C134	0.5957 (2)	0.1800 (2)	0.60985 (17)	0.0481 (7)
H13J	0.6220	0.2335	0.5914	0.072*
H13K	0.5399	0.1874	0.5839	0.072*
H13L	0.6492	0.1298	0.5938	0.072*
C144	0.65055 (19)	0.16092 (19)	0.77505 (18)	0.0446 (7)
H14J	0.7103	0.1151	0.7595	0.067*
H14K	0.6261	0.1497	0.8354	0.067*
H14L	0.6678	0.2186	0.7567	0.067*
C154	0.5303 (2)	0.04458 (18)	0.74791 (19)	0.0509 (7)
H15J	0.4659	0.0465	0.7367	0.076*
H15K	0.5299	0.0185	0.8063	0.076*
H15L	0.5848	0.0088	0.7128	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0380 (4)	0.0410 (4)	0.0310 (4)	−0.0191 (3)	−0.0046 (3)	−0.0041 (3)
O11	0.0621 (13)	0.0559 (13)	0.0321 (11)	−0.0048 (11)	−0.0079 (10)	−0.0004 (10)
O21	0.0582 (12)	0.0401 (11)	0.0489 (12)	−0.0028 (10)	−0.0286 (10)	−0.0006 (9)
N11	0.0275 (10)	0.0430 (12)	0.0342 (12)	−0.0098 (9)	−0.0029 (9)	−0.0132 (10)
N21	0.0373 (11)	0.0282 (11)	0.0312 (12)	−0.0012 (9)	−0.0060 (9)	−0.0092 (9)
N31	0.0481 (13)	0.0372 (13)	0.0369 (13)	−0.0120 (11)	−0.0216 (12)	−0.0015 (10)
C11	0.0322 (13)	0.0346 (14)	0.0317 (14)	−0.0121 (11)	−0.0096 (11)	−0.0094 (11)
C21	0.0254 (12)	0.0385 (14)	0.0366 (14)	−0.0102 (11)	−0.0087 (11)	−0.0105 (11)
C31	0.0308 (13)	0.0340 (14)	0.0395 (15)	−0.0051 (11)	−0.0163 (12)	−0.0084 (11)
C41	0.0378 (13)	0.0337 (14)	0.0299 (14)	−0.0126 (11)	−0.0150 (11)	−0.0034 (11)
C51	0.0345 (13)	0.0330 (13)	0.0295 (14)	−0.0098 (11)	−0.0095 (11)	−0.0076 (11)
C61	0.0340 (13)	0.0284 (13)	0.0303 (13)	−0.0096 (10)	−0.0102 (11)	−0.0072 (10)
C71	0.0267 (13)	0.0450 (16)	0.0435 (16)	−0.0061 (11)	−0.0090 (12)	−0.0128 (12)
C81	0.0428 (15)	0.0392 (15)	0.0421 (16)	−0.0166 (12)	−0.0125 (13)	−0.0067 (12)
C91	0.0441 (16)	0.062 (2)	0.0482 (18)	−0.0079 (14)	−0.0031 (14)	−0.0235 (15)
C101	0.0411 (14)	0.0317 (14)	0.0269 (13)	−0.0072 (11)	−0.0072 (11)	−0.0050 (11)
C111	0.0388 (15)	0.0434 (16)	0.0541 (18)	−0.0070 (13)	−0.0129 (14)	−0.0093 (14)
C121	0.0572 (18)	0.0376 (16)	0.0433 (17)	0.0029 (13)	−0.0026 (14)	−0.0117 (13)
C131	0.0492 (17)	0.0601 (19)	0.0486 (18)	−0.0311 (15)	0.0033 (14)	−0.0107 (15)
C141	0.0523 (17)	0.0473 (17)	0.0373 (16)	−0.0223 (14)	−0.0152 (13)	0.0040 (13)
C151	0.0631 (19)	0.0432 (17)	0.0440 (17)	−0.0240 (15)	−0.0045 (15)	0.0000 (13)
Si2	0.0319 (4)	0.0326 (4)	0.0283 (4)	−0.0095 (3)	−0.0046 (3)	−0.0017 (3)
O22	0.0396 (10)	0.0519 (12)	0.0664 (14)	−0.0135 (9)	−0.0222 (10)	−0.0166 (10)
O12	0.0357 (10)	0.0824 (16)	0.0531 (13)	−0.0224 (10)	0.0006 (10)	−0.0249 (12)
N12	0.0353 (11)	0.0333 (12)	0.0296 (12)	−0.0020 (9)	−0.0073 (9)	−0.0090 (9)
N22	0.0342 (11)	0.0376 (12)	0.0294 (11)	−0.0125 (9)	−0.0013 (9)	−0.0114 (9)
N32	0.0315 (11)	0.0357 (12)	0.0510 (15)	−0.0062 (10)	−0.0185 (11)	−0.0047 (11)
C12	0.0300 (12)	0.0249 (12)	0.0281 (13)	−0.0017 (10)	−0.0115 (10)	−0.0017 (10)
C22	0.0353 (13)	0.0277 (13)	0.0280 (13)	−0.0026 (10)	−0.0144 (11)	−0.0017 (10)
C32	0.0362 (13)	0.0307 (13)	0.0360 (15)	−0.0039 (11)	−0.0189 (12)	−0.0051 (11)
C42	0.0277 (12)	0.0267 (13)	0.0398 (15)	−0.0036 (10)	−0.0135 (11)	−0.0020 (11)
C52	0.0271 (12)	0.0268 (13)	0.0341 (14)	−0.0024 (10)	−0.0073 (11)	−0.0062 (10)
C62	0.0288 (12)	0.0226 (12)	0.0329 (14)	−0.0037 (10)	−0.0100 (11)	−0.0037 (10)
C72	0.0423 (14)	0.0388 (15)	0.0291 (14)	−0.0077 (12)	−0.0133 (12)	−0.0075 (11)
C82	0.0389 (14)	0.0310 (14)	0.0458 (16)	−0.0062 (11)	−0.0147 (12)	−0.0038 (12)
C92	0.0500 (17)	0.0538 (18)	0.0417 (17)	−0.0023 (14)	−0.0064 (14)	−0.0200 (14)
C102	0.0283 (12)	0.0336 (14)	0.0324 (14)	−0.0086 (10)	−0.0036 (11)	−0.0109 (11)
C112	0.0608 (18)	0.0467 (17)	0.0439 (17)	−0.0204 (14)	−0.0210 (15)	−0.0009 (13)
C122	0.0471 (16)	0.0626 (19)	0.0385 (16)	−0.0221 (14)	0.0015 (13)	−0.0243 (14)
C132	0.0572 (17)	0.0414 (16)	0.0322 (15)	−0.0141 (14)	−0.0022 (13)	−0.0023 (12)
C142	0.0322 (14)	0.0485 (17)	0.0450 (17)	−0.0123 (12)	−0.0088 (12)	−0.0023 (13)
C152	0.0505 (16)	0.0435 (16)	0.0461 (17)	−0.0231 (14)	−0.0034 (14)	−0.0072 (13)
Si3	0.0346 (4)	0.0365 (4)	0.0263 (4)	−0.0035 (3)	−0.0043 (3)	−0.0095 (3)
O13	0.0582 (13)	0.0804 (15)	0.0296 (11)	−0.0283 (12)	0.0004 (10)	−0.0157 (10)

O23	0.0571 (12)	0.0539 (12)	0.0385 (11)	−0.0176 (10)	−0.0197 (9)	−0.0101 (9)
N13	0.0325 (11)	0.0365 (12)	0.0299 (12)	−0.0085 (9)	−0.0025 (9)	−0.0052 (9)
N23	0.0349 (11)	0.0464 (13)	0.0340 (12)	−0.0130 (10)	−0.0010 (10)	−0.0147 (10)
N33	0.0446 (13)	0.0355 (12)	0.0320 (12)	−0.0061 (10)	−0.0147 (11)	−0.0060 (10)
C13	0.0274 (12)	0.0260 (12)	0.0265 (13)	0.0008 (10)	−0.0069 (10)	−0.0034 (10)
C23	0.0264 (12)	0.0306 (13)	0.0314 (14)	−0.0008 (10)	−0.0090 (10)	−0.0051 (10)
C33	0.0323 (13)	0.0307 (13)	0.0351 (15)	−0.0036 (11)	−0.0133 (11)	−0.0056 (11)
C43	0.0359 (13)	0.0274 (13)	0.0263 (13)	−0.0025 (10)	−0.0106 (11)	−0.0043 (10)
C53	0.0346 (13)	0.0256 (12)	0.0264 (13)	−0.0040 (10)	−0.0061 (11)	−0.0024 (10)
C63	0.0316 (12)	0.0236 (12)	0.0259 (13)	−0.0018 (10)	−0.0081 (10)	−0.0040 (10)
C73	0.0286 (13)	0.0400 (15)	0.0355 (15)	−0.0058 (11)	−0.0069 (11)	−0.0078 (12)
C83	0.0457 (15)	0.0354 (15)	0.0400 (16)	−0.0045 (12)	−0.0100 (13)	−0.0095 (12)
C93	0.0466 (16)	0.0546 (18)	0.0372 (16)	−0.0215 (14)	−0.0006 (13)	−0.0002 (13)
C103	0.0367 (13)	0.0303 (13)	0.0265 (13)	−0.0086 (11)	−0.0032 (11)	−0.0066 (10)
C113	0.0454 (17)	0.060 (2)	0.073 (2)	0.0055 (15)	−0.0229 (16)	−0.0304 (17)
C123	0.0517 (18)	0.088 (2)	0.0499 (19)	−0.0394 (18)	0.0070 (15)	−0.0251 (17)
C133	0.0449 (16)	0.0478 (17)	0.0378 (16)	−0.0039 (13)	−0.0006 (13)	−0.0165 (13)
C143	0.0492 (16)	0.0581 (18)	0.0330 (15)	−0.0063 (14)	−0.0146 (13)	−0.0084 (13)
C153	0.0602 (19)	0.0467 (17)	0.0481 (18)	−0.0135 (15)	0.0026 (15)	−0.0244 (14)
Si4	0.0293 (4)	0.0376 (4)	0.0333 (4)	−0.0046 (3)	−0.0051 (3)	−0.0135 (3)
O14	0.0360 (10)	0.0555 (13)	0.0556 (14)	−0.0011 (9)	0.0036 (10)	−0.0090 (11)
O24	0.0369 (10)	0.0397 (11)	0.0669 (14)	0.0007 (9)	−0.0191 (10)	−0.0091 (10)
N14	0.0347 (11)	0.0387 (12)	0.0258 (11)	−0.0130 (9)	−0.0053 (9)	−0.0054 (9)
N24	0.0632 (17)	0.0716 (19)	0.0392 (16)	0.0179 (15)	−0.0012 (13)	0.0031 (14)
N34	0.0301 (11)	0.0351 (13)	0.0518 (15)	−0.0024 (10)	−0.0149 (11)	−0.0133 (11)
C14	0.0270 (12)	0.0335 (13)	0.0325 (14)	−0.0093 (10)	−0.0089 (10)	−0.0103 (11)
C24	0.0315 (13)	0.0350 (14)	0.0278 (13)	−0.0097 (11)	−0.0115 (10)	−0.0058 (10)
C34	0.0342 (13)	0.0318 (13)	0.0368 (15)	−0.0064 (11)	−0.0161 (12)	−0.0056 (11)
C44	0.0277 (12)	0.0302 (13)	0.0397 (15)	−0.0056 (10)	−0.0121 (11)	−0.0108 (11)
C54	0.0283 (12)	0.0350 (14)	0.0329 (14)	−0.0110 (11)	−0.0042 (11)	−0.0099 (11)
C64	0.0257 (12)	0.0288 (13)	0.0324 (14)	−0.0080 (10)	−0.0080 (10)	−0.0074 (10)
C74	0.0390 (14)	0.0386 (15)	0.0274 (14)	−0.0102 (11)	−0.0108 (11)	−0.0019 (11)
C84	0.0429 (15)	0.0411 (15)	0.0408 (16)	−0.0109 (12)	−0.0107 (13)	−0.0142 (12)
C94	0.0455 (16)	0.0554 (18)	0.0383 (16)	−0.0216 (14)	−0.0023 (13)	−0.0021 (14)
C104	0.0302 (13)	0.0355 (14)	0.0390 (16)	−0.0069 (11)	−0.0051 (11)	−0.0007 (12)
C114	0.105 (2)	0.097 (2)	0.085 (2)	−0.0003 (16)	−0.0282 (16)	−0.0263 (16)
C124	0.0762 (18)	0.0835 (18)	0.0721 (18)	−0.0036 (15)	−0.0071 (15)	0.0102 (15)
C134	0.0480 (16)	0.0537 (18)	0.0416 (17)	−0.0070 (14)	−0.0013 (13)	−0.0222 (14)
C144	0.0299 (13)	0.0532 (17)	0.0490 (17)	−0.0031 (12)	−0.0113 (13)	−0.0112 (14)
C154	0.0551 (18)	0.0430 (17)	0.0539 (19)	−0.0065 (14)	−0.0052 (15)	−0.0212 (14)

Geometric parameters (Å, °)

Si1—C141	1.869 (3)	Si3—C133	1.864 (3)
Si1—C131	1.870 (3)	Si3—C143	1.869 (3)
Si1—C151	1.887 (3)	Si3—C153	1.885 (3)
Si1—C11	1.921 (3)	Si3—C13	1.916 (2)
O11—N31	1.224 (3)	O13—N33	1.222 (3)
O21—N31	1.234 (3)	O23—N33	1.231 (3)

N11—C81	1.458 (3)	N13—C93	1.461 (3)
N11—C91	1.464 (3)	N13—C83	1.463 (3)
N11—C71	1.466 (3)	N13—C73	1.469 (3)
N21—C111	1.451 (3)	N23—C113	1.440 (4)
N21—C121	1.452 (3)	N23—C103	1.448 (3)
N21—C101	1.455 (3)	N23—C123	1.460 (3)
N31—C41	1.470 (3)	N33—C43	1.471 (3)
C11—C61	1.419 (3)	C13—C63	1.416 (3)
C11—C21	1.423 (3)	C13—C23	1.422 (3)
C21—C31	1.388 (3)	C23—C33	1.393 (3)
C21—C71	1.514 (3)	C23—C73	1.511 (3)
C31—C41	1.376 (3)	C33—C43	1.375 (3)
C31—H31	0.9500	C33—H33	0.9500
C41—C51	1.380 (3)	C43—C53	1.378 (3)
C51—C61	1.393 (3)	C53—C63	1.396 (3)
C51—H51	0.9500	C53—H53	0.9500
C61—C101	1.527 (3)	C63—C103	1.524 (3)
C71—H71A	0.9900	C73—H73A	0.9900
C71—H71B	0.9900	C73—H73B	0.9900
C81—H81A	0.9800	C83—H83A	0.9800
C81—H81B	0.9800	C83—H83B	0.9800
C81—H81C	0.9800	C83—H83C	0.9800
C91—H91A	0.9800	C93—H93A	0.9800
C91—H91B	0.9800	C93—H93B	0.9800
C91—H91C	0.9800	C93—H93C	0.9800
C101—H10A	0.9900	C103—H10E	0.9900
C101—H10B	0.9900	C103—H10F	0.9900
C111—H11A	0.9800	C113—H11G	0.9800
C111—H11B	0.9800	C113—H11H	0.9800
C111—H11C	0.9800	C113—H11I	0.9800
C121—H12A	0.9800	C123—H12G	0.9800
C121—H12B	0.9800	C123—H12H	0.9800
C121—H12C	0.9800	C123—H12I	0.9800
C131—H13A	0.9800	C133—H13G	0.9800
C131—H13B	0.9800	C133—H13H	0.9800
C131—H13C	0.9800	C133—H13I	0.9800
C141—H14A	0.9800	C143—H14G	0.9800
C141—H14B	0.9800	C143—H14H	0.9800
C141—H14C	0.9800	C143—H14I	0.9800
C151—H15A	0.9800	C153—H15G	0.9800
C151—H15B	0.9800	C153—H15H	0.9800
C151—H15C	0.9800	C153—H15I	0.9800
Si2—C132	1.870 (3)	Si4—C134	1.864 (3)
Si2—C142	1.872 (3)	Si4—C144	1.870 (3)
Si2—C152	1.881 (3)	Si4—C154	1.885 (3)
Si2—C12	1.922 (2)	Si4—C14	1.918 (2)
O22—N32	1.232 (3)	O14—N34	1.223 (3)
O12—N32	1.216 (3)	O24—N34	1.233 (3)
N12—C92	1.459 (3)	N14—C84	1.459 (3)

N12—C82	1.459 (3)	N14—C94	1.465 (3)
N12—C72	1.465 (3)	N14—C74	1.470 (3)
N22—C112	1.448 (3)	N24—C114	1.362 (5)
N22—C122	1.453 (3)	N24—C104	1.419 (4)
N22—C102	1.454 (3)	N24—C124	1.483 (4)
N32—C42	1.476 (3)	N34—C44	1.468 (3)
C12—C62	1.414 (3)	C14—C64	1.417 (3)
C12—C22	1.422 (3)	C14—C24	1.422 (3)
C22—C32	1.388 (3)	C24—C34	1.389 (3)
C22—C72	1.507 (3)	C24—C74	1.512 (3)
C32—C42	1.381 (3)	C34—C44	1.380 (3)
C32—H32	0.9500	C34—H34	0.9500
C42—C52	1.378 (3)	C44—C54	1.378 (3)
C52—C62	1.396 (3)	C54—C64	1.394 (3)
C52—H52	0.9500	C54—H54	0.9500
C62—C102	1.529 (3)	C64—C104	1.520 (3)
C72—H72A	0.9900	C74—H74A	0.9900
C72—H72B	0.9900	C74—H74B	0.9900
C82—H82A	0.9800	C84—H84A	0.9800
C82—H82B	0.9800	C84—H84B	0.9800
C82—H82C	0.9800	C84—H84C	0.9800
C92—H92A	0.9800	C94—H94A	0.9800
C92—H92B	0.9800	C94—H94B	0.9800
C92—H92C	0.9800	C94—H94C	0.9800
C102—H10C	0.9900	C104—H10G	0.9900
C102—H10D	0.9900	C104—H10H	0.9900
C112—H11D	0.9800	C114—H11J	0.9800
C112—H11E	0.9800	C114—H11K	0.9800
C112—H11F	0.9800	C114—H11L	0.9800
C122—H12D	0.9800	C124—H12J	0.9800
C122—H12E	0.9800	C124—H12K	0.9800
C122—H12F	0.9800	C124—H12L	0.9800
C132—H13D	0.9800	C134—H13J	0.9800
C132—H13E	0.9800	C134—H13K	0.9800
C132—H13F	0.9800	C134—H13L	0.9800
C142—H14D	0.9800	C144—H14J	0.9800
C142—H14E	0.9800	C144—H14K	0.9800
C142—H14F	0.9800	C144—H14L	0.9800
C152—H15D	0.9800	C154—H15J	0.9800
C152—H15E	0.9800	C154—H15K	0.9800
C152—H15F	0.9800	C154—H15L	0.9800
C141—Si1—C131	110.51 (13)	C133—Si3—C143	110.14 (13)
C141—Si1—C151	108.98 (14)	C133—Si3—C153	101.98 (13)
C131—Si1—C151	102.26 (13)	C143—Si3—C153	109.89 (14)
C141—Si1—C11	110.41 (11)	C133—Si3—C13	114.45 (11)
C131—Si1—C11	114.12 (13)	C143—Si3—C13	110.70 (11)
C151—Si1—C11	110.20 (12)	C153—Si3—C13	109.31 (12)
C81—N11—C91	109.6 (2)	C93—N13—C83	109.5 (2)
C81—N11—C71	111.9 (2)	C93—N13—C73	109.59 (19)

C91—N11—C71	109.5 (2)	C83—N13—C73	111.7 (2)
C111—N21—C121	110.0 (2)	C113—N23—C103	111.6 (2)
C111—N21—C101	111.4 (2)	C113—N23—C123	110.3 (2)
C121—N21—C101	111.3 (2)	C103—N23—C123	110.7 (2)
O11—N31—O21	123.6 (2)	O13—N33—O23	123.3 (2)
O11—N31—C41	118.4 (2)	O13—N33—C43	118.6 (2)
O21—N31—C41	118.0 (2)	O23—N33—C43	118.1 (2)
C61—C11—C21	117.0 (2)	C63—C13—C23	117.0 (2)
C61—C11—Si1	120.90 (18)	C63—C13—Si3	120.53 (17)
C21—C11—Si1	122.10 (18)	C23—C13—Si3	122.38 (17)
C31—C21—C11	120.9 (2)	C33—C23—C13	121.0 (2)
C31—C21—C71	116.4 (2)	C33—C23—C73	116.1 (2)
C11—C21—C71	122.5 (2)	C13—C23—C73	122.7 (2)
C41—C31—C21	119.6 (2)	C43—C33—C23	119.1 (2)
C41—C31—H31	120.2	C43—C33—H33	120.4
C21—C31—H31	120.2	C23—C33—H33	120.4
C31—C41—C51	121.9 (2)	C33—C43—C53	122.3 (2)
C31—C41—N31	119.4 (2)	C33—C43—N33	119.1 (2)
C51—C41—N31	118.7 (2)	C53—C43—N33	118.6 (2)
C41—C51—C61	119.0 (2)	C43—C53—C63	118.8 (2)
C41—C51—H51	120.5	C43—C53—H53	120.6
C61—C51—H51	120.5	C63—C53—H53	120.6
C51—C61—C11	121.2 (2)	C53—C63—C13	121.3 (2)
C51—C61—C101	116.1 (2)	C53—C63—C103	116.1 (2)
C11—C61—C101	122.6 (2)	C13—C63—C103	122.7 (2)
N11—C71—C21	111.54 (19)	N13—C73—C23	111.12 (19)
N11—C71—H71A	109.3	N13—C73—H73A	109.4
C21—C71—H71A	109.3	C23—C73—H73A	109.4
N11—C71—H71B	109.3	N13—C73—H73B	109.4
C21—C71—H71B	109.3	C23—C73—H73B	109.4
H71A—C71—H71B	108.0	H73A—C73—H73B	108.0
N11—C81—H81A	109.5	N13—C83—H83A	109.5
N11—C81—H81B	109.5	N13—C83—H83B	109.5
H81A—C81—H81B	109.5	H83A—C83—H83B	109.5
N11—C81—H81C	109.5	N13—C83—H83C	109.5
H81A—C81—H81C	109.5	H83A—C83—H83C	109.5
H81B—C81—H81C	109.5	H83B—C83—H83C	109.5
N11—C91—H91A	109.5	N13—C93—H93A	109.5
N11—C91—H91B	109.5	N13—C93—H93B	109.5
H91A—C91—H91B	109.5	H93A—C93—H93B	109.5
N11—C91—H91C	109.5	N13—C93—H93C	109.5
H91A—C91—H91C	109.5	H93A—C93—H93C	109.5
H91B—C91—H91C	109.5	H93B—C93—H93C	109.5
N21—C101—C61	112.40 (19)	N23—C103—C63	112.27 (19)
N21—C101—H10A	109.1	N23—C103—H10E	109.2
C61—C101—H10A	109.1	C63—C103—H10E	109.2
N21—C101—H10B	109.1	N23—C103—H10F	109.2
C61—C101—H10B	109.1	C63—C103—H10F	109.2
H10A—C101—H10B	107.9	H10E—C103—H10F	107.9

N21—C111—H11A	109.5	N23—C113—H11G	109.5
N21—C111—H11B	109.5	N23—C113—H11H	109.5
H11A—C111—H11B	109.5	H11G—C113—H11H	109.5
N21—C111—H11C	109.5	N23—C113—H11I	109.5
H11A—C111—H11C	109.5	H11G—C113—H11I	109.5
H11B—C111—H11C	109.5	H11H—C113—H11I	109.5
N21—C121—H12A	109.5	N23—C123—H12G	109.5
N21—C121—H12B	109.5	N23—C123—H12H	109.5
H12A—C121—H12B	109.5	H12G—C123—H12H	109.5
N21—C121—H12C	109.5	N23—C123—H12I	109.5
H12A—C121—H12C	109.5	H12G—C123—H12I	109.5
H12B—C121—H12C	109.5	H12H—C123—H12I	109.5
Si1—C131—H13A	109.5	Si3—C133—H13G	109.5
Si1—C131—H13B	109.5	Si3—C133—H13H	109.5
H13A—C131—H13B	109.5	H13G—C133—H13H	109.5
Si1—C131—H13C	109.5	Si3—C133—H13I	109.5
H13A—C131—H13C	109.5	H13G—C133—H13I	109.5
H13B—C131—H13C	109.5	H13H—C133—H13I	109.5
Si1—C141—H14A	109.5	Si3—C143—H14G	109.5
Si1—C141—H14B	109.5	Si3—C143—H14H	109.5
H14A—C141—H14B	109.5	H14G—C143—H14H	109.5
Si1—C141—H14C	109.5	Si3—C143—H14I	109.5
H14A—C141—H14C	109.5	H14G—C143—H14I	109.5
H14B—C141—H14C	109.5	H14H—C143—H14I	109.5
Si1—C151—H15A	109.5	Si3—C153—H15G	109.5
Si1—C151—H15B	109.5	Si3—C153—H15H	109.5
H15A—C151—H15B	109.5	H15G—C153—H15H	109.5
Si1—C151—H15C	109.5	Si3—C153—H15I	109.5
H15A—C151—H15C	109.5	H15G—C153—H15I	109.5
H15B—C151—H15C	109.5	H15H—C153—H15I	109.5
C132—Si2—C142	110.51 (13)	C134—Si4—C144	110.19 (13)
C132—Si2—C152	102.18 (13)	C134—Si4—C154	102.07 (13)
C142—Si2—C152	109.54 (13)	C144—Si4—C154	109.37 (13)
C132—Si2—C12	114.17 (12)	C134—Si4—C14	114.69 (12)
C142—Si2—C12	110.46 (11)	C144—Si4—C14	110.55 (11)
C152—Si2—C12	109.64 (12)	C154—Si4—C14	109.59 (12)
C92—N12—C82	109.5 (2)	C84—N14—C94	109.5 (2)
C92—N12—C72	109.63 (19)	C84—N14—C74	111.80 (19)
C82—N12—C72	111.9 (2)	C94—N14—C74	109.58 (19)
C112—N22—C122	110.3 (2)	C114—N24—C104	110.7 (3)
C112—N22—C102	111.7 (2)	C114—N24—C124	112.0 (3)
C122—N22—C102	111.29 (19)	C104—N24—C124	111.5 (3)
O12—N32—O22	123.7 (2)	O14—N34—O24	123.1 (2)
O12—N32—C42	118.6 (2)	O14—N34—C44	118.9 (2)
O22—N32—C42	117.7 (2)	O24—N34—C44	118.0 (2)
C62—C12—C22	117.3 (2)	C64—C14—C24	116.9 (2)
C62—C12—Si2	120.74 (16)	C64—C14—Si4	120.50 (17)
C22—C12—Si2	121.97 (18)	C24—C14—Si4	122.63 (18)
C32—C22—C12	120.8 (2)	C34—C24—C14	121.0 (2)

C32—C22—C72	116.2 (2)	C34—C24—C74	116.3 (2)
C12—C22—C72	122.8 (2)	C14—C24—C74	122.4 (2)
C42—C32—C22	119.3 (2)	C44—C34—C24	119.4 (2)
C42—C32—H32	120.3	C44—C34—H34	120.3
C22—C32—H32	120.3	C24—C34—H34	120.3
C52—C42—C32	122.2 (2)	C54—C44—C34	121.8 (2)
C52—C42—N32	118.5 (2)	C54—C44—N34	118.5 (2)
C32—C42—N32	119.3 (2)	C34—C44—N34	119.7 (2)
C42—C52—C62	118.7 (2)	C44—C54—C64	119.1 (2)
C42—C52—H52	120.6	C44—C54—H54	120.5
C62—C52—H52	120.6	C64—C54—H54	120.5
C52—C62—C12	121.3 (2)	C54—C64—C14	121.3 (2)
C52—C62—C102	115.6 (2)	C54—C64—C104	115.8 (2)
C12—C62—C102	123.16 (19)	C14—C64—C104	122.9 (2)
N12—C72—C22	111.90 (19)	N14—C74—C24	111.13 (19)
N12—C72—H72A	109.2	N14—C74—H74A	109.4
C22—C72—H72A	109.2	C24—C74—H74A	109.4
N12—C72—H72B	109.2	N14—C74—H74B	109.4
C22—C72—H72B	109.2	C24—C74—H74B	109.4
H72A—C72—H72B	107.9	H74A—C74—H74B	108.0
N12—C82—H82A	109.5	N14—C84—H84A	109.5
N12—C82—H82B	109.5	N14—C84—H84B	109.5
H82A—C82—H82B	109.5	H84A—C84—H84B	109.5
N12—C82—H82C	109.5	N14—C84—H84C	109.5
H82A—C82—H82C	109.5	H84A—C84—H84C	109.5
H82B—C82—H82C	109.5	H84B—C84—H84C	109.5
N12—C92—H92A	109.5	N14—C94—H94A	109.5
N12—C92—H92B	109.5	N14—C94—H94B	109.5
H92A—C92—H92B	109.5	H94A—C94—H94B	109.5
N12—C92—H92C	109.5	N14—C94—H94C	109.5
H92A—C92—H92C	109.5	H94A—C94—H94C	109.5
H92B—C92—H92C	109.5	H94B—C94—H94C	109.5
N22—C102—C62	112.13 (18)	N24—C104—C64	113.0 (2)
N22—C102—H10C	109.2	N24—C104—H10G	109.0
C62—C102—H10C	109.2	C64—C104—H10G	109.0
N22—C102—H10D	109.2	N24—C104—H10H	109.0
C62—C102—H10D	109.2	C64—C104—H10H	109.0
H10C—C102—H10D	107.9	H10G—C104—H10H	107.8
N22—C112—H11D	109.5	N24—C114—H11J	109.5
N22—C112—H11E	109.5	N24—C114—H11K	109.5
H11D—C112—H11E	109.5	H11J—C114—H11K	109.5
N22—C112—H11F	109.5	N24—C114—H11L	109.5
H11D—C112—H11F	109.5	H11J—C114—H11L	109.5
H11E—C112—H11F	109.5	H11K—C114—H11L	109.5
N22—C122—H12D	109.5	N24—C124—H12J	109.5
N22—C122—H12E	109.5	N24—C124—H12K	109.5
H12D—C122—H12E	109.5	H12J—C124—H12K	109.5
N22—C122—H12F	109.5	N24—C124—H12L	109.5
H12D—C122—H12F	109.5	H12J—C124—H12L	109.5

H12E—C122—H12F	109.5	H12K—C124—H12L	109.5
Si2—C132—H13D	109.5	Si4—C134—H13J	109.5
Si2—C132—H13E	109.5	Si4—C134—H13K	109.5
H13D—C132—H13E	109.5	H13J—C134—H13K	109.5
Si2—C132—H13F	109.5	Si4—C134—H13L	109.5
H13D—C132—H13F	109.5	H13J—C134—H13L	109.5
H13E—C132—H13F	109.5	H13K—C134—H13L	109.5
Si2—C142—H14D	109.5	Si4—C144—H14J	109.5
Si2—C142—H14E	109.5	Si4—C144—H14K	109.5
H14D—C142—H14E	109.5	H14J—C144—H14K	109.5
Si2—C142—H14F	109.5	Si4—C144—H14L	109.5
H14D—C142—H14F	109.5	H14J—C144—H14L	109.5
H14E—C142—H14F	109.5	H14K—C144—H14L	109.5
Si2—C152—H15D	109.5	Si4—C154—H15J	109.5
Si2—C152—H15E	109.5	Si4—C154—H15K	109.5
H15D—C152—H15E	109.5	H15J—C154—H15K	109.5
Si2—C152—H15F	109.5	Si4—C154—H15L	109.5
H15D—C152—H15F	109.5	H15J—C154—H15L	109.5
H15E—C152—H15F	109.5	H15K—C154—H15L	109.5
C141—Si1—C11—C61	−83.6 (2)	C133—Si3—C13—C63	154.31 (18)
C131—Si1—C11—C61	151.23 (18)	C143—Si3—C13—C63	−80.5 (2)
C151—Si1—C11—C61	36.9 (2)	C153—Si3—C13—C63	40.7 (2)
C141—Si1—C11—C21	98.4 (2)	C133—Si3—C13—C23	−23.4 (2)
C131—Si1—C11—C21	−26.8 (2)	C143—Si3—C13—C23	101.8 (2)
C151—Si1—C11—C21	−141.15 (19)	C153—Si3—C13—C23	−137.0 (2)
C61—C11—C21—C31	−6.7 (3)	C63—C13—C23—C33	−7.7 (3)
Si1—C11—C21—C31	171.41 (16)	Si3—C13—C23—C33	170.06 (18)
C61—C11—C21—C71	168.3 (2)	C63—C13—C23—C73	166.5 (2)
Si1—C11—C21—C71	−13.6 (3)	Si3—C13—C23—C73	−15.8 (3)
C11—C21—C31—C41	2.0 (3)	C13—C23—C33—C43	3.3 (3)
C71—C21—C31—C41	−173.2 (2)	C73—C23—C33—C43	−171.3 (2)
C21—C31—C41—C51	3.3 (3)	C23—C33—C43—C53	2.8 (4)
C21—C31—C41—N31	−179.59 (19)	C23—C33—C43—N33	−179.6 (2)
O11—N31—C41—C31	−178.5 (2)	O13—N33—C43—C33	−173.9 (2)
O21—N31—C41—C31	1.2 (3)	O23—N33—C43—C33	5.5 (3)
O11—N31—C41—C51	−1.3 (3)	O13—N33—C43—C53	3.8 (3)
O21—N31—C41—C51	178.4 (2)	O23—N33—C43—C53	−176.8 (2)
C31—C41—C51—C61	−3.7 (3)	C33—C43—C53—C63	−4.1 (4)
N31—C41—C51—C61	179.23 (19)	N33—C43—C53—C63	178.3 (2)
C41—C51—C61—C11	−1.4 (3)	C43—C53—C63—C13	−0.7 (3)
C41—C51—C61—C101	178.7 (2)	C43—C53—C63—C103	178.7 (2)
C21—C11—C61—C51	6.3 (3)	C23—C13—C63—C53	6.4 (3)
Si1—C11—C61—C51	−171.78 (16)	Si3—C13—C63—C53	−171.39 (17)
C21—C11—C61—C101	−173.7 (2)	C23—C13—C63—C103	−173.0 (2)
Si1—C11—C61—C101	8.1 (3)	Si3—C13—C63—C103	9.2 (3)
C81—N11—C71—C21	−56.6 (3)	C93—N13—C73—C23	−178.9 (2)
C91—N11—C71—C21	−178.4 (2)	C83—N13—C73—C23	−57.4 (3)
C31—C21—C71—N11	123.5 (2)	C33—C23—C73—N13	121.9 (2)
C11—C21—C71—N11	−51.7 (3)	C13—C23—C73—N13	−52.6 (3)

C111—N21—C101—C61	−74.6 (2)	C113—N23—C103—C63	−70.9 (3)
C121—N21—C101—C61	162.2 (2)	C123—N23—C103—C63	165.9 (2)
C51—C61—C101—N21	−24.5 (3)	C53—C63—C103—N23	−28.8 (3)
C11—C61—C101—N21	155.5 (2)	C13—C63—C103—N23	150.6 (2)
C132—Si2—C12—C62	152.50 (18)	C134—Si4—C14—C64	154.47 (18)
C142—Si2—C12—C62	−82.2 (2)	C144—Si4—C14—C64	−80.2 (2)
C152—Si2—C12—C62	38.6 (2)	C154—Si4—C14—C64	40.4 (2)
C132—Si2—C12—C22	−25.5 (2)	C134—Si4—C14—C24	−24.0 (2)
C142—Si2—C12—C22	99.8 (2)	C144—Si4—C14—C24	101.3 (2)
C152—Si2—C12—C22	−139.4 (2)	C154—Si4—C14—C24	−138.05 (19)
C62—C12—C22—C32	−7.3 (3)	C64—C14—C24—C34	−7.9 (3)
Si2—C12—C22—C32	170.74 (17)	Si4—C14—C24—C34	170.62 (17)
C62—C12—C22—C72	166.6 (2)	C64—C14—C24—C74	166.5 (2)
Si2—C12—C22—C72	−15.3 (3)	Si4—C14—C24—C74	−15.0 (3)
C12—C22—C32—C42	2.4 (3)	C14—C24—C34—C44	3.2 (3)
C72—C22—C32—C42	−171.9 (2)	C74—C24—C34—C44	−171.5 (2)
C22—C32—C42—C52	3.3 (4)	C24—C34—C44—C54	3.1 (3)
C22—C32—C42—N32	−179.6 (2)	C24—C34—C44—N34	−179.5 (2)
O12—N32—C42—C52	0.1 (3)	O14—N34—C44—C54	1.9 (3)
O22—N32—C42—C52	−179.9 (2)	O24—N34—C44—C54	−178.3 (2)
O12—N32—C42—C32	−177.1 (2)	O14—N34—C44—C34	−175.5 (2)
O22—N32—C42—C32	2.8 (3)	O24—N34—C44—C34	4.2 (3)
C32—C42—C52—C62	−3.7 (4)	C34—C44—C54—C64	−4.3 (3)
N32—C42—C52—C62	179.2 (2)	N34—C44—C54—C64	178.29 (19)
C42—C52—C62—C12	−1.6 (3)	C44—C54—C64—C14	−0.8 (3)
C42—C52—C62—C102	178.0 (2)	C44—C54—C64—C104	179.3 (2)
C22—C12—C62—C52	6.9 (3)	C24—C14—C64—C54	6.7 (3)
Si2—C12—C62—C52	−171.13 (17)	Si4—C14—C64—C54	−171.87 (17)
C22—C12—C62—C102	−172.7 (2)	C24—C14—C64—C104	−173.4 (2)
Si2—C12—C62—C102	9.2 (3)	Si4—C14—C64—C104	8.0 (3)
C92—N12—C72—C22	−177.6 (2)	C84—N14—C74—C24	−58.2 (3)
C82—N12—C72—C22	−55.9 (3)	C94—N14—C74—C24	−179.8 (2)
C32—C22—C72—N12	122.9 (2)	C34—C24—C74—N14	122.5 (2)
C12—C22—C72—N12	−51.3 (3)	C14—C24—C74—N14	−52.2 (3)
C112—N22—C102—C62	−72.7 (2)	C114—N24—C104—C64	−76.1 (3)
C122—N22—C102—C62	163.5 (2)	C124—N24—C104—C64	158.5 (3)
C52—C62—C102—N22	−28.1 (3)	C54—C64—C104—N24	−28.9 (3)
C12—C62—C102—N22	151.5 (2)	C14—C64—C104—N24	151.2 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C101—H10A···O24	0.99	2.66	3.411 (3)	133
C102—H10C···O23	0.99	2.70	3.452 (3)	133
C103—H10E···O22	0.99	2.63	3.402 (3)	135
C104—H10G···O21	0.99	2.59	3.390 (3)	138
C51—H51···N21	0.95	2.39	2.753 (3)	102
C52—H52···N22	0.95	2.41	2.754 (3)	101
C53—H53···N23	0.95	2.43	2.764 (3)	101

C54—H54···N24	0.95	2.42	2.755 (4)	101

Fig. 1

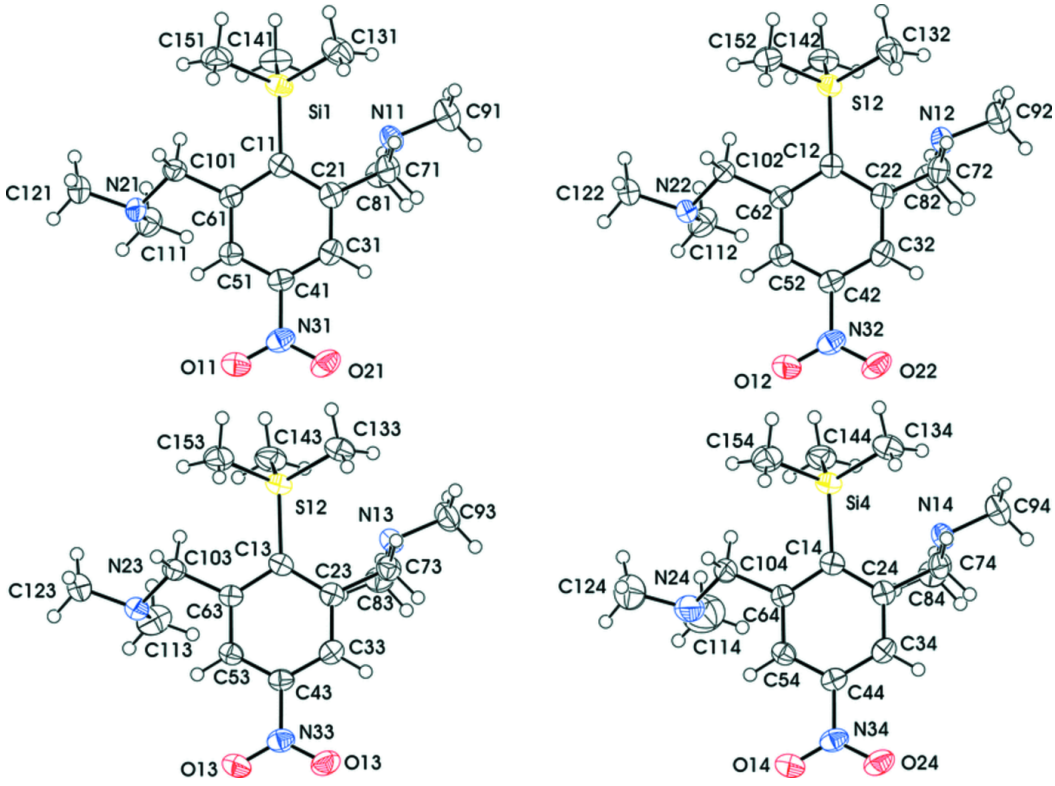


Fig. 2

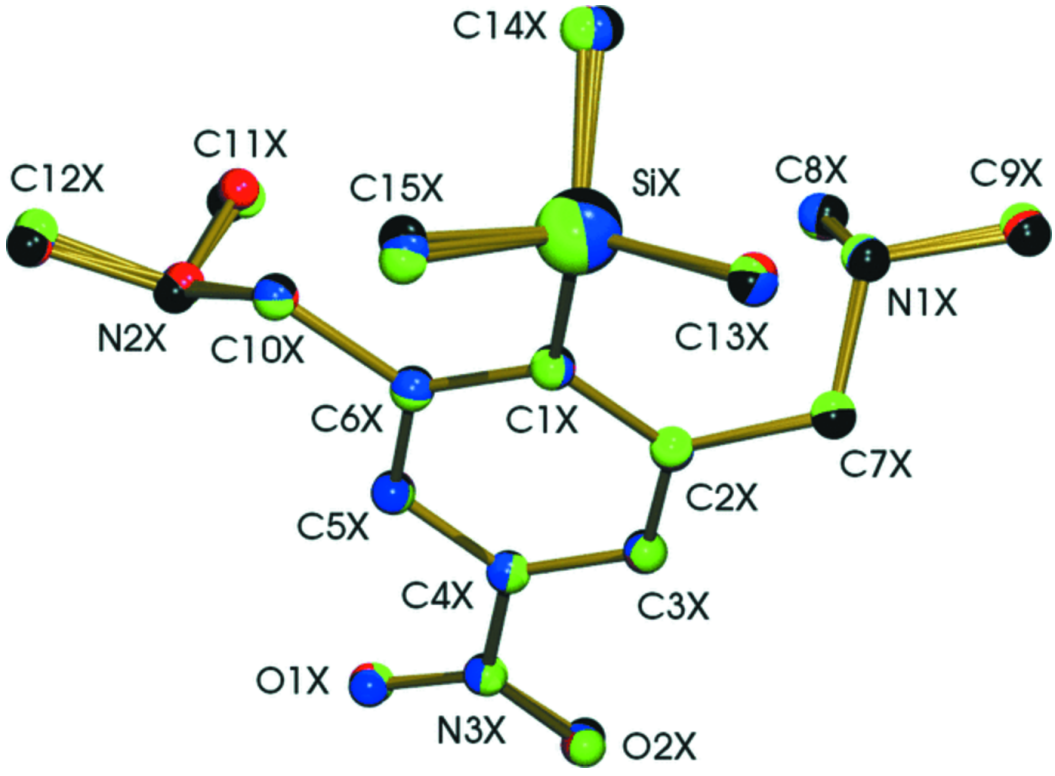
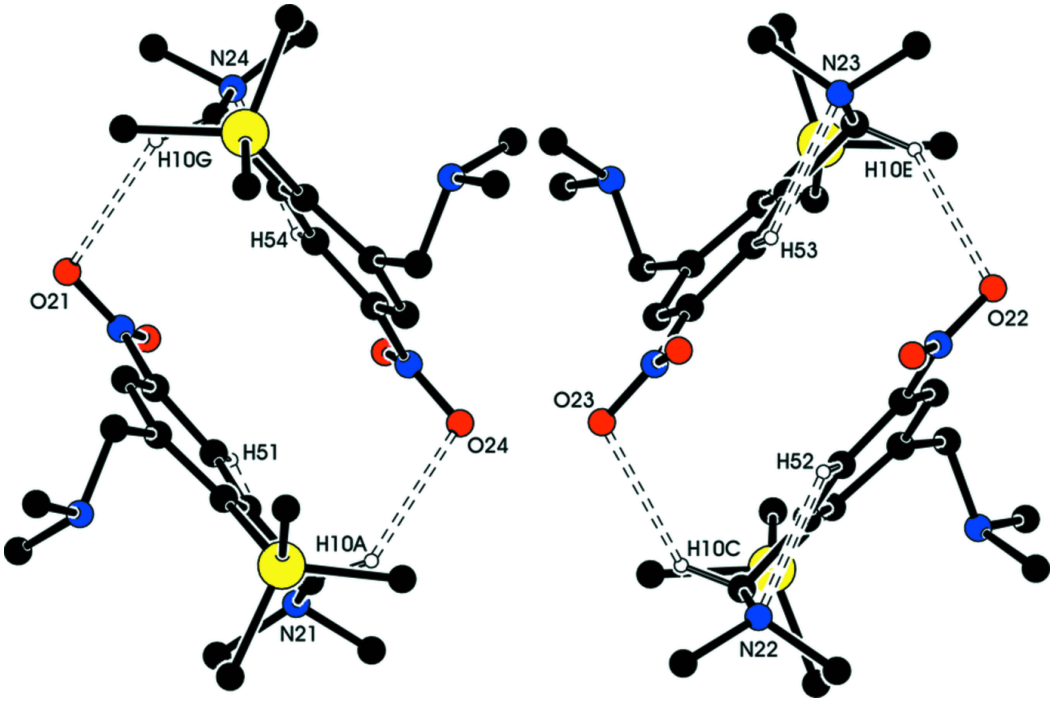

C14X
C11X
C12X
C15X
SiX
C8X
C9X
N2X
C10X
C13X
N1X
C6X
C1X
C7X
C2X
C5X
C4X
C3X
O1X
N3X
O2X

Fig. 3


N24
H10G
H54
O21
H51
O24
H10A
N21
N23
H10E
H53
O22
O23
H52
H10C
N22