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1-[1-(3-Methylphenyl)-5-phenyl-4-phenylsulfonyl-1*H*-pyrazol-3-yl]ethanone

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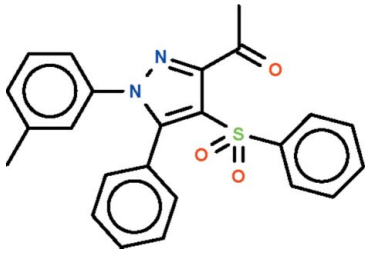
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.041; wR factor = 0.131; data-to-parameter ratio = 18.6.

Both the acetyl and phenyl substituents of the central pyrazole ring in the title compound, $C_{24}H_{20}N_2O_3S$, are twisted with respect to the pyrazole ring, with the twist involving the phenyl ring being greater [67.4 (1) and 29.6 (2)°]. The tolyl substituent is disordered over two positions in a 1:1 ratio; the mean planes of the aromatic ring are aligned at 67.7 (3) and 69.4 (3)° with respect to the pyrazole ring.

Related literature

For the synthesis of this class of pyrazoles, which have been tested as anti-inflammatory agents, see: Nasser *et al.* (2011).



Experimental

Crystal data

$C_{24}H_{20}N_2O_3S$
M_r = 416.48
Monoclinic, $P2_1/n$
a = 10.5717 (4) Å
b = 17.7004 (6) Å
c = 12.8744 (4) Å
β = 115.945 (1)°
V = 2166.30 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 293 K
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2007)
T_{min} = 0.933, T_{max} = 0.966
23603 measured reflections
4951 independent reflections
3490 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.131
S = 1.16
4951 reflections
266 parameters
44 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5108).

References

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supporting information

Acta Cryst. (2011). E**67**, o2922 [doi:10.1107/S1600536811041122]

1-[1-(3-Methylphenyl)-5-phenyl-4-phenylsulfonyl-1*H*-pyrazol-3-yl]ethanone

Mohamed Ghazzali, Hatem A. Abdel-Aziz, Khalid Al-Farhan and Seik Weng Ng

S1. Comment

1-[1-(3-Methylphenyl)-5-phenyl-4-(phenylsulfanyl)-1*H*-pyrazol-3-yl]ethanone (Scheme I) exhibited excellent activity compared with a standard drug, indomethacin, when tested as an anti-inflammatory chemical. The high activity has been rationalized by using molecular docking (Nasser *et al.*, 2011). Both the acetyl and phenyl substituents of the central pyrazole ring are twisted with respect to the pyrazole ring, with the twist involving the phenyl ring being greater (67.4 (1) ° and 29.6 (2) °). The tolyl substituent is disordered over two positions in a 1:1 ratio; the mean planes of the aromatic ring are aligned at 67.7 (3) ° and 69.4 (3) ° (Fig. 1).

S2. Experimental

We have recently reported the synthesis of the compound (Nasser *et al.*, 2011). Crystals were obtained upon recrystallization from ethanol suitable for X-ray structural analysis was obtained by slow evaporation from ethanolic solution at room temperature.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93–0.96 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2–1.5*U*(C).

The tolyl group is disordered over two positions; the occupancy could not be refined, and was assumed to be a 1:1 type of disorder. The benzene rings were refined as rigid hexagons of 1.39 Å sides. The temperature factors of the primed atoms were set to those of the unprimed ones, and all anisotropic temperature factors were restrained to be nearly isotropic. The pair of *N*–C_{tolyl} distances were restrained to within 0.01 Å of each other as were the pair of C_{methyl}–$C_{phenylene}$ bonds.

Omitted because of bad agreement were (0 8 0), (-2 18 8) and (-8 10 13).

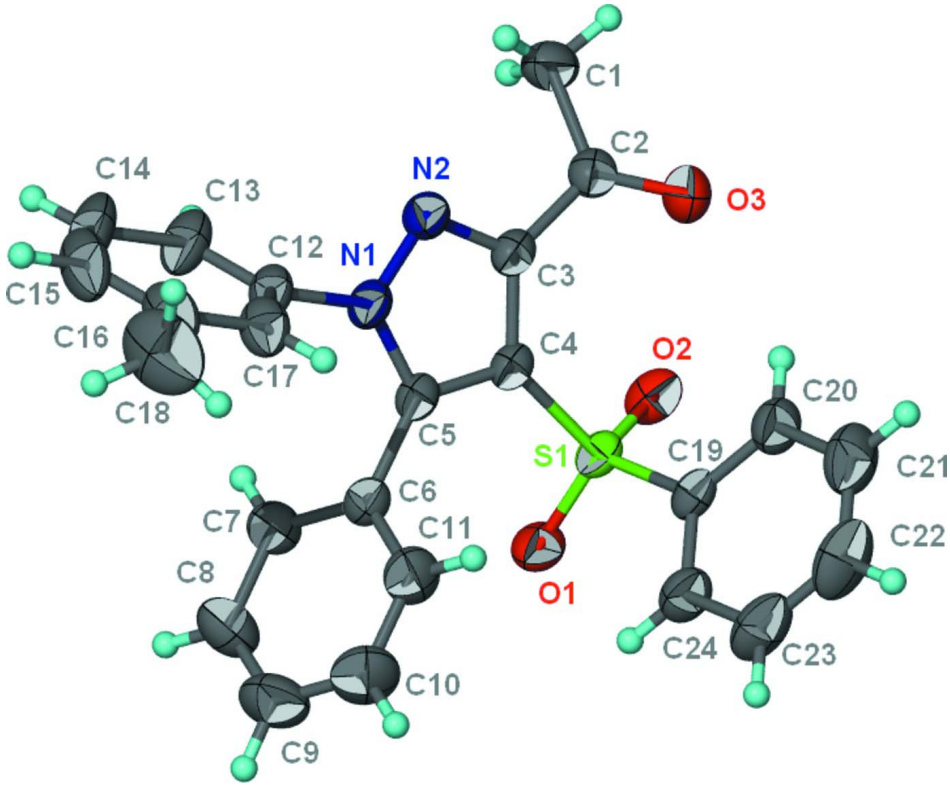

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the title compound at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disordered tolyl component is not shown.

1-[1-(3-Methylphenyl)-5-phenyl-4-phenylsulfonyl-1*H*-pyrazol-3-yl]ethanone

Crystal data

$C_{24}H_{20}N_2O_3S$
$M_r = 416.48$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.5717\ (4)$ Å
$b = 17.7004\ (6)$ Å
$c = 12.8744\ (4)$ Å
$\beta = 115.945\ (1)°$
$V = 2166.30\ (13)$ Å^3
$Z = 4$
$F(000) = 872$
$D_x = 1.277$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 725 reflections
$\theta = 3.1–27.5°$
$\mu = 0.18$ mm^{-1}
$T = 293$ K
Block, yellow
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2007)
$T_{min} = 0.933$, $T_{max} = 0.966$
23603 measured reflections
4951 independent reflections
3490 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -13\rightarrow13$
$k = -22\rightarrow22$
$l = -16\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.131$
$S = 1.16$
4951 reflections
266 parameters
44 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
$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 0.3317P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0235 (19)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.54751 (5)	0.63143 (2)	0.45045 (4)	0.03997 (16)	
O1	0.40174 (15)	0.64090 (7)	0.42277 (13)	0.0545 (4)	
O2	0.64729 (16)	0.62701 (7)	0.56934 (11)	0.0534 (4)	
O3	0.88191 (16)	0.55753 (8)	0.54515 (13)	0.0637 (4)	
N1	0.50448 (17)	0.45192 (8)	0.26398 (13)	0.0440 (4)	
N2	0.63866 (17)	0.43781 (9)	0.34261 (13)	0.0460 (4)	
C1	0.8879 (2)	0.42371 (13)	0.5538 (2)	0.0624 (6)	
H1A	0.9853	0.4310	0.6057	0.094*	
H1B	0.8804	0.3920	0.4909	0.094*	
H1C	0.8409	0.4001	0.5944	0.094*	
C2	0.8211 (2)	0.49846 (11)	0.50784 (17)	0.0452 (4)	
C3	0.67586 (19)	0.49709 (9)	0.41353 (15)	0.0405 (4)	
C4	0.56201 (19)	0.54928 (9)	0.38003 (14)	0.0382 (4)	
C5	0.45247 (19)	0.51785 (9)	0.28374 (15)	0.0388 (4)	
C6	0.3067 (2)	0.54191 (10)	0.21258 (15)	0.0431 (4)	
C7	0.1966 (2)	0.50136 (12)	0.21653 (18)	0.0551 (5)	
H7	0.2151	0.4584	0.2624	0.066*	
C8	0.0593 (2)	0.52496 (16)	0.1521 (2)	0.0722 (7)	
H8	−0.0146	0.4975	0.1542	0.087*	
C9	0.0319 (3)	0.58849 (17)	0.0853 (2)	0.0803 (7)	
H9	−0.0604	0.6048	0.0437	0.096*	
C10	0.1397 (3)	0.62815 (15)	0.0796 (2)	0.0822 (8)	
H10	0.1204	0.6708	0.0331	0.099*	
C11	0.2772 (3)	0.60493 (13)	0.14280 (19)	0.0631 (6)	
H11	0.3501	0.6319	0.1383	0.076*	
C12	0.4517 (7)	0.3942 (4)	0.1774 (6)	0.0362 (12)	0.50
C13	0.4027 (10)	0.3246 (6)	0.1945 (5)	0.0663 (7)	0.50
H13	0.4246	0.3081	0.2690	0.080*	0.50
C14	0.3208 (9)	0.2798 (4)	0.1002 (8)	0.0720 (15)	0.50
H14	0.2880	0.2333	0.1116	0.086*	0.50
C15	0.2879 (7)	0.3045 (4)	−0.0112 (6)	0.0686 (16)	0.50
H15	0.2331	0.2745	−0.0742	0.082*	0.50

C16	0.3369 (10)	0.3741 (6)	−0.0283 (5)	0.0685 (10)	0.50
C17	0.4188 (8)	0.4189 (4)	0.0660 (8)	0.0459 (12)	0.50
H17	0.4516	0.4654	0.0545	0.055*	0.50
C18	0.2992 (15)	0.3922 (5)	−0.1542 (5)	0.1145 (12)	0.50
H18A	0.2297	0.4315	−0.1807	0.172*	0.50
H18B	0.2623	0.3478	−0.2005	0.172*	0.50
H18C	0.3819	0.4087	−0.1608	0.172*	0.50
C12′	0.4183 (7)	0.4036 (4)	0.1680 (6)	0.0362 (12)	0.50
C13′	0.4065 (10)	0.3301 (6)	0.2006 (4)	0.0663 (7)	0.50
H13′	0.4309	0.3190	0.2776	0.080*	0.50
C14′	0.3584 (9)	0.2731 (4)	0.1180 (8)	0.0720 (15)	0.50
H14′	0.3505	0.2239	0.1398	0.086*	0.50
C15′	0.3219 (8)	0.2897 (4)	0.0029 (6)	0.0686 (16)	0.50
H15′	0.2897	0.2516	−0.0524	0.082*	0.50
C16′	0.3337 (10)	0.3633 (6)	−0.0297 (4)	0.0685 (10)	0.50
C17′	0.3819 (8)	0.4203 (4)	0.0529 (8)	0.0459 (12)	0.50
H17′	0.3898	0.4695	0.0312	0.055*	0.50
C18′	0.2985 (14)	0.3918 (2)	−0.1529 (2)	0.1145 (12)	0.50
H18D	0.2052	0.3758	−0.2049	0.172*	0.50
H18E	0.3648	0.3712	−0.1776	0.172*	0.50
H18F	0.3034	0.4459	−0.1527	0.172*	0.50
C19	0.59640 (16)	0.70713 (9)	0.38558 (12)	0.0420 (4)	
C20	0.73709 (16)	0.72002 (10)	0.41591 (12)	0.0567 (5)	
H20	0.8059	0.6889	0.4690	0.068*	
C21	0.7737 (3)	0.78024 (14)	0.3657 (2)	0.0777 (7)	
H21	0.8679	0.7898	0.3853	0.093*	
C22	0.6707 (4)	0.82612 (15)	0.2866 (2)	0.0850 (9)	
H22	0.6961	0.8661	0.2527	0.102*	
C23	0.5320 (3)	0.81318 (13)	0.2580 (2)	0.0755 (7)	
H23	0.4634	0.8446	0.2054	0.091*	
C24	0.4932 (2)	0.75312 (11)	0.30731 (17)	0.0562 (5)	
H24	0.3989	0.7440	0.2878	0.067*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0528 (3)	0.0324 (2)	0.0414 (3)	0.00075 (18)	0.0268 (2)	−0.00099 (17)
O1	0.0550 (9)	0.0472 (8)	0.0739 (10)	0.0037 (6)	0.0399 (8)	−0.0035 (7)
O2	0.0773 (10)	0.0465 (8)	0.0364 (7)	0.0045 (7)	0.0249 (7)	−0.0011 (5)
O3	0.0572 (10)	0.0547 (9)	0.0710 (10)	−0.0084 (7)	0.0205 (8)	−0.0132 (7)
N1	0.0500 (10)	0.0366 (8)	0.0474 (8)	−0.0036 (6)	0.0232 (8)	−0.0090 (6)
N2	0.0470 (9)	0.0415 (9)	0.0519 (9)	−0.0001 (7)	0.0239 (8)	−0.0062 (7)
C1	0.0521 (13)	0.0565 (13)	0.0761 (15)	0.0077 (10)	0.0259 (12)	0.0102 (11)
C2	0.0464 (11)	0.0466 (11)	0.0486 (10)	−0.0017 (8)	0.0264 (9)	−0.0043 (8)
C3	0.0470 (11)	0.0337 (9)	0.0464 (10)	−0.0019 (7)	0.0256 (9)	−0.0020 (7)
C4	0.0474 (10)	0.0319 (9)	0.0406 (9)	−0.0021 (7)	0.0242 (8)	−0.0010 (7)
C5	0.0473 (11)	0.0333 (9)	0.0408 (9)	−0.0027 (7)	0.0238 (8)	−0.0008 (7)
C6	0.0495 (11)	0.0381 (10)	0.0404 (9)	−0.0004 (8)	0.0184 (9)	−0.0012 (7)

C7	0.0516 (13)	0.0572 (13)	0.0562 (12)	0.0001 (9)	0.0234 (11)	0.0081 (9)
C8	0.0483 (14)	0.0915 (18)	0.0703 (15)	0.0003 (12)	0.0199 (12)	0.0094 (13)
C9	0.0616 (17)	0.091 (2)	0.0703 (16)	0.0187 (14)	0.0123 (13)	0.0107 (14)
C10	0.084 (2)	0.0708 (17)	0.0720 (16)	0.0151 (14)	0.0159 (15)	0.0280 (13)
C11	0.0649 (15)	0.0553 (13)	0.0619 (13)	−0.0018 (11)	0.0211 (12)	0.0165 (10)
C12	0.022 (3)	0.0355 (19)	0.0547 (14)	0.007 (2)	0.0206 (17)	−0.0108 (14)
C13	0.0873 (18)	0.0454 (16)	0.0844 (16)	−0.0160 (12)	0.0545 (15)	−0.0206 (12)
C14	0.063 (4)	0.0491 (16)	0.117 (3)	−0.016 (2)	0.051 (3)	−0.0338 (17)
C15	0.037 (4)	0.072 (3)	0.092 (2)	0.001 (3)	0.023 (2)	−0.046 (2)
C16	0.0551 (15)	0.085 (3)	0.0636 (14)	−0.0097 (16)	0.0246 (12)	−0.0338 (14)
C17	0.022 (4)	0.0633 (13)	0.049 (2)	−0.0071 (17)	0.012 (2)	−0.0137 (11)
C18	0.109 (3)	0.164 (3)	0.0582 (16)	−0.006 (2)	0.0247 (17)	−0.0346 (18)
C12′	0.022 (3)	0.0355 (19)	0.0547 (14)	0.007 (2)	0.0206 (17)	−0.0108 (14)
C13′	0.0873 (18)	0.0454 (16)	0.0844 (16)	−0.0160 (12)	0.0545 (15)	−0.0206 (12)
C14′	0.063 (4)	0.0491 (16)	0.117 (3)	−0.016 (2)	0.051 (3)	−0.0338 (17)
C15′	0.037 (4)	0.072 (3)	0.092 (2)	0.001 (3)	0.023 (2)	−0.046 (2)
C16′	0.0551 (15)	0.085 (3)	0.0636 (14)	−0.0097 (16)	0.0246 (12)	−0.0338 (14)
C17′	0.022 (4)	0.0633 (13)	0.049 (2)	−0.0071 (17)	0.012 (2)	−0.0137 (11)
C18′	0.109 (3)	0.164 (3)	0.0582 (16)	−0.006 (2)	0.0247 (17)	−0.0346 (18)
C19	0.0583 (12)	0.0319 (9)	0.0389 (9)	−0.0036 (8)	0.0241 (9)	−0.0048 (7)
C20	0.0614 (14)	0.0467 (11)	0.0677 (13)	−0.0072 (9)	0.0333 (11)	−0.0009 (10)
C21	0.0881 (19)	0.0641 (16)	0.0975 (19)	−0.0226 (14)	0.0560 (17)	−0.0040 (14)
C22	0.134 (3)	0.0551 (15)	0.0825 (18)	−0.0239 (16)	0.0628 (19)	0.0065 (13)
C23	0.112 (2)	0.0456 (13)	0.0597 (14)	−0.0017 (13)	0.0294 (15)	0.0126 (10)
C24	0.0689 (14)	0.0422 (11)	0.0514 (11)	0.0000 (9)	0.0208 (11)	0.0041 (9)

Geometric parameters (Å, º)

S1—O1	1.4316 (14)	C14—H14	0.9300
S1—O2	1.4314 (14)	C15—C16	1.3900
S1—C4	1.7554 (17)	C15—H15	0.9300
S1—C19	1.7713 (15)	C16—C17	1.3900
O3—C2	1.211 (2)	C16—C18	1.525 (6)
N1—N2	1.358 (2)	C17—H17	0.9300
N1—C5	1.361 (2)	C18—H18A	0.9600
N1—C12	1.434 (5)	C18—H18B	0.9600
N1—C12′	1.450 (5)	C18—H18C	0.9600
N2—C3	1.332 (2)	C12′—C13′	1.3900
C1—C2	1.495 (3)	C12′—C17′	1.3900
C1—H1A	0.9600	C13′—C14′	1.3900
C1—H1B	0.9600	C13′—H13′	0.9300
C1—H1C	0.9600	C14′—C15′	1.3900
C2—C3	1.484 (3)	C14′—H14′	0.9300
C3—C4	1.426 (2)	C15′—C16′	1.3900
C4—C5	1.390 (2)	C15′—H15′	0.9300
C5—C6	1.469 (3)	C16′—C17′	1.3900
C6—C11	1.380 (3)	C16′—C18′	1.547 (5)
C6—C7	1.387 (3)	C17′—H17′	0.9300

C7—C8	1.385 (3)	C18′—H18D	0.9600
C7—H7	0.9300	C18′—H18E	0.9600
C8—C9	1.367 (4)	C18′—H18F	0.9600
C8—H8	0.9300	C19—C24	1.381 (2)
C9—C10	1.368 (4)	C19—C20	1.382 (3)
C9—H9	0.9300	C20—C21	1.387 (3)
C10—C11	1.381 (3)	C20—H20	0.9300
C10—H10	0.9300	C21—C22	1.382 (4)
C11—H11	0.9300	C21—H21	0.9300
C12—C13	1.3900	C22—C23	1.366 (4)
C12—C17	1.3900	C22—H22	0.9300
C13—C14	1.3900	C23—C24	1.389 (3)
C13—H13	0.9300	C23—H23	0.9300
C14—C15	1.3900	C24—H24	0.9300

O1—S1—O2	118.81 (9)	C13—C14—C15	120.0
O1—S1—C4	107.23 (8)	C13—C14—H14	120.0
O2—S1—C4	108.48 (8)	C15—C14—H14	120.0
O1—S1—C19	107.36 (8)	C16—C15—C14	120.0
O2—S1—C19	108.37 (8)	C16—C15—H15	120.0
C4—S1—C19	105.89 (7)	C14—C15—H15	120.0
N2—N1—C5	113.22 (14)	C15—C16—C17	120.0
N2—N1—C12	111.9 (3)	C15—C16—C18	114.4 (7)
C5—N1—C12	134.9 (3)	C17—C16—C18	125.6 (7)
N2—N1—C12′	126.1 (3)	C16—C17—C12	120.0
C5—N1—C12′	120.7 (3)	C16—C17—H17	120.0
C3—N2—N1	105.36 (14)	C12—C17—H17	120.0
C2—C1—H1A	109.5	C13′—C12′—C17′	120.0
C2—C1—H1B	109.5	C13′—C12′—N1	113.7 (7)
H1A—C1—H1B	109.5	C17′—C12′—N1	124.2 (7)
C2—C1—H1C	109.5	C12′—C13′—C14′	120.0
H1A—C1—H1C	109.5	C12′—C13′—H13′	120.0
H1B—C1—H1C	109.5	C14′—C13′—H13′	120.0
O3—C2—C3	121.22 (18)	C13′—C14′—C15′	120.0
O3—C2—C1	122.0 (2)	C13′—C14′—H14′	120.0
C3—C2—C1	116.76 (17)	C15′—C14′—H14′	120.0
N2—C3—C4	110.24 (16)	C14′—C15′—C16′	120.0
N2—C3—C2	117.59 (16)	C14′—C15′—H15′	120.0
C4—C3—C2	132.17 (16)	C16′—C15′—H15′	120.0
C5—C4—C3	105.91 (15)	C17′—C16′—C15′	120.0
C5—C4—S1	124.43 (14)	C17′—C16′—C18′	113.1 (7)
C3—C4—S1	129.29 (14)	C15′—C16′—C18′	126.9 (7)
N1—C5—C4	105.25 (16)	C16′—C17′—C12′	120.0
N1—C5—C6	122.09 (16)	C16′—C17′—H17′	120.0
C4—C5—C6	132.64 (16)	C12′—C17′—H17′	120.0
C11—C6—C7	119.18 (19)	C16′—C18′—H18D	109.5
C11—C6—C5	121.16 (18)	C16′—C18′—H18E	109.5
C7—C6—C5	119.66 (16)	H18D—C18′—H18E	109.5

C8—C7—C6	119.9 (2)	C16′—C18′—H18F	109.5
C8—C7—H7	120.0	H18D—C18′—H18F	109.5
C6—C7—H7	120.0	H18E—C18′—H18F	109.5
C9—C8—C7	120.2 (2)	C24—C19—C20	121.21 (13)
C9—C8—H8	119.9	C24—C19—S1	119.32 (14)
C7—C8—H8	119.9	C20—C19—S1	119.46 (6)
C8—C9—C10	120.2 (2)	C19—C20—C21	118.73 (15)
C8—C9—H9	119.9	C19—C20—H20	120.6
C10—C9—H9	119.9	C21—C20—H20	120.6
C9—C10—C11	120.2 (2)	C22—C21—C20	120.3 (2)
C9—C10—H10	119.9	C22—C21—H21	119.8
C11—C10—H10	119.9	C20—C21—H21	119.8
C6—C11—C10	120.3 (2)	C23—C22—C21	120.4 (2)
C6—C11—H11	119.9	C23—C22—H22	119.8
C10—C11—H11	119.9	C21—C22—H22	119.8
C13—C12—C17	120.0	C22—C23—C24	120.1 (2)
C13—C12—N1	123.6 (7)	C22—C23—H23	119.9
C17—C12—N1	114.5 (7)	C24—C23—H23	119.9
C14—C13—C12	120.0	C19—C24—C23	119.2 (2)
C14—C13—H13	120.0	C19—C24—H24	120.4
C12—C13—H13	120.0	C23—C24—H24	120.4

C5—N1—N2—C3	−1.55 (19)	N2—N1—C12—C17	−116.8 (4)
C12—N1—N2—C3	177.1 (5)	C5—N1—C12—C17	61.4 (7)
C12′—N1—N2—C3	179.6 (5)	C12′—N1—C12—C17	71 (3)
N1—N2—C3—C4	0.88 (19)	C17—C12—C13—C14	0.0
N1—N2—C3—C2	−178.29 (14)	N1—C12—C13—C14	163.3 (5)
O3—C2—C3—N2	150.22 (18)	C12—C13—C14—C15	0.0
C1—C2—C3—N2	−29.7 (2)	C13—C14—C15—C16	0.0
O3—C2—C3—C4	−28.7 (3)	C14—C15—C16—C17	0.0
C1—C2—C3—C4	151.39 (19)	C14—C15—C16—C18	177.0 (10)
N2—C3—C4—C5	0.03 (19)	C15—C16—C17—C12	0.0
C2—C3—C4—C5	179.04 (18)	C18—C16—C17—C12	−176.7 (11)
N2—C3—C4—S1	173.15 (13)	C13—C12—C17—C16	0.0
C2—C3—C4—S1	−7.8 (3)	N1—C12—C17—C16	−164.8 (5)
O1—S1—C4—C5	22.34 (17)	N2—N1—C12′—C13′	54.4 (6)
O2—S1—C4—C5	151.81 (14)	C5—N1—C12′—C13′	−124.5 (3)
C19—S1—C4—C5	−92.06 (15)	C12—N1—C12′—C13′	64 (3)
O1—S1—C4—C3	−149.63 (16)	N2—N1—C12′—C17′	−108.7 (6)
O2—S1—C4—C3	−20.16 (18)	C5—N1—C12′—C17′	72.4 (6)
C19—S1—C4—C3	95.97 (16)	C12—N1—C12′—C17′	−99 (3)
N2—N1—C5—C4	1.57 (19)	C17′—C12′—C13′—C14′	0.0
C12—N1—C5—C4	−176.6 (6)	N1—C12′—C13′—C14′	−163.9 (6)
C12′—N1—C5—C4	−179.5 (5)	C12′—C13′—C14′—C15′	0.0
N2—N1—C5—C6	−176.67 (15)	C13′—C14′—C15′—C16′	0.0
C12—N1—C5—C6	5.1 (7)	C14′—C15′—C16′—C17′	0.0
C12′—N1—C5—C6	2.3 (5)	C14′—C15′—C16′—C18′	179.9 (11)
C3—C4—C5—N1	−0.93 (18)	C15′—C16′—C17′—C12′	0.0

S1—C4—C5—N1	−174.47 (12)	C18′—C16′—C17′—C12′	−179.9 (9)
C3—C4—C5—C6	177.05 (17)	C13′—C12′—C17′—C16′	0.0
S1—C4—C5—C6	3.5 (3)	N1—C12′—C17′—C16′	162.1 (6)
N1—C5—C6—C11	−113.8 (2)	O1—S1—C19—C24	−10.71 (16)
C4—C5—C6—C11	68.5 (3)	O2—S1—C19—C24	−140.20 (14)
N1—C5—C6—C7	67.2 (2)	C4—S1—C19—C24	103.59 (15)
C4—C5—C6—C7	−110.5 (2)	O1—S1—C19—C20	167.98 (11)
C11—C6—C7—C8	−0.9 (3)	O2—S1—C19—C20	38.50 (12)
C5—C6—C7—C8	178.2 (2)	C4—S1—C19—C20	−77.71 (12)
C6—C7—C8—C9	−0.6 (4)	C24—C19—C20—C21	−0.3 (2)
C7—C8—C9—C10	1.6 (4)	S1—C19—C20—C21	−178.99 (16)
C8—C9—C10—C11	−1.1 (4)	C19—C20—C21—C22	−0.2 (3)
C7—C6—C11—C10	1.4 (3)	C20—C21—C22—C23	0.7 (4)
C5—C6—C11—C10	−177.7 (2)	C21—C22—C23—C24	−0.7 (4)
C9—C10—C11—C6	−0.4 (4)	C20—C19—C24—C23	0.3 (3)
N2—N1—C12—C13	79.0 (4)	S1—C19—C24—C23	178.96 (16)
C5—N1—C12—C13	−102.8 (6)	C22—C23—C24—C19	0.2 (3)
C12′—N1—C12—C13	−93 (3)		