Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

6′-Amino-3′-methyl-2-oxo-1′-phenyl-1′,3a′,4′,7a′-tetrahydrospiro[1*H*-indole-3(2*H*),4′-pyrano[2,3-*d*]pyrazole]-5′-carbonitrile

S. Etti,[a] G. Shanthi,[b] G. Shanmugam[a]* and P. T. Perumal[b]

[a]Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, and [b]Organic Chemistry Division, Central Leather Research Institute, Adyar, Chennai 600 020, India
Correspondence e-mail: gurushan48@yahoo.com

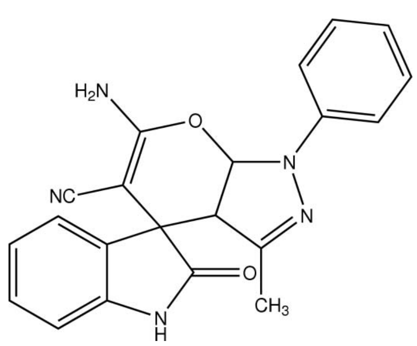
Received 15 November 2007; accepted 1 December 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.118; data-to-parameter ratio = 17.7.

In the crystal structure of the title compound, $C_{21}H_{15}N_5O_2$, the planar indolone unit and the pyran ring are almost perpendicular to each other [dihedral angle = 89.41 (2)°], and the pyrazole and phenyl rings are oriented at an angle of 25.74 (1)°. The molecular packing is stabilized by inter- and intramolecular C—H···O, N—H···O and C—H···π hydrogen bonds.

Related literature

For related literature, see: Houlihan *et al.* (1992); Jeyabharathi *et al.* (2001); Kang *et al.* (2002); Khafagy *et al.* (2002); McSweeney *et al.* (2004), Selvanayagam *et al.* (2005); Usui *et al.* (1998).



Experimental

Crystal data

$C_{21}H_{15}N_5O_2$
M_r = 369.38
Monoclinic, $P2_1/c$
a = 10.0370 (3) Å
b = 21.9705 (6) Å
c = 8.2325 (2) Å
β = 98.761 (1)°
V = 1794.23 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.24 × 0.21 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SAINT*; Bruker, 1999)
T_{min} = 0.978, T_{max} = 0.982
21620 measured reflections
4485 independent reflections
3277 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.118
S = 1.02
4485 reflections
254 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

Cg is the centroid of the pyrazole ring.

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O2	0.93	2.42	2.959 (2)	117
N1—H1···O1^{i}	0.86	1.99	2.819 (2)	161
N3—H3B···O1^{ii}	0.86	2.12	2.880 (1)	148
C6—H6···Cg^{iii}	0.92	2.85	3.771 (3)	173

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x, y-1, z-1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; 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: *SHELXL97* and *PARST97* (Nardelli, 1995).

SE thanks the Council of Scientific and Industrial Research (CSIR), New Delhi, for providing financial assistance as a Senior Research Fellowship (SRF).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2047).

References

Bruker (1999). *SAINT*. Version 6.02. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Houlihan, W. J., Remers, W. A. & Brown, R. K. (1992). *Indoles: Part I*. New York: J. Wiley & Sons.
Jeyabharathi, A., Ponnuswamy, M. N., Amal Raj, A., Raghunathan, R., Razak, I. A., Usman, A., Chantrapromma, S. & Fun, H.-K. (2001). *Acta Cryst.* E**57**, o901–o903.
Kang, T.-H., Matsumoto, K., Murakami, Y., Takayama, H., Kitajima, M., Aimi, N. & Watanabe, H. (2002). *Eur. J. Pharmacol.* **444**, 39–45.
Khafagy, M. M., El-Wahas, A. H. F. A., Eid, F. A. & El-Agrody, A. M. (2002). *Farmaco*, **57**, 715–722.
McSweeney, N., Pratt, A. C., Creaven, B. S., Long, C. & Howie, R. A. (2004). *Acta Cryst.* E**60**, o2025–o2028.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Selvanayagam, S., Rathisuganya, P., Shaherin, B., Velmurugan, D., Ravikumar, K. & Poornachandran, M. (2005). *Acta Cryst.* E**61**, o3693–o3695.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Usui, T., Kondoh, M., Cui, C.-B., Mayumi, T. & Osada, H. (1998). *Biochem. J.* **333**, 543–548.

 doi:10.1107/S1600536807064926

supplementary materials

Acta Cryst. (2008). E**64**, o341 [**doi:10.1107/S1600536807064926**]

6'-Amino-3'-methyl-2-oxo-1'-phenyl-1',3a',4',7a'-tetrahydrospiro[1*H*-indole-3(2*H*),4'-pyrano[2,3-*d*]pyrazole]-5'-carbonitrile

S. Etti, G. Shanthi, G. Shanmugam and P. T. Perumal

Comment

The indole moiety is probably the most well known heterocycle, a common and important feature of a variety of natural products and medicinal agents (Houlihan *et al.*, 1992). Spiro compounds represent an important class of naturally occurring substances characterized by highly pronounced biological properties. The spiro indolone system is the core structure of many pharmacological agents and natural alkaloids (Usui *et al.*, 1998). For example, spirotryprostatin A, a natural alkaloid isolated from the fermentation broth of Aspergillus fumigatus, has been identified as a novel inhibitor of microtubule assembly (Khafagy *et al.*, 2002), and pteropodine and isopteropodine have been shown to modulate the function of muscarinic serotonin receptors (Kang *et al.*, 2002). In view of the above properties of spiro indolone derivatives, the crystal structure analysis of the title compound was undertaken. The indolone and the pyrano pyrazole moities are connected through a spiro junction in the molecule. The dihedral angle between the planar indolone ring and pyrano ring(mean plane calculated through atoms C9,C10,O2,C11, C13) is 89.41 (2)°, which indicates that the rings are perpendicularto each other, also the dihedral angle between the pyrazole ring and the phenyl ring is 25.74 (1)° and the pyrano ring is 3.98 (1)°. The gemoetry of the indolone and pyrano pyrazole moieties are comparable with literature values(Jeyabharathi *et al.*, 2001, Selvanayagam *et al.*,2005, McSweeney *et al.*, 2004), a slight distortion of bond lengths and angles is seen around the C1 atom due to spiro charecter and in the pyrano ring the angle between (C11—O2—C10) 113.87 (1)° which is lower compared to the literature value (McSweeney *et al.*, 2004). The bond length of C9—C14 (sp2-*sp*) 1.42 (2)° is long due to sp2 hybridization. The cyanide group orients with pyrano ring (O2—C10—C19—C14) −178.4 (1)° in -anti-periplanar(-*ap*) conformation, while the amino group orients (C11—O2—C10—N3) 176.1 (1)° in +*ap* conformation. The angle of (C13—C12—C21) 127.83 (1) and (C1—C13—C12) 133.86 (1) is above the normal value due to the steric hindarance of the bulky indolone ring and the methyl group.

The packing of the molecules viewed along C axis is shown in Figure 2 and the hydrogen bond geometry are given in Table 2. The molecular packing is stabilzed by inter and intra molecular C—H.·O, N—H···O and C—H···pi hydrogen bonds.

Experimental

1-methyl isatin (0.161 g, 1 mmol), malononitrile (0.066 g, 1 mmol) and 1-phenyl-3-methyl pyrazolon-5-one (0.174 g, 1 mmol) were added to silica gel impregnated with indium(III) chloride (44 mg, 20 mol°), prepared by adding a solution of InCl3 in a minimum amount of THF to silica gel (2 g, 100–200 mesh activated by heating for 4 h at 150° before use), followed by complete evaporation of solvent under vacuum. The whole mixture was stirred for 5 min for uniform mixing and then irradiated in a microwave oven at 300 W for 3 min. On completion, the reaction mixture was directly charged on a small silica gel column and eluted with a mixture of ethyl acetate-hexane (4:6) to afford the pure product in 88° yield as a white solid. Crystals of (I) were grown by slow evaporation from ethanol.

Figures

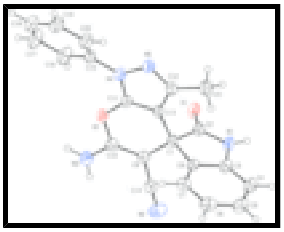


Fig. 1. : The *ORTEP* diagram of the title compound with 30% probability displacement ellipsoids.

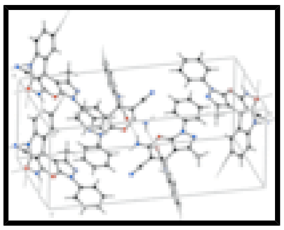


Fig. 2. : Packing of the molecules viewed down *c* axis, the dashed lines represent hydrogen bonds.

6'-Amino-3'-methyl-2-oxo-1'-phenyl-1',3a',4',7a'-tetrahydro- spiro[1*H*-indole-3(2*H*),4'-pyrano[2,3-*d*]pyrazole]-5'-carbonitrile

Crystal data

$C_{21}H_{15}N_5O_2$	F_{000} = 768
M_r = 369.38	D_x = 1.367 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P2ybc	Cell parameters from 4485 reflections
a = 10.0370 (3) Å	θ = 2.7–28.4º
b = 21.9705 (6) Å	μ = 0.09 mm^{-1}
c = 8.2325 (2) Å	*T* = 293 (2) K
β = 98.761 (1)º	Cubic, colourless
V = 1794.23 (8) Å^3	0.24 × 0.21 × 0.20 mm
Z = 4	

Data collection

Bruker Kappa APEXII diffractometer	R_{int} = 0.028
Radiation source: fine-focus sealed tube	θ_{max} = 28.4º
Monochromator: graphite	θ_{min} = 2.7º
T = 293(2) K	*h* = −13→13
ω and φ scans	*k* = −29→29
Absorption correction: multi-scan (SAINT; Bruker, 1999)	*l* = −10→10
T_{min} = 0.978, T_{max} = 0.982	Standard reflections: ?;
21620 measured reflections	every ? reflections
4485 independent reflections	intensity decay: none
3277 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.041$	Calculated $w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 0.3722P]$ where $P = (F_o^2 + 2F_c^2)/3$?
$wR(F^2) = 0.118$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.24$ e Å^{-3}
4485 reflections	$\Delta\rho_{min} = -0.17$ e Å^{-3}
254 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0028 (11)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. 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}
N1	0.94447 (12)	0.45685 (6)	0.30510 (15)	0.0484 (3)
H1	1.0221	0.4718	0.3436	0.058*
N2	0.63637 (18)	0.56417 (7)	0.0884 (2)	0.0705 (4)
N3	0.37828 (13)	0.49908 (6)	0.28737 (17)	0.0560 (4)
H3A	0.3820	0.5318	0.2309	0.067*
H3B	0.3071	0.4910	0.3298	0.067*
N4	0.53791 (11)	0.31470 (5)	0.49407 (14)	0.0416 (3)
N5	0.65120 (12)	0.27975 (6)	0.49024 (16)	0.0467 (3)
O1	0.83478 (10)	0.47928 (5)	0.52173 (12)	0.0524 (3)
O2	0.45453 (9)	0.41161 (4)	0.40050 (12)	0.0434 (2)
C1	0.71934 (12)	0.42403 (6)	0.27907 (15)	0.0354 (3)
C2	0.83874 (13)	0.45672 (6)	0.38640 (16)	0.0400 (3)
C3	0.91361 (14)	0.42960 (6)	0.14910 (17)	0.0423 (3)
C4	0.99616 (17)	0.42282 (8)	0.0305 (2)	0.0555 (4)
H4	1.0852	0.4360	0.0477	0.067*
C5	0.9396 (2)	0.39532 (8)	−0.1154 (2)	0.0611 (5)

H5	0.9915	0.3907	−0.1991	0.073*
C6	0.80860 (19)	0.37474 (7)	−0.13958 (19)	0.0567 (4)
H6	0.7738	0.3561	−0.2384	0.068*
C7	0.72765 (16)	0.38144 (6)	−0.01793 (17)	0.0459 (3)
H7	0.6393	0.3673	−0.0339	0.055*
C8	0.78159 (14)	0.40946 (6)	0.12661 (16)	0.0375 (3)
C9	0.60089 (13)	0.46759 (6)	0.24995 (16)	0.0374 (3)
C10	0.48299 (14)	0.46081 (6)	0.30913 (16)	0.0392 (3)
C11	0.55303 (12)	0.36842 (6)	0.41973 (16)	0.0366 (3)
C12	0.73234 (14)	0.31320 (6)	0.41359 (17)	0.0418 (3)
C13	0.67407 (12)	0.37005 (6)	0.36648 (15)	0.0359 (3)
C14	0.61894 (15)	0.52139 (7)	0.16089 (18)	0.0445 (3)
C15	0.42476 (13)	0.28945 (7)	0.55574 (16)	0.0414 (3)
C16	0.33155 (19)	0.32592 (8)	0.6121 (2)	0.0658 (5)
H16	0.3417	0.3680	0.6131	0.079*
C17	0.2218 (2)	0.29945 (10)	0.6676 (3)	0.0811 (6)
H17	0.1579	0.3241	0.7058	0.097*
C18	0.20561 (18)	0.23795 (9)	0.6674 (2)	0.0682 (5)
H18	0.1310	0.2207	0.7042	0.082*
C19	0.29922 (18)	0.20212 (9)	0.6129 (2)	0.0669 (5)
H19	0.2893	0.1600	0.6138	0.080*
C20	0.40913 (17)	0.22731 (7)	0.5562 (2)	0.0580 (4)
H20	0.4726	0.2023	0.5183	0.070*
C21	0.86622 (16)	0.28962 (8)	0.3862 (2)	0.0615 (5)
H21A	0.8791	0.2494	0.4314	0.092*
H21B	0.9359	0.3160	0.4391	0.092*
H21C	0.8699	0.2883	0.2704	0.092*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0335 (6)	0.0648 (8)	0.0489 (7)	−0.0131 (6)	0.0126 (5)	−0.0126 (6)
N2	0.0949 (12)	0.0515 (8)	0.0673 (9)	−0.0072 (8)	0.0194 (8)	0.0063 (7)
N3	0.0533 (8)	0.0583 (8)	0.0608 (8)	0.0199 (6)	0.0225 (6)	0.0096 (6)
N4	0.0356 (6)	0.0435 (6)	0.0475 (6)	−0.0009 (5)	0.0122 (5)	0.0011 (5)
N5	0.0378 (6)	0.0464 (7)	0.0569 (7)	0.0024 (5)	0.0108 (5)	0.0051 (6)
O1	0.0406 (5)	0.0763 (7)	0.0418 (5)	−0.0155 (5)	0.0111 (4)	−0.0182 (5)
O2	0.0358 (5)	0.0462 (5)	0.0508 (6)	0.0044 (4)	0.0146 (4)	0.0022 (4)
C1	0.0312 (6)	0.0404 (7)	0.0349 (6)	−0.0042 (5)	0.0063 (5)	−0.0047 (5)
C2	0.0334 (7)	0.0466 (7)	0.0407 (7)	−0.0057 (6)	0.0082 (5)	−0.0040 (6)
C3	0.0418 (7)	0.0423 (7)	0.0455 (7)	0.0001 (6)	0.0150 (6)	−0.0029 (6)
C4	0.0509 (9)	0.0594 (9)	0.0623 (10)	0.0043 (7)	0.0280 (8)	−0.0017 (8)
C5	0.0773 (12)	0.0601 (10)	0.0535 (9)	0.0170 (9)	0.0338 (9)	−0.0017 (8)
C6	0.0802 (12)	0.0495 (9)	0.0418 (8)	0.0128 (8)	0.0140 (8)	−0.0073 (6)
C7	0.0544 (9)	0.0417 (7)	0.0412 (7)	0.0015 (6)	0.0064 (6)	−0.0050 (6)
C8	0.0409 (7)	0.0358 (6)	0.0374 (7)	0.0009 (5)	0.0109 (5)	−0.0007 (5)
C9	0.0381 (7)	0.0375 (7)	0.0367 (6)	−0.0006 (5)	0.0057 (5)	−0.0046 (5)
C10	0.0398 (7)	0.0416 (7)	0.0363 (7)	0.0029 (6)	0.0060 (5)	−0.0044 (5)

C11	0.0320 (6)	0.0400 (7)	0.0382 (7)	−0.0002 (5)	0.0066 (5)	−0.0029 (5)
C12	0.0342 (7)	0.0445 (7)	0.0469 (8)	0.0000 (6)	0.0063 (6)	0.0001 (6)
C13	0.0299 (6)	0.0413 (7)	0.0364 (6)	−0.0033 (5)	0.0047 (5)	−0.0028 (5)
C14	0.0482 (8)	0.0430 (8)	0.0429 (7)	−0.0006 (6)	0.0086 (6)	−0.0049 (6)
C15	0.0366 (7)	0.0502 (8)	0.0388 (7)	−0.0049 (6)	0.0099 (5)	−0.0001 (6)
C16	0.0685 (11)	0.0557 (10)	0.0830 (13)	−0.0057 (8)	0.0431 (10)	−0.0117 (9)
C17	0.0702 (12)	0.0807 (14)	0.1060 (16)	0.0021 (10)	0.0569 (12)	−0.0063 (12)
C18	0.0531 (10)	0.0820 (13)	0.0748 (12)	−0.0128 (9)	0.0268 (9)	0.0111 (10)
C19	0.0603 (11)	0.0599 (10)	0.0837 (13)	−0.0114 (9)	0.0218 (9)	0.0131 (9)
C20	0.0517 (9)	0.0494 (9)	0.0772 (11)	0.0013 (7)	0.0237 (8)	0.0091 (8)
C21	0.0414 (8)	0.0590 (10)	0.0872 (13)	0.0085 (7)	0.0196 (8)	0.0120 (9)

Geometric parameters (Å, °)

N1—C2	1.3381 (17)	C6—C7	1.390 (2)
N1—C3	1.4081 (18)	C6—H6	0.9300
N1—H1	0.8600	C7—C8	1.3754 (19)
N2—C14	1.141 (2)	C7—H7	0.9300
N3—C10	1.3366 (18)	C9—C10	1.3548 (18)
N3—H3A	0.8600	C9—C14	1.417 (2)
N3—H3B	0.8600	C11—C13	1.3534 (17)
N4—C11	1.3488 (17)	C12—C13	1.4084 (19)
N4—N5	1.3764 (16)	C12—C21	1.489 (2)
N4—C15	1.4251 (16)	C15—C16	1.366 (2)
N5—C12	1.3258 (17)	C15—C20	1.374 (2)
O1—C2	1.2255 (16)	C16—C17	1.384 (2)
O2—C11	1.3620 (15)	C16—H16	0.9300
O2—C10	1.3716 (16)	C17—C18	1.361 (3)
C1—C13	1.4935 (18)	C17—H17	0.9300
C1—C9	1.5166 (18)	C18—C19	1.353 (3)
C1—C8	1.5189 (17)	C18—H18	0.9300
C1—C2	1.5525 (18)	C19—C20	1.378 (2)
C3—C4	1.3813 (19)	C19—H19	0.9300
C3—C8	1.3824 (19)	C20—H20	0.9300
C4—C5	1.387 (2)	C21—H21A	0.9600
C4—H4	0.9300	C21—H21B	0.9600
C5—C6	1.376 (3)	C21—H21C	0.9600
C5—H5	0.9300		
C2—N1—C3	111.98 (11)	C10—C9—C1	125.48 (12)
C2—N1—H1	124.0	C14—C9—C1	116.69 (11)
C3—N1—H1	124.0	N3—C10—C9	126.49 (13)
C10—N3—H3A	120.0	N3—C10—O2	110.13 (12)
C10—N3—H3B	120.0	C9—C10—O2	123.38 (12)
H3A—N3—H3B	120.0	N4—C11—C13	109.79 (11)
C11—N4—N5	109.11 (10)	N4—C11—O2	122.18 (11)
C11—N4—C15	130.78 (11)	C13—C11—O2	127.99 (12)
N5—N4—C15	119.80 (11)	N5—C12—C13	111.30 (12)
C12—N5—N4	105.73 (11)	N5—C12—C21	120.88 (13)
C11—O2—C10	113.87 (10)	C13—C12—C21	127.82 (13)

C13—C1—C9	106.77 (10)	C11—C13—C12	104.06 (11)
C13—C1—C8	115.12 (11)	C11—C13—C1	122.07 (12)
C9—C1—C8	114.43 (11)	C12—C13—C1	133.86 (11)
C13—C1—C2	111.00 (11)	N2—C14—C9	178.35 (17)
C9—C1—C2	108.46 (10)	C16—C15—C20	119.84 (14)
C8—C1—C2	100.88 (10)	C16—C15—N4	121.12 (14)
O1—C2—N1	126.29 (13)	C20—C15—N4	119.03 (13)
O1—C2—C1	125.13 (11)	C15—C16—C17	119.13 (17)
N1—C2—C1	108.58 (11)	C15—C16—H16	120.4
C4—C3—C8	122.46 (14)	C17—C16—H16	120.4
C4—C3—N1	128.18 (14)	C18—C17—C16	121.16 (17)
C8—C3—N1	109.36 (11)	C18—C17—H17	119.4
C3—C4—C5	116.65 (16)	C16—C17—H17	119.4
C3—C4—H4	121.7	C19—C18—C17	119.31 (16)
C5—C4—H4	121.7	C19—C18—H18	120.3
C6—C5—C4	121.65 (14)	C17—C18—H18	120.3
C6—C5—H5	119.2	C18—C19—C20	120.70 (17)
C4—C5—H5	119.2	C18—C19—H19	119.6
C5—C6—C7	120.77 (15)	C20—C19—H19	119.6
C5—C6—H6	119.6	C15—C20—C19	119.85 (16)
C7—C6—H6	119.6	C15—C20—H20	120.1
C8—C7—C6	118.32 (15)	C19—C20—H20	120.1
C8—C7—H7	120.8	C12—C21—H21A	109.5
C6—C7—H7	120.8	C12—C21—H21B	109.5
C7—C8—C3	120.14 (12)	H21A—C21—H21B	109.5
C7—C8—C1	130.69 (12)	C12—C21—H21C	109.5
C3—C8—C1	109.17 (11)	H21A—C21—H21C	109.5
C10—C9—C14	117.73 (12)	H21B—C21—H21C	109.5

C11—N4—N5—C12	0.01 (15)	C11—O2—C10—N3	176.12 (11)
C15—N4—N5—C12	174.29 (12)	C11—O2—C10—C9	−3.13 (18)
C3—N1—C2—O1	−177.13 (15)	N5—N4—C11—C13	−0.03 (15)
C3—N1—C2—C1	1.82 (17)	C15—N4—C11—C13	−173.48 (13)
C13—C1—C2—O1	−60.38 (18)	N5—N4—C11—O2	177.86 (11)
C9—C1—C2—O1	56.62 (18)	C15—N4—C11—O2	4.4 (2)
C8—C1—C2—O1	177.16 (14)	C10—O2—C11—N4	−174.36 (12)
C13—C1—C2—N1	120.66 (12)	C10—O2—C11—C13	3.11 (19)
C9—C1—C2—N1	−122.35 (12)	N4—N5—C12—C13	0.02 (16)
C8—C1—C2—N1	−1.81 (15)	N4—N5—C12—C21	−179.85 (14)
C2—N1—C3—C4	178.50 (15)	N4—C11—C13—C12	0.04 (15)
C2—N1—C3—C8	−1.03 (18)	O2—C11—C13—C12	−177.69 (13)
C8—C3—C4—C5	0.9 (2)	N4—C11—C13—C1	180.00 (11)
N1—C3—C4—C5	−178.53 (15)	O2—C11—C13—C1	2.3 (2)
C3—C4—C5—C6	−1.3 (3)	N5—C12—C13—C11	−0.03 (16)
C4—C5—C6—C7	0.6 (3)	C21—C12—C13—C11	179.83 (15)
C5—C6—C7—C8	0.4 (2)	N5—C12—C13—C1	−179.99 (13)
C6—C7—C8—C3	−0.7 (2)	C21—C12—C13—C1	−0.1 (3)
C6—C7—C8—C1	179.10 (14)	C9—C1—C13—C11	−6.46 (16)
C4—C3—C8—C7	0.0 (2)	C8—C1—C13—C11	−134.66 (13)
N1—C3—C8—C7	179.58 (13)	C2—C1—C13—C11	111.56 (14)

C4—C3—C8—C1	−179.81 (14)	C9—C1—C13—C12	173.49 (14)
N1—C3—C8—C1	−0.25 (16)	C8—C1—C13—C12	45.3 (2)
C13—C1—C8—C7	61.85 (19)	C2—C1—C13—C12	−68.48 (18)
C9—C1—C8—C7	−62.41 (18)	C10—C9—C14—N2	−176 (100)
C2—C1—C8—C7	−178.61 (14)	C1—C9—C14—N2	8(6)
C13—C1—C8—C3	−118.34 (13)	C11—N4—C15—C16	−29.0 (2)
C9—C1—C8—C3	117.40 (13)	N5—N4—C15—C16	158.13 (15)
C2—C1—C8—C3	1.21 (14)	C11—N4—C15—C20	150.19 (16)
C13—C1—C9—C10	6.56 (17)	N5—N4—C15—C20	−22.7 (2)
C8—C1—C9—C10	135.16 (13)	C20—C15—C16—C17	−0.5 (3)
C2—C1—C9—C10	−113.12 (14)	N4—C15—C16—C17	178.65 (17)
C13—C1—C9—C14	−177.13 (11)	C15—C16—C17—C18	0.2 (3)
C8—C1—C9—C14	−48.53 (16)	C16—C17—C18—C19	0.5 (4)
C2—C1—C9—C14	63.20 (14)	C17—C18—C19—C20	−0.8 (3)
C14—C9—C10—N3	2.5 (2)	C16—C15—C20—C19	0.2 (3)
C1—C9—C10—N3	178.78 (13)	N4—C15—C20—C19	−178.97 (15)
C14—C9—C10—O2	−178.36 (12)	C18—C19—C20—C15	0.5 (3)
C1—C9—C10—O2	−2.1 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O2	0.93	2.42	2.959 (2)	117
N1—H1···O1^{i}	0.86	1.99	2.819 (2)	161
N3—H3B···O1^{ii}	0.86	2.12	2.880 (1)	148
C6—H6···Cg^{iii}	0.92	2.85	3.771 (3)	173

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, *y*−1, *z*−1.

Fig. 1

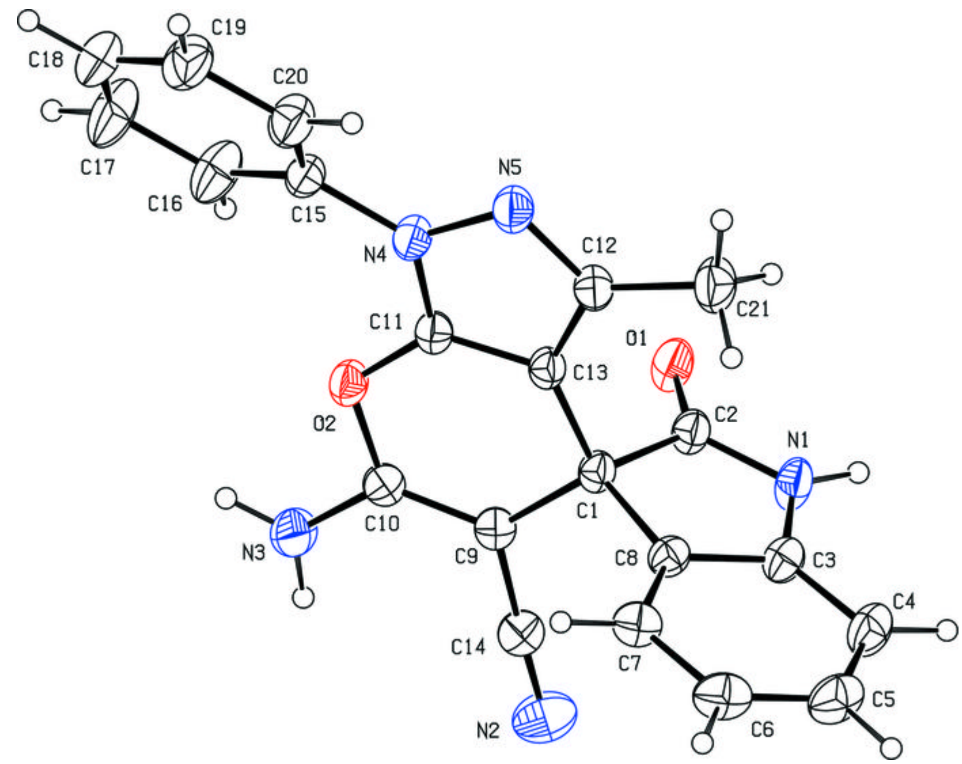
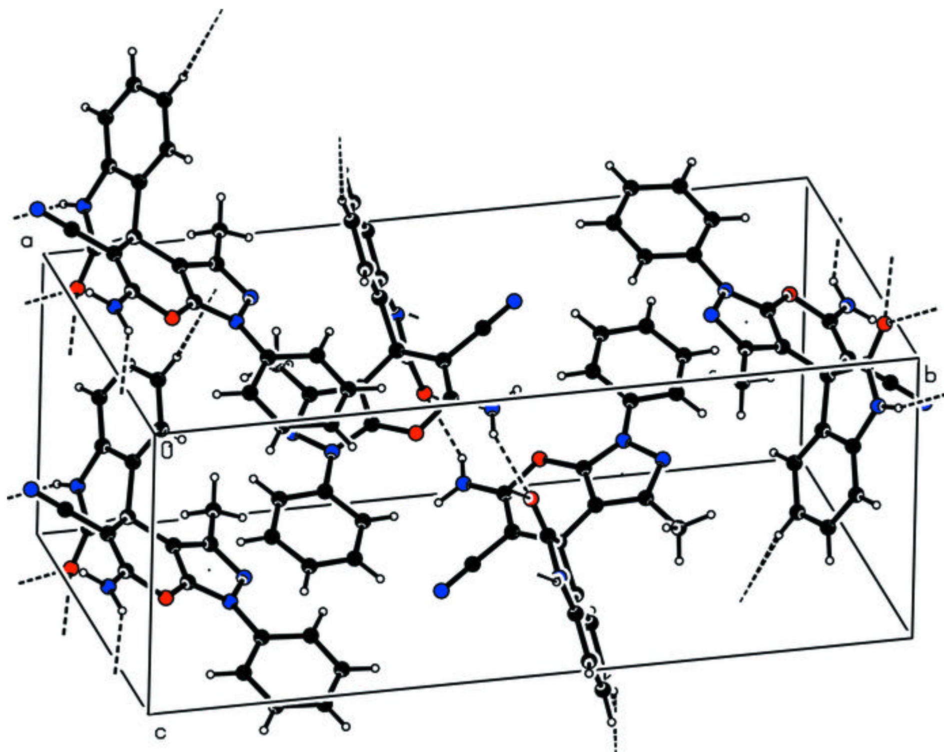

C18
C19
C20
C17
C16
C15
N5
N4
C12
C21
C11
O1
C13
O2
C2
N1
C1
C10
C9
N3
C8
C3
C4
C14
C7
C5
N2
C6

Fig. 2



Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

6′-Amino-3′-methyl-2-oxo-1′-phenyl-1′,3a′,4′,7a′-tetrahydrospiro[1*H*-indole-3(2*H*),4′-pyrano[2,3-*d*]pyrazole]-5′-carbonitrile. Corrigendum

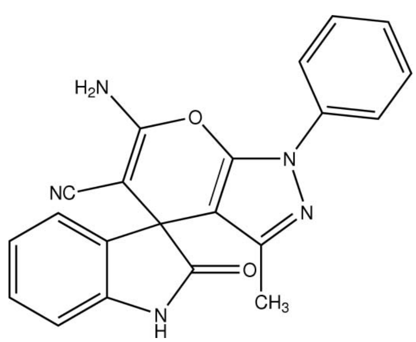
S. Etti,[a] G. Shanthi,[b] G. Shanmugam[a]* and P. T. Perumal[b]

[a]Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, and [b]Organic Chemistry Division, Central Leather Research Institute, Adyar, Chennai 600 020, India
Correspondence e-mail: gurushan48@yahoo.com

Received 22 February 2008; accepted 27 February 2008

The title and chemical structural diagram in Etti, Shanmugam & Perumal [*Acta Cryst.* (2008), E**64**, o341] are corrected.

In the paper by Etti, Shanmugam & Perumal [*Acta Cryst.* (2008), E**64**, o341], the chemical name in the title and the structual diagram are incorrect. The correct title should be '6′-Amino-3′-methyl-2-oxo-1′-phenyl-1′,4′-tetrahydrospiro[1*H*-indole-3(2*H*),4′-pyrano[2,3-*d*]pyrazole]-5′-carbonitrile' and the correct scheme is shown below.



 doi:10.1107/S1600536808005564