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(±)-*N*-[4-Acetyl-5-methyl-5-(4-methylcyclohex-3-enyl)-4,5-dihydro-1,3,4-thiadiazol-2-yl]acetamide

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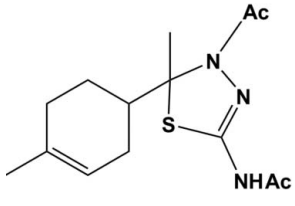
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.113; data-to-parameter ratio = 25.1.

The new title thiadiazole compound, $C_{14}H_{21}N_3O_2S$, was semi-synthesized starting from 1-(4-methylcyclohex-3-enyl)-ethanone, a natural product isolated from *Cedrus atlantica* essential oil. The stereochemistry has been confirmed by single-crystal X-ray diffraction. The thiadiazoline ring is roughly planar, although it may be regarded as having a half-chair conformation. The cyclohexenyl ring has a half-chair conformation. The most interesting feature is the formation of a pseudo-ring formed by four molecules associated through N—H···O hydrogen bonds around a fourfold inversion axis, forming an $R_4^4(28)$ motif.

Related literature

For related literature, see: Aly *et al.* (2007); Beatriz *et al.* (2002); Bernstein *et al.* (1995); Cremer & Pople (1975); Demirbas *et al.* (2005); Etter *et al.* (1990); Farghaly *et al.* (2006); Invidiata *et al.* (1996); Kubota *et al.* (1982); Nizamuddin *et al.* (1999); Ourhriss *et al.* (2005); Paolo *et al.* (2005); Radul *et al.* (2005); Sun *et al.* (1999); Udupi *et al.* (2000).



Experimental

Crystal data

$C_{14}H_{21}N_3O_2S$
M_r = 295.40
Tetragonal, $I4_1/a$
a = 16.6855 (3) Å
c = 21.8961 (8) Å
V = 6096.0 (3) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 180 (2) K
0.29 × 0.24 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: none
87517 measured reflections
4637 independent reflections
3849 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.113
S = 1.11
4637 reflections
185 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1^{i}	0.88	1.95	2.8223 (14)	171

Symmetry code: (i) $y+\frac{1}{4}, -x+\frac{7}{4}, -z+\frac{3}{4}$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2164).

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