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# 2-[(2-Chlorophenyl)(1,2,3,4-tetrahydro-1-oxo-2-naphthyl)methyl]malononitrile

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**Key indicators**

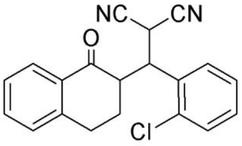
Single-crystal X-ray study
*T* = 193 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.064
*wR* factor = 0.165
Data-to-parameter ratio = 17.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{20}H_{15}ClN_2O_3$, was synthesized by the reaction of 2-(2-chlorobenzylidene)-1-tetralone and malononitrile in dimethylformamide in the presence of KF–montmorillonite as a catalyst. Intermolecular C—H···O and C—H···N hydrogen bonds link adjacent molecules into dimers and propagate chains along the *c* axis.

## Comment

Recently, montmorillonite, in both natural and exchanged forms, has received considerable attention as a catalyst in various organic syntheses because of its environmental compatibility, low cost, high selectivity, reusability and operational simplicity (Hauke *et al.*, 1994). Typical reactions include rearrangements (Chalais *et al.*, 1986), oxidation (Cornelis & Laszlo, 1980) and addition (Braibante *et al.*, 1994). In most previous work, montmorillonite clays have been reported as being used as acid catalysts (Villemin & Martin, 1994; Cornelis *et al.*, 1984). However, we have found that montmorillonite coated with potassium fluoride (KF–montmorillonite), as an alkaline catalyst, results in higher selectivity, lower cost and easier work-up in organic synthesis (Shi *et al.*, 2002). The title compound, (I), was synthesized by the reaction of 2-(2-chlorobenzylidene)-1-tetralone and malononitrile in dimethylformamide in the presence of KF–montmorillonite and its structure is reported here (Fig. 1).



(I)

In the molecule of (I), the fused six-membered C2–C7 ring adopts a half-chair conformation. Atoms C3, C4, C5 and C6 are coplanar, with a maximum deviation of 0.010 (2)Å for atom C5, while atoms C2 and C7 deviate from this plane by 0.130 (2) and −0.564 (2) Å, respectively. Similar conformations were observed in 2-amino-4-phenyl-5,6-dihydrobenzo[*h*]quinazoline (Wang, Shi *et al.*, 2003) and 2-amino-3-cyano-4-(4-methoxyphenyl)-1,4,5,6-tetrahydrobenzo[*h*]chromene (Wang, Li *et al.*, 2003). The plane through C3/C4/C5/C6 is almost parallel to that of the fused benzene ring C4/C5/C8–C11, with a dihedral angle of 1.53 (2)°.

In the crystal structure of (I), intermolecular C20—H20···O1[i] and C12—H12···O1[i] hydrogen bonds link adjacent molecules into inversion-related dimers. Additional C10—H10···N1[ii] interactions form a network structure (Fig. 2; symmetry codes as in Table 1).

## Experimental

The title compound, (I), was prepared by the reaction of 2-(2-chlorobenzylidene)-1-tetralone (0.54 g, 2 mmol) and malononitrile (0.13 g, 2 mmol) in the presence of KF–montmorillonite (0.25 g) in dimethylformamide (10 ml) at room temperature for 9 h (yield 82%; m.p. 453–455 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a solution in dimethylformamide. Elemental analysis, calculated: C 71.75, H 4.52, N 8.37%; found: C 71.84, H 4.47, N 8.52%. IR (KBr, $\nu$, cm$^{-1}$): 3065 (Ar—H), 2950, 2921, 2868 (C—H), 2247 (CN), 1673 (C═O), 1597, 1476, 1435 (phenyl ring).

### *Crystal data*

$C_{20}H_{15}ClN_2O$
$M_r = 334.79$
Monoclinic, $P2_1/c$
$a = 8.2263\ (8)$ Å
$b = 19.3791\ (19)$ Å
$c = 10.6624\ (10)$ Å
$\beta = 94.198\ (3)^\circ$
$V = 1695.2\ (3)$ Å$^3$
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.23$ mm$^{-1}$
$T = 193\ (2)$ K
0.80 × 0.60 × 0.19 mm

### *Data collection*

Rigaku Mercury CCD area-detector diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
$T_{\min} = 0.835$, $T_{\max} = 0.957$
18644 measured reflections
3859 independent reflections
3452 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.024$

### *Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.165$
$S = 1.10$
3859 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.43$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.56$ e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C20—H20···O1$^{\rm i}$ | 0.95 | 2.52 | 3.277 (3) | 136 |
| C20—H20···O1 | 0.95 | 2.46 | 3.227 (4) | 138 |
| C12—H12···O1$^{\rm i}$ | 1.00 | 2.50 | 3.489 (3) | 170 |
| C10—H10···N1$^{\rm ii}$ | 0.95 | 2.62 | 3.417 (3) | 141 |

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

H atoms were positioned geometrically and refined as riding, with C—H = 0.95 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aromatic H, C—H = 1.00 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for CH, and C—H = 0.99 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for $CH_2$.

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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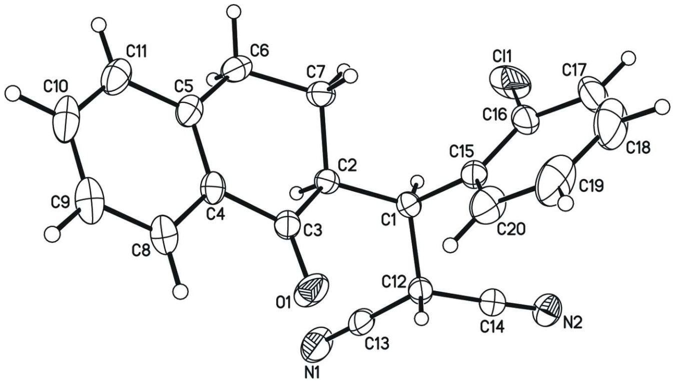

**Figure 1**
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

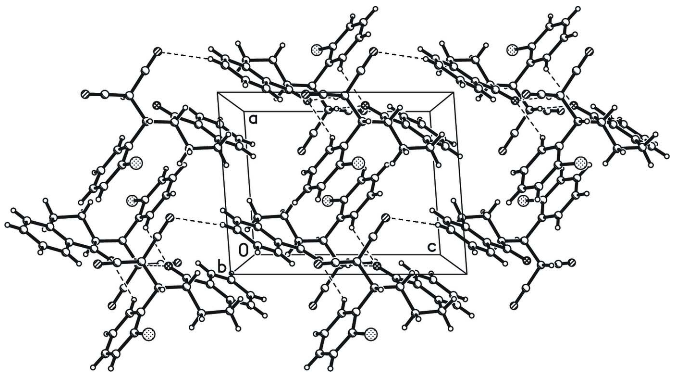

**Figure 2**
A packing diagram for (I), with hydrogen bonds drawn as dashed lines.

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