Journal of Solid State Chemistry **152,** 221–228 (2000)
doi:10.1006/jssc.2000.8685, available online at http://www.idealibrary.com on IDEAL®

C–H···O and C–H···N Hydrogen Bond Networks in the Crystal Structures of Some 1,2-Dihydro-*N*-aryl-4,6-dimethylpyrimidin-2-ones

Meiyappan Muthuraman,*,† Yvette Le Fur,* Muriel Bagieu-Beucher,* René Masse,* Jean-François Nicoud,† Sumod George,‡ Ashwini Nangia,‡ and Gautam R. Desiraju‡,[1]

*Laboratorie de Cristallographie associé à l'Université Joseph Fourier, CNRS, BP166, 38042 Grenoble Cedex, France; †Groupe des Matériaux Organiques, Institut de Physique de Chimie des Matériaux de Strasbourg, CNRS et Université Louis Pasteur (UMR 7504), 23, rue du Loess, 67037 Strasbourg Cedex, France; and ‡School of Chemistry, University of Hyderabad, Hyderabad 500 046, India

A set of three aryl dimethyl pyrimidinones have been studied and their crystal structures described in terms of networks of C–H···O and C–H···N hydrogen bonds. Two of the three molecules in this study differ in the replacement of a chloro group by a methyl group and obey the chloro–methyl exchange rule in that they have nearly identical crystal structures. However, and in contrast to other pairs of compounds so related, the chloro and methyl groups here are not merely isosteric but also form similar polarization-induced Cl···Ph and CH_3···Ph contacts. These conjugated molecules may offer some scope for nonlinear optical studies.

Key Words: **hydrogen bond; supramolecular synthon; nonlinear optical; network; chloro-methyl exchange.**

INTRODUCTION

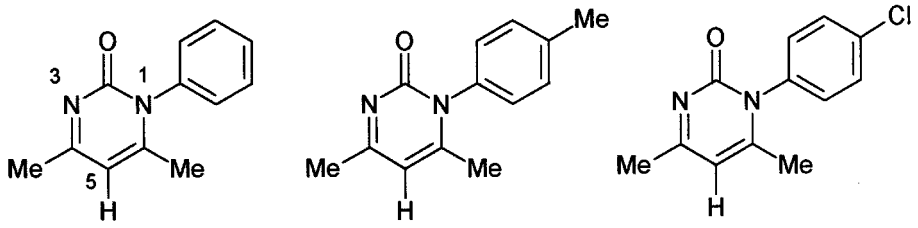
Identification of repetitive patterns in a group of crystal structures is an important endeavor in the design of extended solids. Such robust patterns have been termed *supramolecular synthons* (1) and link molecules, that is *tectons* (2), in one-, two-, and three-dimensional networks. Crystal structures of molecular solids are determined by a convolution of a large number of intermolecular interactions. However, these interactions are generally weak and of variable directionality. Accordingly, small changes in the molecular functionality can often change packing preferences substantially. One therefore attempts to seek out a particular combination of molecular functionalities which leads to a particular supramolecular synthon. If such an attempt is successful, for a synthon of sufficient size, one may access a large number of related crystal structures from a set of related molecular structures (3).

The term *network* has been applied commonly to hydrogen-bonded solids, coordination polymers, and several organic–inorganic mixed varieties (4–9). However, at a formalistic level, all organic crystal structures may be considered to be networks. Indeed, the concept of a supramolecular synthon implies that an organic crystal structure can be represented as a retrosynthetic target, and this is most easily done if it is reduced to a network. Molecular solids assembled with O–H···O and N–H···O hydrogen bonds lend themselves easily to a network description; one of the earliest explicit examples of this is the diamondoid structure of adamantane-1,3,5,7-tetracarboxylic acid (10). Yet, it is also possible to have a network description for solids that contain only weak hydrogen bonds; these include C–H···O, C–H···N, and C–H···π among others (11). An advantage of the network representation is that topological similarities between crystal structures are effectively revealed, so that relationships may be found between crystal structures of widely differing species (12). Many examples are known but we mention here just two, from the Hyderabad group—1,3,5,7-tetrahydroxyadamantane and CsCl have the same network topology (13) while tetrakis(4-bromophenyl)methane and the 1 : 1 molecular complex of tetraphenylmethane and CBr_4 are nearly isostructural (14).

With this backdrop, we move to the present structural study of a set of 1,2-dihydro-*N*-aryl-4,6-dimethylpyrimidin-2-ones, **1–3**. This molecular skeleton is unusually rich in C–H donors and O, N, and π acceptors, and was considered from the viewpoint of new molecules for nonlinear optical (NLO) applications (15). In this latter context, we noted that 1,2-dihydro-*N*-(2-hydroxyethyl)-4,6-dimethylpyrimidin-2-one crystallizes in the space group $P2_1$ with infinite chains of O–H···N hydrogen bonds (16). In the present study, which is exploratory, we report the single-crystal X-ray structures of the *N*-phenyl, *N*-4-tolyl, and *N*-4-chlorophenyl derivatives **1**, **2**, and **3** (see Scheme 1), respectively, and analyze them in terms of networks of C–H···O and C–H···N hydrogen bonds.

[1] To whom correspondence should be addressed. Fax: +91 40 3010567. E-mail: grdch@uohyd.ernet.in

0022-4596/00 $35.00



1 2 3

SCHEME 1

EXPERIMENTAL

Preparation and Characterization

1,2-*Dihydro-N-phenyl*-4,6-*dimethylpyrimidin*-2-*one* 1 (17). Acetyl acetone (2.6 ml, 2.4 g, 24 mmol) and *N*-phenyl urea (2.72 g, 20 mmol) were taken in 25 ml of 95% EtOH and concentrated HCl (5 ml) was added. The reaction mixture was refluxed for 3 h, then cooled in ice, and the precipitated solid was filtered and washed with cold EtOH to provide **1**. HCl (3.85 g). The salt was dissolved in 10 ml of water and neutralized with NaOH solution (0.7 g in 5 ml of water) at 0°C. Extraction of the aqueous layer with chloroform and evaporation of the solvent afforded 2.8 g of phenyl derivative **1**. Mp. 214–215°C. FT-IR (cm^{-1}): 3086, 1651, 1530, 1480, 1334, 1170, 1076, 1005, 949, 779, 634. ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.55–7.15 (m, 5H), 6.16 (s, 1H), 2.42 (s, 3H), 1.97 (s, 3H).

4-*Tolyl derivative* 2. Mp: 190–192°C. FT-IR (partial, cm^{-1}): 1657. ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.30 (d, $J = 8$ Hz, 2H), 7.10 (d, $J = 8$ Hz, 2H), 6.20 (s, 1H), 2.42 (s, 6H), 2.00 (s, 3H).

4-*Chlorophenyl derivative* 3. Mp: 215–216°C. FT-IR (partial, cm^{-1}): 1655. ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.52 (d, $J = 7$ Hz, 2H), 7.13 (d, $J = 7$ Hz, 2H), 6.22 (s, 1H), 2.45 (s, 3H), 2.00 (s, 3H).

Crystal Structure Determination

The cell parameters, space groups, and crystal structures were determined from single-crystal X-ray diffraction data collected at ambient temperature on Nonius-CAD4 diffractometers (Grenoble and Hyderabad) with Mo$K\alpha$ radiation ($\lambda = 0.7107$ Å). Crystal data, experimental conditions, and structure refinement parameters for **1–3** are mentioned in Table 1. No absorption corrections were applied. The structures were solved by direct methods using the SIR92 program (18). Full-matrix least-squares refinements were performed on F using the teXsan software (19). Scattering factors for neutral atoms and f', $\Delta f'$, f'', $\Delta f''$ were taken from the *International Tables for X-ray Crystallography* (20). Some important interatomic distances and hydrogen bonds are summarized in Table 2. Lists of atomic coordinates and complete geometry have been deposited with the Cambridge Crystallographic Data Centre and can be obtained upon request from CCDC, 12 Union Road, Cambridge CB2 1EZ, England (Fax +44 1223 336033; E-mail deposit@ccdc.cam.ac.uk).

RESULTS AND DISCUSSION

The synthesis of *N*-aryl pyrimidinones **1–3** was carried out by condensation of the corresponding *N*-aryl urea with acetyl acetone in the presence of an acid catalyst (17, 21).

TABLE 1
Crystallographic Data on Structures 1–3

	1	2	3
Empirical formula	$C_{12}H_{12}N_2O$	$C_{13}H_{14}N_2O$	$C_{12}H_{11}N_2OCl$
Formula wt	200.24	214.27	234.68
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	*Pbcm*	*Pnma*	*Pnma*
a (Å)	7.13(2)	7.263(1)	7.298(1)
b (Å)	18.104(5)	8.591(2)	8.504(3)
c (Å)	8.612(1)	19.488(4)	19.472(2)
α (°)	90	90	90
β (°)	90	90	90
γ (°)	90	90	90
Z	4	4	4
V (Å^3)	1111(1)	1216(1)	1208(1)
D_{calc} (Mg/m^3)	1.20	1.17	1.29
$F(000)$	424	456	488
θ range (°)	2–30	3–34	3–35
Index range h	0, 10	−10, 10	−11, 11
k	−25, 0	−12, 12	0, 13
l	0, 12	0, 27	0, 31
Mp (K)	487–488	463–465	488–489
R_1	0.058	0.044	0.043
w$R2$	0.046	0.047	0.035
GOF	2.779	5.181	3.067
N-unique	1725	2927	3014
N-observed	674	609	959
Variables	85	91	109
C_k	63.9	63.8	64.2

TABLE 2
Geometry of C–H···O and C–H···N Interactions in Pyrimidinones 1–3

Pyrimidinone	Interaction	H···O/N (Å)	C···O/N (Å)	C–H···O/N (°)
1	C(5)–H···O (*i*)	2.11	3.118(8)	171.5
	C(*p*-Ph)–H···N (*j*)	2.42	3.497(8)	168.5
	C(*o*-Ph)–H···O (*k*)	2.51	3.247(8)	123.6
	C(*m*-Ph)–H···O	2.84	3.413(9)	112.7
	C(*m*-Ph)–H···N	2.93	3.775(8)	134.4
	C(6-Me)–H···O	2.82	3.801(9)	149.5
2	C(5)–H···O (*i*)	2.22	3.306(8)	173.9
	C(*o*-Ph)–H···O (*k*)	2.48	3.226(8)	125.0
	C(*m*-Ph)–H···O	2.73	3.319(8)	113.7
	C(*m*-Ph)–H···N	2.83	3.732(9)	140.2
3	C(5)–H···O (*i*)	2.26	3.445(7)	178.4
	C(*o*-Ph)–H···O (*k*)	2.45	3.171(8)	122.2
	C(*m*-Ph)–H···O	2.72	3.291(8)	112.5
	C(*m*-Ph)–H···N	2.77	3.657(7)	138.8

Note. All C–H distances are neutron-normalized to 1.083 Å.

The three compounds were characterized by their satisfactory NMR and IR spectra. The compounds were recrystallized from chloroform/hexane to afford single crystals suitable for X-ray diffraction: pale yellow for **1**, pale red for **2**, and pink for **3**.

Crystal Structure Analysis

The phenyl pyrimidinone **1** crystallizes in the orthorhombic space group *Pbcm* (No. 57). The heterocyclic ring lies in the mirror plane and the *N*-phenyl ring is bisected by it (Fig. 1a). Translation-related molecules are connected by a linear chain of C–H···O hydrogen bonds along [100] (2.11 Å, 171.5°, interaction *i*) from the C5–H donor to the carbonyl acceptor. A zigzag chain of C–H···N hydrogen bonds (2.42 Å, 168.5°, interaction *j*) from the *p*-phenyl *H* atom to the N3 acceptor connects *b*-glide-related molecules. Thus, a two-dimensional C–H···O/N network of pyrimidinone rings is produced with the *N*-phenyl rings orthogonal to it. Adjacent layers are offset such that the phenyl ring of one molecule approaches the pyrimidinone heterocycle of the next layer in an edge-to-face manner (C–H···O, 2.51 Å, 123.6°, interaction *k*) (Fig. 1b). The activated donor hydrogens (phenyl and sp^2 C–H) and the basic acceptor (carbonyl O atom) mediate self-assembly in the crystal structure. Since the molecule is donor rich, the O atom behaves as a trifurcated acceptor when the weak C–H···O interaction from the methyl donor (2.82 Å, 149.5°, not shown in Fig. 1b) is also considered. The crystallographic data and metrics of hydrogen bonds in **1**, **2**, and **3** are given in Tables 1 and 2.

In order to assess the importance of the (*p*-phenyl) C–H···N interaction in the layered structure of **1**, the crystal structure of the tolyl derivative **2** was next determined. Compound **2** crystallizes in the space group *Pnma* (No. 62) and here too the heterocyclic ring lies in the mirror plane while the tolyl ring is bisected by it. Translation-related molecules are connected by a linear chain of C–H···O hydrogen bonds (2.22 Å, 173.9°, interaction *i*) along [100] (Fig. 2a). Such *a*-glide-related chains are close-packed to produce the *ac*-layer, which in turn is connected to the adjacent layer through C–H···O interactions from the *o*- and *m*-phenyl H atoms to the carbonyl O atom (2.48 Å, 125.0°, interaction *k*; 2.73 Å, 113.7°, not indicated in the figure) (Fig. 2b). There are two types of methyl groups in the tolyl derivative **2**: the C4- and C6-methyl groups are close-packed with van der Waals contacts while the tolyl methyl group points toward the phenyl π-cloud centroid of an adjacent molecule (C···π 3.78 Å). This latter approach geometry is appropriate for electrostatic stabilization of the C–H dipole by the negatively charged surface of the phenyl ring, that is C($\delta-$)-H($\delta+$)···π($\delta-$), though it is difficult to say whether the interaction represents a C–H···π hydrogen bond (11). This is so for two reasons: (i) the interaction is extremely weak and soft; (ii) the exact location of methyl H atoms cannot be determined accurately by X-ray diffraction. Therefore, to better understand the structural role of the tolyl methyl group in **2**, the crystal structure of the chloro analogue **3** was analyzed.

The chloro–methyl exchange rule (22) states that in structures governed by close-packing and shape and size arguments, a methyl group can be replaced in the molecule by a chloro group without a change in crystal structure. This rule follows from the nearly equal volumes of the two groups (Cl 20 Å^3, Me 24 Å^3). In structures wherein the methyl and/or chloro groups participate in intermolecular interactions peculiar to their own distinctive supramolecular characteristics, chloro–methyl exchange is normally not expected. For instance, hexachlorobenzene and hexamethylbenzene have quite different crystal structures because the many Cl···Cl interactions in the former are of the polarization-induced type-II variety (23) and as such inaccessible to methyl groups. In contrast, numerous examples of crystal structures are known in which the close-packed methyl groups can be replaced by type-I van der Waals Cl···Cl interactions (24). However, pyrimidinone **2** is different in that the tolyl methyl group is polarized by the phenyl π-cloud. To our knowledge, the exchange of methyl by chloro groups in such an environment (type-II) has not been studied. For convenience, type-I and type-II geometries for chloro and methyl groups are illustrated in Fig. 4.

In the present instance, pyrimidinones **2** and **3** do exhibit the phenomenon of chloro–methyl exchange. We note that the space group in both cases is the same (*Pnma*) and that the unit cell dimensions are nearly identical. Further, the

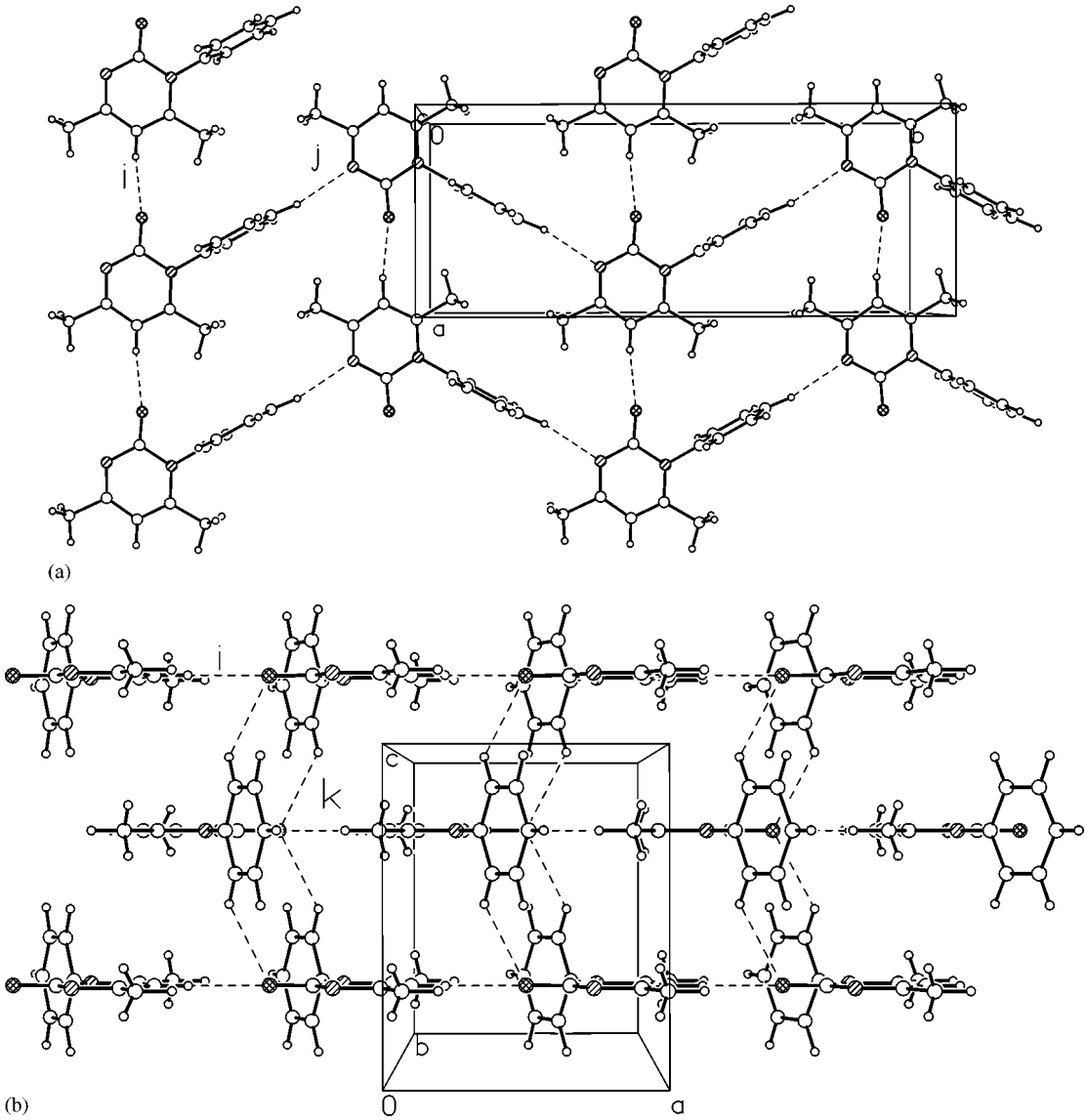


FIG. 1. Crystal structure of phenyl pyrimidinone **1**. (a) View of the *ab*-layer to show the C–H···O and C–H···N hydrogen bond network (interactions *i* and *j*). Notice that the molecules in adjacent chains run antiparallel along [100]. (b) View of the structure down [010]. O, N, and Cl atoms are shaded in Figs. 1, 2, and 3. For a description of the interactions, see text and Table 2.

placement of molecules in the *ac*-layer is identical in the two structures and the packing of the chlorophenyl moiety in **3** is identical to that of the tolyl rings in **2** (Figs. 2 and 3). The metrics of the Cl···π (centroid) interaction in **3** are 3.54 Å and 177.5° (interaction *j* in Fig. 3a). The distances and angles of the other hydrogen bonds in **3** are similar to those found in **2** (Table 2).

In principle, and as mentioned above, chloro–methyl exchange is possible in two distinct situations (Fig. 4): (i) A more common one wherein the groups are related by inversion symmetry so that a Cl group can be replaced by an isosteric Me group. This corresponds to the type-I geometry. (ii) A far less common one wherein the chloro group is present in an L- or T-shaped orientation with respect to a nucleophilic group. This is the type-II geometry. A methyl exchange in such cases would not normally be expected because the methyl group would be expected to behave as an electrophile. However, this is what is seen in the present case. So, the replacement of the Me group in **2** by the Cl group in **3** is not merely isosteric but also leads to the corresponding Cl($\delta+$)···π($\delta-$) interaction. The ability of chlorophenyl (and in general halophenyl) groups to engage in polarization-induced electrophile–nucleophile C–Cl···π contacts has only been appreciated recently (25, 26). Studies

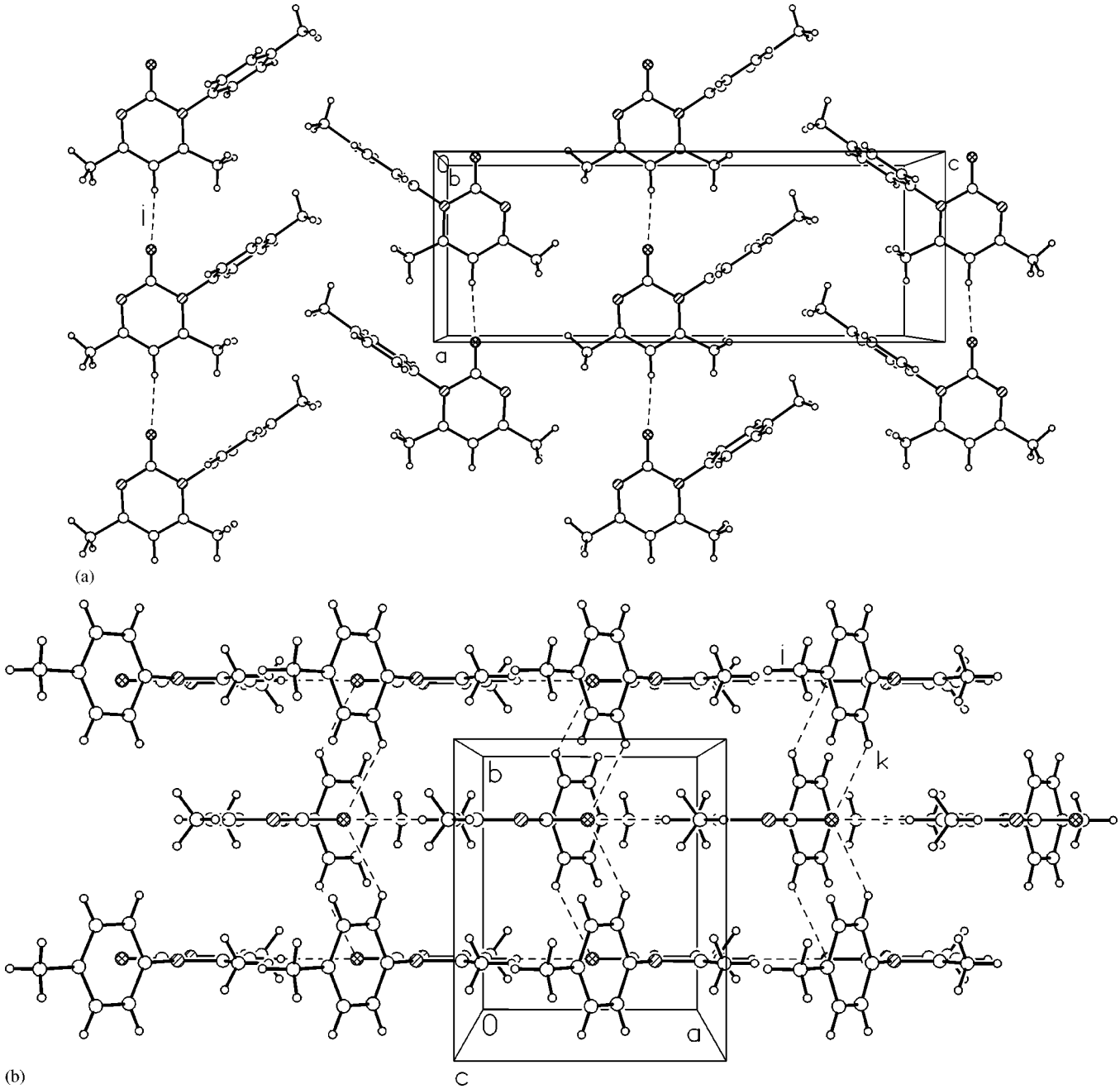


FIG. 2. Crystal structure of tolyl pyrimidinone **2**. View of the *ac*-layer to show the C–H···O chain (interaction *i*) and the T-shaped approach of the tolyl methyl group to the phenyl ring centroid ($H_3C\cdots\pi$ 3.78 Å). Notice the parallel arrangement of molecules along [100]. (b) View of the structure down [001].

of C–H···π hydrogen bonding are also relatively new (11). Pyrimidinones **2** and **3** furnish a rare case of methyl– chloro exchange in which the two groups are not just occupying the same volume but are also involved in comparable electrostatic interactions.

The isostructural Me/Cl pair, **2** and **3**, may be contrasted with the tetraphenylporphyrin crystal structures wherein the 4-chlorophenylporphyrin contains the unusual C–Cl···π contact (25) but the 4-tolyl derivative has a very different crystal packing (27). In 4-tolylporphyrin, the phenyl rings are stacked with offset so as to form a cooperative array of C–H···π interactions. Based on some of these recent examples, it appears that the polarization-type C–Cl···π interaction could also emerge as a useful supramolecular synthon in crystal engineering and complement the well-known steering ability of Cl···Cl interactions (28).

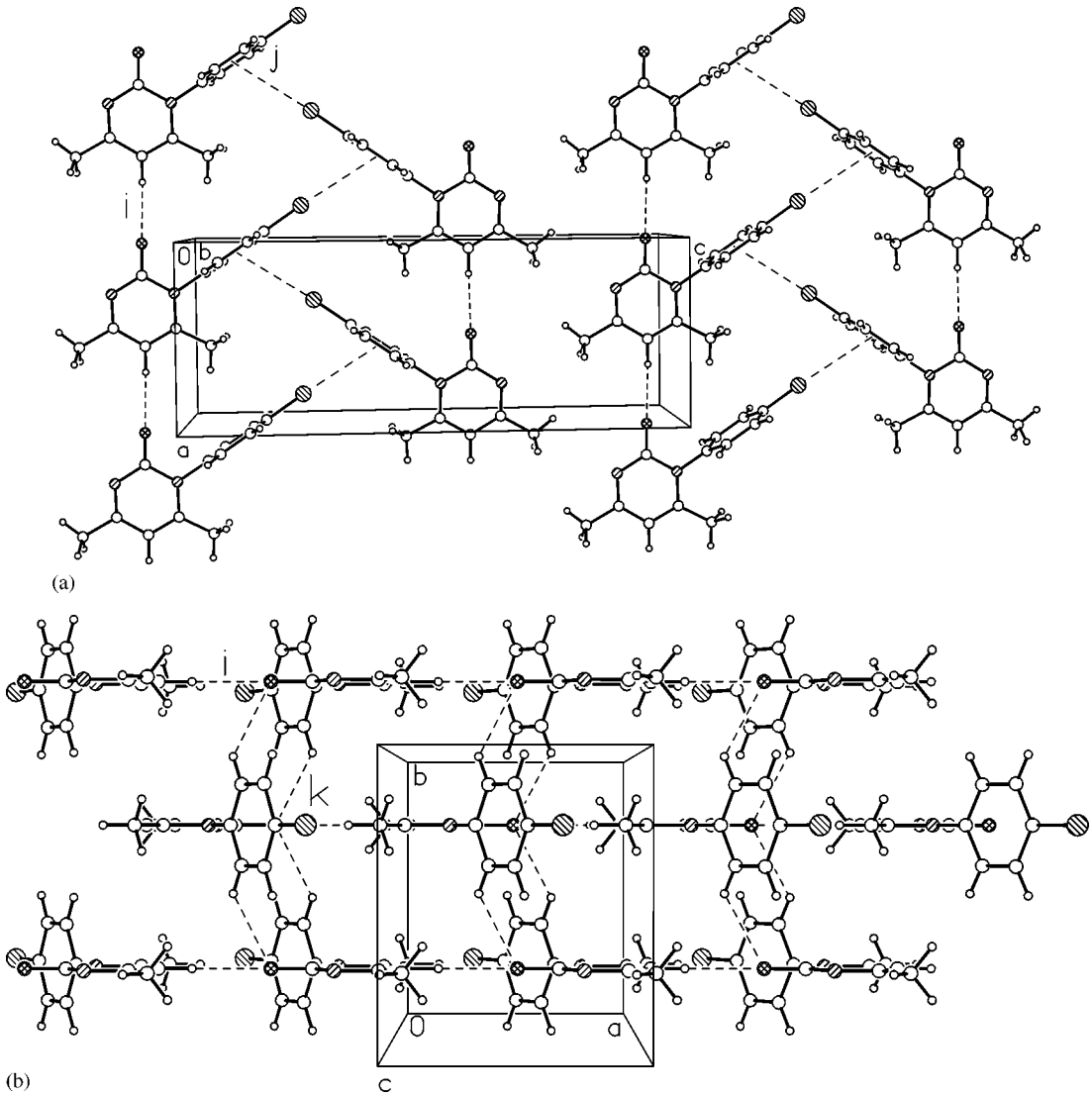


FIG. 3. Crystal structure of chlorophenyl pyrimidinone **3**. View of the *ac*-layer to show the network of C–H···O and C–Cl···π (3.54 Å) interactions (*i* and *j*). Notice the similarity to Fig. 2a. (b) View of the structure down [001]. Compare this with Fig. 2b.

Networks

A comparison of the three crystal structures in this study may be carried out by analyzing the connectivity between molecules within the pyrimidinone layer and in a direction orthogonal to the mirror plane. In **1**, the *ab*-layer is constituted with linear C–H···O and zigzag C–H···N interactions. In **3**, the C–H···O connectivity along [100] is similar to that in **1** while the *ac*-layer is completed through zigzag chains of C–Cl···π interactions. The pyrimidinone layers are connected through C–H···O/N interactions in the three structures and their similarity may be visualized in Figs. 1b, 2b, and 3b. The crystal structure of the methyl derivative **2** is identical to that of the chloro analogue **3** not only in terms of the unit cell parameters; more significantly, the arrangement of molecules and the intermolecular interactions in the two structures are similar. To summarize, the network depiction is an appropriate way to represent these structures.

It is useful to assess the present study in crystal engineering terms. Three structures have been examined and all three have the same one-dimensional arrangement of C–H···O hydrogen bonds. Despite the recurrence of the same pattern, it is difficult to comment on the robustness of this 1D supramolecular synthon because the number of compounds examined is not sufficiently large. However, it seems curious and interesting that in all three cases, the heterocyclic moieties lie on a mirror plane in the crystal,

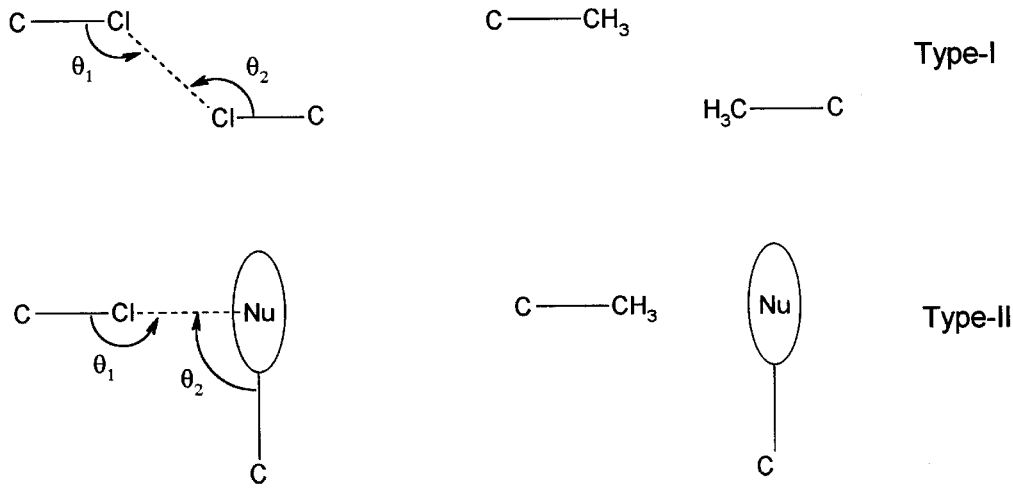


FIG. 4. Type-I and type-II intermolecular geometries formed by halogen atoms. In the type-I geometry, $\theta_1 \approx \theta_2$. In the type-II geometry $\theta_1 \approx 180°$ and $\theta_2 \approx 90°$ with respect to a nucleophilic group, *Nu*. The corresponding methyl group geometries are shown on the right-hand side.

thus necessitating that the phenyl rings be either (a) in the plane, (b) inclined at an arbitrary angle and disordered about the plane, or (c) perpendicular to the plane. In our examples, the last option is favored. Generally, the rings in biphenyl-type systems are inclined because of steric hindrance. However, it is quite unusual to find cases in which the rings are exactly perpendicular (because of the location of the molecule on a special position). The two-dimensional structure follows from the substituent pattern (H, Cl, CH_3). All in all, it is anticipated that other pyrimidinones in this family will have crystal structures that are related to the present ones.

CONCLUSIONS

It is only natural to consider the isolated molecule as a building block of an extended solid-state structure. However, the preferences and protocols of neutral organic molecules in this self-assembly process are far from easy to predict. This difficulty underlies then the need to be able to simplify and analyze crystal structures in terms of networks and eventually in terms of the supramolecular synthons that constitute the networks.

We embarked upon this study in order to assess the NLO potential of *N*-aryl dimethylpyrimidinones. Immediate implications for second-order NLO applications are not apparent in view of the centrosymmetric packing arrangement of the three compounds reported in this paper. However, one may note that the angle made by the phenyl ring to the [100] direction is close to the optically ideal value of 54.7° (15) (Fig. 5). Inspection of Figs. 2a and 3a shows the presence of a 2D polar layer with a potentially chromophoric group aligned at nearly the optimal angle with respect to the polar direction. This is encouraging and could form the basis for future experiments. Substitution of suitable chromophoric groups in the *para* position of the phenyl group and strategies that would favor crystallization in noncentrosymmetric space groups (29, 30) would appear to be reasonable leads for more work on these conjugated molecules.

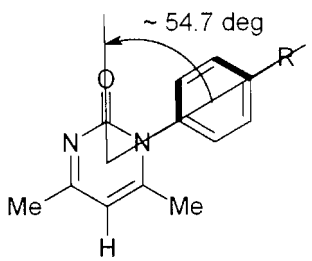


FIG. 5. Orientation of a potential chromophoric aryl group with the [100] direction in the crystal structures of the title compounds. The values of the angles in **1**, **2**, and **3** are 61.3, 56.9, and 56.9°, respectively. The optically ideal value is 54.7°.

ACKNOWLEDGMENTS

We thank the Indo-French Centre for the Promotion of Advanced Research (IFCPAR) for the funding of this project (1708-1).

REFERENCES

1. G. R. Desiraju, *Angew. Chem., Int. Ed. Engl.* **34,** 2311 (1995).
2. P. Brunet, M. Simard, and J. D. Wuest, *J. Am. Chem. Soc.* **119,** 2737 (1997).
3. A. Nangia and G. R. Desiraju, *Top. Curr. Chem.* **198,** 57 (1998), and references cited therein.
4. S. R. Batten and R. Robson, *Angew. Chem., Int. Ed.* **37,** 1460 (1998).

5. O. M Yaghi, H. Li, C. Davis, D. Richardson, and T. L. Groy, *Acc. Chem. Res.* **31,** 474 (1998).
6. N. R. Champness and M. Schröder, *Curr. Opin. Solid State Mater. Sci.* **3,** 419 (1998).
7. M. J. Zaworotko, *Angew. Chem., Int. Ed.* **37,** 1211 (1998).
8. C. B. Aakeröy, *Acta Crystallogr., Sect. B* **53,** 569 (1997).
9. J. Bernstein, R. E. Davis, L. Shimoni, and N.-L. Chang, *Angew. Chem., Int. Ed. Engl.* **34,** 1555 (1995).
10. O. Ermer, *J. Am. Chem. Soc.* **110,** 3747 (1988).
11. G. R. Desiraju and T. Steiner, "The Weak Hydrogen Bond in Structural Chemistry and Biology." Oxford Univ. Press, Oxford, 1999.
12. G. R. Desiraju, *J. Mol. Struct.* **374,** 191 (1996).
13. D. S. Reddy, D. C. Craig, and G. R. Desiraju, *Chem. Commun.* 339 (1995).
14. D. S. Reddy, D. C. Craig, and G. R. Desiraju, *J. Am. Chem. Soc.* **118,** 4090 (1996).
15. J. Zyss and J.-F. Nicoud, *Curr. Opin. Solid State Mater. Sci.* **1,** 533 (1996).
16. I. A. Litvinov, V. E. Kataev, A. T. H. Lenstra, and H. J. Geise, *Acta Crystallogr., Sect. C* **48,** 1286 (1992).
17. R. O. Hutchins and B. E. Maryanoff, *J. Org. Chem.* **37,** 1829 (1972).
18. A. Altomare, M. Cascarano, C. Giacovazzo, and A. J. Guagliardi, *J. Appl. Cryst.* **26,** 343 (1993).
19. Molecular Structure Corp. (1997–1998). teXsan for Windows version 1.03. Single Crystal Structure Analysis Software. Version 1.04. MSC, 3200 Research Forest Drive, Woodlands, TX 77381.
20. "International Tables for Crystallography" (A. J. C. Wilson, Ed.), Vol. C, Table 4268, pp. 6111, 6112. Kluwer Academic, Dordrecht, 1992.
21. P. S. Chandrakala, A. K. Katz, H. L. Carrell, P. R. Sailaja, A. R. Podile, A. Nangia, and G. R. Desiraju, *J. Chem. Soc., Perkin Trans. 1* 2597 (1998).
22. G. R. Desiraju and J. A. R. P. Sarma, *Proc. Ind. Acad. Sci., Chem. Sci.* **96,** 599 (1986).
23. J. A. R. P. Sarma and G. R. Desiraju, *Chem. Phys. Lett.* **117,** 160 (1985).
24. V. R. Pedireddi, J. A. R. P. Sarma, and G. R. Desiraju, *J. Chem. Soc., Perkin Trans. 2*, 311 (1992), and references cited therein.
25. H. Krupitsky, Z. Stein, and I. Goldberg, *J. Incl. Phenom. Mol. Recognit.* **20,** 211 (1995).
26. I. Csöregh, E. Weber, T. Hens, and M. Czugler, *J. Chem. Soc., Perkin Trans. 2* 2733 (1996).
27. P. Dastidar and I. Goldberg, *Acta Crystallogr., Sect. C* **52,** 1976 (1996).
28. J. A. R. P. Sarma and G. R. Desiraju, *Acc. Chem. Res.* **19,** 222 (1986).
29. G. R. Desiraju and T. S. R. Krishna, *Mol. Cryst. Liq. Cryst.* **159,** 277 (1988).
30. J. A. R. P. Sarma, F. H. Allen, V. J. Hoy, J. A. K. Howard, R. Thaimattam, K. Biradha, and G. R. Desiraju, *Chem. Commun.* 101 (1997).