Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

3-{[2-(Trifluoromethyl)phenyl]hydrazono}pentane-2,4-dione

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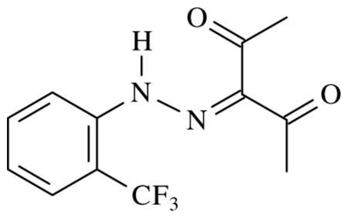
Received 12 September 2007; accepted 17 September 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.145; data-to-parameter ratio = 13.6.

The crystal structure of the title compound, $C_{12}H_{11}F_3N_2O_2$, is stabilized by one N—H···O and two N—H···F intramolecular hydrogen bonds, and by one C—H···F and two C—H···O intermolecular hydrogen bonds. These hydrogen bonds generate $R^4_4(13)S(6)S(6)S(6)R^3_3(20)$ ring motifs in the ac plane. Except for four H atoms of the methyl groups and two F atoms of three trifluoromethyl groups, all atoms are almost in the same plane, and the N—N═C—C(OCH$_3$) torsion angles are 4.1 (3) and −175.25 (14)°.

Related literature

For related structures, see: Sarojini *et al.* (2007); Yathirajan *et al.* (2007); Odabaşoğlu *et al.* (2005*a*,*b*). For related literature, see: Filler & Kabayashi (1992); Sreekumar *et al.* (2003); Narayana *et al.* (2006); Alpaslan *et al.* (2005, 2005*a*,*b*, 2007*a*,*b*); Alpaslan, Özdamar *et al.* (2006); Alpaslan, Odabaşoğlu *et al.* (2006); Etter (1990); Hooper *et al.* (1998); Pottie *et al.* (1998); Vaughan *et al.* (2004).



Experimental

Crystal data

$C_{12}H_{11}F_3N_2O_2$
M_r = 272.23
Monoclinic, $P2_1/c$
a = 8.2941 (4) Å
b = 7.0893 (5) Å
c = 22.2665 (11) Å
β = 109.545 (4)°
V = 1233.81 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 296 K
0.65 × 0.57 × 0.44 mm

Data collection

Stoe IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002) $T_{\min}$ = 0.925, $T_{\max}$ = 0.952
15716 measured reflections
2433 independent reflections
1919 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.145
S = 1.10
2433 reflections
179 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$ = 0.33 e Å^{-3}
$\Delta\rho_{\min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.88 (2)	1.88 (2)	2.568 (2)	133.8 (19)
N1—H1···F3	0.88 (2)	2.46 (2)	2.935 (2)	114.4 (17)
N1—H1···F2	0.88 (2)	2.46 (2)	2.949 (2)	115.9 (17)
C3—H3···O1$^{\rm i}$	0.93	2.63	3.432 (3)	145
C5—H5···O2$^{\rm ii}$	0.93	2.62	3.297 (2)	130
C12—H12C···F1$^{\rm iii}$	0.96	2.75	3.517 (2)	137

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

BKS thanks the AICTE, Government of India, for financial assistance through the Career Award for Young Teachers Scheme. The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDS 2 diffractometer (purchased under grant F.279 of the University Research Fund).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2398).

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supplementary materials

Acta Cryst. (2007). E**63**, o4135-o4136 [**doi:10.1107/S1600536807045631**]

3-{[2-(Trifluoromethyl)phenyl]hydrazono}pentane-2,4-dione

M. Odabasoglu, O. Büyükgüngör, B. K. Sarojini and B. Narayana

Comment

The title compound is used as an intermediate in the synthesis of acetyl cinnoline derivative. Cinnoline derivatives are known for their pharmacological activities (Narayana *et al.*, 2006). The title compound synthesized by coupling 2-trifluoro methyl benzene diazoniumchloride with acetyl acetone [Fig. 4] which further underwent cyclization to yield cinnoline derivative. Recently, fluorinated organic compounds have attracted attention due to the ability of fluorine to act as polar hydrogen or hydroxyl mimic. Therefore, substitution of hydrogen by fluorine has been a strategy in designing molecules for biological activity studies (Filler & Kabayashi, 1992). Owing to the importance of title compound (I), the present paper reports the synthesis and crystal structure of the title compound.

Phenylhydrazono-1,3-diones can exist in four tautomeric forms [Fig. 3]. Our investigations show that, in the solid state, the molecular structure of (I) adopts the keto-hydrazo B form with three intramolecular hydrogen bonds (Fig. 1). This is also indicated by the N—N and C—N bond lengths (Table 1). In (I), the C1—N1, C10—N2 and N1—N2 bond lengths are 1.402 (2) Å, 1.310 (2) Å and 1.3161 (19) Å, respectively. These bonds lengths are common feature of similar systems (Odabaşoğlu *et al.*, 2005*a*,*b*; Alpaslan *et al.*, 2005*a*,*b*; Alpaslan *et al.*, 2005; Alpaslan, Özdamar *et al.*, 2006; Alpaslan, Odabaşoğlu *et al.*, 2006; Alpaslan *et al.*, 2007*a*,*b*).

The N1—N2 single bond of 1.3161 (19) Å is shorter than that observed in 1,2-bis-[1-(3-pyridyl)3-methyltriazen-3-yl]ethane [1.326 (3) Å; Vaughan *et al.*, 2004] and other triazines (Pottie *et al.*, 1998; Hooper *et al.*, 1998). This shortening in the hydrazone group is consistent with the resonance structures shown in Fig. 3, which give to the N1—N2 bond some double-bond character.

The crystal packing is stabilized N—H···F, N—H···O intramolecular and C—H···O, C—H···F intermolecular hydrogen bonds. These hydrogen bonds generate edge-fussed $R_4^4(13)$S(6)S(6)S(6)$R_3^3(20)$ ring motifs in xz plane (Fig. 2) (Etter, 1990). Except the four protons of methyl groups and two fluour atoms of three fluourmethyl group, all atoms are almost in the same plane and the dihedral angle between the aromatic ring and N1/N2/C10/C9 plane in substituted group is 3.77 (8)°. There is no C—H···π and π···π interaction in crystal packing.

Experimental

The title compound (I) was synthesized according to the reported method (Sreekumar *et al.*, 2003) with a yield of 85% (Fig. 4). The compound was purified by recrystallization from ethanol. The initially formed 3-{(*E*)-[2-(trifluoromethyl)phenyl]diazenyl}pentane-2,4-dione underwent enolization to form pentane-2,3,4-trione 3-{[2-(trifluoromethyl)phenyl] hydrazone}. The crystal growth was done in a 8:2 mixture of toluene–acetone by slow evaporation technique [m.p.: 373–375 K]. Analysis for $C_{12}H_{11}F_3N_2O_2$: Found (Calculated): C 52.75 (52.94), H 4.20 (4.04), N 10.39% (10.29%).

Refinement

All C-bound H atoms were refined using the riding model approximation with d(C—H) = 0.93 for aromatic and d(C—H) = 0.96 for methyl C—H [U_{iso}(H) = 1.2 or 1.5U_{eq}(parent atom)]. N-bound H atom was located in Fourier difference map and refined freely due to its taking part in H-bond.

Figures

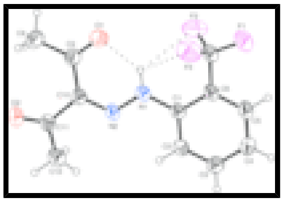

Fig. 1. A view of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level..

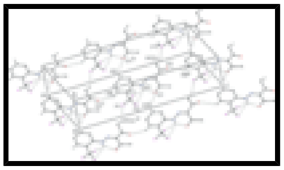

Fig. 2. Part of the crystal structure of (I), showing the formation of $R_4^4(13)S(6)S(6)S(6)R_3^3(20)$ motifs. [Symmetry codes: (i) $x - 1, y, z$; (ii) x, $1/2 - y$,$z + 1/2$; (iii) $x + 1$, $1/2 - y$, $z + 1/2$; (iv) $x + 1, y, z$; (v) x, $1/2 - y$, $z - 1/2$; (vi) $x - 1$, $1/2 - y$, $z - 1/2$].

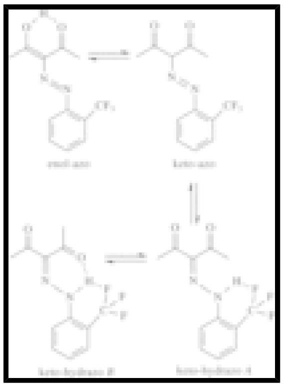

Fig. 3. Tautomerism in the title compound.

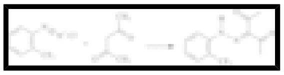

Fig. 4. The formation of the title compound.

3-{[2-(Trifluoromethyl)phenyl]hydrazono}pentane-2,4-dione

Crystal data

$C_{12}H_{11}F_3N_2O_2$

M_r = 272.23

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

a = 8.2941 (4) Å

b = 7.0893 (5) Å

c = 22.2665 (11) Å

β = 109.545 (4)º

F_{000} = 560

D_x = 1.466 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71073 Å

Cell parameters from 15716 reflections

θ = 1.9–28.0º

μ = 0.13 mm^{-1}

T = 296 K

Prism, yellow

V = 1233.81 (12) Å^3	0.65 × 0.57 × 0.44 mm
Z = 4	

Data collection

Stoe IPDS-2 diffractometer	2433 independent reflections
Monochromator: plane graphite	1919 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	R_{int} = 0.040
T = 296 K	θ_{max} = 26.0°
ω scans	θ_{min} = 1.9°
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -10 \rightarrow 10$
T_{min} = 0.925, T_{max} = 0.952	$k = -8 \rightarrow 8$
15716 measured reflections	$l = -27 \rightarrow 27$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.0769P)^2 + 0.1968P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.145	$(\Delta/\sigma)_{\text{max}} < 0.001$
S = 1.10	$\Delta\rho_{\text{max}}$ = 0.33 e Å^{-3}
2433 reflections	$\Delta\rho_{\text{min}}$ = −0.22 e Å^{-3}
179 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.021 (3)
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 > 2sigma(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}

C1	0.4714 (2)	0.2443 (2)	0.48094 (7)	0.0492 (4)
C2	0.6472 (2)	0.2478 (2)	0.49847 (8)	0.0564 (4)
H2	0.7125	0.2667	0.5410	0.068*
C3	0.7275 (3)	0.2239 (3)	0.45425 (10)	0.0658 (5)
H3	0.8463	0.2264	0.4670	0.079*
C4	0.6326 (3)	0.1961 (3)	0.39106 (9)	0.0674 (5)
H4	0.6872	0.1793	0.3611	0.081*
C5	0.4580 (3)	0.1934 (3)	0.37252 (8)	0.0625 (5)
H5	0.3944	0.1747	0.3298	0.075*
C6	0.3743 (2)	0.2181 (2)	0.41629 (8)	0.0530 (4)
C7	0.1812 (3)	0.2184 (3)	0.39347 (8)	0.0637 (5)
C8	0.1589 (3)	0.2857 (4)	0.67265 (11)	0.0830 (7)
H8A	0.0433	0.2401	0.6574	0.100*
H8B	0.1613	0.4092	0.6906	0.100*
H8C	0.2283	0.2015	0.7047	0.100*
C9	0.2271 (2)	0.2953 (3)	0.61862 (9)	0.0603 (5)
C10	0.4125 (2)	0.3127 (2)	0.63042 (8)	0.0513 (4)
C11	0.5375 (2)	0.3573 (3)	0.69423 (8)	0.0580 (5)
C12	0.7209 (3)	0.3113 (4)	0.70645 (10)	0.0794 (6)
H12A	0.7591	0.3724	0.6751	0.095*
H12B	0.7338	0.1773	0.7039	0.095*
H12C	0.7881	0.3545	0.7482	0.095*
N1	0.3891 (2)	0.2659 (2)	0.52622 (7)	0.0523 (4)
N2	0.48311 (18)	0.29271 (19)	0.58622 (6)	0.0504 (4)
O1	0.12893 (18)	0.2806 (3)	0.56407 (7)	0.0824 (5)
O2	0.49197 (19)	0.4327 (2)	0.73475 (6)	0.0792 (5)
F1	0.1151 (2)	0.2002 (3)	0.33166 (6)	0.1288 (7)
F2	0.11712 (17)	0.0876 (2)	0.42020 (8)	0.1040 (5)
F3	0.12016 (18)	0.3783 (2)	0.40798 (8)	0.1052 (5)
H1	0.277 (3)	0.266 (3)	0.5163 (10)	0.073 (7)*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0549 (9)	0.0472 (8)	0.0424 (8)	−0.0006 (7)	0.0123 (7)	0.0008 (6)
C2	0.0553 (10)	0.0638 (10)	0.0458 (9)	−0.0007 (8)	0.0109 (7)	−0.0002 (7)
C3	0.0573 (11)	0.0793 (13)	0.0619 (11)	0.0006 (9)	0.0215 (9)	0.0030 (9)
C4	0.0770 (14)	0.0767 (12)	0.0549 (10)	0.0007 (10)	0.0308 (9)	0.0011 (9)
C5	0.0763 (13)	0.0656 (11)	0.0428 (8)	−0.0012 (9)	0.0161 (8)	−0.0008 (8)
C6	0.0583 (10)	0.0537 (9)	0.0420 (8)	−0.0020 (7)	0.0101 (7)	0.0009 (6)
C7	0.0643 (11)	0.0732 (12)	0.0431 (9)	−0.0004 (9)	0.0040 (8)	0.0012 (8)
C8	0.0678 (13)	0.1169 (19)	0.0717 (14)	−0.0016 (12)	0.0332 (11)	0.0008 (12)
C9	0.0582 (10)	0.0658 (11)	0.0568 (10)	0.0031 (8)	0.0193 (8)	−0.0002 (8)
C10	0.0531 (9)	0.0557 (9)	0.0437 (8)	0.0006 (7)	0.0145 (7)	0.0014 (7)
C11	0.0640 (11)	0.0647 (10)	0.0431 (8)	−0.0043 (8)	0.0152 (8)	0.0035 (7)
C12	0.0618 (12)	0.1099 (17)	0.0566 (11)	−0.0018 (11)	0.0067 (9)	−0.0074 (11)
N1	0.0498 (8)	0.0624 (9)	0.0411 (7)	−0.0011 (6)	0.0103 (6)	−0.0028 (6)
N2	0.0545 (8)	0.0528 (8)	0.0406 (7)	−0.0012 (6)	0.0115 (6)	−0.0007 (5)

O1	0.0520 (8)	0.1283 (14)	0.0622 (8)	−0.0022 (8)	0.0131 (7)	−0.0069 (8)
O2	0.0871 (10)	0.1029 (12)	0.0496 (7)	−0.0062 (8)	0.0253 (7)	−0.0131 (7)
F1	0.0765 (9)	0.237 (2)	0.0541 (7)	−0.0064 (11)	−0.0032 (7)	−0.0179 (10)
F2	0.0668 (8)	0.1121 (12)	0.1195 (12)	−0.0202 (7)	0.0130 (8)	0.0208 (9)
F3	0.0728 (9)	0.1024 (11)	0.1225 (12)	0.0224 (7)	0.0087 (8)	−0.0039 (9)

Geometric parameters (Å, °)

C1—C2	1.378 (3)	C8—C9	1.493 (3)
C1—N1	1.402 (2)	C8—H8A	0.9600
C1—C6	1.407 (2)	C8—H8B	0.9600
C2—C3	1.371 (3)	C8—H8C	0.9600
C2—H2	0.9300	C9—O1	1.220 (2)
C3—C4	1.377 (3)	C9—C10	1.476 (3)
C3—H3	0.9300	C10—N2	1.310 (2)
C4—C5	1.367 (3)	C10—C11	1.486 (2)
C4—H4	0.9300	C11—O2	1.213 (2)
C5—C6	1.384 (3)	C11—C12	1.489 (3)
C5—H5	0.9300	C12—H12A	0.9600
C6—C7	1.509 (3)	C12—H12B	0.9600
C7—F1	1.306 (2)	C12—H12C	0.9600
C7—F2	1.307 (2)	N1—N2	1.3161 (19)
C7—F3	1.325 (2)	N1—H1	0.88 (2)
C2—C1—N1	121.20 (15)	C9—C8—H8B	109.5
C2—C1—C6	118.76 (16)	H8A—C8—H8B	109.5
N1—C1—C6	120.04 (16)	C9—C8—H8C	109.5
C3—C2—C1	121.10 (17)	H8A—C8—H8C	109.5
C3—C2—H2	119.4	H8B—C8—H8C	109.5
C1—C2—H2	119.4	O1—C9—C10	119.55 (17)
C2—C3—C4	120.17 (19)	O1—C9—C8	119.46 (18)
C2—C3—H3	119.9	C10—C9—C8	120.91 (17)
C4—C3—H3	119.9	N2—C10—C9	123.91 (15)
C5—C4—C3	119.73 (18)	N2—C10—C11	113.40 (15)
C5—C4—H4	120.1	C9—C10—C11	122.69 (15)
C3—C4—H4	120.1	O2—C11—C10	120.92 (17)
C4—C5—C6	121.07 (17)	O2—C11—C12	120.94 (17)
C4—C5—H5	119.5	C10—C11—C12	118.12 (16)
C6—C5—H5	119.5	C11—C12—H12A	109.5
C5—C6—C1	119.16 (17)	C11—C12—H12B	109.5
C5—C6—C7	119.25 (16)	H12A—C12—H12B	109.5
C1—C6—C7	121.58 (15)	C11—C12—H12C	109.5
F1—C7—F2	108.57 (18)	H12A—C12—H12C	109.5
F1—C7—F3	106.34 (18)	H12B—C12—H12C	109.5
F2—C7—F3	104.40 (19)	N2—N1—C1	118.68 (15)
F1—C7—C6	112.27 (17)	N2—N1—H1	118.2 (14)
F2—C7—C6	113.16 (16)	C1—N1—H1	123.1 (14)
F3—C7—C6	111.60 (16)	C10—N2—N1	121.07 (15)
C9—C8—H8A	109.5		
N1—C1—C2—C3	179.00 (16)	C5—C6—C7—F3	−121.40 (19)

C6—C1—C2—C3	−0.8 (3)	C1—C6—C7—F3	57.9 (2)
C1—C2—C3—C4	0.1 (3)	O1—C9—C10—N2	−7.9 (3)
C2—C3—C4—C5	0.3 (3)	C8—C9—C10—N2	169.00 (19)
C3—C4—C5—C6	0.0 (3)	O1—C9—C10—C11	171.41 (18)
C4—C5—C6—C1	−0.7 (3)	C8—C9—C10—C11	−11.7 (3)
C4—C5—C6—C7	178.65 (18)	N2—C10—C11—O2	158.23 (18)
C2—C1—C6—C5	1.1 (2)	C9—C10—C11—O2	−21.1 (3)
N1—C1—C6—C5	−178.74 (15)	N2—C10—C11—C12	−20.2 (2)
C2—C1—C6—C7	−178.23 (16)	C9—C10—C11—C12	160.42 (18)
N1—C1—C6—C7	2.0 (2)	C2—C1—N1—N2	1.1 (2)
C5—C6—C7—F1	−2.1 (3)	C6—C1—N1—N2	−179.10 (14)
C1—C6—C7—F1	177.18 (18)	C9—C10—N2—N1	4.1 (3)
C5—C6—C7—F2	121.19 (19)	C11—C10—N2—N1	−175.25 (14)
C1—C6—C7—F2	−59.5 (2)	C1—N1—N2—C10	−179.68 (15)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.88 (2)	1.88 (2)	2.568 (2)	133.8 (19)
N1—H1···F3	0.88 (2)	2.46 (2)	2.935 (2)	114.4 (17)
N1—H1···F2	0.88 (2)	2.46 (2)	2.949 (2)	115.9 (17)
C3—H3···O1^{i}	0.93	2.63	3.432 (3)	145
C5—H5···O2^{ii}	0.93	2.62	3.297 (2)	130
C12—H12C···F1^{iii}	0.96	2.75	3.517 (2)	137

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

Fig. 1

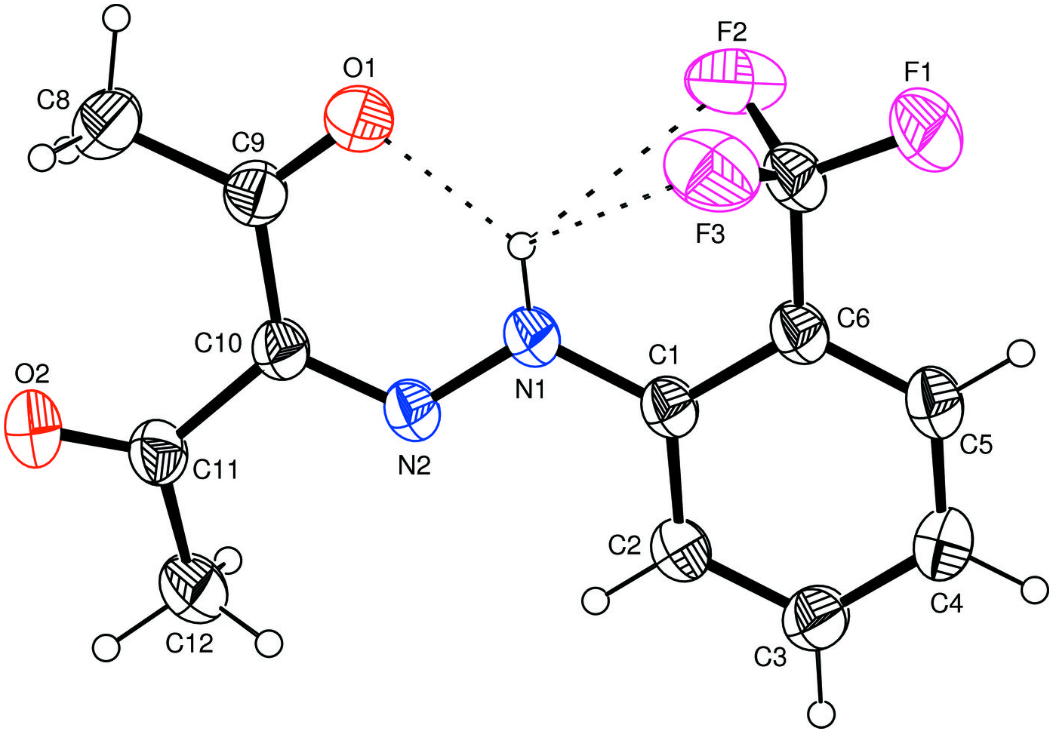

Fig. 2

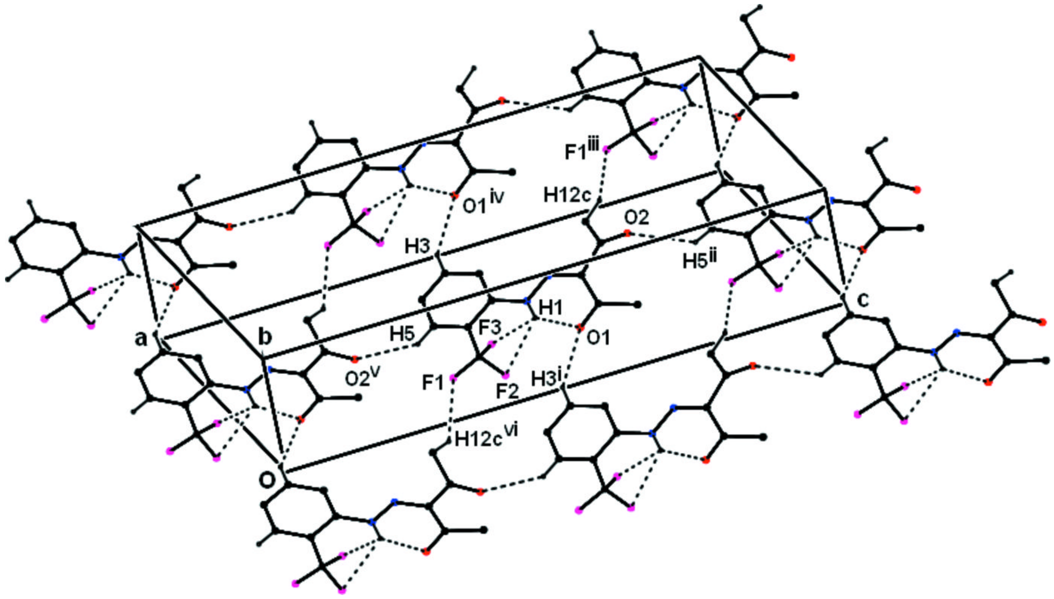

Fig. 3

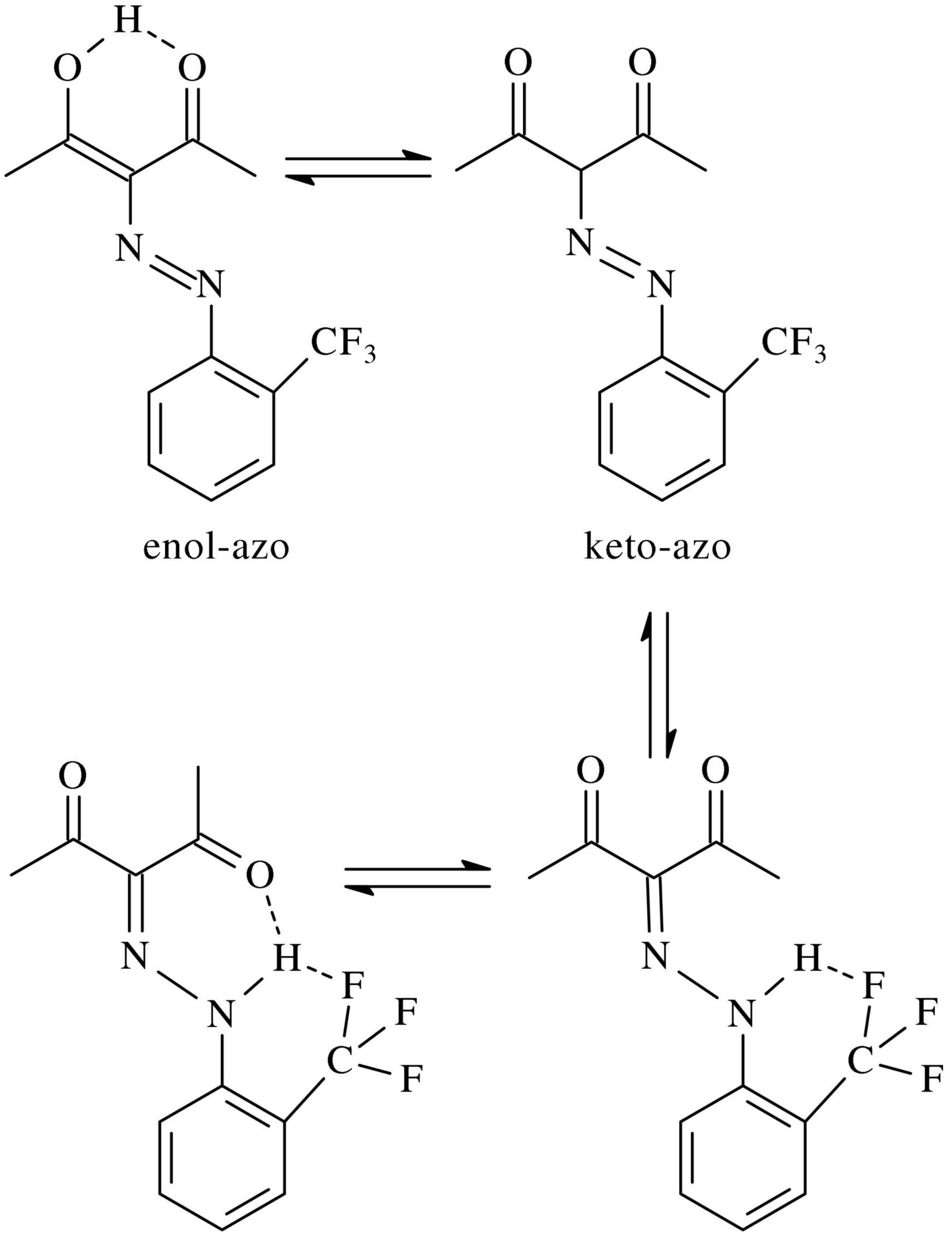

Fig. 4