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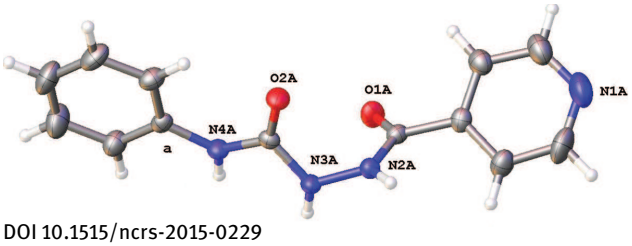
Crystal structure of *N*-phenyl-2-(pyridin-4-ylcarbonyl)hydrazinecarboxamide with Z′ = 4, $C_{13}H_{12}N_4O_2$



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Abstract

$C_{13}H_{12}N_4O_2$, orthorhombic, *Pbca* (no. 61), $a = 16.2353(11)$ Å, $b = 16.8474(12)$ Å, $c = 36.028(2)$ Å, $V = 9854.5(11)$ Å^3, $Z = 32$, $R_{gt}(F) = 0.0903$, $wR_{ref}(F^2) = 0.1773$, $T = 163$ K.

CCDC no.: 1457416

In the figure only one out of four crystallographically independent molecules is shown. Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

Isoniazid (1 g, 7.2 mmol) and phenyl isocyanate (1 g, 8.3 mmol) were mixed in methanol (30 mL) thoroughly and refluxed for 30 min. After the reaction was completed, the resulting mixture was cooled to room temperature. The products were collected by filtration (1.4 g, 80% yield); M.p.:422–424 K. The title compound was recrystallized from a mixture of methanol and dichloromethane (50:50), colourless single crystals were obtained by slow evaporation.

Experimental details

Absorption correction was performed using SADABS (Bruker, 2006). All hydrogen atoms were placed in idealised positions and refined using a riding models with the SHELX program (AFIX 43 option) [18].

Table 1: Data collection and handling.

Crystal:	Colorless, block, size 0.12×0.22×0.35 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.98 cm^{-1}
Diffractometer, scan mode:	Bruker Kappa Duo Apex II Diffractometer, 0.5% φ scans and ω scans
$2\theta_{max}$:	55.95°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	70312, 1181
$N(param)_{refined}$:	686
Programs:	Bruker programs [17], SHELX [18], WinGX [19]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2A)	8*c*	−0.0495	0.2472	0.2743	0.028
H(3A)	8*c*	−0.0810	0.1438	0.2291	0.029
H(4A)	8*c*	−0.0022	0.0543	0.1991	0.030
H(1A)	8*c*	0.1027	0.2295	0.4106	0.058
H(2AA)	8*c*	0.1044	0.1687	0.3543	0.041
H(4AA)	8*c*	−0.1231	0.2524	0.3354	0.046
H(5A)	8*c*	−0.1199	0.3020	0.3959	0.063
H(9A)	8*c*	0.1793	0.1572	0.1775	0.039
H(10A)	8*c*	0.2630	0.1262	0.1277	0.049
H(11A)	8*c*	0.2321	0.0226	0.0891	0.061
H(12A)	8*c*	0.1136	−0.0514	0.0993	0.060
H(13A)	8*c*	0.0297	−0.0226	0.1494	0.041
H(2B)	8*c*	0.4552	0.4780	0.2790	0.030
H(3B)	8*c*	0.5423	0.3611	0.2817	0.033
H(4B)	8*c*	0.6188	0.2915	0.2429	0.031
H(1B)	8*c*	0.2327	0.6096	0.2938	0.047
H(2BA)	8*c*	0.3450	0.5272	0.2948	0.039
H(4BA)	8*c*	0.2654	0.4327	0.1995	0.040
H(5B)	8*c*	0.1553	0.5171	0.2020	0.044
H(9B)	8*c*	0.7691	0.2742	0.2343	0.037
H(10B)	8*c*	0.8742	0.2653	0.1918	0.047
H(11B)	8*c*	0.8553	0.3096	0.1321	0.050
H(12B)	8*c*	0.7286	0.3568	0.1138	0.048

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Table 2: (continued)

Atom	Site	*x*	*y*	*z*	U_{iso}
H(13B)	8*c*	0.6222	0.3665	0.1563	0.041
H(2C)	8*c*	0.1061	0.2746	0.5344	0.037
H(3C)	8*c*	0.2299	0.2996	0.4948	0.040
H(4C)	8*c*	0.2783	0.2450	0.4477	0.039
H(1C)	8*c*	0.1310	0.1053	0.6705	0.056
H(2CA)	8*c*	0.2058	0.1184	0.6171	0.052
H(4CA)	8*c*	0.0512	0.2920	0.5874	0.034
H(5C)	8*c*	−0.0173	0.2727	0.6422	0.040
H(9C)	8*c*	0.3813	0.1905	0.4114	0.040
H(10C)	8*c*	0.4181	0.1036	0.3643	0.048
H(11C)	8*c*	0.3279	0.0061	0.3456	0.054
H(12C)	8*c*	0.2007	−0.0031	0.3726	0.059
H(13C)	8*c*	0.1623	0.0820	0.4197	0.048
H(2D)	8*c*	−0.1502	0.1918	−0.0201	0.045
H(3D)	8*c*	−0.0461	0.2922	−0.0331	0.046
H(4D)	8*c*	0.0276	0.3729	0.0021	0.045
H(1D)	8*c*	−0.0825	−0.0966	0.0589	0.061
H(2DA)	8*c*	−0.0199	0.0269	0.0499	0.047
H(4DA)	8*c*	−0.2024	0.0785	−0.0209	0.053
H(5D)	8*c*	−0.2557	−0.0431	−0.0108	0.068
H(9D)	8*c*	−0.0725	0.4044	0.0877	0.047
H(10D)	8*c*	−0.0318	0.4986	0.1296	0.060
H(11D)	8*c*	0.0731	0.5850	0.1159	0.059
H(12D)	8*c*	0.1365	0.5788	0.0598	0.055
H(13D)	8*c*	0.1007	0.4819	0.0170	0.046

Discussion

Molecules having urea functionality have been reported in a wide range of applications, in particular, metal binding as neutral or anionic ligands [1–6]. These molecules have also been found to be useful in surfactant self-assembies [7] and photo-dimerizing agents in coumarins [8]. These molecules have also received much attention as fundamental synthetic building blocks because of their hydrogen bonding and π-π stacking potential. In particular, Meijer's ureidopyrimidone (UPy) building block [9, 10], with its characteristics of a high dimerization constant and synthetic accessibility, has found widespread applications in supramolecular chemistry, materials science, and catalysis [11, 12]. Zimmerman's ureidodeazapterin and ureidonaphthyridine modules are also successful examples of heterocyclic building blocks [13–16].

Here we report the crystal structure of the title compound, which is based on an amidourea moiety. There are four crystallographically independent molecules in the asymmetric unit of the title structure. The molecules are aligned *via* N—H···O and N—H···N hydrogen bonding interactions. These bonds expand the structure to create an infinite polymeric hydrogen bonded assembly consisting of helical structures. The presence of intermolecular N—H···O N—H···N and weak C—H···O hydrogen bonds link

Table 3: Fractional coordinates and atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1A)	8*c*	0.0172(1)	0.0902(1)	0.30136(6)	0.042(1)	0.022(1)	0.036(1)	0.008(1)	−0.002(1)	−0.003(1)
O(2A)	8*c*	0.0979(1)	0.1924(1)	0.22651(6)	0.026(1)	0.031(1)	0.036(1)	−0.010(1)	0.001(1)	−0.005(1)
N(1A)	8*c*	−0.0088(2)	0.2697(2)	0.40905(9)	0.067(2)	0.061(2)	0.033(2)	−0.013(2)	0.004(2)	−0.007(2)
N(2A)	8*c*	−0.0338(2)	0.1986(2)	0.27255(7)	0.026(1)	0.019(1)	0.026(1)	0.000(1)	−0.001(1)	−0.001(1)
N(3A)	8*c*	−0.0357(2)	0.1601(2)	0.23874(7)	0.019(1)	0.030(2)	0.024(1)	−0.004(1)	−0.004(1)	−0.004(1)
N(4A)	8*c*	0.0379(2)	0.0873(2)	0.19679(7)	0.021(1)	0.026(1)	0.027(1)	−0.009(1)	−0.001(1)	−0.001(1)
C(1A)	8*c*	0.0557(3)	0.2322(3)	0.3958(1)	0.054(2)	0.056(3)	0.034(2)	−0.012(2)	−0.001(2)	−0.005(2)
C(2A)	8*c*	0.0580(2)	0.1969(2)	0.36169(9)	0.037(2)	0.037(2)	0.028(2)	−0.004(2)	0.002(2)	0.001(2)
C(3A)	8*c*	−0.0087(2)	0.2033(2)	0.33840(9)	0.032(2)	0.020(2)	0.027(2)	−0.001(1)	0.007(1)	0.002(1)
C(4A)	8*c*	−0.0773(2)	0.2451(2)	0.3505(1)	0.043(2)	0.032(2)	0.040(2)	0.007(2)	0.007(2)	0.002(2)
C(5A)	8*c*	−0.0737(3)	0.2758(2)	0.3869(1)	0.063(3)	0.040(2)	0.054(3)	0.007(2)	0.027(2)	−0.010(2)
C(6A)	8*c*	−0.0075(2)	0.1595(2)	0.30228(9)	0.020(2)	0.020(2)	0.030(2)	−0.002(1)	0.001(1)	0.001(1)
C(7A)	8*c*	0.0393(2)	0.1490(2)	0.22125(8)	0.022(2)	0.020(2)	0.022(2)	−0.001(1)	−0.005(1)	0.006(1)
C(8A)	8*c*	0.0946(2)	0.0714(2)	0.16811(8)	0.024(2)	0.025(2)	0.025(2)	0.006(1)	0.001(1)	0.004(1)
C(9A)	8*c*	0.1656(2)	0.1153(2)	0.1618(1)	0.027(2)	0.030(2)	0.040(2)	−0.002(2)	0.003(2)	−0.001(2)
C(10A)	8*c*	0.2158(2)	0.0963(2)	0.1320(1)	0.030(2)	0.041(2)	0.052(2)	0.002(2)	0.015(2)	0.006(2)
C(11A)	8*c*	0.1976(3)	0.0347(3)	0.1089(1)	0.051(2)	0.051(3)	0.049(2)	0.010(2)	0.023(2)	−0.005(2)
C(12A)	8*c*	0.1269(3)	−0.0097(2)	0.1151(1)	0.061(3)	0.042(2)	0.048(2)	−0.002(2)	0.015(2)	−0.012(2)
C(13A)	8*c*	0.0762(2)	0.0081(2)	0.1449(1)	0.032(2)	0.031(2)	0.039(2)	−0.001(2)	0.005(2)	−0.004(2)
O(1B)	8*c*	0.3882(1)	0.3545(1)	0.22614(6)	0.029(1)	0.023(1)	0.037(1)	0.004(1)	−0.001(1)	−0.007(1)
O(2B)	8*c*	0.5644(1)	0.4463(1)	0.20838(6)	0.026(1)	0.023(1)	0.034(1)	0.0055(9)	0.002(1)	0.005(1)
N(1B)	8*c*	0.1825(2)	0.5709(2)	0.24826(9)	0.024(1)	0.027(2)	0.056(2)	0.002(1)	0.006(1)	0.004(2)
N(2B)	8*c*	0.4566(2)	0.4365(2)	0.26515(7)	0.021(1)	0.025(1)	0.030(1)	0.006(1)	0.001(1)	−0.005(1)
N(3B)	8*c*	0.5269(2)	0.3900(2)	0.26331(7)	0.020(1)	0.032(2)	0.030(2)	0.007(1)	−0.000(1)	0.007(1)
N(4B)	8*c*	0.6234(2)	0.3298(2)	0.22731(7)	0.021(1)	0.020(1)	0.036(2)	0.001(1)	0.004(1)	0.008(1)
C(1B)	8*c*	0.2392(2)	0.5730(2)	0.2747(1)	0.032(2)	0.036(2)	0.050(2)	0.008(2)	0.006(2)	−0.010(2)

Table 3: (continued)

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(2B)	8*c*	0.3073(2)	0.5241(2)	0.2754(1)	0.028(2)	0.034(2)	0.036(2)	0.003(2)	0.003(2)	−0.005(2)
C(3B)	8*c*	0.3186(2)	0.4706(2)	0.24693(9)	0.018(1)	0.018(2)	0.032(2)	−0.001(1)	0.005(1)	0.001(1)
C(4B)	8*c*	0.2602(2)	0.4682(2)	0.2191(1)	0.024(2)	0.032(2)	0.043(2)	0.002(2)	−0.004(2)	−0.005(2)
C(5B)	8*c*	0.1942(2)	0.5191(2)	0.2210(1)	0.023(2)	0.037(2)	0.050(2)	0.003(2)	−0.007(2)	0.001(2)
C(6B)	8*c*	0.3902(2)	0.4153(2)	0.24480(8)	0.020(2)	0.025(2)	0.025(2)	−0.001(1)	0.003(1)	0.003(1)
C(7B)	8*c*	0.5709(2)	0.3921(2)	0.23075(9)	0.013(1)	0.024(2)	0.032(2)	−0.002(1)	−0.004(1)	−0.001(2)
C(8B)	8*c*	0.6852(2)	0.3237(2)	0.19991(9)	0.019(2)	0.018(2)	0.037(2)	−0.001(1)	0.001(1)	−0.001(1)
C(9B)	8*c*	0.7609(2)	0.2919(2)	0.2101(1)	0.023(2)	0.032(2)	0.038(2)	0.002(2)	−0.000(1)	−0.000(2)
C(10B)	8*c*	0.8237(2)	0.2864(2)	0.1847(1)	0.026(2)	0.040(2)	0.051(2)	0.011(2)	0.002(2)	−0.001(2)
C(11B)	8*c*	0.8121(2)	0.3120(2)	0.1490(1)	0.039(2)	0.037(2)	0.050(2)	0.006(2)	0.018(2)	0.001(2)
C(12B)	8*c*	0.7369(2)	0.3410(2)	0.1383(1)	0.047(2)	0.035(2)	0.037(2)	0.009(2)	0.008(2)	0.006(2)
C(13B)	8*c*	0.6731(2)	0.3469(2)	0.1637(1)	0.030(2)	0.032(2)	0.041(2)	0.008(2)	0.001(2)	0.005(2)
O(1C)	8*c*	0.2568(1)	0.1845(2)	0.55918(7)	0.029(1)	0.047(2)	0.043(1)	0.005(1)	0.004(1)	0.006(1)
O(2C)	8*c*	0.1444(1)	0.1419(2)	0.47860(7)	0.031(1)	0.039(2)	0.046(2)	−0.003(1)	0.008(1)	−0.009(1)
N(1C)	8*c*	0.0502(2)	0.1870(2)	0.66175(8)	0.030(2)	0.043(2)	0.036(2)	−0.004(1)	0.004(1)	0.006(2)
N(2C)	8*c*	0.1542(2)	0.2536(2)	0.53258(7)	0.032(2)	0.031(2)	0.030(2)	0.006(1)	0.012(1)	0.001(1)
N(3C)	8*c*	0.1993(2)	0.2591(2)	0.49961(7)	0.045(2)	0.027(2)	0.028(2)	−0.002(1)	0.015(1)	−0.001(1)
N(4C)	8*c*	0.2495(2)	0.2021(2)	0.44789(7)	0.034(2)	0.032(2)	0.031(2)	−0.000(1)	0.006(1)	−0.001(1)
C(1C)	8*c*	0.1148(2)	0.1436(3)	0.6535(1)	0.043(2)	0.058(3)	0.039(2)	0.008(2)	0.002(2)	0.021(2)
C(2C)	8*c*	0.1603(2)	0.1507(3)	0.6213(1)	0.028(2)	0.057(3)	0.046(2)	0.011(2)	0.005(2)	0.006(2)
C(3C)	8*c*	0.1366(2)	0.2074(2)	0.59525(9)	0.026(2)	0.030(2)	0.024(2)	−0.008(1)	−0.002(1)	−0.001(2)
C(4C)	8*c*	0.0692(2)	0.2531(2)	0.60387(9)	0.029(2)	0.028(2)	0.027(2)	−0.001(2)	0.002(1)	−0.000(2)
C(5C)	8*c*	0.0282(2)	0.2411(2)	0.63697(9)	0.034(2)	0.034(2)	0.031(2)	−0.002(2)	0.005(2)	0.000(2)
C(6C)	8*c*	0.1871(2)	0.2154(2)	0.56083(9)	0.027(2)	0.032(2)	0.029(2)	−0.008(2)	0.003(1)	−0.006(2)
C(7C)	8*c*	0.1924(2)	0.1958(2)	0.47485(9)	0.031(2)	0.031(2)	0.028(2)	0.006(2)	0.003(2)	0.005(2)
C(8C)	8*c*	0.2673(2)	0.1458(2)	0.41977(8)	0.031(2)	0.026(2)	0.021(2)	0.006(1)	0.000(1)	0.002(1)
C(9C)	8*c*	0.3445(2)	0.1517(2)	0.40354(9)	0.034(2)	0.031(2)	0.035(2)	0.000(2)	0.002(2)	0.003(2)
C(10C)	8*c*	0.3667(2)	0.0994(2)	0.3755(1)	0.042(2)	0.035(2)	0.044(2)	0.009(2)	0.019(2)	0.006(2)
C(11C)	8*c*	0.3129(3)	0.0414(2)	0.3643(1)	0.059(3)	0.037(2)	0.039(2)	0.006(2)	0.006(2)	−0.012(2)
C(12C)	8*c*	0.2372(2)	0.0359(3)	0.3805(1)	0.045(2)	0.052(3)	0.050(2)	0.000(2)	−0.002(2)	−0.021(2)
C(13C)	8*c*	0.2137(2)	0.0871(2)	0.4085(1)	0.028(2)	0.045(2)	0.047(2)	−0.001(2)	0.001(2)	−0.014(2)
O(1D)	8*c*	0.0027(1)	0.1607(2)	0.02567(7)	0.029(1)	0.046(2)	0.044(2)	−0.005(1)	0.002(1)	0.002(1)
O(2D)	8*c*	−0.1176(2)	0.3132(2)	0.04439(7)	0.034(1)	0.049(2)	0.043(2)	−0.008(1)	0.011(1)	−0.009(1)
N(1D)	8*c*	−0.1753(2)	−0.0818(2)	0.0241(1)	0.054(2)	0.036(2)	0.070(2)	−0.009(2)	0.005(2)	−0.002(2)
N(2D)	8*c*	−0.1034(2)	0.2015(2)	−0.00988(8)	0.039(2)	0.036(2)	0.039(2)	−0.006(1)	−0.003(1)	0.001(2)
N(3D)	8*c*	−0.0671(2)	0.2753(2)	−0.01266(8)	0.058(2)	0.031(2)	0.025(2)	−0.017(2)	0.001(1)	0.003(1)
N(4D)	8*c*	−0.0059(2)	0.3743(2)	0.02054(8)	0.041(2)	0.035(2)	0.037(2)	0.000(1)	0.004(1)	0.005(1)
C(1D)	8*c*	−0.1059(3)	−0.0607(2)	0.0424(1)	0.073(3)	0.032(2)	0.048(2)	0.018(2)	0.005(2)	0.007(2)
C(2D)	8*c*	−0.0680(2)	0.0135(2)	0.0373(1)	0.040(2)	0.037(2)	0.039(2)	0.004(2)	−0.005(2)	−0.007(2)
C(3D)	8*c*	−0.1047(2)	0.0657(2)	0.01311(9)	0.032(2)	0.025(2)	0.030(2)	0.003(1)	0.005(2)	−0.004(2)
C(4D)	8*c*	−0.1763(2)	0.0437(2)	−0.0048(1)	0.043(2)	0.031(2)	0.059(3)	−0.001(2)	−0.013(2)	−0.011(2)
C(5D)	8*c*	−0.2077(3)	−0.0292(2)	0.0016(1)	0.042(2)	0.035(2)	0.091(3)	−0.003(2)	−0.012(2)	−0.005(2)
C(6D)	8*c*	−0.0640(2)	0.1463(2)	0.0090(1)	0.035(2)	0.040(2)	0.035(2)	0.010(2)	0.007(2)	−0.006(2)
C(7D)	8*c*	−0.0666(2)	0.3215(2)	0.0201(1)	0.037(2)	0.028(2)	0.042(2)	−0.001(2)	−0.005(2)	0.002(2)
C(8D)	8*c*	0.0100(2)	0.4325(2)	0.0478(1)	0.031(2)	0.021(2)	0.040(2)	0.005(1)	−0.012(2)	−0.004(2)
C(9D)	8*c*	−0.0295(2)	0.4387(2)	0.0818(1)	0.030(2)	0.038(2)	0.048(2)	0.002(2)	0.001(2)	−0.011(2)
C(10D)	8*c*	−0.0054(2)	0.4953(3)	0.1068(1)	0.034(2)	0.062(3)	0.055(3)	0.010(2)	−0.001(2)	−0.028(2)
C(11D)	8*c*	0.0570(2)	0.5470(2)	0.0986(1)	0.040(2)	0.044(2)	0.065(3)	0.008(2)	−0.007(2)	−0.030(2)
C(12D)	8*c*	0.0950(2)	0.5427(2)	0.0655(1)	0.036(2)	0.027(2)	0.074(3)	−0.003(2)	−0.014(2)	−0.005(2)
C(13D)	8*c*	0.0731(2)	0.4851(2)	0.0396(1)	0.041(2)	0.034(2)	0.041(2)	0.006(2)	0.003(2)	0.007(2)

the molecules into a complex hydrogen bonded framework. Caused by the complexity a detailed discussion of the hydrogen bonding schemes of all four crystallographically independent molecules cannot be expediently presented.

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References

1. Kala, U. L.; Suma, S.; Kurup, M. R. P.; Krishnan, S.; John, R. P.: Synthesis, spectral characterization and crystal structure of copper(II) complexes of 2-hydroxyacetophenone-N(4)-phenyl semicarbazone. Polyhedron **26** (2007) 1427–1435.
2. Reena, T. A.; Seena, E. B.; Kurup, M. R. P.: Synthesis and spectral studies of cadmium(II) complexes derived from di-2-pyridyl ketone and N^4-phenylsemicarbazide: First structural report of a cadmium(II) complex of semicarbazone. Polyhedron **27** (2008) 1825–1831.
3. Kurup, M. R. P.; Varghese, B.; Sithambaresan, M.; Krishnan, S.; Sheeja, S. R.; Suresh, E.: Synthesis, spectral characterization and crystal structure of copper(II) complexes of 2-benzoylpyridine-N(4)-phenylsemicarbazone. Polyhedron **30** (2011) 70–78.
4. Aiswarya, N.; Sithambaresan, M.; Kurup, M. R. P.; Ng, S. W.: Dichlorido {2-[(*E*)-phenyl(pyridin-2-yl-κ*N*)methylidene]-*N*-phenylhydrazinecarboxamide-κ^2N^2,*O*}copper(II). Acta Crystallogr. **E69** (2013) m588–m589.
5. Wittkopp, A.; Schreiner, P. R.: Metal-free, noncovalent catalysis of Diels–Alder reactions by neutral hydrogen bond donors in organic solvents and in water. Chem. Eur. J. **9** (2003) 407–414.
6. Li, X.; Deng, H.; Luo, S.; Cheng, J.-P.: Organocatalytic three-component reactions of pyruvate, aldehyde and aniline by hydrogenbonding catalysts. Eur J. Org. Chem. **25** (2008) 4350–4356.
7. Vos, M. R. J.; Leclere, P. E. L. G.; Meekes, H.; Vlieg, E.; Nolte, R. J. M.; Sommerdijk, N. A. J. M.: Kinetic switching between two modes of bisurea surfactant self-assembly. Chem. Commun. **46** (2010) 6063–6065.
8. Dawn, S.; Dewal, M. B.; Sobransingh, D.; Paderes, M. C.; Wibowo, A. C.; Smith, M. D.; Krause, J. A.; Pellechia, P. J.; Shimizu, L. S.: Self-assembled phenylethynylene bis-urea macrocycles facilitate the selective photodimerization of coumarin. J. Am. Chem. Soc. **133** (2011) 7025–7032.
9. Beijer, F. H.; Sijbesma, R. P.; Kooijman, H.; Spek, A. L.; Meijer, E. W.: Strong dimerization of ureidopyrimidones via quadruple hydrogen bonding J. Am. Chem. Soc. **120** (1998) 6761–6769.
10. Sontjens, S. H. M.; Sijbesma, R. P.; van Genderen, M. H. P.; Meijer, E. W.: Stability and lifetime of quadruply hydrogen bonded 2-ureido-4[1*H*]-pyrimidinone dimers. J. Am. Chem. Soc. **122** (2000) 7487–7493.
11. Huerta, E.; Metselaar, G. A.; Fragoso, A.; Santos, E.; Bo, C.; de Mendoza, J.: Selective binding and easy separation of C_{70} by nanoscale self-assembled capsules. Angew. Chem., Int. Ed. **46** (2007) 202–205.
12. Scherman, O. A.; Ligthart, G. B. W. L.; Ohkawa, H.; Sijbesma, R. P.; Meijer, E. W.: Olefin metathesis and quadruple hydrogen bonding: a powerful combination in multistep supramolecular synthesis. Proc. Nat. Acad. Sci. U.S.A. **103** (2006) 11850–11855.
13. Corbin, P. S.; Zimmerman, S. C.: Self-association without regard to prototropy. A heterocycle that forms extremely stable quadruply hydrogen-bonded dimers. J. Am. Chem. Soc. **120** (1998) 9710–9711.
14. Corbin, P. S.; Lawless, L. J.; Li, Z.-T.; Ma, Y.; Witmer, M. J.; Zimmerman, S. C.: Discrete and polymeric self-assembled dendrimers: hydrogen bond-mediated assembly with high stability and high fidelity. Proc. Nat. Acad. Sci. U.S.A. **99** (2002) 5099–5104.
15. Corbin, P. S.; Zimmerman, S. C.: Complexation-induced unfolding of heterocyclic ureas: A hydrogen-bonded, sheetlike heterodimer. J. Am. Chem. Soc. **122** (2000) 3779–3780.
16. Mayer, M. F.; Nakashima, S.; Zimmerman, S. C.: Synthesis of a soluble ureido-naphthyridine oligomer that self-associates *via* eight contiguous hydrogen bonds. Org. Lett. **7** (2005) 3005–3008.
17. Bruker: SAINT and SADABS, Bruker AXS Inc., Madison, Wisconsin, USA, 2006.
18. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112–122.
19. Farrugia, L. J.: WinGX suite for small-molecule single-crystal crystallography. J. Appl. Crystallogr. **32** (1999) 837–838.