Electronic Supplementary Material (ESI) for New Journal of Chemistry.
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New J. Chem. ART-02-2014-000212
NH···O and OH···O interactions of glycine derivatives with squaric acid
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Table S1. Experimental bond lengths (Å), bond and torsion angles (°) for the complexes of squaric acid with glycine (**1**), sarcosine (**2**), dimethylglycine (**3**) and betaine (**4**).

Parametrs	**1**		**2**	**3**		**4**	
	A[a]	B[b]		A[a]	B[b]	A[a]	B[b]
Bond lengths							
C(1)-C(2)	1.477(2)		1.496(1)	1.500(2)	1.517(2)	1.494(5)	1.488(5)
C(2)-C(3)	1.447(2)		1.496(2)	1.467(2)	1.490(2)	1.427(5)	1.427(5)
C(3)-C(4)	1.456(2)		1.425(1)	1.415(2)	1.420(2)	1.413(5)	1.430(5)
C(4)-C(1)	1.473(2)		1.423(1)	1.445(2)	1.444(2)	1.482(5)	1.481(5)
O(1)-C(1)	1.242(2)		1.250(1)	1.236(2)	1.235(2)	1.207(4)	1.216(4)
O(2)-C(2)	1.251(2)		1.215(1)	1.218(2)	1.223(2)	1.248(4)	1.240(4)
O(3)-C(3)	1.265(2)		1.247(1)	1.287(2)	1.258(2)	1.314(4)	1.304(4)
O(4)-C(4)	1.249(2)		1.308(1)	1.300(2)	1.318(2)	1.240(4)	1.250(4)
C(5)-C(6)	1.514(2)	1.501(2)	1.507(2)	1.510(2)	1.506(2)	1.498(5)	1.520(5)
C(6)-N(1)	1.476(2)	1.472(2)	1.476(2)	1.487(2)	1.481(2)	1.484(5)	1.512(5)
O(5)-C(5)	1.295(2)	1.312(2)	1.314(2)	1.266(2)	1.305(2)	1.298(4)	1.305(4)
O(6)-C(5)	1.211(2)	1.197(2)	1.201(1)	1.245(2)	1.213(2)	1.207(4)	1.185(4)
N(1)-C(7)			1.476(2)	1.494(2)	1.488(2)	1.498(4)	1.498(5)
N(1)-C(8)				1.491(2)	1.499(2)	1.511(5)	1.489(4)
N(1)-C(9)						1.505(4)	1.506(4)
Bond angles							
C(1)-C(2)-C(3)	89.9(1)		87.7(1)	87.7(1)	88.5(1)	88.9(3)	88.9(3)
C(2)-C(3)-C(4)	91.2(1)		89.4(1)	91.4(1)	89.6(1)	93.3(3)	93.2(3)
C(3)-C(4)-C(1)	89.7(1)		93.4(1)	91.9(1)	94.2(1)	89.9(3)	89.1(3)
C(4)-C(1)-C(2)	89.3(1)		89.4(1)	89.0(1)	87.6(1)	87.9(3)	88.7(3)
O(1)-C(1)-C(2)	135.7(1)		134.2(1)	135.0(1)	136.3(1)	136.0(3)	136.2(4)

O(1)-C(1)-C(4)	135.0(1)		136.4(1)	136.0(1)	136.1(1)	136.1(3)	135.0(3)
O(2)-C(2)-C(1)	136.8(1)		135.9(1)	134.7(1)	136.1(1)	132.4(4)	133.9(4)
O(2)-C(2)-C(3)	133.3(1)		136.4(1)	137.6(1)	135.4(1)	138.7(4)	137.2(3)
O(3)-C(3)-C(2)	132.7(1)		135.8(1)	132.0(1)	135.0(1)	135.2(3)	137.1(3)
O(3)-C(3)-C(4)	136.1(1)		134.9(1)	136.6(1)	135.4(1)	131.5(3)	129.6(3)
O(4)-C(4)-C(1)	135.3(1)		136.9(1)	131.2(1)	135.2(1)	135.1(3)	135.6(3)
O(4)-C(4)-C(3)	135.0(1)		129.7(1)	136.9(1)	130.6(1)	134.9(3)	135.2(3)
N(1)-C(6)-C(5)	109.8(1)	110.4(1)	111.4(1)	113.8(1)	111.2(1)	116.3(3)	114.7(3)
O(5)-C(5)-C(6)	115.5(1)	111.3(1)	111.3(1)	113.8(1)	111.9(1)	111.0(3)	109.0(3)
O(6)-C(5)-C(6)	121.3(1)	122.7(1)	123.3(1)	119.4(1)	121.9(1)	125.2(3)	125.8(4)
O(5)-C(5)-O(6)	123.2(1)	126.0(1)	125.4(1)	126.7(1)	126.1(1)	123.8(3)	125.2(3)
C(6)-N(1)-C(7)			114.2(1)	111.5(1)	112.0(1)	111.9(3)	105.8(3)
C(6)-N(1)-C(8)				110.2(1)	111.2(1)	110.8(3)	111.4(3)
C(7)-N(1)-C(8)				111.5(1)	110.9(1)	109.9(3)	108.6(3)
C(6)-N(1)-C(9)						107.1(3)	111.6(3)
C(7)-N(1)-C(9)						108.5(3)	109.7(3)
C(8)-N(1)-C(9)						108.5(3)	109.5(3)
Torsion angles							
C(1)-C(2)-C(3)-C(4)	-0.4(1)		-1.3(1)	1.0(1)	0.8(1)	-0.1(3)	-1.8(3)
C(2)-C(3)-C(4)-C(1)	0.4(1)		1.3(1)	-1.1(1)	-0.9(1)	0.1(3)	1.8(3)
C(3)-C(4)-C(1)-C(2)	-0.4(1)		-1.3(1)	1.0(1)	0.9(1)	-0.1(3)	-1.7(3)
C(4)-C(1)-C(2)-C(3)	0.4(1)		1.3(1)	-1.0(1)	-0.8(1)	0.1(3)	1.7(3)
O(1)-C(1)-C(2)-C(3)	179.7(2)		-177.2(1)	177.8(2)	178.3(2)	179.0(4)	-175.7(5)
O(1)-C(1)-C(4)-C(3)	-179.7(2)		177.1(2)	-177.7(2)	-178.3(2)	-170.0(4)	175.8(4)
O(1)-C(1)-C(2)-O(2)	-0.4(3)		2.9(2)	-2.2(3)	-2.7(3)	-0.8(7)	2.6(8)
O(1)-C(1)-C(4)-O(4)	1.3(3)		-2.5(3)	2.2(3)	1.4(3)	-0.5(7)	-2.3(7)
O(2)-C(2)-C(1)-C(4)	-179.8(2)		-178.6(2)	179.0(2)	178.2(2)	179.6(4)	-180.0(5)
O(2)-C(2)-C(3)-C(4)	179.8(2)		178.6(2)	-179.0(2)	178.2(2)	-179.6(5)	180.0(5)
O(2)-C(2)-C(3)-O(3)	-1.4(3)		-2.3(3)	1.5(3)	1.1(3)	0.8(8)	0.0(9)
O(3)-C(3)-C(2)-C(1)	178.5(2)		177.8(1)	-178.5(2)	-180.0(2)	-178.9(4)	178.2(4)
O(3)-C(3)-C(4)-C(1)	-178.5(2)		-177.8(1)	178.4(2)	179.9(2)	179.0(4)	-178.2(4)

O(3)-C(3)-C(4)-O(4)	0.5(3)		1.9(2)	-1.5(3)	0.2(3)	0.5(7)	-0.7(7)
O(4)-C(4)-C(1)-C(2)	-179.3(2)		179.1(1)	-179.0(2)	-179.4(2)	178.3(4)	-179.9(4)
O(4)-C(4)-C(3)-C(2)	179.3(2)		-179.1(1)	179.0(2)	179.4(2)	-178.3(4)	-179.8(4)
O(5)-C(5)-C(6)-N(1)	169.1(1)	170.4(1)	178.0(1)	161.8(1)	-166.4(1)	-168.3(3)	167.2(3)
O(6)-C(5)-C(6)-N(1)	-11.8(2)	9.2(2)	-0.5(2)	-21.4(2)	15.4(2)	10.9(6)	-13.9(6)
C(5)-C(6)-N(1)-C(7)			77.2(1)	-80.5(2)	70.1(2)	-61.9(4)	-175.4(3)
C(5)-C(6)-N(1)-C(8)				155.2(1)	-165.2(1)	61.1(4)	-58.5(5)
C(5)-C(6)-N(1)-C(9)						179.3(3)	64.3(4)

[a] Part A - the positions denoted by the unprimed atomic labels
[b] Part B - the positions denoted by the primed atomic labels