

# **Aryl-Perfluoroaryl Stacking Interactions, Hydrogen Bonding and Steric Effects in Controlling the Structure of Supramolecular Assemblies of *N,N'*-Diaryloxalamides**

**Barbara Piotrkowska,<sup>a</sup> Maria Gdaniec<sup>b\*</sup> Maria J. Milewska<sup>a</sup> and Tadeusz Poloński<sup>\*a</sup>**

<sup>a</sup> *Department of Chemistry, Gdańsk University of Technology, 80-952 Gdansk, Poland; E-mail: tadpol@chem.pg.gda.pl*

<sup>b</sup> *Faculty of Chemistry, A. Mickiewicz University, 60-780 Poznań, Poland; E-mail: magdan@amu.edu.pl*

## Supplementary Material

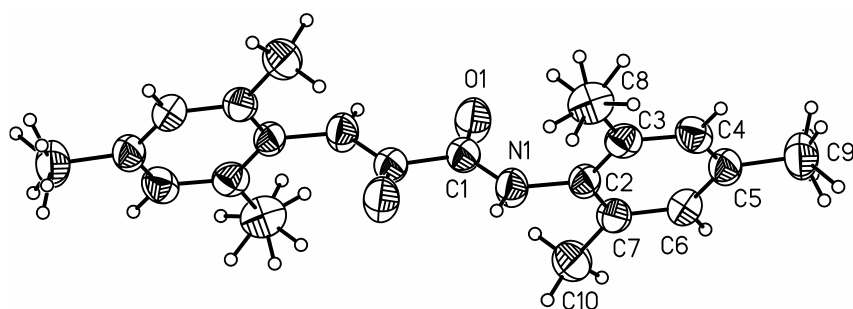


Fig. 1s ORTEP drawing of **2** with displacement ellipsoids shown at the 50% probability level

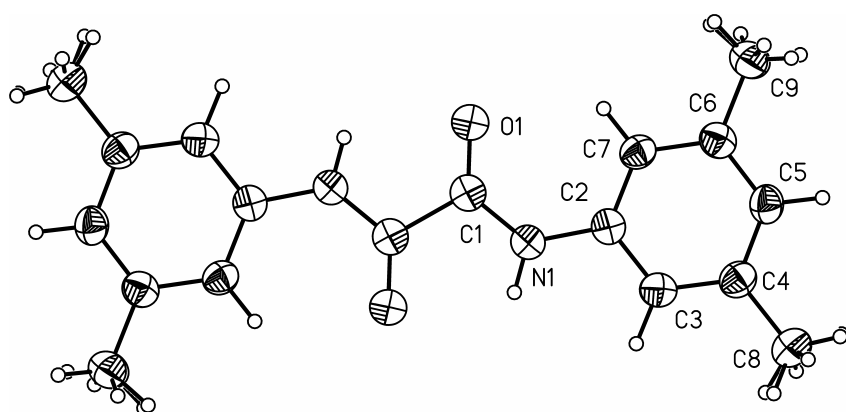


Fig. 2s ORTEP drawing of **4** with displacement ellipsoids shown at the 50% probability level

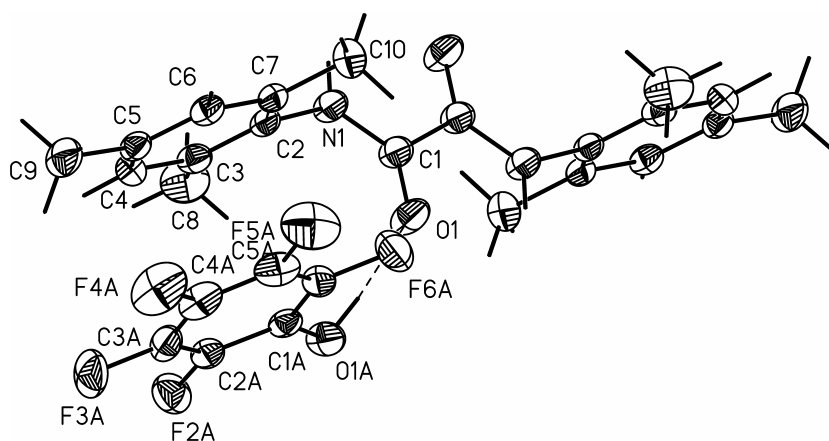


Fig. 3s ORTEP drawing of **2.pfp** with displacement ellipsoids shown at the 50% probability level

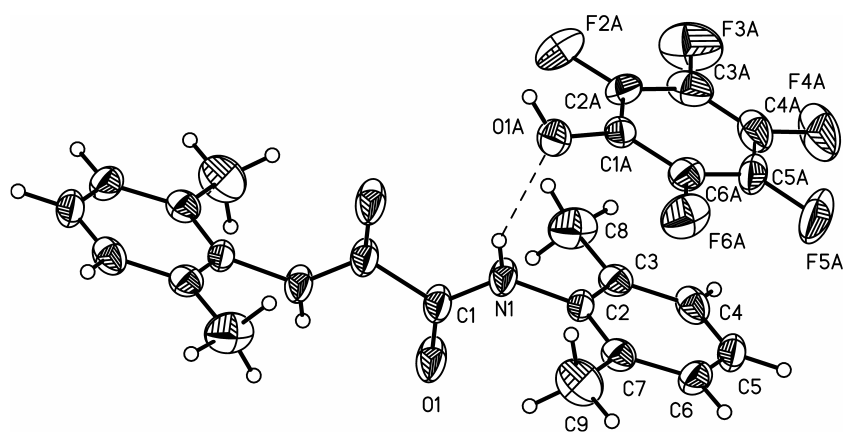


Fig. 4s ORTEP drawing of **3.pfp** with displacement ellipsoids shown at the 50% probability level

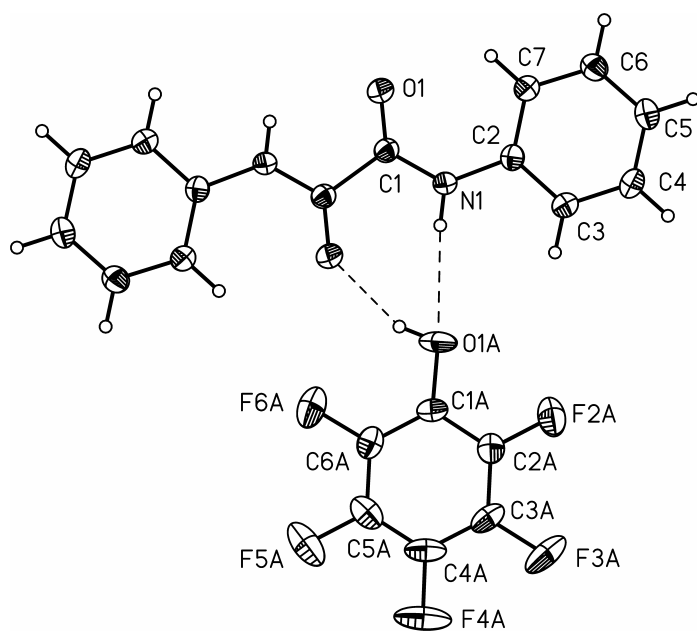


Fig. 5s ORTEP drawing of **1.pfp** with displacement ellipsoids shown at the 50% probability level

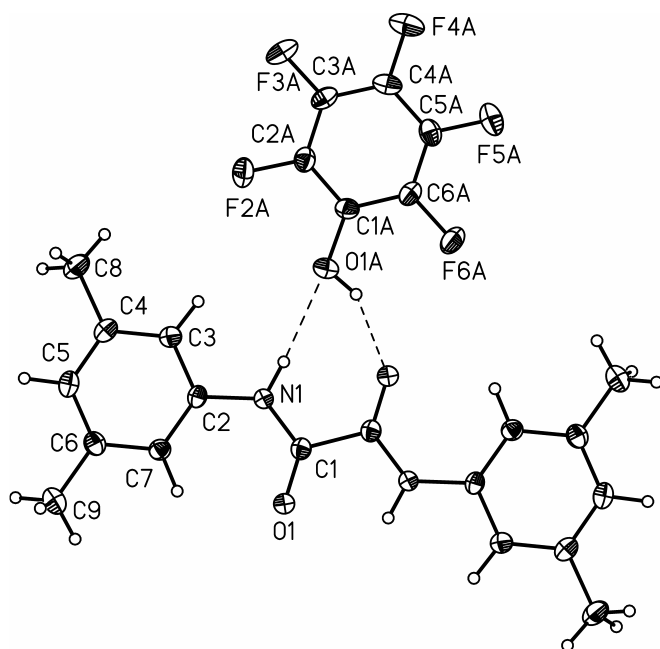


Fig. 6s Ortep drawing of **4.pfp** with displacement ellipsoids shown at the 50% probability level

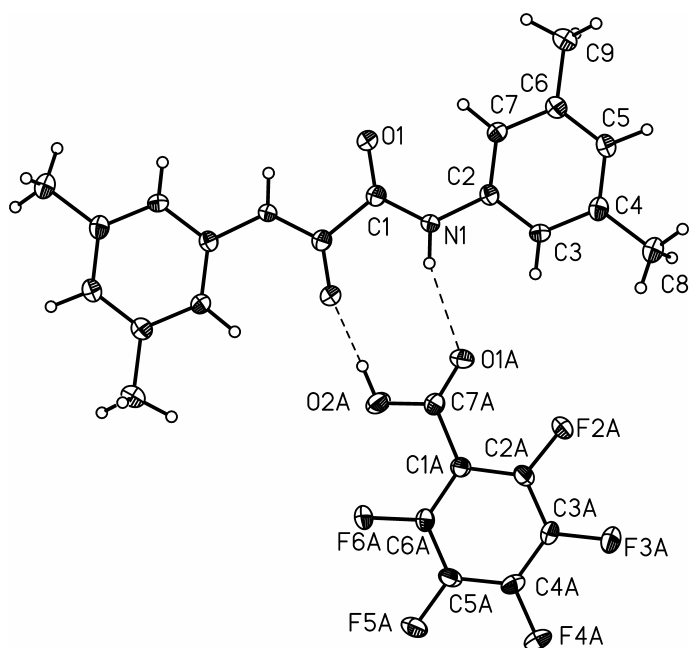


Fig. 7s Ortep drawing of **4.pfba** with displacement ellipsoids shown at the 50% probability level

Table. 1S Geometry of hydrogen bonds and short intramolecular contacts

a) compound **2**

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	<D-H...A (°)
N1 H1N... O1 <sup>(i)</sup>	0.91	2.25	2.684(3)	109

symmetry code: (i) 1-x, 1-y, -z

b) compound **4**

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	<D-H...A (°)
N1 H1... O1 <sup>(i)</sup>	0.90	2.19	2.6602(14)	112
C7 H7 ... O1	0.96	2.31	2.9380(16)	122

symmetry code: (i) -x, 1-y, -z

c) compound **2·pfp**

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	<D-H...A (°)
N1 H1N... O1 <sup>(i)</sup>	0.88	2.26	2.6770(17)	109
O1A H1A... O1	0.88	1.79	2.6524(16)	164
N1 H1N... O1A <sup>(ii)</sup>	0.88	2.33	3.0651(17)	141

symmetry code: (i) 1-x, 1-y, 1-z; (ii) 1+x,y,z

d) compound **3·pfp**

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	<D-H...A (°)
N1 H1A... O1 <sup>(i)</sup>	0.82	2.29	2.6790(19)	110
O1A H1A... O1 <sup>(ii)</sup>	0.81	1.92	2.7278(19)	177
N1 H1A... O1A	0.82	2.42	3.163(2)	152

symmetry code: (i) -x, 2-y, 1-z; (ii) x,-1+y,z

e) compound **4·pfp**

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	<D-H...A (°)
N1 H1N... O1 <sup>(i)</sup>	0.90	2.24	2.6981(15)	111
N1 H1N... O1A	0.90	2.20	3.0953(16)	175
O1A H1O... O1 <sup>(i)</sup>	0.85	1.89	2.6634(16)	151
C7 H7... O1	0.96	2.31	2.8994(17)	119

symmetry code: (i) -x, 1-y, 2-z

f) compound **4·pfba**

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	<D-H...A (°)
N1 H1N... O1 <sup>(i)</sup>	0.87	2.27	2.6945(19)	110
O2A H2O... O1 <sup>(i)</sup>	0.88	1.80	2.663(2)	167
N1 H1N... O1A	0.87	2.20	3.033(2)	160
C7 H7... O1	0.97	2.29	2.866(2)	117

symmetry code: (i) 1-x, 2-y, 1-z

g) compound **1·pfp**

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	<D-H...A (°)
N1 H1N... O1 <sup>(i)</sup>	0.85(2)	2.26(2)	2.698(2)	112.1(19)
N1 H1N... O1A	0.85(2)	2.30(2)	3.122(2)	164(2)
O1A H1A... O1 <sup>(i)</sup>	0.82(6)	1.96(6)	2.730(2)	156(5)
O1A H1A ... F6A	0.82(6)	2.35(5)	2.798(2)	115(4)

symmetry code: (i) 1-x, 2-y, 1-z