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Self-organization of substituted 1,3,4-oxadiazoles in the solid state and at surfaces

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Abstract

Different aspects of the structure formation for a class of molecules containing the diphenyl-1,3,4-oxadiazole fragment are discussed. Starting from the bulk state with the ideal crystal lattice and the derivation of some common packing motifs the formation of liquid-crystalline states are described. This leads to the consideration of structures found in Langmuir–Blodgett films and those obtained by organic molecular beam deposition. These structures may again be compared to those for the bulk crystalline state. Common features as well as characteristic differences due to peculiarities of the individual molecular structures are discussed.

Keywords: Oxadiazoles; Molecular crystals; Liquid crystals; Vacuum deposition; Self-organization

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1. Introduction

The rapid technological development requires the search for advanced materials with specific properties. Organic substances may easily be modified by different chemical procedures. The accordingly changing properties may be

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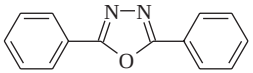
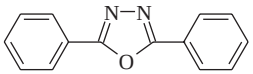
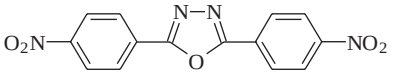
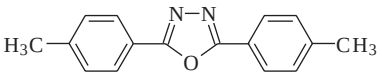
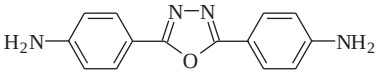
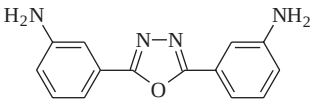
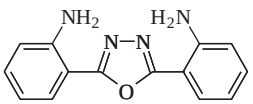
Table 1
Crystal structures and data describing the molecular conformation for selected diphenyloxadiazoles

Compound reference	Molecule (R1 – Oxa – R2)	Structure Space group no.	Molecules per asymmetric unit Notes	Unit cell parameters	Torsion angle [°] R1 – Oxa / Oxa – R2	Interring bond length [Å] R1 – Oxa / Oxa – R2
Ia [32,33]		Monoclinic $P2_1/c$ 14	1 molecule	a=5.188 Å b=18.078 Å c=12.144 Å β=93.19°	1.7 1.0	1.462 1.464
Ib [33]		Monoclinic Cc 9	6 molecules Non-centro-symmetric	a=24.134 Å b=24.099 Å c=12.879 Å β=110.05°	M1: 7.0 / 4.0 M2: 3.3 / 2.3 M3: 8.0 / 5.5 M4: 6.4 / 4.6 M5: 2.7 / 10.0 M6: 1.8 / 11.4	M1: 1.489 / 1.456 M2: 1.454 / 1.469 M3: 1.449 / 1.478 M4: 1.436 / 1.485 M5: 1.446 / 1.438 M6: 1.474 / 1.474
II [35]		*ortho*-Rhombic Pbcn 60	1/2 molecule	a=5.448 Å b=12.758 Å c=19.720 Å	10.7 10.7	1.461 1.461
III [36]		Monoclinic C2/c 15	1/2 molecule	a=11.404 Å b=11.751 Å c=10.870 Å β=116.62°	8.8 8.8	1.454 1.454
IV [37]		*ortho*-Rhombic Pbca 61	1 molecule	a=13.469 Å b=7.968 Å c=22.893 Å	15.4 14.1	1.461 1.463
V [39]		Monoclinic $P2_1/c$ 14	1 molecule	a=12.250 Å b=4.854 Å c=20.452 Å β=98.18°	0.8 0.0	1.478 1.469
VI [39]		Monoclinic C2/c 15	1 molecule	a=27.897 Å b=5.083 Å c=18.092 Å β=107.74°	2.2 1.4	1.452 1.464