

## RACEMIC TWINNING OF 7-CHLORINE-2,3,4a,6-TETRAHYDROFURO[2,3-*b*][1,4]OXATHIIN-6-ONE CRYSTALS

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An unusual type of *rac*-7-chlorine-2,3,4a,6-tetrahydrofuro[2,3-*b*][1,4]oxathiin-6-one crystallization is reported. This compound crystallizes in the form of lamellar conglomerates where each single crystal is not optically pure but is only enantiomerically enriched by one optical antipode and displays optical rotation.

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### INTRODUCTION

Spontaneous separation of racemates upon crystallization associated with the formation of a conglomerate (mechanical mixture of right- and left-handed crystals) has received increasing attention in organic crystal chemistry in the past decades [1-4]. This type of crystallization of chiral compounds allows separating them into enantiomers by a relatively simple method of “resolution by entrainment” or preferential crystallization [5]. Crystallographically, a conglomerate can be formed if the compound crystallizes in one of 65 chiral space groups and all crystallographically independent molecules share the same chirality. However, even these conditions do not always sufficient for enantiomerically pure crystals. This paradox is due to the so-called racemic twinning (lamellar epitaxy) [6, 7], i.e. accurate intergrowth of alternating enantiomeric zones (so-called domains) within each crystal.

The interest in racemic twinning is due to its definite effect on the physicochemical properties of materials. Thus, it was recently shown that this phenomenon decreases the intensity of second-harmonic generation in nonlinear optical materials [8]. It was reported that twins exhibit birefringence [9, 10]. Racemic twinning also affects stereoselectivity of some solid-state reactions [11-13].

In XRD studies, racemic twinning is manifested only in the analysis of intensities of Friedel pairs of reflections ( $hkl$ ) and ( $-h-k-l$ ), for example, using the Flack parameter [14, 15]. In his tutorial, Flack claimed that the noticeable contribution of anomalous scattering begins from silicon atoms in experiments with  $MoK_{\alpha}$  radiation and beginning from oxygen when using  $CuK_{\alpha}$  radiation.

The authors of a recent review paper claim that lamellar racemic twinning relatively rarely occurs during crystallization of chiral molecules and reported only 19 examples of such structures [16]. However, they considered only

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