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Crystal structure and Hirshfeld surface analysis of 3-cyanophenylboronic acid

A. Jaquelin Cárdenas-Valenzuela,[a] Gerardo González-García,[b] Ramón Zárraga-Nuñez,[b] Herbert Höpfl,[c] José J. Campos-Gaxiola[a] and Adriana Cruz-Enríquez[a]*

[a]Facultad de Ingeniería Mochis, Universidad Autónoma de Sinaloa, Fuente de Poseidón y Prol. A. Flores S/N, CP 81223, C.U. Los Mochis, Sinaloa, México, [b]Departamento de Química, División de Ciencias Naturales y Exactas, Campus Guanajuato, Universidad de Guanajuato, Sede Noria Alta, Noria Alta S/N, Col. Noria Alta, CP 36050, Guanajuato, Gto., México, and [c]Centro de Investigaciones Químicas, Instituto de Investigación en Ciencias Básicas y Aplicadas, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, CP 62209, Cuernavaca, Morelos, México. *Correspondence e-mail: cruzadriana@uas.edu.mx

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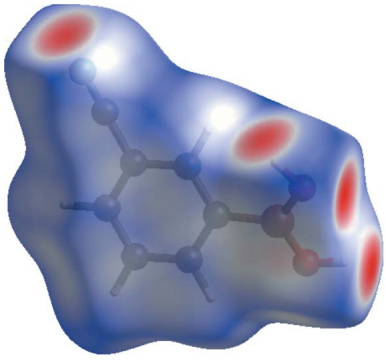
In the title compound, $C_7H_6BNO_2$, the mean plane of the –$B(OH)_2$ group is twisted by 21.28 (6)° relative to the cyanophenyl ring mean plane. In the crystal, molecules are linked by O—H···O and O—H···N hydrogen bonds, forming chains propagating along the [101] direction. Offset π–π and B···π stacking interactions link the chains, forming a three-dimensional network. Hirshfeld surface analysis shows that van der Waals interactions constitute a further major contribution to the intermolecular interactions, with H···H contacts accounting for 25.8% of the surface.

1. Chemical context

Boron-containing compounds and particularly arylboronic acid are an important class of compounds in the fields of organic and medicinal chemistry, and have played a role in the development of modern organic synthesis, macromolecular chemistry, crystal engineering and molecular recognition (Fujita *et al.*, 2008; Severin, 2009). As a result of their peculiar dynamic covalent reactivity with alcohols (Jin *et al.*, 2013), arylboronic acids and their dehydrated derivatives enable the self-assembly of a large variety of architectures resulting from boronate esterification (Takahagi *et al.* 2009) as well as boroxine (Côté *et al.*, 2005) and spiroborate formation (Du *et al.*, 2016).

Boronic acids form neutral and charge-assisted homo- and heterodimeric hydrogen-bonding patterns resembling characteristics similar to those found for carboxylic acids (see Fig. 1*a*). However, the –$B(OH)_2$ moiety contains two O—H



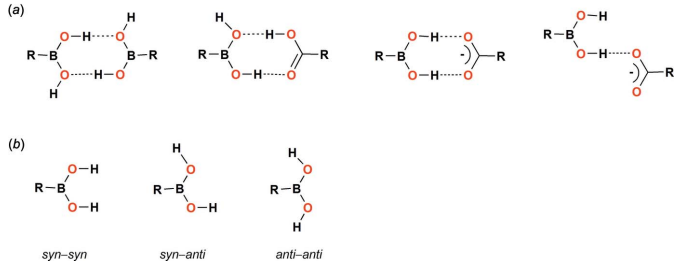


Figure 1
(*a*) Neutral and charge-assisted homo- and heterodimeric hydrogen-bonding motifs involving boronic acids. (*b*) Conformations of the boronic acid moiety.