Cl···Cl Interactions in Dichloromethane

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Dichloromethane, CH_2Cl_2, has been crystallized in a diamond-anvil cell and its structure determined by X-rays at 1.33GPa/293K, and at 1.63GPa/293K. The structures are orthorhombic, space-group *Pbcn*, and isostructural with the low temperature structure [1]. The Cl···Cl intermolecular interactions have been considered as the primary reason for the layer structure of the dichloromethane crystal. The intermolecular distances and molecular geometry of low temperature and high-pressure structures are compared in the Table below.

CH_2Cl_2 at			
T:	153 K	293 K	293 K
P:	0.1 MPa	1.33 GPa	1.63 GPa
	Ref. [1]	This work	This work
C–H	0.99(13) Å	1.01 (9) Å	1.13 (12) Å
C–Cl	1.768(13) Å	1.765 (4) Å	1.769 (5) Å
Cl···Cl	2.932(4) Å	3.360 (3) Å	3.324 (5) Å
∠Cl–C–Cl	112(1) ˚	111.6(3) ˚	111.4 (4) ˚
∠ H–C–H	112(7) ˚	99 (9) ˚	102 (10) ˚

[1] Kawaguchi T., Tanaka K., Takeuchi T., Watanabe T., *Bull. Chem. Soc. Jpn*, 1973, **46**, 62-66.

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