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# Name and address of author for correspondence
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                               'Lorenzo do Canto Visentin'
_publ_contact_author_address
;
Instituto de Qu\'imica
Universidade Federal do Rio de Janeiro
21949-900 Rio de Janeiro-RJ, Brazil.
;
_publ_contact_author_email
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'Andrea Rosane da Silva' .
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Departamento de Qu\'imica-ICE,
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;
'Marcelo Hawrylak Herbst' .
Departamento de Qu\'imica-ICE,
```

```
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21949-900 Rio de Janeiro-RJ, Brazil.
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atom site disorder group Cl2 C 0.3040(2) 0.63286(19) 0.08674(17) 0.0480(4) Uani 1 1 d . . . C13 C 0.3592(2) 0.63187(15) 0.23498(16) 0.0438(4) Uani 1 1 d . . . C15 C 0.5801(3) 0.6038(2) 0.2666(2) 0.0605(5) Uani 1 1 d . . C14 C 0.2153(4) 0.5331(2) 0.3049(2) 0.0645(5) Uani 1 1 d . . . 01 0 0.32623(18) 1.11874(11) 0.49231(11) 0.0496(3) Uani 1 1 d . . . N1 N 0.32296(18) 0.99931(12) 0.41313(12) 0.0392(3) Uani 1 1 d . . . H11B H -0.013(3) 0.6032(19) 0.0740(17) 0.052(4) Uiso 1 1 d . . . H12B H 0.317(3) 0.540(2) 0.0497(18) 0.060(5) Uiso 1 1 d . . . H12A H 0.407(3) 0.6983(18) 0.0486(17) 0.055(5) Uiso 1 1 d . . H11A H 0.068(3) 0.7033(19) -0.037(2) 0.060(5) Uiso 1 1 d . . . H10 H 0.437(4) 1.111(2) 0.540(2) 0.081(7) Uiso 1 1 d . . . H15A H 0.615(3) 0.608(2) 0.356(3) 0.087(7) Uiso 1 1 d . . . H15B H 0.604(3) 0.511(2) 0.2361(19) 0.071(6) Uiso 1 1 d . . . H14A H 0.075(4) 0.566(2) 0.296(2) 0.083(7) Uiso 1 1 d . . . H15C H 0.676(4) 0.675(3) 0.224(2) 0.099(8) Uiso 1 1 d . . . H14B H 0.263(3) 0.532(2) 0.400(2) 0.089(7) Uiso 1 1 d . H14C H 0.220(3) 0.441(2) 0.264(2) 0.084(7) Uiso 1 1 d . . . O3 O 0.34672(15) 0.77394(10) 0.29046(10) 0.0452(3) Uani 1 1 d . . . C1 C 0.1719(2) 0.97625(14) 0.32517(13) 0.0341(3) Uani 1 1 d . . . C2 C 0.1881(2) 0.84616(14) 0.24632(14) 0.0351(3) Uani 1 1 d . . . C3 C 0.0591(2) 0.80624(15) 0.13975(14) 0.0380(3) Uani 1 1 d . . . C4 C -0.1146(2) 0.88588(16) 0.10497(14) 0.0409(4) Uani 1 1 d . . . C10 C -0.0071(2) 1.05705(14) 0.29570(13) 0.0353(3) Uani 1 1 d . . . 02 0 -0.23317(18) 0.85064(13) 0.00816(12) 0.0617(4) Uani 1 1 d . . . C5 C -0.1493(2) 1.00903(15) 0.19046(14) 0.0383(3) Uani 1 1 d . . . C9 C -0.0489(2) 1.17530(15) 0.36925(16) 0.0457(4) Uani 1 1 d . . . H9 H 0.0436 1.2104 0.4378 0.055 Uiso 1 1 calc R . . C11 C 0.0911(3) 0.67900(18) 0.05557(17) 0.0475(4) Uani 1 1 d . . . C6 C -0.3272(2) 1.07613(17) 0.16525(16) 0.0481(4) Uani 1 1 d . . . H6 H -0.4210 1.0429 0.0966 0.058 Uiso 1 1 calc R . . C8 C -0.2261(3) 1.24057(18) 0.34110(17) 0.0531(4) Uani 1 1 d . . . H8 H -0.2508 1.3192 0.3909 0.064 Uiso 1 1 calc R . . C7 C -0.3665(3) 1.19108(18) 0.24037(17) 0.0530(4) Uani 1 1 d . . . H7 H -0.4864 1.2347 0.2233 0.064 Uiso 1 1 calc R . . loop_ _atom_site_aniso_label _atom_site_aniso_U_11 _atom_site_aniso_U_22 atom site aniso U 33 atom site aniso U 23 atom site aniso U 13 _atom_site_aniso_U_12 C12 0.0466(9) 0.0453(9) 0.0512(10) -0.0115(8) 0.0008(7) 0.0051(7) C13 0.0478(9) 0.0303(7) 0.0525(9) -0.0052(6) -0.0013(7) 0.0058(6) $\texttt{C15} \quad \texttt{0.0577(12)} \quad \texttt{0.0487(11)} \quad \texttt{0.0746(14)} \quad \texttt{-0.0050(10)} \quad \texttt{-0.0106(10)} \quad \texttt{0.0195(9)}$ C14 0.0774(15) 0.0486(11) 0.0673(13) 0.0035(9) 0.0097(11) -0.0010(10) 01 0.0491(7) 0.0434(6) 0.0521(7) -0.0189(5) -0.0172(5) 0.0056(5) N1 0.0408(7) 0.0342(6) 0.0400(7) -0.0083(5) -0.0080(5) 0.0006(5) 03 0.0449(6) 0.0369(6) 0.0511(6) -0.0096(5) -0.0164(5) 0.0100(4) $C1 \quad 0.0335(7) \quad 0.0336(7) \quad 0.0335(7) \quad 0.0006(6) \quad -0.0045(6) \quad -0.0008(6)$ $\texttt{C2} \ \texttt{0.0326(7)} \ \texttt{0.0325(7)} \ \texttt{0.0387(8)} \ \texttt{-0.0009(6)} \ \texttt{-0.0045(6)} \ \texttt{0.0007(6)}$ $\texttt{C3} \ \texttt{0.0366(8)} \ \texttt{0.0365(8)} \ \texttt{0.0388(8)} \ -\texttt{0.0060(6)} \ -\texttt{0.0048(6)} \ -\texttt{0.0006(6)}$ $\texttt{C4} \quad \texttt{0.0371(8)} \quad \texttt{0.0454(9)} \quad \texttt{0.0377(8)} \quad \texttt{-0.0033(6)} \quad \texttt{-0.0070(6)} \quad \texttt{-0.0014(6)}$ C10 0.0374(8) 0.0332(7) 0.0344(7) 0.0011(6) -0.0006(6) 0.0003(6) 02 0.0519(7) 0.0733(8) 0.0554(7) -0.0193(6) -0.0256(6) 0.0125(6)

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_geom_special_details

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes. ;

loop_

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C8 H8 0.9300 . ?
C7 H7 0.9300 . ?
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loop_

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C3 C11 H11B 108.3(10) . . ?
C12 C11 H11B 110.4(10) . . ?
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C7 C8 C9 121.07(15) . . ?
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loop_

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C1 C10 C5 C4 -4.0(2) . . . ?
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C13 C12 C11 C3 45.3(2) . . . ?
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