# Vanadium (beta-(dimethylamino)ethyl)cyclopentadienyl complexes with diphenylacetylene ligands

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*Published in:*
Organometallics

*DOI:*
10.1021/om8000718

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; ?
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_chemical_name_common             ?
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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 C   C    0.0033    0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M       'P 21/c'
_symmetry_Int_Tables_number                14

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   2 -x,1/2+y,1/2-z
   3 -x,-y,-z
   4 x,1/2-y,1/2+z


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_cell_length_b                   16.663(3)
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_cell_angle_alpha                90
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_cell_angle_gamma                90
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_computing_cell_refinement        'Bruker SMART'
_computing_data_reduction         'Bruker SAINT'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1997)'
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
```

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 factors based on ALL data will be even larger.
;

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V1 V Uani 1.02896(15) 0.33500(7) 0.36518(7) 1.000 0.0219(4) . .
V2 V Uani 0.74875(16) 0.20963(8) 0.31902(8) 1.000 0.0280(4) . .
Cl1 Cl Uani 0.7484(2) 0.32206(11) 0.41439(11) 1.000 0.0275(6) . .
Cl2 Cl Uani 1.0663(2) 0.19033(11) 0.35758(12) 1.000 0.0315(6) . .
N1 N Uani 1.1828(7) 0.3442(3) 0.4953(3) 1.000 0.0243(17) . .
N2 N Uani 0.6959(8) 0.1076(4) 0.4029(4) 1.000 0.0350(2) . .
C1 C Uani 1.0123(9) 0.4656(4) 0.3233(4) 1.000 0.0267(2) . .
C2 C Uani 0.9583(10) 0.4184(4) 0.2510(4) 1.000 0.0278(2) . .
C3 C Uani 1.0992(9) 0.3706(4) 0.2361(4) 1.000 0.0270(2) . .
C4 C Uani 1.2437(9) 0.3877(4) 0.2997(4) 1.000 0.0278(2) . .
C5 C Uani 1.1920(9) 0.4453(4) 0.3542(4) 1.000 0.0256(2) . .
C6 C Uani 1.2993(10) 0.4688(5) 0.4372(4) 1.000 0.0308(2) . .
C7 C Uani 1.2248(10) 0.4313(4) 0.5096(4) 1.000 0.0293(2) . .
C8 C Uani 1.3493(9) 0.2984(5) 0.5012(5) 1.000 0.0309(3) . .
C9 C Uani 1.0928(10) 0.3166(5) 0.5641(5) 1.000 0.0360(3) . .
C10 C Uani 0.6951(10) 0.1461(5) 0.1950(5) 1.000 0.0352(3) . .
C11 C Uani 0.7187(10) 0.2276(5) 0.1771(5) 1.000 0.0347(3) . .
C12 C Uani 0.5832(10) 0.2719(5) 0.2052(4) 1.000 0.0311(3) . .
C13 C Uani 0.4759(9) 0.2168(4) 0.2404(4) 1.000 0.0289(3) . .
C14 C Uani 0.5441(10) 0.1396(5) 0.2342(5) 1.000 0.0334(3) . .
C15 C Uani 0.4847(12) 0.0646(5) 0.2754(5) 1.000 0.0465(3) . .
C16 C Uani 0.5165(17) 0.0824(8) 0.3761(9) 1.000 0.1143(7) . .
C17 C Uani 0.716(2) 0.1275(7) 0.4944(7) 1.000 0.1007(6) . .
C18 C Uani 0.8152(15) 0.0395(7) 0.4007(9) 1.000 0.0958(6) . .
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H2 H Uiso 0.84489(-) 0.41896(-) 0.21790(-) 1.000 0.0333(-) . .
H3 H Uiso 1.09807(-) 0.33347(-) 0.19152(-) 1.000 0.0324(-) . .
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H8A H Uiso 1.42721(-) 0.31279(-) 0.55305(-) 1.000 0.0463(-) . .
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H9C H Uiso 1.17022(-) 0.32436(-) 0.61770(-) 1.000 0.0540(-) . .
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H16B H Uiso 0.49252(-) 0.03324(-) 0.40656(-) 1.000 0.1372(-) . .
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H17B H Uiso 0.83248(-) 0.15009(-) 0.51337(-) 1.000 0.1510(-) . .
H17C H Uiso 0.70112(-) 0.07868(-) 0.52613(-) 1.000 0.1510(-) . .
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H18B H Uiso 0.93470(-) 0.05561(-) 0.42488(-) 1.000 0.1437(-) . .
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V2 0.0158(7) 0.0354(7) 0.0327(7) -0.0023(6) 0.0042(5) -0.0003(5)
Cl1 0.0137(8) 0.0394(10) 0.0306(10) -0.0044(8) 0.0068(7) 0.0000(8)
Cl2 0.0133(9) 0.0332(10) 0.0479(12) -0.0013(8) 0.0047(8) 0.0023(7)
N1 0.011(3) 0.035(3) 0.027(3) 0.000(3) 0.004(2) -0.002(3)
N2 0.027(4) 0.047(4) 0.031(4) -0.005(3) 0.005(3) 0.011(3)
C1 0.022(4) 0.031(4) 0.029(4) 0.000(3) 0.009(3) 0.006(3)
C2 0.024(4) 0.037(4) 0.021(4) 0.001(3) -0.001(3) -0.008(3)
C3 0.030(4) 0.032(4) 0.021(4) -0.009(3) 0.012(3) -0.007(3)
C4 0.018(4) 0.036(4) 0.031(4) 0.000(3) 0.008(3) -0.003(3)
C5 0.019(4) 0.031(4) 0.028(4) 0.001(3) 0.009(3) -0.003(3)
C6 0.022(4) 0.035(4) 0.035(4) -0.004(3) 0.004(3) -0.005(3)
C7 0.019(4) 0.037(4) 0.030(4) -0.008(3) -0.002(3) 0.005(3)
C8 0.012(4) 0.042(5) 0.038(4) -0.001(4) 0.001(3) 0.002(3)
C9 0.022(4) 0.059(5) 0.027(4) 0.008(4) 0.003(3) -0.006(3)
C10 0.027(4) 0.045(4) 0.032(4) -0.006(4) 0.001(4) 0.013(4)
C11 0.024(4) 0.047(5) 0.033(4) -0.001(4) 0.005(4) -0.003(4)
C12 0.026(4) 0.035(4) 0.032(4) -0.002(3) 0.004(3) 0.006(3)
C13 0.009(4) 0.045(5) 0.031(4) -0.012(4) -0.001(3) 0.000(3)
C14 0.028(4) 0.040(5) 0.032(4) -0.006(4) 0.003(4) -0.000(4)
C15 0.035(5) 0.047(5) 0.052(6) -0.006(4) -0.009(4) -0.014(4)
C16 0.065(9) 0.105(10) 0.167(15) 0.075(10) 0.000(9) -0.042(8)
C17 0.170(15) 0.071(8) 0.063(8) -0.001(7) 0.023(9) -0.031(9)
C18 0.057(8) 0.075(8) 0.163(13) 0.061(9) 0.039(8) 0.023(6)
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 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All su's are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
 distances, angles and torsion angles
;

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 V1      Cl2          2.434(2)  .       .                  yes
 V1      N1           2.251(5)  .       .                  yes
 V1      C1           2.277(7)  .       .                  yes
 V1      C2           2.308(7)  .       .                  yes
 V1      C3           2.326(7)  .       .                  yes
 V1      C4           2.290(7)  .       .                  yes
 V1      C5           2.253(7)  .       .                  yes
 V2      Cl1          2.430(2)  .       .                  yes
 V2      Cl2          2.454(2)  .       .                  yes
 V2      N2           2.258(7)  .       .                  yes
 V2      C10          2.251(8)  .       .                  yes
 V2      C11          2.296(8)  .       .                  yes
 V2      C12          2.312(7)  .       .                  yes
 V2      C13          2.282(7)  .       .                  yes
 V2      C14          2.246(8)  .       .                  yes
 N1      C7           1.496(8)  .       .                  yes
 N1      C8           1.487(9)  .       .                  yes
 N1      C9           1.483(9)  .       .                  yes
 N2      C16          1.446(15)  .       .                  yes
 N2      C17          1.503(13)  .       .                  yes
 N2      C18          1.467(13)  .       .                  yes
 C1      C2           1.417(9)  .       .                  no
 C1      C5           1.438(10)  .       .                  no
 C2      C3           1.403(10)  .       .                  no
 C3      C4           1.419(9)  .       .                  no
 C4      C5           1.408(9)  .       .                  no
 C5      C6           1.511(9)  .       .                  no
 C6      C7           1.525(10)  .       .                  no
 C10     C11          1.407(12)  .       .                  no
 C10     C14          1.424(11)  .       .                  no
 C11     C12          1.418(11)  .       .                  no
 C12     C13          1.42(1)  .       .                  no
 C13     C14          1.400(11)  .       .                  no
 C14     C15          1.524(12)  .       .                  no
 C15     C16          1.639(8)  .       .                  no
 C1      H1           0.9500  .       .                  no
 C2      H2           0.9500  .       .                  no
 C3      H3           0.9500  .       .                  no
 C4      H4           0.9500  .       .                  no
 C6      H6A          0.9900  .       .                  no
 C6      H6B          0.9900  .       .                  no
 C7      H7A          0.9900  .       .                  no
 C7      H7B          0.9900  .       .                  no
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 C8      H8A          0.9800  .       .                  no
 C8      H8B          0.9800  .       .                  no
 C8      H8C          0.9800  .       .                  no
 C9      H9A          0.9800  .       .                  no
 C9      H9B          0.9800  .       .                  no
 C9      H9C          0.9800  .       .                  no
 C10     H10          0.9500  .       .                  no
 C11     H11          0.9500  .       .                  no
 C12     H12          0.9500  .       .                  no
 C13     H13          0.9500  .       .                  no
 C15     H15A         0.9900  .       .                  no
 C15     H15B         0.9900  .       .                  no
 C16     H16A         0.9900  .       .                  no
 C16     H16B         0.9900  .       .                  no
 C17     H17A         0.9800  .       .                  no
 C17     H17B         0.9800  .       .                  no
 C17     H17C         0.9800  .       .                  no
 C18     H18A         0.9800  .       .                  no
 C18     H18B         0.9800  .       .                  no
 C18     H18C         0.9800  .       .                  no

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 Cl1     V1      Cl2          92.78(7)    .       .       . yes
 Cl1     V1      N1           93.43(15)   .       .       . yes
 Cl1     V1      C1           99.93(19)   .       .       . yes
 Cl1     V1      C2          102.1(2)     .       .       . yes
 Cl1     V1      C3          132.03(18)   .       .       . yes
 Cl1     V1      C4          159.64(18)   .       .       . yes
 Cl1     V1      C5          129.57(19)   .       .       . yes
 Cl2     V1      N1           93.81(14)   .       .       . yes
 Cl2     V1      C1          158.90(18)   .       .       . yes
 Cl2     V1      C2          124.74(18)   .       .       . yes
 Cl2     V1      C3           99.17(18)   .       .       . yes
 Cl2     V1      C4          104.76(18)   .       .       . yes
 Cl2     V1      C5          137.02(19)   .       .       . yes
 N1      V1      C1          102.1(2)     .       .       . yes
 N1      V1      C2          136.9(2)     .       .       . yes
 N1      V1      C3          131.4(2)     .       .       . yes
 N1      V1      C4           95.6(2)     .       .       . yes
 N1      V1      C5           78.6(2)     .       .       . yes
 C1      V1      C2           36.0(2)     .       .       . yes
 C1      V1      C3           59.9(2)     .       .       . yes
 C1      V1      C4           60.3(2)     .       .       . yes
 C1      V1      C5           37.0(2)     .       .       . yes
 C2      V1      C3           35.2(3)     .       .       . yes
 C2      V1      C4           59.4(3)     .       .       . yes
 C2      V1      C5           60.4(2)     .       .       . yes
 C3      V1      C4           35.8(2)     .       .       . yes
 C3      V1      C5           60.2(2)     .       .       . yes
 C4      V1      C5           36.1(2)     .       .       . yes
 Cl1     V2      Cl2          92.60(7)    .       .       . yes
 Cl1     V2      N2          100.22(18)   .       .       . yes
 Cl1     V2      C10         155.8(2)     .       .       . yes
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| | | | | | | |
|---|---|---|---|---|---|---|
| Cl1 | V2 | C11 | 121.8(2) | . | . | . yes |
| Cl1 | V2 | C12 | 96.0(2) | . | . | . yes |
| Cl1 | V2 | C13 | 102.57(18) | . | . | . yes |
| Cl1 | V2 | C14 | 135.7(2) | . | . | . yes |
| Cl2 | V2 | N2 | 91.21(17) | . | . | . yes |
| Cl2 | V2 | C10 | 101.2(2) | . | . | . yes |
| Cl2 | V2 | C11 | 101.8(2) | . | . | . yes |
| Cl2 | V2 | C12 | 131.4(2) | . | . | . yes |
| Cl2 | V2 | C13 | 160.72(18) | . | . | . yes |
| Cl2 | V2 | C14 | 131.5(2) | . | . | . yes |
| N2 | V2 | C10 | 99.2(3) | . | . | . yes |
| N2 | V2 | C11 | 134.8(3) | . | . | . yes |
| N2 | V2 | C12 | 133.5(3) | . | . | . yes |
| N2 | V2 | C13 | 97.7(2) | . | . | . yes |
| N2 | V2 | C14 | 78.4(3) | . | . | . yes |
| C10 | V2 | C11 | 36.0(3) | . | . | . yes |
| C10 | V2 | C12 | 60.1(3) | . | . | . yes |
| C10 | V2 | C13 | 60.5(3) | . | . | . yes |
| C10 | V2 | C14 | 36.9(3) | . | . | . yes |
| C11 | V2 | C12 | 35.8(3) | . | . | . yes |
| C11 | V2 | C13 | 60.1(3) | . | . | . yes |
| C11 | V2 | C14 | 60.6(3) | . | . | . yes |
| C12 | V2 | C13 | 36.0(3) | . | . | . yes |
| C12 | V2 | C14 | 60.2(3) | . | . | . yes |
| C13 | V2 | C14 | 36.0(3) | . | . | . yes |
| V1 | Cl1 | V2 | 76.43(6) | . | . | . yes |
| V1 | Cl2 | V2 | 76.16(6) | . | . | . yes |
| V1 | N1 | C7 | 106.2(4) | . | . | . yes |
| V1 | N1 | C8 | 110.1(4) | . | . | . yes |
| V1 | N1 | C9 | 116.3(4) | . | . | . yes |
| C7 | N1 | C8 | 108.9(5) | . | . | . yes |
| C7 | N1 | C9 | 107.6(5) | . | . | . yes |
| C8 | N1 | C9 | 107.6(5) | . | . | . yes |
| V2 | N2 | C16 | 107.3(6) | . | . | . yes |
| V2 | N2 | C17 | 115.4(6) | . | . | . yes |
| V2 | N2 | C18 | 113.0(6) | . | . | . yes |
| C16 | N2 | C17 | 107.3(9) | . | . | . yes |
| C16 | N2 | C18 | 110.2(8) | . | . | . yes |
| C17 | N2 | C18 | 103.5(9) | . | . | . yes |
| V1 | C1 | C2 | 73.2(4) | . | . | . yes |
| V1 | C1 | C5 | 70.6(4) | . | . | . yes |
| C2 | C1 | C5 | 107.1(6) | . | . | . yes |
| V1 | C2 | C1 | 70.8(4) | . | . | . yes |
| V1 | C2 | C3 | 73.1(4) | . | . | . yes |
| C1 | C2 | C3 | 109.1(6) | . | . | . no |
| V1 | C3 | C2 | 71.7(4) | . | . | . yes |
| V1 | C3 | C4 | 70.7(4) | . | . | . yes |
| C2 | C3 | C4 | 107.6(6) | . | . | . no |
| V1 | C4 | C3 | 73.5(4) | . | . | . yes |
| V1 | C4 | C5 | 70.5(4) | . | . | . yes |
| C3 | C4 | C5 | 108.8(6) | . | . | . no |
| V1 | C5 | C1 | 72.4(4) | . | . | . yes |
| V1 | C5 | C4 | 73.4(4) | . | . | . yes |
| V1 | C5 | C6 | 111.9(5) | . | . | . yes |
| C1 | C5 | C4 | 107.5(6) | . | . | . no |
| C1 | C5 | C6 | 127.3(6) | . | . | . no |
| C4 | C5 | C6 | 124.4(6) | . | . | . no |
| C5 | C6 | C7 | 111.0(6) | . | . | . no |
| N1 | C7 | C6 | 112.2(5) | . | . | . yes |
| V2 | C10 | C11 | 73.7(5) | . | . | . yes |
| V2 | C10 | C14 | 71.4(5) | . | . | . yes |

| | | | | | | |
|---|---|---|---|---|---|---|
| C11 | C10 | C14 | 108.1(7) | . | . | . no |
| V2 | C11 | C10 | 70.2(5) | . | . | . yes |
| V2 | C11 | C12 | 72.7(4) | . | . | . yes |
| C10 | C11 | C12 | 108.0(7) | . | . | . no |
| V2 | C12 | C11 | 71.5(4) | . | . | . yes |
| V2 | C12 | C13 | 70.9(4) | . | . | . yes |
| C11 | C12 | C13 | 107.8(7) | . | . | . no |
| V2 | C13 | C12 | 73.2(4) | . | . | . yes |
| V2 | C13 | C14 | 70.6(4) | . | . | . yes |
| C12 | C13 | C14 | 108.3(6) | . | . | . no |
| V2 | C14 | C10 | 71.7(5) | . | . | . yes |
| V2 | C14 | C13 | 73.4(4) | . | . | . yes |
| V2 | C14 | C15 | 113.0(5) | . | . | . yes |
| C10 | C14 | C13 | 108.0(7) | . | . | . no |
| C10 | C14 | C15 | 126.0(7) | . | . | . no |
| C13 | C14 | C15 | 125.3(7) | . | . | . no |
| C14 | C15 | C16 | 106.4(7) | . | . | . no |
| N2 | C16 | C15 | 109.3(9) | . | . | . yes |
| V1 | C1 | H1 | 122.0 | . | . | . no |
| C2 | C1 | H1 | 126.0 | . | . | . no |
| C5 | C1 | H1 | 126.00 | . | . | . no |
| V1 | C2 | H2 | 122.00 | . | . | . no |
| C1 | C2 | H2 | 125.00 | . | . | . no |
| C3 | C2 | H2 | 125.00 | . | . | . no |
| V1 | C3 | H3 | 123.00 | . | . | . no |
| C2 | C3 | H3 | 126.00 | . | . | . no |
| C4 | C3 | H3 | 126.00 | . | . | . no |
| V1 | C4 | H4 | 122.00 | . | . | . no |
| C3 | C4 | H4 | 126.00 | . | . | . no |
| C5 | C4 | H4 | 126.00 | . | . | . no |
| C5 | C6 | H6A | 109.00 | . | . | . no |
| C5 | C6 | H6B | 109.00 | . | . | . no |
| C7 | C6 | H6A | 109.00 | . | . | . no |
| C7 | C6 | H6B | 109.00 | . | . | . no |
| H6A | C6 | H6B | 108.00 | . | . | . no |
| N1 | C7 | H7A | 109.00 | . | . | . no |
| N1 | C7 | H7B | 109.00 | . | . | . no |
| C6 | C7 | H7A | 109.00 | . | . | . no |
| C6 | C7 | H7B | 109.00 | . | . | . no |
| H7A | C7 | H7B | 108.00 | . | . | . no |
| N1 | C8 | H8A | 109.00 | . | . | . no |
| N1 | C8 | H8B | 109.00 | . | . | . no |
| N1 | C8 | H8C | 109.00 | . | . | . no |
| H8A | C8 | H8B | 109.00 | . | . | . no |
| H8A | C8 | H8C | 109.00 | . | . | . no |
| H8B | C8 | H8C | 109.00 | . | . | . no |
| N1 | C9 | H9A | 109.00 | . | . | . no |
| N1 | C9 | H9B | 109.00 | . | . | . no |
| N1 | C9 | H9C | 109.00 | . | . | . no |
| H9A | C9 | H9B | 109.00 | . | . | . no |
| H9A | C9 | H9C | 109.00 | . | . | . no |
| H9B | C9 | H9C | 109.00 | . | . | . no |
| V2 | C10 | H10 | 121.00 | . | . | . no |
| C11 | C10 | H10 | 126.00 | . | . | . no |
| C14 | C10 | H10 | 126.00 | . | . | . no |
| V2 | C11 | H11 | 123.00 | . | . | . no |
| C10 | C11 | H11 | 126.00 | . | . | . no |
| C12 | C11 | H11 | 126.00 | . | . | . no |
| V2 | C12 | H12 | 123.00 | . | . | . no |
| C11 | C12 | H12 | 126.00 | . | . | . no |
| C13 | C12 | H12 | 126.00 | . | . | . no |

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 V2      C13     H13          122.00    .       .       . no
 C12     C13     H13          126.00    .       .       . no
 C14     C13     H13          126.00    .       .       . no
 C14     C15     H15A         110.00    .       .       . no
 C14     C15     H15B         110.00    .       .       . no
 C16     C15     H15A         110.00    .       .       . no
 C16     C15     H15B         110.00    .       .       . no
 H15A    C15     H15B         109.00    .       .       . no
 N2      C16     H16A         110.00    .       .       . no
 N2      C16     H16B         110.00    .       .       . no
 C15     C16     H16A         110.00    .       .       . no
 C15     C16     H16B         110.00    .       .       . no
 H16A    C16     H16B         108.00    .       .       . no
 N2      C17     H17A         109.00    .       .       . no
 N2      C17     H17B         109.00    .       .       . no
 N2      C17     H17C         109.00    .       .       . no
 H17A    C17     H17B         109.00    .       .       . no
 H17A    C17     H17C         109.00    .       .       . no
 H17B    C17     H17C         109.00    .       .       . no
 N2      C18     H18A         109.00    .       .       . no
 N2      C18     H18B         109.00    .       .       . no
 N2      C18     H18C         109.00    .       .       . no
 H18A    C18     H18B         109.00    .       .       . no
 H18A    C18     H18C         109.00    .       .       . no
 H18B    C18     H18C         109.00    .       .       . no


loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
C8      H8B     Cl1   0.9800     2.8300     3.621(7)     139.00   1_655 yes
C9      H9B     Cl1   0.9800     2.8100     3.296(8)     111.00     .   yes
C18     H18B    Cl2   0.9800     2.7600     3.321(12)     117.00     .   yes


_diffrn_measured_fraction_theta_max    2.44
_diffrn_reflns_theta_full              26.02
_diffrn_measured_fraction_theta_full   2.2
_refine_diff_density_max    1.2(1)
_refine_diff_density_min   -0.7

#===END
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