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

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2008

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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_angle_gamma                90
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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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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) . .
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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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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
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 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
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 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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