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

Liu, Guohua; Lu, Xiaoquan; Gagliardo, Marcella; Beetstra, Dirk J.; Meetsma, Auke; Hessen, Bart; Liu, Gaifen

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2008

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

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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-
 factors based on ALL data will be even larger.
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N N Uani -0.1049(4) 0.09668(11) 0.1892(3) 1.000 0.0151(11) . .
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C2 C Uani 0.1280(5) 0.21143(13) 0.3647(4) 1.000 0.0192(14) . .
C3 C Uani 0.0349(5) 0.22464(13) 0.2245(4) 1.000 0.0180(14) . .
C4 C Uani -0.1131(5) 0.20506(13) 0.1778(4) 1.000 0.0174(14) . .
C5 C Uani -0.1107(5) 0.17953(13) 0.2909(4) 1.000 0.0172(14) . .
C6 C Uani -0.2373(5) 0.14899(14) 0.2827(4) 1.000 0.0209(14) . .
C7 C Uani -0.2590(5) 0.11451(14) 0.1711(4) 1.000 0.0202(14) . .
C8 C Uani -0.1399(5) 0.06808(14) 0.0644(4) 1.000 0.0194(14) . .
C9 C Uani -0.0378(5) 0.06939(14) 0.3201(4) 1.000 0.0201(14) . .
C10 C Uani 0.2743(5) 0.13598(12) 0.3450(4) 1.000 0.0168(14) . .
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C12 C Uani 0.5429(5) 0.15905(13) 0.5160(4) 1.000 0.0169(14) . .
C13 C Uani 0.6598(5) 0.16517(12) 0.6520(5) 1.000 0.0192(16) . .
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C22 C Uani 0.3585(5) -0.01490(14) 0.2757(4) 1.000 0.0215(14) . .
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C31 C Uani 0.1141(5) 0.16334(12) 0.0693(4) 1.000 0.0133(12) . .
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H6B H Uiso -0.20743 0.13511 0.37619 1.000 0.0250 . .
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H7B H Uiso -0.31492 0.12742 0.07517 1.000 0.0242 . .
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H8B H Uiso -0.04170 0.05645 0.06932 1.000 0.0292 . .
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H9B H Uiso 0.05750 0.05496 0.32789 1.000 0.0302 . .
H9C H Uiso -0.11478 0.04743 0.31494 1.000 0.0302 . .
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H20 H Uiso 0.71067 0.02394 0.44406 1.000 0.0224 . .
H21 H Uiso 0.57606 -0.04215 0.37492 1.000 0.0218 . .
H22 H Uiso 0.30273 -0.04160 0.24941 1.000 0.0258 . .
H23 H Uiso 0.16565 0.02341 0.18486 1.000 0.0197 . .
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H27 H Uiso -0.09027 0.07591 -0.36240 1.000 0.0260 . .
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H29 H Uiso 0.35334 0.03158 -0.15757 1.000 0.0276 . .
H30 H Uiso 0.38386 0.06780 0.04786 1.000 0.0211 . .
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H34 H Uiso -0.12063 0.26749 -0.26889 1.000 0.0205 . .
H35 H Uiso 0.06848 0.26228 -0.35280 1.000 0.0266 . .
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H37 H Uiso 0.30577 0.17300 -0.05136 1.000 0.0218 . .

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N 0.015(2) 0.0158(18) 0.0138(18) -0.0004(15) 0.0060(16) -0.0008(19)
C1 0.022(3) 0.012(2) 0.012(2) -0.0020(17) 0.0093(19) 0.0061(19)
C2 0.020(3) 0.014(2) 0.024(2) -0.0082(19) 0.010(2) 0.0012(19)
C3 0.024(3) 0.012(2) 0.025(2) -0.0006(19) 0.017(2) 0.0010(19)
C4 0.022(3) 0.015(2) 0.018(2) -0.0002(18) 0.011(2) 0.005(2)
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```
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C36 0.031(3) 0.016(2) 0.033(3) -0.002(2) 0.023(2) 0.001(2)
C37 0.021(3) 0.014(2) 0.022(2) -0.0011(19) 0.012(2) 0.000(2)


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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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 V       C3           2.274(4)    . .  yes
 V       C4           2.264(5)    . .  yes
 V       C5           2.268(5)    . .  yes
 V       C10          1.888(5)    . .  yes
 V       C17          2.360(5)    . .  yes
 V       C24          2.339(5)    . .  yes
 V       C31          1.895(4)    . .  yes
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N	C8	1.489(5)	.	.	yes
N	C9	1.491(5)	.	.	yes
C1	C2	1.404(6)	.	.	yes
C1	C5	1.412(6)	.	.	yes
C2	C3	1.400(5)	.	.	yes
C3	C4	1.405(7)	.	.	no
C4	C5	1.415(6)	.	.	no
C5	C6	1.500(7)	.	.	no
C6	C7	1.526(6)	.	.	no
C10	C11	1.468(6)	.	.	no
C10	C17	1.433(6)	.	.	no
C11	C12	1.409(7)	.	.	no
C11	C16	1.397(6)	.	.	no
C12	C13	1.380(6)	.	.	no
C13	C14	1.394(6)	.	.	no
C14	C15	1.365(7)	.	.	no
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C17	C18	1.508(6)	.	.	no
C17	C24	1.417(5)	.	.	no
C18	C19	1.389(7)	.	.	no
C18	C23	1.406(6)	.	.	no
C19	C20	1.395(6)	.	.	no
C20	C21	1.383(6)	.	.	no
C21	C22	1.386(7)	.	.	no
C22	C23	1.384(6)	.	.	no
C24	C25	1.501(5)	.	.	no
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C25	C26	1.403(6)	.	.	no
C25	C30	1.388(7)	.	.	no
C26	C27	1.384(6)	.	.	no
C27	C28	1.389(8)	.	.	no
C28	C29	1.374(7)	.	.	no
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C6	H6A	0.9900	.	.	no
C6	H6B	0.9900	.	.	no
C7	H7A	0.9900	.	.	no
C7	H7B	0.9900	.	.	no
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
C12	H12	0.9500	.	.	no
C13	H13	0.9500	.	.	no
C14	H14	0.9500	.	.	no
C15	H15	0.9500	.	.	no
C16	H16	0.9500	.	.	no
C19	H19	0.9500	.	.	no

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 C21     H21          0.9500   . .  no
 C22     H22          0.9500   . .  no
 C23     H23          0.9500   . .  no
 C26     H26          0.9500   . .  no
 C27     H27          0.9500   . .  no
 C28     H28          0.9500   . .  no
 C29     H29          0.9500   . .  no
 C30     H30          0.9500   . .  no
 C33     H33          0.9500   . .  no
 C34     H34          0.9500   . .  no
 C35     H35          0.9500   . .  no
 C36     H36          0.9500   . .  no
 C37     H37          0.9500   . .  no

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
 N       V       C1           96.63(14)   .       .       .  yes
 N       V       C2          131.79(16)   .       .       .  yes
 N       V       C3          131.01(16)   .       .       .  yes
 N       V       C4           95.24(15)   .       .       .  yes
 N       V       C5           75.68(15)   .       .       .  yes
 N       V       C10         112.60(15)   .       .       .  yes
 N       V       C17          96.71(15)   .       .       .  yes
 N       V       C24          97.61(14)   .       .       .  yes
 N       V       C31         116.32(15)   .       .       .  yes
 C1      V       C2           35.69(16)   .       .       .  yes
 C1      V       C3           59.78(14)   .       .       .  yes
 C1      V       C4           60.18(14)   .       .       .  yes
 C1      V       C5           36.04(16)   .       .       .  yes
 C1      V       C10          90.56(17)   .       .       .  yes
 C1      V       C17         126.97(15)   .       .       .  yes
 C1      V       C24         158.56(16)   .       .       .  yes
 C1      V       C31         142.41(15)   .       .       .  yes
 C2      V       C3           35.78(14)   .       .       .  yes
 C2      V       C4           59.94(15)   .       .       .  yes
 C2      V       C5           59.89(17)   .       .       .  yes
 C2      V       C10          82.33(16)   .       .       .  yes
 C2      V       C17         116.72(16)   .       .       .  yes
 C2      V       C24         129.88(17)   .       .       .  yes
 C2      V       C31         107.91(16)   .       .       .  yes
 C3      V       C4           36.08(17)   .       .       .  yes
 C3      V       C5           60.20(16)   .       .       .  yes
 C3      V       C10         110.03(16)   .       .       .  yes
 C3      V       C17         132.16(17)   .       .       .  yes
 C3      V       C24         119.55(16)   .       .       .  yes
 C3      V       C31          84.09(16)   .       .       .  yes
 C4      V       C5           36.40(15)   .       .       .  yes
 C4      V       C10         142.24(16)   .       .       .  yes
 C4      V       C17         165.01(16)   .       .       .  yes
 C4      V       C24         133.82(14)   .       .       .  yes
 C4      V       C31          97.30(17)   .       .       .  yes
 C5      V       C10         125.56(16)   .       .       .  yes
 C5      V       C17         157.20(14)   .       .       .  yes
```

C5	V	C24	165.16(15)	.	.	.	yes
C5	V	C31	133.49(17)	.	.	.	yes
C10	V	C17	37.40(15)	.	.	.	yes
C10	V	C24	69.17(16)	.	.	.	yes
C10	V	C31	92.7(2)	.	.	.	yes
C17	V	C24	35.11(14)	.	.	.	yes
C17	V	C31	69.22(17)	.	.	.	yes
C24	V	C31	37.91(16)	.	.	.	yes
V	N	C7	110.0(2)	.	.	.	yes
V	N	C8	116.3(3)	.	.	.	yes
V	N	C9	107.1(3)	.	.	.	yes
C7	N	C8	106.3(3)	.	.	.	yes
C7	N	C9	108.6(3)	.	.	.	yes
C8	N	C9	108.4(3)	.	.	.	yes
V	C1	C2	71.6(2)	.	.	.	yes
V	C1	C5	70.9(2)	.	.	.	yes
C2	C1	C5	107.6(3)	.	.	.	no
V	C2	C1	72.7(2)	.	.	.	yes
V	C2	C3	71.8(2)	.	.	.	yes
C1	C2	C3	108.7(4)	.	.	.	no
V	C3	C2	72.5(2)	.	.	.	yes
V	C3	C4	71.6(2)	.	.	.	yes
C2	C3	C4	108.1(4)	.	.	.	no
V	C4	C3	72.3(3)	.	.	.	yes
V	C4	C5	72.0(3)	.	.	.	yes
C3	C4	C5	107.7(4)	.	.	.	no
V	C5	C1	73.1(3)	.	.	.	yes
V	C5	C4	71.7(3)	.	.	.	yes
V	C5	C6	115.5(3)	.	.	.	yes
C1	C5	C4	107.9(4)	.	.	.	no
C1	C5	C6	125.8(4)	.	.	.	no
C4	C5	C6	125.9(4)	.	.	.	no
C5	C6	C7	108.1(4)	.	.	.	no
N	C7	C6	111.5(4)	.	.	.	yes
V	C10	C11	142.6(3)	.	.	.	yes
V	C10	C17	89.5(3)	.	.	.	yes
C11	C10	C17	127.6(4)	.	.	.	no
C10	C11	C12	119.7(4)	.	.	.	no
C10	C11	C16	122.9(4)	.	.	.	no
C12	C11	C16	117.4(4)	.	.	.	no
C11	C12	C13	121.4(4)	.	.	.	no
C12	C13	C14	119.5(5)	.	.	.	no
C13	C14	C15	120.2(4)	.	.	.	no
C14	C15	C16	120.5(4)	.	.	.	no
C11	C16	C15	121.0(4)	.	.	.	no
V	C17	C10	53.1(2)	.	.	.	yes
V	C17	C18	146.0(3)	.	.	.	yes
V	C17	C24	71.6(3)	.	.	.	yes
C10	C17	C18	119.9(3)	.	.	.	no
C10	C17	C24	116.8(4)	.	.	.	no
C18	C17	C24	123.1(4)	.	.	.	no
C17	C18	C19	118.2(4)	.	.	.	no
C17	C18	C23	124.7(4)	.	.	.	no
C19	C18	C23	117.0(4)	.	.	.	no
C18	C19	C20	121.9(4)	.	.	.	no
C19	C20	C21	120.1(4)	.	.	.	no
C20	C21	C22	118.8(4)	.	.	.	no
C21	C22	C23	121.0(4)	.	.	.	no
C18	C23	C22	121.1(4)	.	.	.	no
V	C24	C17	73.3(3)	.	.	.	yes
V	C24	C25	143.9(3)	.	.	.	yes

V	C24	C31	54.1(2)	.	.	.	yes
C17	C24	C25	123.6(4)	.	.	.	no
C17	C24	C31	118.0(4)	.	.	.	no
C25	C24	C31	118.3(3)	.	.	.	no
C24	C25	C26	121.0(4)	.	.	.	no
C24	C25	C30	121.5(4)	.	.	.	no
C26	C25	C30	117.1(4)	.	.	.	no
C25	C26	C27	121.6(4)	.	.	.	no
C26	C27	C28	120.1(4)	.	.	.	no
C27	C28	C29	119.1(4)	.	.	.	no
C28	C29	C30	120.7(5)	.	.	.	no
C25	C30	C29	121.3(4)	.	.	.	no
V	C31	C24	88.0(3)	.	.	.	yes
V	C31	C32	149.0(3)	.	.	.	yes
C24	C31	C32	123.0(4)	.	.	.	no
C31	C32	C33	122.5(4)	.	.	.	no
C31	C32	C37	120.5(4)	.	.	.	no
C33	C32	C37	117.0(4)	.	.	.	no
C32	C33	C34	121.8(4)	.	.	.	no
C33	C34	C35	119.3(4)	.	.	.	no
C34	C35	C36	119.8(4)	.	.	.	no
C35	C36	C37	120.9(5)	.	.	.	no
C32	C37	C36	121.1(4)	.	.	.	no
V	C1	H1	123.00	.	.	.	no
C2	C1	H1	126.00	.	.	.	no
C5	C1	H1	126.00	.	.	.	no
V	C2	H2	122.00	.	.	.	no
C1	C2	H2	126.00	.	.	.	no
C3	C2	H2	126.00	.	.	.	no
V	C3	H3	122.00	.	.	.	no
C2	C3	H3	126.00	.	.	.	no
C4	C3	H3	126.00	.	.	.	no
V	C4	H4	121.00	.	.	.	no
C3	C4	H4	126.00	.	.	.	no
C5	C4	H4	126.00	.	.	.	no
C5	C6	H6A	110.00	.	.	.	no
C5	C6	H6B	110.00	.	.	.	no
C7	C6	H6A	110.00	.	.	.	no
C7	C6	H6B	110.00	.	.	.	no
H6A	C6	H6B	108.00	.	.	.	no
N	C7	H7A	109.00	.	.	.	no
N	C7	H7B	109.00	.	.	.	no
C6	C7	H7A	109.00	.	.	.	no
C6	C7	H7B	109.00	.	.	.	no
H7A	C7	H7B	108.00	.	.	.	no
N	C8	H8A	109.00	.	.	.	no
N	C8	H8B	109.00	.	.	.	no
N	C8	H8C	109.00	.	.	.	no
H8A	C8	H8B	109.00	.	.	.	no
H8A	C8	H8C	109.00	.	.	.	no
H8B	C8	H8C	109.00	.	.	.	no
N	C9	H9A	109.00	.	.	.	no
N	C9	H9B	109.00	.	.	.	no
N	C9	H9C	109.00	.	.	.	no
H9A	C9	H9B	109.00	.	.	.	no
H9A	C9	H9C	109.00	.	.	.	no
H9B	C9	H9C	109.00	.	.	.	no
C11	C12	H12	119.00	.	.	.	no
C13	C12	H12	119.00	.	.	.	no
C12	C13	H13	120.00	.	.	.	no
C14	C13	H13	120.00	.	.	.	no

```
 C13     C14     H14          120.00              .       .       .          no
 C15     C14     H14          120.00              .       .       .          no
 C14     C15     H15          120.00              .       .       .          no
 C16     C15     H15          120.00              .       .       .          no
 C11     C16     H16          120.00              .       .       .          no
 C15     C16     H16          120.00              .       .       .          no
 C18     C19     H19          119.00              .       .       .          no
 C20     C19     H19          119.00              .       .       .          no
 C19     C20     H20          120.00              .       .       .          no
 C21     C20     H20          120.00              .       .       .          no
 C20     C21     H21          121.00              .       .       .          no
 C22     C21     H21          121.00              .       .       .          no
 C21     C22     H22          119.00              .       .       .          no
 C23     C22     H22          119.00              .       .       .          no
 C18     C23     H23          119.00              .       .       .          no
 C22     C23     H23          119.00              .       .       .          no
 C25     C26     H26          119.00              .       .       .          no
 C27     C26     H26          119.00              .       .       .          no
 C26     C27     H27          120.00              .       .       .          no
 C28     C27     H27          120.00              .       .       .          no
 C27     C28     H28          120.00              .       .       .          no
 C29     C28     H28          120.00              .       .       .          no
 C28     C29     H29          120.00              .       .       .          no
 C30     C29     H29          120.00              .       .       .          no
 C25     C30     H30          119.00              .       .       .          no
 C29     C30     H30          119.00              .       .       .          no
 C32     C33     H33          119.00              .       .       .          no
 C34     C33     H33          119.00              .       .       .          no
 C33     C34     H34          120.00              .       .       .          no
 C35     C34     H34          120.00              .       .       .          no
 C34     C35     H35          120.00              .       .       .          no
 C36     C35     H35          120.00              .       .       .          no
 C35     C36     H36          120.00              .       .       .          no
 C37     C36     H36          120.00              .       .       .          no
 C32     C37     H37          119.00              .       .       .          no
 C36     C37     H37          119.00              .       .       .          no


_diffrn_measured_fraction_theta_max    2.41
_diffrn_reflns_theta_full              24.73
_diffrn_measured_fraction_theta_full   1.21
_refine_diff_density_max    1.12(10)
_refine_diff_density_min   -0.43

#===END
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