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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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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 $F^2 > 2\sigma(F^2)$ 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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C2 C Uani 0.1280(5) 0.21143(13) 0.3647(4) 1.000 0.0192(14) . . .
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C25 C Uani 0.1657(5) 0.09409(12) -0.0317(4) 1.000 0.0128(12) . . .

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 H6B H Uiso -0.20743 0.13511 0.37619 1.000 0.0250 . .
 H7A H Uiso -0.32420 0.09055 0.17883 1.000 0.0242 . .
 H7B H Uiso -0.31492 0.12742 0.07517 1.000 0.0242 . .
 H8A H Uiso -0.20716 0.04403 0.06486 1.000 0.0292 . .
 H8B H Uiso -0.04170 0.05645 0.06932 1.000 0.0292 . .
 H8C H Uiso -0.19387 0.08493 -0.02327 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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 H13 H Uiso 0.75806 0.17699 0.66674 1.000 0.0230 . .
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 H30 H Uiso 0.38386 0.06780 0.04786 1.000 0.0211 . .
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 C35 0.031(3) 0.016(2) 0.022(2) 0.002(2) 0.014(2) -0.004(2)
 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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loop_

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| V | C2 | 2.283(4) | . . | yes |
| 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 |
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| C5 | C6 | 1.500 (7) | . . | no |
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| 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 |
| C15 | C16 | 1.388 (6) | . . | no |
| 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 |
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| C24 | C25 | 1.501 (5) | . . | no |
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| C25 | C26 | 1.403 (6) | . . | no |
| C25 | C30 | 1.388 (7) | . . | no |
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| C36 | C37 | 1.378 (6) | . . | 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 |
| 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 |

| | | | | |
|-----|-----|--------|-----|----|
| C20 | H20 | 0.9500 | . . | no |
| 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 | no |
| C3 | C2 | H2 | 126.00 | . | . | . | no | no |
| V | C3 | H3 | 122.00 | . | . | . | no | no |
| C2 | C3 | H3 | 126.00 | . | . | . | no | no |
| C4 | C3 | H3 | 126.00 | . | . | . | no | no |
| V | C4 | H4 | 121.00 | . | . | . | no | no |
| C3 | C4 | H4 | 126.00 | . | . | . | no | no |
| C5 | C4 | H4 | 126.00 | . | . | . | no | no |
| C5 | C6 | H6A | 110.00 | . | . | . | no | no |
| C5 | C6 | H6B | 110.00 | . | . | . | no | no |
| C7 | C6 | H6A | 110.00 | . | . | . | no | no |
| C7 | C6 | H6B | 110.00 | . | . | . | no | no |
| H6A | C6 | H6B | 108.00 | . | . | . | no | no |
| N | C7 | H7A | 109.00 | . | . | . | no | no |
| N | C7 | H7B | 109.00 | . | . | . | no | no |
| C6 | C7 | H7A | 109.00 | . | . | . | no | no |
| C6 | C7 | H7B | 109.00 | . | . | . | no | no |
| H7A | C7 | H7B | 108.00 | . | . | . | no | no |
| N | C8 | H8A | 109.00 | . | . | . | no | no |
| N | C8 | H8B | 109.00 | . | . | . | no | no |
| N | C8 | H8C | 109.00 | . | . | . | no | no |
| H8A | C8 | H8B | 109.00 | . | . | . | no | no |
| H8A | C8 | H8C | 109.00 | . | . | . | no | no |
| H8B | C8 | H8C | 109.00 | . | . | . | no | no |
| N | C9 | H9A | 109.00 | . | . | . | no | no |
| N | C9 | H9B | 109.00 | . | . | . | no | no |
| N | C9 | H9C | 109.00 | . | . | . | no | no |
| H9A | C9 | H9B | 109.00 | . | . | . | no | no |
| H9A | C9 | H9C | 109.00 | . | . | . | no | no |
| H9B | C9 | H9C | 109.00 | . | . | . | no | no |
| C11 | C12 | H12 | 119.00 | . | . | . | no | no |
| C13 | C12 | H12 | 119.00 | . | . | . | no | no |
| C12 | C13 | H13 | 120.00 | . | . | . | no | no |
| C14 | C13 | H13 | 120.00 | . | . | . | no | 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 |

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_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

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#===END