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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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N N 0.0061 0.0033
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl Cl 0.1484 0.1585
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H H 0.0000 0.0000
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C C 0.0033 0.0016
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2 -y,x-y,z
3 -x+y,-x,z
4 -x,-y,-z
5 y,-x+y,-z
6 x-y,x,-z
7 1/3+x,2/3+y,2/3+z
8 1/3-y,2/3+x-y,2/3+z
9 1/3-x+y,2/3-x,2/3+z
10 1/3-x,2/3-y,2/3-z
11 1/3+y,2/3-x+y,2/3-z
12 1/3+x-y,2/3+x,2/3-z
13 2/3+x,1/3+y,1/3+z
14 2/3-y,1/3+x-y,1/3+z
15 2/3-x+y,1/3-x,1/3+z
16 2/3-x,1/3-y,1/3-z
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18 2/3+x-y,1/3+x,1/3-z

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_computing_data_reduction	'Bruker SAINT'
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_computing_publication_material 'Bruker SHELXTL'
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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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_atom_site_refinement_flags  
V V Uani 0.17014(1) 0.26531(1) 0.05282(3) 1.000 0.0165(11) . .  
Cl Cl Uani 0.13373(2) 0.22855(2) -0.12984(4) 1.000 0.0241(16) . .  
N N Uani 0.17751(8) 0.20036(8) 0.10452(17) 1.000(4) 0.0274(6) . .  
C1 C Uani 0.24031(8) 0.31703(9) 0.14132(2) 1.000(4) 0.0251(7) . .  
C2 C Uani 0.22343(8) 0.34547(9) 0.08376(2) 1.000 0.0257(7) . .  
C3 C Uani 0.22404(8) 0.33874(8) -0.04188(2) 1.000 0.0242(7) . .  
C4 C Uani 0.24190(8) 0.30673(8) -0.06130(2) 1.000 0.0218(7) . .  
C5 C Uani 0.25210(8) 0.29333(9) 0.05073(15) 1.000 0.0228(6) . .  
C6 C Uani 0.26497(9) 0.25478(10) 0.06965(2) 1.000 0.0291(8) . .  
C7 C Uani 0.22136(10) 0.20627(10) 0.03869(2) 1.000 0.0295(8) . .  
C8 C Uani 0.13566(12) 0.15337(10) 0.06903(3) 1.000 0.0377(9) . .  
C9 C Uani 0.18543(12) 0.19781(13) 0.23668(2) 1.000 0.0382(10) . .
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C10 C Uani 0.07218(8) 0.31264(9) 0.20955(19) 1.000 0.0230(6) . . .  
C11 C Uani 0.05630(9) 0.34589(10) 0.21528(2) 1.000 0.0284(7) . . .  
C12 C Uani 0.07693(9) 0.38656(9) 0.14167(2) 1.000 0.0275(7) . . .  
C13 C Uani 0.11240(9) 0.39327(9) 0.05901(2) 1.000 0.0250(7) . . .  
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C16 C Uani 0.12506(7) 0.28403(8) 0.12172(18) 1.000 0.0180(6) . . .  
C17 C Uani 0.11902(8) 0.24560(8) 0.17975(18) 1.000 0.0195(6) . . .  
C18 C Uani 0.09061(8) 0.21539(8) 0.28163(19) 1.000 0.0218(6) . . .  
C19 C Uani 0.10995(10) 0.22542(9) 0.39845(2) 1.000 0.0275(7) . . .  
C20 C Uani 0.08299(12) 0.19711(10) 0.49544(2) 1.000 0.0367(9) . . .  
C21 C Uani 0.03704(12) 0.15848(11) 0.47796(3) 1.000 0.0423(10) . . .  
C22 C Uani 0.01762(11) 0.14791(12) 0.36269(3) 1.000 0.0446(9) . . .  
C23 C Uani 0.04416(9) 0.17589(10) 0.26485(2) 1.000 0.0344(8) . . .  
H1 H Uiso 0.24347(-) 0.31322(-) 0.22344(-) 1.000 0.0313(10) . . .  
H2 H Uiso 0.21390(-) 0.36730(-) 0.12484(-) 1.000 0.0309(10) . . .  
H3 H Uiso 0.21387(-) 0.35410(-) -0.10219(-) 1.000 0.0448(11) . . .  
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H6' H Uiso 0.27566(-) 0.25600(-) 0.15572(-) 1.000 0.0374(10) . . .  
H7 H Uiso 0.21493(-) 0.20569(-) -0.05076(-) 1.000 0.0365(10) . . .  
H7' H Uiso 0.22746(-) 0.17998(-) 0.06271(-) 1.000 0.0353(10) . . .  
H8 H Uiso 0.12930(-) 0.15429(-) -0.01613(-) 1.000 0.0288(10) . . .  
H8' H Uiso 0.10905(-) 0.14987(-) 0.10798(-) 1.000 0.0401(12) . . .  
H8'' H Uiso 0.14219(-) 0.12843(-) 0.09112(-) 1.000 0.0417(11) . . .  
H9 H Uiso 0.19843(-) 0.17632(-) 0.24959(-) 1.000 0.0414(11) . . .  
H9' H Uiso 0.21031(-) 0.23032(-) 0.26554(-) 1.000 0.0588(14) . . .  
H9'' H Uiso 0.15309(-) 0.18522(-) 0.28252(-) 1.000 0.0343(10) . . .  
H10 H Uiso 0.05818(-) 0.28409(-) 0.26028(-) 1.000 0.0299(10) . . .  
H11 H Uiso 0.03095(-) 0.34013(-) 0.26559(-) 1.000 0.0323(10) . . .  
H12 H Uiso 0.06483(-) 0.40916(-) 0.14750(-) 1.000 0.0396(11) . . .  
H13 H Uiso 0.12718(-) 0.42164(-) 0.00843(-) 1.000 0.0197(9) . . .  
H14 H Uiso 0.15198(-) 0.36436(-) -0.00557(-) 1.000 0.0316(10) . . .  
H19 H Uiso 0.14159(-) 0.25076(-) 0.41563(-) 1.000 0.0344(11) . . .  
H20 H Uiso 0.09810(-) 0.20524(-) 0.57270(-) 1.000 0.0446(12) . . .  
H21 H Uiso 0.01797(-) 0.14062(-) 0.54280(-) 1.000 0.0487(12) . . .  
H22 H Uiso -0.01592(-) 0.12384(-) 0.35035(-) 1.000 0.0547(14) . . .  
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loop\_

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N 0.0375(12) 0.0306(11) 0.0224(9) 0.0045(8) 0.0087(8) 0.0232(10)  
C1 0.0208(11) 0.0335(13) 0.0212(10) -0.0099(9) -0.0059(9) 0.0137(10)  
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C3 0.0170(11) 0.0244(12) 0.0296(12) 0.0048(9) 0.0034(9) 0.0092(9)  
C4 0.0178(10) 0.0265(12) 0.0204(10) -0.0012(9) 0.0016(8) 0.0105(9)  
C5 0.0174(10) 0.0313(12) 0.0218(10) -0.0053(9) -0.0020(8) 0.0138(10)  
C6 0.0321(13) 0.0473(16) 0.0207(11) -0.0004(10) 0.0011(10) 0.0295(12)  
C7 0.0413(15) 0.0371(14) 0.0252(11) 0.0047(10) 0.0095(10) 0.0308(13)  
C8 0.0457(17) 0.0270(14) 0.0450(16) 0.0066(12) 0.0156(14) 0.0217(13)  
C9 0.0576(19) 0.0573(19) 0.0242(12) 0.0157(12) 0.0130(12) 0.0472(18)  
C10 0.0250(12) 0.0322(12) 0.0146(9) -0.0013(9) 0.0002(8) 0.0165(10)  
C11 0.0326(13) 0.0464(15) 0.0182(10) -0.0053(10) -0.0010(9) 0.0289(12)

C12 0.0352(13) 0.0379(14) 0.0219(10) -0.0077(10) -0.0075(9) 0.0276(12)  
 C13 0.0281(12) 0.0285(12) 0.0217(10) -0.0021(9) -0.0060(9) 0.0168(10)  
 C14 0.0190(1) 0.0268(12) 0.0171(9) -0.0023(8) -0.0019(8) 0.0121(9)  
 C15 0.0189(10) 0.0244(11) 0.0142(9) -0.0041(8) -0.0044(8) 0.0121(9)  
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 C19 0.0362(14) 0.0302(13) 0.0183(10) -0.0022(9) 0.0021(10) 0.0182(12)  
 C20 0.0597(19) 0.0405(15) 0.0181(11) 0.0031(10) 0.0098(11) 0.0312(14)  
 C21 0.0556(19) 0.0410(16) 0.0329(14) 0.0153(12) 0.0240(13) 0.0261(15)  
 C22 0.0333(15) 0.0412(16) 0.0476(17) 0.0153(14) 0.0118(13) 0.0098(14)  
 C23 0.0280(13) 0.0365(14) 0.0305(13) 0.0068(11) -0.0003(10) 0.0101(11)

\_geom\_special\_details

;

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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loop\_

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V	C2	2.284(3)	.	.	.	.	yes
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V	C4	2.360(3)	.	.	.	.	yes
V	C5	2.305(3)	.	.	.	.	yes
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V	C17	2.003(2)	.	.	.	.	yes
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N	C8	1.479(4)	.	.	.	.	yes
N	C9	1.495(2)	.	.	.	.	yes
C1	C2	1.419(4)	.	.	.	.	no
C1	C5	1.417(3)	.	.	.	.	no
C2	C3	1.410(1)	.	.	.	.	no
C3	C4	1.415(4)	.	.	.	.	no
C4	C5	1.403(3)	.	.	.	.	no
C5	C6	1.496(4)	.	.	.	.	no
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C17	C18	1.467(3)	.	.	.	.	no
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C21	C22	1.386 (2)	.	.	no
C22	C23	1.391 (4)	.	.	no
C1	H1	0.9300 (-)	.	.	no
C2	H2	1.0000 (-)	.	.	no
C3	H3	0.9800 (-)	.	.	no
C4	H4	0.9100 (-)	.	.	no
C6	H6	0.9400 (-)	.	.	no
C6	H6'	1.0100 (-)	.	.	no
C7	H7	1.0100 (-)	.	.	no
C7	H7'	0.9900 (-)	.	.	no
C8	H8	0.9700 (-)	.	.	no
C8	H8'	0.9100 (-)	.	.	no
C8	H8''	0.9500 (-)	.	.	no
C9	H9	0.9700 (-)	.	.	no
C9	H9'	0.9900 (-)	.	.	no
C9	H9''	1.0400 (-)	.	.	no
C10	H10	0.9700 (-)	.	.	no
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C12	H12	0.9800 (-)	.	.	no
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\_geom\_angle\_publ\_flag

C1	V	N	90.69 (5)	.	.	.	yes
C1	V	C1	144.41 (7)	.	.	.	yes
C1	V	C2	126.74 (6)	.	.	.	yes
C1	V	C3	92.71 (6)	.	.	.	yes
C1	V	C4	85.29 (6)	.	.	.	yes
C1	V	C5	111.71 (6)	.	.	.	yes
C1	V	C16	103.43 (7)	.	.	.	yes
C1	V	C17	109.09 (7)	.	.	.	yes
N	V	C1	92.34 (9)	.	.	.	yes
N	V	C2	128.75 (10)	.	.	.	yes
N	V	C3	131.6 (1)	.	.	.	yes
N	V	C4	97.57 (9)	.	.	.	yes
N	V	C5	75.01 (9)	.	.	.	yes
N	V	C16	127.19 (9)	.	.	.	yes
N	V	C17	88.66 (9)	.	.	.	yes
C1	V	C2	36.55 (10)	.	.	.	yes
C1	V	C3	59.70 (8)	.	.	.	yes
C1	V	C4	59.16 (8)	.	.	.	yes
C1	V	C5	36.29 (9)	.	.	.	yes
C1	V	C16	102.76 (10)	.	.	.	yes
C1	V	C17	106.43 (9)	.	.	.	yes
C2	V	C3	35.38 (3)	.	.	.	yes
C2	V	C4	58.74 (9)	.	.	.	yes
C2	V	C5	60.05 (10)	.	.	.	yes

C2	V	C16	81.35 (10)	.	.	.	yes
C2	V	C17	106.30 (9)	.	.	.	yes
C3	V	C4	34.94 (9)	.	.	.	yes
C3	V	C5	59.01 (9)	.	.	.	yes
C3	V	C16	98.73 (9)	.	.	.	yes
C3	V	C17	134.58 (9)	.	.	.	yes
C4	V	C5	34.98 (8)	.	.	.	yes
C4	V	C16	133.65 (9)	.	.	.	yes
C4	V	C17	164.34 (8)	.	.	.	yes
C5	V	C16	138.36 (9)	.	.	.	yes
C5	V	C17	135.92 (9)	.	.	.	yes
C16	V	C17	38.56 (9)	.	.	.	yes
V	N	C7	106.13 (15)	.	.	.	yes
V	N	C8	113.9 (2)	.	.	.	yes
V	N	C9	113.18 (19)	.	.	.	yes
C7	N	C8	108.1 (2)	.	.	.	yes
C7	N	C9	108.0 (3)	.	.	.	yes
C8	N	C9	107.3 (2)	.	.	.	yes
V	C1	C2	73.44 (15)	.	.	.	yes
V	C1	C5	74.40 (15)	.	.	.	yes
C2	C1	C5	108.2 (2)	.	.	.	no
V	C2	C1	70.01 (14)	.	.	.	yes
V	C2	C3	74.94 (14)	.	.	.	yes
C1	C2	C3	107.9 (2)	.	.	.	no
V	C3	C2	69.68 (14)	.	.	.	yes
V	C3	C4	72.87 (13)	.	.	.	yes
C2	C3	C4	107.6 (2)	.	.	.	no
V	C4	C3	72.19 (14)	.	.	.	yes
V	C4	C5	70.36 (15)	.	.	.	yes
C3	C4	C5	109.0 (2)	.	.	.	no
V	C5	C1	69.31 (16)	.	.	.	yes
V	C5	C4	74.66 (16)	.	.	.	yes
V	C5	C6	113.92 (18)	.	.	.	yes
C1	C5	C4	107.4 (2)	.	.	.	no
C1	C5	C6	126.6 (2)	.	.	.	no
C4	C5	C6	125.2 (2)	.	.	.	no
C5	C6	C7	108.6 (3)	.	.	.	no
N	C7	C6	109.9 (2)	.	.	.	yes
C11	C10	C15	120.6 (2)	.	.	.	no
C10	C11	C12	120.3 (3)	.	.	.	no
C11	C12	C13	120.0 (3)	.	.	.	no
C12	C13	C14	119.7 (2)	.	.	.	no
C13	C14	C15	121.2 (2)	.	.	.	no
C10	C15	C14	118.2 (2)	.	.	.	no
C10	C15	C16	120.5 (2)	.	.	.	no
C14	C15	C16	121.3 (2)	.	.	.	no
V	C16	C15	148.42 (17)	.	.	.	yes
V	C16	C17	72.13 (16)	.	.	.	yes
C15	C16	C17	139.1 (2)	.	.	.	no
V	C17	C16	69.31 (14)	.	.	.	yes
V	C17	C18	152.3 (2)	.	.	.	yes
C16	C17	C18	138.2 (3)	.	.	.	no
C17	C18	C19	120.2 (2)	.	.	.	no
C17	C18	C23	121.3 (2)	.	.	.	no
C19	C18	C23	118.5 (2)	.	.	.	no
C18	C19	C20	120.4 (3)	.	.	.	no
C19	C20	C21	120.7 (3)	.	.	.	no
C20	C21	C22	119.6 (3)	.	.	.	no
C21	C22	C23	120.4 (3)	.	.	.	no
C18	C23	C22	120.5 (2)	.	.	.	no
V	C1	H1	118.00 (-)	.	.	.	no



C2	C1	H1	129.00 (-)	.	.	.	no
C5	C1	H1	123.00 (-)	.	.	.	no
V	C2	H2	122.00 (-)	.	.	.	no
C1	C2	H2	126.00 (-)	.	.	.	no
C3	C2	H2	126.00 (-)	.	.	.	no
V	C3	H3	123.00 (-)	.	.	.	no
C2	C3	H3	124.00 (-)	.	.	.	no
C4	C3	H3	128.00 (-)	.	.	.	no
V	C4	H4	121.00 (-)	.	.	.	no
C3	C4	H4	125.00 (-)	.	.	.	no
C5	C4	H4	126.00 (-)	.	.	.	no
C5	C6	H6	110.00 (-)	.	.	.	no
C5	C6	H6'	109.00 (-)	.	.	.	no
C7	C6	H6	111.00 (-)	.	.	.	no
C7	C6	H6'	112.00 (-)	.	.	.	no
H6	C6	H6'	106.00 (-)	.	.	.	no
N	C7	H7	108.00 (-)	.	.	.	no
N	C7	H7'	109.00 (-)	.	.	.	no
C6	C7	H7	108.00 (-)	.	.	.	no
C6	C7	H7'	110.00 (-)	.	.	.	no
H7	C7	H7'	112.00 (-)	.	.	.	no
N	C8	H8	109.00 (-)	.	.	.	no
N	C8	H8'	108.00 (-)	.	.	.	no
N	C8	H8''	108.00 (-)	.	.	.	no
H8	C8	H8'	106.00 (-)	.	.	.	no
H8	C8	H8''	114.00 (-)	.	.	.	no
H8'	C8	H8''	111.00 (-)	.	.	.	no
N	C9	H9	109.00 (-)	.	.	.	no
N	C9	H9'	109.00 (-)	.	.	.	no
N	C9	H9''	110.00 (-)	.	.	.	no
H9	C9	H9'	107.00 (-)	.	.	.	no
H9	C9	H9''	110.00 (-)	.	.	.	no
H9'	C9	H9''	112.00 (-)	.	.	.	no
C11	C10	H10	121.00 (-)	.	.	.	no
C15	C10	H10	118.00 (-)	.	.	.	no
C10	C11	H11	120.00 (-)	.	.	.	no
C12	C11	H11	120.00 (-)	.	.	.	no
C11	C12	H12	118.00 (-)	.	.	.	no
C13	C12	H12	122.00 (-)	.	.	.	no
C12	C13	H13	120.00 (-)	.	.	.	no
C14	C13	H13	120.00 (-)	.	.	.	no
C13	C14	H14	119.00 (-)	.	.	.	no
C15	C14	H14	120.00 (-)	.	.	.	no
C18	C19	H19	123.00 (-)	.	.	.	no
C20	C19	H19	117.00 (-)	.	.	.	no
C19	C20	H20	117.00 (-)	.	.	.	no
C21	C20	H20	123.00 (-)	.	.	.	no
C20	C21	H21	121.00 (-)	.	.	.	no
C22	C21	H21	119.00 (-)	.	.	.	no
C21	C22	H22	120.00 (-)	.	.	.	no
C23	C22	H22	119.00 (-)	.	.	.	no
C18	C23	H23	120.00 (-)	.	.	.	no
C22	C23	H23	119.00 (-)	.	.	.	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   H8   C1   0.9700   2.6300   3.282(2)  125.00   .   yes
```

```
_diffn_measured_fraction_theta_max    2.21
_diffn_refl_theta_full                 28.28
_diffn_measured_fraction_theta_full    1.876
_refine_diff_density_max                0.430
_refine_diff_density_min               -0.280
```

```
###END
```