CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 9 November 2006

Crystal Structure Analysis of:

TA28

(shown below)

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Account Number: JEB.65152-1-DOE.651520

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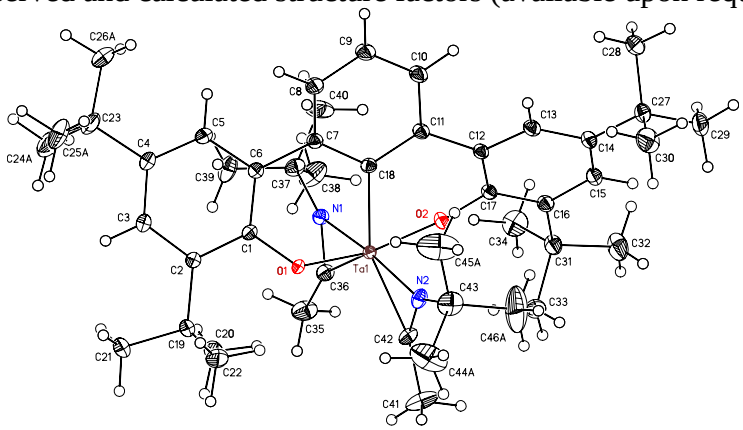


TA28

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 626579. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 626579."

Table 1. Crystal data and structure refinement for TA28 (CCDC 626579).

Empirical formula	$C_{46}H_{67}N_2O_2Ta$
Formula weight	860.97
Crystallization Solvent	Not given
Crystal Habit	Block
Crystal size	0.35 x 0.26 x 0.22 mm^3
Crystal color	Pale yellow

Data Collection

Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 43330 reflections used in lattice determination	2.19 to 45.01°	
Unit cell dimensions	a = 10.1483(3) Å b = 14.5504(4) Å c = 15.6639(4) Å	α= 88.0490(10)° β= 86.7020(10)° γ = 73.7530(10)°
Volume	2216.53(11) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.290 Mg/m^3	
F(000)	892	
θ range for data collection	1.94 to 45.15°	
Completeness to θ = 45.15°	84.2 %	
Index ranges	$-20 \le h \le 18$, $-27 \le k \le 27$, $-28 \le l \le 29$	
Data collection scan type	ω scans at 7 ϕ settings	
Reflections collected	76283	
Independent reflections	31062 [R_{int}= 0.0806]	
Absorption coefficient	2.515 mm^{-1}	
Absorption correction	None	
Max. and min. transmission	0.6076 and 0.4731	

Table 1 (cont.)

Structure solution and Refinement

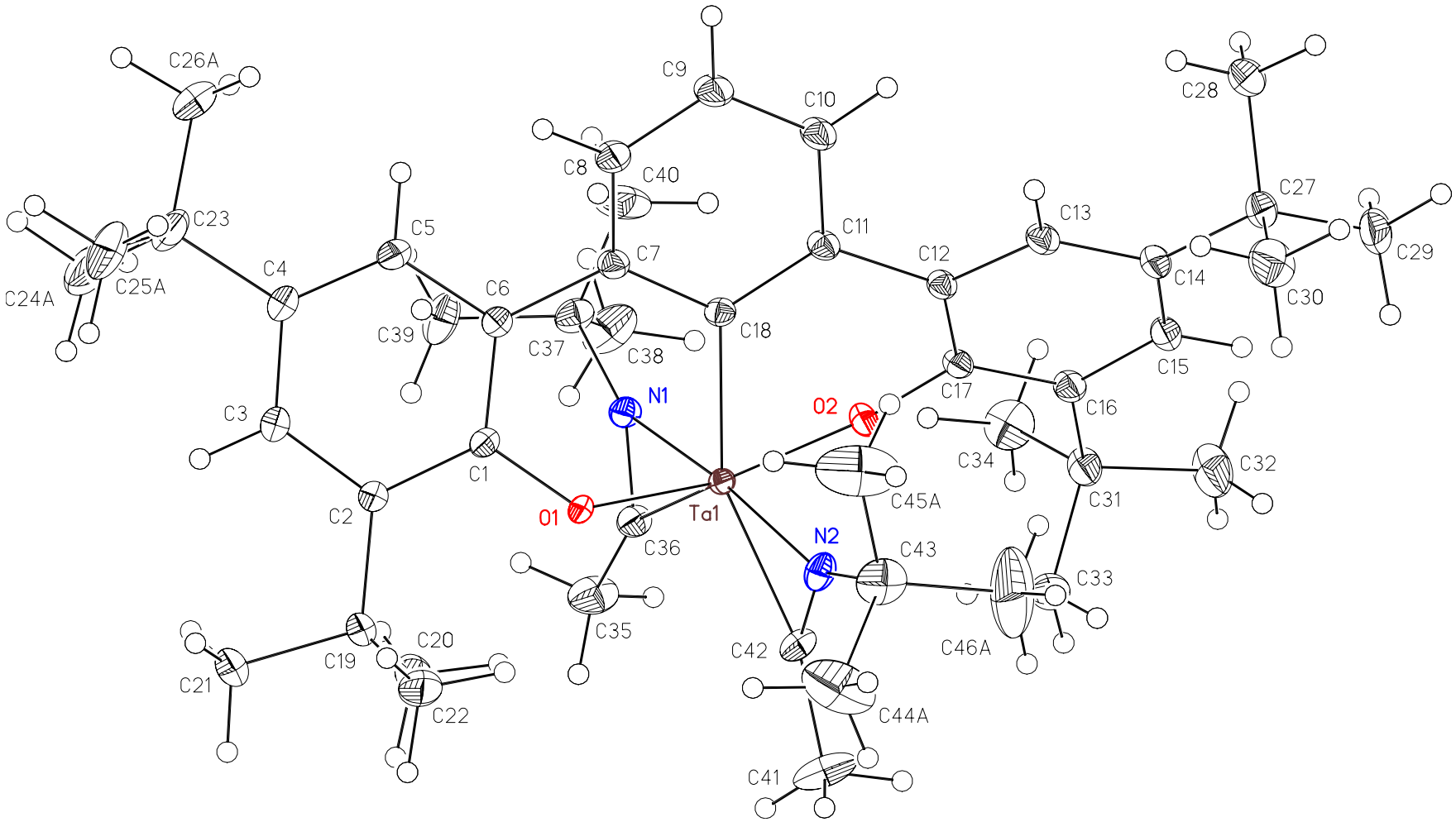
Structure solution program	Bruker XS v6.12
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	31062 / 66 / 506
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.155
Final R indices [I>2σ(I), 25961 reflections]	R1 = 0.0349, *w*R2 = 0.0749
R indices (all data)	R1 = 0.0466, *w*R2 = 0.0778
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.007
Average shift/error	0.000
Largest diff. peak and hole	4.416 and -2.619 e.Å^{-3}

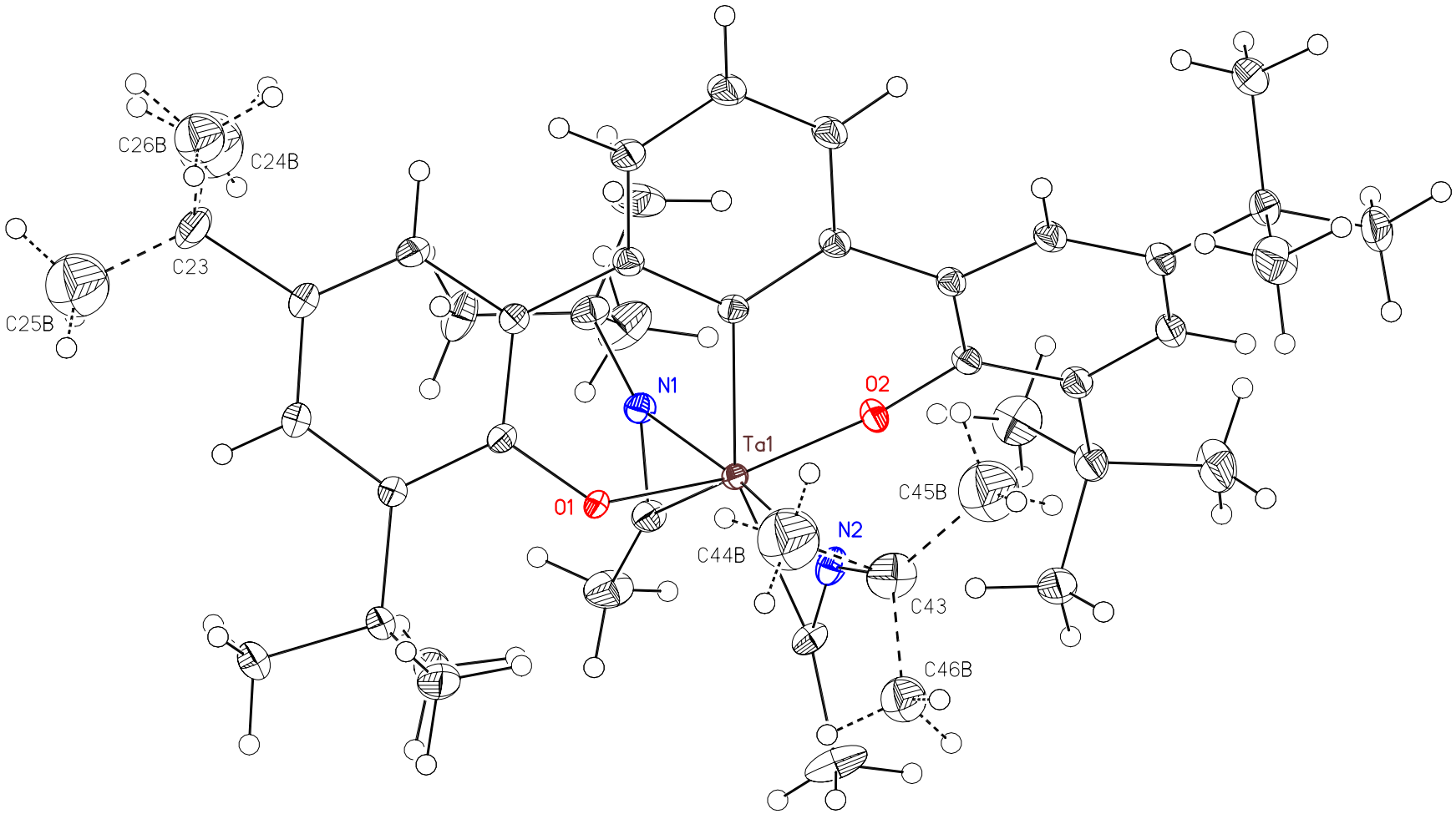
Special Refinement Details

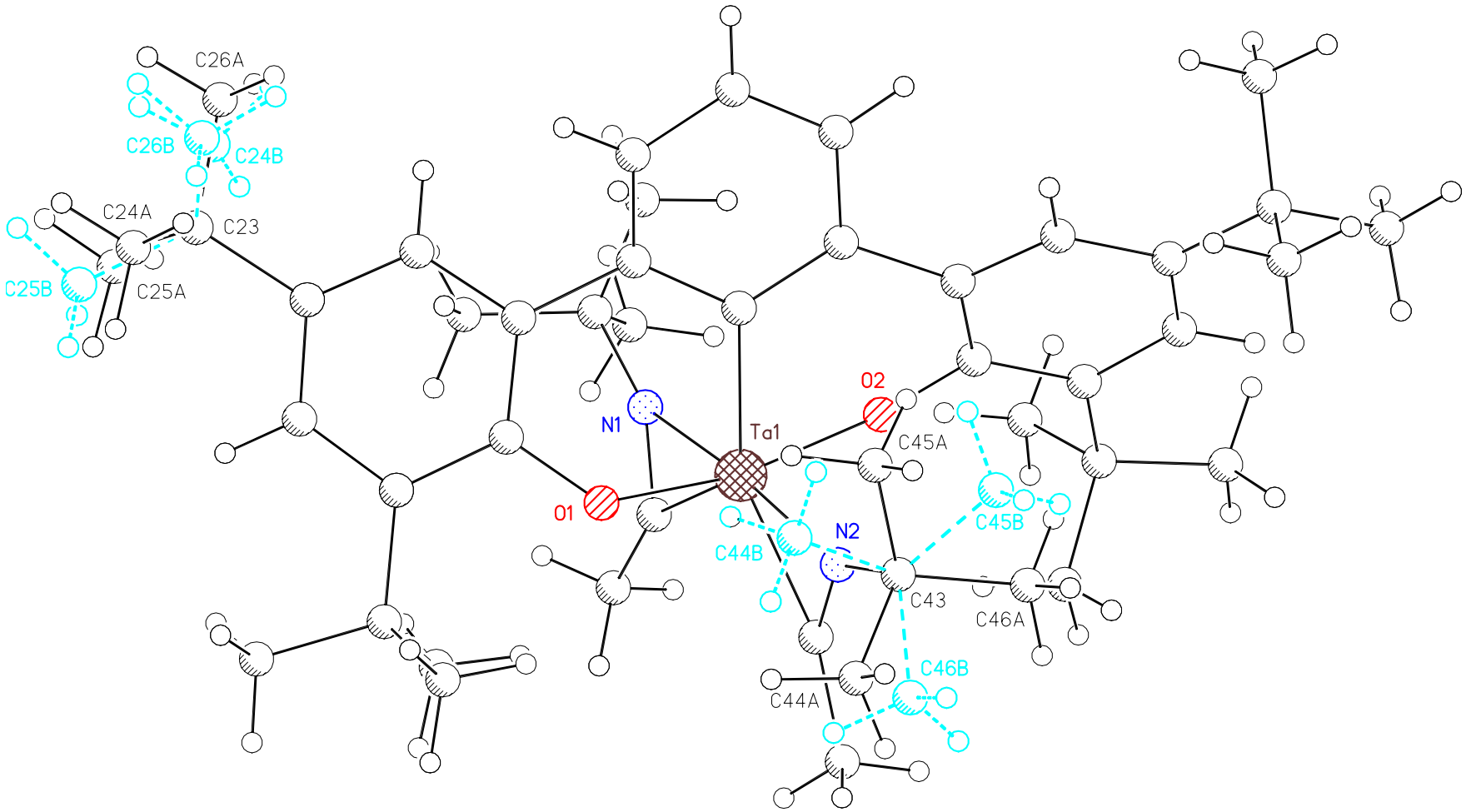
Two tertiary butyl groups exhibit a common type of disorder; rotation about the C-C bond to the central carbon, in this structure the C(24)-C(4) and C(43)-N(2) bond. The disorder was included in the model with the minor component refined isotropically and the C-C distances in both components restrained to be similar without imposing a target value. The relative populations are listed in Table 2 and the distances are listed in Table 4. The third figure illustrates both components together with the minor component in cyan.

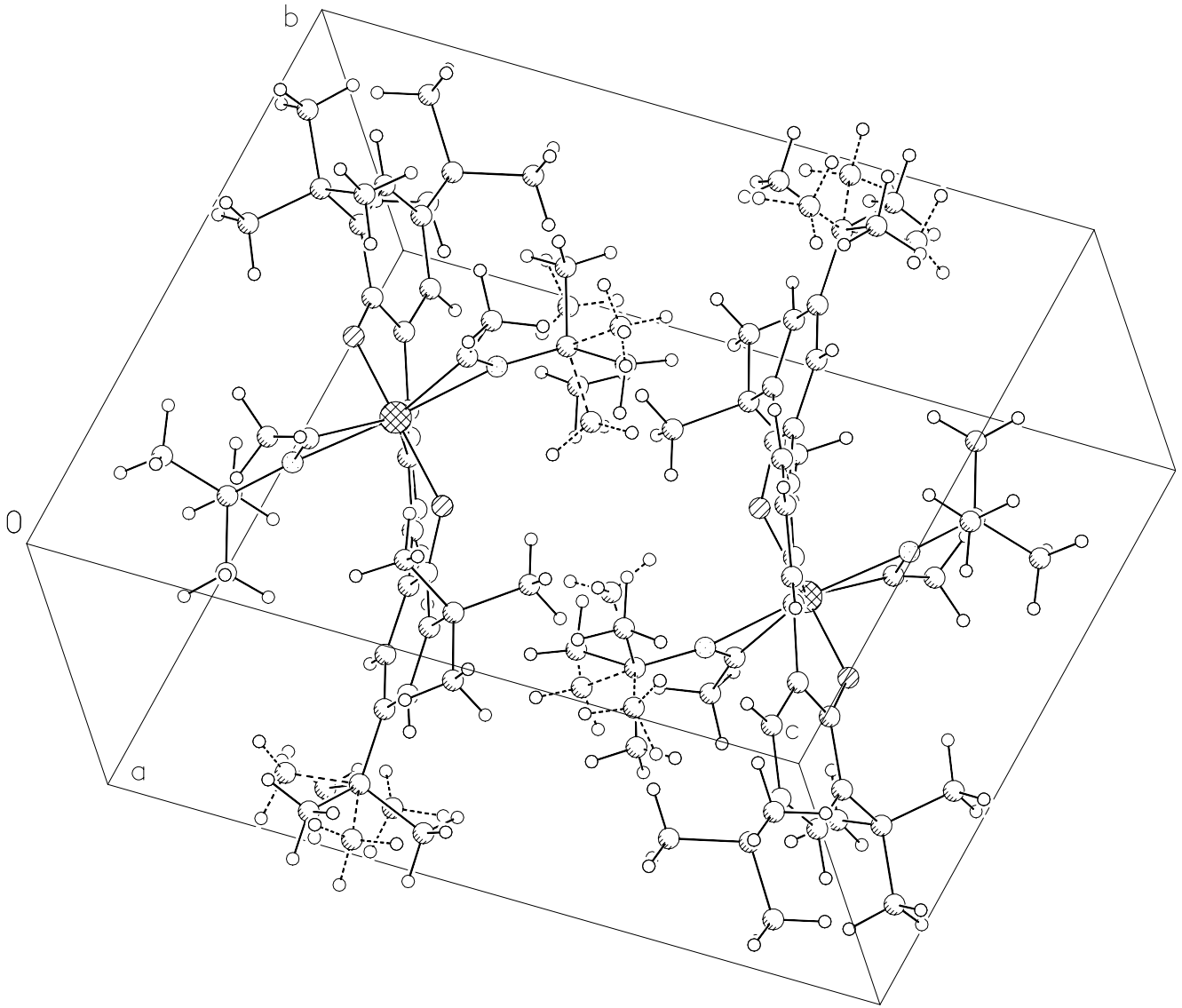
Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not 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.

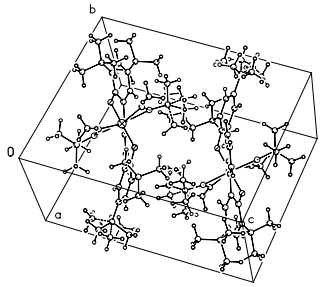
All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C26A
C9
C10
C28
C8
C40
C23
C5
C11
C13
C27
C7
C12
C14
C29
C4
C6
C30
C24A
C25A
C39
C18
C37
C38
C15
N1
C17
O2
C16
C3
C1
C34
C32
C45A
C31
C2
O1
Ta1
C36
N2
C43
C33
C35
C42
C46A
C20
C19
C21
C22
C44A
C41


C26B
C24B
C23
C25B
N1
O2
Ta1
O1
C45B
N2
C44B
C43
C46B


C26A
C26B
C24B
C24A
C23
C25B
C25A
N1
Ta1
O2
C45A
O1
C45B
C44B
N2
C43
C46A
C46B
C44A


b
O
a
c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a
c

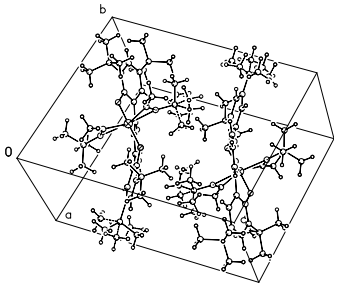
b
0
a

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for TA28 (CCDC 626579). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ta(1)	7042(1)	5215(1)	7361(1)	10(1)	1
O(1)	6257(1)	6158(1)	6479(1)	12(1)	1
O(2)	7394(1)	4223(1)	8247(1)	13(1)	1
N(1)	6602(1)	6263(1)	8342(1)	13(1)	1
N(2)	7758(2)	4179(1)	6372(1)	16(1)	1
C(1)	5105(2)	6900(1)	6515(1)	14(1)	1
C(2)	5153(2)	7788(1)	6141(1)	17(1)	1
C(3)	3978(2)	8561(1)	6245(1)	21(1)	1
C(4)	2789(2)	8488(1)	6703(1)	18(1)	1
C(5)	2767(2)	7594(1)	7035(1)	16(1)	1
C(6)	3896(2)	6774(1)	6931(1)	13(1)	1
C(7)	3774(2)	5819(1)	7254(1)	14(1)	1
C(8)	2437(2)	5714(1)	7341(1)	18(1)	1
C(9)	2199(2)	4899(1)	7722(1)	20(1)	1
C(10)	3299(2)	4154(1)	7976(1)	18(1)	1
C(11)	4660(2)	4204(1)	7835(1)	13(1)	1
C(12)	5766(2)	3341(1)	8102(1)	12(1)	1
C(13)	5519(2)	2438(1)	8136(1)	15(1)	1
C(14)	6442(2)	1621(1)	8466(1)	16(1)	1
C(15)	7654(2)	1725(1)	8773(1)	17(1)	1
C(16)	7997(2)	2593(1)	8727(1)	15(1)	1
C(17)	7054(2)	3389(1)	8360(1)	12(1)	1
C(18)	4922(2)	5052(1)	7485(1)	12(1)	1
C(19)	6461(2)	7903(1)	5647(2)	25(1)	1
C(20)	7678(2)	7703(2)	6226(2)	33(1)	1
C(21)	6254(2)	8928(2)	5284(2)	38(1)	1
C(22)	6820(3)	7229(2)	4884(2)	35(1)	1
C(23)	1557(2)	9383(1)	6812(1)	27(1)	1
C(24A)	933(3)	9663(2)	5945(2)	38(1)	0.819(5)
C(25A)	2032(3)	10226(2)	7098(3)	38(1)	0.819(5)
C(26A)	438(3)	9214(2)	7438(3)	45(1)	0.819(5)
C(24B)	234(8)	9149(10)	6613(9)	35(3)	0.181(5)
C(25B)	1700(20)	10363(7)	6522(14)	57(5)	0.181(5)
C(26B)	1280(20)	9445(16)	7779(3)	62(6)	0.181(5)
C(27)	6104(2)	656(1)	8468(1)	19(1)	1
C(28)	4670(2)	752(1)	8899(2)	25(1)	1
C(29)	7142(2)	-121(1)	8962(2)	29(1)	1
C(30)	6103(3)	339(2)	7543(2)	32(1)	1
C(31)	9359(2)	2678(1)	9060(1)	20(1)	1
C(32)	10168(2)	1743(2)	9501(2)	34(1)	1
C(33)	10288(2)	2889(2)	8312(1)	24(1)	1
C(34)	9092(2)	3475(2)	9721(1)	29(1)	1
C(35)	8815(2)	6741(2)	8251(2)	26(1)	1
C(36)	7802(2)	6223(1)	8024(1)	15(1)	1
C(37)	5749(2)	6806(1)	9068(1)	18(1)	1
C(38)	6639(2)	6773(2)	9832(1)	32(1)	1
C(39)	5116(2)	7834(1)	8759(1)	28(1)	1

C(40)	4616(3)	6334(2)	9312(2)	33(1)	1
C(41)	10187(2)	4316(2)	6130(2)	34(1)	1
C(42)	8763(2)	4508(1)	6523(1)	17(1)	1
C(43)	7596(2)	3471(1)	5752(1)	27(1)	1
C(44A)	8124(5)	3677(3)	4856(1)	46(1)	0.871(5)
C(45A)	6074(3)	3526(3)	5749(2)	52(1)	0.871(5)
C(46A)	8404(5)	2478(2)	6064(2)	63(1)	0.871(5)
C(44B)	6420(20)	4165(16)	5299(16)	55(7)	0.129(5)
C(45B)	7080(30)	2639(13)	6109(17)	52(6)	0.129(5)
C(46B)	8681(16)	3289(14)	5015(9)	29(4)	0.129(5)

Table 3. Selected bond lengths [Å] and angles [°] for TA28 (CCDC 626579).

Ta(1)-O(2)	1.9415(11)	O(2)-Ta(1)-O(1)	166.30(5)
Ta(1)-O(1)	1.9517(11)	O(2)-Ta(1)-N(1)	88.66(5)
Ta(1)-N(1)	2.1414(12)	O(1)-Ta(1)-N(1)	93.03(5)
Ta(1)-N(2)	2.1494(13)	O(2)-Ta(1)-N(2)	91.75(5)
Ta(1)-C(36)	2.1574(15)	O(1)-Ta(1)-N(2)	88.37(5)
Ta(1)-C(42)	2.1576(15)	N(1)-Ta(1)-N(2)	172.36(5)
Ta(1)-C(18)	2.2256(14)	O(2)-Ta(1)-C(36)	96.37(6)
		O(1)-Ta(1)-C(36)	92.68(6)
		N(1)-Ta(1)-C(36)	34.51(5)
		N(2)-Ta(1)-C(36)	137.95(6)
		O(2)-Ta(1)-C(42)	95.39(6)
		O(1)-Ta(1)-C(42)	92.46(6)
		N(1)-Ta(1)-C(42)	137.86(6)
		N(2)-Ta(1)-C(42)	34.52(6)
		C(36)-Ta(1)-C(42)	103.50(6)
		O(2)-Ta(1)-C(18)	83.37(5)
		O(1)-Ta(1)-C(18)	82.98(5)
		N(1)-Ta(1)-C(18)	92.28(5)
		N(2)-Ta(1)-C(18)	95.35(6)
		C(36)-Ta(1)-C(18)	126.52(6)
		C(42)-Ta(1)-C(18)	129.87(6)

Table 4. Bond lengths [Å] and angles [°] for TA28 (CCDC 626579).

Ta(1)-O(2)	1.9415(11)	C(31)-C(33)	1.539(3)
Ta(1)-O(1)	1.9517(11)	C(35)-C(36)	1.498(2)
Ta(1)-N(1)	2.1414(12)	C(37)-C(40)	1.521(3)
Ta(1)-N(2)	2.1494(13)	C(37)-C(39)	1.528(3)
Ta(1)-C(36)	2.1574(15)	C(37)-C(38)	1.532(3)
Ta(1)-C(42)	2.1576(15)	C(41)-C(42)	1.493(3)
Ta(1)-C(18)	2.2256(14)	C(43)-C(44A)	1.5243(15)
O(1)-C(1)	1.3517(18)	C(43)-C(45A)	1.5246(15)
O(2)-C(17)	1.3548(18)	C(43)-C(46B)	1.5253(15)
N(1)-C(36)	1.275(2)	C(43)-C(46A)	1.5265(15)
N(1)-C(37)	1.494(2)	C(43)-C(45B)	1.5250(15)
N(2)-C(42)	1.278(2)	C(43)-C(44B)	1.5254(15)
N(2)-C(43)	1.487(2)		
C(1)-C(6)	1.410(2)	O(2)-Ta(1)-O(1)	166.30(5)
C(1)-C(2)	1.413(2)	O(2)-Ta(1)-N(1)	88.66(5)
C(2)-C(3)	1.397(2)	O(1)-Ta(1)-N(1)	93.03(5)
C(2)-C(19)	1.545(2)	O(2)-Ta(1)-N(2)	91.75(5)
C(3)-C(4)	1.396(2)	O(1)-Ta(1)-N(2)	88.37(5)
C(4)-C(5)	1.390(2)	N(1)-Ta(1)-N(2)	172.36(5)
C(4)-C(23)	1.539(2)	O(2)-Ta(1)-C(36)	96.37(6)
C(5)-C(6)	1.410(2)	O(1)-Ta(1)-C(36)	92.68(6)
C(6)-C(7)	1.498(2)	N(1)-Ta(1)-C(36)	34.51(5)
C(7)-C(8)	1.405(2)	N(2)-Ta(1)-C(36)	137.95(6)
C(7)-C(18)	1.423(2)	O(2)-Ta(1)-C(42)	95.39(6)
C(8)-C(9)	1.384(2)	O(1)-Ta(1)-C(42)	92.46(6)
C(9)-C(10)	1.388(2)	N(1)-Ta(1)-C(42)	137.86(6)
C(10)-C(11)	1.408(2)	N(2)-Ta(1)-C(42)	34.52(6)
C(11)-C(18)	1.420(2)	C(36)-Ta(1)-C(42)	103.50(6)
C(11)-C(12)	1.497(2)	O(2)-Ta(1)-C(18)	83.37(5)
C(12)-C(13)	1.403(2)	O(1)-Ta(1)-C(18)	82.98(5)
C(12)-C(17)	1.411(2)	N(1)-Ta(1)-C(18)	92.28(5)
C(13)-C(14)	1.397(2)	N(2)-Ta(1)-C(18)	95.35(6)
C(14)-C(15)	1.394(2)	C(36)-Ta(1)-C(18)	126.52(6)
C(14)-C(27)	1.535(2)	C(42)-Ta(1)-C(18)	129.87(6)
C(15)-C(16)	1.399(2)	C(1)-O(1)-Ta(1)	129.80(10)
C(16)-C(17)	1.409(2)	C(17)-O(2)-Ta(1)	133.22(10)
C(16)-C(31)	1.543(2)	C(36)-N(1)-C(37)	132.80(13)
C(19)-C(20)	1.530(3)	C(36)-N(1)-Ta(1)	73.43(9)
C(19)-C(22)	1.534(3)	C(37)-N(1)-Ta(1)	153.56(11)
C(19)-C(21)	1.540(3)	C(42)-N(2)-C(43)	132.75(14)
C(23)-C(26A)	1.5242(15)	C(42)-N(2)-Ta(1)	73.09(9)
C(23)-C(25B)	1.5250(15)	C(43)-N(2)-Ta(1)	154.12(12)
C(23)-C(24B)	1.5252(15)	O(1)-C(1)-C(6)	119.45(14)
C(23)-C(25A)	1.5254(15)	O(1)-C(1)-C(2)	118.75(14)
C(23)-C(26B)	1.5255(15)	C(6)-C(1)-C(2)	121.79(14)
C(23)-C(24A)	1.5265(15)	C(3)-C(2)-C(1)	117.37(15)
C(27)-C(29)	1.535(3)	C(3)-C(2)-C(19)	121.37(15)
C(27)-C(30)	1.535(3)	C(1)-C(2)-C(19)	121.25(14)
C(27)-C(28)	1.541(3)	C(4)-C(3)-C(2)	122.94(16)
C(31)-C(34)	1.538(3)	C(5)-C(4)-C(3)	117.81(15)
C(31)-C(32)	1.541(3)	C(5)-C(4)-C(23)	122.64(15)

C(3)-C(4)-C(23)	119.54(15)	C(26A)-C(23)-C(4)	112.53(17)
C(4)-C(5)-C(6)	122.50(15)	C(25B)-C(23)-C(4)	120.0(8)
C(1)-C(6)-C(5)	117.32(14)	C(24B)-C(23)-C(4)	110.0(6)
C(1)-C(6)-C(7)	122.86(14)	C(25A)-C(23)-C(4)	110.37(17)
C(5)-C(6)-C(7)	119.82(14)	C(26B)-C(23)-C(4)	103.6(9)
C(8)-C(7)-C(18)	120.48(14)	C(24A)-C(23)-C(4)	108.60(16)
C(8)-C(7)-C(6)	116.29(14)	C(29)-C(27)-C(14)	111.65(15)
C(18)-C(7)-C(6)	123.22(13)	C(29)-C(27)-C(30)	109.35(17)
C(9)-C(8)-C(7)	120.71(16)	C(14)-C(27)-C(30)	109.51(15)
C(8)-C(9)-C(10)	119.68(15)	C(29)-C(27)-C(28)	107.53(16)
C(9)-C(10)-C(11)	120.95(15)	C(14)-C(27)-C(28)	110.27(14)
C(10)-C(11)-C(18)	120.17(15)	C(30)-C(27)-C(28)	108.45(17)
C(10)-C(11)-C(12)	116.25(14)	C(34)-C(31)-C(32)	107.17(18)
C(18)-C(11)-C(12)	123.54(13)	C(34)-C(31)-C(33)	109.49(16)
C(13)-C(12)-C(17)	117.14(14)	C(32)-C(31)-C(33)	107.08(17)
C(13)-C(12)-C(11)	119.75(13)	C(34)-C(31)-C(16)	110.91(15)
C(17)-C(12)-C(11)	123.06(13)	C(32)-C(31)-C(16)	111.98(15)
C(14)-C(13)-C(12)	122.88(15)	C(33)-C(31)-C(16)	110.08(15)
C(15)-C(14)-C(13)	117.42(14)	N(1)-C(36)-C(35)	130.96(15)
C(15)-C(14)-C(27)	122.95(16)	N(1)-C(36)-Ta(1)	72.06(9)
C(13)-C(14)-C(27)	119.63(15)	C(35)-C(36)-Ta(1)	156.92(13)
C(14)-C(15)-C(16)	122.90(16)	N(1)-C(37)-C(40)	107.69(13)
C(15)-C(16)-C(17)	117.49(14)	N(1)-C(37)-C(39)	108.10(15)
C(15)-C(16)-C(31)	121.44(15)	C(40)-C(37)-C(39)	109.68(18)
C(17)-C(16)-C(31)	121.07(14)	N(1)-C(37)-C(38)	110.01(15)
O(2)-C(17)-C(16)	119.20(13)	C(40)-C(37)-C(38)	109.89(19)
O(2)-C(17)-C(12)	118.97(14)	C(39)-C(37)-C(38)	111.37(16)
C(16)-C(17)-C(12)	121.82(14)	N(2)-C(42)-C(41)	132.08(16)
C(11)-C(18)-C(7)	117.70(13)	N(2)-C(42)-Ta(1)	72.39(9)
C(11)-C(18)-Ta(1)	121.44(11)	C(41)-C(42)-Ta(1)	155.46(14)
C(7)-C(18)-Ta(1)	120.79(10)	N(2)-C(43)-C(44A)	111.18(17)
C(20)-C(19)-C(22)	109.99(18)	N(2)-C(43)-C(45A)	108.02(16)
C(20)-C(19)-C(21)	106.7(2)	C(44A)-C(43)-C(45A)	109.9(2)
C(22)-C(19)-C(21)	106.98(19)	N(2)-C(43)-C(46B)	113.5(8)
C(20)-C(19)-C(2)	111.51(17)	N(2)-C(43)-C(46A)	107.65(17)
C(22)-C(19)-C(2)	109.90(18)	C(44A)-C(43)-C(46A)	110.2(3)
C(21)-C(19)-C(2)	111.64(15)	C(45A)-C(43)-C(46A)	109.7(3)
C(25B)-C(23)-C(24B)	117.3(11)	N(2)-C(43)-C(45B)	117.3(11)
C(26A)-C(23)-C(25A)	110.1(2)	C(46B)-C(43)-C(45B)	118.9(13)
C(25B)-C(23)-C(26B)	105.5(12)	N(2)-C(43)-C(44B)	95.2(11)
C(24B)-C(23)-C(26B)	96.4(11)	C(46B)-C(43)-C(44B)	99.0(13)
C(26A)-C(23)-C(24A)	108.0(2)	C(45B)-C(43)-C(44B)	107.6(16)
C(25A)-C(23)-C(24A)	107.0(2)		

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for TA28 (CCDC 626579). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	90(1)	92(1)	110(1)	-8(1)	3(1)	-26(1)
O(1)	98(4)	97(4)	141(5)	14(3)	10(3)	3(3)
O(2)	147(5)	116(5)	150(5)	29(3)	-28(4)	-54(4)
N(1)	144(5)	122(5)	131(5)	-35(4)	15(4)	-45(4)
N(2)	180(6)	127(5)	142(6)	-40(4)	-17(4)	-6(4)
C(1)	121(5)	129(6)	144(6)	-2(4)	11(4)	-11(4)
C(2)	147(6)	135(6)	213(7)	32(5)	37(5)	-10(5)
C(3)	172(7)	132(7)	279(9)	31(5)	38(6)	0(5)
C(4)	148(6)	144(7)	230(8)	7(5)	6(5)	5(5)
C(5)	122(6)	169(7)	177(7)	-1(5)	11(5)	-20(5)
C(6)	122(5)	132(6)	144(6)	2(4)	-7(4)	-30(4)
C(7)	116(5)	149(6)	138(6)	11(4)	-7(4)	-37(4)
C(8)	107(6)	194(7)	223(7)	32(5)	-25(5)	-42(5)
C(9)	115(6)	239(8)	259(8)	54(6)	-24(5)	-71(5)
C(10)	133(6)	195(7)	219(7)	47(5)	-28(5)	-76(5)
C(11)	115(5)	148(6)	145(6)	11(4)	-23(4)	-58(4)
C(12)	115(5)	126(6)	137(6)	9(4)	-14(4)	-50(4)
C(13)	147(6)	153(6)	175(7)	5(5)	-5(5)	-69(5)
C(14)	174(6)	124(6)	188(7)	1(4)	11(5)	-59(5)
C(15)	160(6)	141(6)	208(7)	34(5)	-10(5)	-49(5)
C(16)	129(6)	160(6)	164(6)	24(5)	-22(5)	-50(5)
C(17)	120(5)	132(6)	127(6)	15(4)	-10(4)	-49(4)
C(18)	101(5)	135(6)	136(6)	-3(4)	-13(4)	-39(4)
C(19)	198(8)	161(8)	355(10)	105(6)	79(7)	-5(6)
C(20)	185(8)	234(9)	580(15)	132(9)	4(9)	-73(7)
C(21)	274(10)	218(10)	575(16)	188(9)	126(10)	-11(7)
C(22)	334(11)	300(11)	327(11)	61(8)	183(9)	11(8)
C(23)	165(7)	183(8)	423(12)	-38(7)	20(7)	25(6)
C(24A)	276(13)	280(14)	482(18)	5(12)	-101(12)	87(10)
C(25A)	302(13)	237(13)	570(20)	-176(12)	62(13)	-15(10)
C(26A)	289(14)	294(15)	640(20)	50(13)	237(15)	76(11)
C(27)	198(7)	123(6)	265(8)	-7(5)	12(6)	-62(5)
C(28)	222(8)	174(8)	367(11)	1(6)	30(7)	-98(6)
C(29)	256(9)	142(8)	463(13)	54(7)	-15(8)	-67(6)
C(30)	428(13)	228(10)	320(11)	-94(7)	62(9)	-147(9)
C(31)	147(6)	190(7)	257(8)	65(6)	-71(6)	-57(5)
C(32)	235(9)	296(11)	504(14)	183(9)	-190(9)	-92(8)
C(33)	143(7)	245(9)	349(10)	52(7)	-19(6)	-64(6)
C(34)	265(9)	366(11)	246(9)	1(7)	-127(7)	-98(8)
C(35)	194(8)	302(10)	332(10)	-111(7)	14(7)	-137(7)
C(36)	135(6)	150(6)	190(7)	-39(5)	0(5)	-58(5)
C(37)	181(7)	190(7)	157(7)	-65(5)	19(5)	-43(5)
C(38)	289(10)	412(12)	185(9)	-108(8)	-29(7)	12(8)
C(39)	316(10)	173(8)	295(10)	-85(6)	-32(8)	24(7)
C(40)	372(11)	384(12)	285(10)	-146(8)	188(9)	-210(9)
C(41)	160(8)	538(15)	282(10)	-148(9)	53(7)	-36(8)
C(42)	134(6)	173(7)	178(7)	-47(5)	16(5)	-8(5)

C(43)	337(10)	296(10)	214(9)	-140(7)	16(7)	-117(8)
C(44A)	720(30)	640(20)	161(11)	-150(12)	84(13)	-420(20)
C(45A)	520(20)	870(30)	339(16)	-310(17)	72(13)	-440(20)
C(46A)	1150(40)	192(14)	510(20)	-110(12)	-170(20)	-74(18)