Supporting Information

for

Semiconducting nanostructured copper sulfide thin films from bidentate copper(II) complexes of *N*-(dialkylcarbamothioyl)-nitrosubstituted benzamides by chemical vapour deposition

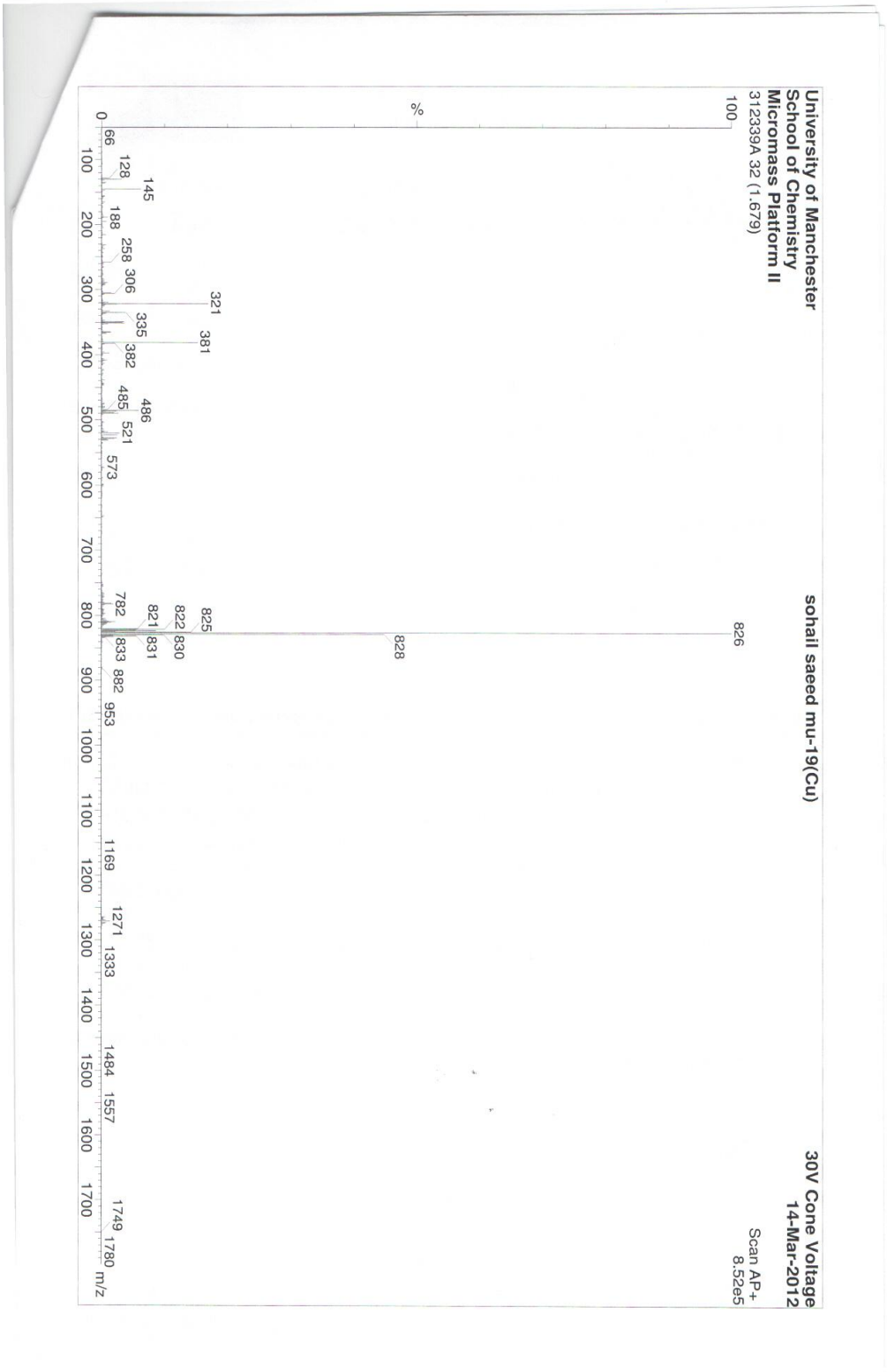
Sohail Saeed,* Naghmana Rashid, Rizwan Hussain, Muhammad Azad Malik, Paul O'Brien and Wing-Tak Wong

***Corresponding author address:**

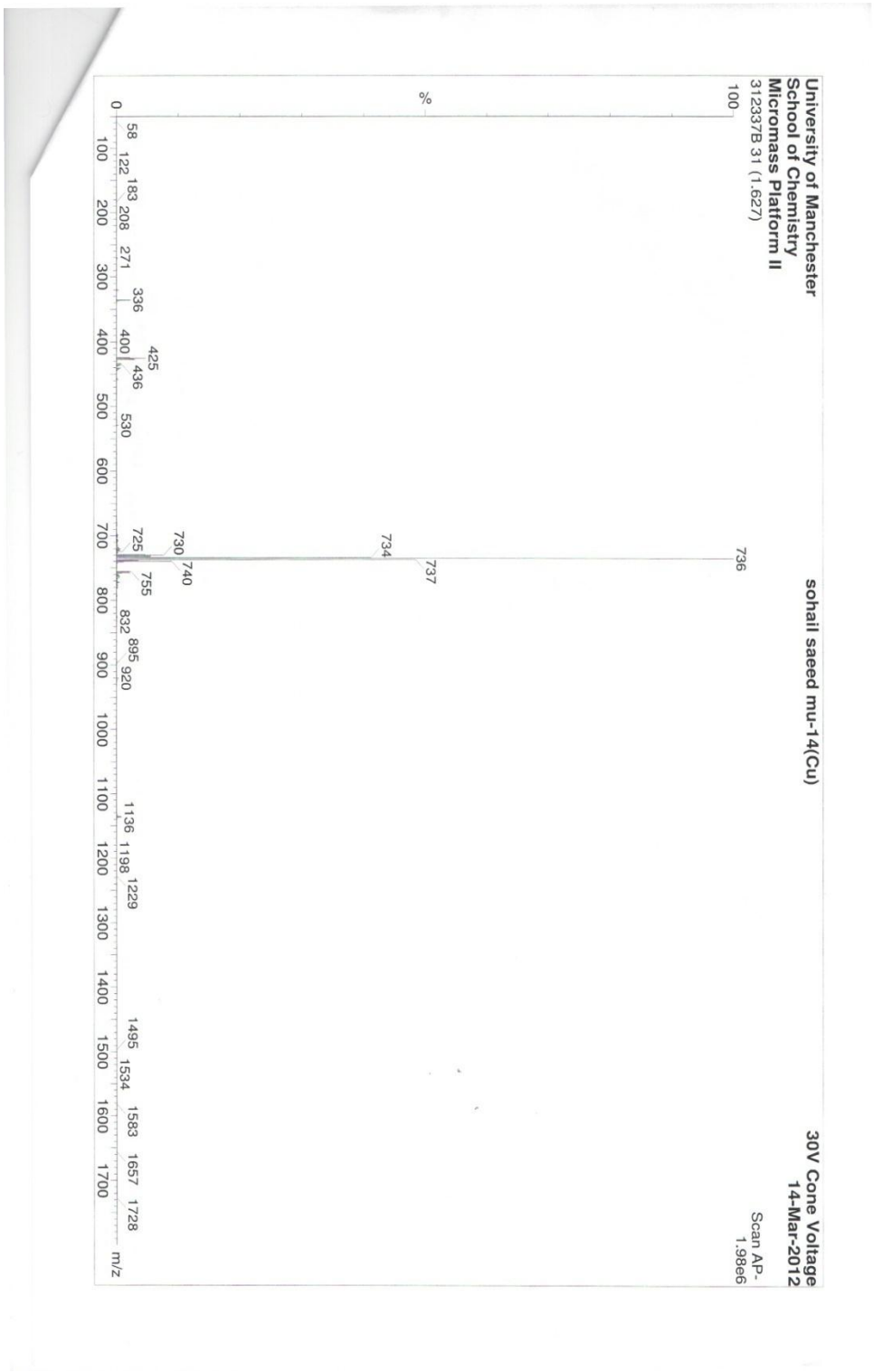
Department of Chemistry, Research Complex, Allama Iqbal Open University, Islamabad - 44000, Pakistan

Fax: +92 51 9250081; Tel.: +92 51 9250081; E-mail: sohail262001@yahoo.com

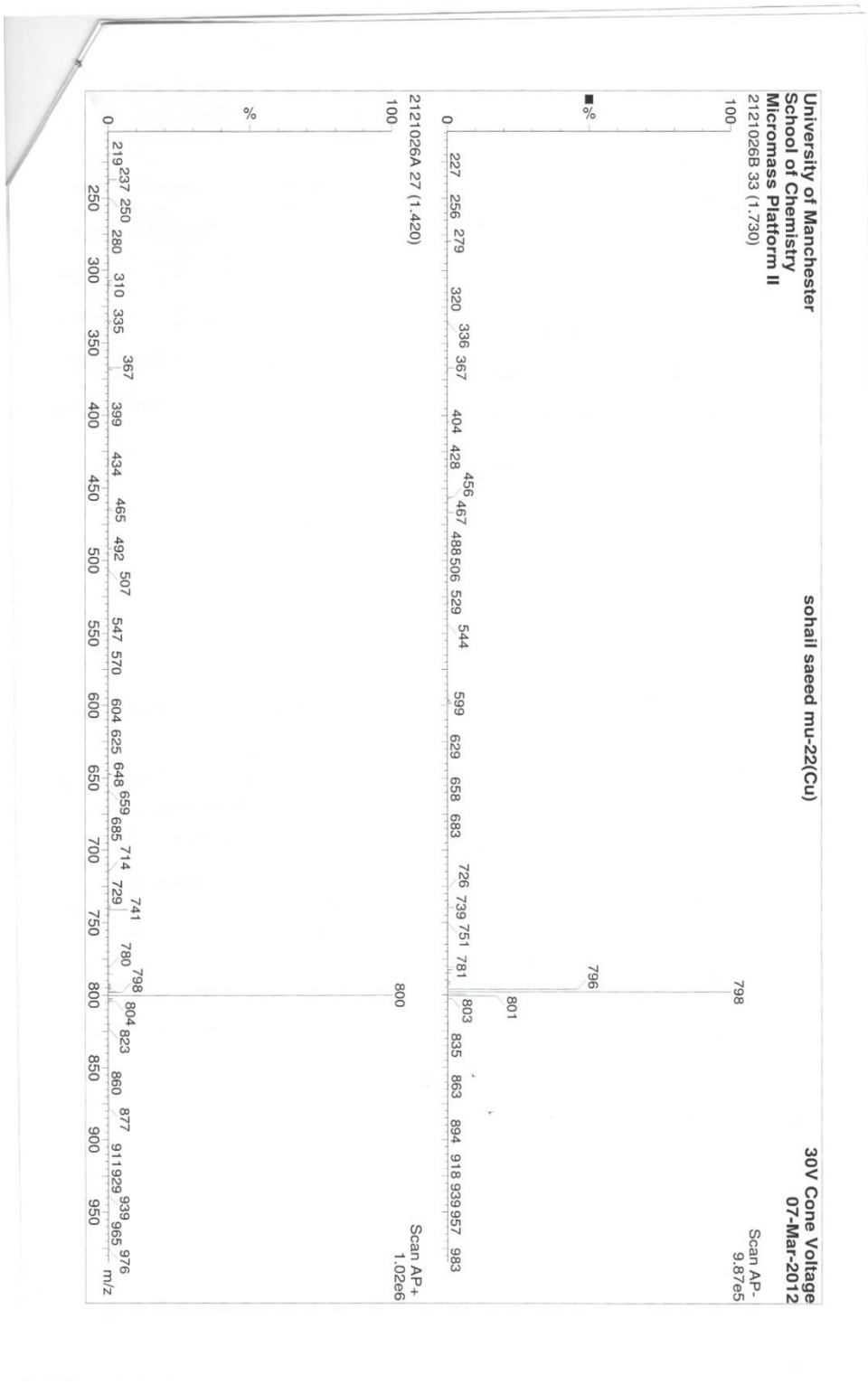
MS-APCI Spectra of copper complex (**1a**)



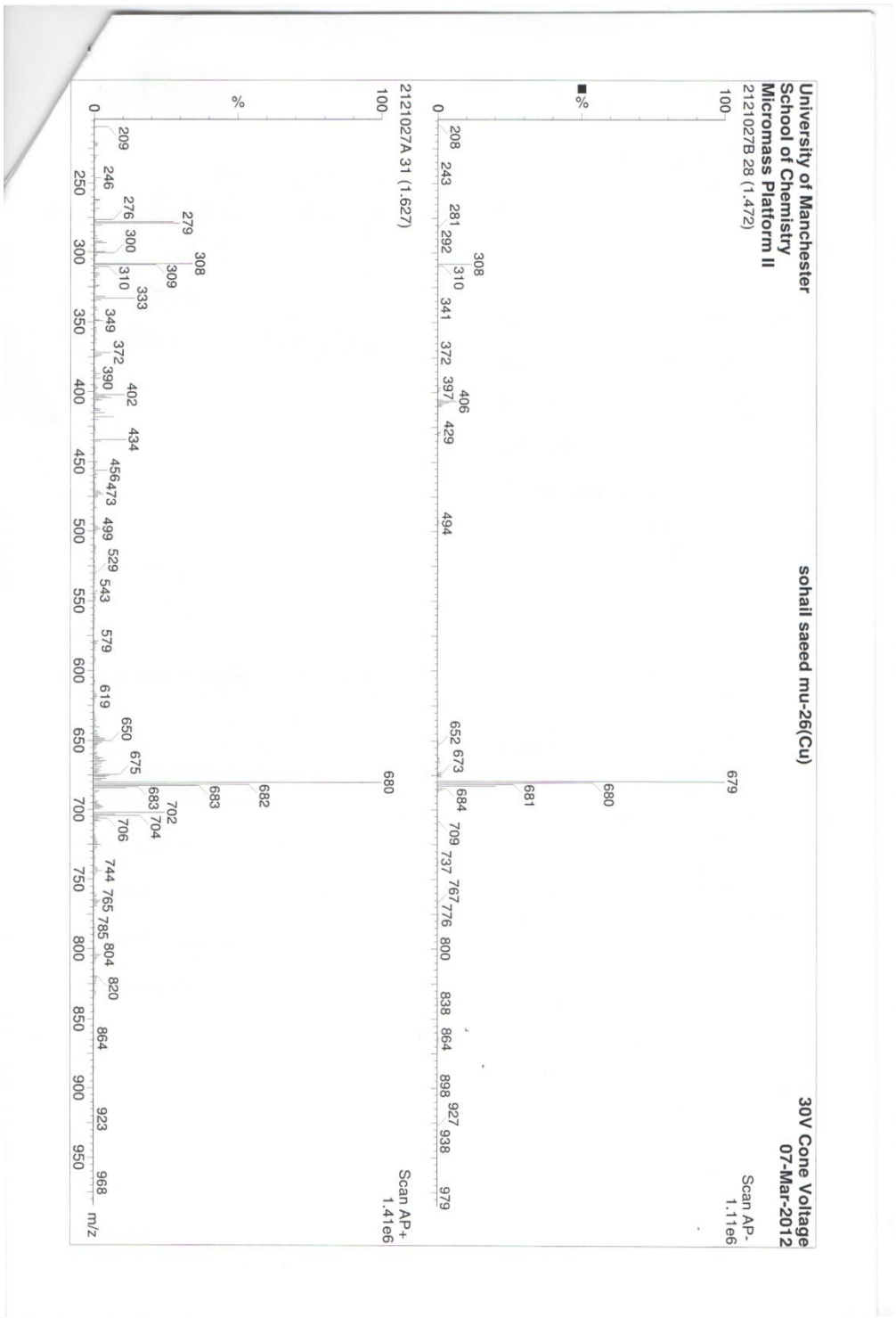
MS-APCI Spectra of copper complex (**2a**)



MS-APCI Spectra of copper complex (**3a**)



MS-APCI Spectra of copper complex (**4a**)



X-Ray Crystallography of 2a

Crystal data

$C_{32}H_{44}CuN_6O_6S_2$	γ = 87.573 (4)°
M_r = 736.39	V = 1828.8 (8) Å^3
Triclinic, P^-1	Z = 2
a = 8.585 (2) Å	Mo $K\alpha$ radiation, λ = 0.71073 Å
b = 12.347 (3) Å	μ = 0.76 mm^{-1}
c = 17.326 (4) Å	T = 300 K
α = 85.325 (4)°	0.50 × 0.10 × 0.08 mm
β = 89.305 (4)°	

Data collection

Bruker SMART 1000 CCD diffractometer	6286 independent reflections
Absorption correction: multi-scan *SADABS* (Sheldrick, 2004)	4382 reflections with $I > 2\sigma(I)$
T_{min} = 0.702, T_{max} = 0.942	R_{int} = 0.021
10157 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.049	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.119	H-atom parameters constrained
S = 1.05	$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2 + 1.3544P]$ where $P = (F_o^2 + 2F_c^2)/3$
6286 reflections	$(\Delta/\sigma)_{max}$ = 0.002
446 parameters	$\Delta\rho_{max}$ = 0.41 e Å^{-3}
6 restraints	$\Delta\rho_{min}$ = -0.37 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.13700 (5)	0.46084 (3)	0.08466 (2)	0.04884 (15)	
S1	0.10537 (12)	0.35834 (8)	-0.01477 (6)	0.0573 (3)	
S2	-0.02149 (12)	0.35095 (8)	0.15728 (5)	0.0584 (3)	
O1	0.2799 (3)	0.55317 (19)	0.02773 (14)	0.0556 (7)	
O2	0.6444 (5)	1.0128 (3)	-0.1032 (2)	0.1072 (13)	
O3	0.7362 (4)	0.9347 (3)	-0.2002 (2)	0.0937 (11)	
O4	0.1785 (3)	0.5477 (2)	0.17061 (14)	0.0615 (7)	
O5	0.2564 (7)	0.9794 (3)	0.3879 (2)	0.158 (2)	
O6	0.1703 (6)	0.8912 (3)	0.4863 (2)	0.1350 (17)	
N1	0.3386 (3)	0.4768 (2)	-0.08949 (16)	0.0477 (7)	
N2	0.6611 (4)	0.9342 (3)	-0.1404 (2)	0.0689 (10)	
N3	0.2607 (4)	0.3268 (2)	-0.14275 (17)	0.0533 (8)	
N4	0.0975 (4)	0.4442 (2)	0.28196 (16)	0.0529 (8)	
N5	0.2060 (6)	0.8989 (3)	0.4194 (2)	0.0879 (12)	
N6	0.0210 (4)	0.2716 (2)	0.30187 (17)	0.0566 (8)	
C1	0.3409 (4)	0.5504 (3)	-0.0388 (2)	0.0449 (8)	
C2	0.4328 (4)	0.6487 (3)	-0.06438 (19)	0.0451 (8)	
C3	0.4321 (4)	0.7354 (3)	-0.0188 (2)	0.0554 (10)	
H3	0.3799	0.7307	0.0286	0.066*	
C4	0.5076 (5)	0.8290 (3)	-0.0425 (2)	0.0604 (10)	
H4	0.5066	0.8876	-0.0120	0.073*	
C5	0.5846 (4)	0.8328 (3)	-0.1129 (2)	0.0520 (9)	
C6	0.5903 (5)	0.7477 (3)	-0.1587 (2)	0.0599 (10)	
H6	0.6447	0.7523	-0.2055	0.072*	
C7	0.5136 (4)	0.6545 (3)	-0.1341 (2)	0.0547 (10)	
H7	0.5163	0.5957	-0.1644	0.066*	
C8	0.2453 (4)	0.3926 (3)	-0.0842 (2)	0.0469 (9)	
C9	0.3776 (5)	0.3477 (3)	-0.2044 (2)	0.0728 (12)	
H9A	0.4111	0.2797	-0.2250	0.087*	
H9B	0.4680	0.3789	-0.1832	0.087*	

C10	0.3066 (7)	0.4283 (5)	-0.2713 (3)	0.1013 (17)	
H10A	0.2136	0.3976	-0.2902	0.122*	
H10B	0.2752	0.4961	-0.2499	0.122*	
C11	0.4100 (8)	0.4515 (6)	-0.3357 (4)	0.129 (2)	
H11A	0.4472	0.3839	-0.3556	0.155*	
H11B	0.4995	0.4879	-0.3183	0.155*	
C12	0.3297 (9)	0.5226 (5)	-0.3996 (3)	0.144 (3)	
H12A	0.3970	0.5290	-0.4442	0.216*	
H12B	0.3064	0.5934	-0.3823	0.216*	
H12C	0.2347	0.4905	-0.4129	0.216*	
C13	0.1529 (5)	0.2413 (3)	-0.1538 (2)	0.0582 (10)	
H13A	0.1441	0.2340	-0.2089	0.070*	
H13B	0.0507	0.2639	-0.1349	0.070*	
C14	0.1980 (5)	0.1303 (3)	-0.1138 (2)	0.0627 (11)	
H14A	0.2938	0.1026	-0.1367	0.075*	
H14B	0.2170	0.1376	-0.0595	0.075*	
C15	0.0708 (5)	0.0503 (3)	-0.1212 (3)	0.0693 (11)	
H15A	0.0531	0.0429	-0.1757	0.083*	
H15B	-0.0251	0.0792	-0.0993	0.083*	
C16	0.1094 (6)	-0.0615 (4)	-0.0811 (3)	0.0875 (15)	
H16A	0.0203	-0.1057	-0.0824	0.131*	
H16B	0.1368	-0.0543	-0.0283	0.131*	
H16C	0.1955	-0.0952	-0.1073	0.131*	
C17	0.1460 (4)	0.5324 (3)	0.2417 (2)	0.0482 (9)	
C18	0.1678 (4)	0.6266 (3)	0.28922 (19)	0.0450 (8)	
C19	0.2114 (4)	0.7257 (3)	0.2533 (2)	0.0529 (9)	
H19	0.2310	0.7322	0.2003	0.063*	
C20	0.2257 (5)	0.8142 (3)	0.2957 (2)	0.0613 (11)	
H20	0.2548	0.8804	0.2717	0.074*	
C21	0.1965 (5)	0.8033 (3)	0.3736 (2)	0.0607 (10)	
C22	0.1562 (6)	0.7062 (3)	0.4112 (2)	0.0734 (13)	
H22	0.1391	0.6999	0.4644	0.088*	

C23	0.1419 (5)	0.6188 (3)	0.3682 (2)	0.0681 (12)	
H23	0.1140	0.5526	0.3929	0.082*	
C24	0.0393 (4)	0.3581 (3)	0.2506 (2)	0.0494 (9)	
C25	0.0695 (5)	0.2742 (3)	0.3827 (2)	0.0663 (12)	
H25A	0.0123	0.2210	0.4147	0.080*	
H25B	0.0417	0.3454	0.3999	0.080*	
C26	0.2400 (6)	0.2512 (4)	0.3945 (2)	0.0788 (13)	
H26A	0.2975	0.3100	0.3688	0.095*	
H26B	0.2714	0.1847	0.3713	0.095*	
C27	0.2805 (8)	0.2393 (5)	0.4804 (3)	0.115 (2)	
H27A	0.2528	0.3072	0.5025	0.137*	
H27B	0.2173	0.1836	0.5061	0.137*	
C28	0.4432 (9)	0.2111 (6)	0.4967 (4)	0.153 (3)	
H28A	0.4603	0.2097	0.5514	0.230*	
H28B	0.5074	0.2643	0.4701	0.230*	
H28C	0.4697	0.1407	0.4793	0.230*	
C29	-0.0512 (5)	0.1721 (3)	0.2829 (2)	0.0672 (12)	
H29A	0.0009	0.1101	0.3112	0.081*	
H29B	-0.0373	0.1638	0.2280	0.081*	
C30	-0.2243 (6)	0.1730 (4)	0.3028 (3)	0.0814 (14)	0.782 (16)
H30A	-0.2357	0.1841	0.3574	0.098*	0.782 (16)
H30B	-0.2740	0.2356	0.2742	0.098*	0.782 (16)
C31	-0.3141 (11)	0.0744 (7)	0.2875 (5)	0.083 (3)	0.782 (16)
H31A	-0.4240	0.0891	0.2977	0.099*	0.782 (16)
H31B	-0.3023	0.0607	0.2334	0.099*	0.782 (16)
C32	-0.2593 (15)	-0.0244 (7)	0.3367 (5)	0.121 (5)	0.782 (16)
H32A	-0.3195	-0.0850	0.3257	0.181*	0.782 (16)
H32B	-0.2719	-0.0115	0.3904	0.181*	0.782 (16)
H32C	-0.1512	-0.0404	0.3258	0.181*	0.782 (16)
C30'	-0.2243 (6)	0.1730 (4)	0.3028 (3)	0.0814 (14)	0.218 (16)
H30C	-0.2872	0.2120	0.2626	0.098*	0.218 (16)
H30D	-0.2471	0.2021	0.3522	0.098*	0.218 (16)

C31'	-0.244 (4)	0.038 (3)	0.3063 (19)	0.079 (10)	0.218 (16)
H31C	-0.2189	0.0104	0.2566	0.095*	0.218 (16)
H31D	-0.1777	0.0004	0.3455	0.095*	0.218 (16)
C32'	-0.415 (4)	0.023 (3)	0.3266 (18)	0.130 (15)	0.218 (16)
H32D	-0.4386	-0.0522	0.3254	0.195*	0.218 (16)
H32E	-0.4793	0.0664	0.2898	0.195*	0.218 (16)
H32F	-0.4363	0.0456	0.3776	0.195*	0.218 (16)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0560 (3)	0.0459 (3)	0.0456 (3)	-0.0145 (2)	0.0076 (2)	-0.00487 (19)
S1	0.0615 (6)	0.0526 (6)	0.0607 (6)	-0.0213 (5)	0.0132 (5)	-0.0149 (5)
S2	0.0679 (7)	0.0570 (6)	0.0511 (6)	-0.0247 (5)	0.0017 (5)	0.0018 (4)
O1	0.0652 (17)	0.0548 (16)	0.0491 (15)	-0.0245 (13)	0.0126 (13)	-0.0093 (12)
O2	0.136 (3)	0.065 (2)	0.125 (3)	-0.044 (2)	0.040 (2)	-0.020 (2)
O3	0.116 (3)	0.076 (2)	0.088 (2)	-0.0336 (19)	0.031 (2)	0.0099 (17)
O4	0.087 (2)	0.0543 (16)	0.0459 (15)	-0.0288 (14)	0.0144 (13)	-0.0078 (12)
O5	0.329 (7)	0.059 (2)	0.091 (3)	-0.055 (3)	-0.011 (3)	-0.010 (2)
O6	0.230 (5)	0.100 (3)	0.084 (3)	-0.050 (3)	0.036 (3)	-0.045 (2)
N1	0.0491 (18)	0.0453 (18)	0.0487 (17)	-0.0070 (14)	0.0036 (14)	-0.0023 (14)
N2	0.072 (2)	0.056 (2)	0.078 (3)	-0.0201 (18)	0.005 (2)	0.0060 (19)
N3	0.058 (2)	0.0482 (19)	0.0552 (19)	-0.0073 (15)	0.0060 (15)	-0.0120 (15)
N4	0.071 (2)	0.0414 (18)	0.0468 (17)	-0.0119 (15)	0.0033 (15)	-0.0006 (14)
N5	0.136 (4)	0.061 (3)	0.070 (3)	-0.018 (2)	-0.007 (3)	-0.011 (2)
N6	0.081 (2)	0.0415 (18)	0.0475 (18)	-0.0148 (16)	0.0035 (16)	-0.0002 (14)
C1	0.040 (2)	0.043 (2)	0.050 (2)	-0.0013 (16)	-0.0017 (16)	0.0018 (17)
C2	0.043 (2)	0.043 (2)	0.049 (2)	-0.0083 (16)	0.0015 (16)	0.0009 (16)
C3	0.060 (2)	0.056 (2)	0.051 (2)	-0.0129 (19)	0.0100 (18)	-0.0020 (18)
C4	0.067 (3)	0.052 (2)	0.064 (3)	-0.014 (2)	0.004 (2)	-0.0107 (19)
C5	0.052 (2)	0.044 (2)	0.059 (2)	-0.0149 (17)	-0.0033 (18)	0.0057 (18)
C6	0.065 (3)	0.059 (3)	0.055 (2)	-0.010 (2)	0.014 (2)	0.0003 (19)
C7	0.062 (2)	0.048 (2)	0.055 (2)	-0.0082 (18)	0.0097 (19)	-0.0066 (17)

C8	0.045 (2)	0.045 (2)	0.050 (2)	-0.0009 (17)	-0.0025 (16)	-0.0016 (17)
C9	0.081 (3)	0.065 (3)	0.075 (3)	-0.010 (2)	0.023 (2)	-0.023 (2)
C10	0.115 (4)	0.113 (4)	0.075 (3)	-0.002 (3)	0.023 (3)	-0.004 (3)
C11	0.138 (6)	0.134 (6)	0.113 (5)	0.006 (4)	0.031 (4)	-0.001 (4)
C12	0.199 (8)	0.128 (6)	0.099 (5)	0.015 (5)	0.008 (5)	0.017 (4)
C13	0.064 (3)	0.058 (3)	0.055 (2)	-0.009 (2)	-0.0028 (19)	-0.0196 (19)
C14	0.066 (3)	0.051 (2)	0.073 (3)	-0.001 (2)	-0.006 (2)	-0.015 (2)
C15	0.078 (3)	0.062 (3)	0.071 (3)	-0.015 (2)	0.001 (2)	-0.012 (2)
C16	0.118 (4)	0.063 (3)	0.083 (3)	-0.016 (3)	-0.001 (3)	-0.007 (2)
C17	0.050 (2)	0.046 (2)	0.049 (2)	-0.0060 (17)	0.0020 (17)	-0.0028 (17)
C18	0.047 (2)	0.040 (2)	0.048 (2)	-0.0070 (16)	-0.0008 (16)	-0.0022 (15)
C19	0.064 (3)	0.049 (2)	0.045 (2)	-0.0109 (19)	0.0009 (18)	0.0017 (17)
C20	0.083 (3)	0.042 (2)	0.059 (2)	-0.016 (2)	-0.006 (2)	0.0046 (18)
C21	0.079 (3)	0.046 (2)	0.059 (2)	-0.012 (2)	-0.004 (2)	-0.0111 (18)
C22	0.114 (4)	0.062 (3)	0.047 (2)	-0.026 (3)	0.012 (2)	-0.009 (2)
C23	0.103 (3)	0.050 (2)	0.052 (2)	-0.026 (2)	0.015 (2)	-0.0021 (19)
C24	0.055 (2)	0.040 (2)	0.052 (2)	-0.0087 (17)	0.0080 (17)	0.0008 (16)
C25	0.098 (4)	0.051 (2)	0.049 (2)	-0.020 (2)	0.003 (2)	0.0039 (18)
C26	0.110 (4)	0.060 (3)	0.065 (3)	-0.008 (3)	-0.012 (3)	0.005 (2)
C27	0.119 (5)	0.128 (5)	0.095 (4)	-0.003 (4)	-0.027 (4)	0.003 (4)
C28	0.146 (7)	0.183 (8)	0.129 (6)	-0.031 (6)	-0.035 (5)	0.018 (5)
C29	0.097 (3)	0.043 (2)	0.062 (3)	-0.015 (2)	0.012 (2)	-0.0021 (18)
C30	0.096 (4)	0.076 (3)	0.074 (3)	-0.028 (3)	0.016 (3)	-0.005 (2)
C31	0.086 (6)	0.086 (6)	0.077 (5)	-0.031 (5)	0.011 (4)	-0.005 (4)
C32	0.192 (12)	0.073 (6)	0.099 (6)	-0.057 (6)	0.007 (6)	0.005 (4)
C30'	0.096 (4)	0.076 (3)	0.074 (3)	-0.028 (3)	0.016 (3)	-0.005 (2)
C31'	0.077 (13)	0.077 (13)	0.083 (12)	-0.011 (9)	-0.001 (9)	-0.004 (9)
C32'	0.08 (3)	0.18 (3)	0.13 (2)	-0.06 (2)	0.011 (18)	0.01 (2)

Geometric parameters (Å, º)

Cu1—O1	1.919 (2)	C14—C15	1.517 (5)
Cu1—O4	1.949 (2)	C14—H14A	0.9700
Cu1—S1	2.2448 (11)	C14—H14B	0.9700
Cu1—S2	2.2610 (10)	C15—C16	1.519 (6)
S1—C8	1.731 (4)	C15—H15A	0.9700
S2—C24	1.715 (4)	C15—H15B	0.9700
O1—C1	1.262 (4)	C16—H16A	0.9600
O2—N2	1.212 (4)	C16—H16B	0.9600
O3—N2	1.212 (4)	C16—H16C	0.9600
O4—C17	1.260 (4)	C17—C18	1.498 (5)
O5—N5	1.190 (5)	C18—C23	1.380 (5)
O6—N5	1.192 (5)	C18—C19	1.391 (5)
N1—C1	1.316 (4)	C19—C20	1.376 (5)
N1—C8	1.335 (4)	C19—H19	0.9300
N2—C5	1.480 (5)	C20—C21	1.366 (5)
N3—C8	1.351 (4)	C20—H20	0.9300
N3—C13	1.459 (5)	C21—C22	1.372 (5)
N3—C9	1.472 (5)	C22—C23	1.370 (5)
N4—C17	1.324 (4)	C22—H22	0.9300
N4—C24	1.350 (4)	C23—H23	0.9300
N5—C21	1.482 (5)	C25—C26	1.493 (6)
N6—C24	1.346 (4)	C25—H25A	0.9700
N6—C29	1.462 (5)	C25—H25B	0.9700
N6—C25	1.468 (5)	C26—C27	1.526 (6)
C1—C2	1.509 (5)	C26—H26A	0.9700
C2—C3	1.380 (5)	C26—H26B	0.9700
C2—C7	1.383 (5)	C27—C28	1.451 (8)
C3—C4	1.380 (5)	C27—H27A	0.9700
C3—H3	0.9300	C27—H27B	0.9700
C4—C5	1.378 (5)	C28—H28A	0.9600
C4—H4	0.9300	C28—H28B	0.9600

C5—C6	1.367 (5)	C28—H28C	0.9600
C6—C7	1.385 (5)	C29—C30	1.522 (6)
C6—H6	0.9300	C29—H29A	0.9700
C7—H7	0.9300	C29—H29B	0.9700
C9—C10	1.576 (6)	C30—C31	1.510 (8)
C9—H9A	0.9700	C30—H30A	0.9700
C9—H9B	0.9700	C30—H30B	0.9700
C10—C11	1.434 (7)	C31—C32	1.494 (16)
C10—H10A	0.9700	C31—H31A	0.9700
C10—H10B	0.9700	C31—H31B	0.9700
C11—C12	1.510 (8)	C32—H32A	0.9600
C11—H11A	0.9700	C32—H32B	0.9600
C11—H11B	0.9700	C32—H32C	0.9600
C12—H12A	0.9600	C31'—C32'	1.52 (5)
C12—H12B	0.9600	C31'—H31C	0.9700
C12—H12C	0.9600	C31'—H31D	0.9700
C13—C14	1.521 (5)	C32'—H32D	0.9600
C13—H13A	0.9700	C32'—H32E	0.9600
C13—H13B	0.9700	C32'—H32F	0.9600
O1—Cu1—O4	84.88 (10)	H15A—C15—H15B	107.7
O1—Cu1—S1	93.14 (8)	C15—C16—H16A	109.5
O4—Cu1—S1	176.40 (9)	C15—C16—H16B	109.5
O1—Cu1—S2	176.75 (9)	H16A—C16—H16B	109.5
O4—Cu1—S2	92.89 (8)	C15—C16—H16C	109.5
S1—Cu1—S2	88.96 (4)	H16A—C16—H16C	109.5
C8—S1—Cu1	107.78 (13)	H16B—C16—H16C	109.5
C24—S2—Cu1	104.65 (12)	O4—C17—N4	129.9 (3)
C1—O1—Cu1	132.5 (2)	O4—C17—C18	116.1 (3)
C17—O4—Cu1	130.7 (2)	N4—C17—C18	114.0 (3)
C1—N1—C8	124.2 (3)	C23—C18—C19	118.5 (3)
O3—N2—O2	123.1 (4)	C23—C18—C17	121.7 (3)

O3—N2—C5	118.0 (4)	C19—C18—C17	119.8 (3)
O2—N2—C5	118.9 (4)	C20—C19—C18	120.4 (3)
C8—N3—C13	122.7 (3)	C20—C19—H19	119.8
C8—N3—C9	120.5 (3)	C18—C19—H19	119.8
C13—N3—C9	116.4 (3)	C21—C20—C19	119.1 (3)
C17—N4—C24	124.6 (3)	C21—C20—H20	120.5
O5—N5—O6	122.8 (4)	C19—C20—H20	120.5
O5—N5—C21	117.6 (4)	C20—C21—C22	122.0 (4)
O6—N5—C21	119.6 (4)	C20—C21—N5	119.6 (4)
C24—N6—C29	123.6 (3)	C22—C21—N5	118.3 (4)
C24—N6—C25	120.7 (3)	C23—C22—C21	118.3 (4)
C29—N6—C25	115.8 (3)	C23—C22—H22	120.9
O1—C1—N1	131.3 (3)	C21—C22—H22	120.9
O1—C1—C2	114.3 (3)	C22—C23—C18	121.6 (4)
N1—C1—C2	114.5 (3)	C22—C23—H23	119.2
C3—C2—C7	119.7 (3)	C18—C23—H23	119.2
C3—C2—C1	119.5 (3)	N6—C24—N4	113.6 (3)
C7—C2—C1	120.8 (3)	N6—C24—S2	118.6 (3)
C4—C3—C2	121.0 (3)	N4—C24—S2	127.7 (3)
C4—C3—H3	119.5	N6—C25—C26	113.6 (3)
C2—C3—H3	119.5	N6—C25—H25A	108.8
C3—C4—C5	117.9 (4)	C26—C25—H25A	108.8
C3—C4—H4	121.1	N6—C25—H25B	108.8
C5—C4—H4	121.1	C26—C25—H25B	108.8
C6—C5—C4	122.6 (3)	H25A—C25—H25B	107.7
C6—C5—N2	118.9 (3)	C25—C26—C27	111.5 (4)
C4—C5—N2	118.5 (4)	C25—C26—H26A	109.3
C5—C6—C7	118.7 (3)	C27—C26—H26A	109.3
C5—C6—H6	120.6	C25—C26—H26B	109.3
C7—C6—H6	120.6	C27—C26—H26B	109.3
C2—C7—C6	120.1 (4)	H26A—C26—H26B	108.0
C2—C7—H7	120.0	C28—C27—C26	114.6 (6)

C6—C7—H7	120.0	C28—C27—H27A	108.6
N1—C8—N3	114.8 (3)	C26—C27—H27A	108.6
N1—C8—S1	129.2 (3)	C28—C27—H27B	108.6
N3—C8—S1	116.0 (3)	C26—C27—H27B	108.6
N3—C9—C10	110.2 (4)	H27A—C27—H27B	107.6
N3—C9—H9A	109.6	C27—C28—H28A	109.5
C10—C9—H9A	109.6	C27—C28—H28B	109.5
N3—C9—H9B	109.6	H28A—C28—H28B	109.5
C10—C9—H9B	109.6	C27—C28—H28C	109.5
H9A—C9—H9B	108.1	H28A—C28—H28C	109.5
C11—C10—C9	114.7 (5)	H28B—C28—H28C	109.5
C11—C10—H10A	108.6	N6—C29—C30	112.2 (3)
C9—C10—H10A	108.6	N6—C29—H29A	109.2
C11—C10—H10B	108.6	C30—C29—H29A	109.2
C9—C10—H10B	108.6	N6—C29—H29B	109.2
H10A—C10—H10B	107.6	C30—C29—H29B	109.2
C10—C11—C12	111.4 (6)	H29A—C29—H29B	107.9
C10—C11—H11A	109.3	C31—C30—C29	118.2 (5)
C12—C11—H11A	109.3	C31—C30—H30A	107.8
C10—C11—H11B	109.3	C29—C30—H30A	107.8
C12—C11—H11B	109.3	C31—C30—H30B	107.8
H11A—C11—H11B	108.0	C29—C30—H30B	107.8
C11—C12—H12A	109.5	H30A—C30—H30B	107.1
C11—C12—H12B	109.5	C32—C31—C30	112.0 (8)
H12A—C12—H12B	109.5	C32—C31—H31A	109.2
C11—C12—H12C	109.5	C30—C31—H31A	109.2
H12A—C12—H12C	109.5	C32—C31—H31B	109.2
H12B—C12—H12C	109.5	C30—C31—H31B	109.2
N3—C13—C14	115.2 (3)	H31A—C31—H31B	107.9
N3—C13—H13A	108.5	C31—C32—H32A	109.5
C14—C13—H13A	108.5	C31—C32—H32B	109.5
N3—C13—H13B	108.5	H32A—C32—H32B	109.5

C14—C13—H13B	108.5	C31—C32—H32C	109.5
H13A—C13—H13B	107.5	H32A—C32—H32C	109.5
C15—C14—C13	111.3 (3)	H32B—C32—H32C	109.5
C15—C14—H14A	109.4	C32'—C31'—H31C	110.9
C13—C14—H14A	109.4	C32'—C31'—H31D	110.9
C15—C14—H14B	109.4	H31C—C31'—H31D	108.9
C13—C14—H14B	109.4	C31'—C32'—H32D	109.5
H14A—C14—H14B	108.0	C31'—C32'—H32E	109.5
C14—C15—C16	113.3 (4)	H32D—C32'—H32E	109.5
C14—C15—H15A	108.9	C31'—C32'—H32F	109.5
C16—C15—H15A	108.9	H32D—C32'—H32F	109.5
C14—C15—H15B	108.9	H32E—C32'—H32F	109.5

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TITL  wt2335w-SS-MU-14Cu_SohailSaeed_10-April-2012
CELL  0.71073 8.58490 12.34710 17.32640 85.325 89.305 87.573
ZERR  2 0.00210 0.00290 0.00410 0.004 0.004 0.004
LATT 1
SFAC N O C H CU S
UNIT 12 12 64 88 2 4
SHEL 8.000000 0.84
OMIT    -2   5   2
OMIT     1  -4   3
OMIT     0   8   5
OMIT     1  -5   9
OMIT    -7  -3   9
OMIT     7   6   4
OMIT    -5  10  10
OMIT    -1 -14  11
OMIT    -9  -2  15
OMIT    -8  -2  17
OMIT    10  -5   5
OMIT     7   0   9
OMIT    -6 -11   2
OMIT     0 -12   9
OMIT     4  -5  15
OMIT    -4   6  17
L.S. 6
FMAP 2
PLAN -20
BOND $H
HTAB
TEMP 27.0
EADP C30 C30'
EXYZ C30 C30'
ISOR 0.01 0.02 C31'
MPLA 3 N2 O2 O3
MPLA 6 C2 C3 C4 C5 C6 C7
MPLA 6 Cu1 S1 C8 N1 C1 O1
MPLA 6 Cu1 S2 C24 N4 C17 O4
MPLA 6 C18 C19 C20 C21 C22 C23
MPLA 3 N5 O5 O6
ACTA
SIZE 0.500 0.100 0.080
LIST 4
WGHT    0.041100    1.354400
FVAR       0.34457   0.78228
CU1   5    0.137004    0.460838    0.084659    11.00000    0.05604
0.04594 =
         0.04559   -0.00487    0.00761   -0.01450
S1    6    0.105367    0.358342   -0.014773    11.00000    0.06151
0.05259 =
         0.06066   -0.01494    0.01322   -0.02126
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S2    6   -0.021492    0.350948    0.157281    11.00000    0.06787
0.05703 =
         0.05106    0.00180    0.00170   -0.02466
O1    2    0.279900    0.553167    0.027728    11.00000    0.06518
0.05483 =
         0.04906   -0.00931    0.01261   -0.02451
O2    2    0.644444    1.012824   -0.103167    11.00000    0.13605
0.06512 =
         0.12487   -0.02044    0.04015   -0.04435
O3    2    0.736184    0.934661   -0.200181    11.00000    0.11626
0.07580 =
         0.08815    0.00989    0.03131   -0.03356
O4    2    0.178505    0.547700    0.170606    11.00000    0.08687
0.05427 =
         0.04586   -0.00785    0.01441   -0.02879
O5    2    0.256401    0.979408    0.387929    11.00000    0.32923
0.05896 =
         0.09083   -0.00983   -0.01121   -0.05510
O6    2    0.170277    0.891231    0.486291    11.00000    0.23050
0.09959 =
         0.08393   -0.04538    0.03568   -0.04976
N1    1    0.338602    0.476768   -0.089490    11.00000    0.04914
0.04528 =
         0.04868   -0.00234    0.00364   -0.00702
N2    1    0.661088    0.934178   -0.140443    11.00000    0.07206
0.05571 =
         0.07846    0.00602    0.00543   -0.02012
N3    1    0.260669    0.326835   -0.142748    11.00000    0.05808
0.04822 =
         0.05524   -0.01196    0.00602   -0.00732
N4    1    0.097533    0.444244    0.281955    11.00000    0.07057
0.04145 =
         0.04681   -0.00060    0.00327   -0.01189
N5    1    0.205981    0.898918    0.419430    11.00000    0.13581
0.06060 =
         0.06970   -0.01142   -0.00702   -0.01796
N6    1    0.020980    0.271639    0.301875    11.00000    0.08130
0.04155 =
         0.04749   -0.00025    0.00350   -0.01481
C1    3    0.340900    0.550426   -0.038751    11.00000    0.04046
0.04338 =
         0.04991    0.00180   -0.00165   -0.00134
C2    3    0.432815    0.648748   -0.064383    11.00000    0.04346
0.04255 =
         0.04892    0.00086    0.00147   -0.00833
C3    3    0.432088    0.735416   -0.018827    11.00000    0.05975
0.05570 =
         0.05101   -0.00203    0.00995   -0.01288
AFIX  43
H3    4    0.379863    0.730665    0.028592    11.00000   -1.20000
AFIX   0
C4    3    0.507627    0.828991   -0.042533    11.00000    0.06747
0.05171 =
         0.06401   -0.01069    0.00353   -0.01400
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AFIX  43
H4    4    0.506602    0.887586   -0.012010    11.00000   -1.20000
AFIX   0
C5    3    0.584615    0.832840   -0.112869    11.00000    0.05172
0.04443 =
         0.05928    0.00568   -0.00326   -0.01494
C6    3    0.590328    0.747719   -0.158694    11.00000    0.06521
0.05932 =
         0.05459    0.00026    0.01397   -0.01003
AFIX  43
H6    4    0.644716    0.752312   -0.205515    11.00000   -1.20000
AFIX   0
C7    3    0.513559    0.654461   -0.134071    11.00000    0.06194
0.04821 =
         0.05470   -0.00658    0.00972   -0.00821
AFIX  43
H7    4    0.516318    0.595652   -0.164424    11.00000   -1.20000
AFIX   0
C8    3    0.245324    0.392583   -0.084230    11.00000    0.04546
0.04527 =
         0.04956   -0.00165   -0.00249   -0.00089
C9    3    0.377579    0.347688   -0.204407    11.00000    0.08100
0.06513 =
         0.07519   -0.02294    0.02272   -0.00992
AFIX  23
H9A   4    0.411051    0.279706   -0.225037    11.00000   -1.20000
H9B   4    0.467985    0.378878   -0.183206    11.00000   -1.20000
AFIX   0
C10   3    0.306622    0.428273   -0.271332    11.00000    0.11466
0.11254 =
         0.07541   -0.00396    0.02317   -0.00224
AFIX  23
H10A  4    0.213578    0.397550   -0.290190    11.00000   -1.20000
H10B  4    0.275218    0.496127   -0.249948    11.00000   -1.20000
AFIX   0
C11   3    0.409998    0.451511   -0.335658    11.00000    0.13781
0.13418 =
         0.11289   -0.00098    0.03116    0.00558
AFIX  23
H11A  4    0.447202    0.383853   -0.355590    11.00000   -1.20000
H11B  4    0.499546    0.487934   -0.318277    11.00000   -1.20000
AFIX   0
C12   3    0.329707    0.522576   -0.399567    11.00000    0.19925
0.12800 =
         0.09905    0.01713    0.00796    0.01512
AFIX 137
H12A  4    0.397000    0.528973   -0.444219    11.00000   -1.50000
H12B  4    0.306370    0.593417   -0.382257    11.00000   -1.50000
H12C  4    0.234705    0.490519   -0.412855    11.00000   -1.50000
AFIX   0
C13   3    0.152884    0.241300   -0.153783    11.00000    0.06422
0.05826 =
         0.05522   -0.01962   -0.00275   -0.00856
AFIX  23
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H13A  4    0.144137    0.234019   -0.208867    11.00000   -1.20000
H13B  4    0.050735    0.263918   -0.134930    11.00000   -1.20000
AFIX   0
C14   3    0.198017    0.130327   -0.113826    11.00000    0.06555
0.05127 =
         0.07298   -0.01470   -0.00590   -0.00077
AFIX  23
H14A  4    0.293789    0.102622   -0.136730    11.00000   -1.20000
H14B  4    0.216980    0.137638   -0.059457    11.00000   -1.20000
AFIX   0
C15   3    0.070826    0.050261   -0.121203    11.00000    0.07781
0.06179 =
         0.07060   -0.01230    0.00078   -0.01544
AFIX  23
H15A  4    0.053073    0.042928   -0.175678    11.00000   -1.20000
H15B  4   -0.025126    0.079246   -0.099251    11.00000   -1.20000
AFIX   0
C16   3    0.109423   -0.061509   -0.081120    11.00000    0.11781
0.06259 =
         0.08340   -0.00655   -0.00077   -0.01631
AFIX 137
H16A  4    0.020295   -0.105708   -0.082425    11.00000   -1.50000
H16B  4    0.136844   -0.054295   -0.028287    11.00000   -1.50000
H16C  4    0.195524   -0.095162   -0.107314    11.00000   -1.50000
AFIX   0
C17   3    0.146006    0.532376    0.241672    11.00000    0.05005
0.04586 =
         0.04875   -0.00281    0.00203   -0.00597
C18   3    0.167830    0.626557    0.289219    11.00000    0.04743
0.03984 =
         0.04799   -0.00222   -0.00079   -0.00703
C19   3    0.211389    0.725681    0.253303    11.00000    0.06445
0.04940 =
         0.04462    0.00173    0.00095   -0.01088
AFIX  43
H19   4    0.230975    0.732209    0.200255    11.00000   -1.20000
AFIX   0
C20   3    0.225703    0.814152    0.295715    11.00000    0.08252
0.04178 =
         0.05939    0.00465   -0.00625   -0.01598
AFIX  43
H20   4    0.254840    0.880445    0.271707    11.00000   -1.20000
AFIX   0
C21   3    0.196528    0.803272    0.373568    11.00000    0.07924
0.04620 =
         0.05873   -0.01115   -0.00359   -0.01177
C22   3    0.156224    0.706178    0.411163    11.00000    0.11414
0.06198 =
         0.04652   -0.00900    0.01220   -0.02616
AFIX  43
H22   4    0.139085    0.699859    0.464412    11.00000   -1.20000
AFIX   0
C23   3    0.141888    0.618774    0.368204    11.00000    0.10287
0.05049 =
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         0.05222   -0.00211    0.01468   -0.02614
AFIX  43
H23   4    0.113996    0.552598    0.392881    11.00000   -1.20000
AFIX   0
C24   3    0.039257    0.358130    0.250582    11.00000    0.05535
0.04020 =
         0.05227    0.00080    0.00804   -0.00868
C25   3    0.069451    0.274236    0.382658    11.00000    0.09835
0.05110 =
         0.04949    0.00393    0.00337   -0.01988
AFIX  23
H25A  4    0.012306    0.221045    0.414668    11.00000   -1.20000
H25B  4    0.041680    0.345396    0.399863    11.00000   -1.20000
AFIX   0
C26   3    0.240025    0.251214    0.394529    11.00000    0.11048
0.05980 =
         0.06530    0.00451   -0.01237   -0.00828
AFIX  23
H26A  4    0.297505    0.309996    0.368827    11.00000   -1.20000
H26B  4    0.271376    0.184735    0.371286    11.00000   -1.20000
AFIX   0
C27   3    0.280493    0.239283    0.480401    11.00000    0.11897
0.12786 =
         0.09525    0.00299   -0.02707   -0.00267
AFIX  23
H27A  4    0.252785    0.307246    0.502519    11.00000   -1.20000
H27B  4    0.217285    0.183630    0.506113    11.00000   -1.20000
AFIX   0
C28   3    0.443221    0.211116    0.496665    11.00000    0.14621
0.18280 =
         0.12883    0.01833   -0.03509   -0.03070
AFIX 137
H28A  4    0.460304    0.209722    0.551397    11.00000   -1.50000
H28B  4    0.507376    0.264259    0.470054    11.00000   -1.50000
H28C  4    0.469670    0.140727    0.479306    11.00000   -1.50000
AFIX   0
C29   3   -0.051184    0.172113    0.282917    11.00000    0.09662
0.04338 =
         0.06206   -0.00212    0.01172   -0.01456
AFIX  23
H29A  4    0.000945    0.110117    0.311158    11.00000   -1.20000
H29B  4   -0.037338    0.163833    0.228034    11.00000   -1.20000
AFIX   0
PART 1
C30   3   -0.224338    0.172959    0.302775    21.00000    0.09596
0.07577 =
         0.07387   -0.00478    0.01614   -0.02817
AFIX  23
H30A  4   -0.235693    0.184076    0.357369    21.00000   -1.20000
H30B  4   -0.273962    0.235640    0.274162    21.00000   -1.20000
AFIX   0
C31   3   -0.314081    0.074431    0.287502    21.00000    0.08639
0.08631 =
         0.07714   -0.00518    0.01112   -0.03063
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AFIX  23
H31A  4   -0.423986    0.089143    0.297662    21.00000   -1.20000
H31B  4   -0.302284    0.060686    0.233371    21.00000   -1.20000
AFIX   0
C32   3   -0.259269   -0.024432    0.336743    21.00000    0.19249
0.07277 =
         0.09942    0.00533    0.00699   -0.05704
AFIX  33
H32A  4   -0.319475   -0.084983    0.325651    21.00000   -1.50000
H32B  4   -0.271899   -0.011451    0.390384    21.00000   -1.50000
H32C  4   -0.151201   -0.040407    0.325845    21.00000   -1.50000
AFIX   0
PART 2
C30'  3   -0.224338    0.172959    0.302775   -21.00000    0.09596
0.07577 =
         0.07387   -0.00478    0.01614   -0.02817
AFIX  23
H30C  4   -0.287244    0.211971    0.262589   -21.00000   -1.20000
H30D  4   -0.247113    0.202077    0.352197   -21.00000   -1.20000
AFIX   0
C31'  3   -0.244489    0.037899    0.306267   -21.00000    0.07702
0.07744 =
         0.08347   -0.00444   -0.00085   -0.01094
AFIX  23
H31C  4   -0.218887    0.010387    0.256603   -21.00000   -1.20000
H31D  4   -0.177689    0.000430    0.345509   -21.00000   -1.20000
AFIX   0
C32'  3   -0.415393    0.023058    0.326647   -21.00000    0.08385
0.18100 =
         0.12583    0.00677    0.01066   -0.05634
AFIX  33
H32D  4   -0.438557   -0.052155    0.325353   -21.00000   -1.50000
H32E  4   -0.479278    0.066369    0.289837   -21.00000   -1.50000
H32F  4   -0.436278    0.045587    0.377623   -21.00000   -1.50000
PART 0
HKLF 4

REM   wt2335w-SS-MU-14Cu_SohailSaeed_10-April-2012
REM R1 =  0.0486 for   4382 Fo > 4sig(Fo)  and  0.0740 for all   6286 data
REM    446 parameters refined using      6 restraints

END

WGHT      0.0368      1.3930
REM Highest difference peak  0.411,  deepest hole -0.374,  1-sigma level
0.053
Q1    1   0.3899  0.3586 -0.2819  11.00000  0.05    0.41
Q2    1   0.1764  0.4041  0.0421  11.00000  0.05    0.39
Q3    1  -0.0007  0.4862  0.0403  11.00000  0.05    0.32
Q4    1   0.0346  0.3160 -0.0162  11.00000  0.05    0.31
Q5    1   0.2616  0.4434  0.1365  11.00000  0.05    0.30
Q6    1   0.2080  0.3805 -0.0334  11.00000  0.05    0.29
Q7    1   0.0368  0.4216  0.1214  11.00000  0.05    0.29
Q8    1   0.2026  0.4675  0.1585  11.00000  0.05    0.28
```

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Q9    1   0.2727  0.4067 -0.3300  11.00000  0.05    0.26
Q10   1   0.0849  0.5170  0.1401  11.00000  0.05    0.25
Q11   1   0.0372  0.5425  0.0268  11.00000  0.05    0.23
Q12   1  -0.0046  0.4843  0.0834  11.00000  0.05    0.23
Q13   1   0.2785  0.4400  0.0815  11.00000  0.05    0.23
Q14   1   0.5030  0.3185 -0.1609  11.00000  0.05    0.23
Q15   1   0.3136  0.1807  0.5372  11.00000  0.05    0.22
Q16   1   0.0126  0.2890  0.1951  11.00000  0.05    0.21
Q17   1   0.1745  0.5255  0.1220  11.00000  0.05    0.21
Q18   1   0.0858  0.3910  0.0524  11.00000  0.05    0.21
Q19   1   0.1763  0.3830  0.1169  11.00000  0.05    0.21
Q20   1  -0.0885  0.4242  0.1652  11.00000  0.05    0.20
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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.

The structure was solved by Patterson methods (<i>DIRDIF-99</i> (Beurskens
et al., 1999)) and expanded using Fourier techniques. All non-H atoms were
refined anisotropically.

The C-bound H atoms are all placed at geometrical positions with C---H =
0.93
0.96 and 0.97\%A for phenyl, methyl and methylene H-atoms respectively.
The C-bound methylene and phenyl H-atoms were refined using riding model
with <i>U</i>~iso~(H) = 1.2<i>U</i>~eq~(Carrier). The methyl H-atoms were
refined using riding model with <i>U</i>~iso~(H) =
1.5<i>U</i>~eq~(Carrier).

One of the n-butyl groups were found to be disordered in two positions
at occupancies of 0.782(16) and 0.218(16) respectively. A total of six
restraints have been used in the refinement. They are relating to
the anisotropic refinement of atom C31' using the isotropic restrains
of standard uncertainty of 0.01., six restraints for each atom.
The refinement command used was:
ISOR 0.01 0.02 C31'
The command is needed to restrain the thermal parameters of the atom C31'
within reasonable range.

Highest peak is 0.41 at (0.3899, 0.3586, 0.7181) [1.12\%A from C10]
Deepest hole is -0.37 at (0.1563, 0.5255, 0.0791) [0.82\%A from Cu1]
;

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S1 S 0.10537(12) 0.35834(8) -0.01477(6) 0.0573(3) Uani 1 1 d . . .
S2 S -0.02149(12) 0.35095(8) 0.15728(5) 0.0584(3) Uani 1 1 d . . .
O1 O 0.2799(3) 0.55317(19) 0.02773(14) 0.0556(7) Uani 1 1 d . . .
O2 O 0.6444(5) 1.0128(3) -0.1032(2) 0.1072(13) Uani 1 1 d . . .
O3 O 0.7362(4) 0.9347(3) -0.2002(2) 0.0937(11) Uani 1 1 d . . .
O4 O 0.1785(3) 0.5477(2) 0.17061(14) 0.0615(7) Uani 1 1 d . . .
O5 O 0.2564(7) 0.9794(3) 0.3879(2) 0.158(2) Uani 1 1 d . . .
O6 O 0.1703(6) 0.8912(3) 0.4863(2) 0.1350(17) Uani 1 1 d . . .
N1 N 0.3386(3) 0.4768(2) -0.08949(16) 0.0477(7) Uani 1 1 d . . .
N2 N 0.6611(4) 0.9342(3) -0.1404(2) 0.0689(10) Uani 1 1 d . . .
N3 N 0.2607(4) 0.3268(2) -0.14275(17) 0.0533(8) Uani 1 1 d . . .
N4 N 0.0975(4) 0.4442(2) 0.28196(16) 0.0529(8) Uani 1 1 d . . .
N5 N 0.2060(6) 0.8989(3) 0.4194(2) 0.0879(12) Uani 1 1 d . . .
N6 N 0.0210(4) 0.2716(2) 0.30187(17) 0.0566(8) Uani 1 1 d . B .
C1 C 0.3409(4) 0.5504(3) -0.0388(2) 0.0449(8) Uani 1 1 d . . .
C2 C 0.4328(4) 0.6487(3) -0.06438(19) 0.0451(8) Uani 1 1 d . . .
C3 C 0.4321(4) 0.7354(3) -0.0188(2) 0.0554(10) Uani 1 1 d . . .
H3 H 0.3799 0.7307 0.0286 0.066 Uiso 1 1 calc R . .
C4 C 0.5076(5) 0.8290(3) -0.0425(2) 0.0604(10) Uani 1 1 d . . .
H4 H 0.5066 0.8876 -0.0120 0.073 Uiso 1 1 calc R . .
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C5 C 0.5846(4) 0.8328(3) -0.1129(2) 0.0520(9) Uani 1 1 d . . .
C6 C 0.5903(5) 0.7477(3) -0.1587(2) 0.0599(10) Uani 1 1 d . . .
H6 H 0.6447 0.7523 -0.2055 0.072 Uiso 1 1 calc R . .
C7 C 0.5136(4) 0.6545(3) -0.1341(2) 0.0547(10) Uani 1 1 d . . .
H7 H 0.5163 0.5957 -0.1644 0.066 Uiso 1 1 calc R . .
C8 C 0.2453(4) 0.3926(3) -0.0842(2) 0.0469(9) Uani 1 1 d . . .
C9 C 0.3776(5) 0.3477(3) -0.2044(2) 0.0728(12) Uani 1 1 d . . .
H9A H 0.4111 0.2797 -0.2250 0.087 Uiso 1 1 calc R . .
H9B H 0.4680 0.3789 -0.1832 0.087 Uiso 1 1 calc R . .
C10 C 0.3066(7) 0.4283(5) -0.2713(3) 0.1013(17) Uani 1 1 d . . .
H10A H 0.2136 0.3976 -0.2902 0.122 Uiso 1 1 calc R . .
H10B H 0.2752 0.4961 -0.2499 0.122 Uiso 1 1 calc R . .
C11 C 0.4100(8) 0.4515(6) -0.3357(4) 0.129(2) Uani 1 1 d . . .
H11A H 0.4472 0.3839 -0.3556 0.155 Uiso 1 1 calc R . .
H11B H 0.4995 0.4879 -0.3183 0.155 Uiso 1 1 calc R . .
C12 C 0.3297(9) 0.5226(5) -0.3996(3) 0.144(3) Uani 1 1 d . . .
H12A H 0.3970 0.5290 -0.4442 0.216 Uiso 1 1 calc R . .
H12B H 0.3064 0.5934 -0.3823 0.216 Uiso 1 1 calc R . .
H12C H 0.2347 0.4905 -0.4129 0.216 Uiso 1 1 calc R . .
C13 C 0.1529(5) 0.2413(3) -0.1538(2) 0.0582(10) Uani 1 1 d . . .
H13A H 0.1441 0.2340 -0.2089 0.070 Uiso 1 1 calc R . .
H13B H 0.0507 0.2639 -0.1349 0.070 Uiso 1 1 calc R . .
C14 C 0.1980(5) 0.1303(3) -0.1138(2) 0.0627(11) Uani 1 1 d . . .
H14A H 0.2938 0.1026 -0.1367 0.075 Uiso 1 1 calc R . .
H14B H 0.2170 0.1376 -0.0595 0.075 Uiso 1 1 calc R . .
C15 C 0.0708(5) 0.0503(3) -0.1212(3) 0.0693(11) Uani 1 1 d . . .
H15A H 0.0531 0.0429 -0.1757 0.083 Uiso 1 1 calc R . .
H15B H -0.0251 0.0792 -0.0993 0.083 Uiso 1 1 calc R . .
C16 C 0.1094(6) -0.0615(4) -0.0811(3) 0.0875(15) Uani 1 1 d . . .
H16A H 0.0203 -0.1057 -0.0824 0.131 Uiso 1 1 calc R . .
H16B H 0.1368 -0.0543 -0.0283 0.131 Uiso 1 1 calc R . .
H16C H 0.1955 -0.0952 -0.1073 0.131 Uiso 1 1 calc R . .
C17 C 0.1460(4) 0.5324(3) 0.2417(2) 0.0482(9) Uani 1 1 d . . .
C18 C 0.1678(4) 0.6266(3) 0.28922(19) 0.0450(8) Uani 1 1 d . . .
C19 C 0.2114(4) 0.7257(3) 0.2533(2) 0.0529(9) Uani 1 1 d . . .
H19 H 0.2310 0.7322 0.2003 0.063 Uiso 1 1 calc R . .
C20 C 0.2257(5) 0.8142(3) 0.2957(2) 0.0613(11) Uani 1 1 d . . .
H20 H 0.2548 0.8804 0.2717 0.074 Uiso 1 1 calc R . .
C21 C 0.1965(5) 0.8033(3) 0.3736(2) 0.0607(10) Uani 1 1 d . . .
C22 C 0.1562(6) 0.7062(3) 0.4112(2) 0.0734(13) Uani 1 1 d . . .
H22 H 0.1391 0.6999 0.4644 0.088 Uiso 1 1 calc R . .
C23 C 0.1419(5) 0.6188(3) 0.3682(2) 0.0681(12) Uani 1 1 d . . .
H23 H 0.1140 0.5526 0.3929 0.082 Uiso 1 1 calc R . .
C24 C 0.0393(4) 0.3581(3) 0.2506(2) 0.0494(9) Uani 1 1 d . . .
C25 C 0.0695(5) 0.2742(3) 0.3827(2) 0.0663(12) Uani 1 1 d . . .
H25A H 0.0123 0.2210 0.4147 0.080 Uiso 1 1 calc R . .
H25B H 0.0417 0.3454 0.3999 0.080 Uiso 1 1 calc R . .
C26 C 0.2400(6) 0.2512(4) 0.3945(2) 0.0788(13) Uani 1 1 d . . .
H26A H 0.2975 0.3100 0.3688 0.095 Uiso 1 1 calc R . .
H26B H 0.2714 0.1847 0.3713 0.095 Uiso 1 1 calc R . .
C27 C 0.2805(8) 0.2393(5) 0.4804(3) 0.115(2) Uani 1 1 d . . .
H27A H 0.2528 0.3072 0.5025 0.137 Uiso 1 1 calc R . .
H27B H 0.2173 0.1836 0.5061 0.137 Uiso 1 1 calc R . .
C28 C 0.4432(9) 0.2111(6) 0.4967(4) 0.153(3) Uani 1 1 d . . .
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H28A H 0.4603 0.2097 0.5514 0.230 Uiso 1 1 calc R . .
H28B H 0.5074 0.2643 0.4701 0.230 Uiso 1 1 calc R . .
H28C H 0.4697 0.1407 0.4793 0.230 Uiso 1 1 calc R . .
C29 C -0.0512(5) 0.1721(3) 0.2829(2) 0.0672(12) Uani 1 1 d . . .
H29A H 0.0009 0.1101 0.3112 0.081 Uiso 1 1 calc R A 1
H29B H -0.0373 0.1638 0.2280 0.081 Uiso 1 1 calc R A 1
C30 C -0.2243(6) 0.1730(4) 0.3028(3) 0.0814(14) Uani 0.782(16) 1 d P B 1
H30A H -0.2357 0.1841 0.3574 0.098 Uiso 0.782(16) 1 calc PR B 1
H30B H -0.2740 0.2356 0.2742 0.098 Uiso 0.782(16) 1 calc PR B 1
C31 C -0.3141(11) 0.0744(7) 0.2875(5) 0.083(3) Uani 0.782(16) 1 d P B 1
H31A H -0.4240 0.0891 0.2977 0.099 Uiso 0.782(16) 1 calc PR B 1
H31B H -0.3023 0.0607 0.2334 0.099 Uiso 0.782(16) 1 calc PR B 1
C32 C -0.2593(15) -0.0244(7) 0.3367(5) 0.121(5) Uani 0.782(16) 1 d P B 1
H32A H -0.3195 -0.0850 0.3257 0.181 Uiso 0.782(16) 1 calc PR B 1
H32B H -0.2719 -0.0115 0.3904 0.181 Uiso 0.782(16) 1 calc PR B 1
H32C H -0.1512 -0.0404 0.3258 0.181 Uiso 0.782(16) 1 calc PR B 1
C30' C -0.2243(6) 0.1730(4) 0.3028(3) 0.0814(14) Uani 0.218(16) 1 d P B 2
H30C H -0.2872 0.2120 0.2626 0.098 Uiso 0.218(16) 1 calc PR B 2
H30D H -0.2471 0.2021 0.3522 0.098 Uiso 0.218(16) 1 calc PR B 2
C31' C -0.244(4) 0.038(3) 0.3063(19) 0.079(10) Uani 0.218(16) 1 d PU B 2
H31C H -0.2189 0.0104 0.2566 0.095 Uiso 0.218(16) 1 calc PR B 2
H31D H -0.1777 0.0004 0.3455 0.095 Uiso 0.218(16) 1 calc PR B 2
C32' C -0.415(4) 0.023(3) 0.3266(18) 0.130(15) Uani 0.218(16) 1 d P B 2
H32D H -0.4386 -0.0522 0.3254 0.195 Uiso 0.218(16) 1 calc PR B 2
H32E H -0.4793 0.0664 0.2898 0.195 Uiso 0.218(16) 1 calc PR B 2
H32F H -0.4363 0.0456 0.3776 0.195 Uiso 0.218(16) 1 calc PR B 2

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S1 0.0615(6) 0.0526(6) 0.0607(6) -0.0149(5) 0.0132(5) -0.0213(5)
S2 0.0679(7) 0.0570(6) 0.0511(6) 0.0018(4) 0.0017(5) -0.0247(5)
O1 0.0652(17) 0.0548(16) 0.0491(15) -0.0093(12) 0.0126(13) -0.0245(13)
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O4 0.087(2) 0.0543(16) 0.0459(15) -0.0078(12) 0.0144(13) -0.0288(14)
O5 0.329(7) 0.059(2) 0.091(3) -0.010(2) -0.011(3) -0.055(3)
O6 0.230(5) 0.100(3) 0.084(3) -0.045(2) 0.036(3) -0.050(3)
N1 0.0491(18) 0.0453(18) 0.0487(17) -0.0023(14) 0.0036(14) -0.0070(14)
N2 0.072(2) 0.056(2) 0.078(3) 0.0060(19) 0.005(2) -0.0201(18)
N3 0.058(2) 0.0482(19) 0.0552(19) -0.0120(15) 0.0060(15) -0.0073(15)
N4 0.071(2) 0.0414(18) 0.0468(17) -0.0006(14) 0.0033(15) -0.0119(15)
N5 0.136(4) 0.061(3) 0.070(3) -0.011(2) -0.007(3) -0.018(2)
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C1 0.040(2) 0.043(2) 0.050(2) 0.0018(17) -0.0017(16) -0.0013(16)
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C7 0.062(2) 0.048(2) 0.055(2) -0.0066(17) 0.0097(19) -0.0082(18)
C8 0.045(2) 0.045(2) 0.050(2) -0.0016(17) -0.0025(16) -0.0009(17)
C9 0.081(3) 0.065(3) 0.075(3) -0.023(2) 0.023(2) -0.010(2)
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C11 0.138(6) 0.134(6) 0.113(5) -0.001(4) 0.031(4) 0.006(4)
C12 0.199(8) 0.128(6) 0.099(5) 0.017(4) 0.008(5) 0.015(5)
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C14 0.066(3) 0.051(2) 0.073(3) -0.015(2) -0.006(2) -0.001(2)
C15 0.078(3) 0.062(3) 0.071(3) -0.012(2) 0.001(2) -0.015(2)
C16 0.118(4) 0.063(3) 0.083(3) -0.007(2) -0.001(3) -0.016(3)
C17 0.050(2) 0.046(2) 0.049(2) -0.0028(17) 0.0020(17) -0.0060(17)
C18 0.047(2) 0.040(2) 0.048(2) -0.0022(15) -0.0008(16) -0.0070(16)
C19 0.064(3) 0.049(2) 0.045(2) 0.0017(17) 0.0009(18) -0.0109(19)
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C29 0.097(3) 0.043(2) 0.062(3) -0.0021(18) 0.012(2) -0.015(2)
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C31 0.086(6) 0.086(6) 0.077(5) -0.005(4) 0.011(4) -0.031(5)
C32 0.192(12) 0.073(6) 0.099(6) 0.005(4) 0.007(6) -0.057(6)
C30' 0.096(4) 0.076(3) 0.074(3) -0.005(2) 0.016(3) -0.028(3)
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PROBLEM: Number of Uiso or Uij Restrained Atom Sites .... 1
RESPONSE: Atom C31' was refined with the isotropic restrains
of standard uncertainty of 0.01., six restraints for each atom.
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PROBLEM: Note: Number of Least-Squares Restraints ....... 6
RESPONSE: Atom C31' was refined with the isotropic restrains
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PROBLEM: The su's on the Cell Angles are Equal .......... 0.00400 Deg.
RESPONSE: It was accidental that The su's on the cell angles are equal.
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PROBLEM: Note: Main Residue Disorder ................... 6 Perc.
RESPONSE: One of the n-butyl groups were found to be disordered in two
positions at occupancies of 0.782(16) and 0.218(16) respectively.

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_publ_contact_author_email             'Sohail262001@yahoo.com'
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# TITLE AND AUTHOR LIST

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# copper (II) complex,
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Department of Chemistry, Research Complex,
Allama Iqbal Open Unicversity,
Islamabad-44000,
Pakistan
;
.
'sohail262002@yahoo.com'
'Wong, Wing-Tak'
;
Department of Chemistry
The University of Hong Kong
Pokfulam Road, Pokfulam,
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P. R. CHINA
;
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There are two molecules of the copper(II) complex,
C~32~H~44~CuN~6~O~6~S~2~, in
the unit cell.

One of the butyl groups was found to be disordered in two positions
at occupancies of 0.782(16) and 0.218(16) respectively.


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Fig. 1. The title molecule was shown at 50% probability thermal ellipsoids with the atom numbering scheme (only the major component was shown).

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The crystal of the copper complex, C~32~H~44~CuN~6~O~6~S~2~, a dark-brown block,
having approximate dimensions of 0.08 mm x 0.10 mm x 0.50 mm was
mounted on glass fiber. All measurements were made on a Bruker
SMART 1000 CCD detector with graphite monochromated Mo---K\a radiation. The crystal-to-detector distance was 50.00 mm.

Indexing was performed from 60 images that were exposed for 10 s for a preliminary unit cell determination. Of which, 52 out of total of 65 reflections were successfully indexed. The crystal-to-detector distance was
50.00 mm.

Cell constants and an orientation matrix for data collection corresponded to a
primitive monoclinic cell with dimensions: a = 8.585(2)\%A,
b = 12.347(3)\%A, c = 17.326(4)\%A, V = 1828.8(8)\%A^3^ \a =85.325(4)\%
\b = 89.305(4)\% \g = 87.573(4)\%.

For Z = 2 and F.W. = 736.40, the calculated density is 1.337
g/cm^3^.
Based on a statistical analysis of intensity distribution, and the
successful
solution and refinement of the structure, the space group was determined
to
be: P -1 (#2).

The data were collected at a temperature of 27(1)\%C to a maximum 2\q
value of
50.0\%. A total of 1421 oscillation images were collected in 4 runs. A
sweep
of data was done using \w scans from 330.0 to 148.2\% in -0.3\% step, at
\c =
54.7\% and \f = 0.0\%. The exposure rate was 35.0 [sec./\%]. The detector
swing angle was -30.00\%. A second sweep was performed using \w scans from
330.0 to 199.5\% in -0.3\% step, at \c = 54.7\% and \f = 90.0\%. The
exposure
rate was 35.0 [sec./\%]. The detector swing angle was -30.00\%. A third
sweep
was performed using \w scans from 330.0 to 261.0\% in -0.3\% step, at \c =
54.7\% and \f = 180.0\%. The exposure rate was 35.0 [sec./\%]. The
detector
swing angle was -30.00\%. A last sweep was performed using \w scans from
330.0
to 285.0\% in -0.3\% step, at \c = 54.7\% and \f = 270.0\%. The exposure
rate was 35.0 [sec./\%]. The detector swing angle was -30.00\%. The
crystal-to-detector distance was 50.00 mm.

Of the 10157 reflections that were collected, 6286 reflections were
unique.
(R~int~ = 0.0211); equivalent reflections were merged.
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_publ_section_exptl_refinement
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The structure was solved by Patterson methods (DIRDIF-99 (Beurskens
et al., 1999)) and expanded using Fourier techniques. All non-H atoms were
refined anisotropically.

The C-bound H atoms are all placed at geometrical positions with C---H =
0.93
0.96 and 0.97\%A for phenyl, methyl and methylene H-atoms respectively.
The C-bound methylene and phenyl H-atoms were refined using riding model
with U~iso~(H) = 1.2U~eq~(Carrier). The methyl H-atoms were
refined using riding model with U~iso~(H) =
1.5U~eq~(Carrier).

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One of the n-butyl groups were found to be disordered in two positions
at occupancies of 0.782(16) and 0.218(16) respectively. A total of six
restraints have been used in the refinement. They are relating to
the anisotropic refinement of atom C31' using the isotropic restrains
of standard uncertainty of 0.01., six restraints for each atom.

Highest peak is 0.41 at (0.3899, 0.3586, 0.7181) [1.12\%A from C10]
Deepest hole is -0.37 at (0.1563, 0.5255, 0.0791) [0.82\%A from Cu1]
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