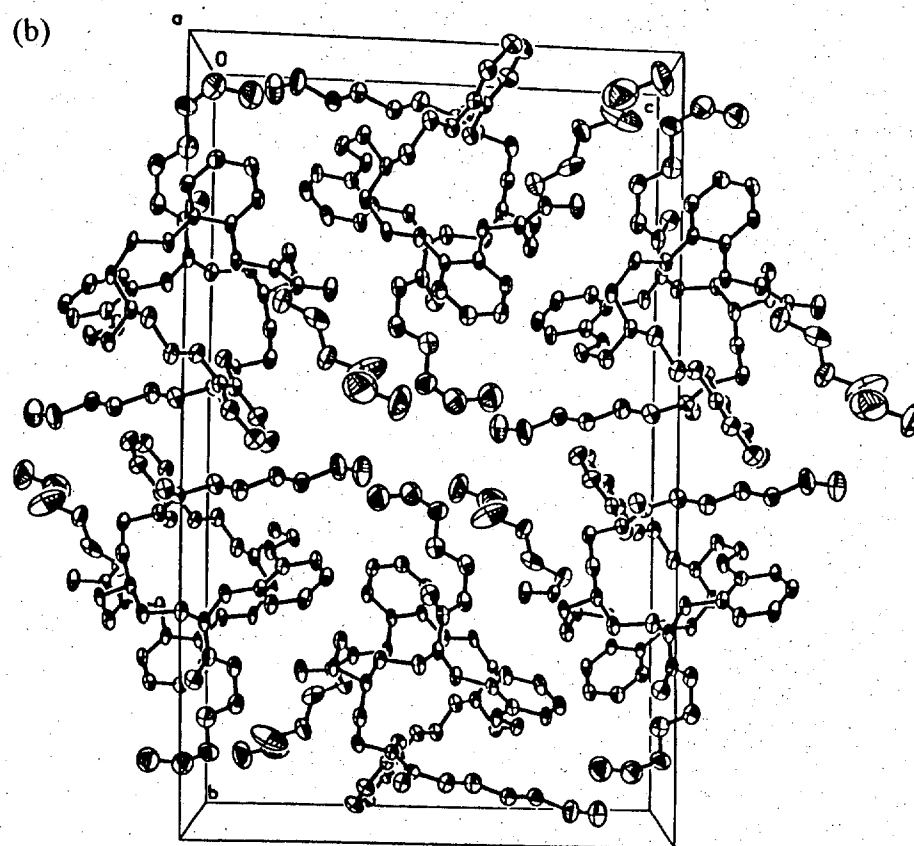
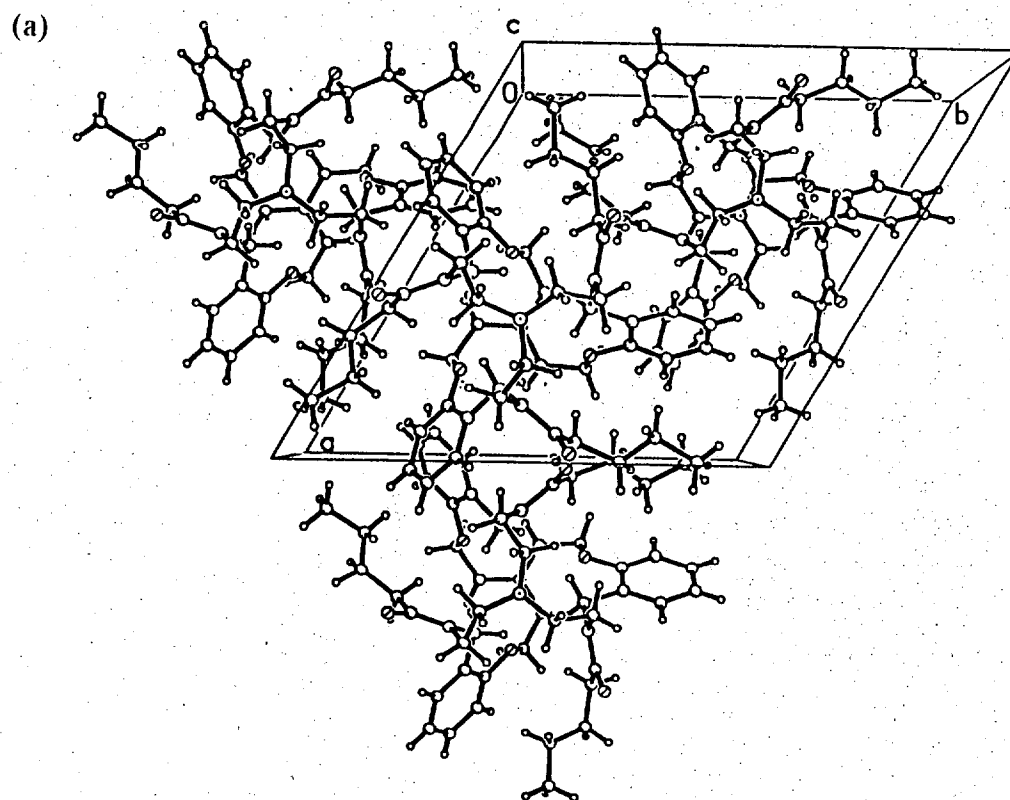


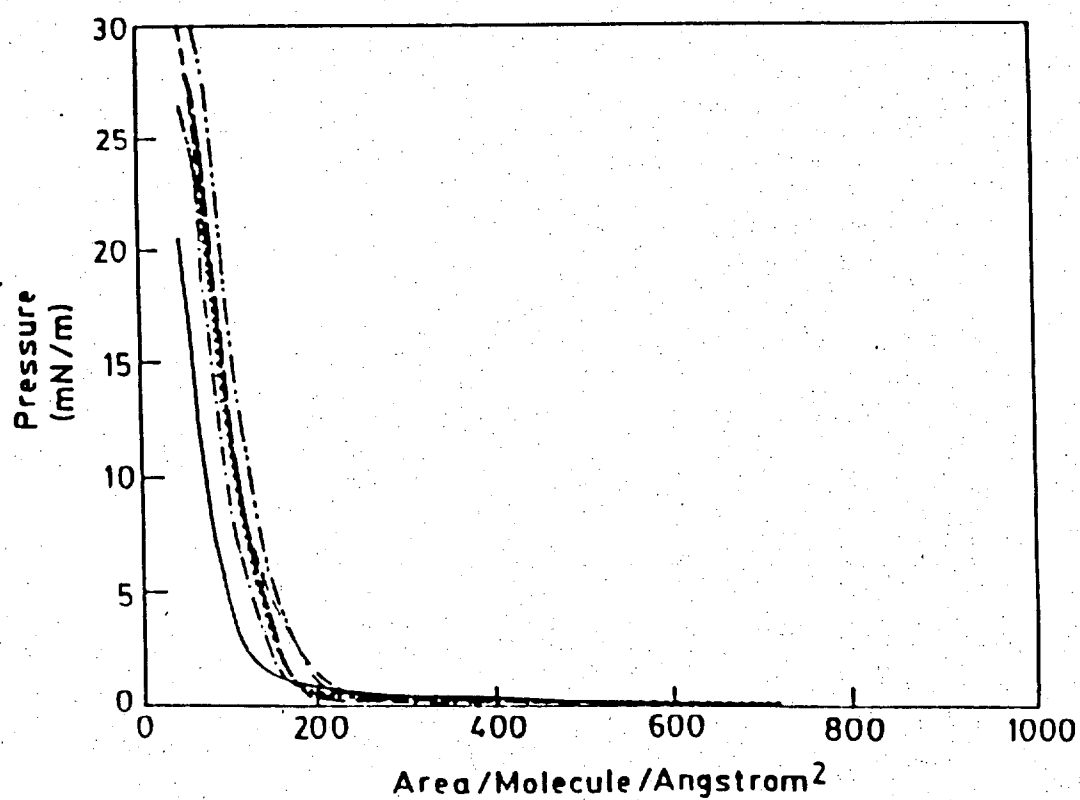
Table 1. Crystal data and structure refinement for  $L_6$  and  $L_5$ 

|                                                       | $L_6$                                                               | $L_5$                                                               |
|-------------------------------------------------------|---------------------------------------------------------------------|---------------------------------------------------------------------|
| Empirical Formula                                     | $C_{48}H_{69}N_5O_6$                                                | $C_{54}H_{80}N_5O_6$                                                |
| Formula Weight                                        | 811.07                                                              | 895.23                                                              |
| Crystal system                                        | Trigonal                                                            | Monoclinic                                                          |
| Space group                                           | $P31c$                                                              | $P2_1/c$                                                            |
| $a/\text{\AA}$                                        | 15.118(2)                                                           | 10.091(3)                                                           |
| $b/\text{\AA}$                                        | 15.118(2)                                                           | 29.994(8)                                                           |
| $c/\text{\AA}$                                        | 11.734(2)                                                           | 18.174(5)                                                           |
| $\alpha/^\circ$                                       | 90                                                                  | 90                                                                  |
| $\beta/^\circ$                                        | 90                                                                  | 94.404(6)                                                           |
| $\gamma/^\circ$                                       | 120                                                                 | 90                                                                  |
| Volume/ $\text{\AA}^3$                                | 2322.5(6)                                                           | 5484(3)                                                             |
| Z                                                     | 2                                                                   | 4                                                                   |
| $D_c/\text{Mg m}^{-3}$                                | 1.160                                                               | 1.084                                                               |
| Absorption coefficient<br>( $\mu$ )/ $\text{mm}^{-1}$ | 0.066                                                               | 0.070                                                               |
| Crystal size/mm                                       | 0.14 x 0.2 x 0.23                                                   | 0.01 x 0.1 x 0.2                                                    |
| Limiting indices                                      | $-18 \leq h \leq 18$<br>$-18 \leq k \leq 18$<br>$-14 \leq l \leq 4$ | $-8 \leq h \leq 11$<br>$-36 \leq k \leq 12$<br>$-23 \leq l \leq 10$ |
| Reflections collected                                 | 13592                                                               | 15444                                                               |
| R                                                     | 0.033                                                               | 0.1048                                                              |
| $R'$                                                  | 0.062                                                               | 0.2660                                                              |
| Goodness of fit on $F^2$                              | 0.813                                                               | 0.925                                                               |
| Largest and mean shift/e.s.d.                         | 0.001, 0.0006                                                       |                                                                     |

Details in common:  $\theta$ -2 $\theta$  scans, range  $0.80 + 0.35 \tan \theta$ ; 2 $\theta$  range 2-50 $^\circ$ ;  
 $R = \sum ||F_o| - |F_c|| / \sum |F_o|$ .  $R' = [ \sum \omega (|F_o| - |F_c|)^2 / \sum \omega (F_o)^2 ]^{1/2}$ ,  $\omega = 1/\sigma(F)$ .

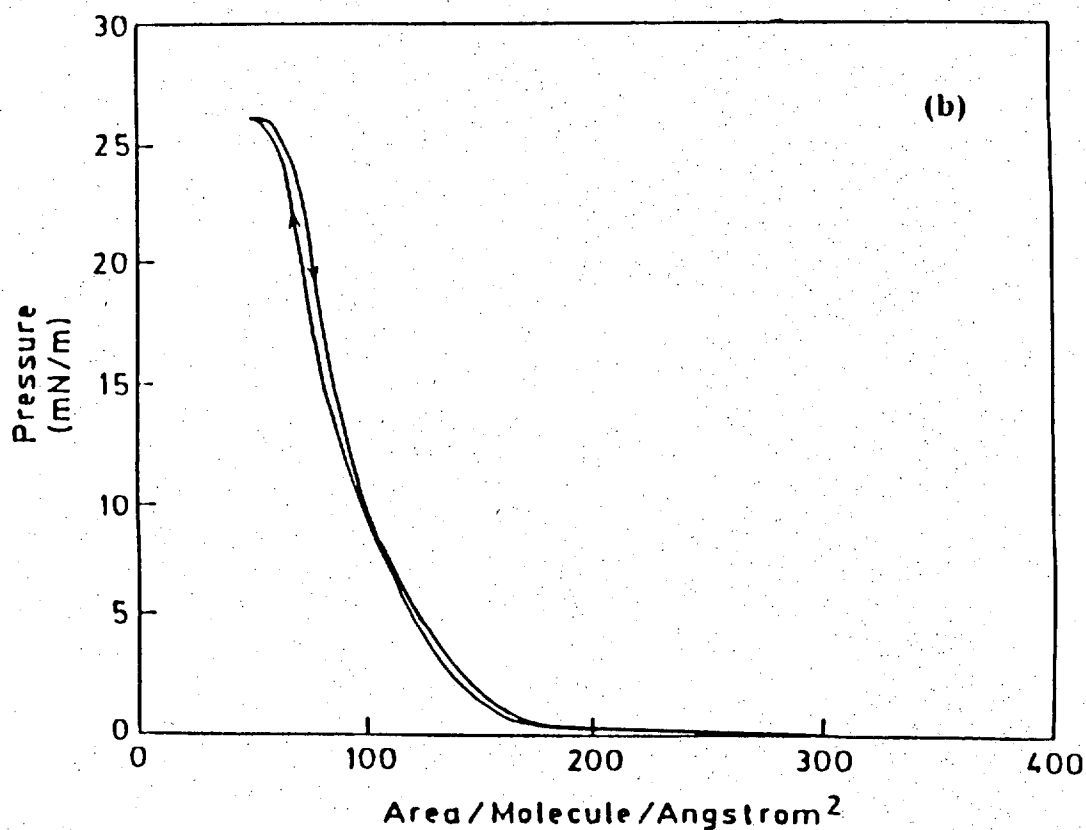
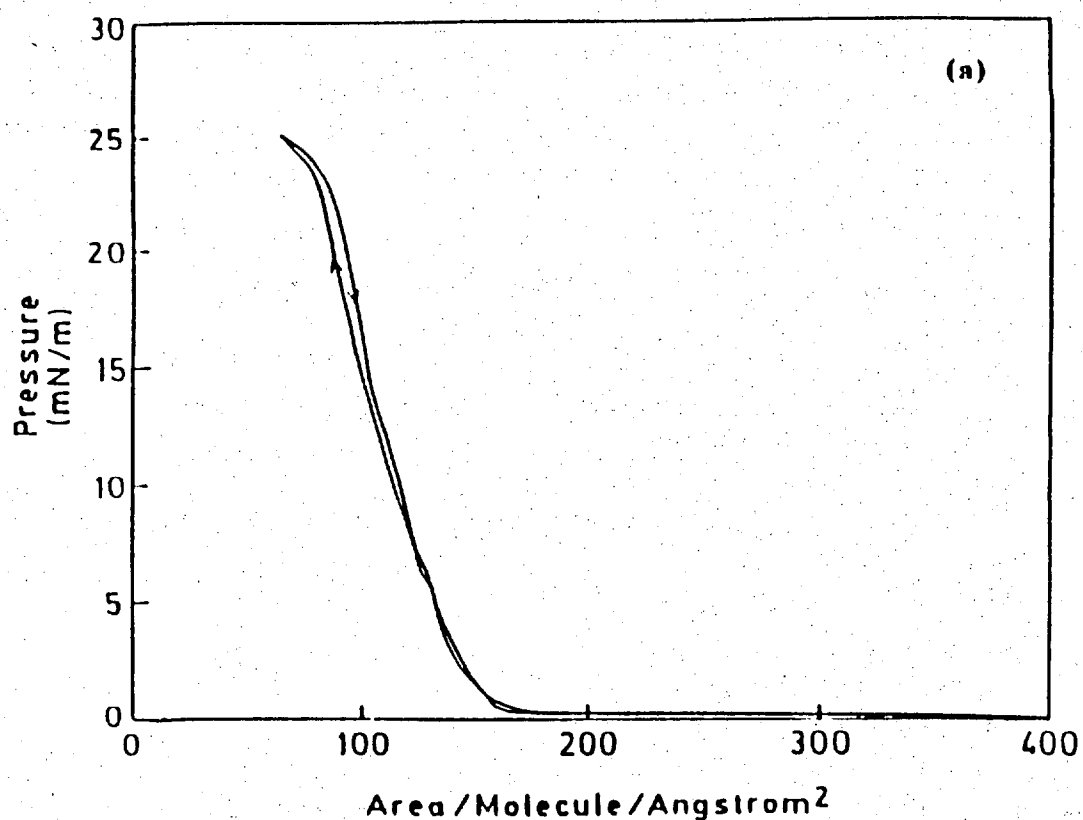


Packing of (a)  $L_5$  and (b)  $L_6$

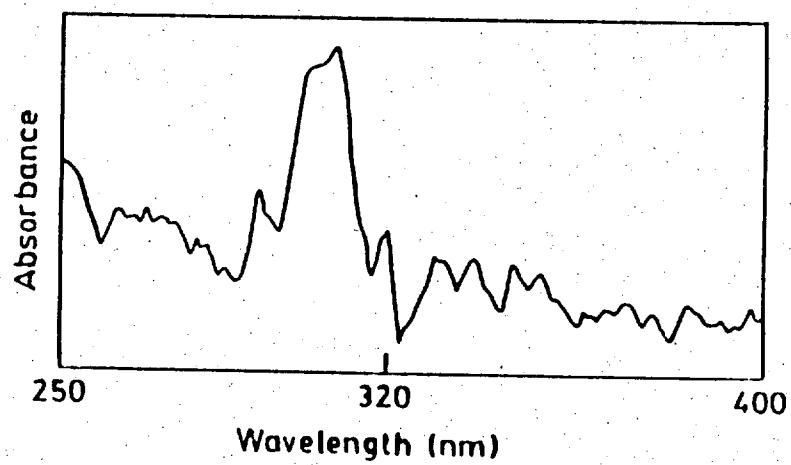


Pressure-area ( $\Pi$ -A) isotherms for Cu(II)-complex of  $L_1 - L_6$ , at 298 K.

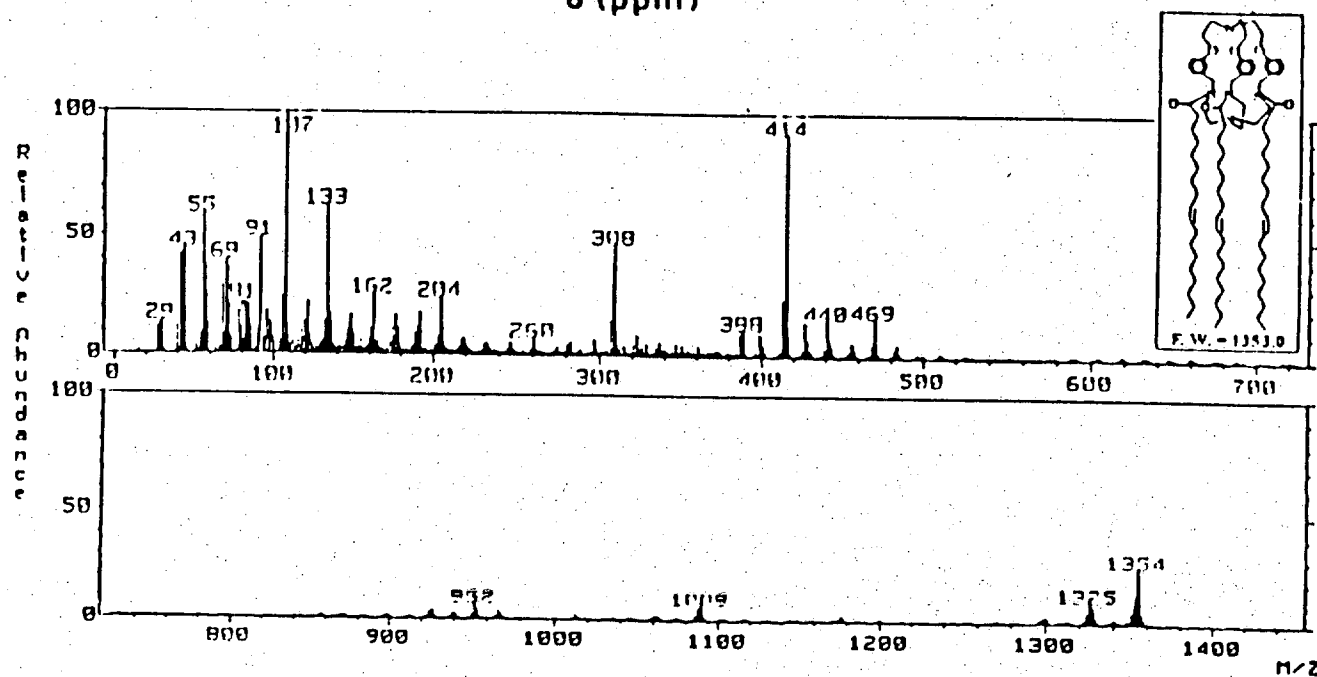
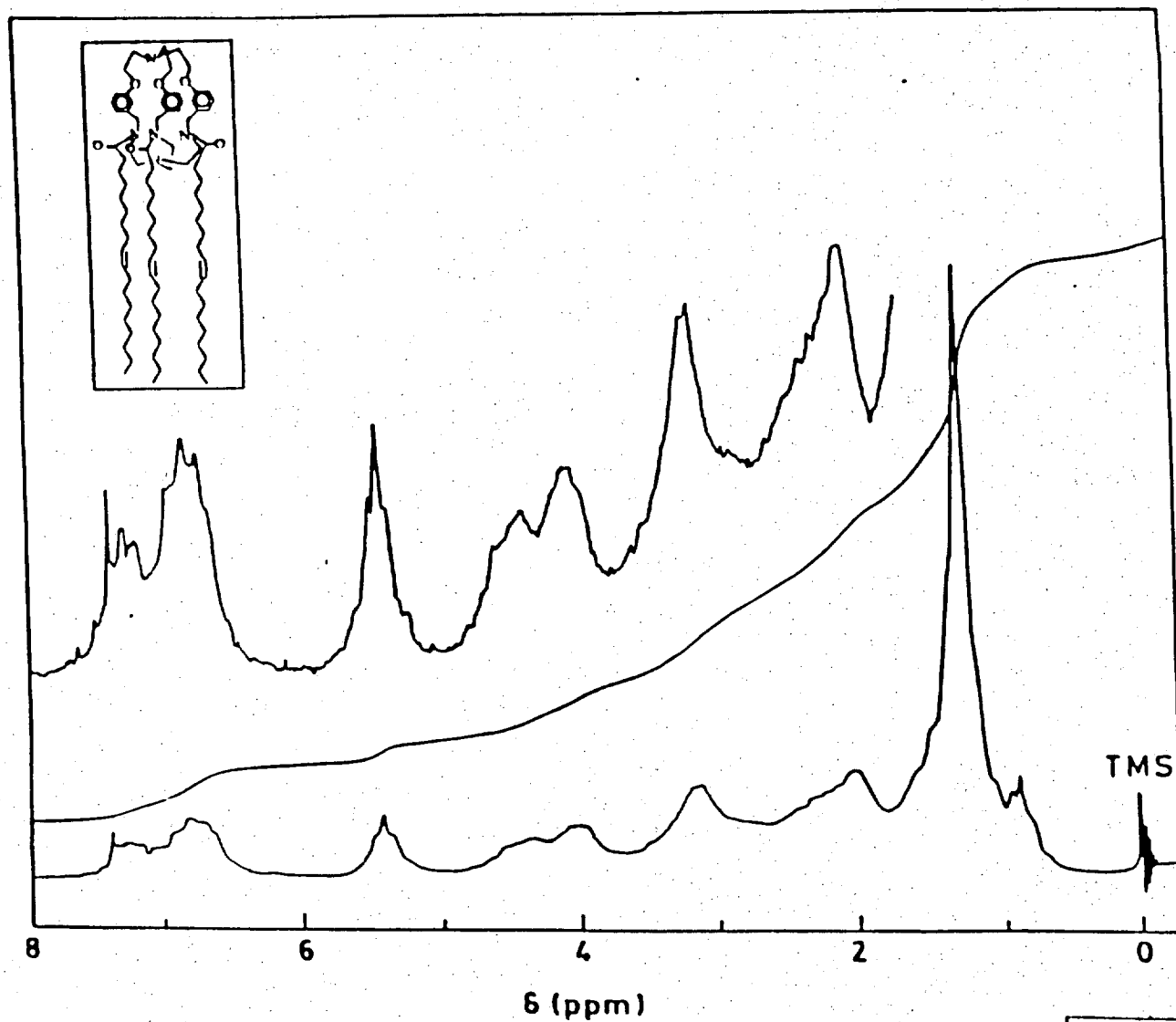
$L_1$  (---),  $L_2$  (-•-),  $L_3$  (•••),  $L_4$  (-••-),  $L_5$  (- - - -),  $L_6$  (—)

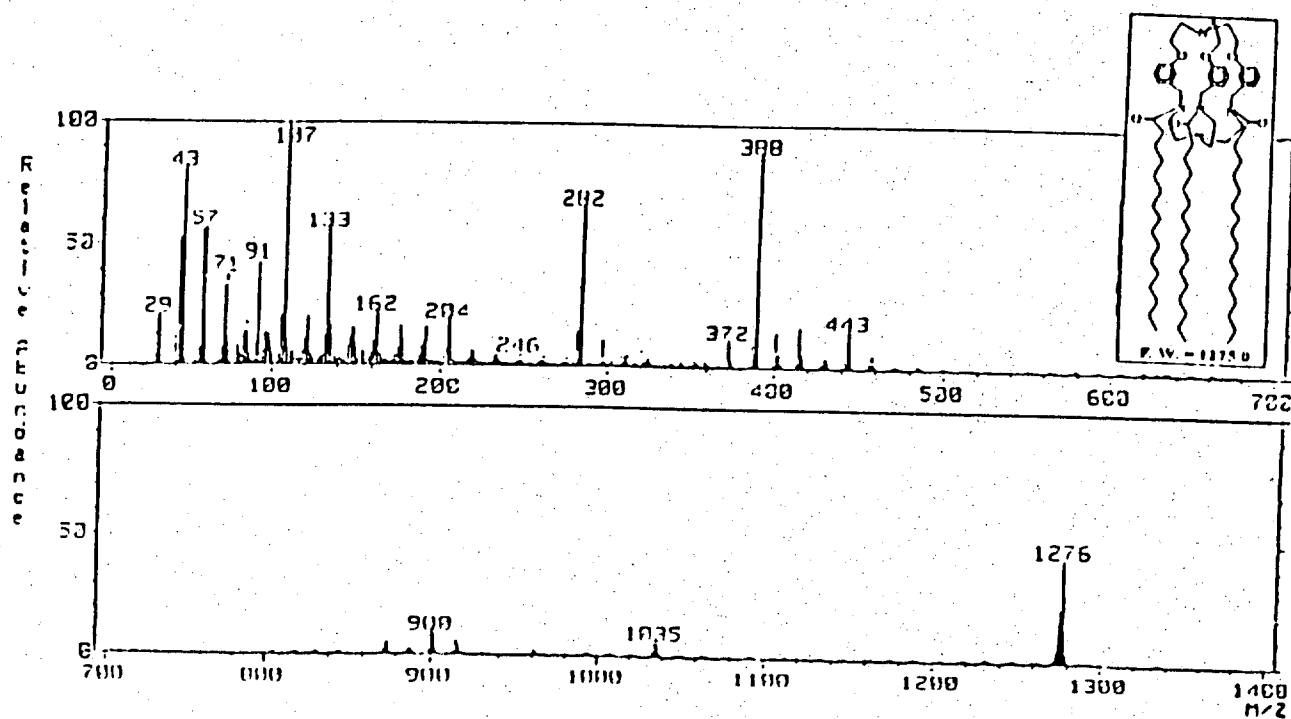
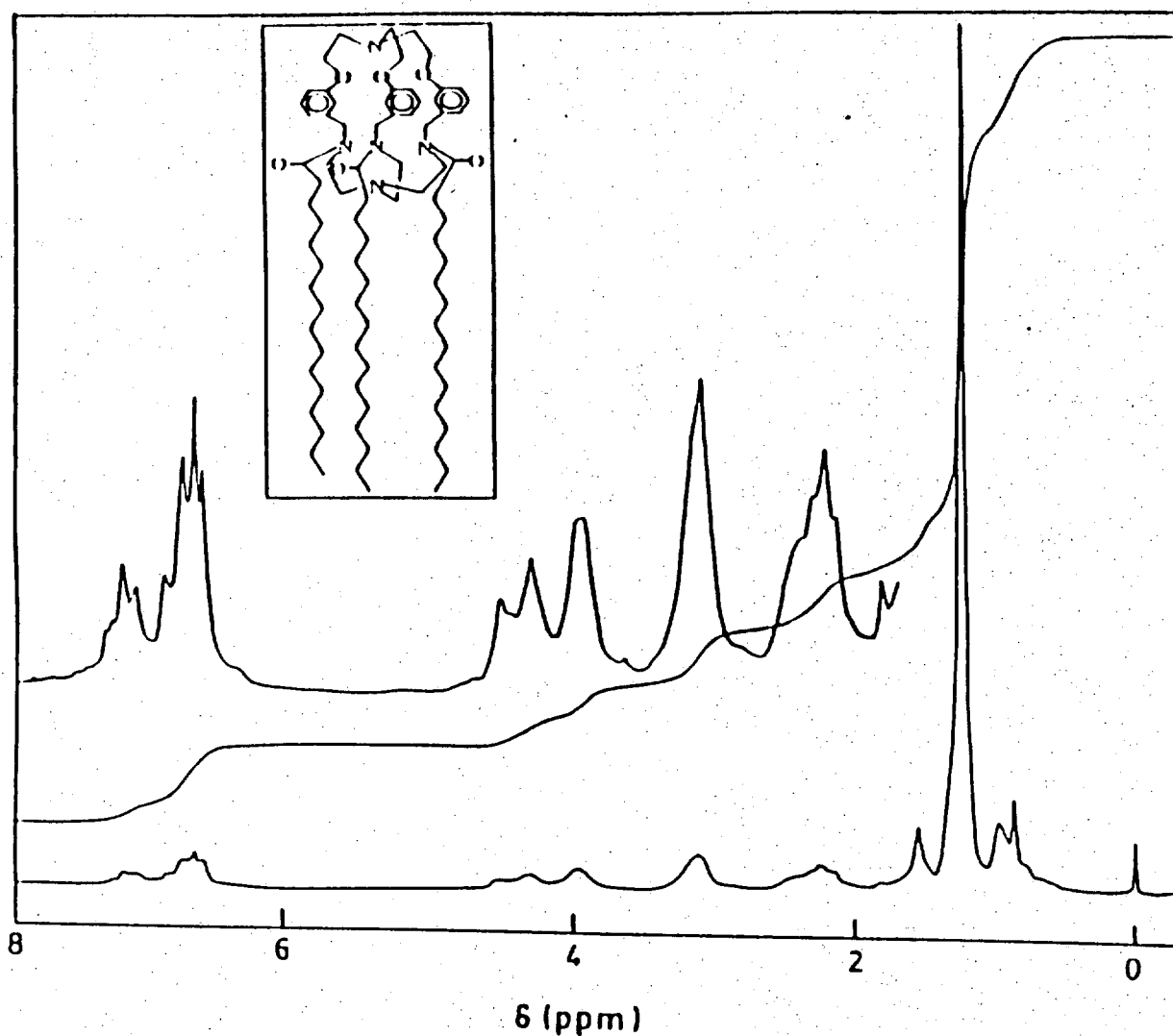


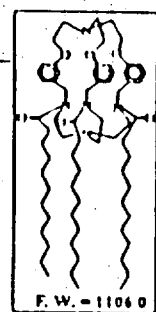
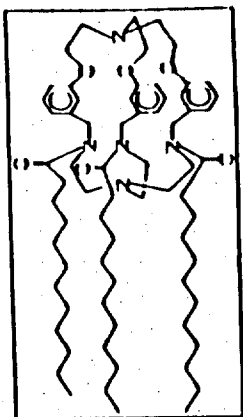
Representative successive compression and expansion cycles (hysteresis) with a monolayer of (a)  $L_2$  and (b) Cu-complex of  $L_2$  at 298 K, showing the reversibility of the compression.

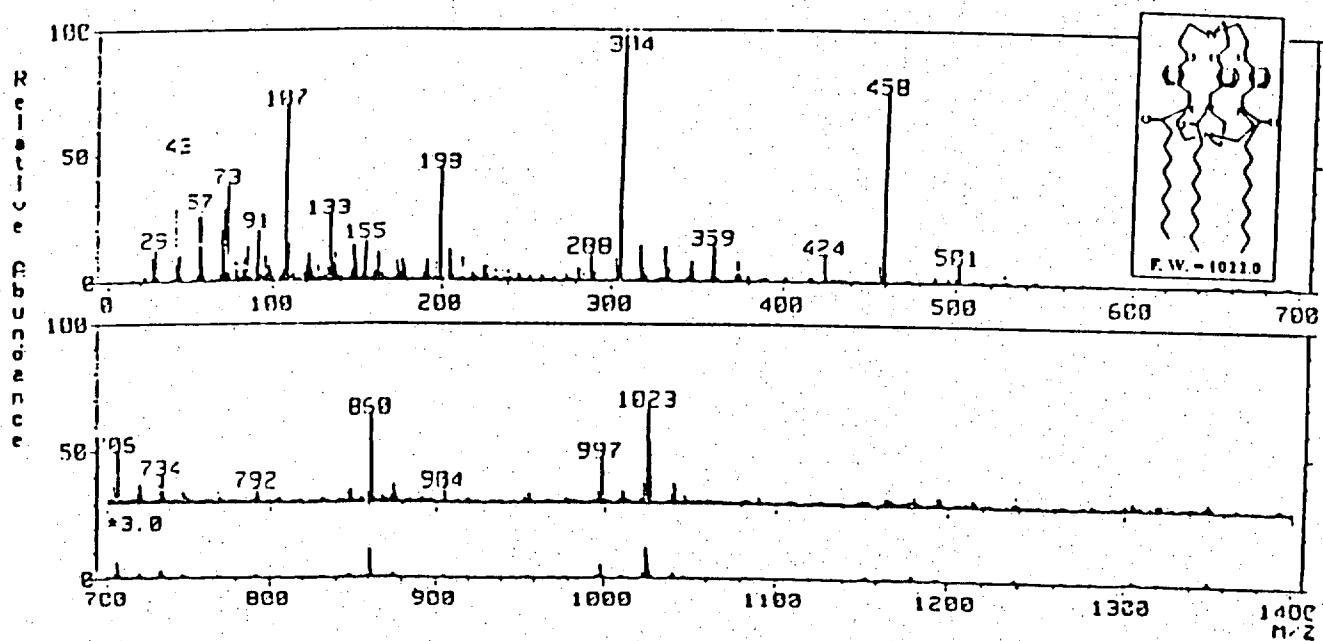
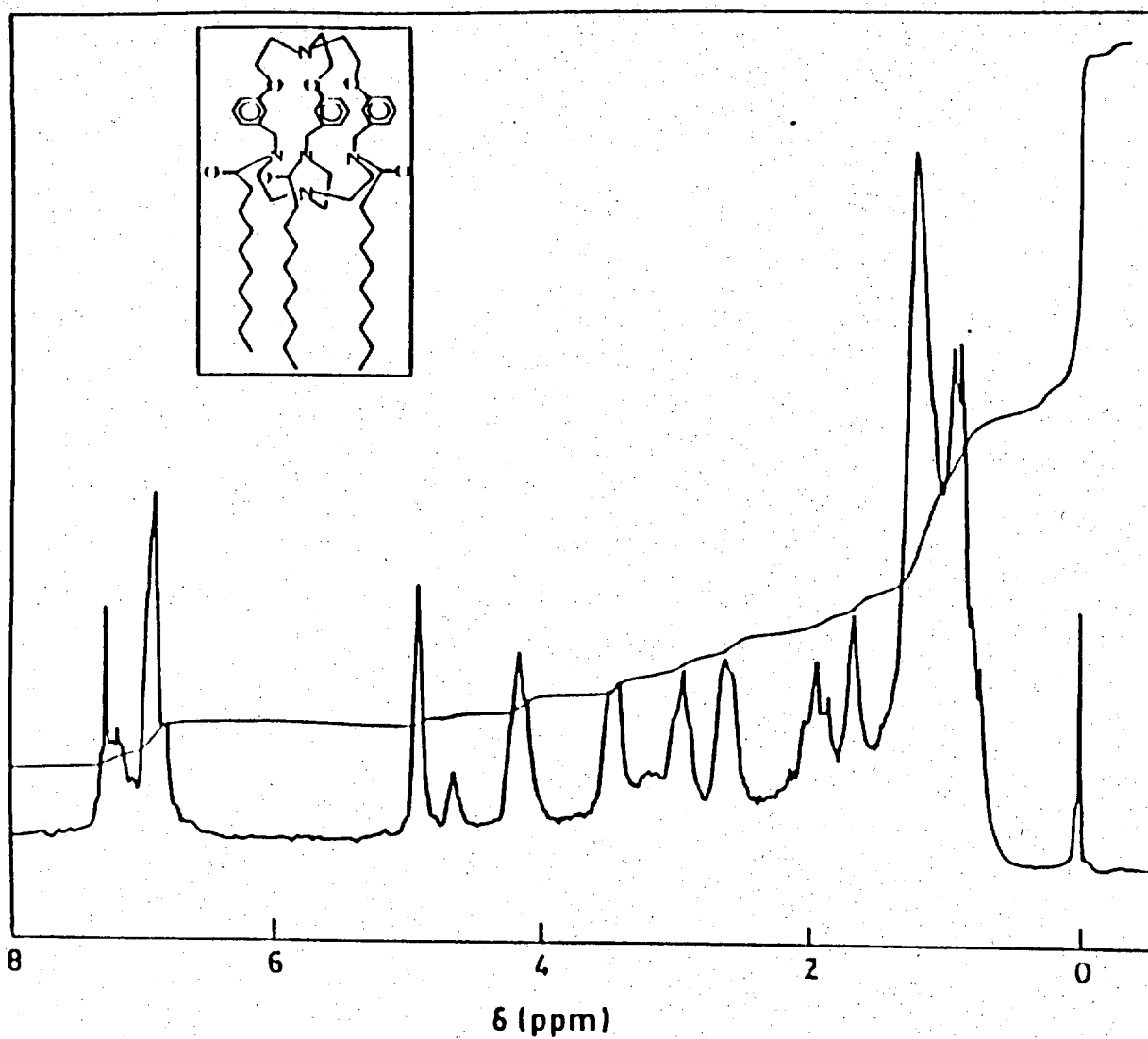


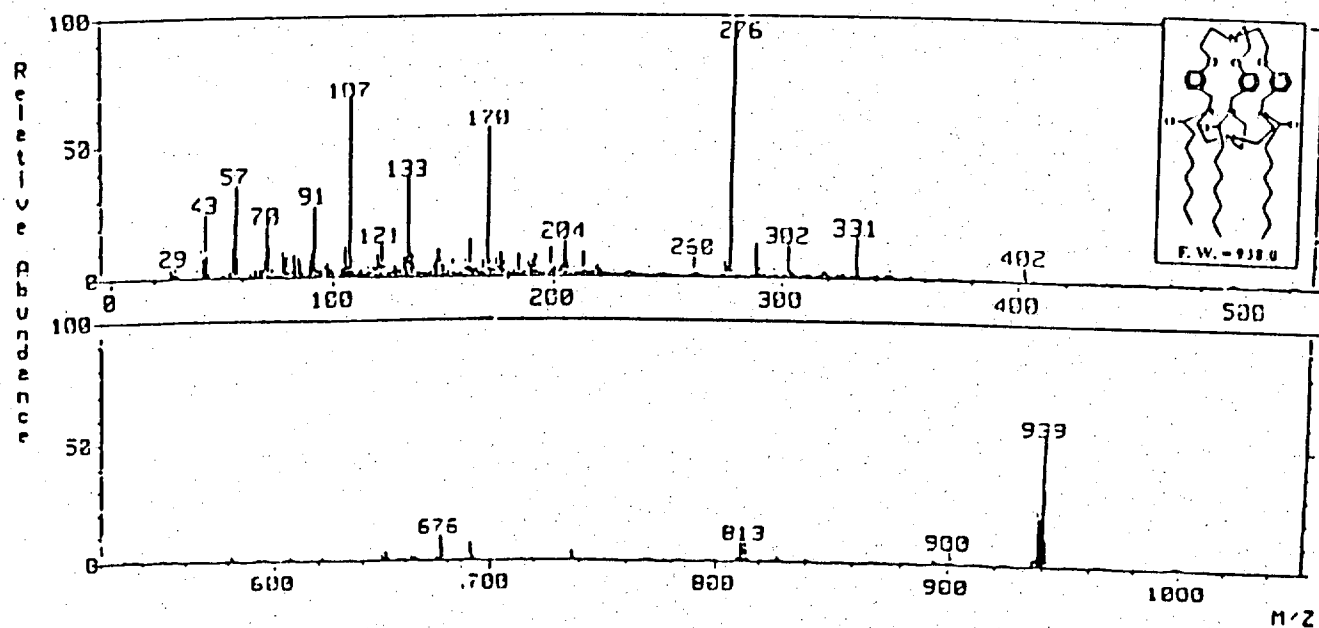
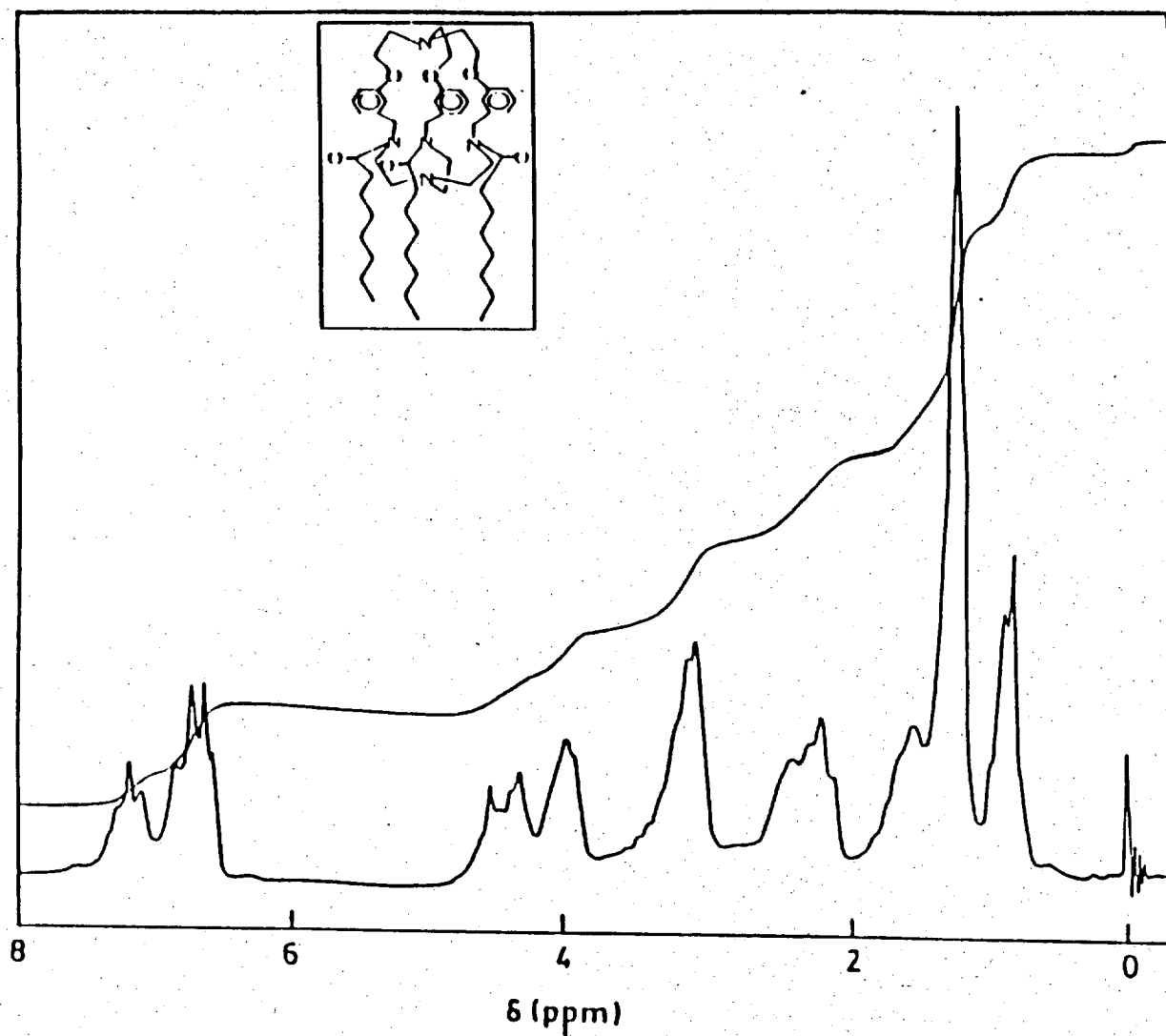
UV-Vis absorption spectra of the LB-film deposited onto quartz plate of  $L_2$ .

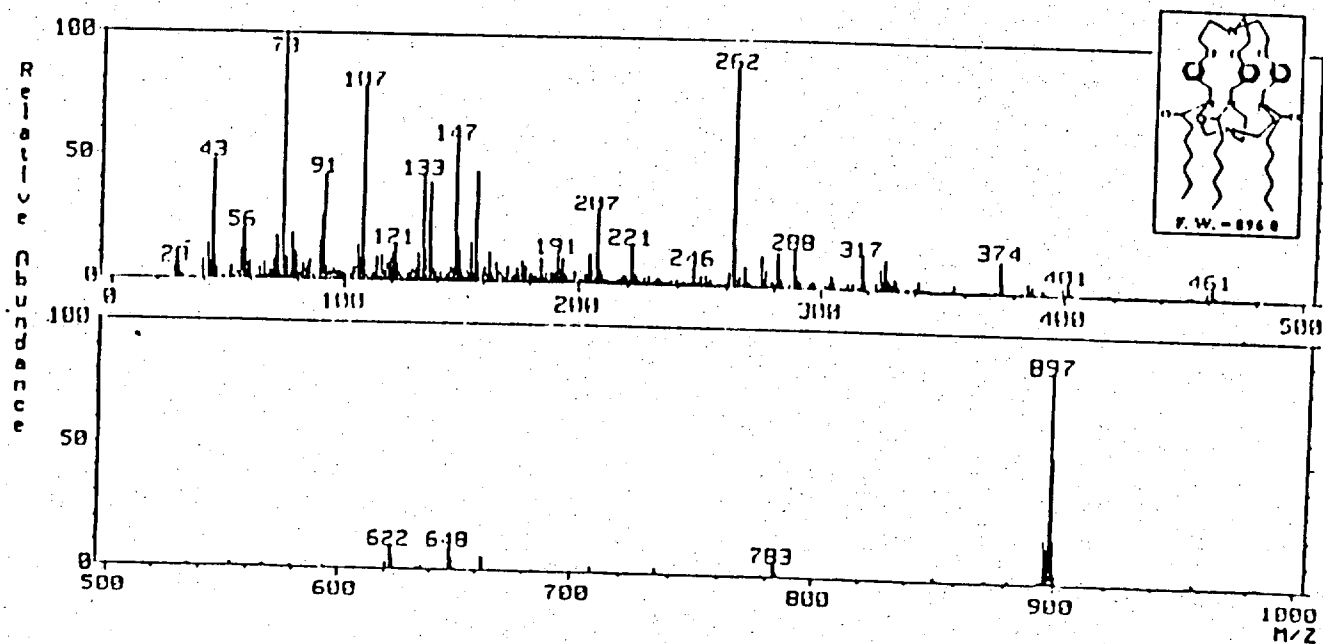
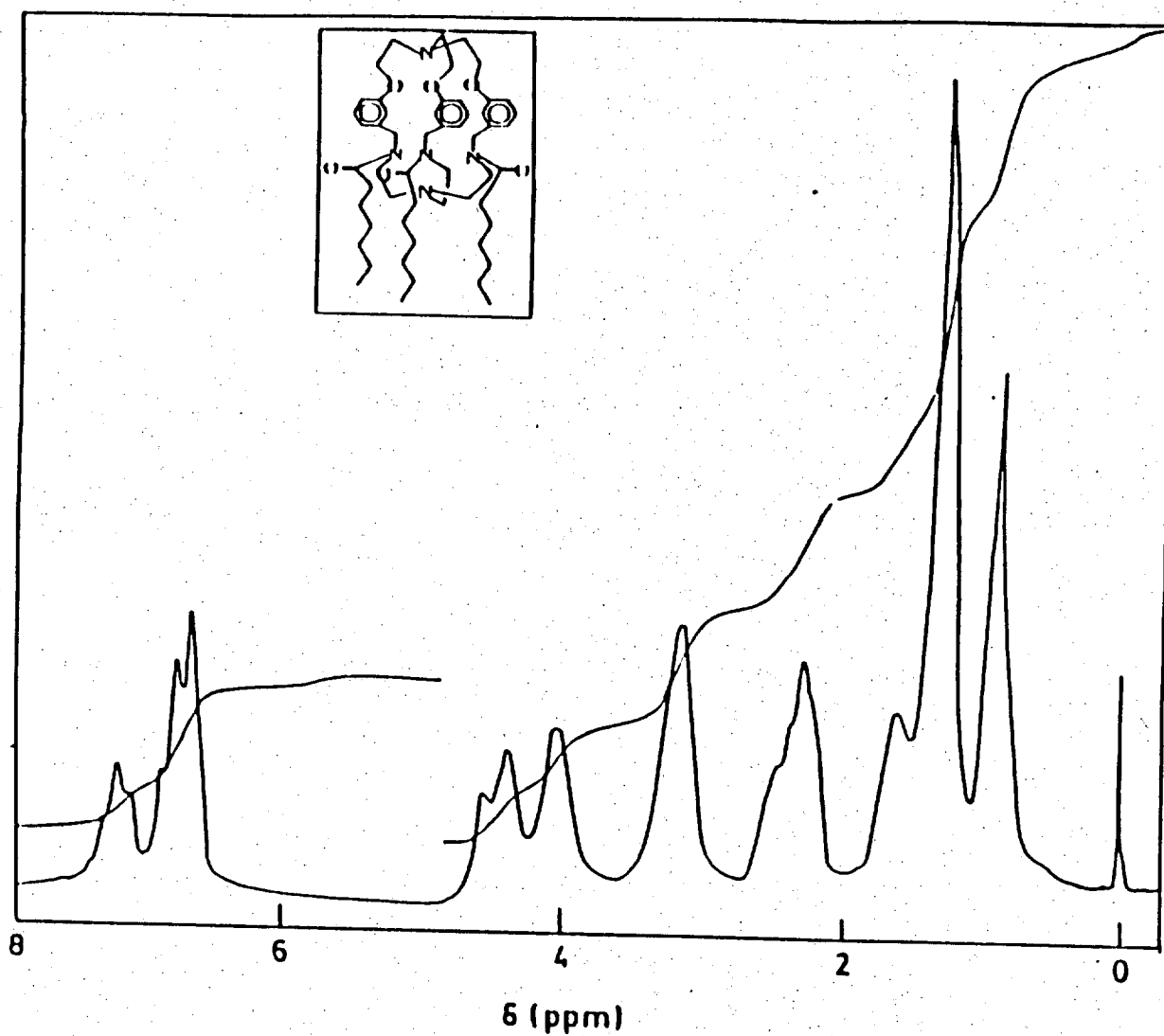












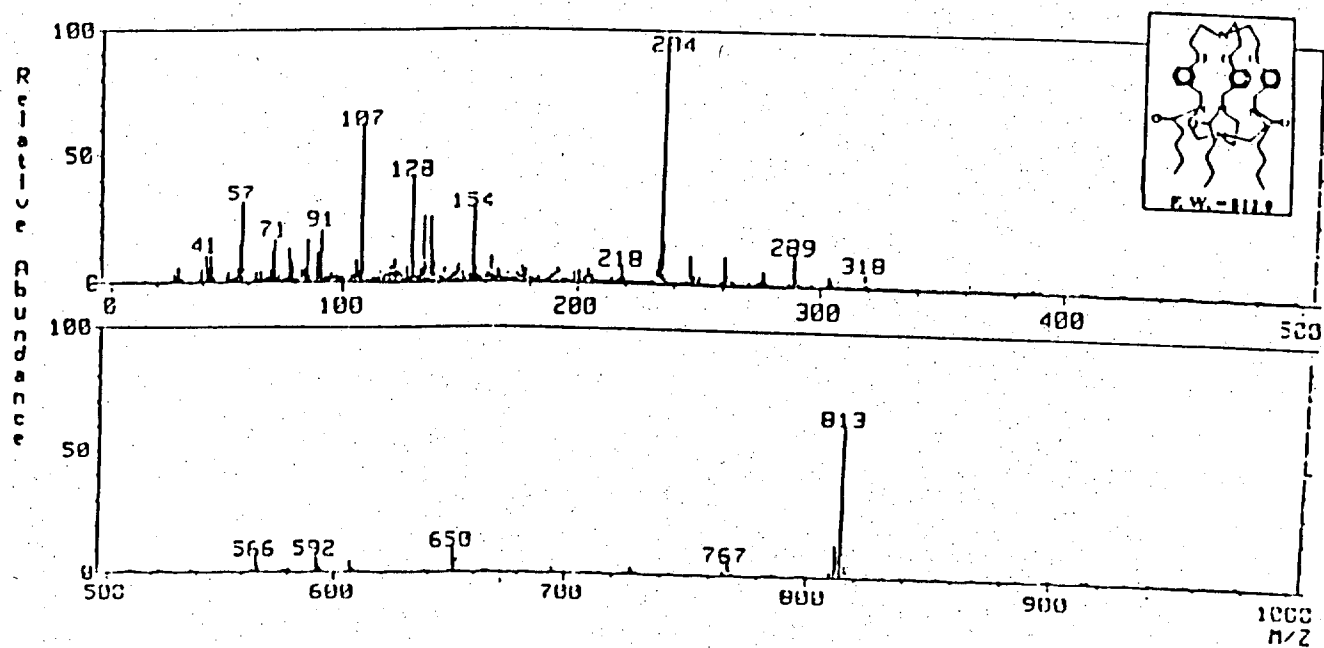
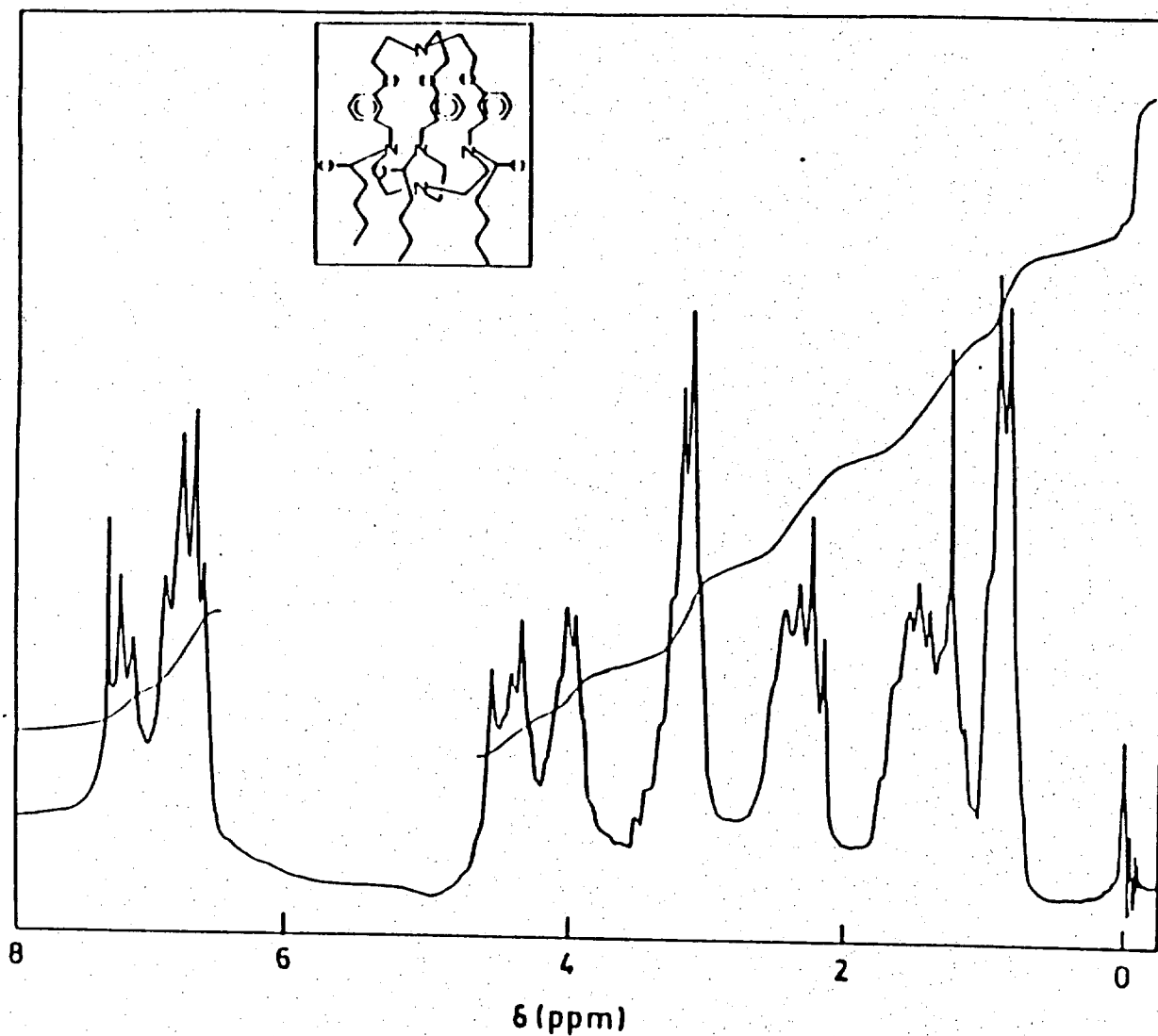


Table 2. Atomic coordinates [ $\times 10^4$ ] and equivalent isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for  $\text{L}_5$ .  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

|        | x         | y        | z       | $U(\text{eq})$ |
|--------|-----------|----------|---------|----------------|
| O(1A)  | 9431(3)   | -1066(1) | 4703(2) | 35(1)          |
| O(2A)  | 15404(3)  | -608(1)  | 4401(2) | 39(1)          |
| O(1B)  | 12255(3)  | -1424(1) | 6471(2) | 36(1)          |
| O(2B)  | 14747(4)  | -3082(1) | 4988(2) | 52(1)          |
| O(1C)  | 9674(3)   | -2408(1) | 5323(2) | 33(1)          |
| O(2C)  | 10561(3)  | -1928(1) | 2117(2) | 49(1)          |
| N(1)   | 9510(4)   | -1563(1) | 6024(2) | 30(1)          |
| N(2)   | 14067(4)  | -1908(1) | 3602(2) | 33(1)          |
| N(1A)  | 13391(4)  | -941(1)  | 4163(2) | 33(1)          |
| N(1B)  | 14161(4)  | -2353(1) | 5174(2) | 32(1)          |
| N(1C)  | 11074(4)  | -2176(1) | 3273(2) | 32(1)          |
| C(1A)  | 8245(5)   | -1461(2) | 5590(2) | 36(1)          |
| C(2A)  | 8256(5)   | -1038(2) | 5136(3) | 36(1)          |
| C(3A)  | 9658(5)   | -700(2)  | 4259(2) | 31(1)          |
| C(4A)  | 8706(5)   | -389(2)  | 4009(3) | 41(1)          |
| C(5A)  | 9041(5)   | -49(2)   | 3531(3) | 43(1)          |
| C(6A)  | 10348(5)  | -21(2)   | 3296(3) | 48(2)          |
| C(7A)  | 11294(5)  | -330(2)  | 3562(3) | 42(1)          |
| C(8A)  | 11001(4)  | -683(2)  | 4031(2) | 31(1)          |
| C(9A)  | 11995(4)  | -1041(2) | 4309(3) | 32(1)          |
| C(10A) | 13827(5)  | -1071(2) | 3428(2) | 39(1)          |
| C(11A) | 14761(5)  | -1480(2) | 3483(3) | 37(1)          |
| C(1RA) | 14258(5)  | -697(2)  | 4599(3) | 32(1)          |
| C(2RA) | 13879(5)  | -542(2)  | 5362(3) | 41(1)          |
| C(3RA) | 15050(5)  | -603(2)  | 5931(3) | 45(1)          |
| C(4RA) | 14782(5)  | -413(2)  | 6693(3) | 43(1)          |
| C(5RA) | 15987(6)  | -475(2)  | 7252(3) | 48(2)          |
| C(6RA) | 15797(9)  | -263(3)  | 8011(3) | 84(2)          |
| C(7RA) | 17056(10) | -304(4)  | 8541(4) | 99(3)          |
| C(1B)  | 99575(5)  | -1178(2) | 6492(2) | 37(1)          |
| C(2B)  | 11249(5)  | -1264(2) | 6948(2) | 34(1)          |
| C(3B)  | 13410(5)  | -1612(2) | 6792(2) | 32(1)          |
| C(4B)  | 13917(5)  | -1517(2) | 7518(2) | 37(1)          |
| C(5B)  | 15111(5)  | -1709(2) | 7774(3) | 42(1)          |
| C(6B)  | 15815(5)  | -1996(2) | 7344(3) | 42(1)          |
| C(7B)  | 15297(5)  | -2088(2) | 6625(2) | 36(1)          |
| C(8B)  | 14092(5)  | -1906(2) | 6343(2) | 32(1)          |
| C(9B)  | 13457(5)  | -2008(2) | 5568(2) | 35(1)          |
| C(10B) | 15307(4)  | -2202(2) | 4761(2) | 33(1)          |
| C(11B) | 15024(5)  | -2247(2) | 3926(2) | 34(1)          |

Contd.

|        |           |          |          |          |
|--------|-----------|----------|----------|----------|
| C(1RB) | 13999(5)  | -2806(2) | 5266(2)  | 37(1)    |
| C(2RB) | 12884(5)  | -2965(2) | 5747(3)  | 43(1)    |
| C(3RB) | 12720(6)  | -3466(2) | 5779(3)  | 50(2)    |
| C(4RB) | 12010(7)  | -3674(2) | 5104(3)  | 61(2)    |
| C(5RB) | 11840(8)  | -4186(2) | 5145(4)  | 72(2)    |
| C(6RB) | 10916(9)  | -4396(3) | 4541(4)  | 99(3)    |
| C(7RB) | 11391(12) | -4333(3) | 3812(5)  | 112(3)   |
| C(1C)  | 9455(5)   | -1989(2) | 6430(2)  | 36(1)    |
| C(2C)  | 8937(5)   | -2387(2) | 5988(2)  | 33(1)    |
| C(3C)  | 9257(5)   | -2716(2) | 4807(2)  | 29(1)    |
| C(4C)  | 8389(5)   | -3077(2) | 4900(3)  | 37(1)    |
| C(5C)  | 8053(5)   | -3377(2) | 4330(3)  | 42(1)    |
| C(6C)  | 8629(5)   | -3326(2) | 3661(3)  | 45(1)    |
| C(7C)  | 9490(5)   | -2964(2) | 3562(2)  | 37(1)    |
| C(8C)  | 9846(5)   | -2659(2) | 4114(2)  | 31(1)    |
| C(9C)  | 10741(5)  | -2252(2) | 4037(2)  | 35(1)    |
| C(10C) | 12269(5)  | -2404(2) | 3019(3)  | 37(1)    |
| C(11C) | 13428(5)  | -2086(2) | 2907(2)  | 34(1)    |
| C(1RC) | 10282(5)  | -1948(2) | 2781(2)  | 34(1)    |
| C(2RC) | 9007(5)   | -1730(2) | 3028(3)  | 48(1)    |
| C(3RC) | 8195(7)   | -1520(2) | 2325(4)  | 67(4)    |
| C(4RC) | 8854(9)   | -1060(2) | 2117(4)  | 69(4)    |
| C(5RC) | 8225(9)   | -893(4)  | 1338(4)  | 157(9)   |
| C(6RC) | 6783(12)  | -695(7)  | 1420(4)  | 169(11)  |
| C(3RD) | 8257(13)  | -1351(2) | 2546(6)  | 58(6)    |
| C(4RD) | 7360(20)  | -1573(4) | 1888(9)  | 710(100) |
| C(5RD) | 6365(14)  | -1210(6) | 1520(10) | 520(70)  |
| C(6RD) | 7166(11)  | -875(5)  | 1040(10) | 89(7)    |
| C(7RC) | 6160(11)  | -529(3)  | 635(5)   | 141(4)   |

Table 3. Bond lengths [Å] and bond angles [°] for L<sub>5</sub>.

|                         |           |                        |          |
|-------------------------|-----------|------------------------|----------|
| O(1A) – C(3A)           | 1.392(5)  | O(1A) – C(2A)          | 1.474(5) |
| O(2A) – C(1RA)          | 1.266(5)  | O(1B) – C(3B)          | 1.383(6) |
| O(1B) – C(2B)           | 1.465(5)  | O(2B) – C(1RB)         | 1.253(6) |
| O(1C) – C(3C)           | 1.359(5)  | O(1C) – C(2C)          | 1.469(5) |
| O(2C) – C(1RC)          | 1.261(5)  | N(1) – C(1C)           | 1.478(6) |
| N(1) – C(1A)            | 1.480(6)  | N(1) – C(1B)           | 1.489(6) |
| N(2) – C(11C)           | 1.473(6)  | N(2) – C(11A)          | 1.486(6) |
| N(2) – C(11B)           | 1.491(6)  | N(1A) – C(1RA)         | 1.351(6) |
| N(1A) – C(9A)           | 1.484(6)  | N(1A) – C(10A)         | 1.489(5) |
| N(1B) – C(1RB)          | 1.378(6)  | N(1B) – C(9B)          | 1.473(6) |
| N(1B) – C(10B)          | 1.496(5)  | N(1C) – C(1RC)         | 1.340(6) |
| N(1C) – C(9C)           | 1.471(5)  | N(1C) – C(10C)         | 1.491(6) |
| C(1A) – C(2A)           | 1.515(7)  | C(3A) – C(4A)          | 1.391(7) |
| C(3A) – C(8A)           | 1.448(6)  | C(4A) – C(5A)          | 1.399(7) |
| C(5A) – C(6A)           | 1.419(7)  | C(6A) – C(7A)          | 1.392(7) |
| C(7A) – C(8A)           | 1.405(7)  | C(8A) – C(9A)          | 1.527(7) |
| C(10A) – C(11A)         | 1.547(7)  | C(1RA) – C(2RA)        | 1.538(6) |
| C(2RA) – C(3RA)         | 1.520(7)  | C(3RA) – C(4RA)        | 1.541(7) |
| C(4RA) – C(5RA)         | 1.534(8)  | C(5RA) – C(6RA)        | 1.544(8) |
| C(6RA) – C(7RA)         | 1.539(11) | C(1B) – C(2B)          | 1.497(7) |
| C(3B) – C(4B)           | 1.406(6)  | C(3B) – C(8B)          | 1.416(6) |
| C(4B) – C(5B)           | 1.383(7)  | C(5B) – C(6B)          | 1.394(7) |
| C(6B) – C(7B)           | 1.396(7)  | C(7B) – C(8B)          | 1.394(7) |
| C(8B) – C(9B)           | 1.533(6)  | C(10B) – C(11B)        | 1.528(6) |
| C(1RB) – C(2RB)         | 1.552(7)  | C(2RB) – C(3RB)        | 1.514(8) |
| C(3RB) – C(4RB)         | 1.508(8)  | C(4RB) – C(5RB)        | 1.547(9) |
| C(1C) – C(2C)           | 1.508(7)  | C(3C) – C(4C)          | 1.411(6) |
| C(3C) – C(8C)           | 1.443(5)  | C(4C) – C(5C)          | 1.393(7) |
| C(5C) – C(6C)           | 1.395(7)  | C(6C) – C(7C)          | 1.411(7) |
| C(7C) – C(8C)           | 1.385(6)  | C(8C) – C(9C)          | 1.533(7) |
| C(10C) – C(11C)         | 1.535(7)  | C(1RC) – C(2RC)        | 1.541(7) |
| C(2RC) – C(3RD)         | 1.591(3)  | C(2RC) – C(3RC)        | 1.593(3) |
| C(3RC) – C(4RC)         | 1.590(4)  | C(4RC) – C(5RC)        | 1.589(3) |
| C(5RC) – C(6RC)         | 1.590(4)  | C(6RC) – C(7RC)        | 1.594(3) |
| C(3RD) – C(4RD)         | 1.591(3)  | C(4RD) – C(5RD)        | 1.591(3) |
| C(5RD) – C(6RD)         | 1.592(3)  | C(6RD) – C(7RD)        | 1.592(3) |
| C(3A) – O(1A) – C(2A)   | 116.0(3)  | C(3B) – O(1B) – C(2B)  | 118.9(3) |
| C(3C) – O(1C) – C(2C)   | 116.6(3)  | C(1C) – N(1) – C(1A)   | 112.5(4) |
| C(1C) – N(1) – C(1B)    | 114.1(3)  | C(1A) – N(1) – C(1B)   | 111.3(4) |
| C(11C) – N(2) – C(11A)  | 111.5(4)  | C(11C) – N(2) – C(11B) | 108.7(3) |
| C(11A) – N(2) – C(11B)  | 110.4(4)  | C(1RA) – N(1A) – C(9A) | 125.8(4) |
| C(1RA) – N(1A) – C(10A) | 116.4(4)  | C(9A) – N(1A) – C(10A) | 117.3(4) |

Contd.

|                          |          |                          |          |
|--------------------------|----------|--------------------------|----------|
| C(1RB) – N(1B) – C(9B)   | 124.6(4) | C(1RB) – N(1B) – C(10B)  | 117.5(4) |
| C(9B) – N(1B) – C(10B)   | 116.7(4) | C(1RC) – N(1C) – C(9C)   | 122.8(4) |
| C(1RC) – N(1C) – C(10C)  | 118.8(3) | C(9C) – N(1C) – C(10C)   | 118.1(4) |
| N(1) – C(1A) – C(2A)     | 115.0(4) | O(1A) – C(2A) – C(1A)    | 106.4(4) |
| C(4A) – C(3A) – O(1A)    | 125.3(4) | C(4A) – C(3A) – C(8A)    | 121.5(4) |
| O(1A) – C(3A) – C(8A)    | 113.1(4) | C(3A) – C(4A) – C(5A)    | 119.4(4) |
| C(4A) – C(5A) – C(6A)    | 120.3(5) | C(7A) – C(6A) – C(5A)    | 119.0(5) |
| C(6A) – C(7A) – C(8A)    | 122.9(4) | C(7A) – C(8A) – C(3A)    | 116.3(4) |
| C(7A) – C(8A) – C(9A)    | 124.5(4) | C(3A) – C(8A) – C(9A)    | 119.1(4) |
| N(1A) – C(9A) – C(8A)    | 114.1(4) | N(1A) – C(10A) – C(11A)  | 111.7(4) |
| N(2) – C(11A) – C(10A)   | 113.8(4) | O(2A) – C(1RA) – N(1A)   | 120.8(4) |
| O(2A) – C(1RA) – C(2RA)  | 119.2(4) | N(1A) – C(1RA) – C(2RA)  | 119.9(4) |
| C(3RA) – C(2RA) – C(1RA) | 110.0(4) | C(2RA) – C(3RA) – C(4RA) | 112.8(4) |
| C(5RA) – C(4RA) – C(3RA) | 111.5(4) | C(4RA) – C(5RA) – C(6RA) | 113.3(5) |
| C(7RA) – C(6RA) – C(5RA) | 119.9(7) | N(1) – C(1B) – C(2B)     | 113.7(4) |
| O(1B) – C(2B) – C(1B)    | 109.5(3) | O(1B) – C(3B) – C(4B)    | 123.2(4) |
| O(1B) – C(3B) – C(8B)    | 116.2(4) | C(4B) – C(3B) – C(8B)    | 120.6(5) |
| C(5B) – C(5B) – C(3B)    | 118.5(4) | C(4B) – C(5B) – C(6B)    | 122.4(5) |
| C(5B) – C(6B) – C(7B)    | 118.5(5) | C(8B) – C(7B) – C(6B)    | 121.3(5) |
| C(7B) – C(8B) – C(3B)    | 118.7(4) | C(7B) – C(8B) – C(9B)    | 123.5(4) |
| C(3B) – C(8B) – C(9B)    | 117.8(4) | N(1B) – C(9B) – C(8B)    | 113.8(4) |
| N(1B) – C(10B) – C(11B)  | 112.2(4) | N(2) – C(11B) – C(10B)   | 113.5(4) |
| O(2B) – C(1RB) – N(1B)   | 121.4(4) | O(2B) – C(1RB) – C(2RB)  | 120.6(5) |
| N(1B) – C(1RB) – C(2RB)  | 117.9(4) | C(3RB) – C(2RB) – C(1RB) | 114.4(4) |
| C(4RB) – C(3RB) – C(2RB) | 115.3(5) | C(3RB) – C(4RB) – C(5RB) | 114.8(5) |
| C(6RB) – C(5RB) – C(4RB) | 116.1(7) | C(7RB) – C(6RB) – C(5RB) | 112.1(8) |
| N(1) – C(1C) – C(2C)     | 116.3(4) | O(1C) – C(2C) – C(1C)    | 107.2(3) |
| O(1C) – C(3C) – C(4C)    | 126.9(4) | O(1C) – C(3C) – C(8C)    | 113.3(4) |
| C(4C) – C(3C) – C(8C)    | 119.7(4) | C(5C) – C(4C) – C(3C)    | 121.6(4) |
| C(4C) – C(5C) – C(6C)    | 118.9(5) | C(5C) – C(6C) – C(7C)    | 119.8(5) |
| C(8C) – C(7C) – C(6C)    | 122.9(4) | C(7C) – C(8C) – C(3C)    | 117.0(4) |
| C(7C) – C(8C) – C(9C)    | 125.6(4) | C(3C) – C(8C) – C(9C)    | 117.3(4) |
| N(1C) – C(9C) – C(8C)    | 112.9(4) | N(1C) – C(10C) – C(11C)  | 113.5(4) |
| N(2) – C(11C) – C(10C)   | 113.5(3) | O(2C) – C(1RC) – N(1C)   | 119.8(4) |
| O(2C) – C(1RC) – C(2RC)  | 120.8(4) | N(1C) – C(1RC) – C(2RC)  | 119.3(4) |
| C(1RC) – C(2RC) – C(3RD) | 121.0(7) | C(1RC) – C(2RC) – C(3RC) | 108.9(7) |
| C(3RD) – C(2RC) – C(3RC) | 23.4(4)  | C(4RC) – C(3RC) – C(2RC) | 109.6(2) |
| C(5RC) – C(4RC) – C(3RC) | 109.8(2) | C(6RC) – C(5RC) – C(4RC) | 109.2(2) |
| C(5RC) – C(6RC) – C(7RC) | 109.5(2) | C(2RC) – C(3RD) – C(4RD) | 109.5(2) |
| C(5RD) – C(4RD) – C(3RD) | 109.5(2) | C(6RD) – C(5RD) – C(4RD) | 109.2(2) |
| C(5RD) – C(6RD) – C(7RC) | 109.4(2) | C(6RD) – C(7RC) – C(6RC) | 35.8(8)  |

Table 4. Anisotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for  $L_5$ . The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^* b^* U_{12}]$

|        | U11    | U22    | U33   | U23    | U13    | U12    |
|--------|--------|--------|-------|--------|--------|--------|
| O(1A)  | 15(2)  | 54(2)  | 37(2) | 8(2)   | 16(1)  | 6(2)   |
| O(2A)  | 10(2)  | 62(2)  | 47(2) | -4(2)  | 8(2)   | -3(2)  |
| O(1B)  | 25(2)  | 63(2)  | 23(2) | -6(1)  | 9(1)   | 3(2)   |
| O(2B)  | 38(2)  | 66(2)  | 55(2) | 0(2)   | 20(2)  | 16(2)  |
| O(1C)  | 26(2)  | 52(2)  | 23(2) | -4(1)  | 16(1)  | -6(2)  |
| O(2C)  | 30(2)  | 92(3)  | 28(2) | 6(2)   | 10(2)  | -7(2)  |
| N(1)   | 17(2)  | 52(2)  | 23(2) | -1(2)  | 8(2)   | -2(2)  |
| N(2)   | 20(2)  | 58(3)  | 22(2) | -3(2)  | 9(2)   | 3(2)   |
| N(1A)  | 18(2)  | 50(2)  | 32(2) | -2(2)  | 11(2)  | -3(2)  |
| N(1B)  | 20(2)  | 56(3)  | 21(2) | 1(2)   | 8(2)   | 4(2)   |
| N(1C)  | 21(2)  | 55(2)  | 20(2) | -2(2)  | 11(2)  | -2(2)  |
| C(1A)  | 14(3)  | 62(3)  | 34(2) | 7(2)   | 12(2)  | 5(2)   |
| C(2A)  | 14(3)  | 63(3)  | 34(3) | 4(2)   | 17(2)  | 8(2)   |
| C(3A)  | 18(3)  | 42(3)  | 32(2) | 0(2)   | 6(2)   | 0(2)   |
| C(4A)  | 24(3)  | 55(3)  | 44(3) | 3(2)   | 13(2)  | 7(2)   |
| C(5A)  | 19(3)  | 54(3)  | 57(3) | 9(2)   | 6(3)   | 11(2)  |
| C(6A)  | 31(4)  | 58(3)  | 58(3) | 17(3)  | 18(3)  | 3(3)   |
| C(7A)  | 23(3)  | 49(3)  | 56(3) | 9(2)   | 16(3)  | 3(2)   |
| C(8A)  | 13(3)  | 48(3)  | 32(2) | -1(2)  | 5(2)   | -2(2)  |
| C(9A)  | 11(3)  | 47(3)  | 38(3) | 6(2)   | 6(2)   | 0(2)   |
| C(10A) | 29(3)  | 62(3)  | 28(2) | 7(2)   | 11(2)  | -6(2)  |
| C(11A) | 23(3)  | 60(3)  | 30(2) | -2(2)  | 12(2)  | -3(2)  |
| C(1RA) | 16(3)  | 41(3)  | 40(3) | -2(2)  | 7(2)   | -4(2)  |
| C(2RA) | 17(3)  | 63(4)  | 45(3) | -9(2)  | 11(3)  | -2(2)  |
| C(3RA) | 30(3)  | 64(4)  | 43(3) | -1(2)  | 21(3)  | 2(3)   |
| C(4RA) | 32(4)  | 56(3)  | 41(3) | -2(2)  | 10(3)  | 1(3)   |
| C(5RA) | 49(4)  | 58(4)  | 40(3) | 4(2)   | 15(3)  | -6(3)  |
| C(6RA) | 105(7) | 107(6) | 39(3) | -10(3) | 9(4)   | 13(5)  |
| C(7RA) | 103(8) | 135(9) | 54(4) | 1(5)   | -21(5) | 0(7)   |
| C(1B)  | 26(3)  | 56(3)  | 29(2) | -4(2)  | 14(2)  | 5(2)   |
| C(2B)  | 18(3)  | 59(3)  | 28(2) | -10(2) | 12(2)  | -1(2)  |
| C(3B)  | 17(3)  | 49(3)  | 29(2) | 2(2)   | 2(2)   | 0(2)   |
| C(4B)  | 33(4)  | 59(3)  | 21(2) | 0(2)   | 4(2)   | -5(3)  |
| C(5B)  | 32(4)  | 65(3)  | 28(3) | 5(2)   | -2(2)  | -12(3) |
| C(6B)  | 25(3)  | 71(4)  | 30(3) | 12(2)  | -2(2)  | -5(3)  |
| C(7B)  | 22(3)  | 58(3)  | 28(2) | 4(2)   | 6(2)   | 0(2)   |
| C(8B)  | 20(3)  | 53(3)  | 24(2) | 4(2)   | 7(2)   | -7(2)  |
| C(9B)  | 22(3)  | 60(3)  | 22(2) | -3(2)  | 3(2)   | 9(2)   |
| C(10B) | 9(3)   | 61(3)  | 29(2) | 4(2)   | 5(2)   | 1(2)   |
| C(11B) | 22(3)  | 53(3)  | 27(2) | -4(2)  | 11(2)  | 0(2)   |

Contd.

|        |          |          |          |           |         |          |
|--------|----------|----------|----------|-----------|---------|----------|
| C(1RB) | 23(3)    | 60(3)    | 28(2)    | 3(2)      | 2(2)    | 8(2)     |
| C(2RB) | 29(4)    | 67(4)    | 34(3)    | 4(2)      | 11(2)   | 2(3)     |
| C(3RB) | 40(4)    | 68(4)    | 44(3)    | 6(3)      | 15(3)   | 4(3)     |
| C(4RB) | 47(4)    | 75(4)    | 60(4)    | 2(3)      | 6(3)    | 5(3)     |
| C(5RB) | 84(6)    | 64(4)    | 68(4)    | -8(3)     | 11(4)   | -20(4)   |
| C(6RB) | 129(8)   | 93(6)    | 80(5)    | 6(4)      | 27(5)   | -23(5)   |
| C(7RB) | 137(11)  | 113(8)   | 86(6)    | 0(5)      | 15(6)   | -31(7)   |
| C(1C)  | 32(3)    | 58(3)    | 20(2)    | 2(2)      | 15(2)   | 6(2)     |
| C(2C)  | 31(3)    | 53(3)    | 18(2)    | 7(2)      | 17(2)   | -2(2)    |
| C(3C)  | 24(3)    | 45(3)    | 19(2)    | 3(2)      | 8(2)    | 0(2)     |
| C(4C)  | 30(3)    | 50(3)    | 32(3)    | 5(2)      | 8(2)    | -5(2)    |
| C(5C)  | 35(3)    | 50(3)    | 40(3)    | 0(2)      | 3(2)    | -12(3)   |
| C(6C)  | 48(4)    | 57(3)    | 29(3)    | -7(2)     | 1(2)    | -2(3)    |
| C(7C)  | 30(3)    | 59(3)    | 22(2)    | -1(2)     | 5(2)    | -5(2)    |
| C(8C)  | 22(3)    | 50(3)    | 21(2)    | 4(2)      | 7(2)    | -2(2)    |
| C(9C)  | 30(3)    | 58(3)    | 18(2)    | -2(2)     | 8(2)    | -4(2)    |
| C(10C) | 22(3)    | 58(3)    | 30(2)    | -4(2)     | 6(2)    | 3(2)     |
| C(11C) | 28(3)    | 56(3)    | 19(2)    | -5(2)     | 9(2)    | 2(2)     |
| C(1RC) | 24(3)    | 53(3)    | 25(2)    | 4(2)      | 4(2)    | -7(2)    |
| C(2RC) | 14(3)    | 82(4)    | 49(3)    | 14(3)     | 7(2)    | 9(3)     |
| C(3RC) | 56(8)    | 60(8)    | 92(9)    | -29(6)    | 44(7)   | 19(7)    |
| C(4RC) | 79(9)    | 83(8)    | 45(6)    | 20(5)     | 17(5)   | 31(6)    |
| C(5RC) | 106(16)  | 126(15)  | 240(20)  | 85(16)    | 25(16)  | 23(13)   |
| C(6RC) | 240(30)  | 125(16)  | 160(20)  | -13(15)   | 90(20)  | 28(18)   |
| C(3RD) | 27(10)   | 62(12)   | 90(13)   | 12(10)    | 39(9)   | 18(8)    |
| C(4RD) | 350(60)  | 910(150) | 940(140) | -880(140) | 510(80) | -510(80) |
| C(5RD) | 760(130) | 720(120) | 110(30)  | 120(50)   | 110(50) | 80(110)  |
| C(6RD) | 83(18)   | 99(16)   | 88(14)   | -15(12)   | 22(13)  | 47(14)   |
| C(7RC) | 195(12)  | 157(9)   | 67(5)    | 32(6)     | -12(6)  | 62(9)    |

Table 5. Hydrogen coordinates [ $\times 10^4$ ] and isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for  $\text{L}_5$ .

|        | x     | y     | z    | U(eq)    |
|--------|-------|-------|------|----------|
| H(17A) | 7533  | -1436 | 5933 | 57(15)   |
| H(17B) | 8019  | -1714 | 5254 | 29(12)   |
| H(34A) | 7434  | -1015 | 4803 | 57(17)   |
| H(34B) | 8317  | -773  | 5461 | 24(11)   |
| H(46A) | 7829  | -407  | 4163 | 67(18)   |
| H(44A) | 8391  | 165   | 3362 | 62(17)   |
| H(50A) | 10573 | 206   | 2963 | 52(15)   |
| H(41A) | 12176 | -301  | 3421 | 55(16)   |
| H(37A) | 11944 | -1077 | 4848 | 36(13)   |
| H(37B) | 11734 | -1328 | 4072 | 30(12)   |
| H(35A) | 14269 | -817  | 3216 | 38(13)   |
| H(35B) | 13037 | -1140 | 3091 | 29(13)   |
| H(45A) | 15222 | -1503 | 3022 | 100(20)  |
| H(45B) | 15446 | -1433 | 3895 | 31(12)   |
| H(38A) | 13618 | -223  | 5338 | 43(14)   |
| H(38B) | 13111 | -717  | 5509 | 37(13)   |
| H(52A) | 15839 | -453  | 5753 | 100(20)  |
| H(52B) | 15254 | -925  | 5981 | 43(14)   |
| H(47A) | 14570 | -92   | 6645 | 27(11)   |
| H(47B) | 14003 | -566  | 6877 | 62(17)   |
| H(49A) | 16777 | -340  | 7049 | 73(19)   |
| H(49B) | 16161 | -797  | 7319 | 74(19)   |
| H(57A) | 15567 | 56    | 7943 | 150(40)  |
| H(57B) | 15047 | -412  | 8233 | 510(150) |
| H(62A) | 16850 | -216  | 9039 | 320(100) |
| H(62B) | 17750 | -108  | 8373 | 180(50)  |
| H(62C) | 17370 | -613  | 8547 | 90(30)   |
| H(19A) | 9278  | -1101 | 6825 | 110(30)  |
| H(19B) | 10097 | -918  | 6170 | 22(11)   |
| H(25A) | 11560 | -986  | 7199 | 31(12)   |
| H(25B) | 11103 | -1490 | 7330 | 36(13)   |
| H(27A) | 13451 | -1326 | 7825 | 58(16)   |
| H(29A) | 15464 | -1642 | 8262 | 120(30)  |
| H(48A) | 16628 | -2126 | 7535 | 49(16)   |
| H(28A) | 15775 | -2278 | 6323 | 44(14)   |
| H(26A) | 12528 | -2105 | 5608 | 25(11)   |
| H(26B) | 13433 | -1730 | 5273 | 36(13)   |
| H(33A) | 16101 | -2382 | 4921 | 21(11)   |
| H(33B) | 15507 | -1887 | 4885 | 34(13)   |
| H(30A) | 15870 | -2219 | 3689 | 24(11)   |
| H(30B) | 14663 | -2548 | 3814 | 24(11)   |

Contd.

|        |       |       |      |            |
|--------|-------|-------|------|------------|
| H(36A) | 13079 | -2851 | 6256 | 73(19)     |
| H(36B) | 12032 | -2831 | 5551 | 49(16)     |
| H(39A) | 13612 | -3603 | 5859 | 42(14)     |
| H(39B) | 12224 | -3540 | 6213 | 100(20)    |
| H(55A) | 12508 | -3603 | 4671 | 33(12)     |
| H(55B) | 11119 | -3537 | 5023 | 41(14)     |
| H(58A) | 12287 | -4359 | 5526 | 170(40)    |
| H(56A) | 10837 | -4720 | 4640 | 120(30)    |
| H(56B) | 10021 | -4263 | 4551 | 2000(1100) |
| H(63A) | 10875 | -4522 | 3454 | 140(40)    |
| H(63B) | 12332 | -4416 | 3824 | 120(40)    |
| H(63C) | 11287 | -4020 | 3667 | 160(40)    |
| H(22A) | 8888  | -1946 | 6845 | 80(20)     |
| H(22B) | 10362 | -2060 | 6645 | 38(14)     |
| H(12A) | 9075  | -2663 | 6281 | 15(10)     |
| H(12B) | 7976  | -2353 | 5851 | 54(17)     |
| H(42A) | 8025  | -3117 | 5362 | 130(30)    |
| H(54A) | 7442  | -3611 | 4396 | 46(14)     |
| H(53A) | 8442  | -3535 | 3274 | 43(14)     |
| H(24A) | 9842  | -2928 | 3095 | 56(15)     |
| H(21A) | 10287 | -1984 | 4214 | 42(13)     |
| H(21B) | 11573 | -2293 | 4355 | 36(14)     |
| H(14A) | 12018 | -2558 | 2547 | 43(14)     |
| H(14B) | 12571 | -2633 | 3386 | 24(11)     |
| H(31A) | 14103 | -2246 | 2640 | 46(14)     |
| H(31B) | 13095 | -1833 | 2594 | 21(10)     |
| H(3RA) | 8200  | -1729 | 1903 | 81         |
| H(3RB) | 7261  | -1470 | 2435 | 81         |
| H(4RA) | 8702  | -834  | 2499 | 82         |
| H(4RB) | 9825  | -1099 | 2099 | 82         |
| H(5RA) | 8800  | -661  | 1142 | 189        |
| H(5RB) | 8167  | -1145 | 985  | 189        |
| H(6RA) | 6840  | -442  | 1772 | 203        |
| H(6RB) | 6207  | -927  | 1616 | 203        |
| H(3RC) | 8914  | -1149 | 2344 | 69         |
| H(3RD) | 7694  | -1173 | 2859 | 69         |
| H(4RC) | 7927  | -1693 | 1515 | 853        |
| H(4RD) | 6844  | -1824 | 2079 | 853        |
| H(5RC) | 5658  | -1359 | 1202 | 628        |
| H(5RD) | 5940  | -1044 | 1909 | 628        |
| H(6RC) | 7634  | -1043 | 670  | 107        |
| H(6RD) | 7838  | -713  | 1364 | 107        |

Table 7. Atomic coordinates [ $\times 10^4$ ] and equivalent isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for  $\text{L}_6$ .  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

|       | x        | y       | z        | U(eq)  |
|-------|----------|---------|----------|--------|
| O(1)  | 4839(1)  | 2232(1) | 6930(1)  | 39(1)  |
| O(2)  | 6094(2)  | 232(1)  | 10678(2) | 58(1)  |
| N(1)  | 6667     | 3333    | 11274(3) | 37(1)  |
| N(2)  | 6667     | 3333    | 5760(3)  | 40(1)  |
| N(3)  | 5686(2)  | 1326(2) | 9856(2)  | 38(1)  |
| C(1)  | 6238(2)  | 2277(2) | 11691(2) | 41(1)  |
| C(2)  | 5351(2)  | 1493(2) | 10980(2) | 41(1)  |
| C(3)  | 6038(2)  | 662(2)  | 9806(2)  | 45(1)  |
| C(4A) | 6355(2)  | 467(2)  | 8652(2)  | 57(1)  |
| C(4B) | 7052(4)  | 27(4)   | 8728(4)  | 91(1)  |
| C(4C) | 8041(4)  | 622(4)  | 9303(5)  | 82(2)  |
| C(4D) | 8627(4)  | 74(5)   | 9382(7)  | 155(3) |
| C(4E) | 7703(17) | 142(17) | 7845(16) | 67(5)  |
| C(4F) | 8635(11) | 91(12)  | 7890(14) | 67(5)  |
| C(5)  | 5434(2)  | 1731(2) | 8861(2)  | 38(1)  |
| C(6)  | 4405(2)  | 996(2)  | 8331(2)  | 36(1)  |
| C(7)  | 3726(2)  | 59(2)   | 8792(2)  | 48(1)  |
| C(8)  | 2796(2)  | -584(2) | 8275(2)  | 55(1)  |
| C(9)  | 2547(2)  | -285(2) | 7272(2)  | 53(1)  |
| C(10) | 3214(2)  | 651(2)  | 6782(2)  | 44(1)  |
| C(11) | 4133(2)  | 1280(2) | 7320(2)  | 36(1)  |
| C(12) | 4772(2)  | 2458(2) | 5759(2)  | 44(1)  |
| C(13) | 5758(2)  | 3382(2) | 5438(2)  | 44(1)  |

Table 8. Bond lengths [ $\text{\AA}$ ] and bond angles [ $^\circ$ ] for  $\text{L}_6$ .

|                            |             |                          |             |
|----------------------------|-------------|--------------------------|-------------|
| O(1) – C(11)               | 1.373 (3)   | O(1) – C(12)             | 1.431(3)    |
| O(2) – C(3)                | 1.238 (3)   | N(1) – C(1)              | 1.475 (3)   |
| N(1) – C(1) #1             | 1.475 (3)   | N(1) – C(1) #2           | 1.475 (3)   |
| N(2) – C(13) #1            | 1.462 (3)   | N(2) – C(13) #2          | 1.462 (3)   |
| N(2) – C(13)               | 1.462 (3)   | N(3) – C(3)              | 1.352 (3)   |
| N(3) – C(5)                | 1.454 (3)   | N(3) – C(2)              | 1.479 (3)   |
| C(1) – C(2)                | 1.520 (3)   | C(3) – C(4A)             | 1.514 (4)   |
| C(4A) – C(4B)              | 1.503 (5)   | C(4B) – C(4E)            | 1.380 (2)   |
| C(4B) – C(4C)              | 1.469 (6)   | C(4C) – C(4D)            | 1.487 (6)   |
| C(4E) – C(4F)              | 1.450 (2)   | C(5) – C(6)              | 1.521 (3)   |
| C(6) – C(7)                | 1.378 (3)   | C(6) – C(11)             | 1.391 (3)   |
| C(7) – C(8)                | 1.387 (4)   | C(8) – C(9)              | 1.378 (4)   |
| C(9) – C(10)               | 1.387 (4)   | C(10) – C(11)            | 1.382 (3)   |
| C(12) – C(13)              | 1.494 (3)   |                          |             |
| C(11) – O(1) – C(12)       | 117.34 (19) | C(1) – N(1) – C(1) #1    | 109.54 (15) |
| C(1) – N(1) – C(1) #2      | 109.54 (15) | C(1) #1 – N(1) – C(1) #2 | 109.54 (15) |
| C(13) #1 – N(2) – C(13) #2 | 113.56 (13) | C(13) #1 – N(2) – C(13)  | 113.56 (13) |
| C(13) #2 – N(2) – C(13)    | 113.56 (13) | C(3) – N(3) – C(5)       | 124.1 (2)   |
| C(3) – N(3) – C(2)         | 117.5 (2)   | C(5) – N(3) – C(2)       | 117.3 (2)   |
| N(1) – C(1) – C(2)         | 113.6 (2)   | N(3) – C(2) – C(1)       | 121.7 (3)   |
| O(2) – C(3) – N(3)         | 120.7 (2)   | O(2) – C(3) – C(4A)      | 121.7 (3)   |
| N(3) – C(3) – C(4A)        | 117.6 (2)   | C(4B) – C(4A) – C(3)     | 113.2 (3)   |
| C(4E) – C(4B) – C(4C)      | 79.8 (9)    | C(4E) – C(4B) – C(4A)    | 120.9 (9)   |
| C(4C) – C(4B) – C(4A)      | 118.7 (4)   | C(4B) – C(4C) – C(4D)    | 113.3 (5)   |
| C(4B) – C(4E) – C(4F)      | 128.1 (17)  | N(3) – C(5) – C(6)       | 114.1 (2)   |
| C(7) – C(6) – C(11)        | 117.9 (2)   | C(7) – C(6) – C(5)       | 123.6 (2)   |
| C(11) – C(6) – C(5)        | 118.4 (2)   | C(6) – C(7) – C(8)       | 121.4 (3)   |
| C(9) – C(8) – C(7)         | 119.4 (3)   | C(8) – C(9) – C(10)      | 120.7 (3)   |
| C(11) – C(10) – C(9)       | 118.7 (3)   | O(1) – C(11) – C(10)     | 123.8 (2)   |
| O(1) – C(11) – C(6)        | 114.3 (2)   | C(10) – C(11) – C(6)     | 121.8 (3)   |
| O(1) – C(12) – C(13)       | 108.0 (2)   | N(2) – C(13) – C(12)     | 114.3 (2)   |

Symmetry transformations used to generate equivalent atoms:

#1  $-y+1, x-y, z$ #2  $-x+y+1, -x+1, z$

Table 9. Anisotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for  $\text{L}_6$ . The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ (ha^*)^2 U_{11} + \dots + 2hka^* b^* U_{12}]$

|       | U11    | U22    | U33     | U23   | U13   | U12   |
|-------|--------|--------|---------|-------|-------|-------|
| O(1)  | 46(1)  | 37(1)  | 32(1)   | 1(1)  | -3(1) | 19(1) |
| O(2)  | 76(2)  | 55(1)  | 53(1)   | 12(1) | 3(1)  | 40(1) |
| N(1)  | 39(1)  | 39(1)  | 31(2)   | 0     | 0     | 20(1) |
| N(2)  | 40(2)  | 40(2)  | 40(2)   | 0     | 0     | 20(1) |
| N(3)  | 42(1)  | 36(1)  | 35(1)   | 2(1)  | -4(1) | 19(1) |
| C(1)  | 50(2)  | 47(2)  | 30(1)   | 4(1)  | -1(1) | 26(2) |
| C(2)  | 38(2)  | 42(2)  | 39(1)   | 9(1)  | 4(1)  | 18(2) |
| C(3)  | 47(2)  | 39(2)  | 45(2)   | 5(1)  | -2(1) | 18(2) |
| C(4A) | 67(2)  | 51(2)  | 57(2)   | -7(2) | 2(2)  | 32(2) |
| C(4B) | 119(4) | 104(4) | 89(3)   | 43(3) | 53(3) | 85(4) |
| C(4C) | 70(4)  | 78(4)  | 113(4)  | 27(3) | 25(3) | 48(3) |
| C(4D) | 88(4)  | 119(5) | 273(10) | 52(6) | 33(5) | 63(4) |
| C(5)  | 41(2)  | 34(2)  | 38(1)   | 5(1)  | 1(1)  | 17(1) |
| C(6)  | 33(2)  | 38(2)  | 35(1)   | 1(1)  | 1(1)  | 16(1) |
| C(7)  | 41(2)  | 50(2)  | 44(2)   | 6(2)  | -3(1) | 17(2) |
| C(8)  | 37(2)  | 53(2)  | 53(2)   | 6(2)  | 0(2)  | 7(2)  |
| C(9)  | 32(2)  | 58(2)  | 57(2)   | -1(2) | -7(2) | 13(2) |
| C(10) | 43(2)  | 52(2)  | 41(2)   | 0(1)  | -3(1) | 26(2) |
| C(11) | 35(2)  | 34(2)  | 38(1)   | -5(1) | -1(1) | 17(2) |
| C(12) | 42(2)  | 49(2)  | 38(2)   | 0(1)  | -9(1) | 21(2) |
| C(13) | 47(2)  | 50(2)  | 33(1)   | 10(1) | -1(1) | 23(2) |

Table 10. Hydrogen coordinates [ $\times 10^4$ ] and isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for  $\text{L}_6$ .

|        | x        | y        | z        | U(eq)   |
|--------|----------|----------|----------|---------|
| H(1A)  | 6003     | 2242     | 12486    | 53(8)   |
| H(1B)  | 6785     | 2099     | 11697    | 38(7)   |
| H(2A)  | 5002     | 838      | 11399    | 39(6)   |
| H(2B)  | 4852     | 1728     | 10866    | 44(7)   |
| H(4AA) | 5735     | -10      | 8219     | 97(11)  |
| H(4AB) | 6730(20) | -660(30) | 9170(30) | 67(12)  |
| H(4BB) | 7200(30) | -180(30) | 7890(40) | 57(12)  |
| H(4CA) | 7925     | 796      | 10081    | 77(14)  |
| H(4CB) | 8455     | 1270     | 8883     | 160(20) |
| H(4DA) | 9236     | 471      | 9853     | 232     |
| H(4DB) | 8834     | -11      | 8617     | 232     |
| H(4DC) | 8197     | -598     | 9728     | 232     |
| H(4EA) | 7905     | 817      | 7507     | 80      |
| H(4EB) | 7270     | -370     | 7268     | 80      |
| H(4FA) | 8909     | 157      | 7118     | 10(20)  |
| H(4FB) | 8486     | -567     | 8215     | 0(20)   |
| H(4FC) | 9138     | 647      | 8368     | 90(60)  |
| H(5A)  | 5973     | 1917     | 8280     | 36(7)   |
| H(5B)  | 5435     | 2364     | 9083     | 38(7)   |
| H(7A)  | 3899     | -151     | 9479     | 42(7)   |
| H(8A)  | 2334     | -1224    | 8609     | 76(10)  |
| H(9A)  | 1913     | -725     | 6913     | 39(7)   |
| H(10A) | 3042     | 857      | 6091     | 40(7)   |
| H(12A) | 4199     | 2590     | 5653     | 51(8)   |
| H(12B) | 4649     | 1872     | 5273     | 59(9)   |
| H(13A) | 5766     | 3478     | 4603     | 49(7)   |
| H(13B) | 5790     | 3987     | 5804     | 64(9)   |