

Table 12

Bond angles (°).

Symmetry transformations used to generate equivalent atoms: (i) $-x, -y, -z$;
(ii) $-x + 1, -y, -z$.

| | HS,HS (LIESST) | HS,LS (50%) | LS,LS (reverse LIESST) |
|--|-------------------|----------------|------------------------------|
| N(411) ⁱ –Fe(1)–N(411) | 180.0 | 180.0 | 180.0 |
| N(411) ⁱ –Fe(1)–N(421) ⁱ | 91.57 (11) | 89.22 (10) | 89.39 (12) |
| N(411)–Fe(1)–N(421) ⁱ | 88.43 (11) | 90.78 (10) | 90.61 (12) |
| N(411) ⁱ –Fe(1)–N(421) | 88.43 (11) | 90.78 (10) | 90.61 (12) |
| N(411)–Fe(1)–N(421) | 91.57 (11) | 89.22 (10) | 89.39 (12) |
| N(421) ⁱ –Fe(1)–N(421) | 180.0 | 180.0 | 180.0 |
| N(411) ⁱ –Fe(1)–N(431) | 89.71 (10) | 89.97 (9) | 90.02 (11) |
| N(411)–Fe(1)–N(431) | 90.29 (10) | 90.03 (9) | 89.98 (11) |
| N(421) ⁱ –Fe(1)–N(431) | 90.83 (10) | 90.27 (10) | 90.54 (12) |
| N(421)–Fe(1)–N(431) | 89.17 (10) | 89.73 (10) | 89.46 (12) |
| N(411) ⁱ –Fe(1)–N(431) ⁱ | 90.29 (10) | 90.03 (9) | 89.98 (11) |
| N(411)–Fe(1)–N(431) ⁱ | 89.71 (10) | 89.97 (9) | 90.02 (11) |
| N(421) ⁱ –Fe(1)–N(431) ⁱ | 89.17 (10) | 89.73 (10) | 89.46 (12) |
| N(421)–Fe(1)–N(431) ⁱ | 90.83 (10) | 90.27 (10) | 90.54 (12) |
| N(431)–Fe(1)–N(431) ⁱ | 180.0 | 180.0 | 180.0 |
| C(111)–N(411)–N(311) | 106.2 (3) | 106.1 (2) | 106.5 (3) |
| C(111)–N(411)–Fe(1) | 127.0 (2) | 128.7 (2) | 127.9 (3) |
| N(311)–N(411)–Fe(1) | 124.7 (2) | 124.5 (2) | 124.8 (2) |
| N(211)–N(311)–N(411) | 109.7 (3) | 109.9 (2) | 109.7 (3) |
| N(311)–N(211)–N(111) | 106.4 (3) | 106.3 (2) | 106.5 (3) |
| C(111)–N(111)–N(211) | 108.7 (3) | 109.0 (2) | 109.1 (3) |
| C(111)–N(111)–C(211) | 130.0 (3) | 129.5 (3) | 129.0 (3) |
| N(211)–N(111)–C(211) | 121.2 (3) | 121.4 (2) | 121.9 (3) |
| N(411)–C(111)–N(111) | 109.0 (3) | 108.8 (3) | 108.2 (3) |
| N(411)–C(111)–H(111) | 123 (3) | 128 (2) | 129 (3) |
| N(111)–C(111)–H(111) | 128 (3) | 124 (2) | 123 (3) |
| N(111)–C(211)–H(21A) | 110 (2) | 112 (2) | 110 (3) |
| N(111)–C(211)–H(21B) | 108 (3) | 108 (3) | 104 (2) |
| H(21A)–C(211)–H(21B) | 108 (4) | 112 (3) | 113 (4) |
| N(111)–C(211)–H(21C) | 105 (2) | 105 (2) | 105 (3) |
| H(21A)–C(211)–H(21C) | 114 (3) | 112 (3) | 114 (4) |
| H(21B)–C(211)–H(21C) | 112 (4) | 107 (3) | 110 (4) |
| C(121)–N(421)–N(321) | 105.7 (3) | 105.8 (2) | 106.4 (3) |
| C(121)–N(421)–Fe(1) | 129.8 (2) | 130.0 (2) | 129.9 (2) |
| N(321)–N(421)–Fe(1) | 124.5 (2) | 124.1 (2) | 123.6 (2) |
| N(221)–N(321)–N(421) | 109.9 (3) | 109.8 (2) | 109.6 (3) |
| N(321)–N(221)–N(121) | 106.9 (3) | 107.3 (2) | 106.8 (3) |
| C(121)–N(121)–N(221) | 108.4 (3) | 108.3 (2) | 108.6 (3) |
| C(121)–N(121)–C(221) | 129.9 (3) | 129.9 (2) | 130.0 (3) |
| N(221)–N(121)–C(221) | 121.5 (3) | 121.6 (2) | 121.2 (3) |
| N(421)–C(121)–N(121) | 109.1 (3) | 108.8 (3) | 108.7 (3) |
| N(421)–C(121)–H(121) | 124 (3) | 125 (2) | 125 (3) |
| N(121)–C(121)–H(121) | 127 (3) | 126 (2) | 127 (3) |
| N(121)–C(221)–H(22A) | 107 (4) | 105 (2) | 108 (4) |
| N(121)–C(221)–H(22B) | 103 (3) | 111 (3) | 112 (3) |
| H(22A)–C(221)–H(22B) | 112 (5) | 108 (4) | 109 (5) |
| N(121)–C(221)–H(22C) | 116 (4) | 113 (3) | 109 (5) |
| H(22A)–C(221)–H(22C) | 114 (6) | 109 (4) | 105 (6) |
| H(22B)–C(221)–H(22C) | 105 (5) | 112 (4) | 114 (5) |
| C(131)–N(431)–N(331) | 105.9 (3) | 105.8 (2) | 105.8 (3) |
| C(131)–N(431)–Fe(1) | 130.0 (2) | 129.9 (2) | 129.3 (3) |
| N(331)–N(431)–Fe(1) | 123.8 (2) | 124.1 (2) | 124.8 (2) |
| N(231)–N(331)–N(431) | 110.7 (3) | 110.2 (2) | 110.7 (3) |
| N(331)–N(231)–N(131) | 106.1 (3) | 106.5 (2) | 106.6 (3) |
| C(131)–N(131)–N(231) | 109.4 (3) | 108.6 (2) | 108.9 (3) |
| C(131)–N(131)–C(231) | 128.9 (3) | 129.8 (3) | 129.0 (3) |
| N(231)–N(131)–C(231) | 121.7 (3) | 121.5 (2) | 122.1 (3) |
| N(431)–C(131)–N(131) | 107.9 (3) | 108.8 (3) | 108.0 (4) |
| N(431)–C(131)–H(131) | 129 (3) | 123 (2) | 121 (2) |
| N(131)–C(131)–H(131) | 123 (3) | 128 (2) | 131 (2) |
| N(131)–C(231)–H(23A) | 108 (3) | 106 (3) | 110 (2) |
| N(131)–C(231)–H(23B) | 108 (2) | 108 (2) | 108 (3) |
| H(23A)–C(231)–H(23B) | 109 (3) | 111 (3) | 104 (4) |
| N(131)–C(231)–H(23C) | 108 (2) | 111 (2) | 110 (2) |
| H(23A)–C(231)–H(23C) | 111 (3) | 113 (3) | 114 (4) |
| H(23B)–C(231)–H(23C) | 113 (3) | 108 (3) | 111 (3) |

Table 12 (continued)

| | HS,HS (LIESST) | HS,LS (50%) | LS,LS (reverse LIESST) |
|--|-------------------|----------------|------------------------------|
| N(422)–Fe(2)–N(422) ⁱⁱ | 180.0 | 180.0 | 180.0 |
| N(422)–Fe(2)–N(432) | 90.14 (11) | 90.81 (9) | 89.34 (13) |
| N(422) ⁱⁱ –Fe(2)–N(432) | 89.86 (11) | 89.19 (9) | 90.66 (13) |
| N(422)–Fe(2)–N(432) ⁱⁱ | 89.86 (11) | 89.19 (9) | 90.66 (13) |
| N(422) ⁱⁱ –Fe(2)–N(432) ⁱⁱ | 90.14 (11) | 90.81 (9) | 89.34 (13) |
| N(432)–Fe(2)–N(432) ⁱⁱ | 180.0 | 180.0 | 180.0 |
| N(422)–Fe(2)–N(412) ⁱⁱ | 90.62 (11) | 88.78 (9) | 91.59 (12) |
| N(422) ⁱⁱ –Fe(2)–N(412) ⁱⁱ | 89.38 (11) | 91.22 (9) | 88.41 (12) |
| N(432)–Fe(2)–N(412) ⁱⁱ | 88.24 (11) | 89.62 (9) | 90.07 (12) |
| N(432) ⁱⁱ –Fe(2)–N(412) ⁱⁱ | 91.76 (11) | 90.38 (9) | 89.93 (12) |
| N(422)–Fe(2)–N(412) | 89.38 (11) | 91.22 (9) | 88.41 (12) |
| N(422) ⁱⁱ –Fe(2)–N(412) | 90.62 (11) | 88.78 (9) | 91.59 (12) |
| N(432)–Fe(2)–N(412) | 91.76 (11) | 90.38 (9) | 89.93 (12) |
| N(432) ⁱⁱ –Fe(2)–N(412) | 88.24 (11) | 89.62 (9) | 90.07 (12) |
| N(412) ⁱⁱ –Fe(2)–N(412) | 180.0 | 180.0 | 180.0 |
| C(112)–N(412)–N(312) | 106.1 (3) | 106.1 (2) | 105.9 (3) |
| C(112)–N(412)–Fe(2) | 129.6 (2) | 130.0 (2) | 130.4 (3) |
| N(312)–N(412)–Fe(2) | 124.2 (2) | 123.7 (2) | 123.7 (2) |
| N(212)–N(312)–N(412) | 109.9 (3) | 109.7 (2) | 110.5 (3) |
| N(312)–N(212)–N(112) | 106.4 (3) | 106.8 (2) | 105.6 (3) |
| C(112)–N(112)–N(212) | 108.9 (3) | 108.8 (2) | 109.4 (3) |
| C(112)–N(112)–C(212) | 129.8 (3) | 129.8 (3) | 129.5 (3) |
| N(212)–N(112)–C(212) | 120.7 (3) | 120.8 (2) | 120.4 (3) |
| N(112)–C(112)–N(412) | 108.7 (3) | 108.7 (3) | 108.6 (3) |
| N(112)–C(112)–H(112) | 126 (3) | 122 (2) | 123 (2) |
| N(412)–C(112)–H(112) | 125 (3) | 129 (2) | 128 (2) |
| N(112)–C(212)–H(21A) | 106 (3) | 106 (2) | 105 (2) |
| N(112)–C(212)–H(21B) | 106 (2) | 108 (2) | 107 (3) |
| H(21A)–C(212)–H(21B) | 114 (3) | 112 (3) | 113 (4) |
| N(112)–C(212)–H(21C) | 111 (3) | 109 (2) | 107 (3) |
| H(21A)–C(212)–H(21C) | 116 (4) | 112 (3) | 122 (4) |
| H(21B)–C(212)–H(21C) | 103 (3) | 111 (3) | 103 (4) |
| C(122)–N(422)–N(322) | 106.1 (3) | 106.5 (2) | 106.1 (3) |
| C(122)–N(422)–Fe(2) | 129.5 (2) | 128.5 (2) | 129.6 (2) |
| N(322)–N(422)–Fe(2) | 123.8 (2) | 124.2 (2) | 124.0 (3) |
| N(222)–N(322)–N(422) | 110.0 (3) | 109.6 (2) | 109.6 (3) |
| N(322)–N(222)–N(122) | 106.5 (3) | 106.7 (2) | 106.9 (3) |
| C(122)–N(122)–N(222) | 108.7 (3) | 108.3 (2) | 108.8 (3) |
| C(122)–N(122)–C(222) | 130.4 (3) | 130.1 (3) | 130.1 (3) |
| N(222)–N(122)–C(222) | 120.8 (3) | 121.5 (2) | 121.2 (3) |
| N(122)–C(122)–N(422) | 108.7 (3) | 108.8 (3) | 108.7 (3) |
| N(122)–C(122)–H(122) | 124 (3) | 127 (2) | 124 (2) |
| N(422)–C(122)–H(122) | 128 (3) | 125 (2) | 128 (2) |
| N(122)–C(222)–H(22A) | 110 (3) | 113 (2) | 109 (3) |
| N(122)–C(222)–H(22B) | 112 (3) | 108 (3) | 117 (3) |
| H(22A)–C(222)–H(22B) | 108 (4) | 116 (3) | 101 (4) |
| N(122)–C(222)–H(23C) | 109 (3) | 104 (2) | 111 (2) |
| H(22A)–C(222)–H(23C) | 110 (4) | 100 (3) | 113 (4) |
| H(22B)–C(222)–H(23C) | 108 (4) | 115 (3) | 106 (4) |
| C(132)–N(432)–N(332) | 106.1 (3) | 106.2 (2) | 105.9 (3) |
| C(132)–N(432)–Fe(2) | 131.0 (2) | 130.5 (2) | 131.1 (3) |
| N(332)–N(432)–Fe(2) | 122.4 (2) | 122.9 (2) | 122.7 (2) |
| N(232)–N(332)–N(432) | 109.9 (3) | 109.9 (2) | 109.4 (3) |
| N(332)–N(232)–N(132) | 106.9 (3) | 106.7 (2) | 107.6 (3) |
| C(132)–N(132)–N(232) | 109.2 (3) | 108.6 (2) | 108.5 (3) |
| C(132)–N(132)–C(232) | 130.2 (3) | 130.4 (3) | 130.3 (4) |
| N(232)–N(132)–C(232) | 120.6 (3) | 120.9 (2) | 121.1 (3) |
| N(132)–C(132)–N(432) | 107.9 (3) | 108.5 (3) | 108.5 (4) |
| N(132)–C(132)–H(133) | 129 (2) | 124 (2) | 128 (2) |
| N(432)–C(132)–H(133) | 124 (2) | 128 (2) | 123 (2) |
| N(132)–C(232)–H(23A) | 109 (3) | 113 (2) | 111 (3) |
| N(132)–C(232)–H(23B) | 111 (3) | 110 (2) | 109 (3) |
| H(23A)–C(232)–H(23B) | 107 (4) | 108 (3) | 108 (4) |
| N(132)–C(232)–H(23C) | 113 (3) | 107 (2) | 111 (2) |
| H(23A)–C(232)–H(23C) | 106 (4) | 109 (3) | 110 (4) |
| H(23B)–C(232)–H(23C) | 111 (4) | 110 (3) | 108 (4) |
| F(11)–B(1)–F(21) | 109.9 (3) | 110.1 (3) | 110.3 (3) |
| F(11)–B(1)–F(41) | 109.8 (3) | 110.1 (3) | 109.2 (3) |
| F(21)–B(1)–F(41) | 110.6 (3) | 110.6 (2) | 108.8 (3) |
| F(11)–B(1)–F(31) | 109.4 (3) | 109.0 (2) | 109.2 (3) |

Table 12 (continued)

| | HS,HS (LIESST) | HS,LS (50%) | LS,LS (reverse LIESST) |
|------------------|-------------------|----------------|------------------------------|
| F(21)–B(1)–F(31) | 108.5 (3) | 108.7 (3) | 110.9 (3) |
| F(41)–B(1)–F(31) | 108.6 (3) | 108.3 (3) | 108.4 (3) |
| F(22)–B(2)–F(42) | 110.3 (3) | 110.0 (2) | 109.8 (3) |
| F(22)–B(2)–F(32) | 109.8 (3) | 109.2 (2) | 109.6 (3) |

Table 13

Bond lengths (Å).

Symmetry transformations used to generate equivalent atoms: (i) $-x, -y, -z$;
(ii) $-x + 1, -y, -z$.

| | HS,HS (LIESST) | HS,LS (50%) | LS,LS (reverse LIESST) |
|----------------------------|-------------------|----------------|------------------------------|
| Fe(1)–N(411) ⁱ | 2.162 (3) | 1.983 (2) | 2.021 (3) |
| Fe(1)–N(411) | 2.162 (3) | 1.983 (2) | 2.021 (3) |
| Fe(1)–N(421) ⁱ | 2.166 (3) | 1.989 (2) | 2.034 (3) |
| Fe(1)–N(421) | 2.166 (3) | 1.989 (2) | 2.034 (3) |
| Fe(1)–N(431) | 2.205 (3) | 2.000 (2) | 2.038 (3) |
| Fe(1)–N(431) ⁱ | 2.205 (3) | 2.000 (2) | 2.038 (3) |
| N(411)–C(111) | 1.318 (4) | 1.315 (4) | 1.320 (4) |
| N(411)–N(311) | 1.371 (4) | 1.375 (3) | 1.367 (4) |
| N(311)–N(211) | 1.298 (4) | 1.297 (3) | 1.292 (4) |
| N(211)–N(111) | 1.362 (4) | 1.356 (3) | 1.354 (4) |
| N(111)–C(111) | 1.315 (4) | 1.322 (4) | 1.319 (5) |
| N(111)–C(211) | 1.467 (4) | 1.464 (4) | 1.466 (4) |
| C(111)–H(111) | 0.91 (4) | 0.90 (3) | 0.92 (5) |
| C(211)–H(21A) | 1.00 (4) | 0.99 (4) | 0.97 (5) |
| C(211)–H(21B) | 0.94 (5) | 0.94 (4) | 0.94 (4) |
| C(211)–H(21C) | 0.91 (4) | 0.91 (4) | 0.85 (4) |
| N(421)–C(121) | 1.323 (5) | 1.321 (4) | 1.315 (5) |
| N(421)–N(321) | 1.372 (4) | 1.376 (3) | 1.376 (4) |
| N(321)–N(221) | 1.292 (4) | 1.289 (4) | 1.288 (5) |
| N(221)–N(121) | 1.355 (4) | 1.351 (3) | 1.361 (4) |
| N(121)–C(121) | 1.322 (4) | 1.331 (4) | 1.321 (5) |
| N(121)–C(221) | 1.464 (5) | 1.458 (4) | 1.464 (5) |
| C(121)–H(121) | 0.87 (5) | 0.88 (4) | 0.79 (4) |
| C(221)–H(22A) | 0.88 (6) | 1.04 (5) | 0.89 (7) |
| C(221)–H(22B) | 0.90 (6) | 0.95 (5) | 0.91 (5) |
| C(221)–H(22C) | 1.03 (8) | 0.99 (5) | 0.97 (8) |
| N(431)–C(131) | 1.334 (5) | 1.325 (4) | 1.331 (5) |
| N(431)–N(331) | 1.363 (4) | 1.368 (3) | 1.363 (4) |
| N(331)–N(231) | 1.295 (4) | 1.292 (3) | 1.281 (4) |
| N(231)–N(131) | 1.351 (4) | 1.358 (3) | 1.353 (5) |
| N(131)–C(131) | 1.328 (4) | 1.322 (4) | 1.328 (5) |
| N(131)–C(231) | 1.466 (4) | 1.462 (4) | 1.468 (5) |
| C(131)–H(131) | 0.91 (4) | 0.84 (3) | 0.90 (4) |
| C(231)–H(23A) | 1.00 (5) | 0.88 (5) | 0.99 (5) |
| C(231)–H(23B) | 1.03 (4) | 0.96 (4) | 0.95 (5) |
| C(231)–H(23C) | 0.91 (4) | 0.91 (3) | 0.91 (4) |
| Fe(2)–N(422) | 2.181 (3) | 2.183 (2) | 2.007 (3) |
| Fe(2)–N(422) ⁱⁱ | 2.181 (3) | 2.183 (2) | 2.007 (3) |
| Fe(2)–N(432) | 2.185 (3) | 2.187 (2) | 2.021 (3) |
| Fe(2)–N(432) ⁱⁱ | 2.185 (3) | 2.187 (2) | 2.021 (3) |
| Fe(2)–N(412) ⁱⁱ | 2.183 (3) | 2.192 (2) | 2.023 (3) |
| Fe(2)–N(412) | 2.183 (3) | 2.192 (2) | 2.023 (3) |
| N(412)–C(112) | 1.321 (4) | 1.318 (4) | 1.319 (4) |
| N(412)–N(312) | 1.369 (4) | 1.374 (3) | 1.373 (4) |
| N(312)–N(212) | 1.299 (4) | 1.299 (3) | 1.296 (4) |
| N(212)–N(112) | 1.355 (4) | 1.347 (3) | 1.359 (4) |
| N(112)–C(112) | 1.324 (5) | 1.330 (4) | 1.322 (5) |
| N(112)–C(212) | 1.463 (4) | 1.462 (4) | 1.468 (5) |
| C(112)–H(112) | 0.95 (5) | 0.84 (4) | 0.87 (4) |
| C(212)–H(21A) | 1.04 (5) | 1.01 (4) | 1.00 (5) |
| C(212)–H(21B) | 0.93 (4) | 0.97 (3) | 1.02 (5) |
| C(212)–H(21C) | 0.99 (5) | 0.94 (4) | 1.00 (5) |
| N(422)–C(122) | 1.320 (5) | 1.311 (4) | 1.321 (5) |
| N(422)–N(322) | 1.368 (4) | 1.368 (3) | 1.369 (4) |

Table 13 (continued)

| | HS,HS (LIESST) | HS,LS (50%) | LS,LS (reverse LIESST) |
|---------------|-------------------|----------------|------------------------------|
| N(322)–N(222) | 1.293 (4) | 1.292 (4) | 1.288 (5) |
| N(222)–N(122) | 1.358 (4) | 1.358 (3) | 1.353 (4) |
| N(122)–C(122) | 1.320 (4) | 1.324 (4) | 1.313 (5) |
| N(122)–C(222) | 1.465 (5) | 1.466 (4) | 1.468 (5) |
| C(122)–H(122) | 0.87 (4) | 0.89 (3) | 0.96 (4) |
| C(222)–H(22A) | 0.91 (5) | 0.88 (4) | 0.89 (4) |
| C(222)–H(22B) | 0.93 (4) | 0.89 (4) | 0.89 (5) |
| C(222)–H(23C) | 0.98 (4) | 1.04 (4) | 1.00 (4) |
| N(432)–C(132) | 1.331 (5) | 1.319 (4) | 1.324 (5) |
| N(432)–N(332) | 1.380 (4) | 1.374 (3) | 1.378 (4) |
| N(332)–N(232) | 1.289 (4) | 1.295 (3) | 1.289 (4) |
| N(232)–N(132) | 1.354 (4) | 1.356 (4) | 1.345 (5) |
| N(132)–C(132) | 1.330 (4) | 1.334 (4) | 1.329 (5) |
| N(132)–C(232) | 1.457 (4) | 1.454 (4) | 1.454 (5) |
| C(132)–H(133) | 0.91 (4) | 0.90 (3) | 0.87 (4) |
| C(232)–H(23A) | 0.94 (4) | 0.96 (4) | 0.97 (4) |
| C(232)–H(23B) | 0.90 (4) | 0.93 (4) | 0.86 (5) |
| C(232)–H(23C) | 0.98 (5) | 0.98 (4) | 1.01 (4) |
| B(1)–F(11) | 1.385 (4) | 1.387 (4) | 1.387 (5) |
| B(1)–F(21) | 1.391 (5) | 1.390 (4) | 1.388 (5) |
| B(1)–F(41) | 1.400 (4) | 1.397 (4) | 1.404 (4) |
| B(1)–F(31) | 1.405 (4) | 1.402 (4) | 1.402 (5) |
| B(2)–F(22) | 1.390 (5) | 1.389 (4) | 1.393 (5) |
| B(2)–F(42) | 1.390 (4) | 1.395 (3) | 1.391 (5) |
| B(2)–F(32) | 1.400 (4) | 1.400 (4) | 1.395 (4) |
| B(2)–F(12) | 1.409 (4) | 1.401 (4) | 1.406 (5) |