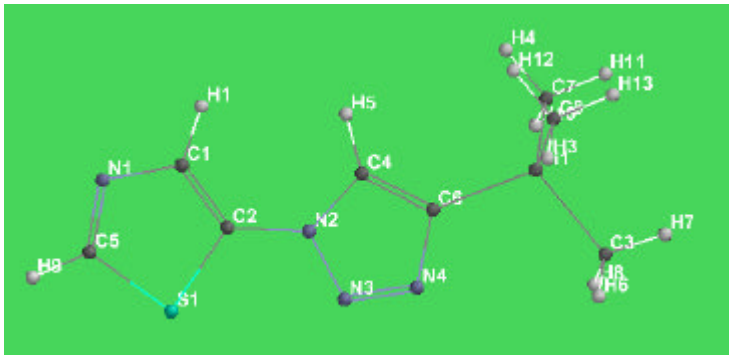
Supplementary Material for Organic & Biomolecular Chemistry


Method: RHF
Basis set: 6-31G(D)
SCF total energy: -1214.1180183 hartrees

NMR shifts (ppm) Calculated at RHF/3-21G* level for the possible isomer

**1,3-Thiazol-5-yl-4'-(trimethylsilyl)-1*H*-1,2,3-triazole 7b**

| | Atom | Isotropic | Rel. Shift | **7b** |
|---|---|---|---|---|
| 1 | S1 | 383.6772 | | |
| 2 | C2 | 65.4192 | **136.301** | **C-5** |
| 3 | C1 | 80.8523 | **120.868** | **C-4** |
| 4 | N1 | -62.7032 | | |
| 5 | C5 | 49.9667 | **151.754** | **C-2** |
| 6 | H9 | 24.3328 | **8.570** | **H-2** |
| 7 | H1 | 24.9679 | **7.935** | **H-4** |
| 8 | N2 | 37.8224 | | |
| 9 | C4 | 74.9921 | **126.729** | **C-5'** |
| 10 | C6 | 63.6898 | **138.031** | **C-4'** |
| 11 | N4 | -128.5687 | | |
| 12 | N3 | -118.8712 | | |
| 13 | H5 | 24.6543 | **8.248** | **H-5'** |
| 14 | Si1 | 453.2683 | | |
| 15 | C3 | 203.4722 | -1.752 | |
| 16 | H6 | 32.0987 | 0.804 | |
| 17 | H7 | 32.7782 | 0.125 | |
| 18 | H8 | 32.0987 | 0.804 | |
| 19 | C7 | 200.5511 | 1.170 | |
| 20 | H4 | 32.7055 | 0.197 | |
| 21 | H10 | 32.6938 | 0.209 | |
| 22 | H11 | 32.6728 | 0.230 | |
| 23 | C8 | 200.5511 | 1.170 | |
| 24 | H3 | 32.6938 | 0.209 | |
| 25 | H12 | 32.7055 | 0.197 | |
| 26 | H13 | 32.6728 | 0.230 | |

Reason for exit: Sucessful completion
Quantum Mechanics Program CPU Time : 002:31:49.9
Quantum Mechanics Program Wall Time: 001:45:53.9

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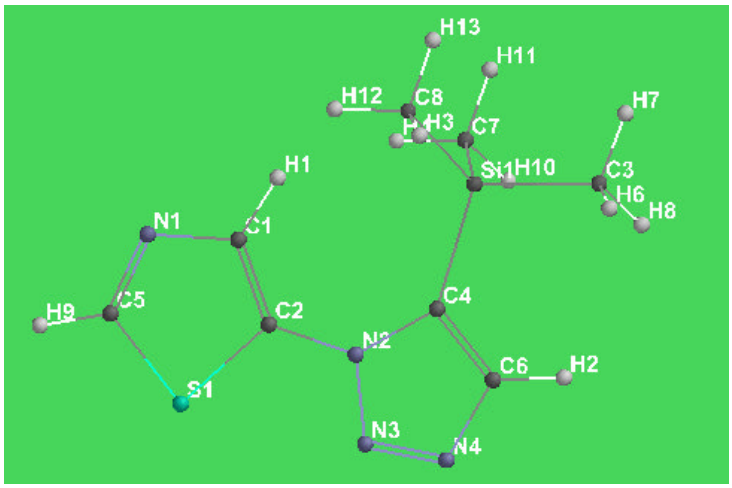


Method: RHF
Basis set: 6-31G(D)
SCF total energy: -1214.1144948 hartrees

NMR shifts (ppm) Calculated at RHF/3-21G* level for the possible isomer

**1,3-Thiazol-5-yl-5'-(trimethylsilyl)-1*H*-1,2,3-triazole 7b**

| | Atom | Isotropic | Rel. Shift | |
|---|---|---|---|---|
| 1 | S1 | 377.3189 | | |
| 2 | C2 | 62.1527 | **139.568** | **C-5** |
| 3 | C1 | 80.8805 | **120.840** | **C-4** |
| 4 | N1 | -61.1238 | | |
| 5 | C5 | 49.4389 | **152.282** | **C-2** |
| 6 | H9 | 24.3508 | **8.552** | **H-2** |
| 7 | H1 | 25.0066 | **7.896** | **H-4** |
| 8 | N2 | 31.8250 | | |
| 9 | C4 | 70.7046 | **131.016** | **C-5'** |
| 10 | C6 | 63.1687 | **138.552** | **C-4'** |
| 11 | N4 | -107.2920 | | |
| 12 | N3 | -133.6348 | | |
| 13 | Si1 | 451.4837 | | |
| 14 | C3 | 202.2337 | -0.513 | |
| 15 | H6 | 32.3831 | 0.520 | |
| 16 | H7 | 32.6220 | 0.281 | |
| 17 | H8 | 32.3831 | 0.520 | |
| 18 | C7 | 202.4650 | -0.744 | |
| 19 | H4 | 32.1289 | 0.774 | |
| 20 | H10 | 32.6725 | 0.230 | |
| 21 | H11 | 32.6074 | 0.295 | |
| 22 | C8 | 202.4650 | -0.744 | |
| 23 | H3 | 32.6725 | 0.230 | |
| 24 | H12 | 32.1289 | 0.774 | |
| 25 | H13 | 32.6074 | 0.295 | |
| 26 | H2 | 25.1413 | **7.761** | **H-4'** |

Reason for exit: Sucessful completion
Quantum Mechanics Program CPU Time : 002:46:41.6
Quantum Mechanics Program Wall Time: 001:58:49.7