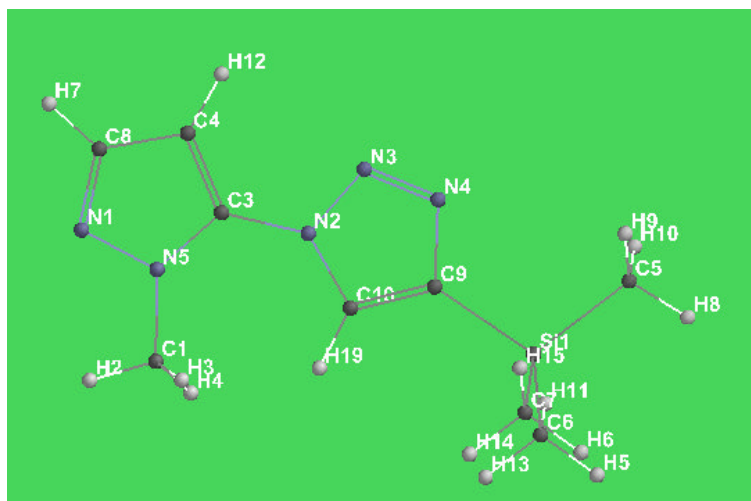




Method: RHF

Basis set: 6-31G(D)

SCF total energy: -910.6552163 hartrees

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

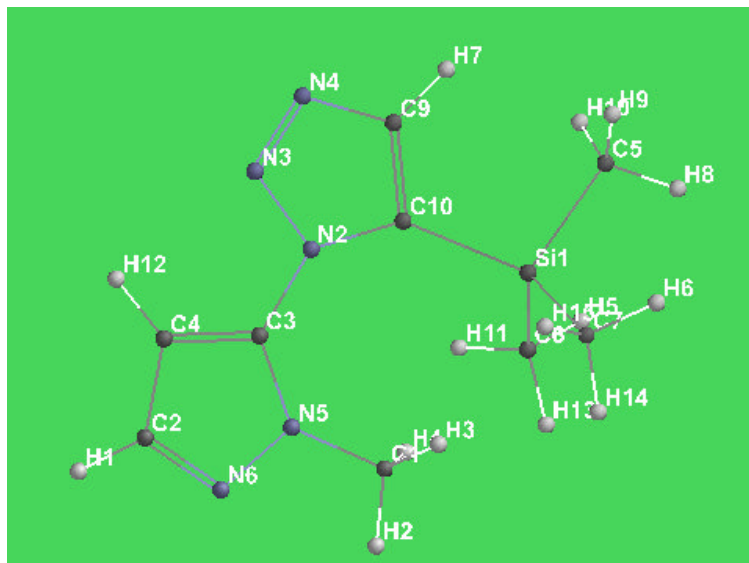
1-(1-Methyl-1H-pyrazol-5-yl)-4'-(trimethylsilyl)1H-1,2,3-triazole 4b

	Atom	Isotropic	Rel.Shift	4b*
1	N5	104.4793		
2	N1	-39.2961		
3	C8	63.7149	138.006	C-3
4	C4	109.5381	92.183	C-4
5	C3	65.0871	136.634	C-5
6	N2	36.4987		
7	N3	-123.3280		
8	N4	-128.1287		
9	C9	64.8244	136.896	C-4'
10	C10	74.6158	127.105	C-5'
11	H19	24.6032	8.299	H-5'
12	C1	164.5448	37.176	
13	H2	28.4154	4.487	
14	H3	29.1854	3.717	
15	H4	29.1854	3.717	
16	H12	25.9866	6.916	H-4
17	Si1	453.3225		
18	C5	203.4277	-1.707	
19	H8	32.7605	0.142	
20	H9	32.0555	0.847	
21	H10	32.0555	0.847	
22	C6	200.4539	1.267	
23	H5	32.6652	0.238	
24	H11	32.6794	0.223	
25	H13	32.7372	0.166	
26	C7	200.4539	1.267	
27	H6	32.6652	0.238	
28	H14	32.7372	0.166	
29	H15	32.6794	0.223	
30	H7	25.2776	7.625	H-3

Reason for exit: Successful completion

Quantum Mechanics Program CPU Time : 002:43:19.8

Quantum Mechanics Program Wall Time: 001:53:51.9



Method: RHF
Basis set: 6-31G(D)
SCF total energy: -910.6317792 hartrees

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

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

Atom	Isotropic	Rel.Shift	4b'
1	N5	104.6584	
2	N6	-38.5053	
3	C2	63.8958	137.825
4	C4	106.4413	95.279
5	C3	61.9564	139.764
6	N2	32.2004	
7	N3	-146.5899	
8	N4	-103.8755	
9	C9	61.8758	139.845
10	C10	70.4934	131.227
11	C1	166.2767	35.444
12	H2	28.5615	4.341
13	H3	29.2091	3.694
14	H4	29.2091	3.694
15	H12	25.7865	7.116
16	Si1	453.3498	
17	C5	196.1582	5.563
18	H8	32.6601	0.243
19	H9	32.2383	0.664
20	H10	32.2383	0.664
21	C6	198.3349	3.386
22	H5	32.4501	0.453
23	H11	32.3649	0.538
24	H13	32.5653	0.337
25	C7	198.3349	3.386
26	H6	32.4501	0.453
27	H14	32.5653	0.337
28	H15	32.3649	0.538
29	H7	25.1312	7.772
30	H1	25.3111	7.592

```
Reason for exit: Successful completion
Quantum Mechanics Program CPU Time : 003:52:21.7
Quantum Mechanics Program Wall Time: 003:28:50.7
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