SUPPLEMANTARY INFORMATION

A Matrix Isolation and Computational Study of the [C, N, F, S] Isomers

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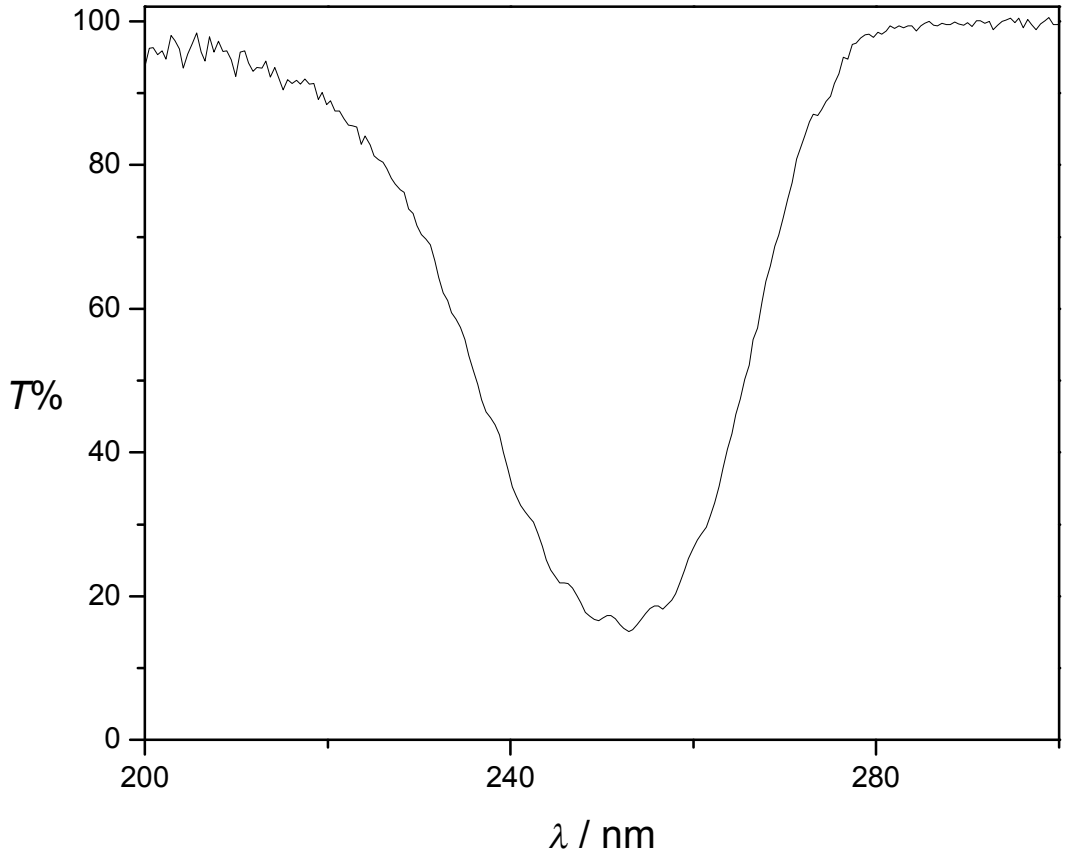

Figure S1. Gas-phase UV spectrum of 3,4-difluoro-1,2,5-thiadiazole (1 atm, in air)

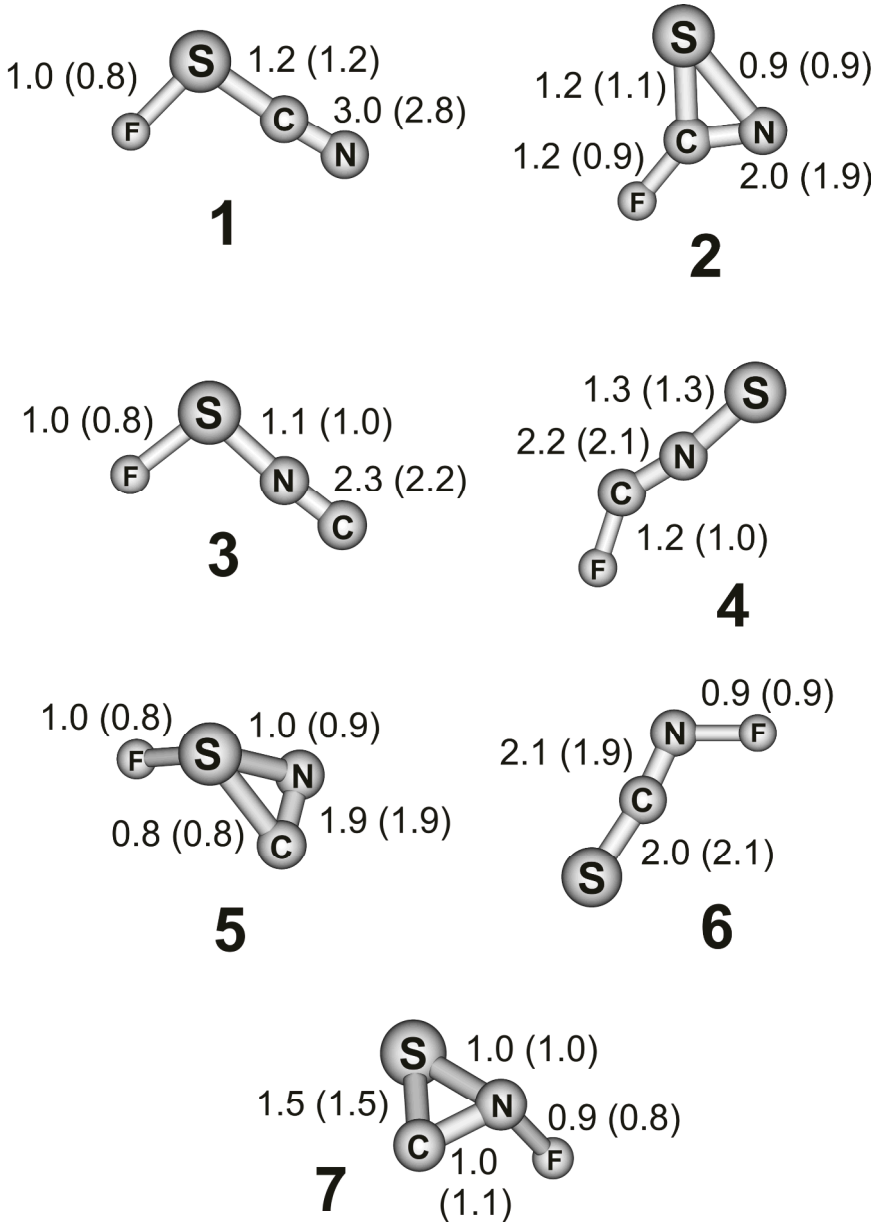

Figure S2. Mayer's bond orders and Wiberg bond indexes (in parenthesis) calculated at the B3LYP/TZ level of theory.

Table S1: Observed vibrational transitions of 3,4-difluoro-1,2,5-thiadiazole in Ar matrix.

$\tilde{\nu}$ /cm^{-1}	A
3776.8	8.8×10^{-3}
3711.6	8.3×10^{-3}
3031.5	1.3×10^{-3}
2778.0	2.3×10^{-3}
2769.6	3.2×10^{-3}
2746.1	5.4×10^{-3}
2741.9	4.8×10^{-3}
2411.6	4.6×10^{-3}
2405.8	1.1×10^{-3}
2396.8	1.8×10^{-3}
2292.6	1.7×10^{-3}
2291.2	1.4×10^{-3}
2153.4	4.1×10^{-3}
2126.2	2.9×10^{-3}
1832.0	4.0×10^{-3}
1820.4	2.2×10^{-3}
1803.7	1.0×10^{-3}
1799.2	3.3×10^{-3}
1643.7	4.1×10^{-3}
1559.6	9.8×10^{-2}
1557.4	1.8×10^{-2}
1554.2	2.0×10^{-2}
1552.4	1.1×10^{-2}
1544.9	3.9×10^{-3}
1522.9	1.1×10^{-2}
1518.2	9.0×10^{-1}
1514.6	3.9×10^{-2}
1501.0	1.1×10^{-2}
1497.4	1.4×10^{-1}
1493.0	3.7×10^{-2}
1485.1	6.3×10^{-2}
1477.9	1.1×10^{-2}
1432.3	3.1×10^{-3}
1423.6	4.0×10^{-3}
1415.4	2.4×10^{-3}
1380.0	4.4×10^{-3}
1377.0	1.0×10^{-1}
1356.6	1.7×10^{-3}
1257.7	8.3×10^{-2}
1212.6	1.0×10^{-1}
1203.3	9.9×10^{-3}
1152.0	1.5×10^{-3}
1118.1	3.1×10^{-3}
894.9	9.2×10^{-2}
892.2	7.1×10^{-3}
888.5	5.7×10^{-3}
884.7	2.9×10^{-3}
882.1	2.6×10^{-2}
869.9	1.6×10^{-1}
864.7	6.6×10^{-3}
777.9	1.6×10^{-2}
609.1	1.1×10^{-2}
606.6	6.3×10^{-2}
536.2	1.2×10^{-1}

Table S2: B3LYP/TZ Vibrational Frequencies (in cm^{-1}) and Infrared Intensities[b] (km mol^{-1}) of [C, N, F, S] isomers.

Molecule	anharmonic frequency (harmonic frequency) [IR intensity]
FCNS	2030 (2095) [69]; 1133 (1154) [488]; 734 (746) [96]; 430 (434) [110]; 326 (322) [1]; 204 (208) [55]
FSCN	2196 (2225) [1]; 762 (771) [100]; 692 (698) [11]; 462 (467) [2]; 397 (398) [2]; 185 (185) [8]
FSNC	2030 (2060) [178]; 768 (777) [115]; 705 (710) [33]; 389 (392) [5]; 294 (294) [0.1]; 152 (149) [3]
FNCS	1837 (1871) [333]; 994 (1014) [101]; 771 (789) [124]; 578 (584) [6]; 420 (423) [1]; 180 (182) [7]
FC(NS)	1798 (1833) [166]; 1134 (1157) [240]; 745 (757) [11]; 508 (513) [9]; 499 (506) [17]; 328 (331) [0.3]
FS(NC)	1653 (1674) [12]; 767 (781) [129]; 626 (649) [15]; 442 (463) [1]; 323 (326) [4]; 282 (290)[3]
FN(SC)	1070 (1095) [14]; 712 (738) [117]; 669 (694) [18]; 632 (646) [85]; 434 (444) [4]; 292 (296) [1]