

**Table S1**

Calculated global reactivity descriptors for 4-methyl-1,2,3-thiadiazole-5-carboxylic acid (4MTCA) (Conf. 1) at B3LYP/6-311++G(d,p) level.

Ionization Potential	<b>IP (eV)</b>	0.93056
Electron Affinity	<b>EA (eV)</b>	10.01468
Electro-negativity	<b>(<math>\chi</math>) (eV)</b>	5.47253
Chemical Potential	<b>(<math>\mu</math>) (eV)</b>	-5.47262
Chemical Hardness	<b>(<math>\eta</math>) (eV)</b>	4.54206
Global Softness	<b>(S) (eV<sup>-1</sup>)</b>	163.01479
Global Electrophilicity Index	<b>(<math>\omega</math>) (eV)</b>	3.29682

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**Table S2**

NHO directionality and "bond bending" (deviations from line of nuclear centers).

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Bond (A-B)	Deviation at A (°)	Deviation at B (°)
C1-C2	1.4	2.4
C1-S3	4.9	8.7
C1-C10	1.9	1.3
C2-C6	1.5	1.2
S3-N4	5.5	6.2
N4-N5	4.0	2.6
C6-H8	1.5	--
C6-H9	1.5	--
C10-O11	4.9	--
C10-O12	--	1.2
O11-H13	2.9	--

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**Table S3**

Thermodynamic properties of 4MTCA calculated at different temperatures using DFT-B3LYP/6-311++G(d,p) method.

T(K)	$C_{p,m}^0$ (cal.mol <sup>-1</sup> K <sup>-1</sup> )	$S_m^0$ (cal.mol <sup>-1</sup> K <sup>-1</sup> )	$\Delta H_m^0$ (kcal.mol <sup>-1</sup> )
100	14.176	68.556	1.204178257
200	22.182	82.189	3.216580378
298.15	29.802	93.282	5.968808536
300	29.938	93.48	6.027793818
400	36.723	103.621	9.568793247
500	42.296	112.88	13.72913814
600	46.736	121.362	18.38772041
700	50.272	129.149	23.44351208

Zero point vibrational energy (Kcal/Mol) (at T=298.15K) = 53.08094

Rotational constants (GHZ): 2.12449 1.40787 0.85116