Electronic Supplementary Material (ESI) for Dalton Transactions.

Energetic Derivatives of 5-(5-Amino-2*H*-1,2,3-triazol-4-yl)-1*H*-tetrazole

Supporting Information

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Contents:

Table S1: Crystallographic data for **2** and **5**.

	2	**5**
Formula	$C_{10}H_{11}N_5O$	$C_3H_4N_8$
M / g mol^{-1}	217.23	152.14
Color	colorless	colorless
Habit	block	block
Crystal size / mm	0.267 × 0.127 × 0.117	0.080 × 0.050 × 0.040
Crystal system	monoclinic	monoclinic
Space Group	$P2_1/c$ (14)	$P2_1/n$ (14)
a / Å	11.731(4)	6.9019(4)
b / Å	7.423(2)	11.6423(7)
c / Å	11.188(4)	8.0685(4)
α / °	90	90
β / °	93.655(3)	113.881(2)
γ / °	90	90
V / Å^3	972.3(5)	592.83(6)
Z	4	4
$\rho_{calc.}$ / g cm^{-3}	1.484	1.705
T / K	173(2)	100(2)
F(000)	456	312
μ / mm^{-1}	0.104	0.131
$\lambda_{MoK\alpha}$ / Å	0.71073	0.71073
θ range / °	4.14–26.37	3.269–26.367
Dataset (h; k; l)	−14:14; −9:9; −12:13	−8:8; −14:14; −9:10
Collected reflections	6884	6279
Independent reflections	1980	1218
Observed reflections	1738	1057
$R_{int.}$	0.0235	0.0217
Parameters	189	116
Restraints	0	0
R_1 (obs.)	0.0318	0.0323
wR_2 (all data)	0.0802	0.0903
S	1.063	1.085
Res. dens. / e Å^{-3}	−0.203:0.240	−0.191:0.348
Solution	SIR97	SIR97
Refinement	SHELXL-97	SHELXL-2013
Absorption correction	multi-scan	multi-scan
CCDC	1406925	1413469

NMR Spectroscopy

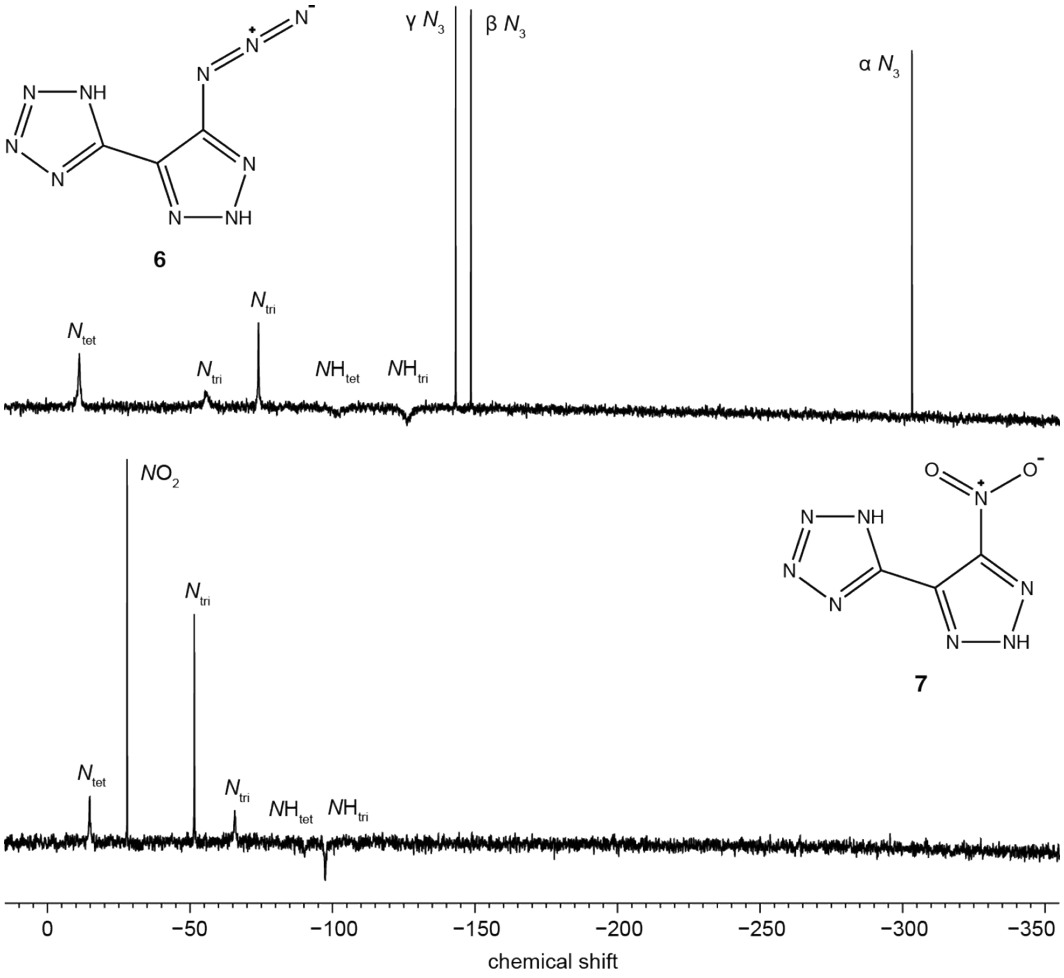

Figure S1: $^{15}N\{^1H\}$ NMR spectra of 5-(5-azido-2*H*-1,2,3-triazol-4-yl)-1*H*-tetrazole (**6**) and 5-(5-nitro-2*H*-1,2,3-triazol-4-yl)-1*H*-tetrazole (**7**) in DMSO-d_6 at room temperature.