Supplementary Material

Synthesis, structure and properties of 2,4,6-triazidopyrimidine-5-carbonitrile

S. V. Chapyshev,* D. V. Korchagin, A. V. Chernyak, and Viktor A. Garanin

Institute of Problems of Chemical Physics, Russian Academy of Sciences, 142432 Chernogolovka, Moscow Region, Russian Federation
Email: Sergei V. Chapyshev – s.chapyshev@mail.ru
*Corresponding author

Table of Contents

I. ^{13}C and ^{15}N NMR spectra of 2,4.6-triazidopyrimidine-5-carbonitrile (9)

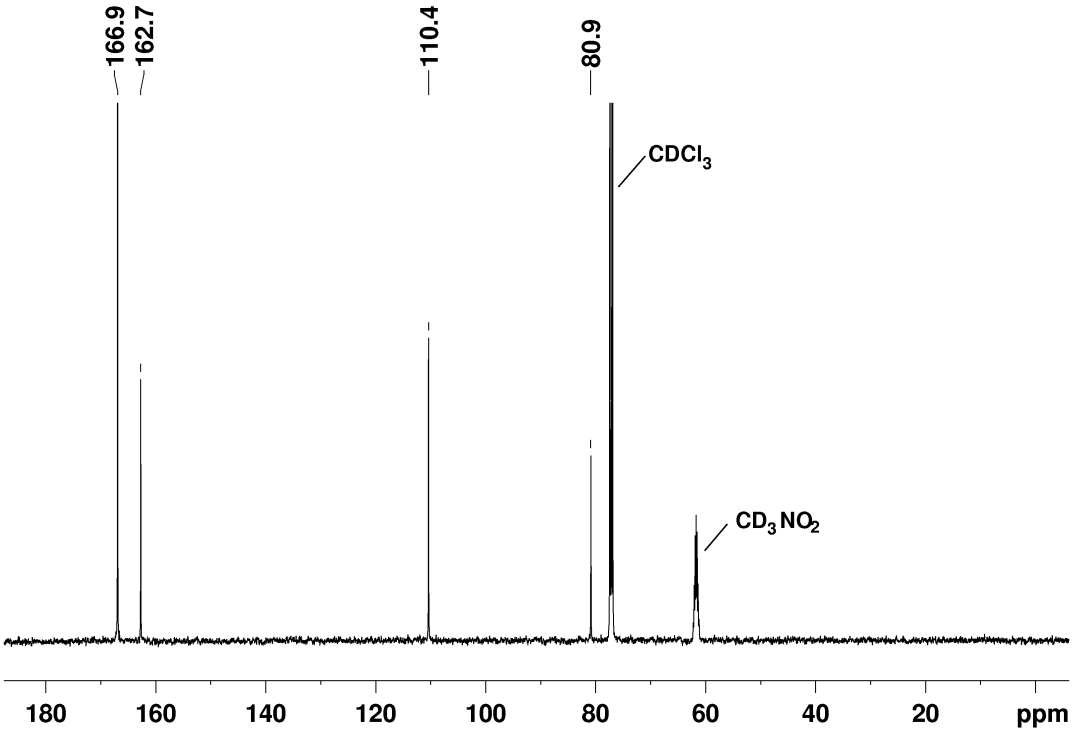


Figure S1: ^{13}C NMR spectrum of triazide **9** ($CDCl_3/CD_3NO_2$).

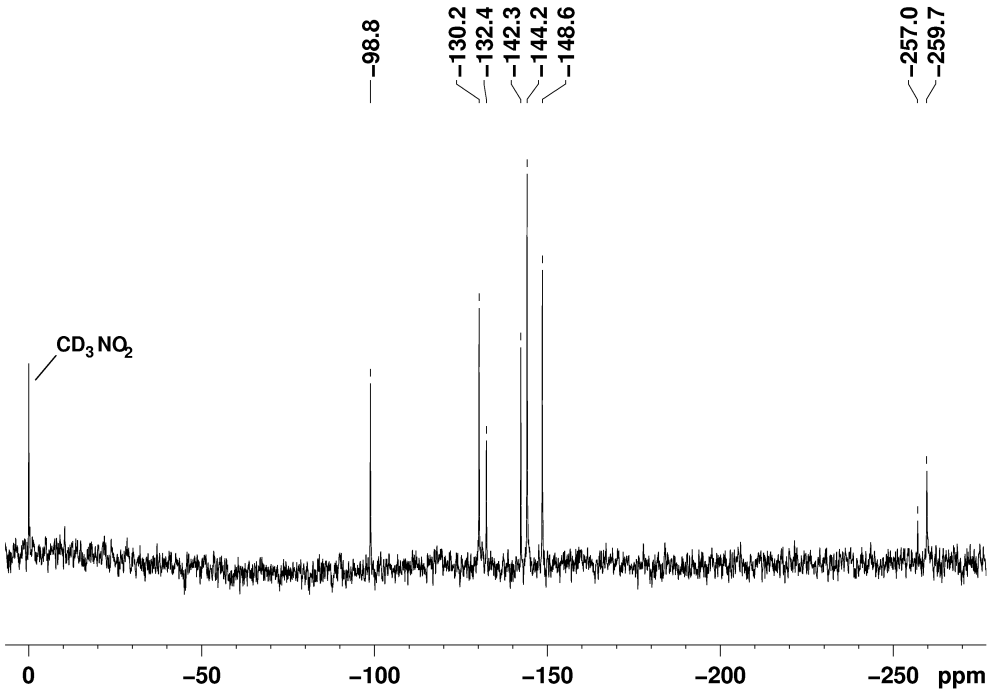


Figure S2: ^{15}N NMR spectrum of triazide **9** ($CDCl_3/CD_3NO_2$).

II. IR and UV spectra of triazide 9

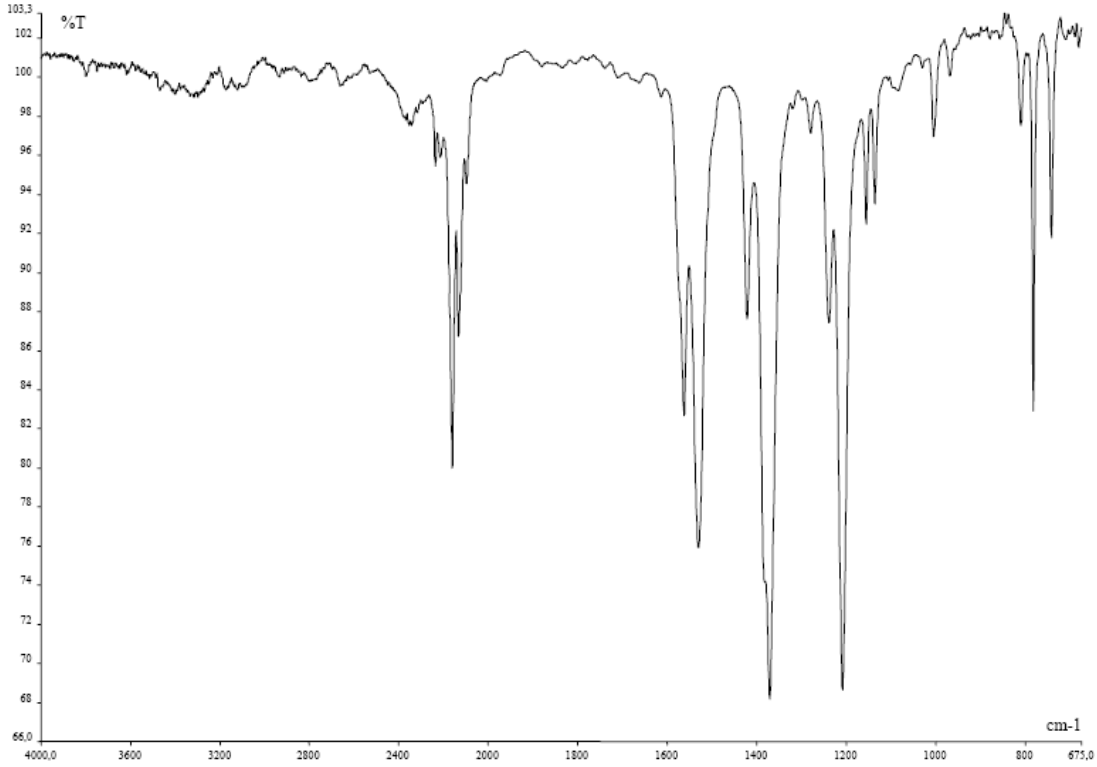


Figure S3: IR spectrum of triazide **9** (microcrystals).

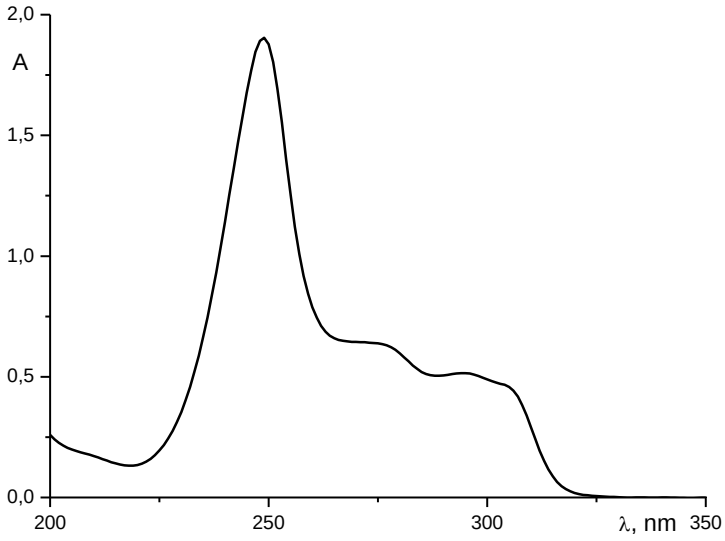


Figure S4: UV spectrum of triazide **9** (MeCN).

III. Electron impact mass-spectrum (EIMS) of triazide 9

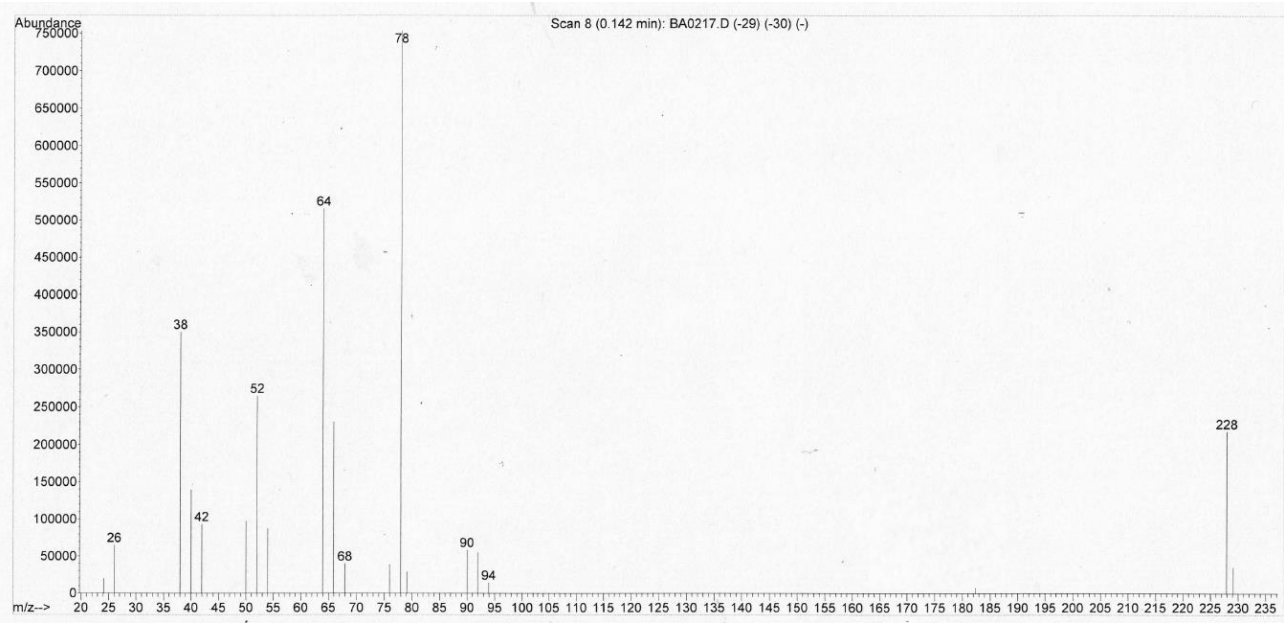


Figure S5: EIMS (70 eV) of triazide **9**.

IV. Theoretical heats of formation of triazides 1 and 9

The isodesmic reactions used to obtain the heats of formation of triazides **1** and **9** at 298 K:

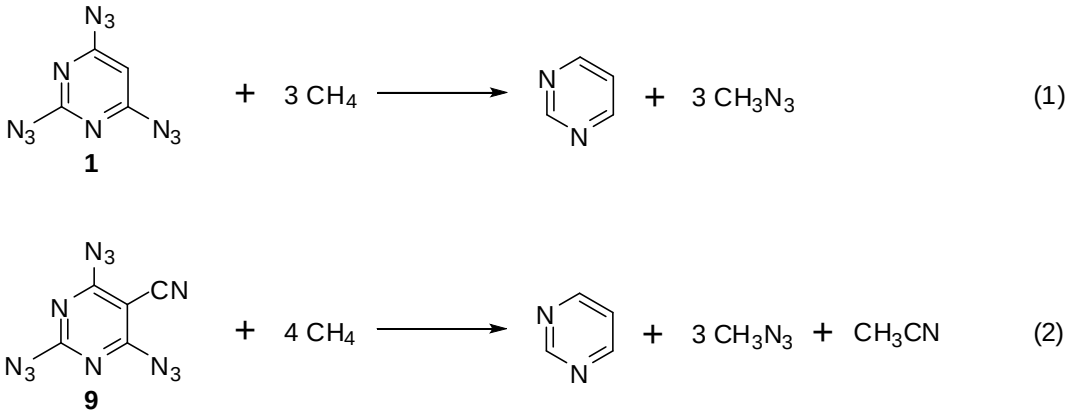
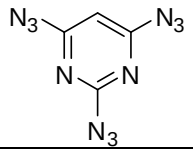


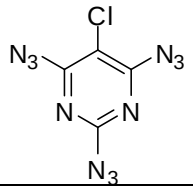
Table S1. CBS-4 calculated enthalpies (a.u.)* and heats of formation (HOFs, kJ mol^{-1}) for the reference compounds for a gas phase at 298 K.

Compound	CBS-4 enthalpy*	HOF
Triazide **1**	–754.120917	1123.61
Triazide **9**	–846.236379	1276.71
CH_4	–40.425402	–74.87[a]
CH_3N_3	–203.803562	296.5[b]
$C_4H_5N_2$	–263.915156	196.65[c]
CH_3CN	–132.542473	74.04[d]

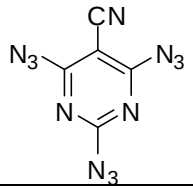
* Montgomery, J. A., Jr.; Frisch, M. J.; Ochterski, J. W.; Petersson, G. A. *J. Chem. Phys.* **2000**, *112*, 6532.
[a] Chase, M. W., Jr. *NIST-JANAF Themochemical Tables, Fourth Edition, J. Phys. Chem. Ref. Data, Monograph 9*, **1998**, 1–1951.
[b] Lide D. R., *Handbook of Chemistry and Physics*, 84ed, CRC Press Boca Raton FL, 2002.
[c] Cox, J. D.; Pilcher, G. *Thermochemistry of Organic and Organometallic Compounds*, Academic Press, New York, 1970, 1-636.
[d] An, X.; Mansson, M. *Enthalpies of combustion and formation of acetonitrile*, *J. Chem. Thermodyn.*, **1983**, *15*, 287–293.

V. Absolute energies and Cartesian coordinates for B3LYP/6-311+G(d) optimized molecular geometries of azides 1, 2 and 9

1 			Charge : 0 Multiplicity : 1 Total energy: -755.3158508 a.u.
7	1.710833000	8.775469000	2.170443000
7	3.117789000	4.974425000	4.767722000
7	1.613297000	7.558798000	1.928449000
7	2.680780000	7.192798000	4.005107000
7	3.741214000	6.760054000	6.064437000
7	2.487241000	3.118963000	3.453469000
7	3.789434000	7.993161000	6.210706000
6	2.557704000	4.502788000	3.650381000
6	2.030712000	5.321410000	2.652330000
7	2.964118000	2.409607000	4.359024000
6	3.146832000	6.299451000	4.880547000
6	2.126258000	6.688171000	2.897189000
7	1.727621000	9.897635000	2.250406000
7	3.351912000	1.645738000	5.087591000
7	3.905896000	9.078718000	6.484421000
1	1.581359000	4.924815000	1.754779000

2 	Charge : 0 Multiplicity : 1 Total energy: -1214.9284658 a.u.

17	3.032479000	6.929477000	2.137899000
7	-2.792762000	2.606723000	1.028368000
7	3.774333000	4.036777000	2.268911000
7	4.603502000	1.828587000	2.417848000
7	4.133603000	2.846149000	2.332679000
7	-0.484152000	2.356015000	1.461866000
7	-2.201067000	7.379807000	1.153213000
7	-0.217918000	4.697247000	1.519012000
7	-1.687024000	2.571855000	1.236034000
7	1.607148000	3.208774000	1.858316000
7	-1.122476000	7.134076000	1.355770000
7	0.096480000	7.035278000	1.585220000
6	1.969639000	5.579248000	1.933706000
6	0.329991000	3.486147000	1.618589000
6	2.421535000	4.253850000	2.014849000
6	0.602690000	5.739992000	1.676720000

9 	Charge : 0 Multiplicity : 1 Total energy: -847.5745632 a.u.

7	0.939862000	-1.236837000	0.000129000
7	-1.223476000	-0.230788000	0.000061000
7	-1.459949000	2.113452000	-0.000008000
7	-2.692123000	1.924244000	0.000010000
7	3.525260000	-0.967257000	0.000001000
7	2.876311000	0.098440000	0.000051000
7	-2.166750000	-2.646051000	0.000080000
7	-3.815526000	1.916088000	-0.000096000
7	-0.923817000	-2.565179000	0.000129000
6	-0.660759000	0.977362000	-0.000004000
7	1.819873000	3.498459000	-0.000033000
6	0.735291000	1.163921000	0.000034000
6	-0.390694000	-1.275320000	0.000105000
7	-3.265555000	-2.883709000	-0.000199000
6	1.493291000	-0.026667000	0.000115000
7	4.242471000	-1.831187000	-0.000284000
6	1.332937000	2.450545000	-0.000003000