

Electronic Supplementary Information:

**Role of substituents in the Hofmann-Löffler-Freytag reaction.
A quantum-chemical case study on nicotine synthesis**

Sofia Shkunnikova,^a Hendrik Zipse^b and Davor Šakić^{*a}

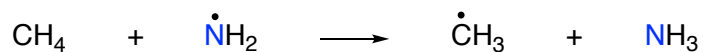
a. University of Zagreb, Faculty of Pharmacy and Biochemistry, Ante Kovačića 1, 10000 Zagreb, Croatia

*b. Department of Chemistry, LMU München, Butenandtstrasse 5-13, D-81377 München,
Germany.*

† Corresponding author: Tel.: +385 1 4818 305; e-mail: dsakic@pharma.unizg.hr

Electronic Supplementary Information (ESI): geometries and energies of all calculated structures.

System 0



1H

15

1

15H

H(kJ/mol)

ΔH(kJ/mol)

NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
1	NulC_rad	-39.804412	-39.773085	-39.789551	0.00	0.00	0.00	exp.	a)
								439.3±0.4	
								kJ/mol	
1H	NulC_neut	-40.469373	-40.434258	-40.454472	-	-	-		
15	NH3_Nrad	-55.849865	-55.829037	-55.835797	0.00	0.00	0.00	exp.	b)
								450.1±0.1	
								kJ/mol	
15H	NH3_neut	-56.509611	-56.494282	-56.504485	-	-	-		
ST_ID1		-80.273785	-80.207343	-80.244023	0.00	0.00	0.00		
MIN_I	Ident_Me_Me_opt_fwd.log	-80.272565	-80.205487	-80.242527	3.20	4.87	3.93		
D1									
TS_ID1	Ident_Me_Me.log	-80.253198	-80.181812	-80.216499	54.05	67.03	72.26		
START	START_Metilamin_nulC	-96.319238	-96.263295	-96.290269	0.00	0.00	0.00		
0									
R0	NH3_TS_nulC_symm_ver1_opt_re v	-96.319532	-96.262693	-96.290107	-0.77	1.58	0.00	0.43	0.00
TS0	NH3_TS_nulC_symm_ver1	-96.302683	-96.245738	-96.268904	43.47	46.10	44.52	56.09	55.67

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)			G3B3	
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP			
P0	NH3_TS_nulC_symm_ver1_opt_fw d	-96.315028	-96.266891	-96.293887	11.05	-9.44	-11.02	-9.50	-9.92
FIN0	FIN_Metilamin_nulC	-96.314023	-96.267367	-96.294036	13.69	-10.69		-9.89	

- a) RSE compared to CH₄/CH₃[•] radical system
b) RSE compared to NH₃/NH₂[•] radical system

1

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H3(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\0,2\C,0,0.,0.,0.000155\H,0,0.,1.082798,-0.00031\H,0,0.937731,-0.541399,-0.00031\H,0,-0.937731,-0.541399,-0.00031\\Version=ES64L-G16RevA.03\State=2-A1\HF=-39.7559614\MP2=-39.8069654\RMSD=3.347e-09\PG=C03V[C3(C1),3SGV(H1)]\\

1H

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C1H4\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\0,1\C,0,0.,0.,0.\H,0,0.631339,0.631339,0.631339\H,0,-0.631339,-0.631339,0.631339\H,0,-0.631339,0.631339,-0.631339\H,0,0.631339,-0.631339,-0.631339\\Version=ES64L-G16RevA.03\State=1-A1\HF=-40.4209215\MP2=-40.4832688\RMSD=1.296e-09\PG=TD[O(C1),4C3(H1)]\\

15

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\H2N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\0,2\N,0,0.,0.,0.14444\H,0,0.,0.804686,-0.505541\H,0,0.,-0.804686,-0.505541\\Version=ES64L-G16RevA.03\State=2-B1\HF=-55.7918729\MP2=-55.8517922\RMSD=1.893e-09\PG=C02V[C2(N1),SGV(H2)]\\

15H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\H3N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\0,1\N,0,0.,0.,0.119349\H,0,0.,0.938581,-0.278482\H,0,-0.812835,-0.469291,-0.278482\H,0,0.812835,-0.469291,-0.278482\\Version=ES64L-G16RevA.03\State=1-A\HF=-56.4579585\MP2=-56.5326192\RMSD=3.740e-09\PG=C03[C3(N1),X(H3)]\\

MIN_ID1

GINC-SL250S-GEN8-06-05\SP\ROB2PLYP-FC\GTMP2large\C2H7(2)\DSAKIC\19-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\0,2\C,0,0.000001,2.15669,0.\H,0,1.082676,2.171163,0.\H,0,0.000344,-0.851133,0.\H,0,-0.541341,2.170888,0.937625\H,0,-0.541341,2.170888,-0.937625\C,0,0.000001,-1.945033,0.\H,0,0.515162,-2.310747,0.892488\H,0,-1.030671,-2.310256,0.\H,0,0.515162,-2.310747,-0.892488\\Version=ES64L-G16RevA.03\State=2-A\HF=-80.1766631\MP2=-80.2903491\RMSD=5.804e-09\PG=CS[SG(C2H3),X(H4)]\\

TS_ID1

GINC-SL230S-GEN8-02-02\SP\ROB2PLYP-FC\GTMP2large\C2H7(2)\DSAKIC\19-Oct-2019\0\#\rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,0,0.,1.348533\H,0,0.,1.050882,1.639313\H,0,0,0.,0.\H,0,0.910091,-0.525441,1.639313\H,0,-0.910091,-0.525441,1.639313\C,0,0,0.,-1.348
533\H,0,0.910091,0.525441,-1.639313\H,0,0.,-1.050882,-1.639313\H,0,-0.910091,0.525441,-1.639313\\Version=ES64L-G16RevA.03\State=2-
A2U\HF=-80.139045\MP2=-80.2623605\RMSD=3.929e-10\PG=D03D[O(H1),C3(C1.C1),3SGD(H2)]\

R0

GINC-SL230S-GEN8-02-03\SP\ROB2PLYP-FC\GTMP2large\C1H6N1(2)\DSAKIC\18-Apr-2019\0\#\rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,1.717595,-0.000135,0.005213\H,0,2.366636,-0.003299,-0.874848\H,0,0.671006,-0.001092,-0.315462\H,0,1.920593,-0.890628,0.607144\H,
0,1.920879,0.894465,0.600928\N,0,-1.866556,-0.000172,-0.142945\H,0,-2.062717,-0.803999,0.476654\H,0,-2.05608,0.806569,0.474927\
\Version=ES64L-G16RevA.03\State=2-A\HF=-96.2126789\MP2=-96.3355371\RMSD=9.101e-09\PG=C01[X(C1H6N1)]\

TS0

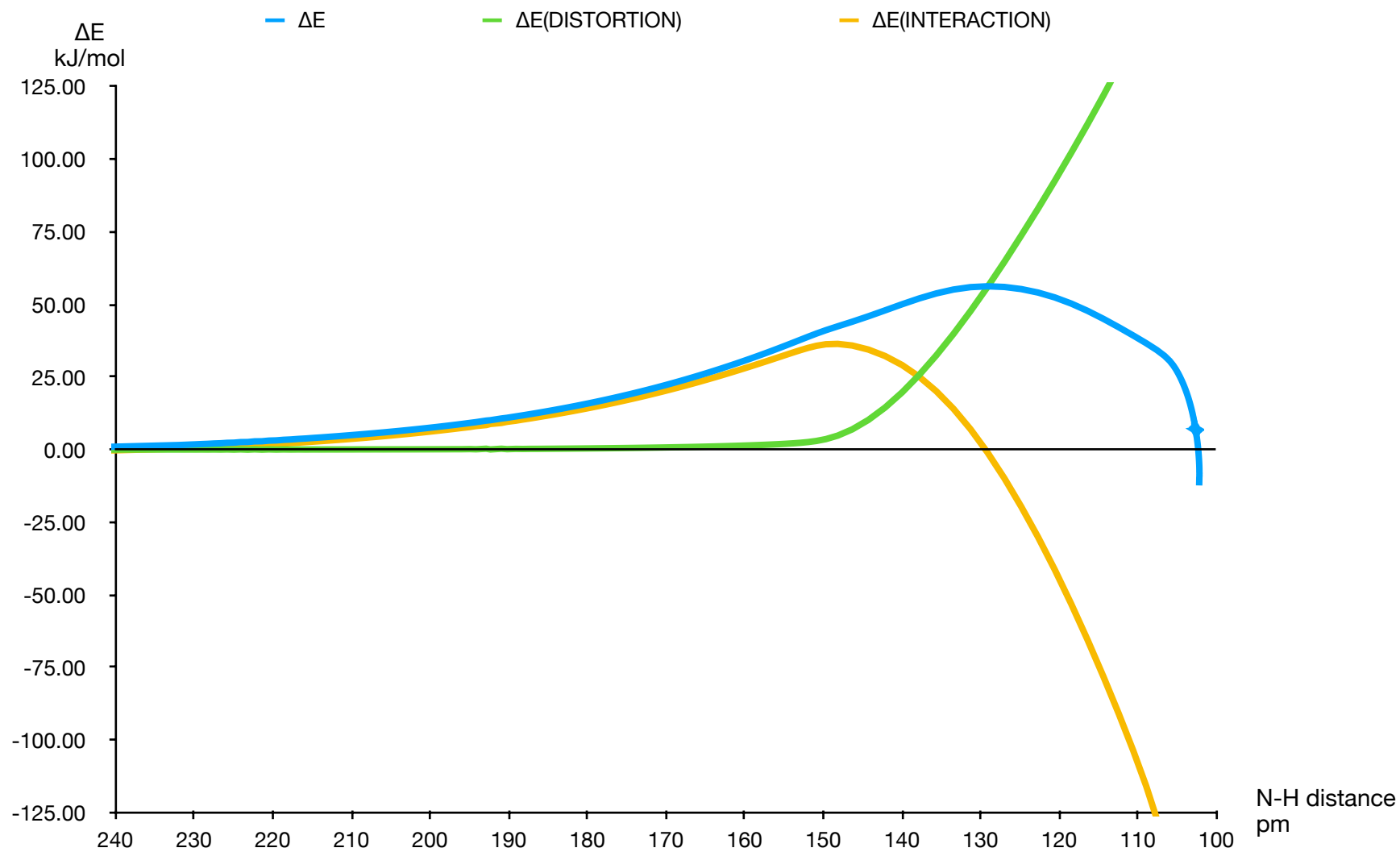
GINC-SL250S-GEN8-09-05\SP\ROB2PLYP-FC\GTMP2large\C1H6N1(2)\DSAKIC\18-Apr-2019\0\#\rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,0.060821,1.264535,0.\H,0,1.094467,1.611763,0.\H,0,0.206656,-0.083119,0.\H,0,-0.48083,1.522521,0.910121\H,0,-0.48083,1.522521,-0.91
0121\N,0,0.060821,-1.322699,0.\H,0,-0.565068,-1.451001,0.806458\H,0,-0.565068,-1.451001,-0.806458\\Version=ES64L-G16RevA.03\State=2-
A\HF=-96.1775047\MP2=-96.3144891\RMSD=4.672e-09\PG=CS[SG(C1H2N1),X(H4)]\

P0

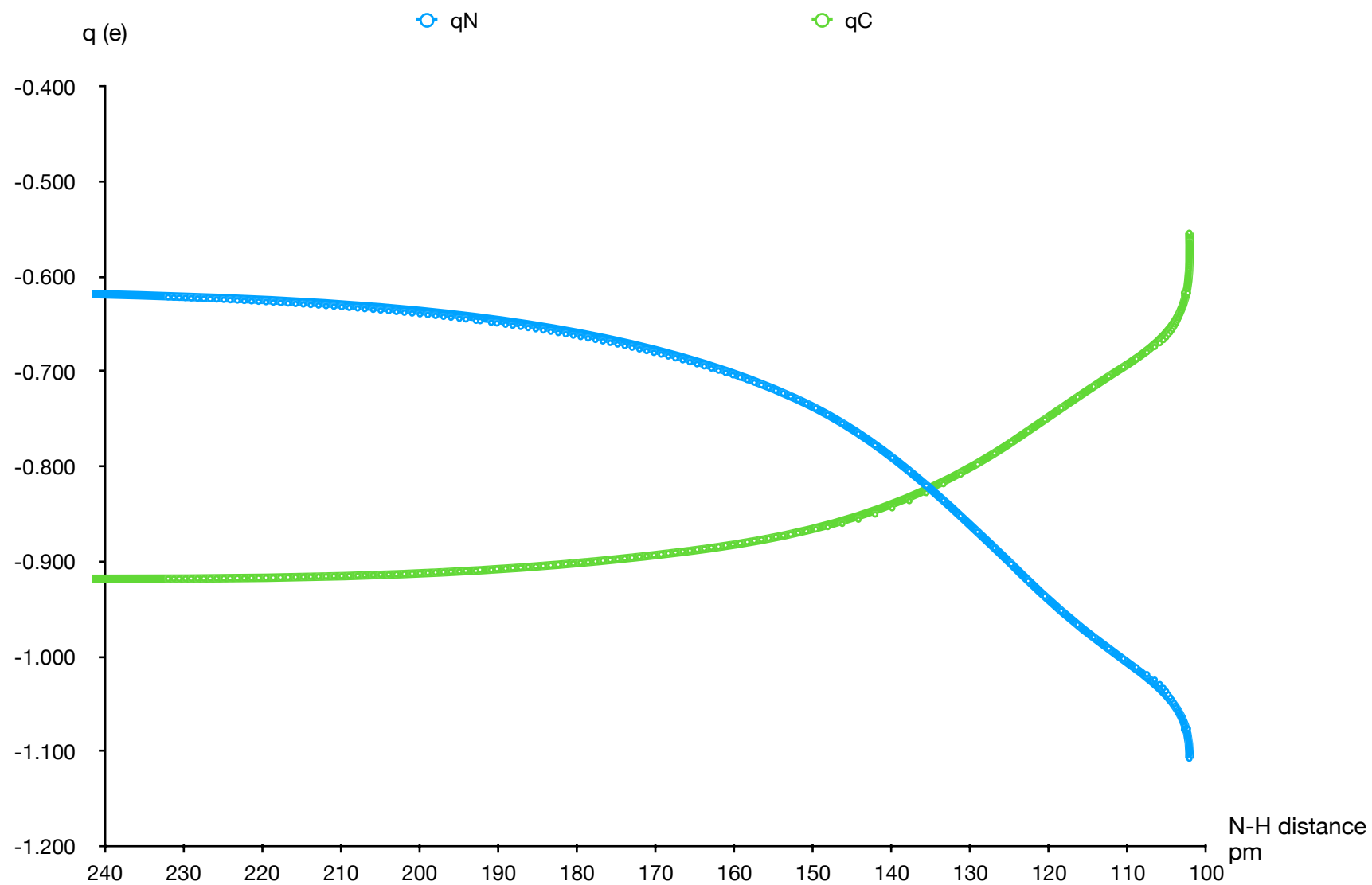
GINC-NX360-M5-02-02\SP\ROB2PLYP-FC\GTMP2large\C1H6N1(2)\DSAKIC\18-Apr-2019\0\#\rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,1.824709,0.,-0.015243\H,0,1.902772,-0.002505,1.065106\H,0,-0.71062,0.000065,0.274939\H,0,1.855982,0.938337,-0.555335\H,0,1.85599
7,-0.935796,-0.559724\N,0,-1.72012,0.000002,0.11593\H,0,-1.905821,0.811864,-0.472584\H,0,-1.905723,-0.811978,-0.47246\\Version=ES64L-
G16RevA.03\State=2-A\HF=-96.2138085\MP2=-96.3402406\RMSD=6.025e-09\PG=C01[X(C1H6N1)]\

Scheme S1. Distortion/Interaction (Activation/Strain) analysis for System 0

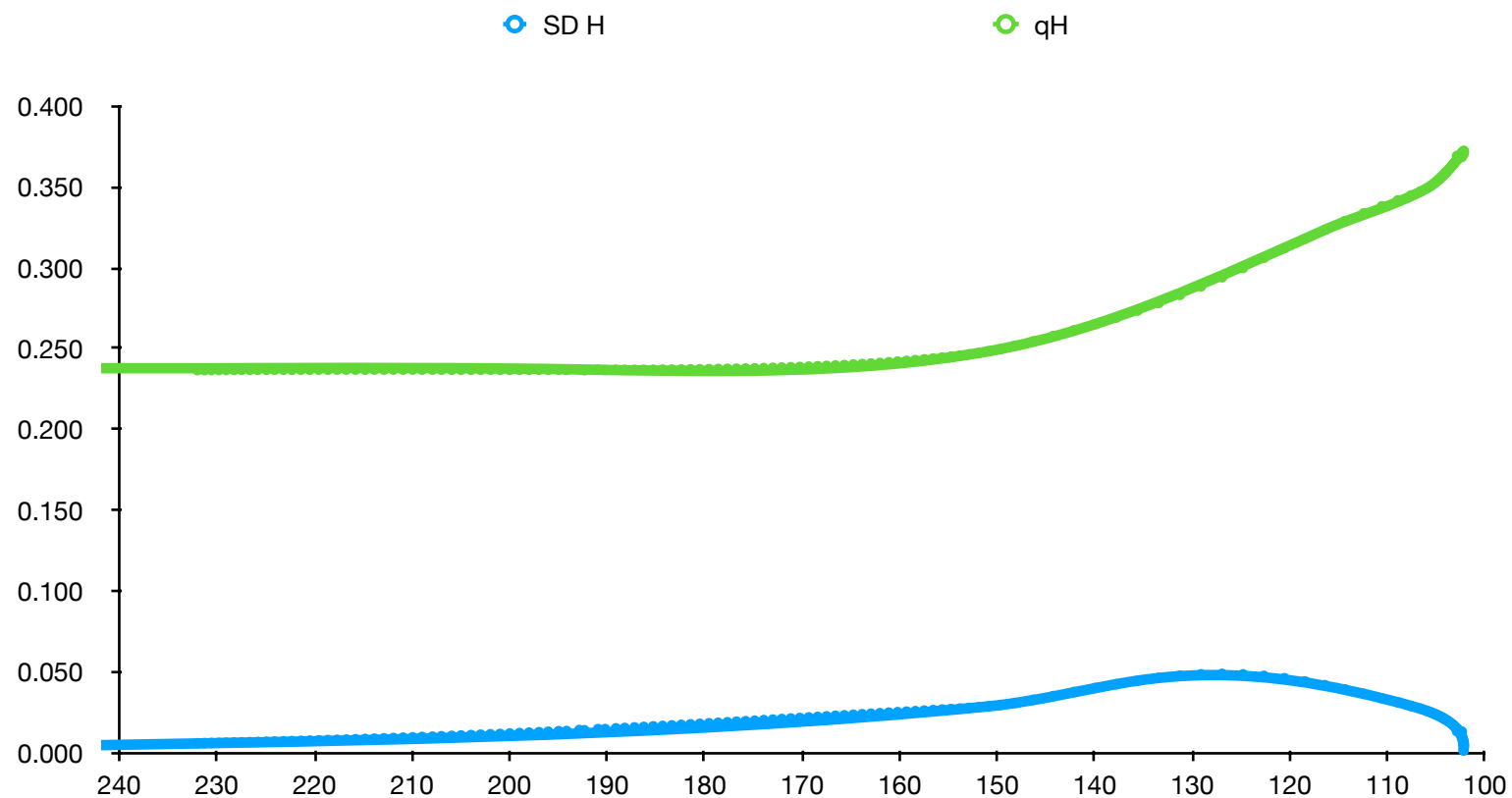
Energies calculated at B2PYLP/GTMP2Large//B3LYP/6-31G(d)



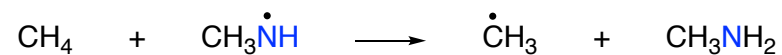
Scheme S2. Overall change of charge of q_N and q_C (NPA) for System 0 along reaction coordinate. Charges calculated at B3LYP/6-31G(d) level of theory using NBO6 program package.



Scheme S3. Overall change of charge and spin distribution of migrating H for System 0 along reaction coordinate. Charges calculated at B3LYP/6-31G(d) level of theory using NBO6 program package.



System 1



1H 16 1 16H

NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)				
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
1	NulC_rad	-39.804412	-39.773085	-39.789551	0.00	0.00	0.00	exp. 439.3±0.4	a)
1H	NulC_neut	-40.469373	-40.434258	-40.454472	-	-	-		
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	exp 425.1±8.4	b)
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-		
START 1	START_Metilamin_nulC	-135.606772	-135.516324	-135.555265	0.00	0.00	0.00		
R1	Metilamino_TS_nulC_CH4_opt_rev	-135.607469	-135.516079	-135.555554	-1.83	0.64	0.00	-0.76	0.00
TS1	Metilamino_TS_nulC_CH4	-135.580629	-135.490641	-135.528212	68.64	67.43	66.79	71.03	71.79
P1	Metilamino_TS_nulC_CH4_opt_fw d	-135.588991	-135.506559	-135.546872	46.68	25.64	24.99	22.04	22.79
FIN1	FIN_Metilamin_nulC	-135.588864	-135.507751	-135.547484	47.02	22.51	20.43		

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

1

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H3(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,0,0,0,0.000155\H,0,0,1.082798,-0.00031\H,0,0.937731,-0.541399,-0.00031\H,0,-0.937731,-0.541399,-0.00031\\Version=ES64L-G16RevA.03\State=2-
A1\HF=-39.7559614\MP2=-39.8069654\RMSD=3.347e-09\PG=C03V[C3(C1),3SGV(H1)]\\

1H

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C1H4\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0,0,0,0\H,0,0.631339,0.631339,0.631339\H,0,-0.631339,-0.631339,0.631339\H,0,-0.631339,0.631339,-0.631339\H,0,0.631339,-0.631339,-0.631339\
\Version=ES64L-G16RevA.03\State=1-A1\HF=-40.4209215\MP2=-40.4832688\RMSD=1.296e-09\PG=TD[O(C1),4C3(H1)]\\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\\

R1

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C2H8N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.957534,0.469282,-0.001936\H,0,-1.273931,1.451316,0.005326\H,0,1.746637,0.025015,-0.001944\C,0,-2.151612,-0.342591,0.000418\H,0,-2.788777,-0.
.131147,-0.876214\H,0,-1.891219,-1.405297,-0.007186\H,0,-2.778314,-0.14125,0.886924\C,0,2.833076,-0.100155,0.000221\H,0,3.139726,-0.67825,-0.876481\H,
0,3.141835,-0.629077,0.906717\H,0,3.317998,0.88019,-0.027428\\Version=ES64L-G16RevA.03\State=2-
A\HF=-135.4414069\MP2=-135.6196444\RMSD=4.180e-09\PG=C01[X(C2H8N1)]\\

TS1

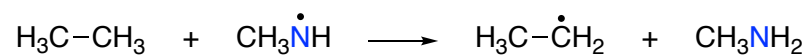
GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C2H8N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.567309,0.740133,-0.149118\H,0,-0.573097,1.258412,0.737464\H,0,0.582922,0.35976,-0.202695\C,0,-1.418557,-0.437646,0.021179\H,0,-2.462974,-0.
107934,0.106629\H,0,-1.343134,-1.07021,-0.869409\H,0,-1.196196,-1.058327,0.904494\C,0,1.855867,-0.180711,0.016206\H,0,2.476217,0.681643,0.260695\H,0,
2.096842,-0.632415,-0.946307\H,0,1.766721,-0.901722,0.828647\\Version=ES64L-G16RevA.03\State=2-
A\HF=-135.3984035\MP2=-135.5905054\RMSD=4.379e-09\PG=C01[X(C2H8N1)]\\

P1

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C2H8N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.91131,0.750412,-0.128633\H,0,-0.990156,1.288754,0.73291\H,0,0.086236,0.568198,-0.250561\C,0,-1.626095,-0.518692,0.022447\H,0,-2.693592,-0.3
16675,0.165483\H,0,-1.527803,-1.09801,-0.902406\H,0,-1.2929,-1.162011,0.856642\C,0,2.490884,-0.153436,0.017365\H,0,2.773715,0.727999,0.579794\H,0,2.59

8377,-0.161036,-1.060437\H,0,2.236557,-1.067339,0.540136\\Version=ES64L-G16RevA.03\State=2-
A\HF=-135.4304007\MP2=-135.6112409\RMSD=3.499e-09\PG=C01[X(C2H8N1)]\

System 2



2H

16

2

16H

NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)				
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	exp	a)
								420.5±1.3	
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-		
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	exp	b)
								425.1±8.4	
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-		
ST_ID2		-158.84409	-158.71846	-158.78112	0.00	0.00	0.00		
MIN_I		-158.84293	-158.71677	-158.78015	3.05	4.42	2.56		
D2									
TS_ID2	Ident_Et_Et.log	-158.82292	-158.69371	-158.75599	55.56	64.97	65.99		
START	START_Metilamin_primC_CH3CH3	-174.88817	-174.76872	-174.82118	0.00	0.00	0.00		
2									
R2	Metilamino_TS_primC_CH3CH3_konf4_o pt_rev	-174.88780	-174.76752	-174.82066	0.97	3.13	0.00	1.36	0.00
TS2	Metilamino_TS_primC_CH3CH3_konf2	-174.86602	-174.74712	-174.79855	58.14	56.71	53.58	59.42	58.06
P2	Metilamino_TS_primC_CH3CH3_opt_fwd	-174.88874	-174.76847	-174.82160	-1.51	0.66	-2.48	-1.11	-2.47
FIN2	FIN_Metilamin_primC_CH3CH3	-174.87776	-174.76647	-174.81866	27.31	5.90	6.61		

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to $\text{NH}_3/\text{NH}_2^\cdot$ radical system

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0.,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0.,0.,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0.,0.,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\\

MIN_ID2

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C4H11(2)\DSAKIC\19-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-1.957865,0.738176,-0.000641\H,0,0.821673,-0.384545,-0.000708\H,0,-1.668414,1.222455,-0.928118\H,0,-1.668148,1.224165,0.92586\C,0,1.86314,-0.7
27834,-0.000495\H,0,2.004154,-1.360386,-0.884846\H,0,2.003472,-1.361351,0.883272\C,0,2.838856,0.451444,0.00052\H,0,2.699039,1.084137,0.884822\H,0,3.8
80583,0.109794,0.00069\H,0,2.699658,1.085149,-0.883153\C,0,-2.934483,-0.386651,0.000541\H,0,-3.979733,-0.027525,0.00088\H,0,-2.825538,-1.021886,-0.886
88\H,0,-2.824636,-1.020815,0.888627\\Version=ES64L-G16RevA.03\State=2-A\HF=-158.6386559\MP2=-158.8629588\RMSD=7.532e-09\PG=C01[X(C4H11)]\\

TS_ID2

GINC-SL250S-GEN8-09-05\SP\ROB2PLYP-FC\GTMP2large\C4H11(2)\DSAKIC\19-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,1.163546,-0.695981,0.000004\H,0,0.000045,-0.000029,0.000105\H,0,1.091808,-1.310737,-0.901534\H,0,1.091869,-1.310946,0.901404\C,0,-1.163526,0.6
95963,0.000001\H,0,-1.091752,1.310735,-0.901521\H,0,-1.091869,1.310865,0.901443\C,0,-2.305501,-0.296975,0.000002\H,0,-2.275493,-0.943325,0.885424\H,0,
-3.283255,0.20724,-0.000094\H,0,-2.275386,-0.943454,-0.885322\C,0,2.305479,0.296994,0.000007\H,0,3.283254,-0.207178,-0.000126\H,0,2.275316,0.943494,-0.
.885302\H,0,2.275471,0.943326,0.885441\\Version=ES64L-G16RevA.03\State=2-A\HF=-158.6005049\MP2=-158.8352301\RMSD=9.161e-09\PG=C01[X(C4H11)]\\

R2

GINC-NX360-M5-04-04\SP\ROB2PLYP-FC\GTMP2large\C3H10N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,1.817451,-0.244681,-0.454391\H,0,2.224011,-0.698608,-1.287055\H,0,-0.887778,-0.548766,0.067191\C,0,2.928071,0.276922,0.30679\H,0,3.523057,0.99
7077,-0.281878\H,0,2.569768,0.77852,1.210791\H,0,3.628127,-0.523574,0.604199\C,0,-1.961694,-0.661898,0.252639\H,0,-2.095847,-0.899728,1.314969\H,0,-2.
313067,-1.527027,-0.322916\C,0,-2.730219,0.605341,-0.130941\H,0,-2.59922,0.844041,-1.193029\H,0,-3.805983,0.49736,0.053013\H,0,-2.382171,1.471284,0.44
4519\Version=ES64L-G16RevA.03\State=2-A\HF=-174.6694681\MP2=-174.902644\RMSD=8.408e-09\PG=C01[X(C3H10N1)]\

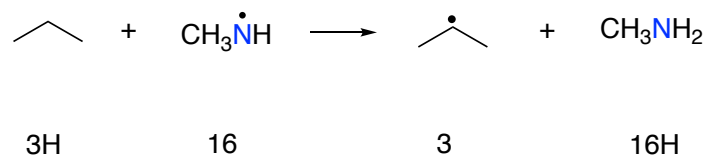
TS2

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C3H10N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.286478,-0.7134,-0.283728\H,0,-1.194326,-0.635361,-1.304238\H,0,-0.088487,-0.773609,0.059517\C,0,-1.816448,0.5582,0.206322\H,0,-2.861398,0.65
7209,-0.120498\H,0,-1.813845,0.553741,1.301609\H,0,-1.281416,1.460036,-0.135474\C,0,1.250993,-0.673266,0.313806\H,0,1.636857,-1.564341,-0.188826\H,0,1
.270685,-0.791945,1.40072\C,0,1.807153,0.636816,-0.194184\H,0,1.308743,1.49683,0.26908\H,0,2.880711,0.73074,0.029895\H,0,1.697639,0.729996,-1.281354\
\Version=ES64L-G16RevA.03\State=2-A\HF=-174.6290171\MP2=-174.8773214\RMSD=5.809e-09\PG=C01[X(C3H10N1)]\

P2

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C3H10N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,1.803253,0.136841,0.46183\H,0,2.152667,0.411733,1.392943\H,0,-0.891836,0.536628,-0.030586\C,0,2.966108,-0.200253,-0.325101\H,0,3.54777,-1.017
61,0.136036\H,0,2.669647,-0.509051,-1.332072\H,0,3.659474,0.654871,-0.410866\C,0,-1.966652,0.685885,-0.182209\H,0,-2.114022,1.048831,-1.20671\H,0,-2.2
94925,1.482089,0.497139\C,0,-2.74897,-0.60691,0.063458\H,0,-2.604948,-0.970775,1.087697\H,0,-3.825677,-0.463124,-0.087493\H,0,-2.423843,-1.403809,-0.6
15786\Version=ES64L-G16RevA.03\State=2-A\HF=-174.6694651\MP2=-174.9026402\RMSD=8.006e-09\PG=C01[X(C3H10N1)]\

System 3



		H(kJ/mol)			ΔH(kJ/mol)				
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
3	SecC_CH3CH2CH3_rad	-118.383469	-118.292442	-118.33473	-36.11	-29.28	-23.68	a)	
3H	SecC_CH3CH2CH3_neut	-119.034676	-118.942464	-118.99063	-	-	-		
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)	
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-		
START 3	START_Metilamin_secC_CH3CH2CH3	-214.172075	-214.024530	-214.09142	0.00	0.00	0.00		
R3	Metilamino_TS_secC_CH3CH2CH3_konf3_opt_rev	-214.168363	-214.026821	-214.09486	9.75	-6.02	0.00	-9.02	0.00
TS3	Metilamino_TS_secC_CH3CH2CH3	-214.153533	-214.006825	-214.07285	48.68	46.48	52.50	48.65	57.67
P3	Metilamino_TS_secC_CH3CH2CH3_konf4_opt_fwd	-214.169298	-214.027859	-214.09375	7.29	-8.74	-2.73	-6.12	2.90
FIN3	FIN_Metilamin_secC_CH3CH2CH3	-214.167921	-214.027108	-214.09266	10.91	-6.77	-3.26		

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

3

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C3H7(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-1.301168,-0.197687,0.00372\H,0,-1.527954,-0.570582,1.020066\H,0,-2.141574,0.440118,-0.29321\H,0,-1.297445,-1.081323,-0.650312\C,0,0.,0.531714,
-0.053087\H,0,0.,1.605526,0.120802\C,0,1.301168,-0.197687,0.00372\H,0,1.297446,-1.08132,-0.650316\H,0,2.141575,0.440119,-0.293206\H,0,1.527952,-0.5705
86,1.020065\\Version=ES64L-G16RevA.03\State=2-A\HF=-118.2245599\MP2=-118.3871301\RMSD=6.982e-09\PG=C01[X(C3H7)]\\

3H

GINC-SL230S-GEN8-02-04\SP\ROB2PLYP-FC\GTMP2large\C3H8\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,-1.277193,-0.259856,0.\H,0,-1.32191,-0.9074,0.88471\H,0,-2.176504,0.367166,-0.000055\H,0,-1.321865,-0.90749,-0.884646\C,0,0.,0.586502,0.\H,0,0.,1.
247338,-0.877617\H,0,0.,1.247369,0.877595\C,0,1.277193,-0.259856,0.000001\H,0,1.321806,-0.90758,-0.884584\H,0,2.176504,0.367166,-0.000179\H,0,1.32196
8,-0.90731,0.884773\\Version=ES64L-G16RevA.03\State=1-A\HF=-118.8790935\MP2=-119.0520308\RMSD=1.564e-09\PG=C01[X(C3H8)]\\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\\

R3

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C4H12N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.985781,-0.128733,0.730835\H,0,-2.07494,-1.112046,0.98248\H,0,-1.004527,0.006404,0.481292\C,0,-2.83043,0.156073,-0.430702\H,0,-3.880918,-0.00
2678,-0.161788\H,0,-2.722886,1.212306,-0.70207\H,0,-2.623318,-0.443512,-1.335632\C,0,1.339913,0.046,-0.443707\H,0,0.858972,0.127301,-1.41742\C,0,1.840
548,-1.297459,-0.022688\H,0,1.19532,-2.107417,-0.381806\H,0,2.853889,-1.500525,-0.415985\H,0,1.914148,-1.376694,1.070303\C,0,1.869019,1.295163,0.1820
76\H,0,1.250411,2.167462,-0.056366\H,0,1.926262,1.20611,1.275207\H,0,2.893752,1.525762,-0.163937\\Version=ES64L-G16RevA.03\State=2-
A\HF=-213.8995952\MP2=-214.1923766\RMSD=6.375e-09\PG=C01[X(C4H12N1)]\\

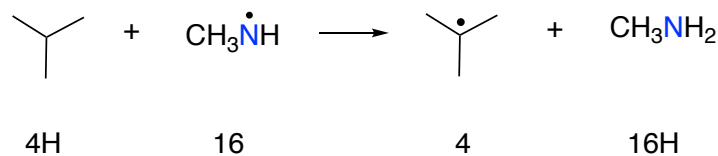
TS3

GINC-NX360-M5-04-04\SP\ROB2PLYP-FC\GTMP2large\C4H12N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,1.459502,-0.608892,-0.518602\H,0,1.51017,-1.553335,-0.115592\H,0,0.295636,-0.26143,-0.136353\C,0,2.412026,0.224101,0.215238\H,0,3.433858,-0.09
6225,-0.034557\H,0,2.308235,1.265625,-0.107708\H,0,2.321343,0.194239,1.314127\C,0,-0.895111,0.051131,0.396173\H,0,-0.69584,0.099569,1.472923\C,0,-1.8
16133,-1.091242,0.017671\H,0,-1.484237,-2.042898,0.448976\H,0,-2.842405,-0.910636,0.373728\H,0,-1.867032,-1.213422,-1.071321\C,0,-1.234849,1.401371,-0
.201677\H,0,-0.499617,2.165562,0.075012\H,0,-1.272318,1.349618,-1.296664\H,0,-2.219909,1.753414,0.143207\\Version=ES64L-G16RevA.03\State=2-
A\HF=-213.8621933\MP2=-214.1669464\RMSD=6.850e-09\PG=C01[X(C4H12N1)]\\

P3

GINC-NX360-M5-02-05\SP\ROB2PLYP-FC\GTMP2large\C4H12N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,2.066472,-0.09293,-0.742461\H,0,2.294864,-1.01973,-1.099029\H,0,1.04847,-0.067855,-0.663699\C,0,2.665424,0.080578,0.582387\H,0,3.757181,0.0451
29,0.493366\H,0,2.404729,1.073205,0.96632\H,0,2.368199,-0.660979,1.345789\C,0,-1.46755,-0.023158,-0.457796\H,0,-1.367827,-0.111824,-1.538574\C,0,-1.65
1212,1.344295,0.115115\H,0,-1.084886,2.099875,-0.440793\H,0,-2.710757,1.660387,0.094059\H,0,-1.339264,1.387,1.167374\C,0,-1.862443,-1.241871,0.310849
\H,0,-1.447658,-2.156617,-0.127778\H,0,-1.533566,-1.183992,1.357293\H,0,-2.960107,-1.373152,0.33957\\Version=ES64L-G16RevA.03\State=2-
A\HF=-213.8997012\MP2=-214.1924726\RMSD=2.587e-09\PG=C01[X(C4H12N1)]\\

System 4



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)			
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
4	TertC_tertbut_min_konf2	-157.673727	-157.553828	-157.610568	-49.60	-38.30	-29.82	a)
4H	TertC_tertbut_konf1	-158.319798	-158.200414	-158.264132	-	-	-	
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-	
START 4	START_Metilamin_tertC	-253.457197	-253.282480	-253.364925	0.00	0.00	0.00	
R4	Metilamino_TS_tertC_tertbut_konf5_opt_rev	-253.456792	-253.281524	-253.365012	1.06	2.51	0.00	0.00
TS4	Metilamino_TS_tertC_tertbut	-253.441200	-253.267696	-253.350080	42.00	38.82	36.31	38.98
P4	Metilamino_TS_tertC_tertbut_konf1_opt_fwd	-253.459128	-253.288765	-253.371157	-5.07	-16.50	-19.01	-16.36
FIN4	FIN_Metilamin_nulC	-253.458179	-253.288494	-253.368501	-2.58	-15.79	-9.39	

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

4

GINC-SL230S-GEN8-02-04\SP\ROB2PLYP-FC\GTMP2large\C4H9(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.000126,-0.000031,0.143769\C,0,0.544018,1.386248,-0.014608\H,0,0.656886,1.67202,-1.078049\H,0,-0.116271,2.136711,0.438597\H,0,1.538065,1.48
7348,0.439607\C,0,0.928713,-1.164194,-0.014617\H,0,0.519163,-2.075955,0.438695\H,0,1.120901,-1.404041,-1.078035\H,0,1.908375,-0.96745,0.43952\C,0,-1.4
72719,-0.222088,-0.014633\H,0,-1.776774,-0.267044,-1.078034\H,0,-1.792249,-1.169266,0.438496\H,0,-2.057411,0.58807,0.439744\\Version=ES64L-
G16RevA.03\State=2-A\HF=-157.4592506\MP2=-157.6784189\RMSD=6.659e-09\PG=C01[X(C4H9)]\\

4H

GINC-SL230S-GEN8-02-03\SP\ROB2PLYP-FC\GTMP2large\C4H10\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0.000066,0.000075,-0.37294\C,0,-0.696425,1.285375,0.09586\H,0,-1.730777,1.334165,-0.265326\H,0,-0.724492,1.336832,1.192403\H,0,-0.172344,2.178
564,-0.265084\C,0,1.461454,-0.039621,0.095857\H,0,1.972812,-0.940029,-0.265337\H,0,2.020908,0.831818,-0.265143\H,0,1.520103,-0.041332,1.192404\C,0,-0.
76507,-1.245842,0.095867\H,0,-0.290012,-2.165947,-0.265196\H,0,-0.795877,-1.295696,1.192395\H,0,-1.800454,-1.238327,-0.265486\H,0,-0.000015,0.000029,-
1.473492\\Version=ES64L-G16RevA.03\State=1-A\HF=-158.109868\MP2=-158.3394261\RMSD=1.501e-09\PG=C01[X(C4H10)]\\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\\

R4

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C5H14N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-2.593,0.529461,0.0069\H,0,-2.947799,1.498357,0.001183\H,0,0.177031,0.114401,0.010164\C,0,-3.754653,-0.32822,0.000929\H,0,-4.387713,-0.14945,-
0.885922\H,0,-3.453219,-1.38004,0.006436\H,0,-4.400853,-0.143922,0.877105\C,0,1.269387,-0.005136,0.001538\C,0,1.884655,1.309351,-0.499719\H,0,1.61864
2,2.149007,0.154098\H,0,2.981046,1.245925,-0.529734\H,0,1.538199,1.551184,-1.511971\C,0,1.610406,-1.166445,-0.943257\H,0,1.147395,-2.102476,-0.607683
\H,0,1.259177,-0.967016,-1.963041\H,0,2.695652,-1.330718,-0.991144\C,0,1.722949,-0.312226,1.435947\H,0,1.452961,0.499922,2.121987\H,0,1.261239,-1.2335
95,1.811432\H,0,2.812783,-0.441741,1.486165\\Version=ES64L-G16RevA.03\State=2-
A\HF=-253.1303225\MP2=-253.475975\RMSD=3.883e-09\PG=C01[X(C5H14N1)]\\

TS4

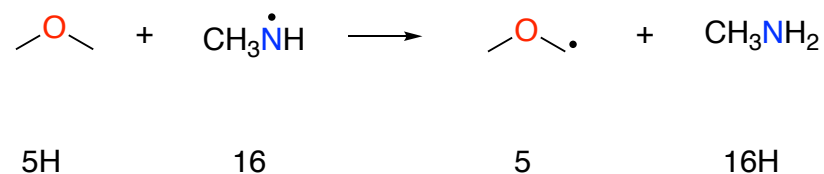
GINC-NX360-M5-02-05\SP\ROB2PLYP-FC\GTMP2large\C5H14N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.647941,0.863832,-0.231916\H,0,-1.671466,1.449846,0.612812\H,0,-0.432059,0.414586,-0.157417\C,0,-2.537483,-0.271045,0.007905\H,0,-3.578185,0
.085674,0.022933\H,0,-2.44991,-0.983763,-0.819428\H,0,-2.369319,-0.817048,0.95165\C,0,0.804325,-0.031759,0.004713\C,0,0.833244,-0.847866,1.286052\H,0,
0.141628,-1.697865,1.2421\H,0,1.839604,-1.258567,1.467269\H,0,0.570323,-0.239396,2.160014\C,0,1.628455,1.24461,0.065246\H,0,1.466557,1.864622,-0.8239

45\H,0,1.379442,1.845422,0.948449\H,0,2.704765,1.015787,0.118445\C,0,1.039668,-0.849424,-1.255324\H,0,0.372188,-1.718072,-1.304986\H,0,0.879127,-0.246377,-2.156303\H,0,2.07363,-1.228772,-1.289738\\Version=ES64L-G16RevA.03\State=2-A\HF=-253.0950145\MP2=-253.4572044\RMSD=5.881e-09\PG=C01[X(C5H14N1)]\\

P4

GINC-NX360-M5-05-03\SP\ROB2PLYP-FC\GTMP2large\C5H14N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,2.127366,0.592035,-0.0606\H,0,2.391932,1.450379,-0.541392\H,0,1.259028,0.281946,-0.495712\C,0,3.17058,-0.419749,-0.245613\H,0,4.094314,-0.078135,0.234642\H,0,2.866011,-1.343857,0.257501\H,0,3.410642,-0.671946,-1.293516\C,0,-1.320203,-0.039129,0.019273\C,0,-0.849728,-1.033789,1.037878\H,0,0.082029,-0.704918,1.514177\H,0,-1.590157,-1.171753,1.848748\H,0,-0.683906,-2.024386,0.595866\C,0,-2.254323,-0.494,-1.060515\H,0,-2.283175,0.212311,-1.900001\H,0,-1.97661,-1.481026,-1.451689\H,0,-3.295142,-0.585564,-0.695015\C,0,-1.293711,1.41325,0.391183\H,0,-0.350366,1.68107,0.882745\H,0,-1.426701,2.061948,-0.483897\H,0,-2.105149,1.670179,1.098507\\Version=ES64L-G16RevA.03\State=2-A\HF=-253.1344654\MP2=-253.4843666\RMSD=3.785e-09\PG=C01[X(C5H14N1)]\\

System 5



		H(kJ/mol)			ΔH(kJ/mol)				
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
5	PrimC_CH3OCH3_rad	-154.29014	-154.21454	-154.231666	-40.96	-37.80	-33.14	a)	
5H	PrimC_CH3OCH3_neut	-154.93950	-154.86132	-154.883965	-	-	-		
16	Metilamin_rad_konf1	-95.137390	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)	
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-		
START 5	START_Metilamin_primC_CH3OCH3	-250.07690	-249.94338	-249.984758	0.00	0.00	0.00		
R5	Metilamino_TS_primC_CH3OCH3_konf5_opt_rev	-250.07618	-249.94889	-249.991057	1.89	-14.46	0.00	-16.54	0.00
TS5	Metilamino_TS_primC_CH3OCH3_konf1	-250.06164	-249.92706	-249.967202	40.05	42.85	57.31	46.09	62.63
P5	Metilamino_TS_primC_CH3OCH3_konf2_opt_fwd	-250.07827	-249.95050	-249.992295	-3.59	-18.69	-4.23	-19.79	-3.25
FIN5	FIN_Metilamin_primC_CH3OCH3	-250.07450	-249.94921	-249.989599	6.06	-15.29	-12.71		

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

5

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C2H5O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-1.203435,0.22891,0.080653\H,0,-2.121745,-0.336837,-0.029801\H,0,-1.151069,1.260952,-0.267316\O,0,-0.090346,-0.541567,-0.045425\C,0,1.137831,0.
168437,0.015604\H,0,1.270915,0.641148,0.997376\H,0,1.934547,-0.559605,-0.150635\H,0,1.18374,0.942796,-0.763765\\Version=ES64L-G16RevA.03\State=2-
A\HF=-154.1036907\MP2=-154.2862229\RMSD=7.403e-09\PG=C01[X(C2H5O1)]\\

5H

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H6O1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,-1.170987,-0.195247,0.\H,0,-2.021921,0.49129,-0.000019\H,0,-1.232474,-0.839748,0.892941\H,0,-1.232449,-0.839774,-0.892924\O,0,0.,0.589929,0.0000
01\C,0,1.170987,-0.195247,0.\H,0,1.23242,-0.839822,-0.892891\H,0,2.021921,0.49129,-0.000088\H,0,1.232503,-0.8397,0.892974\\Version=ES64L-
G16RevA.03\State=1-A\HF=-154.7557241\MP2=-154.9468687\RMSD=1.564e-09\PG=C01[X(C2H6O1)]\\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\\

R5

GINC-SL250S-GEN8-08-03\SP\ROB2PLYP-FC\GTMP2large\C3H10N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.967081,0.263721,0.749627\H,0,-1.759458,-0.505362,1.385435\H,0,-1.117614,0.830299,0.70533\C,0,-2.262195,-0.265591,-0.584895\H,0,-3.142235,-0.
916223,-0.529326\H,0,-2.516226,0.567225,-1.249979\H,0,-1.446403,-0.834094,-1.063284\C,0,1.267149,1.227958,0.040007\H,0,1.694503,1.363123,1.034593\H,0
,1.223278,2.066707,-0.646252\O,0,1.493323,0.045886,-0.589124\C,0,1.637678,-1.074864,0.273793\H,0,1.881975,-1.931596,-0.356978\H,0,2.447247,-0.910467,0
.998622\H,0,0.702119,-1.267767,0.814014\\Version=ES64L-G16RevA.03\State=2-
A\HF=-249.77812\MP2=-250.0914553\RMSD=6.781e-09\PG=C01[X(C3H10N1O1)]\\

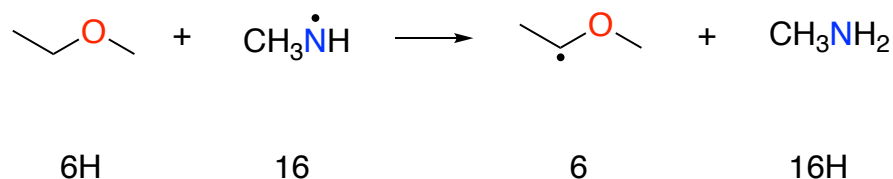
TS5

GINC-NX360-M5-02-05\SP\ROB2PLYP-FC\GTMP2large\C3H10N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.675622,0.279488,0.715783\H,0,-1.370083,-0.4004,1.42502\H,0,-0.552738,0.828388,0.402396\C,0,-2.071159,-0.482751,-0.469194\H,0,-2.923887,-1.13
0831,-0.221639\H,0,-2.396812,0.210599,-1.25226\H,0,-1.27976,-1.122829,-0.893305\C,0,0.672279,1.165443,-0.027637\H,0,1.188747,1.554933,0.861823\H,0,0.4
8949,1.934118,-0.781506\O,0,1.312291,0.08993,-0.621959\C,0,1.786808,-0.873797,0.300512\H,0,2.28877,-1.652717,-0.277813\H,0,2.500715,-0.428891,1.00991
4\H,0,0.959014,-1.321598,0.870474\\Version=ES64L-G16RevA.03\State=2-A\HF=-249.739745\MP2=-250.0637689\RMSD=8.624e-09\PG=C01[X(C3H10N1O1)]\\

P5

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C3H10N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.657294,-0.276416,-0.415099\H,0,-1.838381,-0.416633,-1.407903\H,0,-0.988436,0.493415,-0.358344\C,0,-2.900556,0.083905,0.270837\H,0,-3.604811
, -0.753301,0.209465\H,0,-2.688344,0.252325,1.332377\H,0,-3.413083,0.982677,-0.114397\C,0,1.380896,1.22693,0.155031\H,0,1.16381,1.211638,1.224165\H,0,1
.709261,2.150049,-0.312043\O,0,1.961937,0.128783,-0.386906\C,0,1.653201,-1.10382,0.266626\H,0,2.217853,-1.880319,-0.25361\H,0,1.968555,-1.069156,1.319
184\H,0,0.577887,-1.308128,0.207082\\Version=ES64L-G16RevA.03\State=2-A\HF=-249.7799109\MP2=-250.0932841\RMSD=2.918e-09\PG=C01[X(C3H10N1O1)]\
\

System 6



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)			
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
6	SecC_OCH3_min_konf1	-193.583228	-193.478359	-193.509113	-50.59	-44.65	-38.09	a)
6H	SecC_OCH3_konf2	-194.228920	-194.122527	-194.159528	-	-	-	
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-	
START 6	START_Metilamin_secC_OCH3	-289.366319	-289.204593	-289.260321	0.00	0.00	0.00	
R6	Metilamino_TS_secC_OCH3_konf3_opt_rev	-289.370421	-289.207022	-289.264529	-10.77	-6.38	0.00	-11.05 0.00
TS6	Metilamino_TS_secC_OCH3	-289.352855	-289.190691	-289.245930	35.35	36.50	42.88	37.78 48.83
P6	Metilamino_TS_secC_OCH3_konf3_opt_fwd	-289.371221	-289.214184	-289.269886	-12.87	-25.18	-18.80	-25.11 -14.06
FIN6	FIN_Metilamin_secC_OCH3	-289.367680	-289.213025	-289.267046	-3.57	-22.14	-17.66	

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

6

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C3H7O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.502395,-0.457019,0.096971\H,0,-0.277566,-1.457488,-0.281263\C,0,-1.878961,0.10099,-0.004658\H,0,-2.009067,0.946321,0.682457\H,0,-2.116515,0.470464,-1.017899\H,0,-2.618005,-0.665918,0.250223\O,0,0.495506,0.469151,-0.037279\C,0,1.81099,-0.059251,0.009512\H,0,1.966693,-0.805679,-0.783343\H,0,2.496188,0.777211,-0.144722\H,0,2.016429,-0.526434,0.981826\\Version=ES64L-G16RevA.03\State=2-A\HF=-193.3418817\MP2=-193.5798903\RMSD=4.421e-09\PG=C01[X(C3H7O1)]\\

6H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C3H8O1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\H,0,-0.380766,1.153921,0.887282\C,0,-0.492696,0.506033,-0.000014\H,0,-0.380769,1.153856,-0.887355\C,0,-1.854698,-0.168586,0.000011\H,0,-2.653985,0.580727,0.000039\H,0,-1.969422,-0.800079,-0.886918\H,0,-1.969341,-0.80005,0.886974\O,0,0.50613,-0.498353,-0.00002\C,0,1.812443,0.031412,0.000012\H,0,2.004535,0.649791,0.892668\H,0,2.505752,-0.814119,0.000146\H,0,2.004662,0.649624,-0.892725\\Version=ES64L-G16RevA.03\State=1-A\HF=-193.9910991\MP2=-194.2379073\RMSD=5.976e-09\PG=C01[X(C3H8O1)]\\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962474,-0.000624\H,0,0.97442,0.581813,-0.880942\\Version=ES64L-G16RevA.03\State=2-A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\\Version=ES64L-G16RevA.03\State=1-A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\\

R6

GINC-SL250S-GEN8-10-03\SP\ROB2PLYP-FC\GTMP2large\C4H12N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-2.032213,0.34888,0.553175\H,0,-1.171277,-0.127993,0.242574\H,0,1.730093,0.446164,1.328815\C,0,-3.115072,-0.213877,-0.216114\H,0,-3.207283,-1.303279,-0.056332\H,0,-4.068883,0.254608,0.049525\H,0,-2.952382,-0.082813,-1.300911\C,0,1.693967,0.52491,0.229536\H,0,2.72897,0.42949,-0.139559\C,0,1.090419,1.853308,-0.194937\H,0,1.694922,2.680902,0.192549\H,0,1.060638,1.92926,-1.287005\H,0,0.07122,1.956557,0.190509\O,0,0.903294,-0.533312,-0.303779\C,0,1.412854,-1.811112,0.021192\H,0,1.443175,-1.974106,1.110245\H,0,0.747731,-2.55126,-0.431512\H,0,2.429212,-1.952559,-0.378951\\Version=ES64L-G16RevA.03\State=2-A\HF=-289.0144614\MP2=-289.3783886\RMSD=9.014e-09\PG=C01[X(C4H12N1O1)]\\

TS6

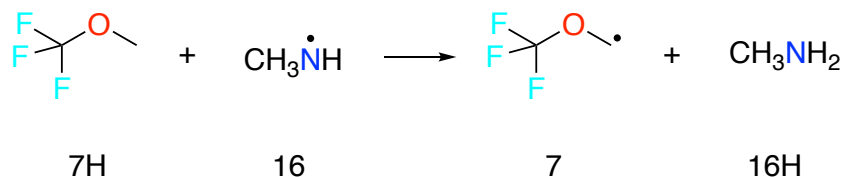
GINC-NX360-M5-05-04\SP\ROB2PLYP-FC\GTMP2large\C4H12N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.788248,-0.011064,0.790087\H,0,-1.683276,-0.929232,1.242659\H,0,-0.535043,0.343756,0.684076\C,0,-2.233318,-0.258845,-0.581937\H,0,-3.209539,-0.764904,-0.568054\H,0,-2.365136,0.698323,-1.098235\H,0,-1.549319,-0.877124,-1.187129\C,0,0.748142,0.558848,0.422361\H,0,1.232325,0.44772,1.405989\C,0,0.83278,1.952049,-0.151584\H,0,0.399476,2.673534,0.548418\H,0,1.874466,2.239419,-0.348424\H,0,0.282612,2.01319,-1.096642\O,0,1.20319,-0.383714,-0.49

6778\C,0,1.358336,-1.68494,0.037639\H,0,0.400109,-2.086056,0.400311\H,0,1.731698,-2.321147,-0.768191\H,0,2.0782,-1.693001,0.869962\\Version=ES64L-G16RevA.03\State=2-A\HF=-288.9768483\MP2=-289.3570859\RMSD=6.681e-09\PG=C01[X(C4H12N1O1)]\\

P6

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C4H12N1O1(2)\DSAKIC\18-Apr-2019\0\#\rob2plyp/gtmp2large maxdisk=20gb\\nekaj\
\0,2\N,0,-2.061188,-0.15071,-0.453185\H,0,-2.231913,-0.091954,-1.455945\H,0,-1.20935,0.386513,-0.281261\C,0,-3.185545,0.438215,0.277809\H,0,-4.089295,-0.152784,0.091543\H,0,-2.980423,0.386892,1.352823\H,0,-3.415682,1.489637,0.031318\C,0,1.22653,0.478899,0.341405\H,0,0.920034,0.362656,1.384712\C,0,1.995576,1.684537,-0.081702\H,0,1.562218,2.587688,0.360919\H,0,3.055471,1.63851,0.223851\H,0,1.982128,1.793381,-1.172952\O,0,1.579959,-0.66906,-0.303805\C,0,0.93667,-1.853096,0.167244\H,0,-0.149894,-1.778609,0.042012\H,0,1.330726,-2.678704,-0.429349\H,0,1.175228,-2.02711,1.226526\\Version=ES64L-G16RevA.03\State=2-A\HF=-289.0178345\MP2=-289.3867953\RMSD=2.573e-09\PG=C01[X(C4H12N1O1)]\\

System 7



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)			
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
7	PrimC_CH3OCF3_rad	-452.045027	-451.946277	-451.889700	-23.59	-17.05	-13.59	a)
7H	PrimC_CH3OCF3_neut	-452.701004	-452.600955	-452.549446	-	-	-	
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-	
START 7	START_Metilamino_TS_primC_CH3OCF3	-547.838403	-547.683021	-547.650239	0.00	0.00	0.00	
R7	Metilamino_TS_primC_CH3OCF3_opt_rev	-547.842422	-547.684934	-547.654185	-10.55	-5.02	0.00	-10.36 0.00
TS7	Metilamino_TS_primC_CH3OCF3_konf4	-547.820293	-547.662712	-547.629182	47.55	53.32	58.34	55.29 65.65
P7	Metilamino_TS_primC_CH3OCF3_opt_fwd	-547.830138	-547.680106	-547.648521	21.70	7.65	12.68	4.51 14.87
FIN7	FIN_Metilamino_TS_primC_CH3OCF3	-547.829479	-547.680943	-547.647633	23.43	5.46	6.84	

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

7

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H2F3O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-1.973326,-0.012315,0.058625\H,0,-2.843376,-0.638025,-0.080324\H,0,-1.963403,1.038242,-0.207409\O,0,-0.799662,-0.723856,-0.100537\C,0,0.364617
,-0.025944,-0.001726\F,0,0.433269,0.968626,-0.909026\F,0,0.518721,0.530625,1.211507\F,0,1.365379,-0.874786,-0.219077\\Version=ES64L-G16RevA.03\State=2-
A\HF=-451.5875758\MP2=-451.9963171\RMSD=3.517e-09\PG=C01[X(C2H2F3O1)]\\

7H

GINC-SL230S-GEN8-02-04\SP\ROB2PLYP-FC\GTMP2large\C2H3F3O1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,1.95396,0.024035,-0.000005\H,0,2.746343,0.771916,-0.0004\H,0,2.025959,-0.597979,-0.896776\H,0,2.026261,-0.597365,0.897169\O,0,0.725322,0.7699
19,-0.000047\C,0,-0.401039,0.034515,0.\F,0,-0.495768,-0.770689,-1.083803\F,0,-0.495688,-0.770666,1.083824\F,0,-1.443951,0.864996,0.000025\\Version=ES64L-
G16RevA.03\State=1-A\HF=-452.2470393\MP2=-452.6654504\RMSD=2.769e-09\PG=C01[X(C2H3F3O1)]\\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\\

R7

GINC-NX360-M5-05-04\SP\ROB2PLYP-FC\GTMP2large\C3H7F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-2.809744,0.540045,-0.322584\H,0,-3.674333,0.60712,-0.880852\H,0,-0.610683,1.600958,-0.227365\C,0,-2.804084,-0.775054,0.274077\H,0,-2.820871,-
1.564025,-0.49772\H,0,-1.909527,-0.912035,0.885584\H,0,-3.698602,-0.939747,0.899406\C,0,0.352507,1.928457,0.17442\H,0,0.296414,2.013652,1.263421\H,0,
0.643068,2.885571,-0.258832\O,0,1.412562,1.013964,-0.18862\C,0,1.135009,-0.287121,-0.045791\F,0,0.188176,-0.724977,-0.912171\F,0,2.249452,-0.988397,-0.
266182\F,0,0.67811,-0.59565,1.196927\\Version=ES64L-G16RevA.03\State=2-
A\HF=-547.2695299\MP2=-547.8050706\RMSD=5.273e-09\PG=C01[X(C3H7F3N1O1)]\\

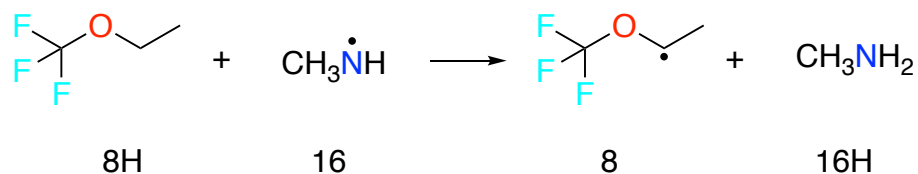
TS7

GINC-NX360-M5-02-05\SP\ROB2PLYP-FC\GTMP2large\C3H7F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-2.498121,0.270447,0.622277\H,0,-2.037657,-0.194057,1.414161\H,0,-1.5819,0.974274,0.196215\C,0,-2.756695,-0.755933,-0.387143\H,0,-3.525635,-1.4
4097,-0.003808\H,0,-3.151572,-0.286219,-1.293848\H,0,-1.87961,-1.362649,-0.659486\C,0,-0.418414,1.541287,-0.294526\H,0,0.04185,2.073113,0.540606\H,0,-0.
.755684,2.190583,-1.100564\O,0,0.4381,0.569714,-0.866731\C,0,1.175631,-0.174049,-0.01527\F,0,0.408089,-0.933963,0.803848\F,0,1.948397,-0.985233,-0.7343
73\F,0,1.962306,0.57778,0.782333\\Version=ES64L-G16RevA.03\State=2-A\HF=-547.227331\MP2=-547.7780005\RMSD=3.395e-09\PG=C01[X(C3H7F3N1O1)]\\

P7

GINC-NX360-M5-04-04\SP\ROB2PLYP-FC\GTMP2large\C3H7F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-3.06674,0.585603,-0.135158\H,0,-3.379816,1.032705,0.725331\H,0,-2.09295,0.865312,-0.255305\C,0,-3.141188,-0.869853,0.015963\H,0,-4.188141,-1.1
64125,0.149839\H,0,-2.78506,-1.343239,-0.905277\H,0,-2.56092,-1.294706,0.853356\C,0,0.35773,1.877859,-0.000622\H,0,0.344006,1.866164,1.083662\H,0,0.29
8652,2.796004,-0.56804\O,0,1.138911,0.934061,-0.635919\C,0,1.273935,-0.274356,-0.021303\F,0,0.09878,-0.924128,0.06857\F,0,2.116558,-1.004555,-0.743317\
F,0,1.759912,-0.15262,1.22871\\Version=ES64L-G16RevA.03\State=2-A\HF=-547.2619191\MP2=-547.8009291\RMSD=4.223e-09\PG=C01[X(C3H7F3N1O1)]\\

System 8



NAME	SYSTEM	H(kJ/mol)			$\Delta H(\text{kJ/mol})$			
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
8	SecC_CH3CH2OCF3_rad	-491.339842	-491.211845	-491.168785	-36.63	-27.37	-21.72	a)
8H	SecC_CH3CH2OCF3_neut	-491.990853	-491.862594	-491.825435	-	-	-	
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-	
START 8	START_Metilamino_TS_secC_OCF3	-587.128252	-586.944660	-586.926228	0.00	0.00	0.00	
R8	Metilamino_TS_secC_OCF3_konf1_opt_rev	-587.129822	-586.949236	-586.931604	-4.12	-12.01	0.00	0.00
TS8	Metilamino_TS_secC_OCF3_konf2	-587.112434	-586.927196	-586.908685	41.53	45.85	57.87	60.17
P8	Metilamino_TS_secC_OCF3_konf3_opt_fwd	-587.131774	-586.946425	-586.929957	-9.25	-4.63	7.38	4.32
FIN8	FIN_Metilamino_TS_secC_OCF3	-587.124294	-586.946511	-586.926718	10.39	-4.86	-1.29	

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

8

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C3H4F3O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-2.813401,-0.195573,-0.012653\H,0,-2.924349,-1.041909,0.675828\H,0,-3.029783,-0.570589,-1.027428\H,0,-3.570842,0.554411,0.235031\C,0,-1.460758
,0.40224,0.092883\H,0,-1.231333,1.406151,-0.251787\O,0,-0.429275,-0.525927,-0.050385\C,0,0.839876,-0.050202,-0.001351\F,0,1.079903,0.856109,-0.972778\F
,0,1.116552,0.547328,1.171963\F,0,1.669791,-1.07893,-0.166055\\Version=ES64L-G16RevA.03\State=2-
A\HF=-490.827488\MP2=-491.2918116\RMSD=4.082e-09\PG=C01[X(C3H4F3O1)]\\

8H

GINC-SL230S-GEN8-02-04\SP\ROB2PLYP-FC\GTMP2large\C3H5F3O1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,-2.777773,0.275059,0.000003\H,0,-2.868211,0.90788,-0.88797\H,0,-2.868203,0.907733,0.888085\H,0,-3.603461,-0.444206,-0.000047\C,0,-1.455062,-0.4
65554,-0.000017\H,0,-1.344343,-1.093771,0.890081\H,0,-1.344359,-1.093816,-0.890088\O,0,-0.404261,0.531932,-0.000051\C,0,0.854954,0.064063,-0.000001\F,
0,1.127932,-0.700652,1.084021\F,0,1.127962,-0.700803,-1.083908\F,0,1.691879,1.103601,-0.000064\\Version=ES64L-G16RevA.03\State=1-
A\HF=-491.4828734\MP2=-491.9568831\RMSD=4.924e-09\PG=C01[X(C3H5F3O1)]\\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\\

R8

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C4H9F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-2.44729,-0.16972,0.151098\H,0,-2.296769,-0.641667,1.040691\H,0,-2.048441,-0.785453,-0.554823\C,0,-3.881187,0.015971,-0.088955\H,0,-4.292517,0.
676683,0.681622\H,0,-4.021928,0.513343,-1.054428\H,0,-4.481738,-0.909351,-0.095552\C,0,0.526664,1.485148,-0.187819\H,0,-0.500104,1.169075,-0.012655\C
,0,1.036819,2.85477,0.057322\H,0,1.295612,3.026214,1.116565\H,0,1.941168,3.056238,-0.530951\H,0,0.272795,3.587257,-0.22102\O,0,1.513053,0.49847,-0.029
591\C,0,1.113842,-0.787047,-0.00534\F,0,2.197411,-1.562912,0.034707\F,0,0.349845,-1.073073,1.075485\F,0,0.384045,-1.131249,-1.092597\\Version=ES64L-
G16RevA.03\State=2-A\HF=-586.5050626\MP2=-587.1000248\RMSD=1.803e-09\PG=C01[X(C4H9F3N1O1)]\\

TS8

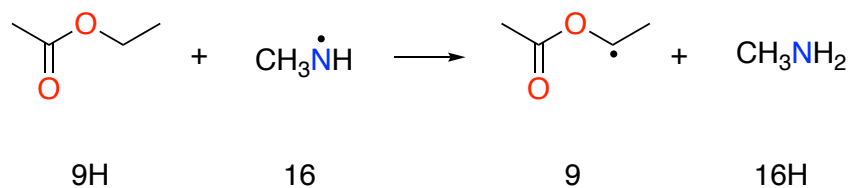
GINC-SL230S-GEN8-02-04\SP\ROB2PLYP-FC\GTMP2large\C4H9F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-2.307405,-0.737181,0.741534\H,0,-1.734562,-1.344606,1.340364\H,0,-1.523844,0.227833,0.585227\C,0,-2.422697,-1.405265,-0.554706\H,0,-3.03807,-
2.308167,-0.433859\H,0,-2.938229,-0.747331,-1.262114\H,0,-1.464905,-1.71638,-0.999228\C,0,-0.551594,1.151188,0.349068\H,0,-0.103272,1.340593,1.328401\
C,0,-1.234657,2.332263,-0.282815\H,0,-2.023551,2.696654,0.38251\H,0,-0.528178,3.152685,-0.468137\H,0,-1.690347,2.054483,-1.23906\O,0,0.408918,0.612907

, -0.560094\C, 0, 1.336609, -0.222331, -0.053193\F, 0, 2.142513, -0.60419, -1.043347\F, 0, 2.085844, 0.355706, 0.910641\F, 0, 0.789363, -1.333058, 0.500017\
\Version=ES64L-G16RevA.03\State=2-A\HF=-586.4652207\MP2=-587.0721704\RMSD=7.357e-09\PG=C01[X(C4H9F3N1O1)]\

P8

GINC-NX360-M5-05-03\SP\ROB2PLYP-FC\GTMP2large\C4H9F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0, 2\N, 0, 2.748339, 0.026985, -0.698843\H, 0, 2.431958, -0.764812, -1.277563\H, 0, 0.659835, 1.187632, -0.572862\C, 0, 3.285858, -0.550021, 0.510378\H, 0, 4.083001, -1.284542, 0.304616\H, 0, 3.686727, 0.23078, 1.164099\H, 0, 2.496622, -1.095211, 1.055847\C, 0, -0.374475, 1.499677, -0.391607\H, 0, -0.923041, 1.508482, -1.339029\C, 0, -0.437296, 2.846123, 0.301254\H, 0, 0.03092, 3.605189, -0.334226\H, 0, -1.473489, 3.142059, 0.492788\H, 0, 0.098939, 2.816756, 1.254705\O, 0, -1.010906, 0.5357, 0.497264\C, 0, -1.098906, -0.722752, 0.055772\F, 0, -1.761605, -1.447908, 0.960208\F, 0, -1.744948, -0.828003, -1.129218\F, 0, 0.118366, -1.308423, -0.129809\\Version=ES64L-G16RevA.03\State=2-A\HF=-586.5051552\MP2=-587.0963353\RMSD=3.110e-09\PG=C01[X(C4H9F3N1O1)]\

System 9



NAME	SYSTEM	H(kJ/mol)			Δ H(kJ/mol)			
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
9	SecC_OCOCH3_ver1_rad	-306.931396	-306.790680	-306.814572	-42.23	-32.55	-25.24	a)
9H	SecC_OCOCH3_neut	-307.580276	-307.439457	-307.469879	-	-	-	
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-	
START 9	START_Metilamino_TS_secC_OCOCH3	-402.717675	-402.521523	-402.570672	0.00	0.00	0.00	
R9	Metilamino_TS_secC_OCOCH3_ver1_opt_fwd	-402.721956	-402.528794	-402.577462	-11.24	-19.09	0.00	0.00
TS9	Metilamino_TS_secC_OCOCH3_ver1	-402.702275	-402.505449	-402.554122	40.43	42.20	61.29	61.28
P9	Metilamino_TS_secC_OCOCH3_ver1_opt_rev	-402.722807	-402.525250	-402.575886	-11.24	-9.79	9.30	4.14
FIN9	FIN_Metilamino_TS_secC_OCOCH3	-402.715850	-402.525346	-402.572505	4.79	-10.04	-4.81	

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

9

GINC-SL230S-GEN8-02-05\SP\ROB2PLYP-FC\GTMP2large\C4H7O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,2.618597,-0.312472,0.062564\H,0,2.76359,-0.655874,1.101844\H,0,3.447189,0.360035,-0.180854\H,0,2.693516,-1.199548,-0.579334\C,0,1.325185,0.38
6366,-0.131176\H,0,1.153859,1.439234,0.053701\O,0,0.211788,-0.425565,-0.06008\C,0,-1.025425,0.162137,0.004495\O,0,-1.193185,1.358696,0.036271\C,0,-2.1
03633,-0.891834,0.020226\H,0,-2.088862,-1.457403,-0.918022\H,0,-1.931293,-1.604477,0.833205\H,0,-3.075164,-0.412204,0.143279\\Version=ES64L-
G16RevA.03\State=2-A\HF=-306.5417503\MP2=-306.9032829\RMSD=6.321e-09\PG=C01[X(C4H7O2)]\\

9H

GINC-NX360-M5-01-06\SP\ROB2PLYP-FC\GTMP2large\C4H8O2\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,2.568185,-0.399519,0.000019\H,0,2.606991,-1.03947,0.887473\H,0,3.455026,0.243642,0.000034\H,0,2.607044,-1.0395,-0.887411\C,0,1.313391,0.45308
,-0.000023\H,0,1.254123,1.09822,-0.882737\H,0,1.254092,1.098281,0.882644\O,0,0.178764,-0.443074,-0.000016\C,0,-1.03893,0.147022,0.000011\O,0,-1.202991
,1.347466,0.000011\C,0,-2.138398,-0.890271,0.000002\H,0,-2.050507,-1.533352,-0.881934\H,0,-2.050438,-1.533449,0.881859\H,0,-3.108006,-0.391374,0.00006
2\\Version=ES64L-G16RevA.03\State=1-A\HF=-307.1960403\MP2=-307.5666196\RMSD=5.502e-09\PG=C01[X(C4H8O2)]\\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\\

R9

GINC-NX360-M5-02-02\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-3.946768,-0.513566,0.272163\H,0,-4.04455,-0.487755,1.371532\H,0,-4.535066,-1.361977,-0.091338\H,0,-4.399508,0.41032,-0.109718\C,0,-2.538008,-0
.647032,-0.170699\H,0,3.662392,0.0008,-1.330174\O,0,-1.755697,0.468825,0.044558\C,0,-0.401555,0.370039,-0.121899\O,0,0.145703,-0.671288,-0.422148\C,0,
0.265913,1.699914,0.106482\H,0,-0.068264,2.413875,-0.65535\H,0,-0.027863,2.10702,1.079682\H,0,1.350254,1.577139,0.052724\H,0,-2.006642,-1.583806,-0.27
9564\N,0,3.239332,0.021078,-0.403562\H,0,2.3454,-0.463777,-0.485648\C,0,4.104942,-0.676685,0.54964\H,0,3.627457,-0.673132,1.53564\H,0,4.339874,-1.7257
45,0.297791\H,0,5.054003,-0.136835,0.645952\\Version=ES64L-G16RevA.03\State=2-
A\HF=-402.2205997\MP2=-402.7125465\RMSD=5.931e-09\PG=C01[X(C5H12N1O2)]\\

TS9

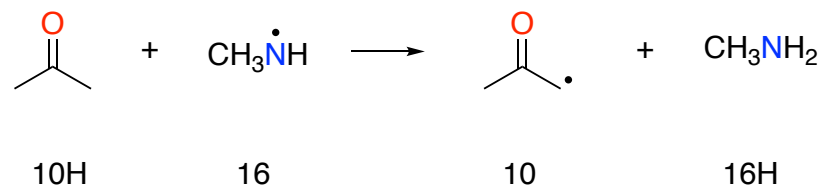
GINC-NX360-M5-05-03\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.83016,2.338113,0.013132\H,0,-0.205384,3.102778,0.495932\H,0,-1.860378,2.473564,0.35865\H,0,-0.803287,2.511821,-1.067799\C,0,-0.357265,0.949
175,0.345865\H,0,-1.134321,0.0602,-0.322286\O,0,0.965098,0.764338,-0.136003\C,0,1.569684,-0.418492,0.140244\O,0,1.035052,-1.317489,0.754205\C,0,2.970
972,-0.447225,-0.419989\H,0,3.563974,0.37216,-0.000548\H,0,3.437438,-1.403437,-0.181229\H,0,2.943079,-0.307206,-1.505708\H,0,-0.439412,0.648955,1.3937

75\N,0,-1.78023,-0.929377,-0.748549\H,0,-1.150968,-1.679748,-0.438097\C,0,-2.997204,-1.029496,0.055306\H,0,-3.538493,-1.941935,-0.232681\H,0,-2.835402,-1.080897,1.144893\H,0,-3.652602,-0.177868,-0.158024\\Version=ES64L-G16RevA.03\State=2-A\HF=-402.1799508\MP2=-402.6834151\RMSD=8.460e-09\PG=C01[X(C5H12N1O2)]\\

P9

GINC-NX360-M5-04-06\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\\nekaj\
\0,2\C,0,-1.498733,2.576427,0.081751\H,0,-2.423282,2.615115,-0.503591\H,0,-0.892682,3.453342,-0.17\H,0,-1.759503,2.633319,1.143505\C,0,-0.714007,1.31328,-0.216518\H,0,0.213384,1.257848,0.359842\O,0,-1.562793,0.18692,0.133063\C,0,-1.06739,-1.041522,-0.093204\O,0,0.036539,-1.261126,-0.554324\C,0,-2.063464,-2.109033,0.297948\H,0,-2.998989,-1.97335,-0.254251\H,0,-1.645048,-3.093378,0.085862\H,0,-2.299765,-2.027412,1.364118\H,0,-0.452758,1.233257,-1.276793\N,0,2.609193,0.391926,0.212096\H,0,1.937657,-0.284496,-0.18086\C,0,3.916913,-0.207709,0.110814\H,0,3.965466,-1.168065,0.654269\H,0,4.175115,-0.4434,-0.936951\H,0,4.686178,0.458728,0.515517\\Version=ES64L-G16RevA.03\State=2-A\HF=-402.2210433\MP2=-402.708311\RMSD=5.983e-09\PG=C01[X(C5H12N1O2)]\\

System 10



		H(kJ/mol)			ΔH(kJ/mol)				
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
10	MIN_primC_Acetyl_rad_ver2symm	-192.41831	-192.320373	-192.343190	-47.31	-35.74	-34.96	a)	
10H	MIN_primC_Acetyl	-193.06525	-192.967934	-192.994795	-	-	-		
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)	
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-		
START 10	START_Metilamin_primC_acetyl	-288.20265	-288.050000	-288.095588	0.00	0.00	0.00		
R10	Metilamino_TS_primC_Acetyl_ver1_opt_rev	-288.20547	-288.051794	-288.098698	-7.42	-4.71	0.00	-8.17	0.00
TS10	Metilamino_TS_primC_Acetyl_ver1	-288.18721	-288.033612	-288.078253	40.52	43.03	47.74	45.51	53.68
P10	Metilamino_TS_primC_Acetyl_ver1_opt_fwd	-288.21019	-288.059253	-288.106642	-19.80	-24.29	-19.58	-29.02	-20.86
FIN10	FIN_Metilamin_primC_acetyl	-288.20276	-288.055039	-288.101123	-0.30	-13.23	-14.53		

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

10

GINC-SL230S-GEN8-02-04\SP\ROB2PLYP-FC\GTMP2large\C3H5O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,0,0.145707,0.\O,0,0.484452,1.286153,0.\C,0,0.887689,-1.091416,0.\H,0,0.692632,-1.712876,0.882681\H,0,0.692632,-1.712876,-0.882681\H,0,1.935631,
-0.785606,0.\C,0,-1.42819,-0.03707,0.\H,0,-1.887284,-1.021495,0.\H,0,-2.06622,0.840301,0.\Version=ES64L-G16RevA.03\State=2-
A\HF=-192.1660687\MP2=-192.397081\RMSD=3.276e-09\PG=CS[SG(C3H3O1),X(H2)]\

10H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C3H6O1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0.000004,0.185333,-0.000023\O,0,0.000041,1.401001,0.000004\C,0,1.29305,-0.614823,0.000005\H,0,1.341138,-1.267755,0.880709\H,0,1.341606,-1.267
025,-0.881214\H,0,2.148527,0.06345,0.000513\C,0,-1.293084,-0.61477,-0.000003\H,0,-1.341272,-1.267677,-0.880716\H,0,-1.341611,-1.266974,0.881217\H,0,-2.
148537,0.063536,-0.000417\Version=ES64L-G16RevA.03\State=1-A\HF=-192.8187398\MP2=-193.0583756\RMSD=3.262e-09\PG=C01[X(C3H6O1)]\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\

R10

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C4H10N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,2.128836,0.002391,-0.327476\H,0,2.079116,0.006338,-1.357372\H,0,-0.085121,-1.316245,0.530902\C,0,3.530222,-0.000829,0.017777\H,0,4.049951,0.8
8165,-0.394232\H,0,3.657811,-0.005432,1.104278\H,0,4.047794,-0.881145,-0.401495\C,0,-1.180677,-1.288254,0.589166\H,0,-1.447804,-1.328299,1.652863\H,0,
-1.60821,-2.149154,0.070576\C,0,-1.681359,-0.000643,-0.041778\O,0,-2.417495,-0.001921,-1.011215\C,0,-1.184685,1.288752,0.588742\H,0,-1.453754,1.329059
,1.65195\H,0,-0.089113,1.319569,0.532389\H,0,-1.613565,2.148138,0.068757\Version=ES64L-G16RevA.03\State=2-
A\HF=-287.8417792\MP2=-288.1978845\RMSD=3.547e-09\PG=C01[X(C4H10N1O1)]\

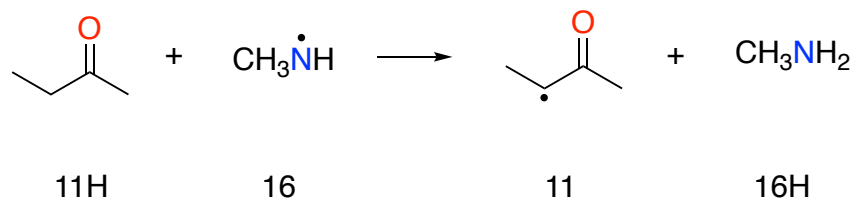
TS10

GINC-SL250S-GEN8-09-05\SP\ROB2PLYP-FC\GTMP2large\C4H10N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.806937,-0.307275,-0.684884\H,0,-1.627716,0.497458,-1.299281\H,0,-0.796454,-0.24346,0.091683\C,0,-3.012065,-0.015951,0.085555\H,0,-3.874249,-
0.040962,-0.596206\H,0,-3.161059,-0.793467,0.841217\H,0,-3.019452,0.96625,0.583349\C,0,0.170096,0.115223,0.946225\H,0,0.132508,-0.712109,1.65917\H,0,-
0.150825,1.070479,1.362393\C,0,1.393481,0.213067,0.109663\O,0,1.759323,1.282369,-0.36144\C,0,2.135868,-1.082745,-0.178794\H,0,2.538082,-1.509975,0.74
845\H,0,1.453543,-1.828175,-0.606468\H,0,2.955315,-0.891626,-0.874496\Version=ES64L-G16RevA.03\State=2-
A\HF=-287.8038041\MP2=-288.1752489\RMSD=2.605e-09\PG=C01[X(C4H10N1O1)]\

P10

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C4H10N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,2.185023,0.201058,-0.503532\H,0,2.562956,0.098619,-1.444247\H,0,1.392918,-0.440519,-0.440469\C,0,3.207128,-0.162215,0.480806\H,0,4.042074,0.5
45504,0.421527\H,0,2.780565,-0.079101,1.486445\H,0,3.621981,-1.180098,0.378811\C,0,-0.919332,1.292642,0.012027\H,0,-1.565235,2.152079,0.169848\H,0,0.
150309,1.435747,-0.128491\C,0,-1.451763,-0.043111,-0.015134\O,0,-0.705605,-1.022014,-0.196552\C,0,-2.947288,-0.239572,0.181972\H,0,-3.267692,0.160368,
1.151825\H,0,-3.5149,0.293497,-0.590625\H,0,-3.185768,-1.303857,0.134496\\Version=ES64L-G16RevA.03\State=2-
A\HF=-287.845792\MP2=-288.2073803\RMSD=4.023e-09\PG=C01[X(C4H10N1O1)]\

System 11



		H(kJ/mol)			ΔH(kJ/mol)				
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
11	SecC_COCH3_min_konf1	-231.713886	-231.586591	-231.622561	-75.74	-62.30	-57.06	a)	
11H	SecC_COCH3_konf2	-232.350000	-232.224035	-232.265748	-	-	-		
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)	
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-		
START 11	START_Metilamin_secC_COCH3	-327.487399	-327.306101	-327.366541	0.00	0.00	0.00		
R11	Metilamino_TS_secC_COCH3_konf2_opt_rev	-327.490088	-327.307747	-327.369598	-7.06	-4.32	0.00	-8.03	0.00
TS11	Metilamino_TS_secC_COCH3_konf2	-327.474943	-327.292832	-327.352955	32.70	34.84	39.16	35.67	43.70
P11	Metilamino_TS_secC_COCH3_konf2_opt_fwd	-327.503578	-327.323757	-327.384356	-42.48	-46.36	-42.03	-46.77	-38.75
FIN11	FIN_Metilamin_secC_COCH3	-327.498338	-327.321257	-327.380494	-28.72	-39.79	-36.63		

a) RSE compared to CH₄/CH₃• radical system

b) RSE compared to NH₃/NH₂• radical system

11

GINC-NX360-M5-04-04\SP\ROB2PLYP-FC\GTMP2large\C4H7O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,0.682365,-0.679806,0.003568\H,0,0.567733,-1.762773,0.006308\C,0,2.050276,-0.099631,-0.002279\H,0,2.626339,-0.434359,0.873032\H,0,2.617245,-0.4
31569,-0.884695\H,0,1.998559,0.991388,-0.000686\C,0,-0.505997,0.142049,0.003298\O,0,-0.429358,1.379401,0.000587\C,0,-1.857826,-0.559741,-0.001078\H,0
,-1.998884,-1.123286,-0.93217\H,0,-1.937016,-1.276038,0.825678\H,0,-2.65202,0.184201,0.086777\Version=ES64L-G16RevA.03\State=2-
A\HF=-231.4049683\MP2=-231.6925923\RMSD=4.524e-09\PG=C01[X(C4H7O1)]\

11H

GINC-SL230S-GEN8-02-03\SP\ROB2PLYP-FC\GTMP2large\C4H8O1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\H,0,-0.599573,-1.425102,-0.872249\C,0,-0.684035,-0.759633,0.000013\H,0,-0.599566,-1.425021,0.872344\C,0,-2.02013,-0.020198,-0.000011\H,0,-2.855039,
-0.728692,0.000041\H,0,-2.110746,0.622466,0.880707\H,0,-2.110783,0.622366,-0.880802\C,0,0.527488,0.16766,-0.000007\O,0,0.409231,1.378382,0.000008\C,0
,1.894369,-0.499297,-0.000012\H,0,2.00927,-1.142961,0.881187\H,0,2.009228,-1.143094,-0.881112\H,0,2.677214,0.261791,-0.000076\Version=ES64L-
G16RevA.03\State=1-A\HF=-232.049052\MP2=-232.3445912\RMSD=4.739e-09\PG=C01[X(C4H8O1)]\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\

R11

GINC-NX360-M5-02-05\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-2.451546,0.027161,-0.358252\H,0,-2.429228,0.05808,-1.388671\H,0,-0.004102,0.909672,0.543695\C,0,-3.810779,0.313841,0.033475\H,0,-4.517628,-0.
418409,-0.394094\H,0,-3.907664,0.297456,1.123013\H,0,-4.137675,1.301974,-0.334462\C,0,1.077441,0.726114,0.626003\H,0,1.271618,0.633057,1.705098\C,0,1
.888157,1.868474,0.017926\H,0,1.651741,2.81804,0.510199\H,0,2.962524,1.685528,0.118222\H,0,1.677157,1.970945,-1.050899\C,0,1.347514,-0.627174,-0.0209
94\O,0,2.116358,-0.751838,-0.957473\C,0,0.582161,-1.807883,0.550515\H,0,0.788431,-1.921599,1.622354\H,0,-0.495262,-1.627113,0.446605\H,0,0.863076,-2.7
23276,0.024935\Version=ES64L-G16RevA.03\State=2-A\HF=-327.0718658\MP2=-327.4839259\RMSD=6.224e-09\PG=C01[X(C5H12N1O1)]\

TS11

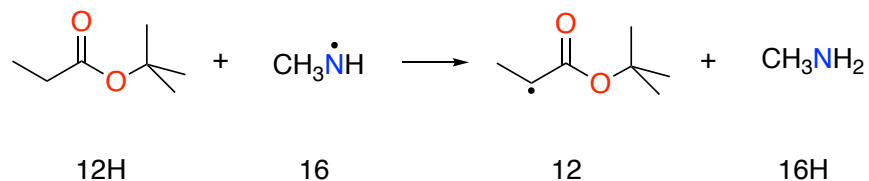
GINC-SL250S-GEN8-09-05\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.736795,-0.917374,-0.493994\H,0,-1.636639,-0.588551,-1.46352\H,0,-0.729147,-0.289995,0.07132\C,0,-2.975374,-0.354174,0.032622\H,0,-3.824209,-
0.844957,-0.466432\H,0,-3.050596,-0.569395,1.103331\H,0,-3.095513,0.730844,-0.117334\C,0,0.20882,0.475971,0.580509\H,0,0.085661,0.202816,1.634927\C,0
, -0.077203,1.927728,0.26709\H,0,-1.087159,2.214786,0.58077\H,0,0.629133,2.587594,0.788556\H,0,0.03618,2.121389,-0.803325\C,0,1.435142,-0.115047,-0.037

561\O,0,2.038842,0.457763,-0.934817\C,0,1.853576,-1.48757,0.462303\H,0,2.126135,-1.446058,1.524373\H,0,1.017054,-2.192001,0.370664\H,0,2.706165,-1.848399,-0.116615\\Version=ES64L-G16RevA.03\State=2-A\HF=-327.0364221\MP2=-327.4643\RMSD=4.300e-09\PG=C01[X(C5H12N1O1)]\\

P11

GINC-NX360-M5-05-03\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O1(2)\DSAKIC\18-Apr-2019\0\#\rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\O,2\N,0,2.73005,-0.178209,0.352241\H,0,3.189705,-0.303642,1.25286\H,0,1.821018,0.243154,0.5487\C,0,3.527254,0.718125,-0.486805\H,0,4.491946,0.249006,
-0.713393\H,0,3.00876,0.870972,-1.439824\H,0,3.732488,1.715009,-0.057706\C,0,-2.367863,-0.200417,-0.264391\H,0,-2.913437,-1.051718,-0.667543\C,0,-3.080
105,1.090913,-0.084954\H,0,-3.494237,1.449272,-1.038832\H,0,-3.937587,0.976615,0.594777\H,0,-2.403161,1.847026,0.318447\C,0,-0.976824,-0.37556,0.0800
42\O,0,-0.319792,0.575646,0.542334\C,0,-0.347598,-1.745426,-0.109094\H,0,-0.766324,-2.271762,-0.973647\H,0,0.736543,-1.644571,-0.214485\H,0,-0.546912,-
2.36288,0.777502\\Version=ES64L-G16RevA.03\State=2-A\HF=-327.0837654\MP2=-327.5019873\RMSD=9.900e-09\PG=C01[X(C5H12N1O1)]\\

System 12



		H(kJ/mol)			ΔH(kJ/mol)			
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
12	SecC_tBoc_rad	-306.934835	-306.792969	-306.817323	-63.18	-51.11	-43.73	
12H	SecC_tBoc_neut	-307.575732	-307.434676	-307.465589	-	-	-	
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-	
START 12	START_Metilamino_TS_secC_tBoc	-402.713131	-402.516742	-402.566382	0.00	0.00	0.00	
R12	Metilamino_TS_secC_tBoc_konf3_o pt_rev	-402.717547	-402.519659	-402.570774	-11.59	-7.66	0.00	-11.53
TS12	Metilamino_TS_secC_tBoc	-402.699819	-402.502657	-402.552203	34.95	36.98	44.64	37.23
P12	Metilamino_TS_secC_tBoc_konf1_o pt_fwd	-402.724709	-402.530231	-402.579565	-30.40	-35.42	-27.76	-34.61
FIN12	FIN_Metilamino_TS_secC_tBoc	-402.719287	-402.527635	-402.575256	-16.16	-28.60	-23.30	

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

12

GINC-SL230S-GEN8-02-07\SP\ROB2PLYP-FC\GTMP2large\C4H7O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,2.533037,0.007014,-0.000085\H,0,3.127751,-0.284426,0.878482\H,0,2.409761,1.092474,0.000436\H,0,3.127017,-0.283483,-0.879504\C,0,1.211175,-0.6
68435,0.000086\H,0,1.143404,-1.752177,-0.000059\C,0,-0.024761,0.089245,0.000075\O,0,-0.105317,1.311182,0.000084\O,0,-1.114991,-0.728383,0.00014\C,0,-
2.377763,-0.052673,-0.000163\H,0,-3.132855,-0.839883,-0.002445\H,0,-2.482442,0.575436,0.889549\H,0,-2.480299,0.578763,-0.887727\Version=ES64L-
G16RevA.03\State=2-A\HF=-306.5446045\MP2=-306.9065767\RMSD=6.303e-09\PG=C01[X(C4H7O2)]\

12H

GINC-SL230S-GEN8-02-04\SP\ROB2PLYP-FC\GTMP2large\C4H8O2\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,2.482922,0.111388,0.000014\H,0,2.520089,0.758039,0.881695\H,0,2.520022,0.758129,-0.881595\H,0,3.373403,-0.525625,-0.000032\C,0,1.21668,-0.742
689,-0.000008\H,0,1.180954,-1.406807,-0.873249\H,0,1.180913,-1.406822,0.873225\C,0,-0.052192,0.088333,-0.00001\O,0,-0.105787,1.298965,-0.000014\O,0,-1.
14865,-0.706131,-0.000011\C,0,-2.408049,-0.015589,0.000018\H,0,-3.170256,-0.795572,-0.000162\H,0,-2.502955,0.613522,0.889322\H,0,-2.50285,0.613813,-0.
889093\Version=ES64L-G16RevA.03\State=1-A\HF=-307.191376\MP2=-307.5621311\RMSD=5.609e-09\PG=C01[X(C4H8O2)]\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\

R12

GINC-SL250S-GEN8-09-05\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,2.79912,-0.10601,-0.473134\H,0,1.887547,-0.426613,-0.113624\H,0,-1.081892,1.719594,-1.356062\C,0,3.794192,-1.001399,0.063876\H,0,3.606013,-2.0
47576,-0.236631\H,0,4.797662,-0.719821,-0.273259\H,0,3.784546,-1.001006,1.168562\C,0,-1.028293,1.60912,-0.263939\H,0,-1.937751,2.082581,0.123973\C,0,0.
.235239,2.271017,0.286007\H,0,0.226076,3.341239,0.054732\H,0,0.294998,2.160028,1.373841\H,0,1.139141,1.833713,-0.146923\C,0,-1.115562,0.125614,0.033
308\O,0,-0.207646,-0.585332,0.419207\O,0,-2.360124,-0.342324,-0.199738\C,0,-2.545234,-1.751984,0.011191\H,0,-2.331938,-2.016268,1.050304\H,0,-3.590977
,-1.947884,-0.227235\H,0,-1.887148,-2.328877,-0.64415\Version=ES64L-G16RevA.03\State=2-
A\HF=-402.2155432\MP2=-402.7030378\RMSD=5.016e-09\PG=C01[X(C5H12N1O2)]\

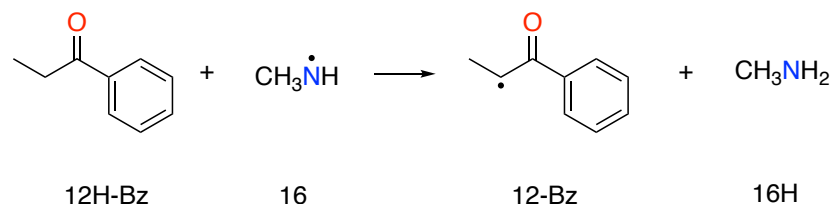
TS12

GINC-SL230S-GEN8-02-04\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.931939,-1.102663,0.796067\H,0,-1.226115,-1.753773,1.165198\H,0,-1.250657,0.002166,0.806082\C,0,-2.171482,-1.463755,-0.599918\H,0,-2.601779,
-2.474938,-0.635527\H,0,-2.898393,-0.771933,-1.03583\H,0,-1.269695,-1.464343,-1.231808\C,0,-0.393479,0.999258,0.656938\H,0,-0.133026,1.201985,1.698086

\C,0,-1.177589,2.089664,-0.042344\H,0,-2.121012,2.28625,0.477461\H,0,-0.609001,3.029458,-0.069588\H,0,-1.392471,1.807895,-1.076901\C,0,0.730914,0.411748,-0.112093\O,0,0.824501,0.391777,-1.327238\O,0,1.638551,-0.185706,0.706482\C,0,2.729175,-0.835589,0.038398\H,0,3.296239,-0.119709,-0.562977\H,0,3.354725,-1.248799,0.830693\H,0,2.36511,-1.632139,-0.617199\\Version=ES64L-G16RevA.03\State=2-A\HF=-402.1775103\MP2=-402.6810809\RMSD=8.038e-09\PG=C01[X(C5H12N1O2)]\\

P12
GINC-SL230S-GEN8-02-04\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\O,2\N,0,-2.810035,-0.041347,-0.509305\H,0,-1.990027,-0.645046,-0.434373\H,0,-3.197797,-0.198302,-1.438384\C,0,-3.799209,-0.407853,0.506558\H,0,-3.360733,-0.265051,1.500319\H,0,-4.665498,0.259941,0.433834\H,0,-4.170911,-1.446154,0.453654\C,0,0.304622,1.212727,-0.074832\H,0,-0.773026,1.285537,-0.209015\C,0,1.127342,2.441081,0.08587\H,0,1.00772,3.104321,-0.784065\H,0,0.7872,3.024344,0.954862\H,0,2.188027,2.215676,0.21013\C,0,0.818281,-0.13951,-0.069333\O,0,0.12188,-1.145749,-0.203633\O,0,2.166723,-0.212679,0.100231\C,0,2.709942,-1.538001,0.111369\H,0,2.506422,-2.04877,-0.834297\H,0,3.784095,-1.413635,0.254877\H,0,2.28009,-2.126669,0.927015\\Version=ES64L-G16RevA.03\State=2-A\HF=-402.2225042\MP2=-402.7151794\RMSD=3.952e-09\PG=C01[X(C5H12N1O2)]\\

System 12-benzoyl



		H(kJ/mol)			ΔH(kJ/mol)				
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
12-Bz	SecC_CH3CH2COPh_rad	-423.38989	-423.155259	-423.224085	-64.24	-51.24	-45.57	a)	
12H-Bz	SecC_CH3CH2COPh_neut	-424.03038	-423.796917	-423.871651	-	-	-		
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)	
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-		
START 12-Bz	START_Metilamino_TS_secC_CH3CH2COPh	-519.16778	-518.878983	-518.972444	0.00	0.00	0.00		
R12-Bz	Metilamino_TS_secC_CH3CH2COPh_konf5_opt_rev	-519.17284	-518.882891	-518.978268	-13.29	-10.26	0.00 -15.29	0.00	
TS12-Bz	Metilamino_TS_secC_CH3CH2COPh_konf5	-519.15792	-518.868294	-518.961936	25.88	28.06	38.33 27.59	42.88	
P12-Bz	Metilamino_TS_secC_CH3CH2COPh_konf5_opt_fwd	-519.18425	-518.897760	-518.991043	-43.24	-49.30	-39.04 -48.83	-33.54	
FIN12-Bz	FIN_Metilamino_TS_secC_CH3CH2COPh	-519.17434	-518.889925	-518.982018	-17.23	-28.73	-25.14		

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

12-Bz

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C9H9O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,2.483064,-1.522127,0.587689\H,0,1.541862,-1.782757,1.077453\H,0,3.295507,-1.605365,1.321548\H,0,2.687496,-2.289093,-0.177205\C,0,2.465686,-0.155217,-0.007885\H,0,3.421716,0.305031,-0.248508\C,0,1.345145,0.731291,-0.20762\C,0,-0.079116,0.267239,-0.093802\C,0,-1.035067,1.184781,0.368134\C,0,-0.500786,-1.008874,-0.494523\C,0,-2.376118,0.822831,0.461813\H,0,-0.704677,2.180888,0.644818\C,0,-1.847869,-1.365925,-0.417103\H,0,0.215612,-1.717162,-0.899931\C,0,-2.78595,-0.455093,0.07051\H,0,-3.105204,1.538226,0.83287\H,0,-2.164159,-2.353304,-0.742785\H,0,-3.833635,-0.736116,0.137743\O,0,1.578944,1.933277,-0.44366\Version=ES64L-G16RevA.03\State=2-A\HF=-422.7798354\MP2=-423.318783\RMSE=7.383e-09\PG=C01[X(C9H9O1)]\

12H-Bz

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C9H10O1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,2.788779,-1.080085,0.787408\H,0,1.963356,-1.633692,1.247581\H,0,3.146846,-0.342932,1.513628\H,0,3.602425,-1.786076,0.590254\C,0,2.353291,-0.383467,-0.516455\H,0,3.202393,0.15502,-0.947148\H,0,2.022526,-1.128483,-1.249127\C,0,1.26774,0.657309,-0.261824\C,0,-0.166178,0.228407,-0.139026\C,0,-1.121261,1.212549,0.165148\C,0,-0.59011,-1.098135,-0.313291\C,0,-2.46592,0.879878,0.29124\H,0,-0.778042,2.233504,0.296344\C,0,-1.938558,-1.432319,-0.185344\H,0,0.126645,-1.878014,-0.549981\C,0,-2.877821,-0.445069,0.116362\H,0,-3.195827,1.649978,0.525917\H,0,-2.255157,-2.462639,-0.322733\H,0,-3.928235,-0.706274,0.214478\O,0,1.574162,1.83315,-0.123066\Version=ES64L-G16RevA.03\State=1-A\HF=-423.4282083\MP2=-423.9744837\RMSE=4.740e-09\PG=C01[X(C9H10O1)]\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962474,-0.000624\H,0,0.97442,0.581813,-0.880942\Version=ES64L-G16RevA.03\State=2-A\HF=-95.0200827\MP2=-95.1355318\RMSE=2.976e-09\PG=C01[X(C1H4N1)]\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\Version=ES64L-G16RevA.03\State=1-A\HF=-95.6745449\MP2=-95.8034231\RMSE=4.406e-09\PG=C01[X(C1H5N1)]\

R12-Bz

GINC-SL230S-GEN8-02-05\SP\ROB2PLYP-FC\GTMP2large\C10H14N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,2.483346,1.811446,-0.241843\H,0,1.77989,2.10425,-0.936373\H,0,1.819361,-0.607198,0.372822\C,0,3.695258,2.533569,-0.546619\H,0,3.53671,3.625587,-0.519305\H,0,4.484518,2.27635,0.166009\H,0,4.053736,2.304145,-1.565348\C,0,1.272645,-1.516101,0.662753\H,0,1.042478,-1.383116,1.730147\C,0,2.128855,-2.762841,0.446672\H,0,3.060732,-2.68962,1.017451\H,0,1.598665,-3.666664,0.761576\H,0,2.380236,-2.887477,-0.61095\C,0,-0.044304,-1.560848,-0.101212\O,0,-0.33382,-2.520301,-0.802483\C,0,-2.859666,1.684491,0.207083\C,0,-1.609048,1.808152,0.815102\C,0,-0.680939,0.769171,0.729225\C,0,-0.997415,-0.404696,0.027586\C,0,-2.255687,-0.516288,-0.584976\C,0,-3.181372,0.518845,-0.495039\H,0,-3.581937,2.493706,0.278886\H,0,-1.35519,2.714205,1.359141\H,0,0.293724,0.886623,1.191137\H,0,-2.481765,-1.429554,-1.1259\H,0,-4.153972,0.420323,-0.96999\Version=ES64L-G16RevA.03\State=2-A\HF=-518.4529017\MP2=-519.1157264\RMSE=5.365e-09\PG=C01[X(C10H14N1O1)]\

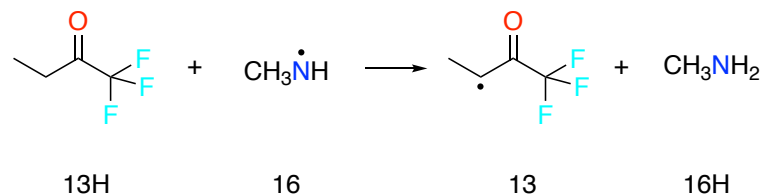
TS12-Bz

GINC-NX360-M5-02-09\SP\ROB2PLYP-FC\GTMP2large\C10H14N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,2.215802,-1.593314,0.560793\H,0,1.942685,-1.309907,1.511273\H,0,1.808177,-0.544446,-0.116937\C,0,3.67348,-1.634802,0.517682\H,0,4.01968,-2.467
98,1.147326\H,0,4.005394,-1.832186,-0.506516\H,0,4.175236,-0.723922,0.88081\C,0,1.484934,0.57382,-0.729754\H,0,1.218023,0.136746,-1.69771\C,0,2.69317,
1.483275,-0.776724\H,0,3.553561,0.976361,-1.226332\H,0,2.48254,2.37884,-1.376182\H,0,2.962779,1.830912,0.224707\C,0,0.304033,1.10765,0.016415\O,0,0.3
97693,2.143782,0.671594\C,0,-3.470178,-0.956073,-0.081071\C,0,-2.323147,-1.613793,-0.528638\C,0,-1.089777,-0.961577,-0.5134\C,0,-0.993502,0.35569,-0.03
7911\C,0,-2.1501,1.002878,0.425114\C,0,-3.381102,0.354762,0.397663\H,0,-4.430841,-1.464221,-0.100605\H,0,-2.387,-2.637207,-0.888319\H,0,-0.20164,-1.494
476,-0.83828\H,0,-2.055438,2.016276,0.801677\H,0,-4.272184,0.867183,0.750535\\Version=ES64L-G16RevA.03\State=2-
A\HF=-518.4173705\MP2=-519.0964018\RMSD=5.020e-09\PG=C01[X(C10H14N1O1)]\\

P12-Bz

GINC-NX360-M5-01-07\SP\ROB2PLYP-FC\GTMP2large\C10H14N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,3.12788,1.409481,-0.546211\H,0,2.877225,2.144952,-1.205376\H,0,3.841387,0.852022,-1.013716\C,0,3.686736,2.006601,0.673773\H,0,2.914967,2.6093
03,1.163072\H,0,3.965351,1.20736,1.368024\H,0,4.571152,2.645986,0.518747\C,0,1.120902,-1.586582,-0.10495\H,0,1.655466,-0.647105,-0.223281\C,0,1.90925
7,-2.847088,-0.078462\H,0,2.491516,-2.965536,-1.004749\H,0,2.644079,-2.832897,0.740561\H,0,1.252996,-3.710991,0.044457\C,0,-0.316665,-1.605141,0.02389
\O,0,-0.91903,-2.688609,0.159871\C,0,-2.691061,1.994165,-0.038745\C,0,-1.30539,2.093036,-0.173407\C,0,-0.50967,0.946487,-0.157134\C,0,-1.098147,-0.3195
58,-0.004627\C,0,-2.492861,-0.407735,0.129763\C,0,-3.283558,0.737454,0.113142\H,0,-3.306146,2.890391,-0.051913\H,0,-0.839914,3.068498,-0.291603\H,0,0.
566304,1.050656,-0.264165\H,0,-2.932484,-1.392667,0.246506\H,0,-4.362085,0.652689,0.218504\\Version=ES64L-G16RevA.03\State=2-
A\HF=-518.4637662\MP2=-519.132432\RMSD=5.574e-09\PG=C01[X(C10H14N1O1)]\\

System 13



		H(kJ/mol)			ΔH (kJ/mol)			
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
13	SecC_COFC3_rad1	-529.444831	-529.292482	-529.253491	-79.76	-57.44	-50.97	a)
13H	SecC_COFC3_neut3	-530.079412	-529.931778	-529.898997	-	-	-	
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-	
START 13	START_Metilamino_TS_secC_COFC3	-625.216811	-625.013844	-624.999790	0.00	0.00	0.00	
R13	Metilamino_TS_secC_COFC3_konf2_opt_rev	-625.221096	-625.016253	-625.004416	-11.25	-6.32	0.00	-12.15 0.00
TS13	Metilamino_TS_secC_COFC3_konf2	-625.205722	-625.000629	-624.986250	29.11	34.70	41.02	35.55 47.69
P13	Metilamino_TS_secC_COFC3_konf2_opt_fwd	-625.231492	-625.028947	-625.014303	-38.54	-39.65	-33.33	-38.10 -25.96
FIN13	FIN_Metilamino_TS_secC_COFC3	-625.229283	-625.027148	-625.011424	-32.75	-34.93	-30.55	

- a) RSE compared to CH₄/CH₃[•] radical system
b) RSE compared to NH₃/NH₂[•] radical system

13

GINC-SL250S-GEN8-03-05\SP\ROB2PLYP-FC\GTMP2large\C4H4F3O1(2)\DSAKIC\24-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-1.637284,0.618216,0.000042\H,0,-2.258058,1.511712,0.000097\C,0,-2.312719,-0.707264,-0.000027\H,0,-2.969706,-0.794708,0.877552\H,0,-2.969749,-
0.794581,-0.877585\H,0,-1.621073,-1.549312,-0.0001\C,0,-0.236666,0.896762,0.000012\O,0,0.214287,2.04882,-0.000024\C,0,0.762454,-0.284188,-0.000006\F,0,
0.579722,-1.067197,1.090232\F,0,0.57981,-1.067118,-1.090286\F,0,2.023755,0.144891,0.000065\\Version=ES64L-G16RevA.03\State=2-
A\HF=-528.860757\MP2=-529.3785739\RMSD=2.522e-09\PG=C01[X(C4H4F3O1)]\\

13H

GINC-NX360-M5-03-06\SP\ROB2PLYP-FC\GTMP2large\C4H5F3O1\DSAKIC\24-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\H,0,1.273523,-1.337341,0.872301\C,0,1.469374,-0.69734,0.000432\H,0,1.273094,-1.337083,-0.871591\C,0,2.901416,-0.16739,0.000051\H,0,3.61369,-0.9979
63,-0.000457\H,0,3.090625,0.451305,-0.882034\H,0,3.09135,0.45073,0.882413\C,0,0.43054,0.401717,0.000553\O,0,0.66611,1.586768,0.00021\C,0,-1.045702,-0.
078637,0.000301\F,0,-1.281832,-0.838853,-1.093142\F,0,-1.282466,-0.843872,1.089522\F,0,-1.902917,0.941182,0.002472\\Version=ES64L-G16RevA.03\State=1-
A\HF=-529.5068992\MP2=-530.0314308\RMSD=2.067e-09\PG=C01[X(C4H5F3O1)]\\

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\\

R13

GINC-NX360-M5-04-04\SP\ROB2PLYP-FC\GTMP2large\C5H9F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-2.63591,1.291693,-0.397827\H,0,-3.275084,1.793096,-1.033037\H,0,-0.285262,1.523326,0.113944\C,0,-3.347623,0.126919,0.073077\H,0,-3.644267,-0.
527082,-0.765069\H,0,-2.721165,-0.450226,0.756842\H,0,-4.282598,0.406044,0.588851\C,0,0.751189,1.408575,0.469599\H,0,0.659342,1.266727,1.556528\C,0,1
.61057,2.626363,0.136906\H,0,1.177356,3.527525,0.581673\H,0,2.630668,2.509066,0.515001\H,0,1.676589,2.775615,-0.945265\C,0,1.30274,0.128989,-0.10419
3\O,0,2.344869,0.015195,-0.707961\C,0,0.414872,-1.134759,0.070627\F,0,-0.216509,-1.135678,1.269556\F,0,-0.537681,-1.151887,-0.888384\F,0,1.128229,-2.259
549,-0.025293\\Version=ES64L-G16RevA.03\State=2-A\HF=-624.5296388\MP2=-625.1714938\RMSD=6.838e-09\PG=C01[X(C5H9F3N1O1)]\\

TS13

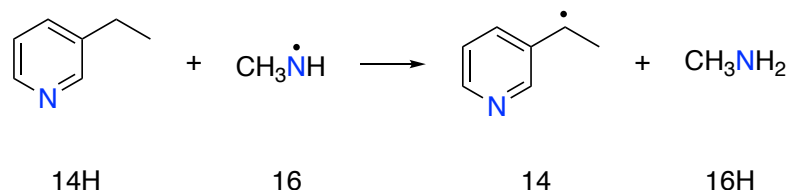
GINC-NX360-M5-05-03\SP\ROB2PLYP-FC\GTMP2large\C5H9F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-2.517133,-0.468908,-0.723127\H,0,-3.309967,0.150623,-0.512122\H,0,-1.496772,0.213616,-0.254587\C,0,-2.678346,-1.686333,0.062674\H,0,-3.495099
,-2.274881,-0.381191\H,0,-1.762417,-2.278564,0.003797\H,0,-2.934804,-1.525053,1.121514\C,0,-0.700149,0.96022,0.478607\H,0,-0.726353,0.445395,1.442998\
C,0,-1.287306,2.358265,0.480451\H,0,-2.30136,2.359316,0.893398\H,0,-0.678122,3.038818,1.088829\H,0,-1.316016,2.767125,-0.533433\C,0,0.600067,0.821245

, -0.208653\O, 0, 1.072893, 1.629917, -0.985659\C, 0, 1.376155, -0.490347, 0.075577\F, 0, 1.622554, -0.615343, 1.400553\F, 0, 0.639013, -1.565612, -0.29828\F, 0, 2.537897, -0.533676, -0.574937\\Version=ES64L-G16RevA.03\State=2-A\HF=-624.4945613\MP2=-625.1513518\RMSD=8.960e-09\PG=C01[X(C5H9F3N1O1)]\\

P13

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C5H9F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\O, 2\N, 0, -3.498351, 0.722374, -0.546056\H, 0, -2.849029, 1.396496, -0.143947\H, 0, -2.940719, 0.182778, -1.205966\C, 0, -3.986984, -0.167682, 0.512566\H, 0, -4.566334, 0.41761, 1.23543\H, 0, -4.667742, -0.906114, 0.074714\H, 0, -3.205632, -0.714333, 1.066317\C, 0, 2.435263, 0.772372, 0.129198\H, 0, 1.996922, 1.757946, 0.25047\C, 0, 3.911479, 0.627175, 0.128505\H, 0, 4.357144, 1.229902, -0.675924\H, 0, 4.336968, 1.011518, 1.066636\H, 0, 4.203522, -0.417002, 0.000663\C, 0, 1.572066, -0.350005, -0.026672\O, 0, 1.963335, -1.516976, -0.172291\C, 0, 0.045692, -0.120042, -0.024601\F, 0, -0.284895, 1.173995, 0.208121\F, 0, -0.478928, -0.465247, -1.216672\F, 0, -0.541557, -0.869917, 0.9217\\Version=ES64L-G16RevA.03\State=2-A\HF=-624.5379192\MP2=-625.1858693\RMSD=5.655e-09\PG=C01[X(C5H9F3N1O1)]\\

System 14



		H(kJ/mol)			ΔH (kJ/mol)			
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
14	b2plyp_MIN_Py_CH_Me_rad_ver3	-326.13059	-325.934634	-325.997351	-84.73	-71.18	-61.03	a)
14H	b2plyp_MIN_Py_CH_Me_neut_ver1	-326.76328	-326.568695	-326.639027	-	-	-	
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-	
START 14		-421.90068	-421.650761	-421.739820	0.00	0.00	0.00	
R14	b2plyp_TS_PyCHMe_NHMe_ver5_opt_rev	-421.90444	-421.654303	-421.742772	-9.88	-9.30	0.00	-7.75
TS14	b2plyp_TS_PyCHMe_NHMe_ver5	-421.88802	-421.637919	-421.723932	33.22	33.72	43.02	41.71
P14	b2plyp_TS_PyCHMe_NHMe_ver5_opt_fwd	-421.92031	-421.672957	-421.760911	-51.54	-58.28	-48.98	-55.37
FIN14		-421.91504	-421.669300	-421.755284	-37.72	-48.67	-40.60	

a) RSE compared to $\text{CH}_4/\text{CH}_3\cdot$ radical system

b) RSE compared to $\text{NH}_3/\text{NH}_2\cdot$ radical system

14

GINC-NX360-M5-01-11\SP\ROB2PLYP-FC\GTMP2large\C7H8N1(2)\DSAKIC\29-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\0,2\C,0,0.56573,1.274432,0.000021\C,0,-0.449573,0.270456,-0.000048\C,0,0.014029,-1.073907,0.00002\C,0,1.377512,-1.32474,0.000017\C,0,2.269971,-0.2463

85,-0.000038\H,0,0.264758,2.322909,0.000038\H,0,-0.696745,-1.895262,0.000096\H,0,1.755864,-2.343275,0.000066\H,0,3.344962,-0.41448,0.000002\C,0,-1.814949,0.634436,-0.000002\C,0,-2.952161,-0.338395,-0.000034\H,0,-3.915428,0.178966,-0.002039\H,0,-2.929452,-0.999128,-0.879882\H,0,-2.931774,-0.996451,0.81912\H,0,-2.047081,1.696808,0.000219\N,0,1.87022,1.039219,-0.000004\\Version=ES64L-G16RevA.03\State=2-A\HF=-325.6464529\MP2=-326.0742938\RMSD=5.715e-09\PG=C01[X(C7H8N1)]\\

14H
GINC-SL230S-GEN8-02-03\SP\ROB2PLYP-FC\GTMP2large\C7H9N1\DSAKIC\29-Oct-2019\0\\#rob2plyp/gtmp2large maxdisk=20gb\\nekaj\
\0,1\C,0,-0.337012,-1.195056,-0.140004\C,0,0.418208,-0.02828,-0.321678\C,0,-0.266732,1.18685,-0.211\C,0,-1.630817,1.183512,0.071979\C,0,-2.273479,-0.044208,0.236866\H,0,0.149193,-2.167505,-0.226586\H,0,0.264684,2.126365,-0.350426\H,0,-2.188135,2.11192,0.159203\H,0,-3.338745,-0.085696,0.458735\C,0,1.905094,-0.089856,-0.590349\H,0,2.149945,-1.050055,-1.061193\H,0,2.179674,0.689438,-1.313002\C,0,2.752267,0.08012,0.683682\H,0,3.821795,0.032387,0.449807\H,0,2.552797,1.044596,1.164336\H,0,2.527063,-0.706475,1.412309\N,0,-1.646207,-1.221924,0.132834\\Version=ES64L-G16RevA.03\State=1-A\HF=-326.2879647\MP2=-326.7225257\RMSD=6.987e-09\PG=C01[X(C7H9N1)]\\

16
GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\\#rob2plyp/gtmp2large maxdisk=20gb\\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962474,-0.000624\H,0,0.97442,0.581813,-0.880942\\Version=ES64L-G16RevA.03\State=2-A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\\

16H
GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\\#rob2plyp/gtmp2large maxdisk=20gb\\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\\Version=ES64L-G16RevA.03\State=1-A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\\

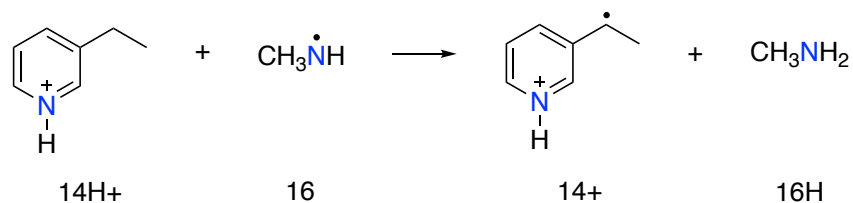
R14
GINC-NX360-M5-01-11\SP\ROB2PLYP-FC\GTMP2large\C8H13N2(2)\DSAKIC\29-Oct-2019\0\\#rob2plyp/gtmp2large maxdisk=20gb\\nekaj\
\0,2\C,0,0.284874,-0.667216,-0.220483\C,0,0.844057,0.518032,0.248673\C,0,2.222346,0.518228,0.47668\C,0,2.467292,-1.631502,-0.175373\C,0,1.106438,-1.759658,-0.436639\H,0,-0.786147,-0.720524,-0.405321\H,0,2.704022,1.420002,0.853006\H,0,3.141702,-2.470062,-0.3346\H,0,0.703723,-2.700989,-0.800007\C,0,0.003375,1.754982,0.466447\H,0,-0.966406,1.460613,0.884656\H,0,0.488454,2.407984,1.202973\C,0,-0.239675,2.545936,-0.831583\H,0,-0.879874,3.415375,-0.643037\H,0,0.70443,2.902744,-1.258598\H,0,-0.734159,1.918636,-1.580852\N,0,-3.301284,-0.091189,0.2043\H,0,-3.332691,0.182862,1.198243\C,0,-4.26918,-1.152763,0.051133\H,0,-4.099215,-1.975949,0.765861\H,0,-5.292083,-0.785451,0.247719\H,0,-4.239035,-1.554778,-0.96596\N,0,3.025587,-0.516909,0.276097\\Version=ES64L-G16RevA.03\State=2-A\HF=-421.3101735\MP2=-421.8604416\RMSD=4.766e-09\PG=C01[X(C8H13N2)]\\

TS14
GINC-NX360-M5-01-05\SP\ROB2PLYP-FC\GTMP2large\C8H13N2(2)\DSAKIC\29-Oct-2019\0\\#rob2plyp/gtmp2large maxdisk=20gb\\nekaj\
\0,2\C,0,0.894915,0.771289,-0.914576\C,0,0.25133,0.492858,0.304192\C,0,0.973081,-0.302323,1.219149\C,0,2.777696,-0.514145,-0.163394\C,0,2.170137,0.265346,-1.149148\H,0,0.403821,1.380311,-1.66809\H,0,0.524547,-0.538268,2.185205\H,0,3.773311,-0.926866,-0.316819\H,0,2.688583,0.471162,-2.081406\C,0,-1.116792,0.949273,0.633105\H,0,-1.951917,0.058782,0.187776\H,0,-1.298066,0.917826,1.71302\C,0,-1.638885,2.22896,-0.002559\H,0,-2.666294,2.4225,0.32147\H,0,-1.025876,3.096923,0.276958\H,0,-1.652296,2.166672,-1.096215\N,0,-2.801335,-0.91415,-0.150377\H,0,-3.165932,-1.166401,0.778235\C,0,-1.984012,-2.0349

83,-0.605554\H,0,-1.198994,-2.355569,0.099007\H,0,-2.635372,-2.904174,-0.782547\H,0,-1.505695,-1.778085,-1.555851\N,0,2.193531,-0.79763,1.009231\
\Version=ES64L-G16RevA.03\State=2-A\HF=-421.2749376\MP2=-421.8425459\RMSD=2.578e-09\PG=C01[X(C8H13N2)]\

P14
GINC-NX360-M5-04-11\SP\ROB2PLYP-FC\GTMP2large\C8H13N2(2)\DSAKIC\29-Oct-2019\0\#\rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,2.040652,-0.914421,-0.118802\C,0,1.306141,0.293808,0.032125\C,0,-0.106768,0.149806,0.173713\C,0,-0.022815,-2.136457,0.026875\C,0,1.368153,-2.1
27248,-0.120424\H,0,3.120523,-0.885149,-0.232056\H,0,-0.73353,1.033426,0.293218\H,0,-0.577523,-3.072193,0.029198\H,0,1.907938,-3.0632,-0.234398\C,0,1.
893889,1.578903,0.046907\H,0,-2.779018,-0.102432,0.428393\H,0,1.226791,2.428751,0.167959\C,0,3.360263,1.841971,-0.093648\H,0,3.576473,2.912625,-0.04
4666\H,0,3.945306,1.349291,0.697691\H,0,3.756366,1.46777,-1.049971\N,0,-3.357349,0.735291,0.516079\H,0,-3.831198,0.665256,1.415258\C,0,-4.347053,0.77
5855,-0.561152\H,0,-5.045749,-0.079298,-0.601152\H,0,-4.947212,1.689569,-0.475979\H,0,-3.825578,0.818885,-1.523846\N,0,-0.749559,-1.011949,0.172034\
\Version=ES64L-G16RevA.03\State=2-A\HF=-421.3252335\MP2=-421.8838332\RMSD=3.291e-09\PG=C01[X(C8H13N2)]\

System 14+



		H(kJ/mol)			ΔH(kJ/mol)				
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
14+	MIN_PyCH2CH3_kationradical_ver2	-326.496612	-326.295183	-326.357190	-90.40	-75.82	-65.75	a)	
14H+	MIN_PyCH2CH3_kation_ver2	-327.127140	-326.927477	-326.997069	-	-	-		
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	b)	
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-		
START 14+		-422.264539	-422.009543	-422.097862	0.00	0.00	0.00		
R14+	TS_PyCH2CH3_kation_NMe_ver1_opt_rev	-422.298311	-422.040012	-422.129821	-88.67	-80.00	0.00	-83.91	0.00
	TS_PyCH2CH3_kation_NMe_opt_rev	-422.278376	-422.021388		-36.33	-31.10	48.90		
TS14+	TS_PyCH2CH3_kation_NMe_ver1	-422.258665	-422.002218	-422.088770	15.42	19.23	99.23	23.87	107.78
	TS_PyCH2CH3_kation_NMe	-422.258340	-422.001890	-422.088346	16.28	20.09	100.09	24.98	108.89
P14+	TS_PyCH2CH3_kation_NMe_ver1_opt_fwd	-422.317091	-422.060187	-422.147131	-137.98	-132.97	-52.97	-129.36	-45.45
	TS_PyCH2CH3_kation_NMe_opt_fwd	-422.293535	-422.039045	-422.126032	-76.13	-77.46	2.54	-73.96	9.95
FIN14+		-422.281064	-422.029849	-422.115123	-43.39	-53.31	-45.32		

- a) RSE compared to CH₄/CH₃[•] radical system
b) RSE compared to NH₃/NH₂[•] radical system

14+
1\1\GINC-SL230S-GEN8-02-01\FOpt\UB3LYP\6-31G(d)\C7H9N1(1+,2)\DSAKIC\24-Sep-2020\0\#optfreqb3lyp/6-31g(d)geom=connectivity\nekaj\
\1,2\C,-0.5549835954,-1.2234046849,0.\C,0.4486022945,-0.2286259157,0.\C,-0.0103201245,1.1261035962,0.\C,-1.3652020662,1.4250375926,0.\C,-2.30260070
15,0.3978056517,0.\H,-2.5411248457,-1.6337123765,0.\H,-0.3300785308,-2.2837948391,0.\H,0.7151721617,1.932234377,0.\H,-1.7093499468,2.4531392974,0.\
H,-3.3751547478,0.5418233886,0.\C,1.8128450825,-0.6060111037,0.\C,2.9524324474,0.3537874778,0.\H,2.9303538207,1.0104293757,0.8821995898\H,3.9080
858749,-0.1730692281,0.\H,2.9303538207,1.0104293757,-0.8821995898\N,-1.852614824,-0.8842446446,0.\H,2.0307343892,-1.6710312401,0.\Version=ES64L-
G16RevC.01\State=2-
A\HF=-326.6496671\S2=0.772452\S2-1=0.\S2A=0.750337\RMSD=7.749e-09\RMSF=4.350e-05\Dipole=-1.2035725,-0.5994815,0.\Quadrupole=10.3951572,1.1987
495,-11.5939067,2.2714911,0.,0.\PG=CS[SG(C7H7N1),X(H2)]\

14H+
1\1\GINC-SL230S-GEN8-02-01\FOpt\RB3LYP\6-31G(d)\C7H10N1(1+)\DSAKIC\24-Sep-2020\0\#optfreqb3lyp/6-31g(d)geom=connectivity\nekaj\
\1,2\C,0.0020834059,-0.9903454083,0.0002250285\C,0.4346127472,0.3301979471,0.0001250166\C,-0.5643120675,1.3230925123,0.0000168877\C,-1.91990533
64,0.9956532664,-0.0000499406\C,-2.2907523575,-0.3389354101,0.0000250869\H,-1.5981112894,-2.2572440281,0.0002423989\H,0.673471716,-1.8393771393
,0.000337918\H,-0.2686726148,2.3690380562,-0.0000484104\H,-2.6853471009,1.7632526575,-0.0001571385\H,-3.316053951,-0.6884598116,-0.000003727\C,1
.9024286131,0.7036772644,0.0003183784\H,2.0806090514,1.3448577018,-0.8732749378\H,2.0806732169,1.3436167783,0.8748206975\C,2.8958825481,-0.460
6224791,-0.0005253872\H,2.7903918133,-1.0897265241,-0.8917952405\H,3.9163919816,-0.0693987522,-0.0000748816\H,2.7901681811,-1.0912172922,0.8896
601429\N,-1.3219400872,-1.2779119991,0.0001581081\Version=ES64L-G16RevC.01\State=1-
A\HF=-327.2951497\RMSD=9.939e-09\RMSF=2.597e-05\Dipole=-1.337942,-0.6458931,0.0002061\Quadrupole=7.5577651,2.6909275,-10.2486926,2.731421,0.000
2865,-0.0009483\PG=C01[X(C7H10N1)]\

16
GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\

16H
GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\

R14+
1\1\GINC-SL250S-GEN8-07-03\FOpt\UB3LYP\6-31G(d)\C8H14N2(1+,2)\DSAKIC\25-Sep-2020\0\#b3lyp/6-31G(d)optfreq\optircreverse\
\1,2\C,0.1906613429,0.4475804586,-0.4295812307\C,1.5257737707,0.0665937097,-0.3304655143\C,1.776510807,-1.2694683471,0.0267646514\C,0.730219353
7,-2.1601579027,0.2688528099\C,-0.575750239,-1.7098744752,0.1522884865\H,-1.8124315623,-0.0951318895,-0.2850196328\H,-0.1158925428,1.4512062276,

-0.7041245821\H,2.803766301,-1.6141912893,0.1097541632\H,0.9215592154,-3.1921028705,0.5405200553\H,-1.4472634023,-2.3321987344,0.3184244653\C,2.6420120057,1.0563122003,-0.5679039691\H,3.4256094133,0.5699056284,-1.1603832037\H,2.2669987513,1.890783125,-1.1707819906\C,3.2460940762,1.5935146693,0.7443845051\H,3.6600508837,0.7843287173,1.3555745614\H,4.0555015422,2.2945134534,0.5213971007\H,2.4953134039,2.1200746362,1.3428663154\N,-0.8057797014,-0.4289536159,-0.191008721\N,-3.4540770222,0.4420746222,-0.4441221891\H,-3.9572809834,0.3851635809,-1.3380433845\C,-4.3265371477,1.0047140107,0.5520981339\H,-4.675777634,2.0041120339,0.2436476641\H,-5.2353269611,0.390271644,0.6642863569\H,-3.8212026706,1.080812407,1.5173151489\\Version=ES64L-G16RevC.01\State=2-

A\HF=-422.5219112\S2=0.75386\S2-1=0.\S2A=0.750011\RMSD=8.978e-09\RMSF=3.332e-06\Dipole=-1.3348426,-0.3365057,-0.2107175\Quadrupole=17.9673777,-4.0048379,-13.9625398,-3.1276988,0.9155687,-1.8513109\PG=C01[X(C8H14N2)]\\

R14+ ver1

1\1\GINC-SL250S-GEN8-05-01\FOpt\UB3LYP\6-31G(d)\C8H14N2(1+,2)\DSAKIC\24-Sep-2020\0\\#b3lyp/6-31G(d)optfreq\loptircreverse\1,2\C,2.0325734856,0.5428800253,0.1724583673\C,0.655636474,0.5698015736,-0.0022696297\C,-0.0013618768,-0.6706886884,-0.1386608561\C,0.7152848458,-1.8681694041,-0.0980110159\C,2.0879018415,-1.8373896789,0.0785907122\H,3.7040149542,-0.6187858644,0.3366253514\H,2.6407769307,1.4308203045,0.2877910941\H,-1.0885149914,-0.6921820352,-0.2788356559\H,0.2125482947,-2.8230684524,-0.202910911\H,2.7203160388,-2.7158545353,0.1219975618\C,-0.1300725768,1.8638806814,-0.0479213122\H,-0.6801165939,1.8822534832,-0.9978047128\H,-0.9022467758,1.8083933066,0.7303912382\C,0.6787629141,3.1530752748,0.1110145767\H,1.4206210336,3.2736187452,-0.686973672\H,0.0086323425,4.0153140579,0.062149937\H,1.1945791512,3.1978666451,1.0772504194\N,2.6956919363,-0.6391957173,0.2070563692\N,-3.2257986537,-0.7393841182,-0.5652615051\H,-3.6552572782,-0.703759783,-1.5008272801\C,-4.2990418087,-0.9027409975,0.3849169869\H,-5.02566153,-0.0759351566,0.3134046318\H,-4.8714032631,-1.8241143071,0.1837471755\H,-3.9114838946,-0.945085359,1.4065141291\\Version=ES64L-G16RevC.01\State=2-

A\HF=-422.5021812\S2=0.753658\S2-1=0.\S2A=0.75001\RMSD=8.318e-09\RMSF=2.207e-06\Dipole=1.630306,-0.7886019,0.0104358\Quadrupole=19.184294,-3.2976258,-15.8866682,-1.9398772,3.2951263,0.2931867\PG=C01[X(C8H14N2)]\\

TS14+

1\1\GINC-SL250S-GEN8-07-03\FTS\UB3LYP\6-31G(d)\C8H14N2(1+,2)\DSAKIC\24-Sep-2020\0\\#opt=(calcfc,ts,noeigentest)frequb3lyp/6-31g(d)geom=connectivity\neka\1,2\C,0.6546146824,0.1109121812,1.0629231823\C,0.2724669945,0.2105980651,-0.282076257\C,1.3060193041,0.0588547915,-1.235089371\C,2.6236990986,-0.1799697705,-0.8477853727\C,2.9376914429,-0.2696143395,0.4983991607\H,2.1676635007,-0.1848053863,2.3883632287\H,-0.0459862697,0.2188735422,1.8826255548\H,1.0684932942,0.1199697744,-2.2916510279\H,3.4088736512,-0.3019076484,-1.5853661026\H,3.9303071417,-0.4542341264,0.888775166\C,-1.1229483489,0.5365865221,-0.615160864\H,-1.825006128,0.0804022469,0.0900311868\H,-1.2015045567,1.7896290088,-0.2010378893\C,-1.5784173968,0.4398617281,-2.0584589414\H,-1.4923693603,-0.5844292863,-2.4462411951\H,-2.6298483996,0.7286845236,-2.140934151\H,-1.0055786185,1.098145549,-2.7218521578\N,1.9384771718,-0.1202262999,1.3994055375\N,-1.3993100992,3.017755595,0.1997667617\H,-2.3949270018,3.0289097854,0.4572185138\C,-1.2160574011,3.9448480532,-0.9084910894\H,-1.914868134,3.7986913222,-1.746397773\H,-1.3788441071,4.9655593744,-0.5325605072\H,-0.1891417204,3.8845930341,-1.2804849627\\Version=ES64L-G16RevC.01\State=2-

A\HF=-422.4772857\S2=0.759857\S2-1=0.\S2A=0.750069\RMSD=8.697e-09\RMSF=1.039e-06\Dipole=1.1681329,-0.7785349,0.9702751\Quadrupole=7.1917004,-6.6461177,-0.5455827,-9.9884895,5.5636818,-4.8105678\PG=C01[X(C8H14N2)]\\

TS14+ ver1

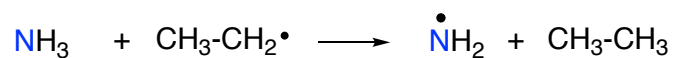
1\1\GINC-SL250S-GEN8-07-03\FTS\UB3LYP\6-31G(d)\C8H14N2(1+,2)\DSAKIC\24-Sep-2020\0\\#opt=(calcfc,ts,noeigentest)freqb3lyp/6-31g(d)geom=connectivity\neka\1,2\C,0.0850237132,-0.8974059818,0.2494214997\C,0.5044522669,0.4086383274,-0.0275980414\C,-0.522934315,1.3689128621,-0.2018657911\C,-1.8672379756,1.0286357864,-0.1011748995\C,-2.218997495,-0.2849400284,0.1765842678\H,-1.4909459114,-2.1548578535,0.5350070047\H,0.7672771457,-1.7249486383,0.394324657\H,-0.2469584342,2.3969153653,-0.4182830332\H,-2.6455474725,1.7709044881,-0.2366775353\H,-3.2369144721,-0.6413798557,0.271110405\C,1

.9221782653,0.7932256532,-0.066441911\H,2.0933718998,1.6023199018,-0.7826608873\H,2.0400116787,1.473133305,1.0688927644\C,2.9874263104,-0.2862658414,-0.1180412052\H,2.9084287187,-0.8967992075,-1.0281534316\H,3.9827041154,0.1666720995,-0.1216813526\H,2.9434878889,-0.9609262558,0.7454546748\N,-1.2315557248,-1.1910959371,0.339108748\N,2.3106435267,2.1924552729,2.1205685294\H,2.906616172,2.9454924529,1.7529922832\C,3.0949170913,1.4306836096,3.0818481317\H,4.0749274055,1.0953258079,2.7086581137\H,3.2894657997,2.0742044296,3.9522415234\H,2.5242682524,0.5637405979,3.4269865453\\Version=ES64L-G16RevC.01\\State=2-
A\HF=-422.4769672\S2=0.759073\S2-1=0.\S2A=0.750058\RMSD=3.355e-09\RMSF=1.489e-06\Dipole=-1.3260853,-1.0697706,-0.3286883\Quadrupole=11.163783,0.1182009,-11.2819839,8.6860979,5.512115,-0.2963385\PG=C01[X(C8H14N2)]\\

P14+
1\1\GINC-NX360-M5-02-08\FOpt\UB3LYP\GTBas1\C8H14N2(1+,2)\DSAKIC\25-Sep-2020\0\#g3b3\nekaj\
\1,2\C,0.1428430573,0.6258984262,-0.1255835217\C,1.4965009245,0.2174808964,-0.0105589493\C,1.7294905207,-1.1875570867,-0.132902459\C,0.6802879196,-2.0672517599,-0.3497827876\C,-0.6208840733,-1.581070915,-0.4505154382\H,-1.8652182541,0.1203104724,-0.4154004168\H,-0.1492388109,1.668123073,-0.0490637058\H,2.7398255207,-1.5727922959,-0.055635781\H,0.8592757408,-3.1326896198,-0.4426396156\H,-1.4890623518,-2.2059963702,-0.6195056857\C,2.4963930109,1.1913283815,0.2099926924\H,2.1618750059,2.2246581951,0.2808622091\H,-3.4427869522,1.6204861654,-0.8999630822\C,3.958233564,0.9571468677,0.3558783027\H,4.5122920301,1.5227654076,-0.4065386725\H,4.309584454,1.3361789619,1.3259950093\H,4.2511006784,-0.0920505846,0.2771698755\N,-0.8420815473,-0.2508815461,-0.3341116233\N,-3.4320205882,0.6725668228,-0.52022447\H,-3.9444169443,0.1104881843,-1.2017953005\C,-4.1561922655,0.6543606168,0.7756271882\H,-5.1871922712,1.0145446951,0.6911395237\H,-4.1736752776,-0.3677061754,1.162284681\H,-3.6234660906,1.2837921875,1.4928820273\\Version=ES64L-G16RevC.01\\State=2-
A\HF=-422.5416107\S2=0.775086\S2-1=0.\S2A=0.750425\RMSD=5.996e-09\RMSF=5.992e-06\Dipole=-1.007423,0.1494398,-0.3181371\Quadrupole=18.345936,-3.4554582,-14.8904778,-1.413062,3.2695654,1.233876\PG=C01[X(C8H14N2)]\\

P14+ ver
1\1\GINC-SL250S-GEN8-07-03\FOpt\UB3LYP\6-31G(d)\C8H14N2(1+,2)\DSAKIC\24-Sep-2020\0\#b3lyp/6-31G(d)optfreq\optircforward\
\1,2\C,1.4979447832,1.6448318804,-0.111822425\C,0.2184846017,1.0561431152,-0.2342002444\C,0.0563503285,-0.2417193956,0.3512696081\C,1.1108943397,-0.8675059546,0.9979683644\C,2.3483344905,-0.2358430245,1.0857115153\H,3.3912459252,1.4478430468,0.5940214972\H,1.7529163778,2.6187348548,-0.508260474\H,-0.9248181858,-0.7299435679,0.2754971548\H,0.9884442738,-1.8494832268,1.4410353374\H,3.2210820409,-0.6531051206,1.571450095\C,-0.8635562121,1.6870716046,-0.8922365581\H,-1.7919133613,1.1217026392,-0.9130733939\H,-3.6368570704,-1.076513441,0.5121349401\C,-0.869563537,3.021807669,-1.5499283095\H,-1.1491998236,2.9229348222,-2.608287858\H,-1.6357878454,3.6659442025,-1.0959692643\H,0.084345884,3.5533837218,-1.50418956\N,2.4854303778,0.9902133792,0.5274530903\N,-2.8936151997,-1.6286075199,0.0837260502\H,-3.1868382958,-1.7640173742,-0.8839627501\C,-2.837650842,-2.945115303,0.7500642471\H,-3.7815322087,-3.5072413149,0.7226157724\H,-2.0658448171,-3.5573440863,0.2729712599\H,-2.5577690242,-2.8058396064,1.7990589053\\Version=ES64L-G16RevC.01\\State=2-
A\HF=-422.5188312\S2=0.77033\S2-1=0.\S2A=0.75028\RMSD=9.709e-09\RMSF=1.599e-06\Dipole=1.6020337,0.7415271,0.1507066\Quadrupole=13.3182553,-1.0948998,-12.2233554,7.5444502,5.9550531,-5.248837\PG=C01[X(C8H14N2)]\\

System 15



15H 2 15 2H

		H(kJ/mol)			ΔH(kJ/mol)			
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
15	NH3_Nrad	-55.849865	-55.829037	-55.835797	0.00	0.00	0.00	a)
15H	NH3_neut	-56.509611	-56.494282	-56.504485	-	-	-	
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-	
ST_ID1 5		-112.359476	-112.323319	-112.340282	0.00	0.00	0.00	
MIN_ID 15	Ident_Am_Am_opt_fwd.log	-112.361979	-112.321771	-112.338626	-6.57	4.06	4.35	
TS_ID1 5	Ident_Am_Am.log	-112.353728	-112.310160	-112.322205	15.09	34.55	47.46	
START 15	START_NH3_TS_primC_CH3CH3	-135.602928	-135.526089	-135.565220	0.00	0.00	0.00	
R15	NH3_TS_primC_CH3CH3_opt_rev	-135.603287	-135.524280	-135.564862	-0.94	4.75	0.00	0.94 0.00
TS15	NH3_TS_primC_CH3CH3	-135.587549	-135.501716	-135.539344	40.38	63.99	59.24	67.94 67.00

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)				
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
P15	NH3_TS_primC_CH3CH3_opt_fwd	-135.599998	-135.514172	-135.555210	7.69	31.29	26.54	26.28	25.34
FIN15	FIN_NH3_TS_primC_CH3CH3	-135.600638	-135.515691	-135.556188	6.01	27.30		23.71	

- a) RSE compared to CH₄/CH₃[•] radical system
b) RSE compared to NH₃/NH₂[•] radical system

15

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\H2N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,0.,0.,0.14444\H,0,0.,0.804686,-0.505541\H,0,0.,-0.804686,-0.505541\Version=ES64L-G16RevA.03\State=2-
B1\HF=-55.7918729\MP2=-55.8517922\RMSD=1.893e-09\PG=C02V[C2(N1),SGV(H2)]\

15H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\H3N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.,0.,0.119349\H,0,0.,0.938581,-0.278482\H,0,-0.812835,-0.469291,-0.278482\H,0,0.812835,-0.469291,-0.278482\Version=ES64L-G16RevA.03\State=1-
A\HF=-56.4579585\MP2=-56.5326192\RMSD=3.740e-09\PG=C03[C3(N1),X(H3)]\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0.,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0.,0.,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0.,0.,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\

MIN_ID15

GINC-NX360-M5-04-10\SP\ROB2PLYP-FC\GTMP2large\H5N2(2)\DSAKIC\19-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\H,0,0.551412,-0.000606,-0.587635\N,0,1.442992,0.000038,-0.082892\N,0,-1.46119,-0.000094,-0.124476\H,0,-1.650419,-0.805536,0.49347\H,0,1.438438,-0.8
16296,0.526705\H,0,1.437811,0.816522,0.526678\H,0,-1.649861,0.806311,0.492359\Version=ES64L-G16RevA.03\State=2-
A\HF=-112.2486818\MP2=-112.3853723\RMSD=5.909e-09\PG=C01[X(H5N2)]\

TS_ID15

GINC-NX360-M5-04-10\SP\ROB2PLYP-FC\GTMP2large\H5N2(2)\DSAKIC\19-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\H,0,0,0.000058,-0.396631\N,0,-1.2197,-0.00001,-0.112863\N,0,1.2197,-0.000009,-0.112863\H,0,1.384777,0.810713,0.494171\H,0,-1.384777,0.810713,0.494
17\H,0,-1.384529,-0.810675,0.494189\H,0,1.384529,-0.810675,0.494188\\Version=ES64L-G16RevA.03\State=2-
A\HF=-112.2176468\MP2=-112.3695882\RMSD=5.227e-09\PG=CS[SG(H1),X(H4N2)]\

R15

GINC-NX360-M5-02-01\SP\ROB2PLYP-FC\GTMP2large\C2H8N1(2)\SSHKUNNI\07-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,2.274019,-0.237239,0.002065\H,0,1.2758,-0.001434,-0.069519\C,0,-1.013007,0.801411,-0.00132\H,0,-0.97129,1.37715,-0.921772\H,0,-0.901985,1.3522
69,0.92852\C,0,-1.568081,-0.58199,0.001352\H,0,-1.221805,-1.158871,0.866797\H,0,-2.672205,-0.578384,0.046578\H,0,-1.294746,-1.133465,-0.905791\H,0,2.61
9579,0.257476,0.843322\H,0,2.735048,0.229403,-0.802791\\Version=ES64L-G16RevA.03\State=2-
A\HF=-135.4464992\MP2=-135.629307\RMSD=5.545e-09\PG=C01[X(C2H8N1)]\

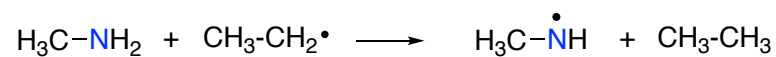
TS15

GINC-NX360-M5-02-05\SP\ROB2PLYP-FC\GTMP2large\C2H8N1(2)\SSHKUNNI\07-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,1.895364,-0.342779,-0.000118\H,0,0.682494,0.077168,-0.000076\C,0,-0.496034,0.682108,0.000061\H,0,-0.491761,1.302053,-0.900751\H,0,-0.491728,1.
301859,0.901006\C,0,-1.523845,-0.428247,-0.000037\H,0,-1.423407,-1.0663,0.884924\H,0,-2.546715,-0.022855,0.000013\H,0,-1.42342,-1.066125,-0.885125\H,0,
2.272959,0.174648,0.805908\H,0,2.273302,0.175839,-0.805217\\Version=ES64L-G16RevA.03\State=2-
A\HF=-135.4091816\MP2=-135.6018075\RMSD=5.958e-09\PG=C01[X(C2H8N1)]\

P15

GINC-NX360-M5-02-05\SP\ROB2PLYP-FC\GTMP2large\C2H8N1(2)\SSHKUNNI\07-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,2.658264,-0.302339,-0.00255\H,0,0.194047,0.010677,-0.004698\C,0,-0.755119,0.561865,0.001135\H,0,-0.768415,1.215441,-0.879518\H,0,-0.763423,1.2
0564,0.889047\C,0,-1.949343,-0.395396,-0.000815\H,0,-1.937133,-1.048222,0.879508\H,0,-2.90039,0.150189,0.004355\H,0,-1.941527,-1.039166,-0.887828\H,0,
2.865561,0.299076,0.812337\H,0,2.870199,0.323927,-0.797276\\Version=ES64L-G16RevA.03\State=2-
A\HF=-135.4406712\MP2=-135.6185879\RMSD=9.797e-09\PG=C01[X(C2H8N1)]\

System 16



16H

2

16

2H

		H(kJ/mol)			ΔH(kJ/mol)			
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
16	Metilamin_rad_konf1	-95.137399	-95.082066	-95.100793	-33.33	-33.20	-30.32	a)
16H	Metilamin_neut_konf1	-95.784452	-95.734666	-95.757933	-	-	-	
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-	
ST_ID1 6		-190.921851	-190.816732	-190.858726	0.00	0.00	0.00	
MIN_ID 16	Ident_MeAm_MeAm_opt_fwd	-190.926451	-190.819440	-190.862763	-12.08	-7.11	-10.60	
TS_ID1 6	Ident_MeAm_MeAm	-190.913681	-190.804034	-190.842694	21.45	33.34	42.09	
START1 6	START_Metilamin_primC_CH3CH3	-174.877769	-174.766473	-174.818668	0.00	0.00	0.00	
R16	Metilamino_TS_primC_CH3CH3_opt_fwd	-174.888748	-174.768470	-174.821606	-28.83	-5.24	0.00	0.00

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)				
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
TS16	Metilamino_TS_primC_CH3CH3_konf2	-174.866026	-174.747121	-174.798551	30.83	50.81	56.05	52.82	60.53
P16	Metilamino_TS_primC_CH3CH3_konf4_opt_rev	-174.887803	-174.767527	-174.820666	-26.34	-2.77	2.48	-5.25	2.47
FIN16	FIN_Metilamin_primC_CH3CH3	-174.888172	-174.768720	-174.821184	-27.31	-5.90		-6.61	

- a) RSE compared to CH₄/CH₃[•] radical system
b) RSE compared to NH₃/NH₂[•] radical system

16

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H4N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.806218,-0.153391,-0.000033\H,0,-1.203068,0.799038,0.000049\C,0,0.628679,0.012503,-0.000044\H,0,0.97408,0.580347,0.88201\H,0,1.126022,-0.962
474,-0.000624\H,0,0.97442,0.581813,-0.880942\Version=ES64L-G16RevA.03\State=2-
A\HF=-95.0200827\MP2=-95.1355318\RMSD=2.976e-09\PG=C01[X(C1H4N1)]\

16H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C1H5N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.752153,-0.00001,0.125912\H,0,1.142991,-0.812381,-0.348136\H,0,1.143104,0.812443,-0.347903\C,0,-0.705576,-0.000002,-0.017564\H,0,-1.115609,-0.
881958,0.486886\H,0,-1.115732,0.881416,0.48768\H,0,-1.086373,0.000564,-1.054525\Version=ES64L-G16RevA.03\State=1-
A\HF=-95.6745449\MP2=-95.8034231\RMSD=4.406e-09\PG=C01[X(C1H5N1)]\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0,0,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0,0,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\

MIN_ID16

GINC-SL230S-GEN8-02-05\SP\ROB2PLYP-FC\GTMP2large\C2H9N2(2)\DSAKIC\19-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\H,0,0.505496,0.376705,0.482811\C,0,2.340544,0.114094,-0.394908\H,0,3.151365,-0.623424,-0.367615\H,0,1.951925,0.130069,-1.419371\H,0,2.784665,1.10
5774,-0.194017\C,0,-2.047615,-0.568637,-0.194331\H,0,-1.172184,-1.218402,-0.1152\H,0,-2.833382,-0.929002,0.492823\H,0,-2.47279,-0.651048,-1.210095\N,0,
1.271492,-0.297877,0.515708\N,0,-1.667714,0.791869,0.108865\H,0,-2.516476,1.37078,0.020099\H,0,1.617356,-0.292143,1.473987\Version=ES64L-
G16RevA.03\State=2-A\HF=-190.6981713\MP2=-190.944073\RMSD=6.120e-09\PG=C01[X(C2H9N2)]\

TS_ID16

GINC-SL230S-GEN8-02-01\SP\ROB2PLYP-FC\GTMP2large\C2H9N2(2)\DSAKIC\19-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\H,0,0.000023,0.822958,-0.349499\C,0,-1.687541,-0.633224,0.021219\H,0,-2.770933,-0.648041,0.211343\H,0,-1.505937,-1.179612,-0.910047\H,0,-1.212391,
-1.196223,0.844935\C,0,1.687534,-0.63323,0.021209\H,0,1.505919,-1.179596,-0.910067\H,0,2.770926,-0.64806,0.211327\H,0,1.212381,-1.196241,0.844916\N,0,
-1.233797,0.74077,-0.123472\N,0,1.233804,0.740772,-0.123453\H,0,1.393278,1.226363,0.765516\H,0,-1.393277,1.226383,0.765485\Version=ES64L-
G16RevA.03\State=2-A\HF=-190.6597571\MP2=-190.9234608\RMSD=3.676e-09\PG=C01[X(C2H9N2)]\

R16

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C3H10N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,1.803253,0.136841,0.46183\H,0,2.152667,0.411733,1.392943\H,0,-0.891836,0.536628,-0.030586\C,0,2.966108,-0.200253,-0.325101\H,0,3.54777,-1.017
61,0.136036\H,0,2.669647,-0.509051,-1.332072\H,0,3.659474,0.654871,-0.410866\C,0,-1.966652,0.685885,-0.182209\H,0,-2.114022,1.048831,-1.20671\H,0,-2.2
94925,1.482089,0.497139\C,0,-2.74897,-0.60691,0.063458\H,0,-2.604948,-0.970775,1.087697\H,0,-3.825677,-0.463124,-0.087493\H,0,-2.423843,-1.403809,-0.6
15786\Version=ES64L-G16RevA.03\State=2-A\HF=-174.6694651\MP2=-174.9026402\RMSD=8.006e-09\PG=C01[X(C3H10N1)]\

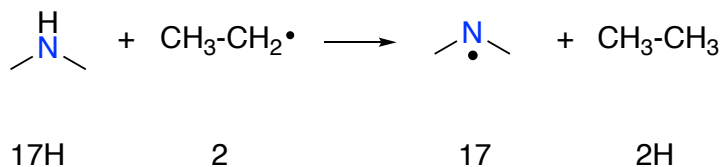
TS16

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C3H10N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.286478,-0.7134,-0.283728\H,0,-1.194326,-0.635361,-1.304238\H,0,-0.088487,-0.773609,0.059517\C,0,-1.816448,0.5582,0.206322\H,0,-2.861398,0.65
7209,-0.120498\H,0,-1.813845,0.553741,1.301609\H,0,-1.281416,1.460036,-0.135474\C,0,1.250993,-0.673266,0.313806\H,0,1.636857,-1.564341,-0.188826\H,0,1
.270685,-0.791945,1.40072\C,0,1.807153,0.636816,-0.194184\H,0,1.308743,1.49683,0.26908\H,0,2.880711,0.73074,0.029895\H,0,1.697639,0.729996,-1.281354\
\Version=ES64L-G16RevA.03\State=2-A\HF=-174.6290171\MP2=-174.8773214\RMSD=5.809e-09\PG=C01[X(C3H10N1)]\

P16

GINC-NX360-M5-04-04\SP\ROB2PLYP-FC\GTMP2large\C3H10N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,1.817451,-0.244681,-0.454391\H,0,2.224011,-0.698608,-1.287055\H,0,-0.887778,-0.548766,0.067191\C,0,2.928071,0.276922,0.30679\H,0,3.523057,0.99
7077,-0.281878\H,0,2.569768,0.77852,1.210791\H,0,3.628127,-0.523574,0.604199\C,0,-1.961694,-0.661898,0.252639\H,0,-2.095847,-0.899728,1.314969\H,0,-2.
313067,-1.527027,-0.322916\C,0,-2.730219,0.605341,-0.130941\H,0,-2.59922,0.844041,-1.193029\H,0,-3.805983,0.49736,0.053013\H,0,-2.382171,1.471284,0.44
4519\Version=ES64L-G16RevA.03\State=2-A\HF=-174.6694681\MP2=-174.902644\RMSD=8.408e-09\PG=C01[X(C3H10N1)]\

System 17



		H(kJ/mol)			ΔH(kJ/mol)				
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
17	MIN_CH3_NMe_radical	-134.426151	-134.338330	-134.370339	-56.10	-57.63	-53.14	a)	
17H	MIN_CH3_NMe_neutral	-135.064531	-134.981626	-135.018786	-	-	-		
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)	
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-		
ST_ID1 7		-269.490682	-269.319956	-269.389125	0.00	0.00	0.00		
MIN_ID 17	Ident_DiMeAm_DiMeAm_opt_fwd	-269.495755	-269.323207	-269.394310	-13.31	-8.54	-13.61		
TS_ID1 7	Ident_DiMeAm_DiMeAm	-269.481379	-269.309311	-269.377557	24.43	27.95	30.37		
START1 7	START_Metilamino_TS_CH3_NMe_secC	-214.157848	-214.013433	-214.079521	0.00	0.00	0.00		
R17	Metilamino_TS_CH3_NMe_secC_opt_rev	-214.158364	-214.013108	-214.080543	-1.35	0.85	0.00	-2.68	0.00
TS17	Metilamino_TS_CH3_NMe_secC	-214.148997	-213.998817	-214.065100	23.24	38.37	37.52	37.86	40.55
P17	Metilamino_TS_CH3_NMe_secC_opt_fwd	-214.176727	-214.023876	-214.090514	-49.57	-27.42	-28.27	-28.86	-26.18

		H(kJ/mol)			ΔH (kJ/mol)		
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
FIN17	FIN_Metilamino_TS_CH3_NMe_s ecC	-214.176924	-214.024984	-214.090730	-50.08	-30.33	-29.43

- a) RSE compared to CH₄/CH₃[•] radical system
b) RSE compared to NH₃/NH₂[•] radical system

17

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H6N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.000027,0.638865,0.00002\C,0,1.192834,-0.17191,-0.000007\H,0,1.232144,-0.833693,-0.883764\H,0,2.084311,0.462725,-0.000089\H,0,1.232191,-0.83
3555,0.883879\C,0,-1.192804,-0.171879,0.000027\H,0,-1.231585,-0.834882,0.882963\H,0,-2.084304,0.462681,0.001336\H,0,-1.232751,-0.832596,-0.884584\
\Version=ES64L-G16RevA.03\State=2-A\HF=-134.2501386\MP2=-134.421668\RMSD=5.024e-09\PG=C01[X(C2H6N1)]\

17H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H7N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,-0.000036,0.565598,-0.150153\C,0,1.213405,-0.222753,0.020536\H,0,1.277141,-0.967325,-0.78247\H,0,2.090061,0.42871,-0.060049\H,0,1.273703,-0.76
8095,0.98252\H,0,-0.000028,1.327509,0.524598\C,0,-1.213387,-0.222792,0.020547\H,0,-1.272954,-0.769294,0.981912\H,0,-2.08999,0.428907,-0.058557\H,0,-1.
277792,-0.96632,-0.783376\Version=ES64L-G16RevA.03\State=1-A\HF=-134.8957687\MP2=-135.0799509\RMSD=4.375e-09\PG=C01[X(C2H7N1)]\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0.,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0.,0.,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0.,0.,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\

MIN_ID17

GINC-SL250S-GEN8-09-01\SP\ROB2PLYP-FC\GTMP2large\C4H13N2(2)\DSAKIC\19-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\H,0,0.6286,-0.000131,-0.267185\C,0,2.265518,-1.211717,-0.159478\H,0,3.175622,-1.28961,0.449894\H,0,1.643598,-2.087136,0.057094\H,0,2.576494,-1.266
416,-1.221736\C,0,2.266089,1.211062,-0.162532\H,0,1.644965,2.087366,0.052716\H,0,3.17669,1.289547,0.446015\H,0,2.576323,1.263331,-1.225118\C,0,-1.721
51,0.001932,1.231909\H,0,-2.286599,-0.881271,1.578545\H,0,-0.731615,0.00248,1.695555\H,0,-2.286284,0.886413,1.57583\C,0,-2.849909,-0.001279,-0.885681\

H,0,-2.702975,-0.002807,-1.969764\H,0,-3.451962,-0.884514,-0.609071\H,0,-3.451977,0.882726,-0.611566\N,0,1.540905,0.000287,0.190706\N,0,-1.579763,-0.000282,-0.204493\\Version=ES64L-G16RevA.03\State=2-A\HF=-269.1496171\MP2=-269.5072738\RMSD=3.315e-09\PG=C01[X(C4H13N2)]\\

TS_ID17

GINC-SL250S-GEN8-09-03\SP\ROB2PLYP-FC\GTMP2large\C4H13N2(2)\ROOT\19-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\H,0,-0.000033,-0.000109,-0.659789\C,0,-1.962165,-0.930989,-0.342514\H,0,-3.038356,-0.719276,-0.442576\H,0,-1.682112,-1.629292,-1.137782\H,0,-1.823873,-1.430777,0.63464\C,0,-1.387084,1.184174,0.647349\H,0,-0.749713,2.067513,0.539588\H,0,-2.432254,1.527811,0.690631\H,0,-1.16881,0.708362,1.623176\C,0,1.961913,0.93108,-0.342584\H,0,3.038125,0.719584,-0.442869\H,0,1.681562,1.629392,-1.13774\H,0,1.823708,1.430756,0.634638\C,0,1.38736,-1.184234,0.647256\H,0,0.750151,-2.067694,0.539541\H,0,2.432605,-1.527666,0.690377\H,0,1.169129,-0.708508,1.623135\N,0,-1.20944,0.300539,-0.486558\N,0,1.2094,-0.30058,-0.486587\\Version=ES64L-G16RevA.03\State=2-A\HF=-269.1099496\MP2=-269.4873371\RMSD=5.433e-09\PG=C01[X(C4H13N2)]\\

R17

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C4H12N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-1.726692,1.211324,-0.199246\H,0,-2.820651,1.27844,-0.253845\H,0,-1.367194,2.089136,0.348607\H,0,-1.341267,1.2695,-1.236413\N,0,-1.351064,0.000199,0.516338\H,0,-0.34123,0.000514,0.666308\C,0,2.156979,0.001043,0.764706\H,0,2.09448,-0.924077,1.330604\C,0,2.665637,-0.000638,-0.635926\H,0,2.338506,-0.889611,-1.18827\H,0,2.338183,0.886814,-1.190519\H,0,3.770163,-0.000479,-0.669855\C,0,-1.726085,-1.211755,-0.19816\H,0,-1.340724,-1.270614,-1.235317\H,0,-1.366031,-2.088888,0.350418\H,0,-2.820014,-1.27954,-0.252597\H,0,2.094186,0.927566,1.328271\\Version=ES64L-G16RevA.03\State=2-A\HF=-213.8859155\MP2=-214.1780414\RMSD=8.220e-09\PG=C01[X(C4H12N1)]\\

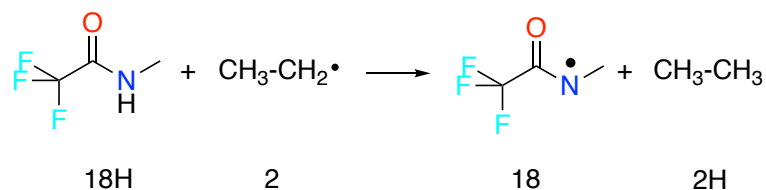
TS17

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C4H12N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,1.353918,1.204972,0.209338\H,0,2.444616,1.300244,0.31339\H,0,0.99198,2.083007,-0.335896\H,0,0.927078,1.221363,1.229186\N,0,1.053369,-0.000204,-0.548357\H,0,-0.155201,-0.00072,-0.747491\C,0,-1.552182,-0.001209,-0.763072\H,0,-1.75748,-0.905777,-1.34178\C,0,-2.101303,0.000642,0.643\H,0,-1.780778,-0.884769,1.205309\H,0,-1.781381,0.887891,1.202747\H,0,-3.202529,0.000271,0.646466\C,0,1.354769,-1.204356,0.210626\H,0,0.927972,-1.219946,1.230504\H,0,0.993422,-2.083227,-0.333653\H,0,2.445535,-1.298763,0.314747\H,0,-1.758028,0.901562,-1.344382\\Version=ES64L-G16RevA.03\State=2-A\HF=-213.8537024\MP2=-214.1584453\RMSD=9.848e-09\PG=C01[X(C4H12N1)]\\

P17

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C4H12N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,2.186823,1.185195,0.096448\H,0,2.959793,1.239024,-0.690763\H,0,1.566169,2.084083,0.038439\H,0,2.725892,1.189716,1.060492\N,0,1.372708,0.003621,-0.046557\H,0,-1.31587,0.050389,-0.552908\C,0,-2.399419,0.066627,-0.715921\H,0,-2.650291,-0.759975,-1.391921\C,0,-3.163997,-0.049348,0.605354\H,0,-2.919991,-0.983036,1.125873\H,0,-2.916601,0.776979,1.282266\H,0,-4.249191,-0.033294,0.447763\C,0,2.158816,-1.202884,0.029204\H,0,2.697609,-1.273981,0.990786\H,0,1.517236,-2.082321,-0.07823\H,0,2.930326,-1.2307,-0.760784\H,0,-2.647371,1.000235,-1.235623\\Version=ES64L-G16RevA.03\State=2-A\HF=-213.8995222\MP2=-214.1889045\RMSD=7.439e-09\PG=C01[X(C4H12N1)]\\

System 18



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)			
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
18	MIN_CF3_CO_NMe_trans_radical	-545.481415	-545.334657	-545.285037	9.79	15.86	16.39	a)
18H	MIN_CF3_CO_NMe_cis_neutral	-546.144889	-546.005947	-545.959961	-	-	-	
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-	
START 18	START_Metilamino_TS_CF3CO_NMe_secC	-625.238206	-625.037757	-625.020707	0.00	0.00	0.00	
R18	Metilamino_TS_CF3CO_NMe_secC_opt_rev	-625.241603	-625.039201	-625.024811	-8.92	-3.82	0.00	0.00
TS18	Metilamino_TS_CF3CO_NMe_secC	-625.220335	-625.012687	-624.996897	46.92	65.82	69.64	73.30
P18	Metilamino_TS_CF3CO_NMe_secC_opt_fwd	-625.232179	-625.020527	-625.007069	15.82	45.23	49.05	46.59
FIN18	FIN_Metilamino_TS_CF3CO_NMe_secC	-625.232188	-625.021317	-625.005428	15.80	43.16	40.10	

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

18

GINC-SL230S-GEN8-02-05\SP\ROB2PLYP-FC\GTMP2large\C3H3F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,0.47449,0.395918,-0.051124\O,0,0.729074,1.594959,-0.042717\N,0,1.39306,-0.592131,-0.277194\C,0,2.751172,-0.349315,0.125839\H,0,3.039236,-1.163
76,0.80784\H,0,3.404206,-0.446303,-0.751266\H,0,2.903036,0.619918,0.612612\C,0,-0.981197,-0.110206,0.018535\F,0,-1.050436,-1.243282,0.743455\F,0,-1.767
12,0.809101,0.588497\F,0,-1.448808,-0.370596,-1.214906\\Version=ES64L-G16RevA.03\State=2-
A\HF=-544.8820129\MP2=-545.4088476\RMSD=5.762e-09\PG=C01[X(C3H3F3N1O1)]\\

18H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C3H4F3N1O1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0.458984,-0.413521,0.000022\O,0,0.669722,-1.613695,0.000006\N,0,1.390488,0.569235,0.000018\H,0,1.072104,1.527393,-0.000041\C,0,2.816483,0.286
755,-0.000009\H,0,3.296093,0.70376,-0.892281\H,0,3.296229,0.704338,0.891919\H,0,2.938224,-0.797056,0.000338\C,0,-1.001374,0.098975,0.000002\F,0,-1.075
132,1.457668,-0.000128\F,0,-1.647919,-0.342654,-1.087336\F,0,-1.647883,-0.342433,1.087443\\Version=ES64L-G16RevA.03\State=1-
A\HF=-545.5575659\MP2=-546.0950232\RMSD=8.371e-09\PG=C01[X(C3H4F3N1O1)]\\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0,0,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0,0,0,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\\

R18

GINC-SL250S-GEN8-09-05\SP\ROB2PLYP-FC\GTMP2large\C5H9F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,0.017623,1.349219,0.221451\C,0,-0.025439,2.792443,0.052436\H,0,-0.135721,3.298001,1.018563\C,0,1.118854,0.626095,-0.085105\O,0,2.179247,1.058
35,-0.504515\C,0,0.930536,-0.901464,0.085538\F,0,0.464908,-1.443493,-1.062241\F,0,0.032668,-1.201206,1.059801\F,0,2.085,-1.492776,0.390344\H,0,0.912554,
3.103733,-0.408626\H,0,-0.861184,3.077999,-0.595235\H,0,-0.814875,0.87366,0.558266\C,0,-3.022726,-0.070195,0.62923\H,0,-3.660264,0.757011,0.929621\C,0
,-3.065816,-0.593211,-0.766031\H,0,-3.248201,0.20274,-1.497239\H,0,-2.13565,-1.105562,-1.036307\H,0,-3.878279,-1.330605,-0.89404\H,0,-2.591354,-0.67304
9,1.42341\\Version=ES64L-G16RevA.03\State=2-A\HF=-624.5486928\MP2=-625.1950446\RMSD=3.821e-09\PG=C01[X(C5H9F3N1O1)]\\

TS18

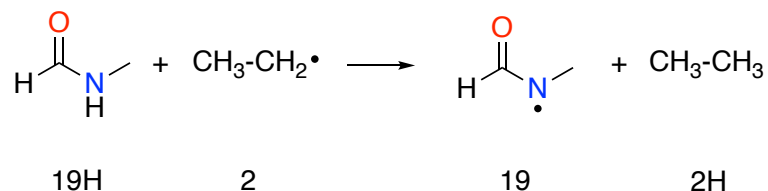
GINC-SL250S-GEN8-10-03\SP\ROB2PLYP-FC\GTMP2large\C5H9F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.540412,1.087879,0.555195\C,0,-1.308642,2.273903,0.206839\H,0,-0.791214,3.15684,0.598455\C,0,0.630966,0.884556,-0.102598\O,0,1.226078,1.737
046,-0.748676\C,0,1.245002,-0.524918,0.063411\F,0,0.684148,-1.373708,-0.836334\F,0,1.026908,-1.041501,1.289532\F,0,2.559867,-0.500574,-0.157887\H,0,-1.4
28567,2.404372,-0.875695\H,0,-2.287412,2.209467,0.688949\H,0,-1.341954,0.000776,0.627521\C,0,-2.173507,-0.962029,0.592534\H,0,-2.928912,-0.635384,1.3

13511\C,0,-2.674162,-1.162521,-0.818051\H,0,-3.200036,-0.278812,-1.196353\H,0,-1.851331,-1.397404,-1.499805\H,0,-3.383285,-2.002496,-0.853962\H,0,-1.569284,-1.78078,0.989813\\Version=ES64L-G16RevA.03\State=2-A\HF=-624.5038806\MP2=-625.1631466\RMSD=3.560e-09\PG=C01[X(C5H9F3N1O1)]\\

P18

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C5H9F3N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,0.06461,1.289165,0.540869\C,0,-0.267834,2.62481,0.127026\H,0,-0.32215,3.269534,1.013262\C,0,1.159621,0.698728,-0.02983\O,0,2.153973,1.300993,
-0.416898\C,0,1.129378,-0.843689,0.010171\F,0,-0.085639,-1.30213,-0.355278\F,0,1.388055,-1.288037,1.251699\F,0,2.041339,-1.349411,-0.825575\H,0,0.42250
7,3.041825,-0.613853\H,0,-1.287306,2.590343,-0.287343\H,0,-2.378334,-0.184813,1.142378\C,0,-3.213621,-0.667902,0.623879\H,0,-4.131508,-0.445239,1.1802
62\C,0,-3.311384,-0.193366,-0.827924\H,0,-3.490041,0.887945,-0.885568\H,0,-2.386218,-0.409801,-1.373276\H,0,-4.13313,-0.687162,-1.359288\H,0,-3.048624,-
1.750015,0.674975\\Version=ES64L-G16RevA.03\State=2-A\HF=-624.5308667\MP2=-625.1763186\RMSD=3.572e-09\PG=C01[X(C5H9F3N1O1)]\\

System 19



		H(kJ/mol)			ΔH(kJ/mol)			
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
19	FormylINMe_rad	-208.459329	-208.362995	-208.374634	-1.30	4.44	2.25	
19H	FormylINMe_neut	-209.118581	-209.029932	-209.044178	-	-	-	
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-	
START 19	START_FormylINMe_TS_primC_CH3C H3	-288.211898	-288.061739	-288.104913	0.00	0.00	0.00	
R19	FormylINMe_TS_primC_CH3CH3_opt _rev	-288.216051	-288.063666	-288.108478	-10.90	-5.06	0.00	-9.36
TS19	FormylINMe_TS_primC_CH3CH3	-288.194869	-288.037532	-288.080367	44.71	63.56	68.61	64.45
P19	FormylINMe_TS_primC_CH3CH3_opt _fwd	-288.207274	-288.044767	-288.091972	12.14	44.56	49.62	33.98
FIN19	FIN_FormylINMe_TS_primC_CH3CH3	-288.210102	-288.049649	-288.095025	4.72	31.74	25.96	

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

19

GINC-SL250S-GEN8-06-07\SP\ROB2PLYP-FC\GTMP2large\C2H4N1O1(2)\SSHKUNNI\07-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,0.497947,-0.730544,-0.135604\C,0,1.425783,0.354492,0.051066\H,0,2.189332,0.016464,0.76763\H,0,1.959859,0.527799,-0.893311\H,0,0.964083,1.2840
33,0.400974\C,0,-0.834139,-0.456792,0.079406\H,0,-1.440787,-1.35421,0.282925\O,0,-1.338498,0.65669,-0.048978\Version=ES64L-G16RevA.03\State=2-
A\HF=-208.1865884\MP2=-208.4286809\RMSD=3.081e-09\PG=C01[X(C2H4N1O1)]\

19H

GINC-NX360-M5-03-04\SP\ROB2PLYP-FC\GTMP2large\C2H5N1O1\SSHKUNNI\07-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,0.399232,-0.406725,0.000144\C,0,1.751542,0.115199,-0.000083\H,0,1.705593,1.208175,0.000547\H,0,2.30812,-0.202117,0.8902\H,0,2.307503,-0.20120
4,-0.891064\C,0,-0.735478,0.347869,0.000038\H,0,-0.510162,1.434349,0.000232\O,0,-1.86969,-0.095138,-0.000084\H,0,0.255461,-1.409434,0.000023\
\Version=ES64L-G16RevA.03\State=1-A\HF=-208.8580904\MP2=-209.1103066\RMSD=3.293e-09\PG=C01[X(C2H5N1O1)]\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0.,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0.,0.,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0.,0.,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\

R19

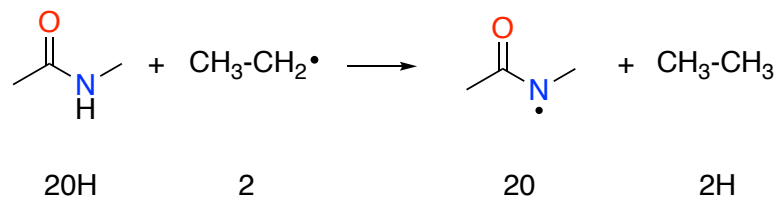
GINC-SL250S-GEN8-06-05\SP\ROB2PLYP-FC\GTMP2large\C4H10N1O1(2)\SSHKUNNI\07-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.101593,-0.334055,0.016479\H,0,-0.136494,-0.656868,-0.034437\C,0,-2.163013,-1.313772,0.135099\H,0,-3.124993,-0.793483,0.16852\H,0,-2.176626,-
1.999562,-0.720961\H,0,-2.06434,-1.905765,1.053251\C,0,2.202237,-1.042219,-0.370186\H,0,1.926348,-0.98946,-1.42079\H,0,2.413414,-2.030032,0.030705\C,0
,2.628978,0.191814,0.348826\H,0,2.728687,0.021348,1.426508\H,0,3.610022,0.548491,-0.012409\H,0,1.915751,1.010597,0.190134\C,0,-1.291707,1.009309,-0.0
47351\H,0,-2.365661,1.282725,0.004292\O,0,-0.409241,1.84745,-0.149813\Version=ES64L-G16RevA.03\State=2-
A\HF=-287.850058\MP2=-288.2109433\RMSD=4.509e-09\PG=C01[X(C4H10N1O1)]\

TS19

GINC-SL250S-GEN8-09-01\SP\ROB2PLYP-FC\GTMP2large\C4H10N1O1(2)\SSHKUNNI\07-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,0.969054,0.320429,-0.377906\H,0,-0.362243,0.491844,-0.584691\C,0,1.611272,1.445516,0.274268\H,0,2.633243,1.164222,0.563045\H,0,1.674175,2.292
29,-0.41519\H,0,1.087135,1.768881,1.185293\C,0,-1.620044,0.604732,-0.658261\H,0,-1.834791,0.026997,-1.560852\H,0,-1.766181,1.676601,-0.826542\C,0,-2.2
49277,0.057294,0.601891\H,0,-1.968601,0.642501,1.485367\H,0,-3.346263,0.086063,0.527297\H,0,-1.947591,-0.981785,0.761576\C,0,1.177642,-0.957948,0.052
24\H,0,2.194955,-1.083257,0.491389\O,0,0.416903,-1.903116,-0.075273\Version=ES64L-G16RevA.03\State=2-
A\HF=-287.8061053\MP2=-288.1791246\RMSD=5.460e-09\PG=C01[X(C4H10N1O1)]\

P19
GINC-SL230S-GEN8-02-04\SP\ROB2PLYP-FC\GTMP2large\C4H10N1O1(2)\SSHKUNNI\07-Oct-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.210997,-0.416285,0.108941\H,0,1.687439,-1.461747,-0.148669\C,0,-2.302525,-1.349321,0.131628\H,0,-3.301214,-0.913862,-0.026186\H,0,-2.114815
,-2.118921,-0.631761\H,0,-2.283005,-1.881134,1.094309\C,0,2.606308,-0.917159,-0.392068\H,0,2.587846,-0.707201,-1.468323\H,0,3.457349,-1.581969,-0.2000
81\C,0,2.701486,0.375156,0.422193\H,0,2.759409,0.162422,1.496598\H,0,3.592806,0.954675,0.152891\H,0,1.821533,1.004857,0.25638\C,0,-1.560314,0.893735,
-0.116007\H,0,-2.638094,1.123101,-0.25586\O,0,-0.720251,1.789913,-0.163295\\Version=ES64L-G16RevA.03\State=2-
A\HF=-287.830627\MP2=-288.19167\RMSD=3.451e-09\PG=C01[X(C4H10N1O1)]\\

System 20



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)			
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
20	MIN_CH3_CO_NMe_trans_radical	-247.755775	-247.631576	-247.657536	-5.33	0.42	-0.57	a)
20H	MIN_CH3_CO_NMe_cis_neutral	-248.413491	-248.296980	-248.326006	-	-	-	
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-	
START 20	START_Metilamino_TS_CH3CO_NMe_secC	-327.506808	-327.328787	-327.386741	0.00	0.00	0.00	
R20	Metilamino_TS_CH3CO_NMe_secC_opt_fwd	-327.508513	-327.329650	-327.389258	-4.48	-2.27	0.00	-6.61 0.00
TS20	Metilamino_TS_CH3CO_NMe_secC	-327.489103	-327.304570	-327.363187	46.48	63.58	65.85	61.84 68.45
P20	Metilamino_TS_CH3CO_NMe_secC_opt_rev	-327.505936	-327.316958	-327.377861	2.29	31.06	33.32	23.31 29.92
FIN20	FIN_Metilamino_TS_CH3CO_NMe_secC	-327.506548	-327.318230	-327.377927	0.68	27.72	23.14	

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

20

GINC-NX360-M5-01-06\SP\ROB2PLYP-FC\GTMP2large\C3H6N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,0.466907,-0.145468,-0.034089\O,0,0.373344,-1.372268,-0.038952\N,0,-0.633144,0.656463,-0.296805\C,0,-1.919363,0.181221,0.142195\H,0,-2.351564,0
.950566,0.800256\H,0,-2.593002,0.111372,-0.722425\H,0,-1.880177,-0.780948,0.664941\C,0,1.779297,0.591321,0.103329\H,0,2.087202,0.978702,-0.874801\H,0
,1.676329,1.450905,0.774423\H,0,2.545424,-0.09013,0.478247\\Version=ES64L-G16RevA.03\State=2-
A\HF=-247.430047\MP2=-247.7268335\RMSD=8.051e-09\PG=C01[X(C3H6N1O1)]\\

20H

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C3H7N1O1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,-0.483447,0.168265,0.000015\O,0,-0.422076,1.391314,-0.000075\N,0,0.62528,-0.635099,-0.000707\H,0,0.499007,-1.636254,0.000713\C,0,1.975525,-0.1
0352,0.000272\H,0,1.892179,0.984264,-0.00121\H,0,2.528642,-0.420193,0.892897\H,0,2.53025,-0.422732,-0.890366\C,0,-1.817033,-0.5669,0.000191\H,0,-1.724
527,-1.657979,-0.000361\H,0,-2.387804,-0.259885,0.881915\H,0,-2.388364,-0.259109,-0.880908\\Version=ES64L-G16RevA.03\State=1-
A\HF=-248.0993459\MP2=-248.4070522\RMSD=3.994e-09\PG=C01[X(C3H7N1O1)]\\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0,0,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0,0,0,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\\

R20

GINC-SL250S-GEN8-10-03\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.638198,0.591978,0.085827\C,0,-1.055796,1.974238,-0.049758\H,0,-2.132243,1.971963,-0.22775\C,0,-1.517327,-0.449888,-0.014651\O,0,-2.715832,-
0.300818,-0.225032\C,0,-0.903987,-1.83398,0.154238\H,0,-0.844136,2.546399,0.862098\H,0,-0.55382,2.462423,-0.894426\H,0,0.341432,0.396912,0.259652\C,0,
2.743021,0.203252,0.677931\H,0,2.591923,-0.493229,1.498323\C,0,3.363465,-0.254717,-0.597255\H,0,3.03817,-1.264939,-0.871761\H,0,3.132258,0.419382,-1.4
30365\H,0,4.464985,-0.29042,-0.520276\H,0,-1.403837,-2.341027,0.985404\H,0,-1.101923,-2.41923,-0.74919\H,0,0.174442,-1.820591,0.341492\H,0,2.710535,1.
261632,0.923233\\Version=ES64L-G16RevA.03\State=2-A\HF=-327.0905927\MP2=-327.5064851\RMSD=2.550e-09\PG=C01[X(C5H12N1O1)]\\

TS20

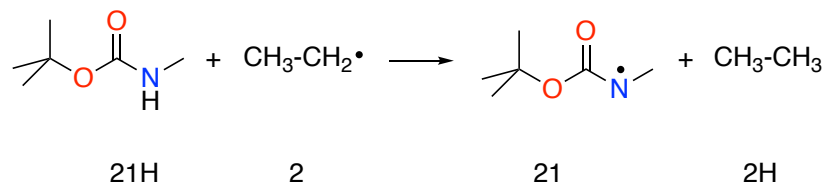
GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-0.361656,0.550335,-0.326329\C,0,-0.707809,1.938044,-0.05377\H,0,-1.409666,2.288474,-0.818631\C,0,-1.311794,-0.40805,-0.055129\O,0,-2.49338,-0.
106694,0.100098\C,0,-0.833482,-1.849101,-0.033117\H,0,-1.182611,2.081255,0.925122\H,0,0.199974,2.544498,-0.121662\H,0,0.824771,0.263467,0.136709\C,0,
1.987457,0.078497,0.699953\H,0,1.816789,-0.734183,1.41084\C,0,2.961186,-0.236707,-0.412466\H,0,2.681602,-1.1509,-0.947988\H,0,3.017062,0.578569,-1.141

859\H,0,3.974225,-0.389971,-0.011707\H,0,-0.639078,-2.156784,1.001776\H,0,-1.627594,-2.489119,-0.424674\H,0,0.079871,-1.993936,-0.615987\H,0,2.169938,1.023741,1.218748\\Version=ES64L-G16RevA.03\State=2-A\HF=-327.0468573\MP2=-327.4761423\RMSD=4.690e-09\PG=C01[X(C5H12N1O1)]\

P20

GINC-NX360-M5-04-04\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O1(2)\DSAKIC\18-Apr-2019\0\#\rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\O,2\N,0,-0.76747,0.545904,0.189086\C,0,-1.135047,1.922033,0.396354\H,0,-0.604384,2.550133,-0.331994\C,0,-1.785284,-0.350677,-0.103844\O,0,-2.771198,0.001313,-0.749814\C,0,-1.515826,-1.781575,0.298747\H,0,-2.213138,2.105914,0.333098\H,0,-0.75643,2.222219,1.385184\H,0,1.937945,-0.344749,0.221652\C,0,2.978915,-0.687267,0.234311\H,0,3.024499,-1.640417,-0.306282\C,0,3.914118,0.349168,-0.393868\H,0,3.641924,0.551112,-1.436415\H,0,3.874026,1.301994,0.147048\H,0,4.956163,0.008471,-0.384667\H,0,-1.167328,-1.835188,1.335884\H,0,-2.423831,-2.375021,0.175571\H,0,-0.721568,-2.197923,-0.331387\H,0,3.252737,-0.888472,1.277021\\Version=ES64L-G16RevA.03\State=2-A\HF=-327.0791491\MP2=-327.4938518\RMSD=2.585e-09\PG=C01[X(C5H12N1O1)]\

System 21



		H(kJ/mol)			ΔH(kJ/mol)				
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
21	MIN_Boc_NMe_ver1_rad	-440.835932	-440.614070	-440.675656	-3.12	-1.15	1.63	a)	
21H	MIN_Boc_NMe_ver1_neut	-441.494490	-441.278878	-441.344965	-	-	-		
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)	
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-		
START 21	START_Metilamino_TS_Boc_NMe_secC	-520.587807	-520.310685	-520.405700	0.00	0.00	0.00		
R21	Metilamino_TS_Boc_NMe_secC_opt_fwd	-520.590041	-520.311821	-520.409847	-5.87	-2.98	0.00	-10.89	0.00
TS21	Metilamino_TS_Boc_NMe_secC	-520.570906	-520.287269	-520.383593	44.37	61.48	64.46	58.04	68.93
P21	Metilamino_TS_Boc_NMe_secC_opt_rev	-520.586289	-520.299795	-520.397053	3.99	28.59	31.57	22.70	33.59
FIN21	FIN_Metilamino_TS_Boc_NMe_secC	-520.586705	-520.300724	-520.396047	2.89	26.15	25.34		

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

21

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C6H12N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,1.015135,0.12873,-0.185833\O,0,1.054066,1.343661,-0.052552\O,0,-0.073463,-0.649699,-0.172724\C,0,-1.422834,-0.084992,0.039888\C,0,-2.309918,-1
.331163,0.001867\H,0,-2.027614,-2.031505,0.794475\H,0,-3.358571,-1.049641,0.144013\H,0,-2.214247,-1.843603,-0.960514\C,0,-1.496972,0.597403,1.409544\
H,0,-1.190881,-0.097716,2.199136\H,0,-0.8584,1.48165,1.448264\H,0,-2.530082,0.902849,1.609305\C,0,-1.767269,0.868489,-1.10841\H,0,-1.656353,0.359358,-
2.071778\H,0,-2.809396,1.193728,-1.0131\H,0,-1.12317,1.749362,-1.097235\C,0,3.319755,-0.332456,0.286773\H,0,3.382516,-1.058309,1.115803\H,0,4.213813,-
0.470648,-0.329445\H,0,3.297518,0.676776,0.715925\N,0,2.143237,-0.634294,-0.487946\\Version=ES64L-G16RevA.03\State=2-
A\HF=-440.2633778\MP2=-440.8041665\RMSD=5.302e-09\PG=C01[X(C6H12N1O2)]\\

21H

GINC-NX360-M5-02-02\SP\ROB2PLYP-FC\GTMP2large\C6H13N1O2\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,-0.985161,-0.106175,-0.000063\O,0,-1.016739,-1.326783,-0.000035\O,0,0.130036,0.671679,-0.000072\C,0,1.469976,0.069376,0.000015\C,0,2.385781,1.
296749,0.000039\H,0,2.207509,1.912301,0.887913\H,0,3.435308,0.984077,0.000078\H,0,2.207572,1.912285,-0.887858\C,0,1.675744,-0.759953,1.272576\H,0,1.
483761,-0.147101,2.160414\H,0,1.009154,-1.623455,1.288249\H,0,2.712687,-1.111663,1.320211\C,0,1.675863,-0.760003,-1.272496\H,0,1.484001,-0.147172,-2.
160374\H,0,2.712795,-1.111761,-1.320005\H,0,1.009237,-1.623476,-1.288208\C,0,-3.436884,0.17812,0.000097\H,0,-3.990374,0.497953,0.891746\H,0,-3.990871,
0.49866,-0.890981\H,0,-3.367137,-0.910534,-0.000345\N,0,-2.086428,0.700712,-0.000137\H,0,-1.926941,1.697058,-0.000027\\Version=ES64L-
G16RevA.03\State=1-A\HF=-440.9319773\MP2=-441.4834862\RMSD=2.478e-09\PG=C01[X(C6H13N1O2)]\\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0,0,0,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0,0,0,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\\

R21

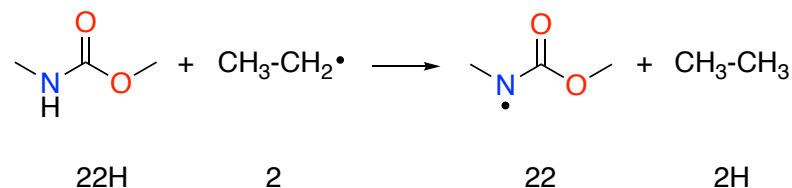
GINC-NX360-M5-02-05\SP\ROB2PLYP-FC\GTMP2large\C8H18N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.040231,1.171807,0.033865\O,0,0.715381,2.092097,0.306904\O,0,0.320259,-0.132044,-0.144879\C,0,1.727142,-0.541173,-0.040698\C,0,1.662547,-2.
044367,-0.326548\H,0,1.247328,-2.231658,-1.322414\H,0,2.666702,-2.479309,-0.283531\H,0,1.034116,-2.553748,0.411581\C,0,2.566506,0.172852,-1.106726\H,
0,2.143374,-0.001537,-2.102408\H,0,2.602291,1.24715,-0.921195\H,0,3.588454,-0.223125,-1.09781\C,0,2.24923,-0.283051,1.37733\H,0,1.606313,-0.777412,2.1
14356\H,0,3.260509,-0.693243,1.479392\H,0,2.27745,0.785703,1.593828\H,0,-1.907238,0.457292,-0.385696\C,0,-2.06818,2.564179,-0.030247\H,0,-2.877991,2.5
19127,0.707916\H,0,-1.337115,3.307827,0.289964\H,0,-2.49071,2.876322,-0.994119\N,0,-1.38683,1.290392,-0.133357\C,0,-2.85951,-1.705902,-0.708874\H,0,-3.
852825,-1.603816,-1.136914\C,0,-2.677269,-2.136615,0.705845\H,0,-3.465868,-1.745673,1.35971\H,0,-2.706104,-3.236903,0.802992\H,0,-1.706536,-1.810792,1

.096574\H,0,-2.020871,-1.735751,-1.398601\\Version=ES64L-G16RevA.03\State=2-
A\HF=-519.9225838\MP2=-520.5831902\RMSE=1.507e-09\PG=C01[X(C8H18N1O2)]\\

TS21
GINC-SL250S-GEN8-08-01\SP\ROB2PLYP-FC\GTMP2large\C8H18N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.215355,-1.016692,-0.122491\O,0,0.361524,-2.082607,0.047038\O,0,0.36567,0.206157,-0.145908\C,0,1.819421,0.355438,0.022716\C,0,2.013251,1.87
1364,-0.071563\H,0,1.452125,2.383576,0.717077\H,0,3.073238,2.12331,0.039137\H,0,1.667931,2.245455,-1.04093\C,0,2.248326,-0.159425,1.401517\H,0,1.6725
82,0.339062,2.189497\H,0,2.099723,-1.237202,1.482913\H,0,3.308916,0.063782,1.563878\C,0,2.555511,-0.355524,-1.118318\H,0,2.194051,0.007152,-2.086829\
H,0,3.628562,-0.142127,-1.053636\H,0,2.407603,-1.435261,-1.067812\H,0,-2.066572,0.203507,0.070259\C,0,-2.383606,-2.052317,0.000676\H,0,-3.434836,-1.78
5312,-0.139422\H,0,-2.154608,-2.899231,-0.655524\H,0,-2.219184,-2.379246,1.036136\N,0,-1.563673,-0.916649,-0.39417\C,0,-2.563131,1.260116,0.626897\H,0,
-3.588817,0.969733,0.872913\C,0,-2.43348,2.365225,-0.394756\H,0,-3.005135,2.142696,-1.302273\H,0,-2.810599,3.316998,0.008541\H,0,-1.386662,2.513184,-0
.677873\H,0,-1.955785,1.388961,1.526039\\Version=ES64L-G16RevA.03\State=2-
A\HF=-519.8799139\MP2=-520.5534537\RMSE=5.972e-09\PG=C01[X(C8H18N1O2)]\\

P21
GINC-NX360-M5-01-07\SP\ROB2PLYP-FC\GTMP2large\C8H18N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.593469,1.167846,-0.215289\O,0,-1.59522,1.575452,-0.785871\O,0,-0.372279,-0.069769,0.24194\C,0,-1.394433,-1.131419,0.118668\C,0,-0.71553,-2.3
2231,0.798125\H,0,-0.485854,-2.092285,1.843433\H,0,-1.375741,-3.195539,0.771336\H,0,0.218801,-2.57654,0.287735\C,0,-2.666244,-0.725782,0.870377\H,0,-2
.430479,-0.471505,1.909639\H,0,-3.152998,0.129029,0.397584\H,0,-3.368038,-1.567118,0.878748\C,0,-1.656267,-1.420654,-1.362517\H,0,-0.718152,-1.658937,
-1.874988\H,0,-2.323109,-2.285479,-1.453229\H,0,-2.122556,-0.566154,-1.855875\H,0,2.903281,0.424606,0.150465\C,0,0.319756,3.306214,0.378065\H,0,0.5055
35,3.359583,1.46451\H,0,1.045687,3.970778,-0.101632\H,0,-0.704502,3.646073,0.184095\N,0,0.550608,1.949422,-0.046799\C,0,3.820205,-0.169788,0.227125\H
,0,4.618095,0.376616,-0.290164\C,0,3.628143,-1.565536,-0.370976\H,0,3.355443,-1.509805,-1.431476\H,0,4.541937,-2.167138,-0.29591\H,0,2.829839,-2.11144
4,0.146055\H,0,4.095575,-0.227598,1.287252\\Version=ES64L-G16RevA.03\State=2-
A\HF=-519.9122938\MP2=-520.5714976\RMSE=4.188e-09\PG=C01[X(C8H18N1O2)]\\

System 22



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)			
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
22	MIN_OCH3_CO_NMe_trans_radical	-322.972694	-322.833850	-322.848137	-8.03	-4.51	-1.48	a)
22H	MIN_OCH3_CO_NMe_trans_neutral	-323.629382	-323.497376	-323.516262	-	-	-	
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-	
START 22	START_Metilamino_TS_OCH3_CO_NMe_trans	-402.722699	-402.529183	-402.576997	0.00	0.00	0.00	
R22	Metilamino_TS_OCH3_CO_NMe_trans_opt_rev	-402.726557	-402.531315	-402.580957	-10.13	-5.60	0.00	-10.40 0.00
TS22	Metilamino_TS_OCH3_CO_NMe_trans	-402.705661	-402.505261	-402.553569	44.73	62.81	68.40	61.51 71.91
P22	Metilamino_TS_OCH3_CO_NMe_trans_opt_fwd	-402.723143	-402.519925	-402.570104	-1.17	24.31	29.90	18.10 28.49
FIN22	FIN_Metilamino_TS_OCH3_CO_NMe_trans	-402.723467	-402.520504	-402.568528	-2.02	22.79	22.24	

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

22

GINC-SL230S-GEN8-02-05\SP\ROB2PLYP-FC\GTMP2large\C3H6N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,0.010928,0.097968,-0.131496\O,0,-0.064065,1.316858,-0.113242\N,0,1.179632,-0.616221,-0.374535\C,0,2.363081,-0.095638,0.259579\H,0,2.577812,-0.723505,1.141221\H,0,3.217601,-0.200962,-0.417279\H,0,2.254674,0.944146,0.589972\O,0,-1.038212,-0.735078,-0.021375\C,0,-2.308696,-0.090283,0.164433\H,0,-3.027928,-0.899774,0.290472\H,0,-2.292344,0.551866,1.04943\H,0,-2.560907,0.515252,-0.710232\\Version=ES64L-G16RevA.03\State=2-A\HF=-322.5650964\MP2=-322.9357826\RMSD=7.323e-09\PG=C01[X(C3H6N1O2)]\\

22H

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C3H7N1O2\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0.067119,0.522872,0.010793\O,0,0.720771,1.549842,-0.037435\N,0,-1.295654,0.472198,0.083419\H,0,-1.734218,1.371601,-0.047993\C,0,-2.103514,-0.730103,-0.040017\H,0,-1.707625,-1.512349,0.610819\H,0,-3.123702,-0.49802,0.277195\H,0,-2.134562,-1.118394,-1.067289\O,0,0.603889,-0.727521,0.021546\C,0,2.03609,-0.757488,-0.004018\H,0,2.304745,-1.814943,-0.001927\H,0,2.418681,-0.267116,-0.90314\H,0,2.450799,-0.256415,0.87497\\Version=ES64L-G16RevA.03\State=1-A\HF=-323.232603\MP2=-323.6139446\RMSD=8.299e-09\PG=C01[X(C3H7N1O2)]\\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,0,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\\Version=ES64L-G16RevA.03\State=2-A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0,0,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0,0,-0.765285\H,0,1.02099,-0.000292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\\Version=ES64L-G16RevA.03\State=1-A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\\

R22

GINC-NX360-M5-05-04\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.746814,-0.192343,-0.078523\O,0,-0.272637,-1.312749,-0.193865\N,0,-0.032359,0.96409,-0.068939\C,0,-0.582515,2.289496,0.158214\H,0,-0.962121,2.414672,1.180414\H,0,0.210509,3.022301,-0.010964\H,0,-1.401057,2.495591,-0.537431\O,0,-2.080169,0.055254,0.04627\C,0,-2.907563,-1.113365,0.021452\H,0,-3.929261,-0.74868,0.138625\H,0,-2.799326,-1.646855,-0.926954\H,0,-2.647724,-1.791424,0.838911\H,0,0.974032,0.840303,-0.09367\C,0,3.274728,0.269581,-0.36292\H,0,3.851623,1.103846,0.027238\H,0,3.008795,0.307672,-1.41655\C,0,3.175227,-1.016686,0.38362\H,0,3.954983,-1.730064,0.061758\H,0,3.302233,-0.872367,1.462359\H,0,2.20789,-1.503757,0.208535\\Version=ES64L-G16RevA.03\State=2-A\HF=-402.2246267\MP2=-402.7146461\RMSD=4.144e-09\PG=C01[X(C5H12N1O2)]\\

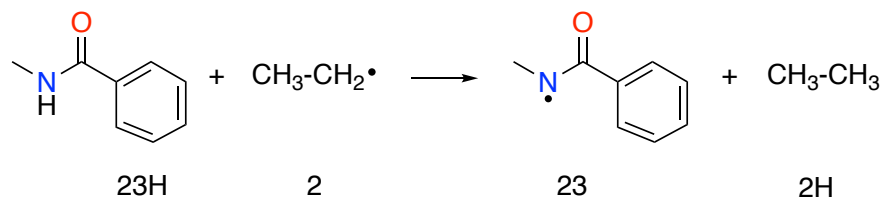
TS22

GINC-SL250S-GEN8-08-03\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,0.663945,-0.1381,0.338327\O,0,0.43065,-1.294938,0.644769\N,0,-0.189706,0.923799,0.556119\C,0,-0.096478,2.110584,-0.280093\H,0,-0.127337,1.905194,-1.359193\H,0,-0.915837,2.785633,-0.016875\H,0,0.849183,2.62048,-0.063367\O,0,1.84596,0.269545,-0.205431\C,0,2.834894,-0.761922,-0.327956\H,0,3.710

063,-0.27552,-0.761358\H,0,3.077653,-1.184301,0.651003\H,0,2.47866,-1.563991,-0.979987\H,0,-1.426541,0.429901,0.540095\C,0,-2.598578,-0.067885,0.391012\H,0,-3.231593,0.815223,0.259324\H,0,-2.747494,-0.52613,1.372165\C,0,-2.594834,-1.039624,-0.764761\H,0,-3.57014,-1.541165,-0.851589\H,0,-2.402607,-0.536389,-1.719571\H,0,-1.83265,-1.810701,-0.617355\\Version=ES64L-G16RevA.03\State=2-A\HF=-402.1804229\MP2=-402.6832118\RMSD=5.996e-09\PG=C01[X(C5H12N1O2)]\\

P22
GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O2(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\\nekaj\
\0,2\C,0,-0.975162,0.202829,0.070895\O,0,-0.618065,-0.146766,1.185746\N,0,-0.335377,1.178826,-0.686298\C,0,0.024178,2.377842,0.026491\H,0,0.085197,2.227052,1.111016\H,0,0.967981,2.769674,-0.364874\H,0,-0.749576,3.138827,-0.174187\O,0,-1.968301,-0.368754,-0.628774\C,0,-2.64242,-1.447944,0.040489\H,0,-3.437693,-1.756153,-0.638327\H,0,-1.950387,-2.274242,0.222993\H,0,-3.058327,-1.112879,0.994567\H,0,2.130411,-0.33741,-1.34135\C,0,2.82369,-1.00208,-0.812883\H,0,3.765577,-1.017863,-1.374128\H,0,2.401439,-2.013335,-0.849894\C,0,3.03709,-0.544015,0.632268\H,0,3.706492,-1.223631,1.172894\H,0,3.485922,0.456167,0.669829\H,0,2.087271,-0.503622,1.176227\\Version=ES64L-G16RevA.03\State=2-A\HF=-402.2144491\MP2=-402.7035121\RMSD=6.636e-09\PG=C01[X(C5H12N1O2)]\\

System 23



		H(kJ/mol)			ΔH(kJ/mol)				
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
23	MIN_Ph_CO_NMe_trans_radical	-439.440854	-439.207933	-439.265785	-14.06	-6.36	-4.20	a)	
23H	MIN_Ph_CO_NMe_cis_neutral	-440.095243	-439.870757	-439.932873	-	-	-		
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)	
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-		
START 23	START_Metilamino_TS_PhCO_NMe_secC	-519.188560	-518.902564	-518.993608	0.00	0.00	0.00		
R23	Metilamino_TS_PhCO_NMe_secC_opt_fwd	-519.190467	-518.904138	-518.99815	-5.01	-4.13	0.00	-11.93	0.00
TS23	Metilamino_TS_PhCO_NMe_secC	-519.172193	-518.880713	-518.974112	42.97	57.37	61.50	51.19	63.11
P23	Metilamino_TS_PhCO_NMe_secC_opt_rev	-519.190694	-518.893439	-518.986437	-5.60	23.96	28.09	18.83	30.75
FIN23	FIN_Metilamino_TS_PhCO_NMe_secC	-519.191627	-518.894587	-518.986176	-8.05	20.94	19.51		

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

23

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C8H8N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-2.108472,-1.383151,-0.047562\C,0,-0.731734,-1.180667,-0.129852\C,0,-0.209942,0.120308,-0.069573\C,0,-1.078784,1.212822,0.06954\C,0,-2.452664,
1.006515,0.150247\C,0,-2.969201,-0.292036,0.092482\H,0,-2.510815,-2.391184,-0.098082\H,0,-0.053841,-2.018591,-0.252185\H,0,-0.656035,2.211506,0.112046
\H,0,-3.123201,1.854608,0.258346\H,0,-4.042417,-0.452025,0.155086\C,0,1.254603,0.379977,-0.129673\O,0,1.730708,1.516137,-0.218758\N,0,2.070467,-0.7449
31,-0.171981\C,0,3.415413,-0.588344,0.312267\H,0,3.589084,-1.369977,1.067071\H,0,4.116608,-0.802928,-0.506606\H,0,3.626361,0.40147,0.730996\
\Version=ES64L-G16RevA.03\State=2-A\HF=-438.8127959\MP2=-439.3597608\RMSD=5.642e-09\PG=C01[X(C8H8N1O1)]\

23H

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C8H9N1O1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,-2.177373,-1.357463,0.139094\C,0,-0.795759,-1.173935,0.20171\C,0,-0.243065,0.105824,0.050717\C,0,-1.096645,1.19973,-0.143704\C,0,-2.475423,1.0
15201,-0.213735\C,0,-3.018996,-0.26462,-0.075591\H,0,-2.596146,-2.351973,0.267416\H,0,-0.155957,-2.028291,0.40705\H,0,-0.654188,2.186323,-0.234013\H,0,
-3.128025,1.869427,-0.372736\H,0,-4.094997,-0.408603,-0.126172\C,0,1.234242,0.385756,0.110865\O,0,1.669142,1.501123,0.384106\N,0,2.059504,-0.678186,-
0.147918\C,0,3.502324,-0.515881,-0.199053\H,0,3.781694,0.267031,0.506973\H,0,3.989027,-1.454185,0.083494\H,0,3.853025,-0.218453,-1.196752\H,0,1.66007
1,-1.490624,-0.594493\Version=ES64L-G16RevA.03\State=1-A\HF=-439.4793372\MP2=-440.0371852\RMSD=7.138e-09\PG=C01[X(C8H9N1O1)]\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0,0,0,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0,0,0,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\

R23

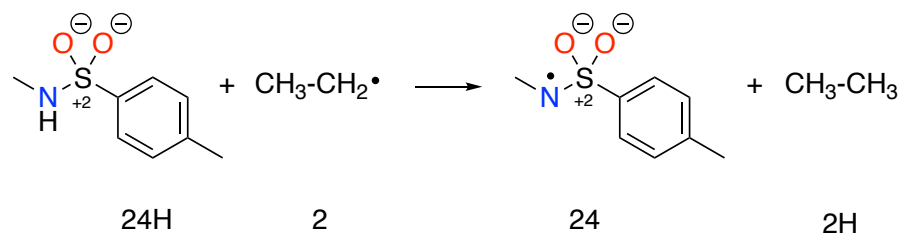
GINC-SL250S-GEN8-08-03\SP\ROB2PLYP-FC\GTMP2large\C10H14N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,1.651429,-0.931971,-0.358624\C,0,2.885237,-1.690233,-0.238747\H,0,3.201186,-1.811109,0.806411\C,0,0.457083,-1.505372,-0.015611\O,0,0.373963,-2
.68173,0.331129\H,0,2.735558,-2.686271,-0.659835\H,0,3.674775,-1.176142,-0.79355\H,0,1.725698,0.079762,-0.371637\C,0,2.504302,2.395377,-0.131589\H,0,3
.524176,2.049177,0.0139\C,0,1.689983,2.859273,1.027079\H,0,0.615215,2.790771,0.822292\H,0,1.903912,2.281966,1.933694\H,0,1.898925,3.916738,1.269448\
C,0,-0.757835,-0.620796,-0.0984\C,0,-1.880462,-0.996468,0.650705\C,0,-0.824966,0.526299,-0.90196\C,0,-3.039772,-0.224615,0.621122\H,0,-1.820407,-1.9018
01,1.245864\C,0,-1.989259,1.295227,-0.93743\H,0,0.018357,0.804473,-1.527641\C,0,-3.095976,0.925236,-0.170755\H,0,-3.902192,-0.520902,1.212274\H,0,-2.0
35859,2.175696,-1.572942\H,0,-4.001855,1.525102,-0.198137\H,0,2.220798,2.666617,-1.145291\Version=ES64L-G16RevA.03\State=2-
A\HF=-518.4705055\MP2=-519.1373076\RMSD=5.692e-09\PG=C01[X(C10H14N1O1)]\

TS23

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C10H14N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,1.679936,-0.474476,-0.756806\C,0,3.034926,-0.978891,-0.573705\H,0,3.300182,-1.140074,0.479021\C,0,0.687638,-1.135629,-0.053797\O,0,0.905521,-2
.198072,0.531257\H,0,3.125681,-1.942757,-1.086332\H,0,3.734325,-0.276676,-1.035776\H,0,1.677808,0.801852,-0.513684\C,0,1.829869,2.041565,-0.103659\H,
0,2.800043,2.308221,-0.532596\C,0,1.760382,2.083188,1.403884\H,0,0.79535,1.717851,1.77084\H,0,2.55271,1.482103,1.863978\H,0,1.880785,3.11418,1.76854
8\C,0,-0.682591,-0.532857,-0.105606\C,0,-1.604769,-0.904875,0.883\C,0,-1.079113,0.351698,-1.119055\C,0,-2.895416,-0.381257,0.873537\H,0,-1.289767,-1.60
9448,1.646187\C,0,-2.374939,0.867816,-1.131964\H,0,-0.377997,0.607808,-1.906702\C,0,-3.282406,0.507623,-0.133277\H,0,-3.602206,-0.668501,1.647404\H,0,
-2.679461,1.544053,-1.92639\H,0,-4.291232,0.911966,-0.143798\H,0,1.008582,2.54505,-0.619256\\Version=ES64L-G16RevA.03\State=2-
A\HF=-518.4282154\MP2=-519.1087276\RMSD=4.402e-09\PG=C01[X(C10H14N1O1)]\\

P23
GINC-NX360-M5-02-05\SP\ROB2PLYP-FC\GTMP2large\C10H14N1O1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,0.905971,-1.328343,0.365015\C,0,1.564122,-2.530732,0.800771\H,0,0.925575,-3.420193,0.781469\C,0,-0.389719,-1.464123,-0.122932\O,0,-0.751214,-2
.507947,-0.674679\H,0,2.451899,-2.697774,0.17455\H,0,1.944516,-2.350632,1.817203\H,0,2.922587,0.528278,-0.600459\C,0,3.685059,1.230537,-0.956442\H,0,
4.182423,0.772749,-1.819756\C,0,4.690675,1.57208,0.146116\H,0,4.195683,2.031021,1.010142\H,0,5.211434,0.675838,0.503507\H,0,5.452628,2.27574,-0.2091
82\C,0,-1.257822,-0.259595,-0.023042\C,0,-2.596212,-0.364833,-0.430184\C,0,-0.778082,0.957718,0.483332\C,0,-3.44483,0.733534,-0.330758\H,0,-2.948033,-1
.314473,-0.820368\C,0,-1.631898,2.055098,0.582841\H,0,0.26122,1.03607,0.783651\C,0,-2.963726,1.944905,0.176616\H,0,-4.480846,0.649019,-0.647062\H,0,-1
.257465,2.997894,0.971989\H,0,-3.62719,2.802325,0.253588\H,0,3.16809,2.128576,-1.314861\\Version=ES64L-G16RevA.03\State=2-
A\HF=-518.461892\MP2=-519.1268735\RMSD=4.050e-09\PG=C01[X(C10H14N1O1)]\\

System 24



		H(kJ/mol)			ΔH(kJ/mol)				
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
24	MIN_Tos_NMe_ver2_rad	-913.951715	-913.642973	-913.675801	-29.25	-31.73	-18.61	a)	
24H	MIN_Tos_NMe_ver3_neut	-914.60032	-914.296134	-914.337399	-	-	-		
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)	
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-		
START 24	START_Metilamino_TS_Tos_NMe_secC	-993.693637	-993.327941	-993.398134	0.00	0.00	0.00		
R24	Metilamino_TS_Tos_NMe_secC_opt_rev	-993.697886	-993.329502	-993.402027	-11.16	-4.10	0.00	-10.22	0.00
TS24	Metilamino_TS_Tos_NMe_secC	-993.685171	-993.312266	-993.383363	22.23	41.15	45.25	38.78	49.00
P24	Metilamino_TS_Tos_NMe_secC_opt_fwd	-993.706734	-993.329212	-993.401187	-34.39	-3.34	0.76	-8.02	2.21
FIN24	FIN_Metilamino_TS_Tos_NMe_secC	-993.702488	-993.329627	-993.396192	-23.24	-4.43	5.10		

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

24

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C8H10N1O2S1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\S,0,1.568228,0.001594,-0.402757\O,0,1.968322,-1.27395,-1.016996\O,0,1.968869,1.282902,-1.004436\C,0,-0.202395,0.000972,-0.184326\C,0,-0.882665,-1.
215381,-0.11097\C,0,-2.265228,-1.20525,0.055859\C,0,-2.976534,0.,0.149614\C,0,-2.26586,1.205394,0.059398\C,0,-0.882896,1.216546,-0.107383\H,0,-0.33671
5,-2.148479,-0.199902\H,0,-2.802442,-2.148999,0.107169\H,0,-2.803391,2.148735,0.113556\H,0,-0.337297,2.150113,-0.193423\C,0,-4.471637,-0.001813,0.3603
26\H,0,-4.93462,0.905574,-0.040292\H,0,-4.943197,-0.86603,-0.118777\H,0,-4.716186,-0.048843,1.429809\N,0,2.112649,-0.007424,1.213668\C,0,3.561404,-0.00
4612,1.292792\H,0,3.978912,0.883358,0.79572\H,0,3.849996,-0.00885,2.346018\H,0,3.982096,-0.886874,0.788159\\Version=ES64L-G16RevA.03\State=2-
A\HF=-913.1242843\MP2=-913.8258572\RMSD=2.787e-09\PG=C01[X(C8H10N1O2S1)]\\

24H

GINC-NX360-M5-01-06\SP\ROB2PLYP-FC\GTMP2large\C8H11N1O2S1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\S,0,1.698773,0.415664,0.323419\O,0,2.005318,1.837123,0.156924\O,0,2.137913,-0.362594,1.482501\C,0,-0.085839,0.231827,0.202379\C,0,-0.830775,1.191
418,-0.488277\C,0,-2.209245,1.030233,-0.603479\C,0,-2.861199,-0.077729,-0.041447\C,0,-2.092436,-1.019162,0.656285\C,0,-0.711542,-0.873376,0.782927\H,0,
-0.335728,2.064463,-0.901243\H,0,-2.791595,1.783192,-1.129145\H,0,-2.58203,-1.873566,1.117299\H,0,-0.125477,-1.588609,1.350318\C,0,-4.352693,-0.256311
, -0.196174\H,0,-4.773607,-0.844546,0.625447\H,0,-4.870891,0.70781,-0.225519\H,0,-4.591367,-0.782171,-1.130272\N,0,2.367773,-0.335013,-1.026469\H,0,2.18
5554,0.217776,-1.860153\C,0,2.21033,-1.780827,-1.189097\H,0,1.176021,-2.093484,-1.394623\H,0,2.849058,-2.09921,-2.017638\H,0,2.559829,-2.269851,-0.277
995\\Version=ES64L-G16RevA.03\State=1-A\HF=-913.7807658\MP2=-914.4933547\RMSD=7.179e-09\PG=C01[X(C8H11N1O2S1)]\\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0.,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0.,0.,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0.,0.,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\\

R24

GINC-SL250S-GEN8-08-01\SP\ROB2PLYP-FC\GTMP2large\C10H16N1O2S1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,5.037304,0.859148,0.40063\H,0,5.397913,1.561834,-0.361323\H,0,5.675747,-0.028556,0.362282\H,0,5.183289,1.339597,1.375203\C,0,3.586321,0.5081
88,0.172663\C,0,3.207354,-0.776659,-0.231355\C,0,2.583972,1.47738,0.350062\C,0,1.867063,-1.097579,-0.45605\H,0,3.968939,-1.538783,-0.376204\C,0,1.2448
6,1.176055,0.130819\H,0,2.86081,2.481838,0.661675\C,0,0.895082,-0.117685,-0.268357\H,0,1.572025,-2.090046,-0.779251\H,0,0.475862,1.929844,0.263615\S,
0,-0.825225,-0.506772,-0.585584\O,0,-1.434285,0.589828,-1.349791\O,0,-0.875788,-1.887071,-1.088955\C,0,-1.393872,-1.573024,1.817956\H,0,-0.337595,-1.77
1306,2.022306\H,0,-1.882997,-1.33853,2.767352\H,0,-1.844897,-2.473477,1.384273\N,0,-1.505956,-0.389273,0.957121\H,0,-2.471614,-0.061437,0.840588\C,0,-
4.714513,0.487687,0.481481\H,0,-5.113115,0.391755,1.488323\C,0,-4.502178,1.828964,-0.132365\H,0,-4.251781,2.586902,0.618558\H,0,-3.701633,1.800813,-0.
880362\H,0,-5.412156,2.181827,-0.650239\H,0,-4.761284,-0.395913,-0.15025\\Version=ES64L-G16RevA.03\State=2-
A\HF=-992.7718897\MP2=-993.5934369\RMSD=2.051e-09\PG=C01[X(C10H16N1O2S1)]\\

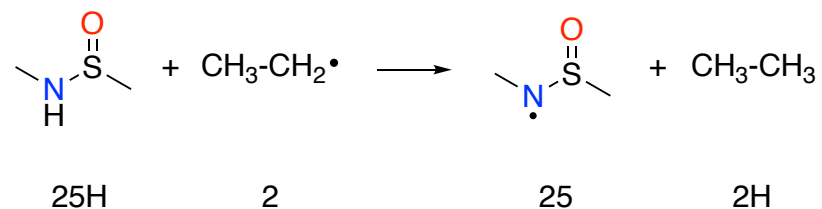
TS24

GINC-NX360-M5-01-07\SP\ROB2PLYP-FC\GTMP2large\C10H16N1O2S1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,5.000947,0.669111,0.471705\H,0,5.475037,1.134197,-0.402387\H,0,5.549888,-0.251018,0.694004\H,0,5.134553,1.357061,1.314179\C,0,3.539201,0.393
437,0.211988\C,0,3.083364,-0.906011,-0.041689\C,0,2.607519,1.444924,0.198506\C,0,1.736452,-1.16065,-0.302993\H,0,3.791156,-1.731235,-0.040015\C,0,1.26
1497,1.210982,-0.060482\H,0,2.94511,2.460571,0.391005\C,0,0.834893,-0.09729,-0.308346\H,0,1.384749,-2.164648,-0.515548\H,0,0.546119,2.026292,-0.07977
8\S,0,-0.897868,-0.405897,-0.649771\O,0,-1.428821,0.710311,-1.441814\O,0,-1.020076,-1.789389,-1.138574\C,0,-1.535756,-1.435729,1.728265\H,0,-0.497766,-
1.641598,2.018989\H,0,-2.106217,-1.235509,2.639825\H,0,-1.935732,-2.32322,1.223634\N,0,-1.569234,-0.219594,0.909028\H,0,-2.809109,0.074641,0.695333\C,
0,-4.099799,0.283562,0.466189\H,0,-4.563958,-0.079805,1.387721\C,0,-4.233557,1.760879,0.196887\H,0,-3.925574,2.358775,1.061619\H,0,-3.625929,2.053646,
-0.664064\H,0,-5.281364,2.016371,-0.024448\H,0,-4.307827,-0.369673,-0.384016\\Version=ES64L-G16RevA.03\State=2-
A\HF=-992.7364152\MP2=-993.5710909\RMSD=4.583e-09\PG=C01[X(C10H16N1O2S1)]\\

P24

GINC-SL250S-GEN8-10-03\SP\ROB2PLYP-FC\GTMP2large\C10H16N1O2S1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,4.646654,1.302554,0.365067\H,0,5.198175,1.31727,-0.584282\H,0,5.253481,0.74713,1.087013\H,0,4.568127,2.338819,0.710218\C,0,3.284954,0.67493,
0.187472\C,0,3.081977,-0.687221,0.448092\C,0,2.20022,1.438227,-0.270374\C,0,1.834892,-1.279673,0.25963\H,0,3.912037,-1.294205,0.800638\C,0,0.946693,0.
865309,-0.466299\H,0,2.340787,2.495769,-0.479709\C,0,0.77532,-0.493015,-0.192408\H,0,1.682218,-2.336449,0.450484\H,0,0.114316,1.456856,-0.832344\S,0,-
0.824862,-1.243024,-0.434625\O,0,-1.549336,-0.497268,-1.47724\O,0,-0.649086,-2.69905,-0.542501\C,0,-2.893987,-1.534846,1.143508\H,0,-2.80277,-2.625319,
1.037184\H,0,-3.329842,-1.28811,2.113772\H,0,-3.560944,-1.184775,0.341194\N,0,-1.59806,-0.89004,1.04553\H,0,-2.590338,1.954773,1.346356\C,0,-3.291391,
2.618548,0.827107\H,0,-3.426604,3.512749,1.446984\C,0,-2.782351,2.975415,-0.571797\H,0,-1.829158,3.516266,-0.520081\H,0,-2.624326,2.075352,-1.176002\
H,0,-3.492914,3.617692,-1.105257\H,0,-4.258541,2.104029,0.777062\\Version=ES64L-G16RevA.03\State=2-
A\HF=-992.7733168\MP2=-993.5936953\RMSD=6.964e-09\PG=C01[X(C10H16N1O2S1)]\\

System 25



		H(kJ/mol)			ΔH(kJ/mol)			
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3	
25	MIN_CH3SO_NMe_ver1_rad	-725.650518	-725.382063	-725.424962	-69.13	-69.04	-63.79	a)
25H	MIN_CH3SO_NMe_ver1_neut	-726.283934	-726.021011	-726.069353	-	-	-	
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-	
START 25	START_Metilamino_TS_CH3SO_NMe_ver3	-805.377251	-805.052818	-805.130088	0.00	0.00	0.00	
R25	Metilamino_TS_CH3SO_NMe_ver1_opt_fwd	-805.379716	-805.053839	-805.134009	-6.47	-2.68	0.00	0.00
TS25	Metilamino_TS_CH3SO_NMe_ver3	-805.367065	-805.037806	-805.117233	26.74	39.41	42.09	33.75
P25	Metilamino_TS_CH3SO_NMe_ver1_opt_rev	-805.400401	-805.067624	-805.145867	-60.78	-38.87	-36.19	-41.43
FIN25	FIN_Metilamino_TS_CH3SO_NMe_ver3	-805.401291	-805.068717	-805.145353	-63.12	-41.74	-40.08	

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

25

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C5H12N1O1S1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\S,0,-0.492075,-0.472827,-0.578182\O,0,-0.81215,-1.721574,0.203826\C,0,1.177385,0.208052,0.07892\C,0,1.014492,0.456349,1.579189\C,0,2.175457,-0.920
74,-0.19814\C,0,1.50925,1.476271,-0.706066\H,0,0.333326,1.290562,1.770607\H,0,0.629722,-0.438465,2.078707\H,0,1.990959,0.699491,2.016541\H,0,2.274958
,-1.11806,-1.271596\H,0,3.161211,-0.62904,0.18359\H,0,1.872769,-1.846867,0.298746\H,0,2.489589,1.847686,-0.381096\H,0,1.568091,1.280684,-1.782833\H,0,
0.765759,2.258085,-0.536101\N,0,-1.438515,0.844749,-0.275439\C,0,-2.758793,0.550581,0.252972\H,0,-3.156533,1.467223,0.698721\H,0,-3.442679,0.253727,-
0.558614\H,0,-2.753924,-0.263528,0.990455\\Version=ES64L-G16RevA.03\State=2-
A\HF=-725.0715381\MP2=-725.562703\RMSD=4.179e-09\PG=C01[X(C5H12N1O1S1)]\\

25H

GINC-NX360-M5-02-02\SP\ROB2PLYP-FC\GTMP2large\C5H13N1O1S1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\S,0,-0.478874,-0.513173,-0.47446\O,0,-0.550999,-1.834642,0.253173\C,0,1.179093,0.257088,0.015822\C,0,1.280656,0.324532,1.541878\C,0,2.218657,-0.72
4095,-0.547372\C,0,1.289849,1.630355,-0.650615\H,0,0.650638,1.117293,1.960415\H,0,0.995846,-0.635644,1.985684\H,0,2.314592,0.542624,1.835463\H,0,2.13
5479,-0.815678,-1.637084\H,0,3.22719,-0.36057,-0.317391\H,0,2.098123,-1.718578,-0.108307\H,0,2.282203,2.054067,-0.451223\H,0,1.173521,1.557003,-1.7385
69\H,0,0.53261,2.321206,-0.271682\N,0,-1.494283,0.669446,0.280983\H,0,-1.386686,0.58928,1.294157\C,0,-2.911478,0.51897,-0.088575\H,0,-3.352396,-0.4372
23,0.22489\H,0,-3.475235,1.337012,0.370393\H,0,-3.006597,0.609888,-1.174488\\Version=ES64L-G16RevA.03\State=1-
A\HF=-725.7168638\MP2=-726.2154505\RMSD=3.885e-09\PG=C01[X(C5H13N1O1S1)]\\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0,0,0,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0,0,0,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\\

R25

GINC-NX360-M5-02-05\SP\ROB2PLYP-FC\GTMP2large\C7H18N1O1S1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\S,0,0.77728,0.795045,-0.623164\O,0,-0.042883,0.229424,-1.763408\C,0,1.554212,-0.692412,0.247908\C,0,0.46325,-1.683903,0.657529\C,0,2.469334,-1.309
73,-0.82063\C,0,2.360383,-0.174265,1.441515\H,0,-0.140364,-1.306113,1.489372\H,0,-0.192842,-1.902579,-0.191457\H,0,0.923401,-2.624442,0.984572\H,0,3.2
38406,-0.600591,-1.149932\H,0,2.978547,-2.186953,-0.404159\H,0,1.893926,-1.62407,-1.696112\H,0,2.894888,-1.009698,1.910886\H,0,3.108634,0.564112,1.12
9108\H,0,1.711886,0.289643,2.188828\N,0,-0.239831,1.313969,0.674592\H,0,-1.026771,0.661591,0.752975\C,0,-0.745702,2.683607,0.487302\H,0,-1.391347,2.8
02972,-0.393822\H,0,-1.313672,2.963077,1.380043\H,0,0.10189,3.368972,0.396779\C,0,-3.223537,-0.259978,-0.22568\H,0,-2.460202,-0.252022,-0.998601\H,0,-
3.764582,0.666624,-0.049359\C,0,-3.753707,-1.542734,0.317749\H,0,-4.571001,-1.94418,-0.308405\H,0,-2.981274,-2.320022,0.35453\H,0,-4.169522,-1.42372,1.
326342\\Version=ES64L-G16RevA.03\State=2-A\HF=-804.7079354\MP2=-805.3151337\RMSD=4.818e-09\PG=C01[X(C7H18N1O1S1)]\\

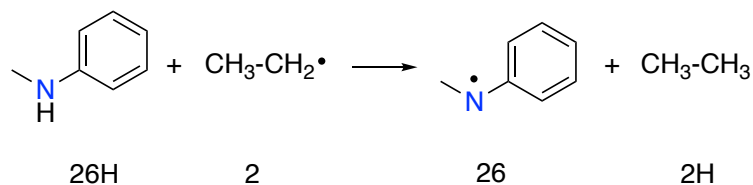
TS25

GINC-NX360-M5-04-04\SP\ROB2PLYP-FC\GTMP2large\C7H18N1O1S1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\S,0,-0.376662,0.67031,0.706888\O,0,0.180043,-0.292677,1.735612\C,0,-1.707496,-0.268918,-0.246882\C,0,-1.13965,-1.567993,-0.818417\C,0,-2.776237,-0.568265,0.816416\C,0,-2.247353,0.664973,-1.333163\H,0,-0.463696,-1.375328,-1.656189\H,0,-0.602212,-2.124271,-0.043336\H,0,-1.959459,-2.197937,-1.185616\H,0,-3.172177,0.352671,1.260928\H,0,-3.612842,-1.103261,0.351589\H,0,-2.368593,-1.189883,1.61884\H,0,-3.081632,0.175386,-1.851151\H,0,-2.625415,1.601552,-0.905997\H,0,-1.475127,0.908834,-2.067043\N,0,0.727772,0.970105,-0.576454\H,0,1.449963,-0.051956,-0.786343\C,0,1.68682,2.027247,-0.214797\H,0,2.241077,1.837716,0.715144\H,0,2.402007,2.128037,-1.036968\H,0,1.15357,2.979233,-0.112632\C,0,2.406395,-1.017017,-0.94166\H,0,2.944472,-0.653306,-1.821689\H,0,1.792807,-1.889318,-1.173849\C,0,3.209941,-1.121469,0.330967\H,0,3.92992,-1.951842,0.265698\H,0,3.787843,-0.210483,0.524065\H,0,2.556819,-1.301458,1.189841\\Version=ES64L-G16RevA.03\State=2-A\HF=-804.6732484\MP2=-805.2940916\RMSD=4.277e-09\PG=C01[X(C7H18N1O1S1)]\\

P25

GINC-SL250S-GEN8-10-03\SP\ROB2PLYP-FC\GTMP2large\C7H18N1O1S1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\S,0,0.982815,0.670405,0.683385\O,0,2.009598,1.753023,0.468875\C,0,1.633471,-0.918172,-0.177186\C,0,1.863447,-0.580626,-1.65089\C,0,2.952237,-1.216298,0.543377\C,0,0.60072,-2.024561,0.031136\H,0,0.916125,-0.410467,-2.170633\H,0,2.488478,0.312631,-1.749101\H,0,2.380795,-1.415867,-2.139318\H,0,2.792654,-1.432603,1.605857\H,0,3.418022,-2.097652,0.086487\H,0,3.647334,-0.37601,0.460223\H,0,0.988671,-2.956046,-0.40069\H,0,0.411344,-2.205418,1.095306\H,0,-0.348085,-1.78478,-0.453675\N,0,-0.439549,0.842654,-0.138468\H,0,-2.937869,-0.552396,0.353934\C,0,-0.767257,2.202569,-0.529418\H,0,0.106766,2.770561,-0.875622\H,0,-1.528034,2.154345,-1.314037\H,0,-1.201959,2.754448,0.31955\C,0,-3.924896,-1.012063,0.478663\H,0,-4.112301,-1.112705,1.554343\H,0,-3.878196,-2.023651,0.05771\C,0,-5.017805,-0.18128,-0.198762\H,0,-6.005967,-0.639859,-0.075332\H,0,-5.069003,0.829665,0.222447\H,0,-4.833247,-0.080849,-1.274851\\Version=ES64L-G16RevA.03\State=2-A\HF=-804.7206406\MP2=-805.3298775\RMSD=5.772e-09\PG=C01[X(C7H18N1O1S1)]\\

System 26



NAME	SYSTEM	H(kJ/mol)				ΔH(kJ/mol)			
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
26	MIN_Ph_NMe_ver1_radical	-326.12550	-325.92875	-325.99267	-77.89	-71.93	-69.16	a)	
26H	MIN_Ph_NMe_ver1_neutral	-326.75558	-326.56660	-326.63502	-	-	-		
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)	
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-		
START 26	START_Metilamino_TS_Ph_NMe_secC	-405.84890	-405.59840	-405.69575	0.00	0.00	0.00		
R26	Metilamino_TS_Ph_NMe_secC_opt_rev	-405.85038	-405.59932	-405.69920	-3.88	0.00	-2.41	0.00	-9.06
TS26	Metilamino_TS_Ph_NMe_secC	-405.83984	-405.58416	-405.68347	23.78	27.65	37.40	39.81	32.26
P26	Metilamino_TS_Ph_NMe_secC_opt_fwd	-405.87613	-405.61448	-405.71348	-71.50	-67.62	-42.21	-39.81	-46.54
FIN26	FIN_Metilamino_TS_Ph_NMe_secC	-405.87628	-405.61540	-405.71306	-71.88	-44.63	-45.44		

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

26

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C7H8N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\N,0,-1.785633,-0.720322,0.000012\C,0,-2.831266,0.280158,-0.000003\H,0,-2.783506,0.934138,-0.885739\H,0,-3.804183,-0.219442,-0.000005\H,0,-2.783545,
0.934085,0.885759\C,0,-0.50384,-0.295523,-0.000012\C,0,0.498663,-1.31515,0.000004\C,0,-0.059618,1.064734,-0.000001\C,0,1.846196,-0.999318,-0.000003\H,
0,0.153684,-2.344446,-0.000002\C,0,1.293607,1.365675,0.000003\H,0,-0.78727,1.869497,0.000025\C,0,2.254344,0.343318,-0.000003\H,0,2.589948,-1.791671,0.
000005\H,0,1.613883,2.404564,0.000007\H,0,3.311901,0.592166,0.000002\\Version=ES64L-G16RevA.03\State=2-
A\HF=-325.641233\MP2=-326.0686159\RMSD=2.561e-09\PG=C01[X(C7H8N1)]\\

26H

GINC-SL230S-GEN8-02-05\SP\ROB2PLYP-FC\GTMP2large\C7H9N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\N,0,1.792651,-0.608982,-0.151432\C,0,2.835924,0.364369,0.108313\H,0,2.741014,0.860865,1.088369\H,0,3.804142,-0.141595,0.067298\H,0,2.837796,1.141
482,-0.664798\C,0,0.443617,-0.273562,-0.060952\C,0,-0.522959,-1.29841,-0.00652\C,0,0.000948,1.061757,-0.057414\C,0,-1.878565,-0.995809,0.044008\H,0,-0.
196208,-2.336769,-0.010646\C,0,-1.363846,1.35103,-0.011553\H,0,0.718241,1.875002,-0.09254\C,0,-2.314799,0.333041,0.040688\H,0,-2.601801,-1.806574,0.08
6965\H,0,-1.681024,2.391147,-0.011275\H,0,-3.374626,0.566728,0.079981\H,0,2.001981,-1.541912,0.177248\\Version=ES64L-G16RevA.03\State=1-
A\HF=-326.286298\MP2=-326.7206305\RMSD=5.092e-09\PG=C01[X(C7H9N1)]\\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0,0,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0,0,0,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\\

R26

GINC-NX360-M5-04-04\SP\ROB2PLYP-FC\GTMP2large\C9H14N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,0.490314,0.45524,-0.307827\C,0,0.553569,-0.897784,-0.704767\C,0,1.686915,-1.662068,-0.452636\C,0,2.794287,-1.10699,0.197054\C,0,2.739892,0.229
627,0.589683\C,0,1.605937,1.007333,0.349524\H,0,-0.295356,-1.335522,-1.225802\H,0,1.706531,-2.70213,-0.769591\H,0,3.679078,-1.706043,0.391318\H,0,3.58
8814,0.681093,1.097805\H,0,1.591255,2.042969,0.672521\N,0,-0.644452,1.202304,-0.606057\H,0,-1.483002,0.644323,-0.73584\C,0,-0.880894,2.49272,0.010144
\H,0,-1.86675,2.850554,-0.298686\H,0,-0.847661,2.468831,1.112479\H,0,-0.141017,3.226063,-0.332232\C,0,-3.456248,-0.751088,-0.34684\H,0,-4.192268,0.0432
55,-0.435262\C,0,-3.054801,-1.272837,0.990325\H,0,-3.091746,-0.494302,1.760441\H,0,-3.724797,-2.08427,1.326666\H,0,-2.041098,-1.691726,0.976455\H,0,-3.
244641,-1.324143,-1.245824\\Version=ES64L-G16RevA.03\State=2-A\HF=-405.2768447\MP2=-405.8200719\RMSD=3.546e-09\PG=C01[X(C9H14N1)]\\

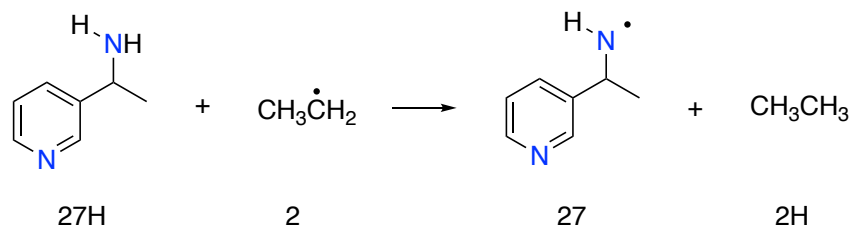
TS26

GINC-NX360-M5-05-04\SP\ROB2PLYP-FC\GTMP2large\C9H14N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,0.28746,0.409443,-0.381928\C,0,0.737856,-0.819892,-0.91859\C,0,1.988704,-1.325945,-0.59234\C,0,2.841768,-0.616637,0.262295\C,0,2.414939,0.6019

53,0.790131\C,0,1.150309,1.108118,0.489598\H,0,0.086,-1.357362,-1.601954\H,0,2.309148,-2.27474,-1.015389\H,0,3.824508,-1.00889,0.507863\H,0,3.06838,1.165694,1.451522\H,0,0.841906,2.055158,0.918948\N,0,-0.961844,0.878257,-0.786098\H,0,-1.807835,0.015464,-0.642641\C,0,-1.471036,2.088131,-0.157715\H,0,-2.498724,2.247667,-0.496535\H,0,-1.465232,2.07026,0.94456\H,0,-0.873598,2.949359,-0.482351\C,0,-2.782848,-0.916802,-0.210814\H,0,-3.704871,-0.332111,-0.262876\C,0,-2.402379,-1.42027,1.157729\H,0,-2.415453,-0.616281,1.90319\H,0,-3.100294,-2.196834,1.508853\H,0,-1.399562,-1.863002,1.157923\H,0,-2.720098,-1.650771,-1.018614\\Version=ES64L-G16RevA.03\State=2-A\HF=-405.243927\MP2=-405.7999164\RMSD=5.870e-09\PG=C01[X(C9H14N1)]\\

P26
GINC-NX360-M5-04-05\SP\ROB2PLYP-FC\GTMP2large\C9H14N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\\nekaj\
\0,2\C,0,0.78713,0.331431,-0.071467\C,0,0.81852,-1.096783,-0.134262\C,0,2.010094,-1.794039,-0.036761\C,0,3.219761,-1.102041,0.127261\C,0,3.219917,0.299465,0.192307\C,0,2.03484,1.011905,0.096055\H,0,-0.130852,-1.607415,-0.261666\H,0,2.009501,-2.879543,-0.087279\H,0,4.155248,-1.649104,0.203869\H,0,4.15909,0.83193,0.319478\H,0,2.055377,2.095321,0.148649\N,0,-0.428658,0.908874,-0.177127\H,0,-2.858778,-0.349816,-0.479262\C,0,-0.504959,2.352999,-0.120025\H,0,-1.549435,2.659811,-0.221646\H,0,-0.122239,2.752666,0.832782\H,0,0.072575,2.832864,-0.926372\C,0,-3.850969,-0.809245,-0.554504\H,0,-4.311495,-0.462884,-1.487753\C,0,-4.721382,-0.459146,0.655337\H,0,-4.865206,0.624391,0.742243\H,0,-5.714534,-0.918927,0.585506\H,0,-4.262377,-0.804444,1.589223\H,0,-3.713971,-1.894244,-0.641537\\Version=ES64L-G16RevA.03\State=2-A\HF=-405.290503\MP2=-405.8360192\RMSD=4.466e-09\PG=C01[X(C9H14N1)]\\

System 27



		H(kJ/mol)			ΔH(kJ/mol)				
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
27	MIN_Py_NH_ver1_radical	-381.43829	-381.22418	-381.29533	-26.53	-25.88	-22.21	a)	
27H	MIN_Py_NH_ver1_neutral	-382.08793	-381.87957	-381.95556	-	-	-		
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)	
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-		
START 27	START_MIN_Py_NH_ver1_neutral	-461.18124	-460.91138	-461.01630	0.00	0.00	0.00		
R27	TS_Py_NH_ethane_opt_fwd	-461.18286	-460.91206	-461.01846	-4.23	0.00	-1.78	0.00	0.00
TS27	TS_Py_NH_ethane	-461.16797	-460.89177	-460.99167	34.85	39.08	51.50	53.28	64.66
P27	TS_Py_NH_ethane_opt_rev	-461.18871	-460.90983	-461.01623	-19.61	-15.38	4.07	5.85	0.17
FIN27	FIN_MIN_Py_NH_ver1_radical	-461.18906	-460.91084	-461.01572	-20.52	1.42	1.51		

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

27

1\1\GINC-SL230S-GEN8-02-05\FOpt\UB3LYP\6-31G(d)\C7H9N2(2)\DSAKIC\12-Jul-2020\0\#opt freq b3lyp/6-31g(d)\nekaj\
\0,2\C,0.2456407297,-0.5472756464,-0.2694493356\C,0.9698895495,0.590754897,0.1061961481\C,0.2398586581,1.7584668301,0.3633311898\C,-1.147078492
9,1.7307262289,0.242888315\C,-1.7614108898,0.5341959921,-0.1323186169\H,0.7739227418,-1.477017908,-0.4835149847\H,0.7540755769,2.6725192958,0.6
480984007\H,-1.7438622813,2.6178825926,0.434027494\H,-2.8439166646,0.4773284145,-0.2347001301\C,2.491213434,0.5656865977,0.21418333\H,2.823769
0151,-0.4203669506,-0.1593790437\C,2.9911037079,0.7366565373,1.654221086\H,2.6076318275,-0.0595239855,2.3009571898\H,4.0853924475,0.7115375454
,1.6731445821\H,2.6689890828,1.7003725488,2.0625965261\N,3.0670534135,1.6022057093,-0.6335949621\N,-1.0859029716,-0.592608606,-0.3866351946\H,2
.7345189058,1.400550417,-1.5902071139\Version=ES64L-G16RevC.01\State=2-
A\HF=-381.5957173\S2=0.753333\S2-1=0.\S2A=0.750008\RMSD=8.208e-09\RMSF=8.190e-06\Dipole=-0.0281953,0.2079449,0.1294707\Quadrupole=-0.8562314,
-0.4512679,1.3074992,-6.9601948,-0.7442606,0.3673483\PG=C01[X(C7H9N2)]\

27H

1\1\GINC-SL250S-GEN8-09-01\FOpt\RB3LYP\6-31G(d)\C7H10N2\DSAKIC\12-Jul-2020\0\#opt freq b3lyp/6-31g(d)\nekaj\
\0,1\C,0.2720468108,-0.5499740394,-0.1460520013\C,0.9757002982,0.6396812244,0.0749380273\C,0.2219333121,1.8089844279,0.2242031184\C,-1.16745306
86,1.7321136526,0.1581239812\C,-1.7599814702,0.4863596478,-0.0560828165\H,0.8204513728,-1.4829668668,-0.2838388067\H,0.7313047751,2.7560646215,
0.3751617405\H,-1.7834760605,2.6203211588,0.2677370769\H,-2.8434751003,0.3915067691,-0.1122932259\C,2.4918779782,0.6415471973,0.1758374858\H,2.
8527059312,-0.2866337726,-0.3037266628\C,2.9518400045,0.6092841571,1.6422310135\H,2.5565191653,-0.2731165683,2.1552689151\H,4.0471891658,0.575
3995869,1.7033242502\H,2.6060069557,1.5052079498,2.1681008496\N,3.0307852952,1.8549183084,-0.4579085562\N,-1.0611746099,-0.6447643384,-0.21019
28974\H,2.8191066218,1.8469136076,-1.4550018985\H,4.0466685429,1.8573522662,-0.3769451633\Version=ES64L-G16RevC.01\State=1-
A\HF=-382.2602418\RMSD=4.706e-09\RMSF=2.107e-05\Dipole=0.8165705,0.4403168,-0.098824\Quadrupole=3.6060608,-3.1282158,-0.477845,-4.5812286,-1.92
35009,-0.771814\PG=C01[X(C7H10N2)]\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0,0,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0,0,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\

R27

1\1\GINC-SL230S-GEN8-02-05\FOpt\UB3LYP\6-31G(d)\C9H15N2(2)\DSAKIC\12-Jul-2020\0\#b3lyp/6-31G(d)optfreq\optircreverse\
\0,2\C,-2.4971299734,0.7374896812,-0.4561178877\C,-1.1480459805,0.3704309913,-0.3797063761\C,-0.8472312043,-0.8349301476,0.2681982231\C,-1.88667
00928,-1.6007537297,0.7895677155\C,-3.1958348343,-1.1362002531,0.6471928187\H,-2.7759832411,1.6699955619,-0.9481269532\H,0.1847508423,-1.161583
6207,0.3644105393\H,-1.6897192275,-2.5398344009,1.2985193066\H,-4.0319562597,-1.7107002455,1.0426045345\C,-0.0501878454,1.2550828429,-0.9620825
565\H,-0.5356249739,2.1896836202,-1.298736597\C,0.6629333975,0.6155383966,-2.1598820195\H,-0.0432726741,0.4031055464,-2.9693138531\H,1.43829942

14,1.2911212465,-2.5351189087\H,1.1458826217,-0.3223490336,-1.8660144972\N,0.9204894495,1.5845763322,0.0729266313\N,-3.5075735,0.0125380262,0.0357313613\H,0.3922448848,2.0538300552,0.8252887157\H,3.1199226058,0.1304074066,0.9177069779\C,3.9144109211,-0.5260330071,1.291531389\H,4.1719055146,-0.1943831966,2.3046312499\H,3.5044662683,-1.5403744908,1.3750142166\C,5.1381086984,-0.4981557414,0.372146389\H,5.9389964509,-1.1464705678,0.747119112\H,4.8854131791,-0.8372297914,-0.6394784434\H,5.5462545518,0.5154845192,0.2855489119\\Version=ES64L-G16RevC.01\State=2-A\HF=-461.4277907\S2=0.753459\S2-1=0.\S2A=0.750009\RMSD=9.443e-09\RMSF=7.429e-05\Dipole=0.0268145,-0.1285956,-0.0222389\Quadrupole=-8.5977556,5.8451478,2.7526078,0.409315,-1.2399542,-2.041326\PG=C01[X(C9H15N2)]\\

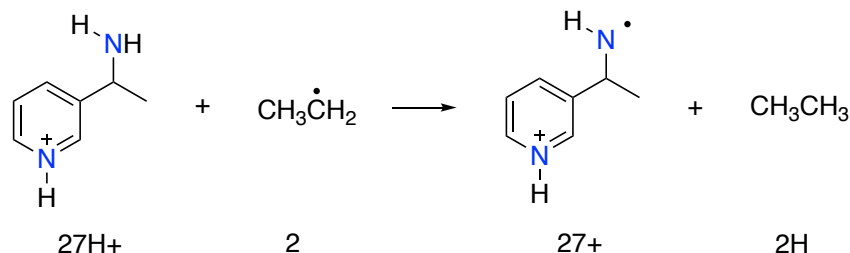
TS27

1\1\GINC-SL250S-GEN8-04-01\FTS\UB3LYP\6-31G(d)\C9H15N2(2)\DSAKIC\12-Jul-2020\0\#opt=(calcf,ts,noeigentest)freqb3lyp/6-31g(d)\nekaj\0,2\C,0.5003333902,1.354407497,-1.6062943277\C,0.9561811922,1.3264142755,-0.2831403369\C,0.1174000195,1.8774324013,0.6937699758\C,-1.1121045991,2.4066783507,0.310569326\C,-1.4646466135,2.3703724123,-1.0403159417\H,1.1260652025,0.9459590966,-2.400786729\H,0.4388079738,1.8975717471,1.7311277517\H,-1.7869651291,2.8426977092,1.0417322871\H,-2.4191328399,2.7753512867,-1.373408012\C,2.3045406986,0.7168439327,0.0725764889\H,2.8346138388,0.5303294784,-0.8777786903\C,2.1483589369,-0.6259151213,0.8011439223\H,1.5832327132,-1.3374556989,0.1900542827\H,3.1296255974,-1.0623970547,1.0192111419\H,1.6219103757,-0.4850260482,1.7507651878\N,3.0314280054,1.6573202511,0.9415199329\N,-0.6784102787,1.8564843982,-1.9931518298\H,3.1751460879,2.5198190394,0.4007513762\H,4.2169761438,1.2491475055,1.0514483148\C,5.5287475143,0.9009309275,0.9795394004\H,6.0190642882,1.8114242436,1.3348643365\H,5.5825175264,0.106203481,1.7286146902\C,5.9028778692,0.4835179581,-0.4237431554\H,6.9623263389,0.1916334843,-0.4830179928\H,5.3156630611,-0.3781710369,-0.7630651558\H,5.7541091462,1.297592274,-1.1430166139\\Version=ES64L-G16RevC.01\State=2-A\HF=-461.4019264\S2=0.757383\S2-1=0.\S2A=0.750027\RMSD=7.564e-09\RMSF=1.109e-05\Dipole=0.6117685,-0.0846552,0.3659965\Quadrupole=3.6523088,0.9506275,-4.6029363,-1.7124158,-5.3451606,0.7771583\PG=C01[X(C9H15N2)]\\

P27

1\1\GINC-SL230S-GEN8-02-07\FOpt\UB3LYP\6-31G(d)\C9H15N2(2)\DSAKIC\12-Jul-2020\0\#b3lyp/6-31G(d)optfreq\optircforward\0,2\C,-1.8562733158,1.0403383201,-0.7408520263\C,-1.0417875333,0.0232696091,-0.2295911039\C,-1.6654920762,-0.970838684,0.5323918987\C,-3.042786539,-0.9076733732,0.7317642812\C,-3.754258703,0.1500394781,0.1625617167\H,-1.40963108,1.8446749762,-1.3272048087\H,-1.064488957,-1.764958861,0.965275464\H,-3.5590727217,-1.661660903,1.3195454543\H,-4.8320143116,0.228456499,0.2987443608\C,0.4493612436,-0.0046274469,-0.5215650138\H,0.7425232255,1.0187950681,-0.8200932153\C,0.7646856413,-0.9341593246,-1.7049354384\H,0.2266440232,-0.6179698362,-2.6044152221\H,1.8390931124,-0.9220662301,-1.9273037436\H,0.4753661528,-1.9628605618,-1.4662024766\N,1.1813882918,-0.4847846136,0.6594364635\N,-3.1804401769,1.117576163,-0.5627307339\H,1.0527894969,0.1695504084,1.4307302779\H,2.182952726,-0.4991872385,0.4562840591\C,4.6670303512,-0.1638831232,0.0665047786\H,4.7633355806,-1.1702576714,0.4638227249\H,4.5645505489,-0.0671066994,-1.0107147792\C,5.0282931365,1.0178376299,0.8994431382\H,6.1151098896,1.2155155815,0.8769608655\H,4.5403526732,1.9334773078,0.5440971401\H,4.7613273208,0.8727665257,1.9529399381\\Version=ES64L-G16RevC.01\State=2-A\HF=-461.4208963\S2=0.753738\S2-1=0.\S2A=0.750009\RMSD=6.992e-09\RMSF=1.173e-06\Dipole=1.1764416,-0.1592964,0.2962932\Quadrupole=1.9312083,-1.9228415,-0.0083668,6.0850805,-2.3296441,0.4300047\PG=C01[X(C9H15N2)]\\

System 27+



		H(kJ/mol)			$\Delta\text{H}(\text{kJ/mol})$		
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
27+	MIN_PyCHMeNH2_katrad	-381.803467	-381.583378		-19.96	-19.98	a)
27H+	MIN_PyCHMeNH2_kation	-382.455610	-382.241014	-382.315960	-	-	-
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-
START 27+		-461.548927	-461.272821	-461.376695	0.00	0.00	0.00
R27+	TS_PyCHMeNH2_katrad_opt_rev	-461.552496	-461.276611		-9.37	0.00	-9.95
TS27+	TS_PyCHMeNH2_katrad	-461.535347	-461.254673		35.65	45.02	47.65
P27+	TS_PyCHMeNH2_katrad_opt_fwd	-461.555096	-461.272173		-16.20	-6.83	1.70
FIN27+		-461.554240	-461.270032		-13.95	7.32	

a) RSE compared to $\text{CH}_4/\text{CH}_3^\bullet$ radical system

b) RSE compared to $\text{NH}_3/\text{NH}_2^\bullet$ radical system

27+
 1\1\GINC-NX360-M5-02-08\FOpt\UB3LYP\6-31G(d)\C7H10N2(1+,2)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp\6-31g(d)\nekaj\
 \1,2\C,0.2391269224,-0.5476856449,0.0331398438\C,0.9054221359,0.669382118,0.0006530977\C,0.1228352231,1.834998137,-0.0441604821\C,-1.272452007,
 1.7633388405,-0.0386439671\C,-1.8873243188,0.5245097738,-0.0006924356\H,0.7421802539,-1.5081355507,0.0537475702\H,0.6332978334,2.7912612329,-0.
 0984066843\H,-1.8809793673,2.6600590011,-0.0706236886\H,-2.9600198751,0.3734950157,0.0003503077\C,2.4316613318,0.7284439642,0.0193748485\H,2.8

154077223,-0.0419612356,-0.6721113811\C,2.9855921319,0.3970940294,1.4348865973\H,2.6415425326,-0.5867865663,1.7701940144\H,4.0790970394,0.3839
040076,1.4106722542\H,2.6597488373,1.1487239449,2.1593136026\N,2.8583280577,2.0374592432,-0.4025587896\N,-1.1135210121,-0.5835821476,0.0309429
791\H,3.8842058913,2.0165916736,-0.4778964593\H,-1.5702696728,-1.4924708267,0.048489272\Version=ES64L-G16RevC.01\State=2-
A\HF=-381.9751801\S2=0.753411\S2-1=0.\S2A=0.750009\RMSD=9.740e-09\RMSF=1.273e-05\Dipole=-1.4624816,-1.3877939,0.0170431\Quadrupole=12.7637903
,-1.2484173,-11.515373,2.5951767,1.3015266,0.5258182\PG=C01[X(C7H10N2)]\

27H+

1\1\GINC-SL250S-GEN8-07-03\FOpt\RB3LYP\6-31G(d)\C7H11N2(1+)\DSAKIC\02-Oct-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,1\C,0.2987332793,-0.5867855033,-0.0935042659\C,0.9837575746,0.6119740576,0.045180122\C,0.2188507554,1.7872778642,0.1366793304\C,-1.176538994
4,1.7406074599,0.1086389842\C,-1.810639256,0.5170724695,-0.0239818245\H,0.7894306828,-1.5492444987,-0.1885541896\H,0.7506915894,2.7309951516,0.
2121204389\H,-1.7719413534,2.6436272605,0.1834427438\H,-2.8853589306,0.3863375547,-0.0615152754\C,2.5084460116,0.645817881,0.1274601284\H,2.88
72601859,-0.2439854879,-0.4034807405\C,2.9508113933,0.5401758221,1.5987358082\H,2.5582989658,-0.3644276105,2.0729879374\H,4.0438061182,0.50001
54036,1.6533648265\H,2.6074265108,1.4113601604,2.1663279181\N,2.9812236297,1.9065583907,-0.4372322069\N,-1.0549546028,-0.5989126007,-0.1222169
534\H,3.0164183465,1.8706101718,-1.4542155708\H,3.9232826655,2.1114149811,-0.1131462711\H,-1.5257616516,-1.4941817674,-0.2305643697\
\Version=ES64L-G16RevC.01\State=1-
A\HF=-382.6420491\RMSD=4.724e-09\RMSF=4.702e-06\Dipole=-1.4625219,-1.1285616,-0.438371\Quadrupole=11.6251562,-1.3601944,-10.2649619,4.1601588,0
.7774908,1.002402\PG=C01[X(C7H11N2)]\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0,0,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0,0,0,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\

R27+

1\1\GINC-NX360-M5-01-03\FOpt\UB3LYP\6-31G(d)\C9H16N2(1+,2)\DSAKIC\25-Sep-2020\0\#b3lyp/6-31G(d)optfreq\optircreverse\
\1,2\C,2.0350220217,1.1586870831,0.4557751924\C,1.0168193141,0.2837053658,0.1049277715\C,1.3841497985,-0.9110387903,-0.5373988001\C,2.724771403
4,-1.2083416614,-0.7911209666\C,3.7021659105,-0.3032226678,-0.4141551255\H,1.8629619547,2.1135575928,0.9402692155\H,0.5870724391,-1.582282797,-
0.8431782695\H,3.0142621803,-2.1307778775,-1.2819015197\H,4.7635778656,-0.4462957403,-0.5766266861\C,-0.4425617301,0.5922904337,0.4321011286\H,
-0.5406861776,1.6902277271,0.4915310996\C,-0.7928661889,0.014654327,1.8164270941\H,-0.1353430902,0.4109198249,2.5964514005\H,-1.8231118809,0.28
00452126,2.0735176489\H,-0.710293514,-1.077182827,1.8076876041\N,-1.2922677641,-0.018960668,-0.5834736634\N,3.3255438513,0.8446880866,0.1913739
085\H,-1.3188701412,0.5474135851,-1.4297459598\H,-2.256227048,-0.0946935859,-0.2478933118\C,-4.5883281139,-0.0974882308,0.3148666875\H,-4.453250
0018,-1.0346836281,0.8495867045\H,-4.5902608662,0.8088695603,0.9160573688\C,-5.2250908016,-0.0962776391,-1.0329143401\H,-6.3228141516,-0.184475
8595,-0.9520772773\H,-5.0307823045,0.8329970379,-1.5812607436\H,-4.8921411761,-0.9410666702,-1.6469991794\H,4.0467972116,1.5112388059,0.4562400

183\\Version=ES64L-G16RevC.01\\State=2-
A\\HF=-461.8057238\\S2=0.753535\\S2-1=0.\\S2A=0.750009\\RMSD=2.237e-09\\RMSF=1.180e-06\\Dipole=3.5167458,0.8124744,0.0282278\\Quadrupole=25.9593828,-
10.5126204,-15.4467624,2.863313,0.0161089,3.2994234\\PG=C01[X(C9H16N2)]\\

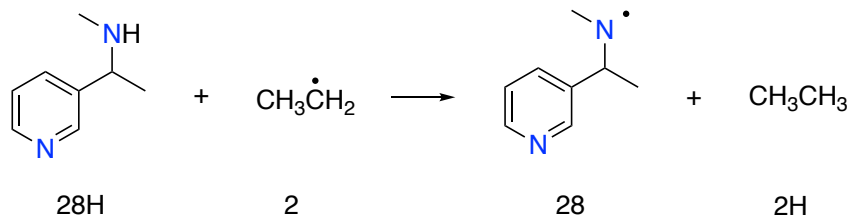
TS27+

1\\1\\GINC-SL250S-GEN8-07-03\\FTS\\UB3LYP\\6-31G(d)\\C9H16N2(1+,2)\\DSAKIC\\25-Sep-2020\\0\\#opt=(calcfc,ts,noeigentest)freqb3lyp/6-31g(d)\\nekaj\\
\\1,2\\C,0.3322382477,1.2861078893,-1.6694935877\\C,0.9328896342,1.3428330793,-0.4204748376\\C,0.205346148,1.9469058207,0.621902694\\C,-1.0778646491
,2.4503281192,0.4034905961\\C,-1.6328238249,2.3643254188,-0.8629315965\\H,0.8070082776,0.853704826,-2.5429915279\\H,0.6760238929,2.0298015334,1.59
65086435\\H,-1.6456107543,2.9118738004,1.2034820414\\H,-2.617077169,2.7339221157,-1.1240985694\\C,2.3277753584,0.7749890811,-0.174330184\\H,2.7933
54823,0.5969758384,-1.1579868363\\C,2.2236272043,-0.5715582838,0.5632328148\\H,1.6047200596,-1.2837079482,0.008064919\\H,3.2192283457,-1.00765799
45,0.6819973201\\H,1.7935551078,-0.4302485337,1.5601003506\\N,3.0382493423,1.7540704444,0.6535927362\\N,-0.9128378177,1.7911790706,-1.8509457458\\
H,3.3371030363,2.5300418723,0.0500399074\\H,4.2201700278,1.2644961595,0.9602929869\\C,5.4564461773,0.878730268,1.1413415586\\H,5.9034397291,1.785
2175108,1.5585294916\\H,5.338043355,0.1101435131,1.910245326\\C,6.0730724961,0.4035147256,-0.1534255219\\H,7.1099199202,0.0804241878,0.016655605
7\\H,5.5393901204,-0.4559062477,-0.5764472232\\H,6.1058680987,1.1971283897,-0.908345331\\H,-1.3219501275,1.7394513739,-2.7808720807\\Version=ES64L-
G16RevC.01\\State=2-
A\\HF=-461.7833514\\S2=0.757026\\S2-1=0.\\S2A=0.750025\\RMSD=9.271e-09\\RMSF=8.052e-07\\Dipole=-2.7725242,0.6483605,-1.7619041\\Quadrupole=17.5404108
, -12.7415565,-4.7988543,-9.011104,9.4490886,-1.1426872\\PG=C01[X(C9H16N2)]\\

P27+

1\\1\\GINC-SL230S-GEN8-02-08\\FOpt\\UB3LYP\\6-31G(d)\\C9H16N2(1+,2)\\DSAKIC\\29-Sep-2020\\0\\#b3lyp/6-31G(d)optfreq\\optircforward\\
\\1,2\\C,-2.0334450405,-1.1893126726,-0.2592816165\\C,-1.2135651834,-0.0855805032,-0.0698633299\\C,-1.8326463525,1.1716611402,0.0257024312\\C,-3.22219
17927,1.2953918842,-0.050945392\\C,-3.9943379471,0.1623795458,-0.235800019\\H,-1.6623984808,-2.2031646446,-0.3610899525\\H,-1.1984227906,2.0442720
946,0.1454448526\\H,-3.7049741113,2.2631950071,0.0246959002\\H,-5.074854685,0.1638958384,-0.3127530274\\C,0.3020412572,-0.242247728,0.0359359426\\
H,0.6315939565,-0.9495545029,-0.7450343894\\C,0.7045469768,-0.85113009,1.4100087788\\H,0.2128801257,-1.8162590352,1.5707442905\\H,1.7861562585,-1.
0101633097,1.4389822973\\H,0.4266482186,-0.1756647399,2.2239784286\\N,0.9247278211,1.0416362622,-0.1539478648\\N,-3.3756519647,-1.0355342697,-0.33
59412994\\H,1.9415747613,0.887301978,-0.187139484\\H,6.6046747738,-0.1408756973,0.4951526478\\C,6.059582881,0.0870423734,-0.426733529\\H,6.3387443
08,1.0991129029,-0.7378177619\\H,6.4054770687,-0.6072363189,-1.1996371443\\C,4.5471117667,-0.0299651983,-0.2162954838\\H,4.0054929265,0.1975582016
, -1.1443136172\\H,4.2678535236,-1.0444896009,0.0950945128\\H,4.2069249646,0.6669562157,0.5611351659\\H,-3.9469462402,-1.8645181327,-0.4818573374\\
\\Version=ES64L-G16RevC.01\\State=2-
A\\HF=-461.8075311\\S2=0.753405\\S2-1=0.\\S2A=0.750008\\RMSD=9.802e-09\\RMSF=1.576e-06\\Dipole=-4.0541183,-1.1768883,-0.1437621\\Quadrupole=26.427808
1,-8.7625166,-17.6652915,3.4764363,2.921761,1.584466\\PG=C01[X(C9H16N2)]\\

System 28



		H(kJ/mol)			ΔH(kJ/mol)				
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3		
28	MIN_Py_NMe_ver1_radical	-420.72485	-420.47882	-	-49.48	-49.41	1104147.13	a)	
28H	MIN_Py_NMe_ver1_neutral	-421.36575	-421.12524	-421.21643	-	-	-		
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82	b)	
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-		
START 28	START_MIN_Py_NMe_ver1_neutral	-500.45907	-500.15705	-500.27717	0.00	0.00	0.00		
R28	TS_Py_NMe_ethane_opt_fwd	-500.45551	-500.15244	-500.27470	9.34	0.00	12.10	0.00	0.00
TS28	TS_Py_NMe_ethane	-500.44372	-500.13642	-500.25807	40.30	30.96	54.16	42.07	50.15
P28	TS_Py_NMe_ethane_opt_rev	-500.47080	-500.16015	-	-30.81	-40.15	-8.14	-20.24	
FIN28	FIN_MIN_Py_NMe_ver1_radical	-500.47562	-500.16547	-79.720391	-43.47	-22.11			

a) RSE compared to CH₄/CH₃[•] radical system

b) RSE compared to NH₃/NH₂[•] radical system

28

1\1\GINC-SL230S-GEN8-02-05\FOpt\UB3LYP\6-31G(d)\C8H11N2(2)\DSAKIC\12-Jul-2020\0\#opt freq b3lyp/6-31g(d)\nekaj\
\0,2\C,-0.6729056826,0.0054887904,-0.3914212951\C,0.3852633922,0.9207810401,-0.2777472431\C,0.1015903802,2.2625782474,-0.5426847349\C,-1.1907729
635,2.6261695932,-0.9199084156\C,-2.161129007,1.6286999692,-1.0085632299\H,-0.5005322855,-1.0462353853,-0.1722412755\H,0.8846288191,3.013305777
7,-0.4590979467\H,-1.442018191,3.6604853112,-1.1365896759\H,-3.1814740266,1.8746288104,-1.2985874281\C,1.7879051968,0.4565404944,0.1136151174\H
,2.389381879,1.3624408244,0.3090231756\C,2.4595641806,-0.3465240239,-1.0120492127\H,2.5320003113,0.2529885751,-1.9259737838\H,3.4680055229,-0.6
491597823,-0.7102907958\H,1.884393599,-1.2513854185,-1.2311172924\N,1.6906986921,-0.3832672581,1.3029717249\N,-1.9180473703,0.3374613148,-0.747
4458998\C,1.7667057444,0.3743156673,2.5275093551\H,2.7405099801,0.8875335172,2.6172452492\H,0.9953734029,1.1625115189,2.5666056664\H,1.638426
066,-0.2855961136,3.390615481\\Version=ES64L-G16RevC.01\State=2-
A\HF=-420.9122585\S2=0.753639\S2-1=0.\S2A=0.75001\RMSD=5.757e-09\RMSF=4.125e-06\Dipole=0.6876273,1.0996789,0.1076381\Quadrupole=-1.039028,0.3
058927,0.7331353,-1.6677733,0.4157671,-0.0238433\PG=C01[X(C8H11N2)]\\

28H

1\1\GINC-SL250S-GEN8-03-05\FOpt\RB3LYP\6-31G(d)\C8H12N2\DSAKIC\12-Jul-2020\0\#opt freq b3lyp/6-31g(d)\nekaj\
\0,1\C,-0.6241603418,0.0878482058,-0.1181849633\C,0.4618141955,0.9691322363,-0.2228139039\C,0.1931387886,2.2567384127,-0.6928786827\C,-1.1114081
878,2.6010961589,-1.0433918399\C,-2.1107430337,1.6381153492,-0.9049843627\H,-0.4571635558,-0.9159710142,0.2659672356\H,0.9987967499,2.983478429
6,-0.7810002989\H,-1.3510950869,3.595145712,-1.4100996473\H,-3.1417601138,1.869903108,-1.1684847271\C,1.8797690849,0.5255009786,0.1123728464\H,
2.4784211922,1.4440312814,0.279359541\C,2.503945508,-0.2295134748,-1.0727966552\H,2.4904388896,0.3867645008,-1.9769602792\H,3.5474768014,-0.494
3057464,-0.8586287908\H,1.9471327541,-1.1508148151,-1.2733353133\N,1.893564712,-0.341786786,1.2926220498\N,-1.8833551977,0.3999749202,-0.447667
6059\C,1.6444319035,0.3568637821,2.5504824069\H,2.3232707626,1.210943714,2.7327678985\H,0.61882905,0.7396853366,2.5613623453\H,1.746256881,-0.
3483310506,3.3814589698\H,2.7972992342,-0.8075265891,1.3409134269\\Version=ES64L-G16RevC.01\State=1-
A\HF=-421.5676462\RMSD=4.553e-09\RMSF=9.037e-06\Dipole=1.0915124,0.613992,0.0336617\Quadrupole=-0.5042444,0.5419633,-0.0377189,-3.9052277,1.378
7329,-1.7879321\PG=C01[X(C8H12N2)]\\

2

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0.795115,
0,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\\Version=ES64L-G16RevA.03\State=2-
A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\\

2H

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
\0,1\C,0,0,0,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0,0,-0.765285\H,0,1.02099,-0.000
292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\\Version=ES64L-G16RevA.03\State=1-
A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\\

R28

1\1\GINC-SL250S-GEN8-09-01\FOpt\UB3LYP\6-31G(d)\C10H17N2(2)\DSAKIC\13-Jul-2020\0\#b3lyp/6-31G(d)optfreq\optircforward\
\0,2\C,-2.0359189687,1.2228813485,0.0520970051\C,-1.144579507,0.161836185,0.2500476032\C,-1.6992735208,-1.1246026181,0.3037266603\C,-3.074018210
8,-1.2861519996,0.1678091023\C,-3.863486104,-0.1498220263,-0.0228640573\H,-1.6713426379,2.2458840072,-0.0033803646\H,-1.0397486863,-1.9769362023

,0.436411399\H,-3.529543174,-2.271868542,0.205885408\H,-4.943459549,-0.2377730283,-0.1345958818\C,0.3616347715,0.3458897242,0.4413685699\H,0.5684841561,0.1302681123,1.5005761925\C,0.8587042099,1.7806016069,0.1793013125\H,0.4154591932,2.4938991699,0.8828086408\H,1.9462131411,1.8186053083,0.3105826646\H,0.6280418202,2.1221736975,-0.8352731679\N,1.0874223041,-0.7030719799,-0.2954515291\N,-3.3638190198,1.0878099336,-0.0828949012\H,2.0469649819,-0.7369502573,0.0512611599\C,4.4001513789,-0.7863743389,0.9478052897\H,4.0375632634,-0.5034437311,1.9320776543\H,4.3338955704,-1.8379833311,0.6834855801\C,5.2754991133,0.1359822843,0.170866356\H,6.3282562241,0.0733107845,0.5005248639\H,5.2708100039,-0.1006538843,-0.8996707383\H,4.9754560527,1.1838771696,0.2917534698\C,1.1003284361,-0.5681915889,-1.7505642731\H,0.0730919632,-0.5987218691,-2.1291670765\H,1.5722239644,0.3528492206,-2.133581079\H,1.6364428299,-1.4225561552,-2.1774558629\Version=ES64L-G16RevC.01\State=2-A\HF=-500.7242789\S2=0.753735\S2-1=0.\S2A=0.750009\RMSD=5.697e-09\RMSF=1.191e-06\Dipole=1.2857743,-0.3861596,0.1247594\Quadrupole=1.1205362,-0.6204254,-0.5001108,5.53617,-0.0993889,0.4514383\PG=C01[X(C10H17N2)]\

TS28

1\1\GINC-SL230S-GEN8-02-06\FTS\UB3LYP\6-31G(d)\C10H17N2(2)\DSAKIC\12-Jul-2020\0\#opt=(calcf,ts,noeigentest)freqb3lyp/6-31g(d)\nekaj\

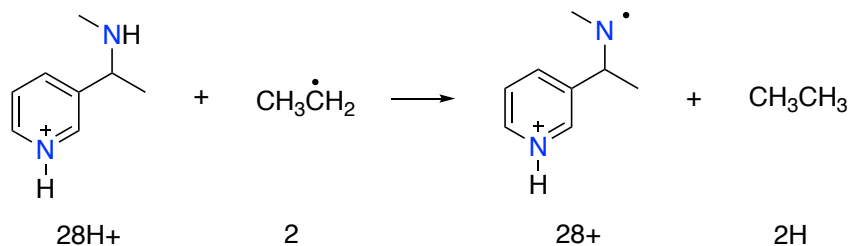
\0,2\C,-0.6855303743,0.0680644857,-0.306843529\C,0.5518926869,0.7103861903,-0.4278392952\C,0.5330520991,2.0401128938,-0.8729265191\C,-0.681839076,2.6453936108,-1.1744689671\C,-1.8541466467,1.9020990207,-1.0158483029\H,-0.7409870078,-0.963277735,0.0329743839\H,1.4687098688,2.5839277369,-0.963570516\H,-0.7253547495,3.6731859604,-1.5237958609\H,-2.8242757751,2.3437697233,-1.2397868061\C,1.8931491501,0.0407141422,-0.1140031255\H,2.4675146205,0.0360158415,-1.0520323818\C,1.7732892101,-1.4232262197,0.3430054874\H,1.3160167882,-2.0387915824,-0.4393150586\H,2.768960493,-1.830117654,0.5476220226\H,1.1706382126,-1.5330214193,1.2502025533\N,2.6521132102,0.940279353,0.777142854\N,-1.8676885946,0.6361220359,-0.5898305841\H,3.840055255,0.6015520256,0.714657671\C,5.1354435179,0.1076885222,0.682847635\H,5.1394101845,-0.5198901959,-0.2125651726\H,5.6873157456,1.0372355713,0.5194699881\C,5.4663809987,-0.6143972783,1.9676526063\H,6.5025414702,-0.986728018,1.9607295506\H,5.3679957824,0.0422861126,2.83979645\H,4.8165343804,-1.4832464952,2.1268671499\C,2.2588361352,0.896732765,2.180076282\H,1.213098119,1.2198399984,2.2723048046\H,2.3424058419,-0.0907052824,2.6619104681\H,2.8782666936,1.6042891805,2.7408276423\Version=ES64L-G16RevC.01\State=2-A\HF=-500.707304\S2=0.757433\S2-1=0.\S2A=0.750027\RMSD=4.296e-09\RMSF=3.841e-06\Dipole=0.9242048,0.0025066,0.1544946\Quadrupole=-4.33129,3.1731096,1.1581803,-3.7300581,0.2991259,-1.8764426\PG=C01[X(C10H17N2)]\

P28

1\1\GINC-SL230S-GEN8-02-07\FOpt\UB3LYP\6-31G(d)\C10H17N2(2)\DSAKIC\13-Jul-2020\0\#b3lyp/6-31G(d)optfreq\optircreverse\

\0,2\C,-2.2880083972,0.9563141844,-0.2759511369\C,-1.1378134754,0.3255821988,0.212189122\C,-1.2772890956,-1.0001797256,0.6463734241\C,-2.5220177859,-1.6169395243,0.578701382\C,-3.5991703734,-0.8854808605,0.0726882323\H,-2.2473334346,1.9872217961,-0.6202882446\H,-0.4125555341,-1.5354317066,1.0309118937\H,-2.6600408251,-2.6417081423,0.9112112968\H,-4.5889396075,-1.3344044969,0.0040448713\C,0.2406329263,0.986104297,0.2760486305\H,0.6277299961,0.8127686306,1.2887717088\C,0.2416513919,2.5085198481,0.0458738818\H,-0.3796670593,3.0070353223,0.7973353718\H,1.2630452908,2.890835926,0.1391677592\H,-0.1331269118,2.7829622493,-0.9449146433\N,1.1738408072,0.2894316564,-0.617667453\N,-3.4958903664,0.3787402858,-0.3481182017\H,3.3427390537,-0.9737852008,0.4527213797\C,4.2218141425,-1.4382994285,0.9138967987\H,4.1329004381,-1.3226186391,2.0011257102\H,4.187481491,-2.5126542551,0.6956137259\C,5.5194506241,-0.8114075369,0.3971587772\H,6.4020354285,-1.2729243309,0.8559780799\H,5.6131212057,-0.928482786,-0.6889699911\H,5.5576326554,0.262399482,0.6156385695\C,0.9026545636,0.4612611392,-2.0271918597\H,-0.157802254,0.5953263789,-2.2867359265\H,1.4476414105,1.3493244078,-2.3908732068\H,1.3028516951,-0.3983001693,-2.5758219517\Version=ES64L-G16RevC.01\State=2-A\HF=-500.7402761\S2=0.75377\S2-1=0.\S2A=0.750011\RMSD=4.003e-09\RMSF=1.030e-06\Dipole=0.1041209,0.0311233,0.0197755\Quadrupole=-7.8839996,5.2851166,2.598883,5.0037933,-2.3572254,-1.1863265\PG=C01[X(C10H17N2)]\

System 28+



		H(kJ/mol)			ΔH(kJ/mol)		
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
28+	MIN_PyCHMeNHMe_katrad_ver	-421.08901	-420.83828		-31.91	-35.23	a)
	MIN_PyCHMeNHMe_katrad	-421.09558	-420.84353				
28H+	MIN_PyCHMeNHMe_kation	-421.73660	-421.49011		-		
	confMIN_PyCHMeNHMe_kation_000	-421.73491	-421.48858				
	confMIN_PyCHMeNHMe_kation_009	-421.72618	-421.48018				
2	PrimC_CH3CH3_rad_konf	-79.093317	-79.031807	-79.060735	-19.70	-16.61	-13.82
2H	PrimC_CH3CH3_neut	-79.750773	-79.686654	-79.720391	-	-	-
START 28+		-500.82991	-500.52191	-79.060735	0.00	0.00	0.00
R28+	TS_PyCHMeNHMe_katrad_opt_rev	-500.82800	-500.51829		5.02	0.00	9.51
TS28+	TS_PyCHMeNHMe_katrad	-500.81450	-500.50082		40.48	35.46	55.37
P28+	TS_PyCHMeNHMe_katrad_opt_fwd	-500.84329	-500.52794		-35.12	-40.14	-15.83

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
FIN28+		-500.83978	-500.52493	-79.720391	-25.90	-7.93	

- a) RSE compared to CH₄/CH₃[·] radical system
b) RSE compared to NH₃/NH₂[·] radical system

28+
1\1\GINC-SL250S-GEN8-07-03\FOpt\UB3LYP\6-31G(d)\C8H12N2(1+,2)\DSAKIC\02-Oct-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,2\C,-0.91185,-1.08637,0.525907\C,-0.215447,0.080886,0.237194\C,-0.950193,1.143354,-0.307976\C,-2.32397,1.027284,-0.543641\C,-2.966255,-0.157008,-0.234417H,-0.439674,-1.971324,0.937065\H,-0.449168,2.073442,-0.554055\H,-2.892409,1.848172,-0.965749\H,-4.024252,-0.336043,-0.382136\C,1.298927,0.102826,0.449658\H,1.514278,-0.472816,1.36795\C,1.872888,1.521632,0.652273\H,1.342608,2.047838,1.452745\H,2.926003,1.45522,0.934752\H,1.810765,2.110546,-0.268252\N,1.880666,-0.56045,-0.703909\N,-2.239452,-1.170424,0.288947\C,3.273098,-0.905797,-0.537542\H,3.895559,-0.085898,-0.9341\H,3.581698,-1.085992,0.503875\H,3.497257,-1.785897,-1.14906\H,-2.714345,-2.041971,0.512967\Version=ES64L-G16RevC.01\State=2-A\HF=-421.2895977\S2=0.753805\S2-1=0.\S2A=0.750011\RMSD=4.349e-09\RMSF=7.539e-07\Dipole=-2.1706378,-0.5421377,0.6190771\Quadrupole=15.3316603,-2.028746,-13.3029143,4.0035489,1.5497411,-3.7682685\PG=C01[X(C8H12N2)]\

28+ ver
1\1\GINC-SL230S-GEN8-02-07\FOpt\UB3LYP\6-31G(d)\C8H12N2(1+,2)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,2\C,-0.9666851691,0.2378999722,-0.011320674\C,0.1212679615,1.0819721667,-0.2030422075\C,-0.0589434967,2.1888863578,-1.04472067\C,-1.2856567802,2.4263109269,-1.6712699269\C,-2.3348542637,1.5513455563,-1.4537509033\H,-0.9097065005,-0.6245223715,0.6416177855\H,0.764615176,2.8786435373,-1.2097193592\H,-1.4298516713,3.2827008921,-2.319994572\H,-3.3183778328,1.6560436449,-1.8953604435\C,1.4489640072,0.7840696328,0.4861926727\H,1.8176450081,1.7246353695,0.9323312751\C,2.5064054911,0.3132739226,-0.5516170063\H,2.6238104354,1.0513150238,-1.3513617609\H,3.4759810463,0.1858969025,-0.063732215\H,2.2067848969,-0.6409942942,-0.9947915706\N,1.2381008674,-0.2199398498,1.4999121932\N,-2.1381324762,0.4938361764,-0.6346318429\C,2.3245723062,-0.3702698763,2.4341551971\H,2.9697950623,-1.2011547684,2.1023840152\H,2.9562678074,0.5228440775,2.5503391609\H,1.9205218073,-0.6671235863,3.407925958\H,-2.9147639427,-0.1431710629,-0.4718286553\Version=ES64L-G16RevC.01\State=2-A\HF=-421.297196\S2=0.75383\S2-1=0.\S2A=0.750011\RMSD=3.276e-09\RMSF=3.024e-06\Dipole=-1.7180688,0.4238896,-0.9085416\Quadrupole=11.5744746,-6.048483,-5.5259916,-0.5881147,9.1619469,-5.5380194\PG=C01[X(C8H12N2)]\

28H+
1\1\GINC-NX360-M5-04-09\FOpt\RB3LYP\6-31G(d)\C8H13N2(1+)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,1\C,-0.6305715826,0.1439552078,0.0353818485\C,0.4412492401,0.9913717318,-0.2195681736\C,0.1652284277,2.2052068268,-0.8652373832\C,-1.1374761557,2.5394059169,-1.2468210835\C,-2.1677220285,1.6568457275,-0.9755041048\H,-0.4941887156,-0.8004607206,0.5501253434\H,0.9765430957,2.8995687983,-1.0686730133\H,-1.3553312076,3.477014564,-1.7454465429\H,-3.2056525314,1.8332131274,-1.2301934494\C,1.8552666585,0.5612653883,0.1652361074\H,2.4071912168,1.478803571,0.4391618698\C,2.553704287,-0.0698772777,-1.0536822775\H,2.5486956621,0.6055479897,-1.9144415911\H,3.5976685095,-0.29151095,-0.8087297533\H,2.0577444486,-1.0030795418,-1.3413926991\N,1.796653946,-0.3923137968,1.2669229892\N,-1.8783035409,0.4956627468,-0.3449760876\C,1.7100960815,0.2187747264,2.5977179932\H,2.5199336658,0.9361591947,2.8063192342\H,0.7565006451,0.7487129539,2.7058349703\H,1.7377442865,-0.5688038556,3.3549352122\H,2.6056998508,-1.0063861352,1.2242584717\H,-2.6405552594,-0.1468760835,-0.1411798407\Version=ES64L-

G16RevC.01\State=1-
 A\HF=-421.9527371\RMSD=3.871e-09\RMSF=1.073e-05\Dipole=-1.7810048,0.325324,-0.6063449\Quadrupole=11.1648274,-4.0633724,-7.101455,-2.0775673,5.0844447,-4.9649346\PG=C01[X(C8H13N2)]\\
 28H+ ver1
 1\1\GINC-SL250S-GEN8-06-07\FOpt\RB3LYP\6-31G(d)\C8H13N2(1+)\DSAKIC\02-Oct-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
 \1,1\C,-0.029800267,-0.0080362081,0.0908657912\C,1.351662106,-0.0586910149,-0.0265184598\C,2.0427399258,1.1640997958,-0.0614640704\C,1.3614144423,2.3787988061,0.0379634562\C,-0.017575498,2.3726855285,0.1623107641\H,-0.6611461113,-0.8895889527,0.1106246027\H,3.1211286225,1.1305929778,-0.1863056026\H,1.8899267806,3.3252178628,0.0152622182\H,-0.6282378554,3.2640577565,0.2401738369\C,2.0966421587,-1.3921069499,-0.0763301994\H,1.3896369451,-2.1506101651,-0.4621742004\C,2.5099681335,-1.8050853156,1.3486753566\H,1.6462461188,-1.8593757834,2.0182168654\H,2.9780568952,-2.7948064924,1.3256396544\H,3.2289351043,-1.0910489008,1.7640554041\N,3.2734673269,-1.2545016909,-0.9212430646\N,-0.6628459032,1.1855802519,0.1822595552\C,3.0132386,-1.3611685163,-2.3593674552\H,2.4899982911,-2.2882140141,-2.6461964885\H,2.4055950512,-0.5125613266,-2.6941994568\H,3.9632181115,-1.3166923204,-2.897613671\H,3.9704225834,-1.94043819,-0.6435903798\H,-1.6769915621,1.1873928618,0.2624555433\Version=ES64L-
 G16RevC.01\State=1-
 A\HF=-421.9509938\RMSD=8.472e-09\RMSF=4.091e-06\Dipole=-1.9218127,1.1339604,0.4040926\Quadrupole=6.0095475,4.7062205,-10.7157681,-8.6406222,-3.1004187,1.7054021\PG=C01[X(C8H13N2)]\\
 28H+ ver2
 1\1\GINC-SL250S-GEN8-07-05\FOpt\RB3LYP\6-31G(d)\C8H13N2(1+)\DSAKIC\02-Oct-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
 \1,1\C,-0.0155313808,-0.0315585727,0.1936410842\C,1.3680466626,-0.0883444945,0.065021386\C,2.0373275738,1.1419059506,-0.0923662708\C,1.3350977244,2.3488729928,-0.1426722077\C,-0.0419256139,2.3403807026,-0.0078796098\H,-0.6341485028,-0.9118014197,0.3321584224\H,3.1199767923,1.1601285926,-0.1561149007\H,1.8514822031,3.2937264845,-0.269513923\H,-0.6637159131,3.2271081759,-0.0185577932\C,2.0719434832,-1.4526344692,0.0169514848\H,1.3667712755,-2.1855444444,0.4273858322\C,3.3350858348,-1.4987798327,0.8842000319\H,3.0966118363,-1.2770957257,1.9292617674\H,3.7616340972,-2.5034112035,0.8275362642\H,4.1038790464,-0.7919395906,0.5566116838\N,2.3328682019,-1.8854584625,-1.3555250076\N,-0.6668958796,1.1532592003,0.1612991554\C,3.2231102915,-1.0958556204,-2.1968178215\H,2.8987919068,-0.053217452,-2.3748914859\H,4.2285875119,-1.0729462605,-1.7668180448\H,3.2976589474,-1.58754294,-3.1702209184\H,1.4677741929,-2.102123101,-1.842173138\H,-1.6776302918,1.1506714901,0.278684009\Version=ES64L-
 G16RevC.01\State=1-
 A\HF=-421.9422649\RMSD=9.675e-09\RMSF=1.156e-05\Dipole=-2.1301758,1.6346809,0.3478252\Quadrupole=7.4486312,1.5514823,-9.0001135,-5.0993373,-2.842335,1.0683608\PG=C01[X(C8H13N2)]\

2
 GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C2H5(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
 \0,2\C,0,-0.694243,0.000008,-0.000769\H,0,-1.109259,0.887906,-0.493472\H,0,-1.109282,-0.887356,-0.494432\H,0,-1.095121,-0.000568,1.029127\C,0,0,0.795115,0,-0.023114\H,0,1.354194,-0.927422,0.051034\H,0,1.354237,0.927393,0.051039\Version=ES64L-G16RevA.03\State=2-
 A\HF=-78.989782\MP2=-79.0963583\RMSD=5.565e-09\PG=C01[X(C2H5)]\

2H
 GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C2H6\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2large maxdisk=20gb\nekaj\
 \0,1\C,0,0,0,0.765285\H,0,0.510242,0.884349,1.16453\H,0,-1.02099,-0.000292,1.16453\H,0,0.510748,-0.884057,1.16453\C,0,0,0,-0.765285\H,0,1.02099,-0.000292,-1.16453\H,0,-0.510748,-0.884057,-1.16453\H,0,-0.510242,0.884349,-1.16453\Version=ES64L-G16RevA.03\State=1-
 A1\HF=-79.6490727\MP2=-79.7663021\RMSD=7.090e-09\PG=D03[C3(C1.C1),X(H6)]\

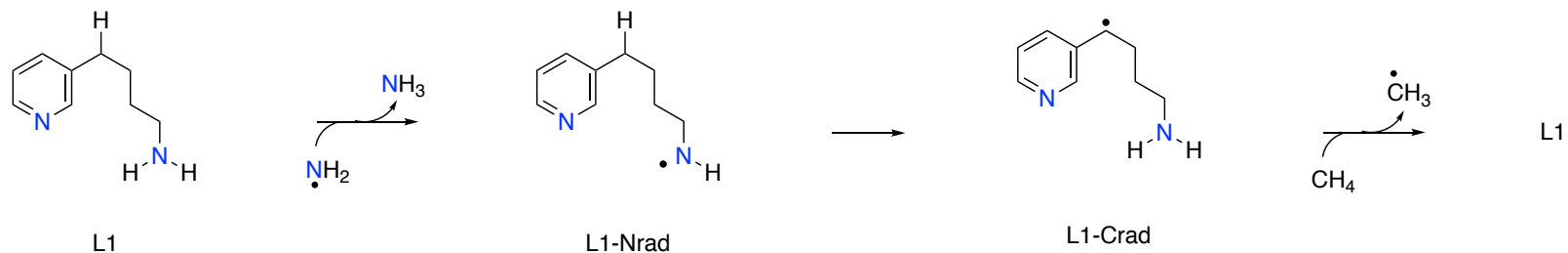
R28+
1\1\GINC-NX360-M5-05-04\FOpt\UB3LYP\6-31G(d)\C10H18N2(1+,2)\DSAKIC\25-Sep-2020\0\#\b3lyp/6-31G(d)optfreq\optircreverse\
\1,2\C,2.0033181578,1.1954961971,-0.1840545413\C,1.0569546181,0.181101778,-0.2120833945\C,1.5342538719,-1.1411524018,-0.1443128094\C,2.89974922
66,-1.416799869,-0.0641425611\C,3.8000235894,-0.3652067858,-0.0396779711\H,1.7597918437,2.2493803179,-0.2222967261\H,0.797755825,-1.9388860691,-
0.1361046532\H,3.2676302558,-2.4355521472,-0.017148073\H,4.8750307513,-0.4815397833,0.026715918\C,-0.4505357365,0.4386824228,-0.3305975018\H,-0.
699880733,0.1977192192,-1.3744419858\C,-0.8444908661,1.9091205509,-0.0991419562\H,-0.4188732199,2.5696597912,-0.8634572017\H,-1.9322725268,2.00
24761103,-0.1658662733\H,-0.5378609425,2.2740598411,0.8870963787\N,-1.1505579057,-0.5612205784,0.4739535704\N,3.3235847057,0.8963379813,-0.0990
939056\H,-2.082604763,-0.7144597124,0.0821153202\C,-4.2105512084,-1.0288142476,-0.8984690542\H,-3.8073069352,-1.0472543079,-1.9084638052\H,-4.21
32336871,-1.9753564681,-0.3631767551\C,-5.1392977232,0.0618713812,-0.4870948265\H,-6.1599009798,-0.1229154038,-0.8659862374\H,-5.2253484104,0.14
19902235,0.6027096914\H,-4.8361788874,1.0371846782,-0.8864786334\C,-1.2448026754,-0.2949818857,1.911404763\H,-0.2409062799,-0.2332204092,2.3486
032178\H,-1.7870211703,0.6254746321,2.1750904864\H,-1.755783198,-1.1373027736,2.3853946876\H,3.988097003,1.665883718,-0.0748951678\
\Version=ES64L-G16RevC.01\State=2-
A\HF=-501.1109889\S2=0.753542\S2-1=0.\S2A=0.750009\RMSD=3.970e-09\RMSF=1.597e-06\Dipole=3.5066617,0.6631518,-0.2036586\Quadrupole=26.5061175,
-8.8501735,-17.655944,3.3466136,-0.0861729,-0.605763\PG=C01[X(C10H18N2)]\

TS28+
1\1\GINC-SL250S-GEN8-07-03\FTS\UB3LYP\6-31G(d)\C10H18N2(1+,2)\DSAKIC\25-Sep-2020\0\#\opt=(calcf,ts,noeigentest)freqb3lyp/6-31g(d)\nekaj\
\1,2\C,-0.6987325021,0.0138676464,-0.3896411264\C,0.5401282656,0.6374341129,-0.4036338566\C,0.5760947861,1.985963738,-0.8080644832\C,-0.58543998
5,2.6589535964,-1.1879265985\C,-1.796963525,1.9888023558,-1.1500998776\H,-0.8524570149,-1.0167565381,-0.0971864766\H,1.5339629856,2.4957631013,-
0.7963565405\H,-0.5582635625,3.6948133753,-1.5064702914\H,-2.7484747696,2.4316032655,-1.4187418844\C,1.8417738365,-0.0592671903,0.0081461509\H,
2.4364503179,-0.1336037386,-0.9145889185\C,1.6422201556,-1.4876144088,0.5381157084\H,1.2262675373,-2.1447475956,-0.2342507971\H,2.6099901372,-1
.9061066108,0.8276890206\H,0.9889334333,-1.524822175,1.4165937149\N,2.5662564035,0.8954586702,0.8584045356\N,-1.8124381689,0.6991325454,-0.754
0197585\H,3.8097428568,0.6298830759,0.7279228445\C,5.0991735233,0.2775483203,0.6135489578\H,5.1291489775,-0.2327253374,-0.3537194234\H,5.56125
57444,1.2666205479,0.5550915377\C,5.5310637713,-0.5615082652,1.7916736024\H,6.5986709658,-0.8127060611,1.7085996435\H,5.4012228514,-0.03270931
17,2.7421835552\H,4.9854752249,-1.5106425451,1.8478890966\C,2.2701789193,0.8221966233,2.2863084163\H,1.2155654526,1.0811567828,2.4622788723\H,
2.4528009787,-0.1581961411,2.7498170445\H,2.8804543378,1.5674228693,2.8037136097\H,-2.7051726545,0.2128402421,-0.7239517881\Version=ES64L-
G16RevC.01\State=2-
A\HF=-501.0920877\S2=0.757144\S2-1=0.\S2A=0.750027\RMSD=6.005e-09\RMSF=1.676e-06\Dipole=-3.2249739,0.2826044,-1.1557249\Quadrupole=19.6623679
,-7.714248,-11.9481199,-5.2696336,11.3247438,-4.560679\PG=C01[X(C10H18N2)]\

P28+
1\1\GINC-SL230S-GEN8-02-03\FOpt\UB3LYP\6-31G(d)\C10H18N2(1+,2)\DSAKIC\25-Sep-2020\0\#\b3lyp/6-31G(d)optfreq\optircforward\
\1,2\C,1.3020828124,0.912650453,-1.0400227051\C,0.6529692891,0.502883756,0.1154291812\C,0.8496566948,-0.8240318046,0.5333788153\C,1.6817984667,
-1.6861510544,-0.1844894967\C,2.3092501483,-1.2260453937,-1.3287369683\H,1.2085406047,1.9080773054,-1.4598527205\H,0.3207523288,-1.1635093314,1
.4177906399\H,1.8387389989,-2.7104432697,0.134183856\H,2.9643825576,-1.8247112554,-1.9498737155\C,-0.2276317378,1.4677973593,0.9030737872\H,-0.
7302999734,2.1443531026,0.1899603126\C,0.6465138014,2.3451333298,1.8441857128\H,1.4118370057,2.8829912272,1.2753943204\H,0.0206897364,3.08198
84286,2.3540948686\H,1.1405736421,1.7228238312,2.5963715682\N,-1.1896919076,0.7054633564,1.6597374818\N,2.0971500122,0.0511079761,-1.716814636
6\H,-2.3679967025,-0.9660210571,-0.3673534805\C,-2.6439490248,-1.3540948004,-1.3563781978\H,-2.4538581754,-0.5632379037,-2.0930814536\H,-1.97107
95153,-2.1896278435,-1.5864869912\C,-4.1079053452,-1.7997186085,-1.3900325146\H,-4.3811200242,-2.1896668964,-2.3762872368\H,-4.299725379,-2.5900
635784,-0.6563088561\H,-4.7831205602,-0.9668248329,-1.1651875026\C,-2.2807275961,1.4802906178,2.1951542592\H,-2.0435702725,1.7625071967,3.23484

91253\H,-2.5059514953,2.4020276139,1.6378788438\H,-3.1747269243,0.8501185647,2.2450307812\H,2.5510335344,0.3810335114,-2.5652200776\
\Version=ES64L-G16RevC.01\State=2-
A\HF=-501.1264577\S2=0.753844\S2-1=0.\S2A=0.750012\RMSD=6.858e-09\RMSF=1.500e-06\Dipole=2.8656909,0.4474705,-1.2242123\Quadrupole=3.9989122,-
2.7062338,-1.2926784,-5.0236803,-12.9819639,3.1171703\PG=C01[X(C10H18N2)]\

System L1



		H(kJ/mol)			ΔH(kJ/mol)		
NAME	SYSTEM	B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.789551	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.454472	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.835797	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.504485	-	-	-
L1-H	Loef_neut_konf_xx04_OnlyH	-460.651585	-460.387236				
L1-Nrad	Loeffler_Nrad_OnlyH	-460.004971	-459.734877		-34.48	-33.83	
L1-Crad	Loeffler_C5rad_OnlyH	-460.019005	-459.753101		-85.02	-70.99	
	Loef_neut_konf_xx17_OnlyH	-460.650915	-460.386763				
	Loef_neut_konf_xx50_OnlyH	-460.647376	-460.383436				
L1-Nrad	Loeffler_Nrad_OnlyH	-460.004971	-459.734877		0.00	0.00	
R-L1	Loeffler_TS_Ndown_eqNMe_eqC5Py_OnlyH_rad_opt_rev	-460.003591	-459.733088		3.62	4.70	
TS-L1	Loeffler_TS_Ndown_eqNMe_eqC5Py_OnlyH_rad	-459.987262	-459.717491		46.49	45.65	
P-L1	Loeffler_TS_Ndown_eqNMe_eqC5Py_OnlyH_rad_opt_fwd	-460.017189	-459.751013		-32.08	-42.37	
L1-Crad	Loeffler_C5rad_OnlyH	-460.019005	-459.753101		-36.85	-47.85	

1

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C1H3(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,0,0,0,0.000155\H,0,0,1.082798,-0.00031\H,0,0.937731,-0.541399,-0.00031\H,0,-0.937731,-0.541399,-0.00031\\Version=ES64L-G16RevA.03\State=2-
A1\HF=-39.7559614\MP2=-39.8069654\RMSD=3.347e-09\PG=C03V[C3(C1),3SGV(H1)]\\

1H

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C1H4\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,1\C,0,0,0,0,0.631339,0.631339,0.631339\H,0,-0.631339,-0.631339,0.631339\H,0,-0.631339,0.631339,-0.631339\H,0,0.631339,-0.631339,-0.631339\
\Version=ES64L-G16RevA.03\State=1-A1\HF=-40.4209215\MP2=-40.4832688\RMSD=1.296e-09\PG=TD[O(C1),4C3(H1)]\\

15

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\H2N1(2)\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\N,0,0,0,0,0.14444\H,0,0,0.804686,-0.505541\H,0,0,-0.804686,-0.505541\\Version=ES64L-G16RevA.03\State=2-
B1\HF=-55.7918729\MP2=-55.8517922\RMSD=1.893e-09\PG=C02V[C2(N1),SGV(H2)]\\

15H

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\H3N1\DSAKIC\18-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,1\N,0,0,0,0,0.119349\H,0,0,0.938581,-0.278482\H,0,-0.812835,-0.469291,-0.278482\H,0,0.812835,-0.469291,-0.278482\\Version=ES64L-G16RevA.03\State=1-
A\HF=-56.4579585\MP2=-56.5326192\RMSD=3.740e-09\PG=C03[C3(N1),X(H3)]\\

L1-H

GINC-NX360-M5-05-03\SP\ROB2PLYP-FC\GTMP2large\C9H14N2\DSAKIC\06-May-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,1\C,0,1.995664,-1.198985,0.097932\C,0,1.274625,-0.053581,0.462545\C,0,1.922789,1.175562,0.29693\C,0,3.218753,1.205885,-0.213529\C,0,3.831846,-0.002
945,-0.545614\H,0,1.537849,-2.181675,0.21788\H,0,1.416645,2.099174,0.571028\H,0,3.747059,2.145459,-0.348378\H,0,4.844144,-0.018038,-0.946673\N,0,3.23
9238,-1.193518,-0.394603\C,0,-0.144052,-0.150067,0.974724\H,0,-0.307245,0.60537,1.754972\H,0,-0.2952,-1.127123,1.452196\C,0,-1.20097,0.036423,-0.13301
\H,0,-1.037784,-0.720293,-0.91299\H,0,-1.044929,1.010838,-0.61711\C,0,-2.63826,-0.054223,0.391779\H,0,-2.811118,0.706243,1.164222\H,0,-2.786131,-1.0297
17,0.880568\C,0,-3.692349,0.121403,-0.703586\H,0,-3.51578,-0.627578,-1.49856\H,0,-3.564957,1.106196,-1.171918\H,0,-5.229435,-0.862237,0.223258\N,0,-5.0
4326,0.07604,-0.130435\H,0,-5.733243,0.238891,-0.862254\\Version=ES64L-G16RevA.03\State=1-
A\HF=-460.0060987\MP2=-460.619929\RMSD=4.824e-09\PG=C01[X(C9H14N2)]\\

L1-Nrad

GINC-NX360-M5-01-01\SP\ROB2PLYP-FC\GTMP2large\C9H13N2(2)\DSAKIC\06-May-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,1.927657,-1.193766,0.121993\C,0,1.21104,-0.039548,0.467226\C,0,1.859972,1.184725,0.271858\C,0,3.152611,1.20218,-0.247643\C,0,3.76134,-0.01440
6,-0.558681\H,0,1.469338,-2.172967,0.265981\H,0,1.357379,2.114761,0.530429\H,0,3.681664,2.137769,-0.405226\H,0,4.770846,-0.039715,-0.966141\N,0,3.167
787,-1.20054,-0.378914\C,0,-0.204516,-0.123274,0.990234\H,0,-0.366308,0.657387,1.745507\H,0,-0.351,-1.084072,1.500636\C,0,-1.267207,0.022579,-0.117838
\H,0,-1.104843,-0.759841,-0.872689\H,0,-1.115624,0.980261,-0.636382\C,0,-2.700683,-0.057682,0.417034\H,0,-2.869248,0.728395,1.165149\H,0,-2.857255,-1.0
13505,0.934474\C,0,-3.759902,0.080108,-0.67877\H,0,-3.616445,-0.702708,-1.448927\H,0,-3.622782,1.034527,-1.22408\N,0,-5.098782,0.00795,-0.140745\H,0,-5
.740629,0.102349,-0.943593\\Version=ES64L-G16RevA.03\State=2-A\HF=-459.3520027\MP2=-459.9522681\RMSD=5.668e-09\PG=C01[X(C9H13N2)]\\

L1-Crad

GINC-NX360-M5-02-07\SP\ROB2PLYP-FC\GTMP2large\C9H13N2(2)\DSAKIC\06-May-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-2.260229,-1.254658,0.020382\C,0,-1.233592,-0.264496,0.11311\C,0,-1.676386,1.08554,0.036926\C,0,-3.027265,1.352805,-0.121889\C,0,-3.930824,0.2
86784,-0.202391\H,0,-1.977023,-2.3066,0.075853\H,0,-0.961803,1.900186,0.107371\H,0,-3.387654,2.376118,-0.181661\H,0,-4.996324,0.468599,-0.326812\N,0,-
3.552448,-1.003375,-0.131196\C,0,0.113656,-0.659122,0.271218\H,0,0.309184,-1.727654,0.351233\C,0,1.293481,0.257082,0.38522\H,0,1.403087,0.597841,1.43
0913\H,0,1.127333,1.171804,-0.201713\C,0,2.609883,-0.403218,-0.055432\H,0,2.517242,-0.728507,-1.101947\H,0,2.794096,-1.308692,0.536139\C,0,3.820446,0.
521355,0.082868\H,0,3.927217,0.82059,1.133928\H,0,3.633767,1.450431,-0.488888\N,0,5.049133,-0.1812,-0.304416\H,0,5.025111,-0.381272,-1.304065\H,0,5.8
53958,0.42676,-0.161143\\Version=ES64L-G16RevA.03\State=2-A\HF=-459.3635652\MP2=-459.9707951\RMDS=2.938e-09\PG=C01[X(C9H13N2)]\\

R-L1

GINC-SL230S-GEN8-02-02\SP\ROB2PLYP-FC\GTMP2large\C9H13N2(2)\DSAKIC\06-May-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-2.815311,-0.958012,-0.472898\C,0,-3.661649,0.312887,-0.338671\C,0,-0.542344,-0.267994,0.57536\C,0,-1.309512,-0.723981,-0.684914\H,0,-3.48466,0
.978086,-1.206213\H,0,-4.734661,0.046853,-0.407153\H,0,-2.976093,-1.582404,0.416153\H,0,-3.203944,-1.52593,-1.328879\H,0,-0.667309,-1.029952,1.355932\
H,0,-1.164813,0.01557,-1.486384\H,0,-0.853979,-1.653702,-1.050913\N,0,-3.441073,1.02521,0.899389\H,0,-0.997097,0.646607,0.96993\C,0,0.929166,-0.051465
,0.30833\C,0,1.860422,-1.086625,0.473955\C,0,1.429987,1.174566,-0.143656\N,0,3.170934,-0.982706,0.22702\H,0,1.522319,-2.058464,0.835836\C,0,2.791899,1
.307282,-0.40698\H,0,0.756834,2.018518,-0.281341\C,0,3.618853,0.201124,-0.208787\H,0,3.207568,2.249049,-0.754265\H,0,4.688206,0.267526,-0.403896\H,0,-
4.01046,1.884016,0.845895\\Version=ES64L-G16RevA.03\State=2-A\HF=-459.3493454\MP2=-459.950502\RMDS=4.964e-09\PG=C01[X(C9H13N2)]\\

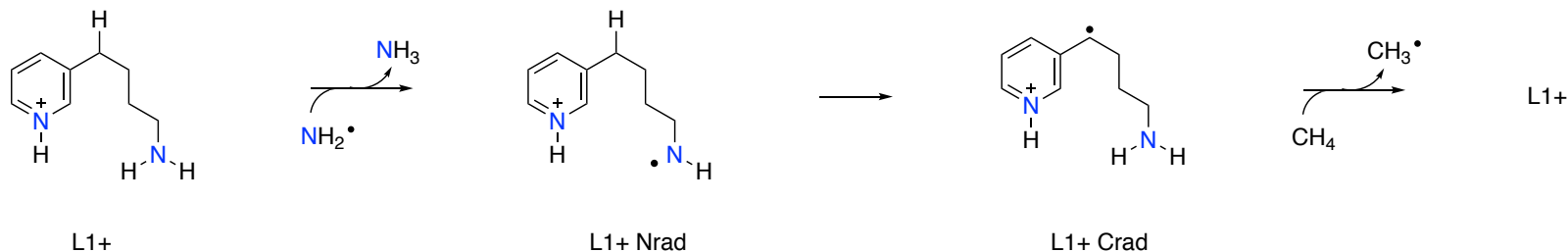
TS-L1

GINC-SL230S-GEN8-02-06\SP\ROB2PLYP-FC\GTMP2large\C9H13N2(2)\DSAKIC\06-May-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-3.057126,0.058947,-0.768065\C,0,-3.178579,0.405292,0.724743\C,0,-0.657088,-0.641345,-0.427384\C,0,-1.603543,0.239226,-1.240721\H,0,-2.937971,
1.471956,0.869716\H,0,-4.225265,0.272422,1.042483\H,0,-3.371344,-0.982445,-0.916864\H,0,-3.734364,0.691552,-1.353666\H,0,-0.744602,-1.697423,-0.706519
\H,0,-1.329791,1.297537,-1.141627\H,0,-1.520406,-0.000565,-2.310501\N,0,-2.344571,-0.503421,1.516913\H,0,-1.295132,-0.693204,0.696957\C,0,0.752159,-0.2
46479,-0.219515\C,0,1.752214,-1.236868,-0.12145\C,0,1.182686,1.08246,-0.059566\N,0,3.045622,-1.001413,0.101929\H,0,1.473044,-2.284401,-0.239007\C,0,2.
529051,1.346687,0.172329\H,0,0.472129,1.902879,-0.113343\C,0,3.422223,0.276523,0.246084\H,0,2.883676,2.366093,0.296102\H,0,4.481634,0.448631,0.4282
21\H,0,-1.910941,0.034152,2.277421\\Version=ES64L-G16RevA.03\State=2-A\HF=-459.3134238\MP2=-459.9303689\RMDS=2.647e-09\PG=C01[X(C9H13N2)]\\

P-L1

GINC-SL230S-GEN8-02-01\SP\ROB2PLYP-FC\GTMP2large\C9H13N2(2)\DSAKIC\06-May-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-2.981769,0.656312,-0.514661\C,0,-3.332371,-0.178845,0.722679\C,0,-0.506759,0.082075,-0.834403\C,0,-1.522535,1.154179,-0.57993\H,0,-3.094664,0.
41148,1.628655\H,0,-4.418087,-0.336065,0.732879\H,0,-3.21099,0.065921,-1.411006\H,0,-3.640273,1.534696,-0.531551\H,0,-0.819826,-0.746495,-1.467309\H,0
, -1.288455,1.702946,0.343176\H,0,-1.460209,1.90516,-1.387768\N,0,-2.70294,-1.504641,0.692218\H,0,-1.698246,-1.413061,0.835558\C,0,0.831726,0.071604,-0.
379624\C,0,1.688629,-1.020952,-0.72312\C,0,1.42809,1.088266,0.418512\N,0,2.954976,-1.144521,-0.353345\H,0,1.284588,-1.826983,-1.336984\C,0,2.752687,0.
962551,0.806859\H,0,0.851886,1.95894,0.716723\C,0,3.48053,-0.163441,0.40439\H,0,3.227683,1.727522,1.414993\H,0,4.521613,-0.28662,0.695484\H,0,-3.0486
36,-2.063794,1.470831\\Version=ES64L-G16RevA.03\State=2-A\HF=-459.3611838\MP2=-459.9697589\RMDS=6.896e-09\PG=C01[X(C9H13N2)]\\

System L1+



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.789551	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.454472	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.835797	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.504485	-	-	-
L1+H	MIN_L1_H+	-461.017451	-460.747753	-460.850892			
L1+ Nrad	TS_L1_H+_opt_rev	-460.374498	-460.097913	-460.197636	-44.09	-40.45	-40.52
	MIN_L1_H+_Nrad (extended chain)	-460.368726	-460.095101	-460.192349			
L1+ Crad	TS_L1_H+_opt_fwd	-460.393867	-460.120614	-460.216396	-108.64	-89.36	-79.88
	MIN_L1_H+_Crad (extended chain)	-460.385693	-460.113852	-460.209144			
L1+ Nrad		-460.374498	-460.097913	-460.197636	0.00	0.00	0.00
R-L1+	TS_L1_H+_opt_rev	-460.374498	-460.097913	-460.197636	0.00	0.00	0.00
TS-L1+	TS_L1_H+	-460.357085	-460.080396	-460.175914	45.72	45.99	57.03
P-L1+	TS_L1_H+_opt_fwd	-460.393867	-460.120614	-460.216396	-50.85	-59.60	-49.25
L1+ Crad		-460.393867	-460.120614	-460.216396	-50.85	-59.60	-49.25

L1+H

```

1\1\GINC-NX360-M5-02-08\FOpt\RB3LYP\6-31G(d)\C9H15N2(1+)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,1\C,2.0127013745,-1.2412019033,0.1561556451\C,1.2632648112,-0.1095495939,0.4596214457\C,1.879636887,1.1362121416,0.2383838697\C,3.1795014497
,1.2266814533,-0.2623147561\C,3.8764774125,0.064672442,-0.5466932818\H,1.6438051062,-2.2515334133,0.2912168244\H,1.3316126769,2.0457280365,0.46
88833237\H,3.6535830214,2.1873968378,-0.4281471813\H,4.8876721864,0.037605356,-0.9339452764\N,3.2709609839,-1.1226771783,-0.3280345949\C,-0.152
6494777,-0.2245342118,0.9649231086\H,-0.3076502517,0.517594958,1.7570785107\H,-0.3020749355,-1.2090203615,1.4229917711\C,-1.2015971684,-0.00743
91375,-0.1514342808\H,-1.0533867578,-0.7592710254,-0.9388535884\H,-1.0311082597,0.9709036873,-0.6224519878\C,-2.6349396888,-0.0791165539,0.38734
20754\H,-2.7851872784,0.6738645108,1.1705877683\H,-2.798712567,-1.0583096726,0.8608729762\C,-3.6951867989,0.1413447823,-0.6982829357\H,-3.55205
66973,-0.6034879076,-1.5039994238\H,-3.5392886666,1.1269788997,-1.1551596495\H,-5.2939179221,-0.8096150079,0.1672655134\N,-5.0282798136,0.13776
64162,-0.097575217\H,-5.7211363955,0.4479976122,-0.7755878523\H,3.7883076592,-1.9745134765,-0.5331163263\Version=ES64L-G16RevC.01\State=1-
A\HF=-461.2643773\RMSD=4.928e-09\RMSF=7.555e-06\Dipole=4.1143261,-0.9382317,-0.6004901\Quadrupole=22.8991313,-5.8875084,-17.0116229,-0.9637347,
-0.4940776,-0.2188957\PG=C01[X(C9H15N2)]\

```

L1+ Nrad

```

1\1\GINC-SL230S-GEN8-02-01\FOpt\UB3LYP\6-31G(d)\C9H14N2(1+,2)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,2\C,-2.3055659333,-1.2873766581,-0.0753253129\C,-1.2624151169,-0.3701207269,0.0376132939\C,-1.6246284645,0.9846056735,0.1223726645\C,-2.96482
90365,1.3835573235,0.0969571096\C,-3.956183005,0.4269246348,-0.015048171\H,-2.1462902485,-2.3575005933,-0.1500742904\H,-0.8507610044,1.73939121
89,0.208620831\H,-3.2387550183,2.4303988561,0.1629868994\H,-5.0171431305,0.6427819673,-0.0431938492\N,-3.5906571355,-0.8725834687,-0.0972512601
\C,0.1678645087,-0.8725927799,0.0655706842\H,0.3149304724,-1.5282824025,-0.8036653493\C,1.264878475,0.1994471967,0.084128746\H,1.1519306947,0.8
330102198,0.9754849715\H,1.1561351327,0.8574011089,-0.7900404159\C,2.6635985217,-0.429918741,0.0814510616\H,2.7894824077,-1.0610375429,-0.8075
120969\H,2.7797771644,-1.0905229647,0.9501119899\C,3.7960676187,0.6016464602,0.1048516661\H,3.704249991,1.254149608,0.9940462305\H,3.71225433
33,1.2849207218,-0.761761457\N,5.0785026272,-0.0604181872,0.0986767735\H,5.7970898557,0.6786718888,0.1161656391\H,-4.3207500536,-1.5764738365,-
0.1813632892\H,0.2809245938,-1.5222616965,0.9450796211\Version=ES64L-G16RevC.01\State=2-
A\HF=-460.599417\S2=0.753277\S2-1=0.\S2A=0.750008\RMSD=9.846e-09\RMSF=6.180e-06\Dipole=-4.5306558,0.1234825,-0.1045292\Quadrupole=22.5451349,
-5.6736424,-16.8714926,10.5801139,1.419697,0.9853221\PG=C01[X(C9H14N2)]\

```

L1+ Crad

```

1\1\GINC-SL230S-GEN8-02-01\FOpt\UB3LYP\6-31G(d)\C9H14N2(1+,2)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,2\C,-2.2050041411,-1.2634239663,0.3038226554\C,-1.1573170271,-0.3114477,0.3431208453\C,-1.4885698658,0.9958025253,-0.1412105342\C,-2.75967488
32,1.2886925785,-0.6100078873\C,-3.7446171779,0.3056029761,-0.6182088229\H,-2.0781233105,-2.2858365378,0.6407398997\H,-0.7308587421,1.770934767
2,-0.1408229143\H,-3.003056569,2.2804069381,-0.9743500021\H,-4.7591601853,0.4494422501,-0.9655712323\N,-3.4182550812,-0.9309682153,-0.1583235493
\C,0.1054430303,-0.6980963158,0.8449318489\H,0.2049177804,-1.7358326707,1.1594288409\C,1.3301103376,0.1392234151,0.9371070723\H,1.7591683783,0.
0133600027,1.9416865743\H,1.1114499232,1.2063669975,0.8203722054\C,2.4006717476,-0.2953799316,-0.1026866512\H,2.0082110089,-0.1366252381,-1.11
59225858\H,2.6088328911,-1.3667995255,-0.0093870837\C,3.7208742215,0.4717529153,0.0691780668\H,4.1246054517,0.2610765612,1.0667526192\H,3.5200
191694,1.5585334197,0.0338588974\N,4.6875345017,0.001439599,-0.917177935\H,4.5193577444,0.4309364344,-1.824542377\H,5.6343035941,0.2536443104,
-0.6446977766\H,-4.138323837,-1.6499203696,-0.1649660738\Version=ES64L-G16RevC.01\State=2-
A\HF=-460.6188968\S2=0.772427\S2-1=0.\S2A=0.750335\RMSD=9.175e-09\RMSF=2.126e-06\Dipole=-3.4073456,-0.1836873,-0.0393554\Quadrupole=24.435244
5,-8.4119615,-16.0232829,9.824454,3.8913044,-4.2104083\PG=C01[X(C9H14N2)]\

```

R-L1+

1\1\GINC-NX360-M5-04-07\FOpt\UB3LYP\6-31G(d)\C9H14N2(1+,2)\DSAKIC\25-Sep-2020\0\#b3lyp/6-31G(d)optfreq\optircreverse\
\1,2\C,-2.970030514,-0.6322197923,-0.6640492825\C,-3.4219207021,0.7194773438,-0.0817792332\C,-0.5891223673,-1.0982131817,0.1845081657\C,-1.473692
408,-0.6736638449,-1.023042755\H,-3.5017851212,1.4568405333,-0.906165753\H,-4.4435761412,0.6390185552,0.3233261306\H,-3.2020637811,-1.436269292
2,0.0460030273\H,-3.5730207069,-0.8318165027,-1.5568628689\H,-0.5089911231,-2.1900705004,0.2248552513\H,-1.1628809591,0.3155560081,-1.382281145
8\H,-1.2984887959,-1.368620239,-1.8519907728\N,-2.4965524228,1.275869336,0.8787798188\H,-1.0762283095,-0.7705768214,1.1067068562\C,0.7816126417,
-0.4757774862,0.1535887971\C,1.9184577489,-1.1964432902,-0.186731765\C,0.9541587353,0.8878855943,0.4664831489\N,3.1306181317,-0.5905479484,-0.2
110815277\H,1.9041731765,-2.2506294638,-0.4385848592\C,2.216797045,1.4805267457,0.43368077\H,0.0712301877,1.4627848721,0.739865981\C,3.3164667
03,0.7135173541,0.0853971079\H,2.3547909367,2.5274639763,0.6791825207\H,4.3315377576,1.0882844355,0.0354018808\H,-2.9863639411,2.0401972566,1.
3639065846\H,3.9419842289,-1.1501616478,-0.461982078\Version=ES64L-G16RevC.01\State=2-
A\HF=-460.6067729\S2=0.753585\S2-1=0.\S2A=0.75001\RMSD=7.025e-09\RMSF=3.120e-06\Dipole=2.6580349,-0.0992302,-0.1685115\Quadrupole=22.867182,-
6.1266055,-16.7405765,-4.3155115,-1.4967223,3.272133\PG=C01[X(C9H14N2)]\

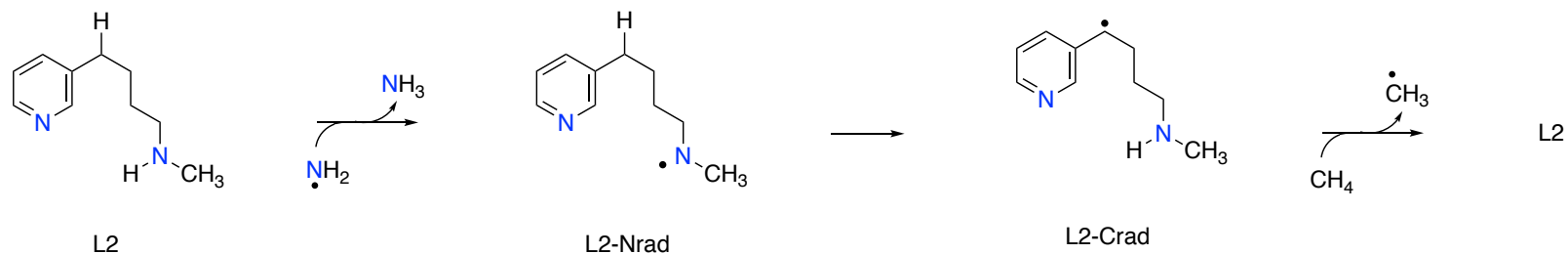
TS-L1+

1\1\GINC-SL250S-GEN8-07-03\FTS\UB3LYP\6-31G(d)\C9H14N2(1+,2)\DSAKIC\24-Sep-2020\0\#opt=(calcfc,ts,noeigentest)freqb3lyp/6-31g(d)\nekaj\
\1,2\C,-3.0605241445,0.0670789182,-0.7670590896\C,-3.218327488,0.329131225,0.7386055792\C,-0.6552603863,-0.5941389797,-0.4517381963\C,-1.6074996
517,0.3288929129,-1.2079545901\H,-3.0713849295,1.398250153,0.9571170498\H,-4.2489398471,0.0841907655,1.0427830836\H,-3.3341771327,-0.9725473399
,-0.984948378\H,-3.748152525,0.7085922301,-1.3267191329\H,-0.7687643175,-1.6389313761,-0.7601370201\H,-1.3687616202,1.3839865704,-1.0218821215\H
,-1.5095024354,0.1724481455,-2.2905374721\N,-2.3252531726,-0.5438520615,1.4958107096\H,-1.2718446225,-0.6972615185,0.6901440137\C,0.7544585436,-
0.2394079606,-0.2492422883\C,1.6997389302,-1.2584108878,-0.0596645071\C,1.2553031876,1.0843441314,-0.1780608353\N,2.9938066419,-0.9692566891,0.
1810473756\H,1.4428337045,-2.3107725546,-0.0976640622\C,2.6001927296,1.3434745699,0.0724226779\H,0.5795140281,1.9196596003,-0.3254486149\C,3.4
830193351,0.2899989085,0.255119707\H,2.971289829,2.3609256729,0.122569773\H,4.5422228669,0.3987492118,0.449594146\H,-1.9817081446,-0.041364456
9,2.3236693771\H,3.6393264611,-1.7454465507,0.306393176\Version=ES64L-G16RevC.01\State=2-
A\HF=-460.5839852\S2=0.760375\S2-1=0.\S2A=0.750072\RMSD=9.261e-09\RMSF=5.968e-06\Dipole=2.7153442,-0.05497,0.1783045\Quadrupole=19.2506389,-5.
7272349,-13.523404,-6.2938143,2.5953633,1.4003927\PG=C01[X(C9H14N2)]\

P-L1+

1\1\GINC-SL250S-GEN8-01-05\FOpt\UB3LYP\6-31G(d)\C9H14N2(1+,2)\DSAKIC\25-Sep-2020\0\#b3lyp/6-31G(d)optfreq\optircforward\
\1,2\C,-3.1116007927,0.3546380947,-0.6267962273\C,-3.1519875657,0.1082712818,0.8825168993\C,-0.6636729404,-0.2487719983,-0.8909093962\C,-1.71109
58475,0.7896000734,-1.1070210827\H,-2.8483836292,1.0201321455,1.4106554726\H,-4.1862109417,-0.1083802311,1.1910282321\H,-3.4164792762,-0.556670
1234,-1.1598650208\H,-3.8384782221,1.1291409208,-0.8953309315\H,-0.9135357213,-1.259690409,-1.201616507\H,-1.4416458285,1.7390260442,-0.62991336
25\H,-1.7710055758,0.997888919,-2.1883380948\N,-2.2057897016,-0.955075687,1.2437361312\H,-2.018518973,-0.9535568381,2.2445532502\C,0.6619995013,
-0.0322248692,-0.460500473\C,1.5525823445,-1.1307132092,-0.3975454004\C,1.2163939122,1.2323923989,-0.0680163087\N,2.8199800949,-0.9705549888,0.
0041668962\H,1.2545741664,-2.1375868941,-0.6658602331\C,2.5346154934,1.3452599584,0.3412731389\H,0.5934079807,2.1187843228,-0.0950397495\C,3.3
572897911,0.2223684259,0.3788810113\H,2.9437117036,2.3057181971,0.6341952889\H,4.3955321034,0.2221567635,0.6816688036\H,-2.5969664353,-1.86960
93085,1.0215376694\H,3.4178913597,-1.7927419894,0.0285649935\Version=ES64L-G16RevC.01\State=2-
A\HF=-460.6272473\S2=0.769458\S2-1=0.\S2A=0.75025\RMSD=7.532e-09\RMSF=7.391e-06\Dipole=1.8521961,-0.8684674,0.277944\Quadrupole=16.9708557,-4.
0054957,-12.96536,-2.8655733,0.8971136,0.2321836\PG=C01[X(C9H14N2)]\

System L2



NAME	SYSTEM	H(kJ/mol)			Δ H(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.789551	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.454472	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.835797	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.504485	-	-	-
L2	Loef_neut_konf_xx04	-499.931260	-499.634006	-499.752434			
	Loef_neut_konf_xx17	-499.930461	-499.633412	-499.752176			
	Loef_neut_konf_xx50	-499.926933	-499.630189	-499.750205			
L2-Nrad	Loef_Nrad_konf_xx16	-499.29336	-498.990993	-499.104017	-57.36	-58.37	-53.22
L2-Crad	Loeffler_C5rad_konf_xx17	-499.298696	-498.999893	-499.110579	-85.06	-71.05	-60.56
L2-Nrad	Loef_Nrad_konf_xx16	-499.29336	-498.990993	-499.104017	0.00	0.00	0.00
R-L2	Loeffler_TS_Ndown_eqNMe_eqC5Py_rad_opt_fwd	-499.292086	-498.989258	-499.102981	3.34	4.56	2.72
TS-L2	Loeffler_TS_Ndown_eqNMe_eqC5Py_rad	-499.271374	-498.97035	-	57.72	54.20	
P-L2	Loeffler_TS_Ndown_eqNMe_eqC5Py_rad_opt_rev	-499.296904	-498.997979	-499.109721	-9.30	-18.34	-14.98
L2-Crad	Loeffler_C5rad_konf_xx17	-499.298696	-498.999893	-499.110579	-14.01	-23.37	-17.23

L2

GINC-NX360-M5-03-10\SP\ROB2PLYP-FC\GTMP2large\C10H16N2\DSAKIC\19-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,1\C,0,2.571294,-1.192183,-0.034476\C,0,1.859881,-0.091542,0.462664\C,0,2.482176,1.157559,0.358575\C,0,3.744777,1.249941,-0.223048\C,0,4.351268,0.08
169,-0.686521\H,0,2.133295,-2.188815,0.032841\H,0,1.982389,2.047922,0.735186\H,0,4.252769,2.20595,-0.312861\H,0,5.337841,0.115379,-1.146241\N,0,3.783
04,-1.126837,-0.597051\C,0,0.475739,-0.252065,1.048213\H,0,0.350989,0.436047,1.895037\H,0,0.36521,-1.266471,1.453491\C,0,-0.647764,0.004627,0.023201\
H,0,-0.523696,-0.684956,-0.823155\H,0,-0.532841,1.016825,-0.38926\C,0,-2.049827,-0.151149,0.623241\H,0,-2.182298,0.543387,1.462952\H,0,-2.154855,-1.164
759,1.040267\C,0,-3.168502,0.093531,-0.39179\H,0,-3.04418,-0.593637,-1.253942\H,0,-3.076918,1.110902,-0.797991\H,0,-4.573559,-0.941343,0.64862\C,0,-5.5
81511,0.19253,-0.704623\H,0,-5.554558,-0.465579,-1.594195\H,0,-6.536202,0.036026,-0.191499\H,0,-5.562088,1.229145,-1.062158\N,0,-4.483967,-0.015115,0.
232806\\Version=ES64L-G16RevA.03\State=1-A\HF=-499.2270301\MP2=-499.8963029\RMSD=4.015e-09\PG=C01[X(C10H16N2)]\\

L2-Nrad

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C10H15N2(2)\DSAKIC\19-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,2.508097,-1.192175,0.029266\C,0,1.805789,-0.062601,0.47179\C,0,2.433045,1.175793,0.295599\C,0,3.691362,1.230356,-0.300081\C,0,4.288497,0.0358
09,-0.70477\H,0,2.066198,-2.181502,0.154073\H,0,1.940638,2.087666,0.627925\H,0,4.203183,2.177519,-0.445017\H,0,5.271405,0.039598,-1.17346\N,0,3.71534
2,-1.163269,-0.545751\C,0,0.425495,-0.184726,1.075323\H,0,0.305277,0.557452,1.875823\H,0,0.317095,-1.170145,1.546831\C,0,-0.704421,0.00363,0.042567\H
,0,-0.583381,-0.740074,-0.757749\H,0,-0.591383,0.986377,-0.437398\C,0,-2.101811,-0.116142,0.659813\H,0,-2.228526,0.631227,1.454246\H,0,-2.218934,-1.096
996,1.139193\C,0,-3.226632,0.063922,-0.362552\H,0,-3.127345,-0.682475,-1.174638\H,0,-3.132393,1.046829,-0.864362\C,0,-5.597708,0.107662,-0.703021\H,0,-
5.543472,-0.657,-1.498108\H,0,-6.568046,0.023095,-0.204435\H,0,-5.547736,1.086807,-1.211624\N,0,-4.528607,-0.047809,0.252193\\Version=ES64L-
G16RevA.03\State=2-A\HF=-498.5818432\MP2=-499.2382945\RMSD=2.855e-09\PG=C01[X(C10H15N2)]\\

L2-Crad

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C10H15N2(2)\DSAKIC\19-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,2.883614,-1.219773,0.003497\C,0,1.820765,-0.271071,-0.111225\C,0,2.210889,1.095897,-0.049986\C,0,3.549111,1.41686,0.116115\C,0,4.492049,0.387
405,0.218573\H,0,2.641406,-2.282466,-0.039918\H,0,1.466437,1.881628,-0.13728\H,0,3.869567,2.453925,0.164916\H,0,5.548683,0.611643,0.34923\N,0,4.16395
3,-0.917101,0.162081\C,0,0.491053,-0.719317,-0.274702\H,0,0.337357,-1.795562,-0.341407\C,0,-0.721737,0.149298,-0.412234\H,0,-0.837203,0.4676,-1.464196
\H,0,-0.595437,1.079344,0.160046\C,0,-2.015175,-0.553319,0.031615\H,0,-1.915836,-0.856647,1.084096\H,0,-2.158293,-1.475092,-0.546192\C,0,-3.257672,0.32
3503,-0.131064\H,0,-3.365014,0.612399,-1.186428\H,0,-3.121849,1.26923,0.433743\C,0,-5.676962,0.407189,0.131786\H,0,-5.645413,1.368249,0.679974\H,0,-5.
853779,0.637396,-0.925778\H,0,-6.536117,-0.166355,0.49499\N,0,-4.466784,-0.396983,0.254909\H,0,-4.370306,-0.706735,1.22103\\Version=ES64L-
G16RevA.03\State=2-A\HF=-498.5845167\MP2=-499.2471856\RMSD=2.207e-09\PG=C01[X(C10H15N2)]\\

R-L2

GINC-SL250S-GEN8-02-07\SP\ROB2PLYP-FC\GTMP2large\C10H15N2(2)\DSAKIC\19-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,2.229886,-1.564606,0.412809\C,0,3.243007,-0.418189,0.516687\C,0,0.10955,-0.429102,-0.564941\C,0,0.758868,-1.167264,0.626093\H,0,3.116723,0.11
0102,1.482397\H,0,4.266923,-0.838085,0.554015\H,0,2.348094,-2.052282,-0.563953\H,0,2.501765,-2.312326,1.169985\H,0,0.165852,-1.076198,-1.450219\H,0,0.
67681,-0.544119,1.528923\H,0,0.172779,-2.072418,0.833809\N,0,3.168421,0.521043,-0.577828\H,0,0.697346,0.463022,-0.803824\C,0,-1.330885,-0.057927,-0.2
9944\C,0,-2.382832,-0.91311,-0.657392\C,0,-1.684877,1.135779,0.339605\N,0,-3.678005,-0.670063,-0.427349\H,0,-2.160467,-1.850708,-1.168464\C,0,-3.02769,
1.411423,0.589524\H,0,-0.912633,1.844442,0.632502\C,0,-3.984307,0.477669,0.189671\H,0,-3.330167,2.332545,1.079817\H,0,-5.043213,0.659126,0.368051\C,0
,4.081182,1.625139,-0.411735\H,0,5.121789,1.279305,-0.28188\H,0,4.038145,2.288594,-1.280615\H,0,3.835941,2.213271,0.490416\\Version=ES64L-
G16RevA.03\State=2-A\HF=-498.5791579\MP2=-499.2365841\RMSD=3.170e-09\PG=C01[X(C10H15N2)]\\

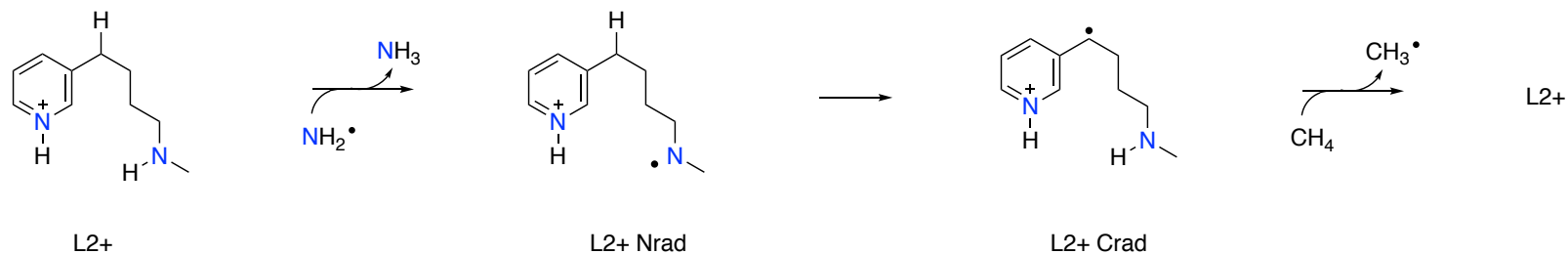
TS-L2

GINC-SL250S-GEN8-04-01\SP\ROB2PLYP-FC\GTMP2large\C10H15N2(2)\DSAKIC\19-Apr-2019\0\#\rob2plyp\gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,2.804712,-1.267285,0.114544\C,0,3.020143,0.232497,0.3643\C,0,0.43365,-0.809701,-0.623562\C,0,1.320798,-1.632676,0.307973\H,0,2.758746,0.47062
7,1.413167\H,0,4.086237,0.483187,0.24189\H,0,3.118734,-1.506482,-0.909756\H,0,3.435481,-1.852054,0.794121\H,0,0.483811,-1.164149,-1.659104\H,0,1.0509
58,-1.455626,1.356769\H,0,1.169391,-2.707058,0.130089\N,0,2.25078,1.016,-0.597075\H,0,1.182677,0.263079,-0.757369\C,0,-0.937529,-0.433018,-0.234858\C,
0,-1.93209,-0.278903,-1.22589\C,0,-1.336901,-0.153542,1.085239\N,0,-3.189784,0.099349,-0.999117\H,0,-1.677557,-0.484718,-2.266188\C,0,-2.646942,0.24093
4,1.339663\H,0,-0.630315,-0.242561,1.905779\C,0,-3.536632,0.354936,0.270443\H,0,-2.976111,0.458629,2.351904\H,0,-4.567795,0.66249,0.435335\C,0,1.8120
54,2.296918,-0.071873\H,0,2.68641,2.954301,0.053596\H,0,1.133349,2.777175,-0.783771\H,0,1.311436,2.234761,0.911015\\Version=ES64L-
G16RevA.03\State=2-A\HF=-498.5382206\MP2=-499.2127766\RMSD=7.332e-09\PG=C01[X(C10H15N2)]\\

P-L2

GINC-SL250S-GEN8-02-03\SP\ROB2PLYP-FC\GTMP2large\C10H15N2(2)\DSAKIC\19-Apr-2019\0\#\rob2plyp\gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,2.49983,-1.48197,-0.316101\C,0,3.051387,-0.244258,0.401018\C,0,0.078235,-0.797211,-0.797299\C,0,0.995309,-1.755638,-0.100292\H,0,2.827936,-0.3
22,1.486012\H,0,4.146909,-0.253316,0.317151\H,0,2.708538,-1.389832,-1.389755\H,0,3.056531,-2.357257,0.042464\H,0,0.395082,-0.449251,-1.779664\H,0,0.78
7163,-1.784218,0.977888\H,0,0.786068,-2.776734,-0.465855\N,0,2.583901,1.008051,-0.185498\H,0,1.567121,1.041543,-0.130878\C,0,-1.185491,-0.356451,-0.34
1153\C,0,-1.954553,0.541971,-1.145814\C,0,-1.7862,-0.739751,0.891043\N,0,-3.145424,1.026318,-0.825394\H,0,-1.543965,0.865967,-2.103046\C,0,-3.031875,-0
.235138,1.229405\H,0,-1.27544,-1.426085,1.559578\C,0,-3.677487,0.642347,0.350196\H,0,-3.50866,-0.515526,2.164594\H,0,-4.655696,1.052781,0.591735\C,0,3
.135986,2.184291,0.476773\H,0,4.220348,2.218149,0.314413\H,0,2.704692,3.088797,0.035382\H,0,2.963194,2.217242,1.569568\\Version=ES64L-
G16RevA.03\State=2-A\HF=-498.582024\MP2=-499.2463007\RMSD=6.183e-09\PG=C01[X(C10H15N2)]\\

System L2+



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.789551	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.454472	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.835797	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.504485	-	-	-
L2+	MIN_L2_H+	-500.296824	-499.994433	-500.111890			
L2+ Nrad	TS_L2_H+_opt_fwd	-499.663474	-499.356494	-499.468431	-69.30	-71.69	-66.24
	MIN_L2_H+_Nrad (extended chain)	-499.658535	-499.352799	-499.463020			
L2+ Crad	TS_L2_H+_opt_rev	-499.672477	-499.367162	-499.477768	-106.63	-89.01	-80.86
	MIN_L2_H+_Crad (extended chain)	-499.664813	-499.360281	-499.469908			
L2+ Nrad		-499.663474	-499.356494	-499.468431	0.00	0.00	0.00
R-L2+	TS_L2_H+_opt_fwd	-499.663474	-499.356494	-499.468431	0.00	0.00	0.00
TS-L2+	TS_L2_H+	-499.644084	-499.335943	-499.445386	50.91	53.96	60.50
P-L2+	TS_L2_H+_opt_rev	-499.672477	-499.367162	-499.477768	-23.64	-28.01	-24.51
L2+ Crad		-499.672477	-499.367162	-499.477768	-23.64	-28.01	-24.51

L2+

1\1\GINC-SL230S-GEN8-02-01\FOpt\RB3LYP\6-31G(d)\C10H17N2(1+)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,1\C,2.5999776915,-1.2294064274,0.0380860765\C,1.846939181,-0.139120948,0.4606146267\C,2.4235995853,1.1332747358,0.2897468994\C,3.6895281374,
1.2886208736,-0.2776056248\C,4.391952566,0.1655223833,-0.6802321012\H,2.2602839159,-2.2551726557,0.1247880435\H,1.8716521627,2.0117670629,0.61
2677775\H,4.1332357293,2.2695327755,-0.4046730585\H,5.3787839934,0.1890683056,-1.1261355387\N,3.8247474275,-1.0481927268,-0.5085316328\C,0.465
4537458,-0.3221124195,1.0363453059\H,0.3392272902,0.3657331309,1.8808572305\H,0.3650398017,-1.3365387221,1.4391746056\C,-0.649387406,-0.064594
5959,-0.0050330886\H,-0.5285682815,-0.7622752207,-0.845035202\H,-0.5285543186,0.9449923183,-0.421980114\C,-2.0490291434,-0.2075586634,0.60392359
99\H,-2.1725620556,0.4941108773,1.4379993358\H,-2.1609863412,-1.2175063207,1.025288539\C,-3.1679274724,0.04777037,-0.4117628584\H,-3.0622643361,
-0.6513546934,-1.2671347422\H,-3.054525759,1.0583796648,-0.8285177836\H,-4.6129916498,-0.9532530853,0.609685755\C,-5.5773015838,0.3087252916,-0.
663990282\H,-5.6132052416,-0.3043719853,-1.5829293295\H,-6.5238753352,0.1836782992,-0.1300554271\H,-5.5017677427,1.3596249414,-0.96615544\N,-4.4
709240489,-0.0170512789,0.2332325897\H,4.346255738,-1.871561727,-0.8008183791\Version=ES64L-G16RevC.01\State=1-
A\HF=-500.5733885\RMSD=6.398e-09\RMSF=3.169e-06\Dipole=5.1633354,-0.8526047,-0.5568281\Quadrupole=29.179938,-9.0738502,-20.1060878,-1.4059063,-
4.8506313,0.3660778\PG=C01[X(C10H17N2)]\

L2+ Nrad (extended chain)

1\1\GINC-NX360-M5-02-08\FOpt\UB3LYP\6-31G(d)\C10H16N2(1+,2)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,2\C,2.5305162731,-1.2352153374,0.1052142133\C,1.7944383001,-0.111172174,0.464665617\C,2.3923274727,1.1402895607,0.2259875976\C,3.661848645,1.
2435120689,-0.3452647787\C,4.3466312526,0.0886360311,-0.68330307\H,2.1740187964,-2.2489838245,0.2478732314\H,1.8546610232,2.044146349,0.499154
7066\H,4.122069417,2.2085564802,-0.5244445199\H,5.3347893516,0.0715851907,-1.1265925854\N,3.7592552041,-1.1043464391,-0.4468098654\C,0.4103449
001,-0.2412635267,1.0485100527\H,0.2975542048,0.4871541761,1.8603036732\H,0.2921726152,-1.2335464636,1.4986281564\C,-0.7040306402,-0.015064794
4,-0.0007130646\H,-0.5865447317,-0.7428013702,-0.8157341243\H,-0.5791418877,0.9785833555,-0.4540120686\C,-2.1001452326,-0.1379531182,0.619092393
\H,-2.2146080393,0.588146267,1.4338720149\H,-2.2252907871,-1.1306739104,1.0696851329\C,-3.2318412681,0.0822144986,-0.3911619157\H,-3.1465426341,
-0.6389588794,-1.2266919211\H,-3.1414894071,1.081941422,-0.8577335678\C,-5.6157947057,0.1534755142,-0.6517132542\H,-5.591628692,-0.5669643171,-1
.487940969\H,-6.5651370624,0.0418019963,-0.1215161084\H,-5.5809561263,1.1590967421,-1.1058902573\N,-4.5139081526,-0.054461186,0.2550698463\H,4.2
680080809,-1.9510259214,-0.6911342547\Version=ES64L-G16RevC.01\State=2-
A\HF=-499.9200919\S2=0.753632\S2-1=0.\S2A=0.75001\RMSD=9.715e-09\RMSF=1.053e-05\Dipole=5.145442,-0.4768967,-0.9045474\Quadrupole=27.9955516,-
8.6237036,-19.371848,-5.9619859,-0.7807034,1.0887756\PG=C01[X(C10H16N2)]\

L2+ Crad (extended chain)

1\1\GINC-NX360-M5-02-08\FOpt\UB3LYP\6-31G(d)\C10H16N2(1+,2)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,2\C,2.809589135,-1.2349940506,-0.2892327035\C,1.7397898166,-0.3084179366,-0.3415139553\C,2.0272931935,1.0000220129,0.1670585265\C,3.27923782
34,1.3174506948,0.6701493245\C,4.2876512411,0.3585885099,0.6896184265\H,2.7161956065,-2.255522192,-0.6424107689\H,1.2512195687,1.7567174411,0.1
57905858\H,3.4893568408,2.3099306733,1.0526552051\H,5.2898315022,0.5225282978,1.0630124998\N,4.002954451,-0.8792259907,0.2062656031\C,0.49943
61767,-0.7191180726,-0.8787399142\H,0.433683809,-1.7542759404,-1.2102765082\C,-0.7421529517,0.0904582307,-0.9947178283\H,-1.1276817731,-0.015437
7811,-2.0191468637\H,-0.5555208762,1.1584863103,-0.8387289512\C,-1.8430829041,-0.3990642964,-0.0131734804\H,-1.4903477867,-0.2680069508,1.018742
6194\H,-2.024896182,-1.470434899,-0.1519114462\C,-3.167326489,0.3510863767,-0.2129406795\H,-3.5274882326,0.1748027364,-1.2351524288\H,-2.9956325
958,1.4436728805,-0.1291301967\C,-5.5245016457,0.3279255616,0.4259517454\H,-5.615846705,1.4285351151,0.4068248983\H,-5.8537848015,-0.0536470762
, -0.5469589013\H,-6.2088295656,-0.0612446891,1.1852729619\N,-4.1733042351,-0.1571098201,0.7037409756\H,-3.9184930059,0.086933056,1.6591928339\H,
4.7402771156,-1.5803611414,0.2208178482\Version=ES64L-G16RevC.01\State=2-
A\HF=-499.9276937\S2=0.772477\S2-1=0.\S2A=0.750336\RMSD=8.925e-09\RMSF=8.493e-07\Dipole=4.5329049,-0.3100082,0.1707485\Quadrupole=29.7897532,
-11.7900991,-17.9996541,-8.349707,3.7791447,3.7195132\PG=C01[X(C10H16N2)]\

R-L2+

1\1\GINC-SL250S-GEN8-07-03\FOpt\UB3LYP\6-31G(d)\C10H16N2(1+,2)\DSAKIC\25-Sep-2020\0\#b3lyp/6-31G(d)optfreq\optircforward\
\1,2\C,2.7112887887,-1.0124951719,-0.4063528658\C,3.1088524953,0.1138238991,0.5652510096\C,0.3015991403,-0.5613157208,-1.1865710051\C,1.2346664
716,-1.4317149285,-0.2958613393\H,3.1282157331,-0.2971384008,1.5929824793\H,4.1413589914,0.4414175761,0.3592455315\H,2.9341978915,-0.708105317
1,-1.4370537021\H,3.3563328587,-1.8733831742,-0.1970269508\H,0.2221230273,-0.9975107491,-2.1882790648\H,0.9204934616,-1.3620067107,0.7533596581
\H,1.1144061119,-2.4832248555,-0.580227311\N,2.1757258437,1.2206638364,0.584384582\H,0.7501332295,0.4301984766,-1.2921052522\C,-1.0672241688,-0.
3731574883,-0.5891837749\C,-2.1939563353,-1.0114356451,-1.0896815207\C,-1.2472746708,0.4686841294,0.5271215102\N,-3.4038210566,-0.8176367767,-0.
509999154\H,-2.1734078549,-1.6750754242,-1.9464677121\C,-2.5071270335,0.6482248177,1.0986267392\H,-0.3708067306,0.9783141991,0.9239208384\C,-3.
5966732511,-0.0156841011,0.5589094759\H,-2.6511489741,1.2989727208,1.9537283618\H,-4.6089848595,0.0645105908,0.9358805715\C,2.775041634,2.4398
734598,1.0711438496\H,3.5727511004,2.7805924603,0.3899422428\H,2.0267943768,3.2329072011,1.1548905623\H,3.2521812959,2.2928718271,2.054834806
3\H,-4.2077545163,-1.2997557302,-0.9045175657\Version=ES64L-G16RevC.01\State=2-
A\HF=-499.9256969\S2=0.753896\S2-1=0.\S2A=0.750012\RMSD=7.314e-09\RMSF=4.101e-06\Dipole=-3.1644367,-0.5854218,-0.1832839\Quadrupole=23.948074
7,-11.8739742,-12.0741005,7.3281609,3.1960466,6.4882566\PG=C01[X(C10H16N2)]\

TS-L2+

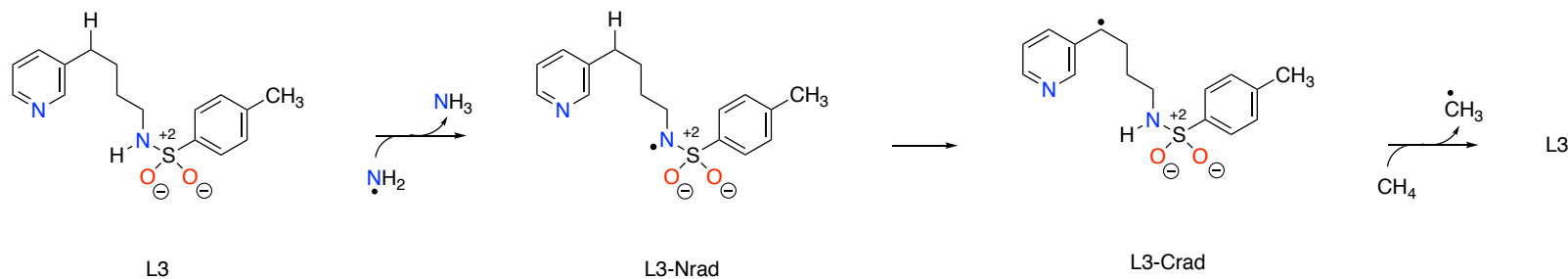
1\1\GINC-SL250S-GEN8-07-03\FTS\UB3LYP\6-31G(d)\C10H16N2(1+,2)\DSAKIC\25-Sep-2020\0\#freqb3ly/6-31g(d)opt=(calcfc,ts,noeigentest)\nekaj\
\1,2\C,2.7926098431,-1.2653735142,0.1137125653\C,3.0642014414,0.2327796076,0.3084990499\C,0.4171130459,-0.8087964474,-0.5757969565\C,1.31069340
05,-1.5865022412,0.3872575729\H,2.9273346106,0.5132845052,1.3675363235\H,4.1127667277,0.4566952819,0.0564217609\H,3.0529659366,-1.5525020708,-
0.9124093916\H,3.4356230395,-1.8436221592,0.7844280502\H,0.5032189031,-1.1739234642,-1.6046418689\H,1.0843744671,-1.332191838,1.4307310794\H,1.
1346418294,-2.6657170104,0.2852702552\N,2.2210167456,1.0223674778,-0.5796808972\H,1.1543983498,0.288688505,-0.7369758356\C,-0.9584973477,-0.459
3529271,-0.2315807737\C,-1.8969566235,-0.251178007,-1.2562928786\C,-1.4406422801,-0.2559244883,1.0883837646\N,-3.1597777837,0.1253457982,-0.9774
550749\H,-1.6574146751,-0.3839286064,-2.3050112041\C,-2.7531728937,0.1336545591,1.3350801227\H,-0.7739376352,-0.4114654669,1.9293553334\C,-3.62
83224748,0.3274348485,0.2760629031\H,-3.1074542646,0.2835897008,2.3487424293\H,-4.6642803744,0.6239809014,0.3758390888\C,1.8988715357,2.344627
424,-0.0800405516\H,2.8149113075,2.9532779464,-0.0902684161\H,1.1694069251,2.8276078941,-0.7362636406\H,1.5252024126,2.3479239595,0.9575025995
\H,-3.7996773484,0.2552762616,-1.7573013794\Version=ES64L-G16RevC.01\State=2-
A\HF=-499.9006176\S2=0.760071\S2-1=0.\S2A=0.750069\RMSD=8.674e-09\RMSF=4.359e-06\Dipole=-2.6976466,0.2467623,-0.212146\Quadrupole=19.6640779,
-12.5724493,-7.0916287,-2.1120576,6.0970034,0.7826316\PG=C01[X(C10H16N2)]\

P-L2+

1\1\GINC-SL250S-GEN8-07-03\FOpt\UB3LYP\6-31G(d)\C10H16N2(1+,2)\DSAKIC\25-Sep-2020\0\#b3lyp/6-31G(d)optfreq\optircreverse\
\1,2\C,2.8125169691,-1.0225624037,0.1747576529\C,2.8607030692,0.2915575278,0.9611312882\C,0.4172613062,-0.6811898639,-0.5655892165\C,1.38096269
62,-1.59033075,0.1211718427\H,2.5210246566,0.10984171,1.9876024191\H,3.9007447343,0.6508445979,1.0244707921\H,3.1873449822,-0.8686932031,-0.845
2138044\H,3.4784908446,-1.7568285869,0.641153306\H,0.7356909703,-0.2725539577,-1.5209454017\H,1.047650142,-1.8362053147,1.1363528899\H,1.40873
23986,-2.545245531,-0.4297087549\N,1.9731474965,1.2919918821,0.36154756\H,1.618616382,1.9226078305,1.0758570321\C,-0.9274232316,-0.4578163862,-
0.2037331749\C,-1.7466510135,0.3309474549,-1.0474485614\C,-1.5733910639,-0.9707361917,0.9730564004\N,-3.0294544524,0.5659356299,-0.7439852343\H
, -1.379527858,0.7731971225,-1.9663374032\C,-2.9033712632,-0.6969481419,1.2425465623\H,-1.010699919,-1.5887122481,1.6630183578\C,-3.6522079923,0.
0873154371,0.3680300753\H,-3.380417402,-1.0909813348,2.132999009\H,-4.6940763743,0.3452493053,0.4996868616\C,2.5626513316,2.0676635487,-0.7308
805093\H,2.8199231399,1.4070347104,-1.565158594\H,1.8350522557,2.8004083711,-1.092890396\H,3.4779913929,2.6039606484,-0.4343641662\H,-3.572982
1976,1.1345991371,-1.3882248325\Version=ES64L-G16RevC.01\State=2-

A\HF=-499.9355436\S2=0.768428\S2-1=0.\S2A=0.750227\RMSD=8.462e-09\RMSF=6.709e-06\Dipole=-2.1898666,0.5644091,-0.3841138\Quadrupole=17.5421094
,-9.7465692,-7.7955402,-2.6478792,2.7199885,-4.3774057\PG=C01[X(C10H16N2)]\

System L3



NAME		SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
			B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad		-39.804412	-39.773085	-39.789551	0.00	0.00	0.00
1H	NulC_neut		-40.469373	-40.434258	-40.454472	-	-	-
15	NH3_Nrad		-55.849865	-55.829037	-55.835797	0.00	0.00	0.00
15H	NH3_neut		-56.509611	-56.494282	-56.504485	-	-	-
L3	Loeffler_R1Tos_TS_Ndown_eqNMe_eqC5Py_neutL2		-1279.465162	-1278.947022				
L3-Nrad	Loeffler_R1Tos_TS_Ndown_eqNMe_eqC5Py_NradL2		-1278.818339	-1278.291709		-33.93	-26.08	
L3-Crad	Loeffler_R1Tos_TS_Ndown_eqNMe_eqC5Py_CradL2		-1278.832760	-1278.311236		-85.48	-66.65	
R-L3	Loeffler_R1Tos_TS_Ndown_eqNMe_eqC5Py_rad_opt_rev		-1278.823113	-1278.295686	-	0.00	0.00	
	Loeffler_R1Tos_TS_Ndown_axNMe_axC5Py_rad_opt_fwd		-1278.820965	-1278.293996		5.64	4.44	
	Loeffler_R1Tos_TS_Ndown_eqNMe_axC5Py_rad_opt_rev		-1278.820927	-1278.293500		5.74	5.74	
	Loeffler_R1Tos_TS_Ndown_axNMe_eqC5Py_rad_opt_fwd		-1278.821157	-1278.292800		5.14	7.58	
TS-L3	Loeffler_R1Tos_TS_Ndown_eqNMe_eqC5Py_rad		-1278.806202	-1278.283898	-	44.40	30.95	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
	Loeffler_R1Tos_TS_Ndown_axNMe_eqC5Py_rad	-1278.806508	-1278.282828		43.60	33.76	
	Loeffler_R1Tos_TS_Ndown_eqNMe_axC5Py_rad	-1278.804629	-1278.281861		48.53	36.30	
	Loeffler_R1Tos_TS_Ndown_axNMe_axC5Py_rad	-1278.803103	-1278.280604		52.54	39.60	
P-L3	Loeffler_R1Tos_TS_Ndown_axNMe_eqC5Py_rad_opt_rev	-1278.834351	-1278.312065	-	-29.51	-43.00	
	Loeffler_R1Tos_TS_Ndown_eqNMe_eqC5Py_rad_opt_fwd	-1278.833251	-1278.311736		-26.62	-42.14	
	Loeffler_R1Tos_TS_Ndown_eqNMe_axC5Py_rad_opt_fwd	-1278.832034	-1278.311082		-23.42	-40.42	
	Loeffler_R1Tos_TS_Ndown_axNMe_axC5Py_rad_opt_rev	-1278.831486	-1278.310589		-21.98	-39.13	
L3-Crad	Loeffler_R1Tos_TS_Ndown_eqNMe_eqC5Py_CradL2	-1278.832760	-1278.311236				

L3

GINC-SL250S-GEN8-09-01\SP\ROB2PLYP-FC\GTMP2large\C16H20N2O2S1\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\neka\0,1\C,0,0.944088,2.269421,0.116287\C,0,-0.244531,1.358195,0.452169\C,0,2.878276,0.707894,-0.662533\C,0,2.342172,1.691053,0.40106\H,0,-0.136395,0.972006,1.46987\H,0,-1.176769,1.943624,0.413819\H,0,0.876573,2.594283,-0.932957\H,0,0.810414,3.178697,0.717152\H,0,2.902494,1.219443,-1.634868\H,0,2.336435,1.195879,1.381679\H,0,3.051772,2.524425,0.487293\N,0,-0.31039,0.188867,-0.437299\C,0,4.261214,0.19777,-0.328078\C,0,5.412243,0.860034,-0.776413\C,0,4.457362,-0.93729,0.466846\N,0,6.665817,0.488123,-0.494557\H,0,5.311384,1.743096,-1.409076\C,0,5.754505,-1.343931,0.77279\H,0,3.600504,-1.497758,0.835006\C,0,6.822361,-0.598526,0.271569\H,0,5.936842,-2.223752,1.383292\H,0,7.849395,-0.88728,0.490162\S,0,-1.28189,-1.124406,-0.021563\O,0,-0.924956,-1.475682,1.354204\O,0,-1.144786,-2.060643,-1.138593\C,0,-2.984083,-0.548432,-0.005026\C,0,-3.536974,-0.048798,1.175725\C,0,-3.732664,-0.584446,-1.184602\C,0,-4.847658,0.426715,1.16583\H,0,-2.953862,-0.055827,2.090512\C,0,-5.040419,-0.106303,-1.175272\H,0,-3.298747,-1.002338,-2.087284\C,0,-5.618699,0.406634,-0.004212\H,0,-5.280912,0.81269,2.085319\H,0,-5.626019,-0.138607,-2.090933\C,0,-7.048809,0.891341,0.000837\H,0,-7.745313,0.056452,0.153841\H,0,-7.224865,1.614504,0.803413\H,0,-7.315183,1.364858,-0.950012\H,0,-0.433011,0.412532,-1.423045\H,0,2.185142,-0.132734,-0.761943\Version=ES64L-G16RevA.03\State=1-A\HF=-1278.1093118\MP2=-1279.3083215\RMSD=2.846e-09\PG=C01[X(C16H20N2O2S1)]\

L3-Nrad

GINC-SL250S-GEN8-09-01\SP\ROB2PLYP-FC\GTMP2large\C16H19N2O2S1(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\neka\0,2\C,0,-0.814918,-2.210623,1.586671\C,0,0.483087,-1.726317,0.913172\C,0,-2.751208,-1.227183,0.173563\C,0,-1.980328,-1.208317,1.51075\H,0,0.811657,-0.775497,1.356713\H,0,1.282179,-2.45974,1.122381\H,0,-1.107433,-3.173973,1.15107\H,0,-0.564792,-2.400037,2.638675\H,0,-3.229399,-2.208922,0.057512\H,0,-1.601581,-0.193757,1.697332\H,0,-2.685285,-1.420851,2.324954\N,0,0.355617,-1.678648,-0.529103\C,0,-3.791273,-0.133655,0.090976\C,0,-5.099072,-0.330717,0.553693\C,0,-3.484459,1.131322,-0.425043\N,0,-6.060237,0.599954,0.542016\H,0,-5.387905,-1.304654,0.951699\C,0,-4.47217,2.114192,-0.448401\H,0,-2.486025,1.331448,-0.807645\C,0,-5.738665,1.801776,0.04732\H,0,-4.268029,3.103522,-0.848351\H,0,-6.53333,2.546631,0.044066\S,0,1.04759,-0.364113,-1.352806\O,0,0.056848,0.717292,-1.205983\O,0,1.429766,-0.873951,-2.668854\C,0,2.544824,0.138948,-0.505971\C,0,2.516575,1.223322,0.373323\C,0,3.730579,-0.561654,-0.747849\C,0,3.692147,1.60094,1.020746\H,0,1.591526,1.768799,0.527463\C,0,4.892435,-0.171659,-0.088392\H,0,3.741146,-1.384678,-1.455143\C,0,4.8937

24,0.913004,0.803069\H,0,3.676233,2.447564,1.702403\H,0,5.817473,-0.711668,-0.274608\C,0,6.169312,1.346257,1.484296\H,0,6.764124,1.992094,0.825153\H,0,5.964469,1.911644,2.398619\H,0,6.795591,0.486936,1.746192\H,0,-2.046151,-1.122729,-0.656819\\Version=ES64L-G16RevA.03\\State=2-A\\HF=-1277.4487102\\MP2=-1278.6388638\\RMSD=5.521e-09\\PG=C01[X(C16H19N2O2S1)]\\

L3-Crad

GINC-SL250S-GEN8-09-01\SP\ROB2PLYP-FC\GTMP2large\C16H19N2O2S1(2)\SSHKUNNI\13-Oct-2019\0\\#rob2plyp/gtmp2largemaxdisk=20gb\\nekaj\\
\0,2\C,0,-0.781068,-2.622024,-0.407157\C,0,0.013344,-1.760198,0.580707\C,0,-2.708094,-1.063646,-1.047889\C,0,-2.303678,-2.367545,-0.426063\H,0,-0.399493,-1.857121,1.594692\H,0,1.046519,-2.122527,0.61713\H,0,-0.366803,-2.488122,-1.414593\H,0,-0.61379,-3.670932,-0.13196\H,0,-2.693368,-2.456187,0.595756\H,0,-2.769444,-3.193789,-0.991273\N,0,0.064117,-0.353803,0.143758\C,0,-3.809321,-0.253176,-0.679533\C,0,-4.703575,-0.566908,0.389297\C,0,-4.093621,0.9531,-1.381551\N,0,-5.741159,0.179553,0.751756\H,0,-4.557549,-1.477674,0.966354\C,0,-5.171538,1.733405,-1.005192\H,0,-3.452995,1.251301,-2.208289\C,0,-5.969814,1.312455,0.067387\H,0,-5.400732,2.658359,-1.526469\H,0,-6.824326,1.903805,0.38968\N,0,1.021187,0.705569,1.058549\O,0,1.095342,0.275022,2.46152\O,0,0.531599,2.041971,0.70382\C,0,2.644737,0.459113,0.340227\C,0,3.644371,-0.152231,1.093756\C,0,2.898117,0.913548,-0.957533\C,0,4.912034,-0.318848,0.532655\H,0,3.428489,-0.481181,2.104557\C,0,4.166271,0.739544,-1.499774\H,0,2.111707,1.399368,-1.525701\C,0,5.193073,0.121947,-0.76535\H,0,5.694626,-0.795902,1.117292\H,0,4.368102,1.091182,-2.508866\C,0,6.570294,-0.039559,-1.363352\H,0,7.08477,0.927376,-1.434514\H,0,7.19539,-0.703112,-0.758254\H,0,6.519765,-0.452069,-2.377597\H,0,-2.136794,-0.747934,-1.920787\H,0,-0.858493,0.075995,0.060942\\Version=ES64L-G16RevA.03\\State=2-A\\HF=-1277.4651886\\MP2=-1278.6584117\\RMSD=2.340e-09\\PG=C01[X(C16H19N2O2S1)]\\

R-L3

GINC-SL250S-GEN8-06-03\SP\ROB2PLYP-FC\GTMP2large\C16H19N2O2S1(2)\DSAKIC\21-Apr-2019\0\\#rob2plyp/gtmp2largemaxdisk=20gb\\nekaj\\
\0,2\C,0,1.572675,2.870744,-1.338912\C,0,0.281181,3.001012,-0.50897\C,0,2.269018,0.387093,-1.136387\C,0,2.584249,1.854885,-0.780994\H,0,0.517641,3.261771,0.531278\H,0,-0.315195,3.833452,-0.918762\H,0,1.311798,2.625658,-2.376189\H,0,2.0313,3.867731,-1.353813\H,0,2.356181,0.257978,-2.223196\H,0,2.640229,1.961347,0.310661\H,0,3.584315,2.099752,-1.161675\N,0,-0.567662,1.825259,-0.640158\H,0,1.225268,0.170915,-0.882947\C,0,3.174111,-0.594923,-0.428781\C,0,4.280365,-1.165576,-1.070894\C,0,2.95812,-0.958534,0.906948\N,0,5.136284,-2.020967,-0.499165\H,0,4.482806,-0.91882,-2.114018\C,0,3.837426,-1.848195,1.520237\H,0,2.108587,-0.549423,1.449859\C,0,4.908902,-2.34857,0.778303\H,0,3.695678,-2.152376,2.553544\H,0,5.614935,-3.045782,1.227359\N,0,-1.258942,1.342976,0.834808\O,0,-2.02574,2.461469,1.401688\O,0,-0.174216,0.719396,1.615237\C,0,-2.398105,0.073045,0.313306\C,0,-3.736697,0.404836,0.103382\C,0,-1.938684,-1.232796,0.130102\C,0,-4.621633,-0.590194,-0.307202\H,0,-4.075053,1.422137,0.268089\C,0,-2.838333,-2.211963,-0.281564\H,0,-0.898342,-1.47693,0.316824\C,0,-4.189967,-1.908813,-0.505883\H,0,-5.665964,-0.338236,-0.473139\H,0,-2.486701,-3.230221,-0.427645\C,0,-5.161377,-2.987287,-0.921426\H,0,-5.541199,-3.530579,-0.046116\H,0,-6.025503,-2.568385,-1.446473\H,0,-4.685907,-3.723145,-1.578305\\Version=ES64L-G16RevA.03\\State=2-A\\HF=-1277.4533329\\MP2=-1278.6429407\\RMSD=3.622e-09\\PG=C01[X(C16H19N2O2S1)]\\

TS-L3

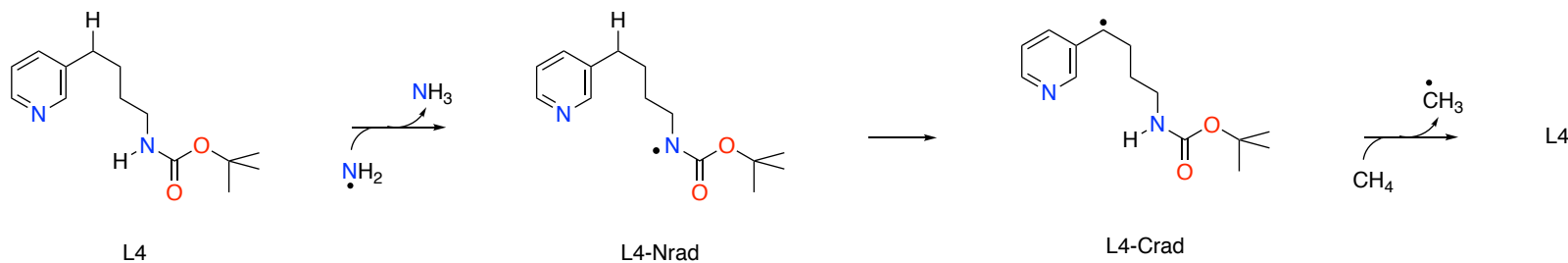
GINC-NX360-M5-01-06\SP\ROB2PLYP-FC\GTMP2large\C16H19N2O2S1(2)\DSAKIC\21-Apr-2019\0\\#rob2plyp/gtmp2largemaxdisk=20gb\\nekaj\\
\0,2\C,0,1.007354,3.186375,-0.21812\C,0,-0.136925,2.265814,0.239279\C,0,2.471728,1.223872,-0.823387\C,0,2.368894,2.506439,-0.002613\H,0,-0.062817,2.091186,1.320675\H,0,-1.102331,2.752001,0.037892\H,0,0.876252,3.435451,-1.278962\H,0,0.951727,4.124522,0.345584\H,0,2.567336,1.426787,-1.895946\H,0,2.502914,2.289382,1.064309\H,0,3.180326,3.191752,-0.287136\N,0,-0.093875,1.010972,-0.526636\H,0,1.243824,0.845284,-0.782433\C,0,3.34609,0.122275,-0.379791\C,0,4.186217,-0.530913,-1.303668\C,0,3.378028,-0.349006,0.945238\N,0,5.0164,-1.530014,-1.001956\H,0,4.187011,-0.207457,-2.344751\C,0,4.233662,-1.393515,1.273137\H,0,2.715168,0.07236,1.695793\C,0,5.033684,-1.948052,0.270714\H,0,4.272855,-1.785272,2.2851\H,0,5.711136,-2.77004,0.495622\N,0,-0.516626,-0.39626,0.334459\O,0,-0.241021,-0.256846,1.777897\O,0,0.065887,-1.508316,-0.422424\C,0,-2.295424,-0.416517,0.119246\C,0,-3.12515,-0.029152,1.171186\C,0,-2.828893,-0.823128,-1.107507\C,0,-4.507516,-0.048142,0.986135\H,0,-2.689515,0.265555,2.119953\C,0,-4.209816,-0.834554,-1.273187\H,0,-2.166541,-1.132316,-1.909168\C,0,-5.070467,-0.448941,-0.232373\H,0,-5.159022,0.248626,1.80441\H,0,-4.630238,-1.151208,-2.224741\C,0,-6.568137,-0.493556,-0.419479\H,

0,-6.944264,-1.521581,-0.334958\H,0,-7.08528,0.108428,0.334072\H,0,-6.859097,-0.124511,-1.409162\\Version=ES64L-G16RevA.03\State=2-A\HF=-1277.419411\MP2=-1278.6255813\RMSD=1.334e-09\PG=C01[X(C16H19N2O2S1)]\\

P-L3

GINC-SL230S-GEN8-02-06\SP\ROB2PLYP-FC\GTMP2large\C16H19N2O2S1(2)\DSAKIC\21-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\\nekaj\0,2\C,0,-1.817078,2.98301,-0.279873\C,0,-0.67003,2.509962,-1.187121\C,0,-2.75102,0.74057,0.517288\C,0,-3.026109,2.025999,-0.203354\H,0,-1.05246,2.282672,-2.190304\H,0,0.070539,3.305785,-1.29425\H,0,-1.430206,3.17655,0.728044\H,0,-2.165052,3.948935,-0.669742\H,0,-2.124075,0.808178,1.404866\H,0,-3.402987,1.839216,-1.218115\H,0,-3.838462,2.561618,0.31822\N,0,0.065818,1.303439,-0.757626\H,0,-0.552875,0.507898,-0.595312\C,0,-3.268766,-0.53517,0.193783\C,0,-2.910325,-1.663298,0.99855\C,0,-4.14138,-0.813818,-0.896069\N,0,-3.321079,-2.906657,0.795993\H,0,-2.24485,-1.505219,1.847933\C,0,-4.573859,-2.113181,-1.10916\H,0,-4.472493,-0.014533,-1.5523\C,0,-4.143557,-3.128602,-0.246714\H,0,-5.241855,-2.347515,-1.933425\H,0,-4.468285,-4.156767,-0.392142\S,0,1.106485,1.464071,0.5737\O,0,0.434599,1.046606,1.816367\O,0,1.697756,2.802418,0.463983\C,0,2.352259,0.231741,0.203999\C,0,2.417197,-0.929968,0.969857\C,0,3.26261,0.464697,-0.831245\C,0,3.402485,-1.876531,0.683475\H,0,1.710593,-1.082398,1.778374\C,0,4.237469,-0.488747,-1.10089\H,0,3.205773,1.380889,-1.409693\C,0,4.323733,-1.673572,-0.350078\H,0,3.455122,-2.785579,1.277156\H,0,4.947288,-0.312907,-1.90574\C,0,5.40026,-2.690044,-0.646783\H,0,5.449416,-2.918243,-1.717756\H,0,6.388713,-2.314979,-0.351886\H,0,5.227055,-3.62668,-0.108495\\Version=ES64L-G16RevA.03\State=2-A\HF=-1277.4651594\MP2=-1278.6593405\RMSD=1.946e-09\PG=C01[X(C16H19N2O2S1)]\\

System L4



NAME	SYSTEM	H(kJ/mol)			Δ H(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.789551	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.454472	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.835797	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.504482	-	-	-
L4	Loeffler_R1Boc_TS_Ndown_eqNMe_eqC5Py_neutL3	-806.359648	-805.930328				
L4-Nrad	Loeffler_R1Boc_TS_Ndown_eqNMe_eqC5Py_NradL3	-805.701761	-805.265828		-4.88	-1.96	
L4-Crad	Loeffler_R1Boc_TS_Ndown_eqNMe_eqC5Py_CradL3	-805.723610	-805.293343		-75.94	-63.51	
R-L4	Loeffler_R1Boc_TS_Ndown_axNMe_axC5Py_rad_opt_fwd	-805.702606	-805.26555	-	0.00	0.00	
	Loeffler_R1Boc_TS_Ndown_eqNMe_eqC5Py_rad_opt_rev	-805.70161	-805.264878		2.61	1.76	
TS-L4	Loeffler_R1Boc_TS_Ndown_eqNMe_eqC5Py_rad	-805.692121	-805.258487	-	27.53	18.54	
	Loeffler_R1Boc_TS_Ndown_axNMe_axC5Py_rad	-805.690469	-805.257061		31.87	22.29	
P-L4	Loeffler_R1Boc_TS_Ndown_eqNMe_eqC5Py_rad_opt_fwd	-805.726954	-805.297131	-	-63.93	-82.92	
	Loeffler_R1Boc_TS_Ndown_axNMe_axC5Py_rad_opt_rev	-805.726222	-805.295954		-62.00	-79.83	

NAME	SYSTEM	H(kJ/mol)				ΔH (kJ/mol)	
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
	Loeffler_R1Boc_TS_Ndown_eqNMe_axC5Py_rad_opt_rev	-805.726382	-805.295246		-62.42	-77.97	
	Loeffler_R1Boc_TS_Ndown_axNMe_eqC5Py_rad_opt_rev	-805.725145	-805.293455		-59.18	-73.26	
	Loeffler_R1Boc_TS_Ndown_axNMe_eqC5Py_rad_opt_fwd	-805.725145	-805.293455		-59.18	-73.26	
L4-Crad	Loeffler_R1Boc_TS_Ndown_eqNMe_eqC5Py_CradL3	-805.723610	-805.293343		-55.15	-72.97	

L4

GINC-SL230S-GEN8-02-02\SP\ROB2PLYP-FC\GTMP2large\C14H22N2O2\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \O,1\C,0,0.528815,3.331607,-0.047472\C,0,-0.903164,3.046992,0.437773\C,0,1.605843,1.086827,-0.793003\C,0,1.556776,2.223774,0.250498\H,0,-0.88498,2.767
 331,1.495019\H,0,-1.501597,3.962804,0.350287\H,0,0.517999,3.562917,-1.122497\H,0,0.846314,4.254562,0.457063\H,0,1.955826,1.494692,-1.75071\H,0,1.3455
 08,1.797248,1.239045\H,0,2.558685,2.667552,0.316013\N,0,-1.611816,1.98368,-0.262293\C,0,2.504767,-0.051275,-0.366896\C,0,3.758679,-0.260428,-0.953338
 \C,0,2.126438,-0.934409,0.653055\N,0,4.609167,-1.235335,-0.608661\H,0,4.094093,0.399457,-1.754537\C,0,2.996319,-1.955643,1.026811\H,0,1.1609,-0.814337
 ,1.140487\C,0,4.223003,-2.063695,0.368332\H,0,2.731313,-2.658218,1.812052\H,0,4.92657,-2.850998,0.635751\C,0,-1.815664,0.744042,0.271071\O,0,-1.33889
 3,0.356347,1.329239\O,0,-2.609941,0.02812,-0.564742\C,0,-3.041106,-1.338095,-0.23021\C,0,-1.828903,-2.269419,-0.12675\C,0,-3.872585,-1.323152,1.056932\
 C,0,-3.90956,-1.713516,-1.434176\H,0,-1.216757,-2.201824,-1.032769\H,0,-1.211602,-2.01712,0.736352\H,0,-2.169758,-3.305945,-0.024382\H,0,-4.713466,-0.62
 753,0.95924\H,0,-4.279189,-2.323278,1.244823\H,0,-3.264086,-1.025038,1.912324\H,0,-4.30986,-2.724961,-1.308761\H,0,-4.749337,-1.018544,-1.536849\H,0,-3
 .322927,-1.685276,-2.358241\H,0,-2.077344,2.184974,-1.135497\H,0,0.594959,0.705706,-0.969271\\Version=ES64L-G16RevA.03\State=1-
 A\HF=-805.2601287\MP2=-806.2991452\RMSD=4.288e-09\PG=C01[X(C14H22N2O2)]\\

L4-Nrad

GINC-SL230S-GEN8-02-04\SP\ROB2PLYP-FC\GTMP2large\C14H21N2O2(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \O,2\C,0,-0.658462,2.845515,-0.265245\C,0,0.712467,2.263669,-0.617136\C,0,-1.96542,0.743957,0.53134\C,0,-1.853203,1.901444,-0.484747\H,0,0.696644,1.836
 348,-1.637459\H,0,1.478271,3.056027,-0.648771\H,0,-0.637616,3.192452,0.776104\H,0,-0.802195,3.737344,-0.889683\H,0,-2.024663,1.167961,1.542282\H,0,-1.
 807517,1.487327,-1.50278\H,0,-2.778582,2.490779,-0.443012\N,0,1.163693,1.258341,0.317704\C,0,-3.170996,-0.130778,0.27485\C,0,-4.408305,0.139215,0.876
 751\C,0,-3.122097,-1.227438,-0.592818\N,0,-5.526265,-0.566557,0.674439\H,0,-4.495521,0.976049,1.570901\C,0,-4.274159,-1.978132,-0.818746\H,0,-2.186321,
 -1.492538,-1.081044\C,0,-5.449348,-1.60666,-0.164819\H,0,-4.263231,-2.837004,-1.483924\H,0,-6.368983,-2.169767,-0.316794\C,0,2.484889,0.836794,0.15029
 6\O,0,3.42468,1.61525,0.117054\O,0,2.538251,-0.500529,0.131669\C,0,3.829354,-1.221247,0.058925\C,0,4.557835,-0.858642,-1.238797\C,0,4.662195,-0.90858
 4,1.305556\C,0,3.387619,-2.685945,0.047718\H,0,3.911557,-1.043568,-2.103966\H,0,4.864663,0.188705,-1.242566\H,0,5.450415,-1.485415,-1.343379\H,0,4.089
 921,-1.133299,2.211966\H,0,5.563022,-1.532508,1.308441\H,0,4.962945,0.140213,1.327477\H,0,4.263692,-3.341108,-0.00009\H,0,2.822755,-2.926095,0.95393\
 H,0,2.752426,-2.89247,-0.819702\H,0,-1.051349,0.141304,0.508515\\Version=ES64L-G16RevA.03\State=2-
 A\HF=-804.5932492\MP2=-805.6197635\RMSD=2.660e-09\PG=C01[X(C14H21N2O2)]\\

L4-Crad

GINC-SL230S-GEN8-02-03\SP\ROB2PLYP-FC\GTMP2large\C14H21N2O2(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,0.590242,3.271602,-0.633415\C,0,1.887822,2.508627,-0.320876\C,0,-1.274246,1.717176,0.180196\C,0,-0.619205,2.388655,-0.98861\H,0,2.145637,1.85
2761,-1.15439\H,0,2.707395,3.232576,-0.213325\H,0,0.333228,3.925736,0.212114\H,0,0.804032,3.938485,-1.479301\H,0,-1.094249,2.134884,1.168238\H,0,-0.3
11094,1.641793,-1.735136\H,0,-1.362793,3.022411,-1.50385\N,0,1.835847,1.685063,0.877748\C,0,-2.166254,0.624705,0.095781\C,0,-2.754647,0.087158,1.2820
07\C,0,-2.550271,-0.007205,-1.119983\N,0,-3.605886,-0.927644,1.318828\H,0,-2.492918,0.532184,2.242591\C,0,-3.438992,-1.071416,-1.085073\H,0,-2.155497,0
.345565,-2.068219\C,0,-3.943314,-1.500477,0.147961\H,0,-3.747485,-1.567906,-2.001076\H,0,-4.643566,-2.331354,0.203963\C,0,1.860909,0.317999,0.97005\O,
0,1.884964,-0.266646,2.041445\O,0,1.853018,-0.255946,-0.257046\C,0,1.941679,-1.718875,-0.405363\C,0,3.264777,-2.223256,0.180703\C,0,0.725763,-2.39334,
0.237854\C,0,1.919199,-1.898385,-1.925772\H,0,4.10997,-1.694924,-0.274817\H,0,3.294621,-2.074898,1.261143\H,0,3.377582,-3.292249,-0.03255\H,0,-0.20208
9,-1.984556,-0.175718\H,0,0.749692,-3.468339,0.024904\H,0,0.724042,-2.247733,1.318712\H,0,1.983507,-2.961631,-2.179705\H,0,0.991416,-1.498365,-2.34808
\H,0,2.764202,-1.379865,-2.391081\H,0,1.850019,2.136412,1.78159\Version=ES64L-G16RevA.03\State=2-
A\HF=-804.6147156\MP2=-805.6478958\RMSD=1.437e-09\PG=C01[X(C14H21N2O2)]\

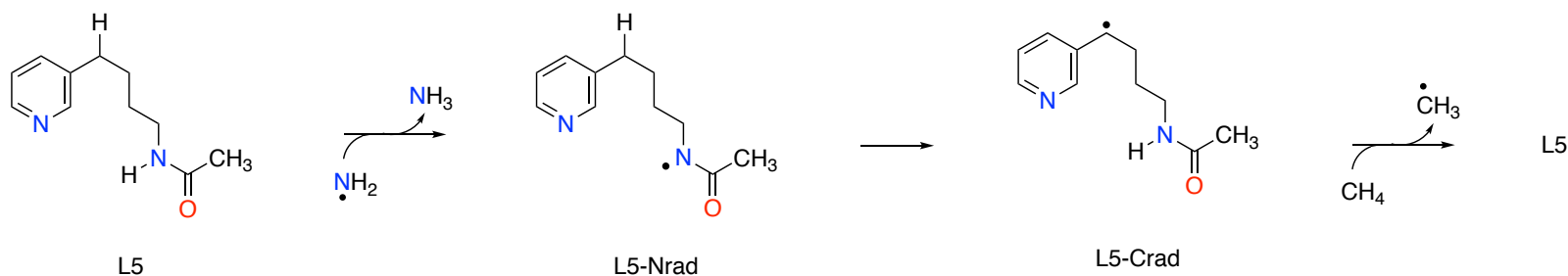
R-L4
GINC-NX360-M5-03-10\SP\ROB2PLYP-FC\GTMP2large\C14H21N2O2(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,0.135091,2.887424,0.296703\C,0,-1.211685,2.385655,0.89529\C,0,-2.402097,2.339389,-0.074142\C,0,-2.388264,1.206503,-1.124937\H,0,0.817179,3.13
8592,1.118544\H,0,-1.05752,1.407045,1.366104\H,0,-1.451427,3.085275,1.70594\H,0,-3.320661,2.252181,0.522647\H,0,-2.470809,3.302,-0.599402\H,0,-3.22667
1,1.374452,-1.814374\H,0,-0.069853,3.795245,-0.285867\N,0,0.737128,1.918277,-0.588772\H,0,-1.469474,1.275445,-1.717271\C,0,-2.501004,-0.181182,-0.5312
11\C,0,-1.400794,-1.04862,-0.512837\C,0,-3.690008,-0.659365,0.033102\N,0,-1.410349,-2.280039,0.016321\H,0,-0.45673,-0.725389,-0.943485\C,0,-3.723677,-1.
93963,0.581328\H,0,-4.582895,-0.036866,0.038034\C,0,-2.558711,-2.708568,0.552976\H,0,-4.633458,-2.338223,1.021319\H,0,-2.548079,-3.711753,0.976596\C,
0,1.815845,1.209112,-0.052397\O,0,2.674795,1.726371,0.647801\O,0,1.799812,-0.052749,-0.500911\C,0,2.805355,-1.050351,-0.064129\C,0,4.190673,-0.627015
,-0.561061\C,0,2.747646,-1.208968,1.458196\C,0,2.332667,-2.327779,-0.761698\H,0,4.175295,-0.473787,-1.645507\H,0,4.521516,0.293838,-0.077808\H,0,4.913
785,-1.420327,-0.340471\H,0,1.730133,-1.463724,1.773272\H,0,3.410894,-2.026267,1.762318\H,0,3.065011,-0.297354,1.968405\H,0,3.012574,-3.152188,-0.520
861\H,0,1.322701,-2.601615,-0.438796\H,0,2.327964,-2.192861,-1.848394\Version=ES64L-G16RevA.03\State=2-
A\HF=-804.5904404\MP2=-805.6204522\RMSD=4.084e-09\PG=C01[X(C14H21N2O2)]\

TS-L4
GINC-NX360-M5-01-06\SP\ROB2PLYP-FC\GTMP2large\C14H21N2O2(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,0.911305,3.610737,-0.140279\C,0,-0.50719,3.129174,0.20686\C,0,1.672343,1.273984,-0.701029\C,0,1.953773,2.514244,0.143759\H,0,-0.611845,2.9643
59,1.288651\H,0,-1.23116,3.909431,-0.068052\H,0,0.950159,3.892452,-1.200557\H,0,1.135467,4.511037,0.442725\H,0,1.925638,1.433037,-1.755563\H,0,1.9290
95,2.271557,1.213264\H,0,2.964376,2.89173,-0.066148\N,0,-0.817563,1.92831,-0.558594\H,0,0.423524,1.321766,-0.779111\C,0,2.072647,-0.072869,-0.238232\
C,0,2.389748,-1.069751,-1.184192\C,0,2.112701,-0.461843,1.111815\N,0,2.721433,-2.326962,-0.888152\H,0,2.372385,-0.819233,-2.245016\C,0,2.461411,-1.768
815,1.438882\H,0,1.871618,0.246432,1.899191\C,0,2.754963,-2.664417,0.408657\H,0,2.504389,-2.091702,2.475069\H,0,3.027113,-3.694887,0.630105\C,0,-1.67
4074,1.018528,0.033769\O,0,-2.489048,1.311521,0.899305\O,0,-1.511443,-0.196357,-0.53218\C,0,-2.325168,-1.350877,-0.118861\C,0,-2.083038,-1.661114,1.36
2554\C,0,-3.803167,-1.084189,-0.423842\C,0,-1.78074,-2.474321,-1.00519\H,0,-1.012548,-1.800505,1.549759\H,0,-2.454084,-0.856257,1.999689\H,0,-2.599556,
-2.589096,1.632785\H,0,-3.93076,-0.819948,-1.479283\H,0,-4.388116,-1.989794,-0.226694\H,0,-4.192052,-0.272505,0.19305\H,0,-2.30831,-3.410202,-0.792362\
H,0,-1.919651,-2.230994,-2.063489\H,0,-0.711925,-2.628252,-0.825814\Version=ES64L-G16RevA.03\State=2-
A\HF=-804.5634207\MP2=-805.6075476\RMSD=3.881e-09\PG=C01[X(C14H21N2O2)]\

P-L4

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C14H21N2O2(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,1.132432,3.482822,-0.262471\C,0,-0.350278,3.299045,0.095489\C,0,2.008336,1.123865,-0.693899\C,0,2.051525,2.330478,0.191295\H,0,-0.460066,3.17
7024,1.17632\H,0,-0.905048,4.202526,-0.192132\H,0,1.240013,3.63485,-1.34625\H,0,1.466161,4.416123,0.210418\H,0,1.913604,1.308435,-1.76359\H,0,1.80938
8,2.065437,1.227774\H,0,3.085947,2.716907,0.214258\N,0,-0.986847,2.142124,-0.507565\H,0,-1.208827,2.141185,-1.492486\C,0,2.165109,-0.221584,-0.293799
\C,0,2.163055,-1.257766,-1.278779\C,0,2.334713,-0.656473,1.050522\N,0,2.303753,-2.552002,-1.02868\H,0,2.03637,-0.981141,-2.326481\C,0,2.485861,-2.0082
73,1.316053\H,0,2.340144,0.063275,1.862662\C,0,2.466091,-2.922261,0.255926\H,0,2.61666,-2.361263,2.33525\H,0,2.582124,-3.988742,0.4375\C,0,-1.373583,1
.048614,0.218081\O,0,-1.179481,0.912093,1.416502\O,0,-1.997561,0.171393,-0.605887\C,0,-2.574887,-1.080879,-0.090837\C,0,-1.474441,-1.97572,0.486985\C,
0,-3.668606,-0.767049,0.936015\C,0,-3.177875,-1.708559,-1.350569\H,0,-0.694462,-2.156568,-0.259671\H,0,-1.019945,-1.518999,1.367083\H,0,-1.903119,-2.94
3452,0.772274\H,0,-4.417751,-0.095262,0.501937\H,0,-4.173744,-1.693911,1.2306\H,0,-3.246515,-0.298289,1.826367\H,0,-3.6508,-2.665089,-1.104466\H,0,-3.9
35395,-1.049595,-1.787808\H,0,-2.401473,-1.889764,-2.100837\\Version=ES64L-G16RevA.03\State=2-
A\HF=-804.6180543\MP2=-805.6517132\RMSD=5.099e-09\PG=C01[X(C14H21N2O2)]\\

System L5



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.78955	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.45447 -	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.83579	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.50448 -	-	-	-
L5	Loeffler_R1acetyl_TS_Ndown_eqNMe_eqC5Py_neutL4	-613.278185	-612.947571				
L5-Nrad	Loeffler_R1acetyl_TS_Ndown_eqNMe_eqC5Py_NradL4	-612.620196	-612.281581		-4.61	1.96	
L5-Crad	Loeffler_R1acetyl_TS_Ndown_eqNMe_eqC5Py_CradL4	-612.646514	-612.315028		-87.40	-75.17	
R-L5	Loeffler_R1acetyl_TS_Ndown_eqNMe_axC5Py_rad_opt_rev	-612.620643	-612.281806	-	0.00	0.00	
	Loeffler_R1acetyl_TS_Ndown_eqNMe_eqC5Py_rad_opt_fwd	-612.620195	-612.281581		1.18	0.59	
	Loeffler_R1acetyl_TS_Ndown_axNMe_eqC5Py_rad_opt_rev	-612.620501	-612.281354		0.37	1.19	
	Loeffler_R1acetyl_TS_Ndown_axNMe_axC5Py_ver1_rad_opt_rev	-612.619555	-612.280927		2.86	2.31	
TS-L5	Loeffler_R1acetyl_TS_Ndown_eqNMe_eqC5Py_rad	-612.610971	-612.275640	-	25.39	16.19	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
	Loeffler_R1acetyl_TS_Ndown_eqNMe_axC5Py_rad	-612.608787	-612.273502		31.13	21.80	
	Loeffler_R1acetyl_TS_Ndown_axNMe_axC5Py_ver1_rad	-612.608059	-612.272967		33.04	23.21	
	Loeffler_R1acetyl_TS_Ndown_axNMe_axC5Py_rad	-612.608059	-612.272967		33.04	23.21	
P-L5	Loeffler_R1acetyl_TS_Ndown_eqNMe_eqC5Py_rad_opt_rev	-612.646514	-612.315027	-	-67.92	-87.22	
	Loeffler_R1acetyl_TS_Ndown_eqNMe_axC5Py_rad_opt_fwd	-612.645661	-612.313691		-65.68	-83.71	
	Loeffler_R1acetyl_TS_Ndown_axNMe_axC5Py_rad_opt_fwd	-612.644699	-612.313100		-63.16	-82.16	
	Loeffler_R1acetyl_TS_Ndown_axNMe_axC5Py_ver1_rad_opt_fw d	-612.644699	-612.313099		-63.16	-82.16	
L5-Crad	Loeffler_R1acetyl_TS_Ndown_eqNMe_eqC5Py_CradL4	-612.646514	-612.315028		-67.92	-87.22	

L5

GINC-SL250S-GEN8-06-01\SP\ROB2PLYP-FC\GTMP2large\C11H16N2O1\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\

\0,1\C,0,1.538328,-2.242025,0.178201\C,0,2.684828,-1.338813,0.673635\C,0,-0.256456,-0.451357,-0.438739\C,0,0.111629,-1.705357,0.381402\H,0,2.404773,-0.831544,1.60077\H,0,3.564022,-1.960165,0.888329\H,0,1.701715,-2.48561,-0.882043\H,0,1.617939,-3.193846,0.720788\H,0,-0.076405,-0.652832,-1.503658\H,0,-0.040448,-1.487911,1.447681\H,0,-0.596679,-2.50696,0.132095\N,0,3.09147,-0.290965,-0.256537\C,0,-1.696395,-0.03831,-0.234887\C,0,-2.729273,-0.56334,-1.023609\C,0,-2.066214,0.864512,0.76833\N,0,-4.025779,-0.267709,-0.878881\H,0,-2.489791,-1.261681,-1.826917\C,0,-3.411385,1.186968,0.937834\H,0,-1.302676,1.312257,1.401145\C,0,-4.350414,0.594201,0.093045\H,0,-3.727792,1.88759,1.705456\H,0,-5.410095,0.823266,0.196336\C,0,2.919182,1.043232,-0.015548\O,0,2.325881,1.470878,0.970194\C,0,3.492794,1.979487,-1.069789\H,0,2.674712,2.557212,-1.511703\H,0,4.164096,2.690247,-0.578793\H,0,4.037894,1.46882,-1.870139\H,0,0.394481,0.377305,-0.146564\H,0,3.597634,-0.567644,-1.085656\Version=ES64L-G16RevA.03\State=1-A\HF=-612.4274933\MP2=-613.2218598\RMSD=4.658e-09\PG=C01[X(C11H16N2O1)]\

L5-Nrad

GINC-SL250S-GEN8-05-01\SP\ROB2PLYP-FC\GTMP2large\C11H15N2O1(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\

\0,2\C,0,1.435924,2.24837,-0.157965\C,0,2.601533,1.292444,-0.45977\C,0,-0.426725,0.591327,0.552803\C,0,0.036308,1.678241,-0.438246\H,0,2.562648,0.912831,-1.491506\H,0,3.539694,1.869951,-0.385495\H,0,1.507682,2.577303,0.886586\H,0,1.57941,3.139334,-0.782302\H,0,-0.406352,1.004288,1.569268\H,0,0.002729,1.277362,-1.461478\H,0,-0.689737,2.501465,-0.413647\N,0,2.720114,0.235843,0.516517\C,0,-1.810995,0.068843,0.243215\C,0,-2.941058,0.570321,0.903677\C,0,-2.035424,-0.911569,-0.730034\N,0,-4.198652,0.182615,0.664539\H,0,-2.817738,1.328905,1.677478\C,0,-3.336947,-1.331287,-0.995437\H,0,-1.196478,-1.344737,-1.271446\C,0,-4.382646,-0.753494,-0.273955\H,0,-3.539653,-2.093283,-1.742592\H,0,-5.412785,-1.05704,-0.45384\C,0,3.332596,-0.939498,0.102687\O,0,4.167828,-0.940593,-0.801112\C,0,2.99971,-2.163385,0.926051\H,0,3.438085,-3.048977,0.462127\H,0,3.398901,-2.046667,1.939966\H,0,1.915164,-2.288721,1.020566\H,0,0.291928,-0.238335,0.549665\Version=ES64L-G16RevA.03\State=2-A\HF=-611.7575213\MP2=-612.5407901\RMSD=4.983e-09\PG=C01[X(C11H15N2O1)]\

L5-Crad

GINC-SL250S-GEN8-04-05\SP\ROB2PLYP-FC\GTMP2large\C11H15N2O1(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-2.565528,-1.709097,0.010945\C,0,-3.094267,-0.266378,0.037413\C,0,-0.027298,-1.653064,0.301467\C,0,-1.170934,-1.870528,-0.640338\H,0,-3.200521,
,0.108486,-0.983688\H,0,-4.087594,-0.250857,0.504607\H,0,-2.546268,-2.123171,1.02929\H,0,-3.298179,-2.307493,-0.546704\H,0,-0.085371,-2.189549,1.24932
6\H,0,-1.102014,-1.214374,-1.514221\H,0,-1.103096,-2.90193,-1.02671\N,0,-2.239555,0.691519,0.722198\C,0,1.158212,-0.920284,0.067508\C,0,2.197498,-0.934
465,1.050109\C,0,1.423128,-0.138412,-1.092876\N,0,3.354147,-0.294885,0.951556\H,0,2.046012,-1.516244,1.960767\C,0,2.632458,0.531242,-1.198584\H,0,0.6
75911,-0.040973,-1.872585\C,0,3.569964,0.427809,-0.163812\H,0,2.852535,1.137484,-2.072846\H,0,4.52625,0.943338,-0.224604\C,0,-1.459203,1.594069,0.050
977\O,0,-1.432667,1.663588,-1.174235\C,0,-0.61248,2.505381,0.924553\H,0,0.441262,2.239889,0.791116\H,0,-0.739165,3.535667,0.580999\H,0,-0.85821,2.449
352,1.989894\H,0,-2.171656,0.647593,1.72879\\Version=ES64L-G16RevA.03\State=2-
A\HF=-611.7857879\MP2=-612.5752561\RMSD=2.549e-09\PG=C01[X(C11H15N2O1)]\\

R-L5

GINC-NX360-M5-02-09\SP\ROB2PLYP-FC\GTMP2large\C11H15N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,0.682902,-1.801496,-0.944147\C,0,2.073836,-1.146456,-0.900806\C,0,-0.451844,-0.818403,1.194651\C,0,0.048164,-2.065835,0.430654\H,0,2.783354,-1
.732913,-0.29923\H,0,2.476458,-1.145239,-1.929154\H,0,0.014411,-1.191783,-1.562952\H,0,0.800576,-2.762068,-1.461368\H,0,0.774205,-2.595285,1.063904\H,
0,-0.798784,-2.751366,0.295923\N,0,2.031126,0.240783,-0.501729\H,0,0.375059,-0.107487,1.314859\H,0,-0.741022,-1.133706,2.205384\C,0,-1.6236,-0.119888,
0.539949\C,0,-2.938885,-0.528138,0.805576\C,0,-1.46177,0.941198,-0.358822\N,0,-4.031563,0.015706,0.259905\H,0,-3.116991,-1.342103,1.509858\C,0,-2.5885
8,1.523387,-0.938039\H,0,-0.462344,1.296387,-0.598006\C,0,-3.846936,1.025671,-0.599912\H,0,-2.494747,2.34968,-1.63714\H,0,-4.748106,1.456716,-1.033475
\C,0,3.174721,0.760601,0.093617\O,0,4.287664,0.300802,-0.156773\C,0,2.957243,1.989442,0.94727\H,0,3.889954,2.259048,1.446154\H,0,2.624815,2.824,0.319
525\H,0,2.173416,1.813791,1.692724\\Version=ES64L-G16RevA.03\State=2-A\HF=-611.7569117\MP2=-612.54124\RMSD=6.518e-09\PG=C01[X(C11H15N2O1)]\\

TS-L5

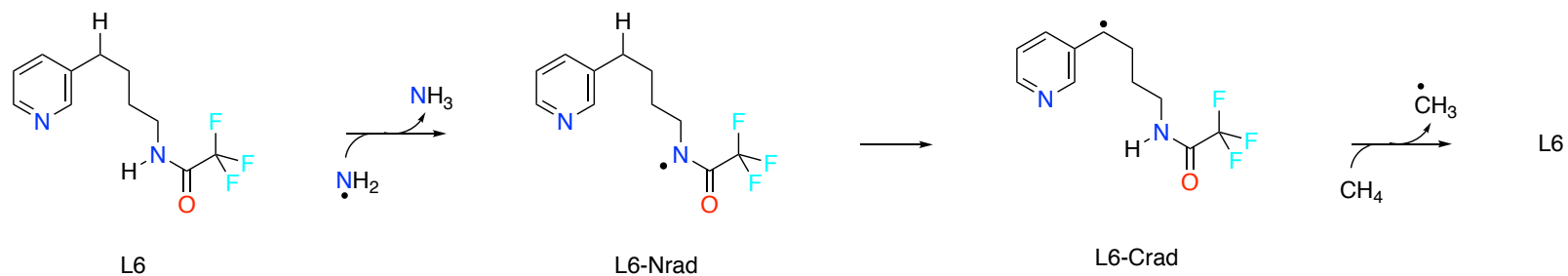
GINC-SL230S-GEN8-02-07\SP\ROB2PLYP-FC\GTMP2large\C11H15N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,2.169021,-2.172664,-0.018397\C,0,2.791922,-0.795331,0.258167\C,0,-0.058975,-1.164239,-0.625366\C,0,0.658816,-2.16771,0.274466\H,0,2.762162,-0.
556555,1.330833\H,0,3.851684,-0.810658,-0.032156\H,0,2.340336,-2.448099,-1.067292\H,0,2.674339,-2.92327,0.599612\H,0,-0.092991,-1.505801,-1.666428\H,
0,0.500079,-1.922111,1.331977\H,0,0.239892,-3.172414,0.121891\N,0,2.116619,0.226643,-0.533479\H,0,0.82828,-0.275176,-0.720689\C,0,-1.34312,-0.56,-0.205
572\C,0,-2.33943,-0.28783,-1.165979\C,0,-1.636778,-0.18916,1.11892\N,0,-3.519713,0.27506,-0.903696\H,0,-2.160898,-0.556216,-2.207567\C,0,-2.863567,0.39
8174,1.409351\H,0,-0.912336,-0.35368,1.911665\C,0,-3.770892,0.610399,0.368817\H,0,-3.11474,0.692266,2.424195\H,0,-4.738017,1.070931,0.562208\C,0,2.12
6851,1.521456,-0.053033\O,0,2.943715,1.886853,0.790805\C,0,1.155797,2.475619,-0.722306\H,0,1.169298,3.431042,-0.194881\H,0,1.450683,2.636629,-1.7653
83\H,0,0.136287,2.074081,-0.728613\\Version=ES64L-G16RevA.03\State=2-A\HF=-611.7309853\MP2=-612.5299814\RMSD=5.508e-09\PG=C01[X(C11H15N2O1)]\\
\

P-L5

GINC-SL230S-GEN8-02-02\SP\ROB2PLYP-FC\GTMP2large\C11H15N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,2.565354,-1.70921,-0.011082\C,0,3.094245,-0.266538,-0.037097\C,0,0.02709,-1.653141,-0.301717\C,0,1.170709,-1.870843,0.640049\H,0,3.200273,0.10
8103,0.984112\H,0,4.087712,-0.251067,-0.503995\H,0,2.546168,-2.122989,-1.029552\H,0,3.297937,-2.307817,0.546436\H,0,0.085105,-2.189492,-1.249653\H,0,1
.101721,-1.214961,1.514131\H,0,1.102877,-2.902363,1.026117\N,0,2.239895,0.691621,-0.721965\H,0,2.172633,0.648176,-1.728619\C,0,-1.158342,-0.920272,-0.
067649\C,0,-2.197609,-0.934181,-1.050276\C,0,-1.423205,-0.138583,1.09286\N,0,-3.354199,-0.294512,-0.951643\H,0,-2.04616,-1.515824,-1.961029\C,0,-2.6324
84,0.531158,1.198663\H,0,-0.676012,-0.041366,1.872619\C,0,-3.56997,0.428006,0.163856\H,0,-2.852528,1.137242,2.073045\H,0,-4.526212,0.943613,0.22471\C

,0,1.459355,1.59407,-0.050805\O,0,1.432309,1.663219,1.174418\C,0,0.613136,2.505718,-0.924521\H,0,-0.440703,2.240342,-0.791629\H,0,0.739824,3.535917,-0.580702\H,0,0.859349,2.449866,-1.989762\\Version=ES64L-G16RevA.03\State=2-A\HF=-611.7857884\MP2=-612.5752552\RMSD=2.540e-09\PG=C01[X(C11H15N2O1)]\\

System L6



NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.78955	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.45447	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.83579	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.50448	-	-	-
L6	Loeffler_R1COCF3_TS_Ndown_eqNMe_eqC5Py_neutL5	-911.010463	-910.656441				
L6-Nrad	Loeffler_R1COCF3_TS_Ndown_eqNMe_eqC5Py_NradL5	-910.348188	-909.985333		6.64	15.39	
L6-Crad	Loeffler_R1COCF3_TS_Ndown_eqNMe_eqC5Py_CradL5	-910.377001	-910.023338		-82.70	-73.70	
R-L6	Loeffler_R1COCF3_TS_Ndown_eqNMe_axC5Py_rad_opt_rev	-910.347874	-909.985345	-	0.00	0.00	
	Loeffler_R1COCF3_TS_Ndown_eqNMe_eqC5Py_rad_opt_rev	-910.348189	-909.985334		-0.83	0.03	
	Loeffler_R1COCF3_TS_Ndown_axNMe_eqC5Py_rad_opt_rev	-910.346301	-909.984923		4.13	1.11	
	Loeffler_R1COCF3_TS_Ndown_axNMe_axC5Py_rad_opt_fwd	-910.346771	-909.983850		2.90	3.93	
TS-L6	Loeffler_R1COCF3_TS_Ndown_eqNMe_eqC5Py_rad	-910.341277	-909.983531	-	17.32	4.76	
	Loeffler_R1COCF3_TS_Ndown_eqNMe_axC5Py_rad	-910.339616	-909.981520		21.68	10.04	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
	Loeffler_R1COCF3_TS_Ndown_axNMe_axC5Py_rad	-910.338049	-909.980671		25.80	12.27	
	Loeffler_R1COCF3_TS_Ndown_axNMe_eqC5Py_rad	-910.335853	-909.977657		31.56	20.18	
P-L6	Loeffler_R1COCF3_TS_Ndown_eqNMe_eqC5Py_rad_opt_fwd	-910.377776	-910.023167	-	-78.51	-99.30	
	Loeffler_R1COCF3_TS_Ndown_eqNMe_axC5Py_rad_opt_fwd	-910.376973	-910.022754		-76.40	-98.22	
	Loeffler_R1COCF3_TS_Ndown_axNMe_axC5Py_rad_opt_rev	-910.376174	-910.021826		-74.30	-95.78	
	Loeffler_R1COCF3_TS_Ndown_axNMe_eqC5Py_rad_opt_fwd	-910.372227	-910.016111		-63.94	-80.78	
L6-Crad	Loeffler_R1COCF3_TS_Ndown_eqNMe_eqC5Py_CradL5	-910.377001	-910.023338		-76.47	-99.75	

L6

GINC-SL250S-GEN8-08-05\SP\ROB2PLYP-FC\GTMP2large\C11H13F3N2O1\SSHKUNNI\15-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \0,1\C,0,-0.605279,2.983042,-0.001071\C,0,-1.925675,2.401689,0.53094\C,0,1.005706,1.09463,-0.777052\C,0,0.652453,2.14161,0.30364\H,0,-1.854519,2.23773,
 1.609379\H,0,-2.744108,3.108343,0.352661\H,0,-0.688206,3.165414,-1.082176\H,0,-0.501921,3.972415,0.463967\H,0,1.241987,1.617871,-1.713347\H,0,0.52811
 9,1.637193,1.26939\H,0,1.514275,2.811178,0.416154\N,0,-2.313377,1.119116,-0.056469\C,0,2.170638,0.219198,-0.374458\C,0,3.476411,0.500232,-0.795336\C,
 0,1.997387,-0.89212,0.460074\N,0,4.556843,-0.211444,-0.453794\H,0,3.657982,1.350551,-1.454256\C,0,3.10912,-1.646873,0.826765\H,0,1.003196,-1.159306,0.
 811462\C,0,4.363605,-1.266077,0.347171\H,0,3.00761,-2.51653,1.469706\H,0,5.253411,-1.834243,0.614543\C,0,-2.074489,-0.06328,0.552273\O,0,-1.551674,-0.
 227617,1.643509\C,0,-2.462602,-1.300722,-0.290381\F,0,-3.229116,-0.979022,-1.364253\F,0,-1.342862,-1.888783,-0.756473\F,0,-3.132977,-2.189593,0.445998\
 H,0,-2.745809,1.104671,-0.969796\H,0,0.13807,0.460542,-0.986747\\Version=ES64L-G16RevA.03\State=1-
 A\HF=-909.8848024\MP2=-910.9098098\RMSD=5.260e-09\PG=C01[X(C11H13F3N2O1)]\\

L6-Nrad

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C11H12F3N2O1(2)\SSHKUNNI\15-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \0,2\C,0,-0.37646,2.971396,-0.05892\C,0,-1.692616,2.322914,0.412917\C,0,1.155131,1.002236,-0.727732\C,0,0.885469,2.153084,0.263358\H,0,-1.702038,2.174
 452,1.501179\H,0,-2.511834,3.024813,0.17718\H,0,-0.43679,3.170264,-1.136064\H,0,-0.317974,3.944994,0.442766\H,0,1.341522,1.433544,-1.720439\H,0,0.814
 488,1.753098,1.284614\H,0,1.753,2.825399,0.264906\N,0,-2.006025,1.113875,-0.306088\C,0,2.321487,0.133253,-0.314622\C,0,3.644987,0.53559,-0.544887\C,0,
 2.138249,-1.091002,0.336766\N,0,4.726126,-0.159988,-0.178448\H,0,3.839919,1.475033,-1.06394\C,0,3.251861,-1.833171,0.726414\H,0,1.132614,-1.461655,0.5
 21279\C,0,4.520997,-1.324433,0.4504\H,0,3.140168,-2.789452,1.229352\H,0,5.41376,-1.87606,0.740698\C,0,-2.670286,0.132413,0.377273\O,0,-3.402026,0.321
 935,1.342571\C,0,-2.568355,-1.26643,-0.268415\F,0,-1.27657,-1.568119,-0.545093\F,0,-3.045609,-2.201117,0.556617\F,0,-3.256885,-1.311188,-1.419929\H,0,0.2
 57455,0.3816,-0.830017\\Version=ES64L-G16RevA.03\State=2-A\HF=-909.2095832\MP2=-910.2237358\RMSD=3.461e-09\PG=C01[X(C11H12F3N2O1)]\\

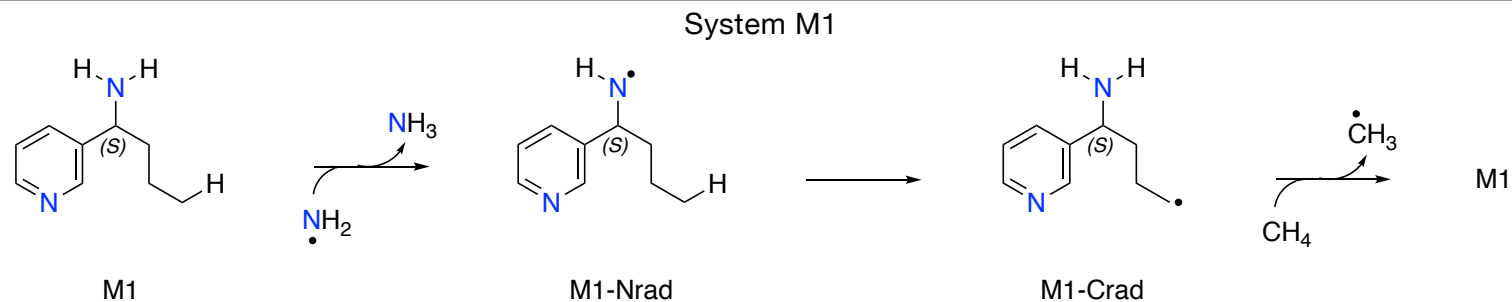
L6-Crad

GINC-SL250S-GEN8-10-01\SP\ROB2PLYP-FC\GTMP2large\C11H12F3N2O1(2)\SSHKUNNI\15-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-2.035931,2.67408,-0.271729\C,0,-2.773153,1.402463,0.173165\C,0,0.39655,2.00462,-0.677665\C,0,-0.562006,2.765035,0.186563\H,0,-2.778773,1.3296
89,1.263538\H,0,-3.816177,1.444016,-0.164298\H,0,-2.088589,2.774594,-1.365115\H,0,-2.596098,3.524057,0.139334\H,0,0.302335,2.170371,-1.751395\H,0,-0.4
89472,2.455313,1.235128\H,0,-0.27863,3.83115,0.167046\N,0,-2.181194,0.160015,-0.309112\C,0,1.457556,1.170218,-0.259513\C,0,2.325449,0.595233,-1.24001
1\C,0,1.750438,0.831438,1.091428\N,0,3.352365,-0.200071,-0.98013\H,0,2.146193,0.821845,-2.29222\C,0,2.822753,-0.001414,1.366209\H,0,1.130492,1.204754,
1.899665\C,0,3.597317,-0.495209,0.30998\H,0,3.059389,-0.27844,2.389516\H,0,4.443819,-1.151711,0.500079\C,0,-1.518368,-0.691124,0.508691\O,0,-1.352359,
-0.557363,1.709985\C,0,-0.957134,-1.947381,-0.19979\F,0,-1.158864,-1.914569,-1.544229\F,0,0.358322,-2.056612,0.014611\F,0,-1.559056,-3.049414,0.27374\H,
0,-2.198254,-0.048736,-1.297528\\Version=ES64L-G16RevA.03\State=2-A\HF=-909.2428032\MP2=-910.2624484\RMSD=3.574e-09\PG=C01[X(C11H12F3N2O1)]\\

R-L6
GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C11H12F3N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,0.483176,2.382943,-0.746382\C,0,-1.023304,2.105831,-0.917857\C,0,1.136242,0.849232,1.26127\C,0,0.993571,2.2809,0.699955\H,0,-1.635554,2.74744
1,-0.26944\H,0,-1.287132,2.358246,-1.960207\H,0,1.048932,1.711012,-1.401625\H,0,0.654711,3.403556,-1.109608\H,0,0.328659,2.856605,1.359103\H,0,1.9732
34,2.774406,0.751115\N,0,-1.349231,0.710131,-0.776841\H,0,0.176148,0.323408,1.203383\H,0,1.376758,0.928076,2.329992\C,0,2.198543,0.021217,0.570551\C
,0,1.863151,-1.022342,-0.303839\C,0,3.563172,0.263326,0.770684\N,0,2.752888,-1.783343,-0.953372\H,0,0.814536,-1.255317,-0.481488\C,0,4.504439,-0.51783
4,0.105319\H,0,3.884518,1.052284,1.44829\C,0,4.048917,-1.525863,-0.746508\H,0,5.569365,-0.355184,0.245145\H,0,4.755801,-2.156724,-1.283468\C,0,-2.5774
43,0.395029,-0.265189\O,0,-3.561999,1.126363,-0.296293\C,0,-2.703754,-1.066005,0.215761\F,0,-3.736692,-1.19354,1.054779\F,0,-1.583165,-1.4592,0.861042\F
,0,-2.892348,-1.890018,-0.82826\\Version=ES64L-G16RevA.03\State=2-A\HF=-909.2087429\MP2=-910.2237172\RMSD=2.849e-09\PG=C01[X(C11H12F3N2O1)]\\

TS-L6
GINC-NX360-M5-01-09\SP\ROB2PLYP-FC\GTMP2large\C11H12F3N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-1.028349,3.168368,-0.290671\C,0,-1.998626,2.13147,0.293905\C,0,0.736861,1.425388,-0.742212\C,0,0.434139,2.754629,-0.05601\H,0,-1.924553,2.093
093,1.389864\H,0,-3.031755,2.419253,0.054757\H,0,-1.215744,3.277262,-1.366632\H,0,-1.227728,4.140643,0.173108\H,0,0.759843,1.528878,-1.83346\H,0,0.61
9273,2.686766,1.023112\H,0,1.110822,3.530758,-0.440205\N,0,-1.751749,0.822662,-0.299832\H,0,-0.344239,0.837026,-0.616153\C,0,1.825534,0.552312,-0.253
013\C,0,2.571348,-0.214843,-1.172097\C,0,2.154927,0.397985,1.10486\N,0,3.558446,-1.047638,-0.843671\H,0,2.350102,-0.133032,-2.236252\C,0,3.180929,-0.4
68551,1.464048\H,0,1.61227,0.943734,1.871607\C,0,3.851944,-1.168506,0.458067\H,0,3.456246,-0.607095,2.50527\H,0,4.656182,-1.858601,0.706301\C,0,-2.16
2862,-0.267872,0.400177\O,0,-2.93924,-0.25052,1.349692\C,0,-1.723561,-1.626008,-0.190057\F,0,-0.533525,-1.548464,-0.828838\F,0,-1.609887,-2.540961,0.781
645\F,0,-2.635186,-2.064566,-1.077954\\Version=ES64L-G16RevA.03\State=2-
A\HF=-909.1874878\MP2=-910.2168715\RMSD=8.414e-09\PG=C01[X(C11H12F3N2O1)]\\

P-L6
GINC-NX360-M5-03-10\SP\ROB2PLYP-FC\GTMP2large\C11H12F3N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-0.445864,2.953656,-0.347597\C,0,-1.109331,2.195557,0.812634\C,0,1.322744,1.235355,-1.027242\C,0,1.05192,2.633158,-0.562253\H,0,-0.52822,2.328
977,1.734117\H,0,-2.112938,2.588903,0.989201\H,0,-1.008489,2.756271,-1.268769\H,0,-0.54253,4.028051,-0.143795\H,0,0.778243,0.911838,-1.914066\H,0,1.60
0323,2.858261,0.360539\H,0,1.433106,3.339601,-1.317914\N,0,-1.271501,0.766309,0.569759\H,0,-0.448614,0.182003,0.511685\C,0,2.215463,0.299306,-0.4563
5\C,0,2.326096,-1.008004,-1.030507\C,0,3.041345,0.539363,0.679218\N,0,3.120501,-1.970751,-0.588038\H,0,1.714403,-1.249205,-1.900593\C,0,3.872889,-0.46
6863,1.143547\H,0,3.027593,1.505222,1.175061\C,0,3.88562,-1.703541,0.48659\H,0,4.512532,-0.303396,2.006268\H,0,4.529935,-2.509784,0.830201\C,0,-2.473
352,0.219402,0.269502\O,0,-3.543651,0.801501,0.219305\C,0,-2.424705,-1.303214,-0.005279\F,0,-1.153855,-1.78384,-0.03782\F,0,-3.088284,-1.969988,0.95086
9\F,0,-2.994093,-1.577584,-1.186606\\Version=ES64L-G16RevA.03\State=2-
A\HF=-909.2438276\MP2=-910.2623524\RMSD=1.634e-09\PG=C01[X(C11H12F3N2O1)]\\



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.789551	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.454472	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.835797	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.504485	-	-	-
M1	Muniz_neut_konf_Honly_xx01	-460.654728	-460.390899				
M1-Nrad	Muniz_Nrad_konf_Honly	-460.005199	-459.735480		-26.82	-25.80	-
M1-Crad	Muniz_C5rad_konf_Honly	-459.995512	-459.733941		-15.08	-11.07	
M1-Nrad	Muniz_Nrad_konf_Honly	-460.005199	-459.735480		0.00	0.00	
R-M1	Muniz_TS_Ndown_eqHonly_eqPy_rad_opt_rev	-459.996034	-459.733395		24.06	5.47	-
TS-M1	Muniz_TS_Ndown_eqHonly_eqPy_rad	-459.980631	-459.712713		64.50	59.77	-
P-M1	Muniz_TS_Ndown_eqHonly_eqPy_rad_opt_fwd	-460.002728	-459.732136		6.49	8.78	-
M1-Crad	Muniz_C5rad_konf_Honly	-459.995512	-459.733941		25.43	4.04	-

M1H

GINC-NX360-M5-01-11\SP\ROB2PLYP-FC\GTMP2large\C9H14N2\DSAKIC\01-May-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,1\C,0,-1.194087,-0.479478,-1.159083\C,0,-0.601554,0.391636,-0.237721\C,0,-1.270735,0.586165,0.976769\C,0,-2.462913,-0.094075,1.210905\C,0,-2.952215,-0.948053,0.220003\H,0,-0.71708,-0.647395,-2.125334\H,0,-0.859683,1.275321,1.708554\H,0,-3.008522,0.034833,2.141529\H,0,-3.881613,-1.495297,0.371536\
N,0,-2.338125,-1.143664,-0.952313\C,0,0.713016,1.089156,-0.542216\H,0,0.902984,0.973925,-1.625592\H,0,1.486057,2.980004,-0.351915\C,0,1.905509,0.450565,0.202263\H,0,1.709831,0.505189,1.281293\H,0,2.79287,1.075532,0.017483\C,0,2.220118,-0.992261,-0.207687\H,0,1.345807,-1.627699,-0.018343\H,0,2.398574,-1.033144,-1.291804\C,0,3.435719,-1.563995,0.529667\H,0,3.274776,-1.568403,1.614628\H,0,3.639988,-2.594865,0.219372\H,0,4.33747,-0.971253,0.331865\
\N,0,0.615244,2.499503,-0.128886\H,0,-0.118443,2.964416,-0.662283\\Version=ES64L-G16RevA.03\State=1-A\HF=-460.0073378\MP2=-460.6231531\RMSD=4.453e-09\PG=C01[X(C9H14N2)]\\

M1-Nrad

GINC-NX360-M5-02-11\SP\ROB2PLYP-FC\GTMP2large\C9H13N2(2)\DSAKIC\01-May-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-1.115414,-0.575045,-1.098122\C,0,-0.606113,0.42606,-0.263794\C,0,-1.350967,0.748723,0.875335\C,0,-2.533357,0.058734,1.129651\C,0,-2.936479,-0.931793,0.231764\H,0,-0.579772,-0.844255,-2.009272\H,0,-1.010961,1.543533,1.532787\H,0,-3.137824,0.285959,2.003184\H,0,-3.855793,-1.490487,0.401185\N,0,-2.248758,-1.250089,-0.870784\C,0,0.703433,1.126311,-0.579712\H,0,0.923624,0.995846,-1.654949\C,0,1.913912,0.50661,0.194564\H,0,1.722441,0.610186,1.270182\H,0,2.803146,1.113514,-0.028086\C,0,2.205853,-0.959455,-0.148883\H,0,1.326272,-1.573644,0.077177\H,0,2.37804,-1.052434,-1.230446\C,0,3.420305,-1.503438,0.611478\H,0,3.264351,-1.452843,1.695842\H,0,3.611026,-2.550522,0.351318\H,0,4.326928,-0.931289,0.379456\N,0,0.613552,2.535122,-0.253283\H,0,1.467924,2.970959,-0.633592\\Version=ES64L-G16RevA.03\State=2-A\HF=-459.350513\MP2=-459.9529258\RMSD=1.234e-09\PG=C01[X(C9H13N2)]\\

M1-Crad

GINC-NX360-M5-02-07\SP\ROB2PLYP-FC\GTMP2large\C9H13N2(2)\DSAKIC\01-May-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-0.984746,-0.73853,-0.986427\C,0,-0.418184,0.299559,-0.235562\C,0,-1.220204,0.857214,0.768446\C,0,-2.507838,0.368468,0.970169\C,0,-2.961731,-0.671172,0.154942\H,0,-0.400128,-1.205785,-1.779301\H,0,-0.843761,1.670717,1.385974\H,0,-3.15108,0.782112,1.741738\H,0,-3.964347,-1.076377,0.283339\N,0,-2.220787,-1.22333,-0.811516\C,0,0.995081,0.79787,-0.523782\H,0,1.356961,0.25671,-1.407397\C,0,1.973781,0.503314,0.629191\H,0,1.62646,1.015733,1.538382\H,0,2.935842,0.957561,0.361796\C,0,2.169572,-0.992908,0.935751\H,0,2.803497,-1.066769,1.839586\H,0,1.210873,-1.447208,1.219156\C,0,2.789135,-1.763854,-0.182131\H,0,3.57897,-1.321704,-0.78408\H,0,2.604051,-2.826614,-0.301133\N,0,1.080869,2.231822,-0.852009\H,0,0.797934,2.788874,-0.045439\H,0,0.414952,2.453531,-1.591535\\Version=ES64L-G16RevA.03\State=2-A\HF=-459.3455932\MP2=-459.9512527\RMSD=6.447e-09\PG=C01[X(C9H13N2)]\\

R-M1

GINC-NX360-M5-01-11\SP\ROB2PLYP-FC\GTMP2large\C9H13N2(2)\DSAKIC\01-May-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-3.956039,-0.284311,-0.201286\C,0,-0.792187,0.061934,0.545391\C,0,-1.570884,0.541585,-0.700924\C,0,-3.056257,0.880566,-0.45147\H,0,-3.836321,-1.19972,-0.774795\H,0,-4.883573,-0.158695,0.349783\H,0,-1.073304,1.440277,-1.084726\H,0,-1.484971,-0.227158,-1.479911\H,0,-3.133923,1.600672,0.376583\H,0,-3.418563,1.431354,-1.340962\H,0,-2.254535,-1.265361,1.084399\N,0,-1.24543,-1.27841,0.935722\H,0,-0.960685,0.819811,1.335591\C,0,0.702723,0.039252,0.262303\C,0,1.515447,1.135277,0.565199\C,0,1.319801,-1.06491,-0.343729\C,0,2.872299,1.092007,0.250886\H,0,1.088459,2.013104,1.047198\H,0,0.724018,-1.944297,-0.575106\C,0,3.374518,-0.058006,-0.358645\H,0,3.529009,1.92705,0.477988\H,0,4.429711,-0.129067,-0.619117\N,0,2.621413,-1.124907,-0.653284\H,0,-0.813736,-1.545124,1.819654\\Version=ES64L-G16RevA.03\State=2-A\HF=-459.3450558\MP2=-459.9506933\RMSD=2.914e-09\PG=C01[X(C9H13N2)]\\

TS-M1

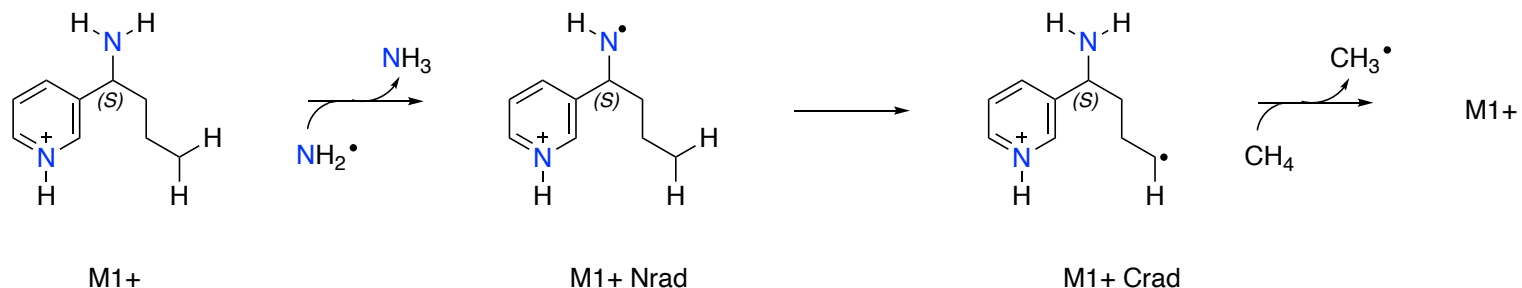
GINC-NX360-M5-01-07\SP\ROB2PLYP-FC\GTMP2large\C9H13N2(2)\DSAKIC\01-May-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-3.659573,-0.469742,0.021226\C,0,-0.811803,0.198118,0.472944\C,0,-1.552038,0.620454,-0.818362\C,0,-3.056308,0.806022,-0.538872\H,0,-3.888101,-

1.2419,-0.717803\H,0,-4.454962,-0.354737,0.759361\H,0,-1.10954,1.544406,-1.207618\H,0,-1.400779,-0.157822,-1.578054\H,0,-3.186446,1.629127,0.176479\H,0,-3.56735,1.113524,-1.463368\H,0,-2.581284,-1.012876,0.61439\N,0,-1.356246,-1.092315,0.92677\H,0,-0.967826,1.003578,1.211551\C,0,0.69094,0.085184,0.239605\C,0,1.547105,1.153548,0.517704\C,0,1.267189,-1.076971,-0.293382\C,0,2.908643,1.028779,0.246242\H,0,1.151571,2.073342,0.944945\H,0,0.636694,-1.939258,-0.495374\C,0,3.368695,-0.171549,-0.294878\H,0,3.599689,1.840817,0.453975\H,0,4.425551,-0.306479,-0.520649\N,0,2.571213,-1.213763,-0.561594\H,0,-1.379091,-1.092234,1.952568\\Version=ES64L-G16RevA.03\State=2-A\HF=-459.3077022\MP2=-459.9249825\RMSD=2.939e-09\PG=C01[X(C9H13N2)]\\

P-M1

GINC-NX360-M5-02-06\SP\ROB2PLYP-FC\GTMP2large\C9H13N2(2)\DSAKIC\01-May-2019\0\\#rob2plyp/gtmp2largemaxdisk=20gb\\nekaj\\0,2\C,0,-3.974759,-0.362086,0.029306\C,0,-0.766965,0.273859,0.463484\C,0,-1.596035,0.224924,-0.83522\C,0,-3.068627,0.648,-0.684491\H,0,-3.981312,-1.322196,-0.500665\H,0,-5.006927,0.005778,0.070287\H,0,-1.11146,0.889145,-1.562566\H,0,-1.537588,-0.790536,-1.249331\H,0,-3.109495,1.61609,-0.162692\H,0,-3.469841,0.835522,-1.689579\H,0,-3.636657,-0.561762,1.050024\N,0,-1.162699,-0.775297,1.393463\H,0,-0.923563,1.262427,0.934765\C,0,0.732653,0.145593,0.195744\C,0,1.615466,1.214354,0.373359\C,0,1.278101,-1.073956,-0.235906\C,0,2.970874,1.031489,0.104437\H,0,1.244826,2.179021,0.713649\H,0,0.628888,-1.936797,-0.374183\C,0,3.399056,-0.224807,-0.325348\H,0,3.681954,1.843228,0.227861\H,0,4.450634,-0.405549,-0.542202\N,0,2.575473,-1.267405,-0.493408\H,0,-0.657457,-0.579661,2.272064\\Version=ES64L-G16RevA.03\State=2-A\HF=-459.3471118\MP2=-459.9494931\RMSD=2.276e-09\PG=C01[X(C9H13N2)]\\

System M1+



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.789551	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.454472	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.835797	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.504485	-	-	-
M1+	MIN_M1H+	-461.023443	-460.753541	-460.859104			
M1+ Nrad	MIN_M1+_Nrad	-460.371759	-460.096368		-21.17	-21.19	
M1+ Crad	TS_M1+_opt_rev	-460.369092	-460.099137		-27.86	-17.77	
	MIN_M1+_Crad	-460.361308	-460.093392	-460.194674			
M1+ Nrad		-460.371759	-460.096368		0.00	0.00	
R-M1+	TS_M1+_opt_fwd	-460.371773	-460.095799		-0.04	1.49	
TS-M1+	TS_M1+	-460.352942	-460.078466		49.40	47.00	
P-M1+	TS_M1+_opt_rev	-460.369092	-460.099137		7.00	-7.27	
M1+ Crad		-460.369092	-460.099137		7.00	-7.27	

M1+
 1\1\GINC-NX360-M5-03-06\FOpt\RB3LYP\6-31G(d)\C9H15N2(1+)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
 \1,1\C,-1.1038533597,-0.55601165,-1.1367070855\C,-0.6012596322,0.3987209764,-0.2643234511\C,-1.3438064846,0.664659426,0.8994663769\C,-2.52780463

92,-0.0239520734,1.1707855623\C,-2.9806394089,-0.9726813142,0.2699005166\H,-0.6224921481,-0.8256297599,-2.0698046171\H,-0.9769583806,1.4369591274,1.5685554374\H,-3.1015822804,0.1739897083,2.0691591471\H,-3.8894349259,-1.5489702051,0.3944569013\N,-2.2584509562,-1.2033019263,-0.8484329834\C,0.7110093169,1.1244096702,-0.5414739486\H,0.9100257691,1.0521534576,-1.6246346504\H,1.4919886273,2.9273366304,0.0523377896\C,1.8879938529,0.4381691519,0.1943647526\H,1.6951502571,0.4756519078,1.2749138916\H,2.7760541604,1.0597976272,0.0159728278\C,2.1945639434,-0.9982270563,-0.2457168881\H,1.3326005822,-1.6489620762,-0.0394614142\H,2.3503449024,-1.0217173635,-1.3337274967\C,3.4310810745,-1.5703971525,0.4569916174\H,3.2979740213,-1.5867291808,1.544718342\H,3.6290118773,-2.5954894053,0.128731371\H,4.3225360996,-0.9721323911,0.2381086046\N,0.576384474,2.4988397226,-0.0614497332\H,0.0569928852,3.0746888707,-0.7213778084\H,-2.6013033379,-1.8933732321,-1.5124142216\\Version=ES64L-G16RevC.01\State=1-A\HF=-461.26984\RMSD=3.265e-09\RMSF=1.042e-05\Dipole=-2.4012787,-0.6652695,-0.832252\Quadrupole=9.7754492,-3.720086,-6.0553631,9.1952028,-0.1576143,2.1287713\PG=C01[X(C9H15N2)]\\

M1+ Nrad

1\1\GINC-NX360-M5-01-03\FOpt\UB3LYP\6-31G(d)\C9H14N2(1+,2)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
1,2\C,-1.0299322118,-0.6472656192,-1.040296526\C,-0.5993006495,0.4162098595,-0.260450794\C,-1.4313891371,0.8210445531,0.7976088548\C,-2.6320892497,0.1587875594,1.0619278267\C,-3.0109370734,-0.9021685493,0.2581270905\H,-0.4798400744,-1.026639927,-1.8936066897\H,-1.1279371926,1.6774202187,1.391345022\H,-3.2759230801,0.4660320256,1.8782529622\H,-3.9259021473,-1.4682841503,0.3842061985\N,-2.2026298876,-1.2649782933,-0.762182144\C,0.71769496,1.1291445325,-0.5393473542\H,0.9429675592,1.0497387806,-1.6165881467\C,1.9167081406,0.4661624713,0.2249351034\H,1.7146567972,0.5206783846,1.3015905864\H,2.7948037435,1.0964268758,0.0371821687\C,2.2335450358,-0.9768724745,-0.1902106308\H,1.3783898158,-1.6305938508,0.0317576598\H,2.3904791058,-1.0187056403,-1.2773929414\C,3.4759272041,-1.5187799135,0.5267372456\H,3.3416058248,-1.5132112451,1.6142297219\H,3.6831152489,-2.5488448267,0.2202991495\H,4.3611447349,-0.9166933585,0.2944814142\N,0.5825064544,2.5039790824,-0.1297572669\H,1.4126315017,3.0088661533,-0.4688117915\H,-2.4923406235,-2.0363183581,-1.358622719\\Version=ES64L-G16RevC.01\State=2-A\HF=-460.6034757\S2=0.753512\S2-1=0.\S2A=0.750009\RMSD=5.328e-09\RMSF=2.398e-05\Dipole=-2.1219403,-1.1757463,-0.6919176\Quadrupole=12.083869,-5.9174086,-6.1664604,9.44122,-1.5174951,3.2980743\PG=C01[X(C9H14N2)]\\

M1+ Crad

1\1\GINC-SL230S-GEN8-02-07\FOpt\UB3LYP\6-31G(d)\C9H14N2(1+,2)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
1,2\C,-0.7775930032,-0.8774525297,-0.7647995362\C,-0.4015396508,0.3467920517,-0.2203467478\C,-1.3647294074,1.0233245459,0.5434322928\C,-2.6361381846,0.484384679,0.756247723\C,-2.9560233139,-0.7361078066,0.187911056\H,-0.106140242,-1.4855577069,-1.3622679557\H,-1.1177857694,1.9936943617,0.9642085613\H,-3.3772851694,1.0064225884,1.3508915993\H,-3.9173240729,-1.2248441716,0.2891103209\N,-2.018955814,-1.3705746942,-0.5516289402\C,1.0077948782,0.9054753042,-0.4696610082\H,1.3516462721,0.4643686099,-1.4135025546\C,1.9953506497,0.4608586748,0.6362862453\H,1.6940589695,0.9182225701,1.5891953425\H,2.9607962519,0.9028556284,0.3664810124\C,2.1483137462,-1.0581034203,0.825438597\H,2.9148151978,-1.2118642726,1.606162196\H,1.2328681314,-1.4906310516,1.2563136855\C,2.5384944073,-1.8020809115,-0.4101072803\H,3.2089010011,-1.3460475297,-1.1346522008\H,2.443980889,-2.8838631131,-0.4448939097\N,1.0844575869,2.344259899,-0.6143785998\H,0.9808400266,2.85551189,0.2569751229\H,0.4618781018,2.7277664321,-1.3188883858\H,-2.2600320421,-2.2641066974,-0.9747965258\\Version=ES64L-G16RevC.01\State=2-A\HF=-460.5927331\S2=0.75362\S2-1=0.\S2A=0.750009\RMSD=5.066e-09\RMSF=2.348e-06\Dipole=-2.6740611,-0.8487915,-0.0798145\Quadrupole=8.0837544,0.2393815,-8.3231359,3.0159525,0.4602721,4.9991215\PG=C01[X(C9H14N2)]\\

R-M1+

1\1\GINC-SL230S-GEN8-02-03\FOpt\UB3LYP\6-31G(d)\C9H14N2(1+,2)\DSAKIC\25-Sep-2020\0\#b3lyp/6-31G(d)optfreq\optircforward\
1,2\C,-3.9651393092,-0.4671818338,-0.5333862607\C,-0.7825652135,0.051898349,0.7305706819\C,-1.651647196,0.6903286966,-0.414396016\C,-3.1600924701,0.7682091426,-0.1099571919\H,-3.8986200652,-0.6210907479,-1.6162862822\H,-5.0227303936,-0.3431245212,-0.2803079256\H,-1.2513188809,1.69816378

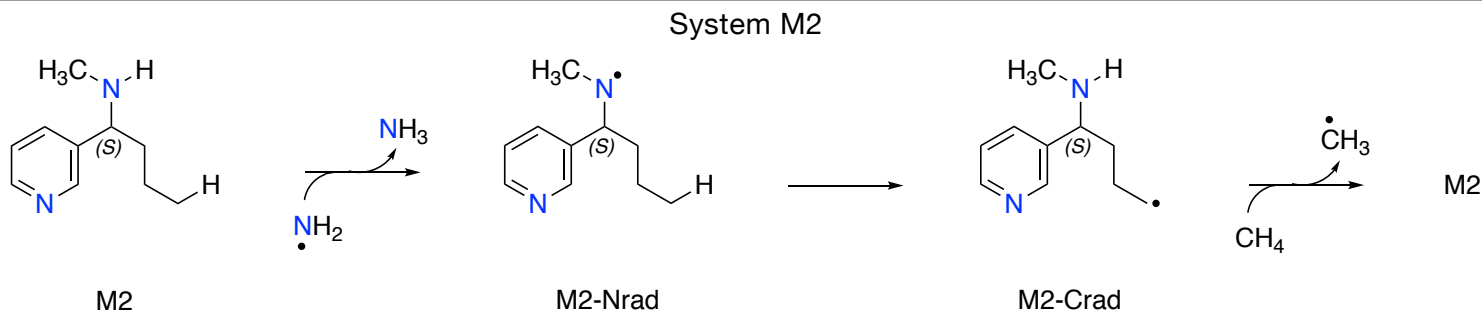
73,-0.5807209707\H,-1.4779759974,0.1232745632,-1.3368644834\H,-3.3122974034,0.9803968113,0.9580093031\H,-3.561139617,1.6398355319,-0.6403844603
\H,-3.6169421868,-1.3892629755,-0.0534159652\N,-1.1771277485,-1.2988090023,1.0211013113\H,-0.9077114698,0.7019990236,1.6136890217\C,0.689861995
8,0.0682117802,0.3350129465\C,1.4408248769,1.2501181868,0.2597140145\C,1.3366537256,-1.1229961088,0.024527822\C,2.7843709804,1.2276153448,-0.12
52209203\H,0.9759800598,2.1998313174,0.5107197328\H,0.8328201131,-2.0802400822,0.0844368861\C,3.3778731092,0.0168022474,-0.4339759667\H,3.3686
934287,2.1388697165,-0.1819697499\H,4.4109197035,-0.096401968,-0.7393472276\N,2.6355486384,-1.1099452255,-0.3470494568\H,-2.0904453833,-1.26507
35164,1.4885795278\H,3.0787637031,-1.999600517,-0.5652853705\\Version=ES64L-G16RevC.01\State=2-
A\HF=-460.6035958\S2=0.753581\S2-1=0.\S2A=0.75001\RMSD=5.461e-09\RMSF=4.948e-06\Dipole=2.8060719,0.0160892,-0.2283947\Quadrupole=18.6492372,-
5.5173338,-13.1319034,-3.9386424,-5.0255535,1.9304283\PG=C01[X(C9H14N2)]\\

TS-M1+

1\1\GINC-NX360-M5-04-11\FTS\UB3LYP\6-31G(d)\C9H14N2(1+,2)\DSAKIC\25-Sep-2020\0\#opt=(calcfc,ts,noeigentest)freqb3lyp/6-31g(d)\nekaj\
\1,2\C,-3.5958423784,-0.5462310912,-0.1751036853\C,-0.8149314901,0.1922617381,0.5652016644\C,-1.5443497815,0.8011365649,-0.6691341142\C,-3.06086
18882,0.8521548126,-0.4181469122\H,-3.7131216518,-1.1648841525,-1.0683897527\H,-4.4409178334,-0.6380432912,0.5080259331\H,-1.1430528281,1.79953
09909,-0.8776043207\H,-1.3331842298,0.1747792029,-1.5459582565\H,-3.2682951243,1.4987859878,0.4434915917\H,-3.553309131,1.3148644781,-1.2846590
14\H,-2.5562839203,-1.1077510839,0.3938404469\N,-1.3434442964,-1.1406309517,0.8682016979\H,-0.928037174,0.9017106778,1.3992760745\C,0.678319548
4,0.0811088797,0.2666396683\C,1.5385997667,1.1885720016,0.286110797\C,1.2297599808,-1.1536104314,-0.0582065528\C,2.896663811,1.0520699368,-0.01
65814802\H,1.1465297858,2.1678834811,0.5479218232\H,0.6299927878,-2.0563925381,-0.0673352499\C,3.3935355312,-0.1969611355,-0.3428470639\H,3.56
61871696,1.904427529,0.0033679364\H,4.4292192463,-0.3967785927,-0.5890462438\N,2.5449676251,-1.2501697972,-0.3525754982\H,-1.5423310613,-1.2039
480275,1.8712302363\H,2.916160646,-2.1682506182,-0.5862799354\\Version=ES64L-G16RevC.01\State=2-
A\HF=-460.5795602\S2=0.757002\S2-1=0.\S2A=0.750026\RMSD=5.176e-09\RMSF=1.853e-06\Dipole=2.5298578,-0.2245662,-0.087862\Quadrupole=17.5148569,
-5.1234263,-12.3914305,-4.5238151,-3.5888195,1.9304346\PG=C01[X(C9H14N2)]\\

P-M1+

1\1\GINC-NX360-M5-03-06\FOpt\UB3LYP\6-31G(d)\C9H14N2(1+,2)\DSAKIC\25-Sep-2020\0\#b3lyp/6-31G(d)optfreq\optircreverse\
\1,2\C,-4.0257364066,-0.3104836689,-0.3652462885\C,-0.9155019508,0.0409161476,0.5728363388\C,-1.6646648867,0.6634745455,-0.6326555124\C,-3.16879
41412,0.9135679353,-0.3787526349\H,-3.9647798052,-1.0215251638,-1.1861654604\H,-4.9028975638,-0.3640071221,0.2714841444\H,-1.1865720703,1.61872
8,-0.8812134366\H,-1.533207369,0.0074752453,-1.5037177438\H,-3.2945381104,1.4798944486,0.5534126173\H,-3.5162055353,1.5891489991,-1.1810237059\
H,-2.3373667785,-1.4298899791,0.5931993589\N,-1.342152456,-1.3380044388,0.804621374\H,-1.0885892221,0.7009736082,1.43992463\C,0.5854954922,0.05
94317178,0.2953438731\C,1.3753296691,1.2074838376,0.455277975\C,1.2161700825,-1.0915067807,-0.1638647216\C,2.7400332486,1.1928774132,0.1532576
26\H,0.9205951531,2.1227516995,0.8257893616\H,0.6712235713,-2.0206631583,-0.2864617361\C,3.3165156163,0.0234533192,-0.3094971529\H,3.354236509
1,2.0772397417,0.2790734551\H,4.3637765408,-0.0814206447,-0.5653270379\N,2.5364070953,-1.0724520456,-0.4503921284\H,-1.2220834807,-1.5962862235
,1.7827779039\H,2.9660357981,-1.9320724331,-0.7846920986\\Version=ES64L-G16RevC.01\State=2-
A\HF=-460.6007184\S2=0.753714\S2-1=0.\S2A=0.750009\RMSD=8.073e-09\RMSF=1.647e-05\Dipole=2.6412126,-0.2517019,-0.0238882\Quadrupole=17.5842023
, -5.4419564,-12.1422459,-3.0558421,-3.8393718,2.0735508\PG=C01[X(C9H14N2)]\\



NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.789551	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.454472	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.835797	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.504485	-	-	-
M2	Muniz_neut_konf_xx01	-499.933183	-499.637289				
M2-Nrad	Muniz_Nrad_konf_xx01	-499.292883	-498.991306	-	-51.06	-50.57	
M2-Crad	Muniz_C5rad_konf_xx05	-499.273518	-498.980083	-	-13.90	-10.42	-
M2-Nrad	Muniz_Nrad_konf_xx01	-499.292883	-498.991306	-	0.00	0.00	-
R-M2	Muniz_TS_Ndown_eqMe_eqPy_rad_opt_rev	-499.290204	-498.987926	-	7.03	8.87	-
TS-M2	Muniz_TS_Ndown_eqMe_eqPy_rad	-499.263358	-498.964156	-	77.52	71.28	-
P-M2	Muniz_TS_Ndown_eqMe_eqPy_rad_opt_fwd	-499.275032	-498.980233	-	46.87	29.07	-
M2-Crad	Muniz_C5rad_konf_xx05	-499.273518	-498.980083	-	50.84	29.47	-

M2

GINC-NX360-M5-01-07\SP\ROB2PLYP-FC\GTMP2large\C10H16N2\DSAKIC\19-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,1\C,0,-1.139745,-0.628861,-1.180856\C,0,-0.578961,0.092817,-0.121348\C,0,-1.233074,0.021862,1.114261\C,0,-2.379107,-0.759866,1.232242\C,0,-2.838697,
-1.447298,0.106506\H,0,-0.674614,-0.588088,-2.16635\H,0,-0.847435,0.591773,1.954767\H,0,-2.912213,-0.835265,2.175912\H,0,-3.7316,-2.068261,0.164551\N,
0,-2.239088,-1.388092,-1.087763\C,0,0.697711,0.901475,-0.298149\H,0,0.878129,1.00054,-1.387668\H,0,1.477389,2.640438,0.410919\C,0,1.9221,0.183916,0.31
2375\H,0,1.745777,0.045963,1.387623\H,0,2.788639,0.857516,0.223495\C,0,-0.340559,3.128339,-0.362572\H,0,-1.364096,2.741824,-0.326732\H,0,-0.332401,4.
100588,0.140694\H,0,-0.078912,3.284296,-1.425624\C,0,2.274071,-1.1583,-0.338923\H,0,1.425786,-1.847486,-0.245632\H,0,2.431035,-1.010129,-1.416776\C,0,
3.523135,-1.800456,0.274157\H,0,3.385335,-1.991355,1.345465\H,0,3.754039,-2.757315,-0.207182\H,0,4.400891,-1.151557,0.164144\N,0,0.555231,2.214485,0.
342369\Version=ES64L-G16RevA.03\State=1-A\HF=-499.2270004\MP2=-499.8991755\RMSD=2.557e-09\PG=C01[X(C10H16N2)]\

M2-Nrad

GINC-NX360-M5-03-03\SP\ROB2PLYP-FC\GTMP2large\C10H15N2(2)\DSAKIC\19-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-1.36319,-0.29831,-1.193037\C,0,-0.673462,0.281729,-0.122664\C,0,-1.365215,0.417987,1.086191\C,0,-2.678175,-0.037779,1.169317\C,0,-3.260547,-0.
612997,0.037789\H,0,-0.86928,-0.406346,-2.159233\H,0,-0.879185,0.893435,1.932658\H,0,-3.24571,0.05467,2.091011\H,0,-4.285601,-0.979486,0.069366\N,0,-2
.624197,-0.743846,-1.131548\C,0,0.769921,0.736967,-0.273895\H,0,1.007614,0.790322,-1.35158\C,0,1.773649,-0.26618,0.371137\H,0,1.523284,-0.366351,1.434
714\H,0,2.77579,0.18223,0.32609\C,0,1.775315,2.927298,-0.355425\H,0,2.016908,3.808294,0.24724\H,0,2.714081,2.459041,-0.699622\H,0,1.247067,3.264411,-
1.265024\C,0,1.804239,-1.644742,-0.300198\H,0,0.806403,-2.098107,-0.258122\H,0,2.043514,-1.525914,-1.366385\C,0,2.823043,-2.587205,0.350047\H,0,2.5908
5,-2.751888,1.409178\H,0,2.829308,-3.56458,-0.145294\H,0,3.839071,-2.177656,0.293391\N,0,0.94597,2.017748,0.392412\Version=ES64L-G16RevA.03\State=2-
A\HF=-498.5796126\MP2=-499.2387693\RMSD=4.407e-09\PG=C01[X(C10H15N2)]\

M2-Crad

GINC-SL250S-GEN8-08-03\SP\ROB2PLYP-FC\GTMP2large\C10H15N2(2)\DSAKIC\19-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-1.029196,-0.542665,-1.117542\C,0,-0.435306,0.097881,-0.02268\C,0,-1.237226,0.271599,1.112088\C,0,-2.550518,-0.190649,1.103596\C,0,-3.028582,-
0.818011,-0.049005\H,0,-0.446483,-0.700154,-2.025485\H,0,-0.840723,0.767208,1.996571\H,0,-3.194387,-0.06922,1.970123\H,0,-4.05071,-1.19143,-0.091179\N,
0,-2.28875,-0.996449,-1.148589\C,0,1.01175,0.588265,-0.079619\H,0,1.37533,0.409158,-1.100699\C,0,1.928779,-0.192162,0.883981\H,0,1.575781,-0.049357,1.
915707\H,0,2.923426,0.266604,0.827087\C,0,0.484813,2.902611,-0.762155\H,0,-0.608018,2.75818,-0.808548\H,0,0.683144,3.944023,-0.487983\H,0,0.884245,2.
743476,-1.770803\C,0,2.031721,-1.70052,0.590692\H,0,2.62708,-2.156704,1.404174\H,0,1.040649,-2.16741,0.663664\C,0,2.650175,-2.019539,-0.729724\H,0,3.4
84268,-1.430962,-1.103369\H,0,2.413801,-2.940928,-1.252275\N,0,1.185049,2.024404,0.171405\H,0,0.900047,2.240973,1.125515\Version=ES64L-
G16RevA.03\State=2-A\HF=-498.5651032\MP2=-499.2269957\RMSD=6.963e-09\PG=C01[X(C10H15N2)]\

R-M2

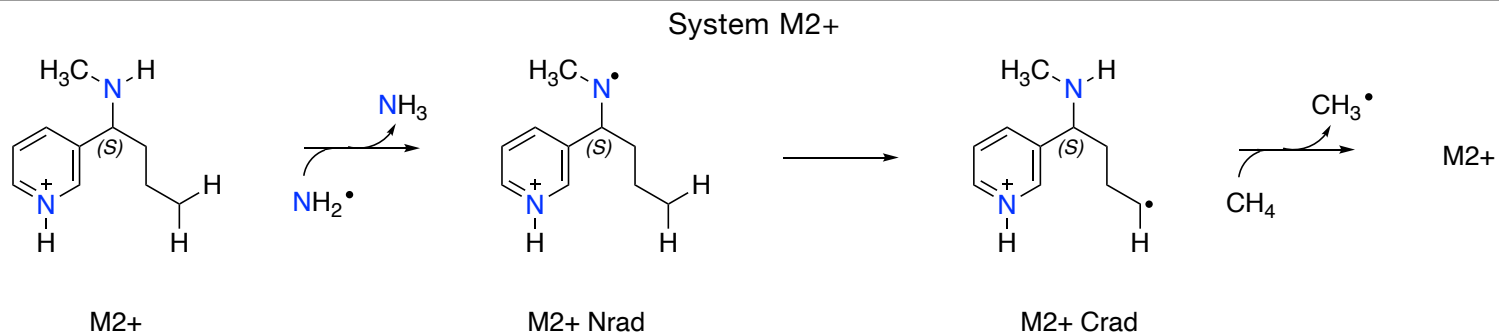
GINC-NX360-M5-03-10\SP\ROB2PLYP-FC\GTMP2large\C10H15N2(2)\DSAKIC\19-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,3.847589,-0.430615,-0.45301\C,0,0.680272,0.108589,0.376135\C,0,1.417751,-1.204898,0.029148\C,0,2.901842,-1.248198,0.434293\H,0,3.803725,-0.77
6977,-1.492492\H,0,4.884456,-0.528204,-0.109946\H,0,0.886718,-2.019239,0.539066\H,0,1.315722,-1.387778,-1.04843\H,0,2.997472,-0.92131,1.480571\H,0,3.2
25444,-2.297702,0.420659\H,0,3.58572,0.631694,-0.458407\N,0,1.147093,1.207992,-0.458378\C,0,1.068984,2.486109,0.206296\H,0,0.035671,2.709864,0.52228
6\H,0,1.68498,2.504242,1.122416\H,0,1.408447,3.282447,-0.46265\H,0,0.842961,0.319857,1.449585\C,0,-0.828315,-0.039718,0.168453\C,0,-1.713729,-0.12526
3,1.245611\C,0,-1.377041,-0.107021,-1.12179\C,0,-3.076289,-0.28914,0.998546\H,0,-1.340076,-0.068531,2.265825\H,0,-0.72534,-0.021412,-1.988697\C,0,-3.50
7341,-0.352541,-0.326164\H,0,-3.789585,-0.362173,1.814512\H,0,-4.56375,-0.47885,-0.558052\N,0,-2.68065,-0.260814,-1.3761\Version=ES64L-
G16RevA.03\State=2-A\HF=-498.5758376\MP2=-499.2352643\RMSD=2.530e-09\PG=C01[X(C10H15N2)]\

TS-M2

GINC-NX360-M5-04-06\SP\ROB2PLYP-FC\GTMP2large\C10H15N2(2)\DSAKIC\19-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,3.534886,-0.140041,-0.488181\C,0,0.699578,-0.100147,0.377895\C,0,1.342541,-1.352654,-0.263285\C,0,2.856059,-1.394893,0.027323\H,0,3.730882,-0.118725,-1.563068\H,0,4.369515,0.247817,0.097707\H,0,0.846423,-2.251111,0.120972\H,0,1.16565,-1.323052,-1.346442\H,0,3.007287,-1.485779,1.111221\H,0,3.291213,-2.299186,-0.424217\H,0,2.486871,0.741161,-0.410571\N,0,1.3185,1.100707,-0.192119\C,0,1.353809,2.223109,0.734346\H,0,0.32969,2.588528,0.893766\H,0,1.773266,1.978465,1.726384\H,0,1.935748,3.040583,0.297018\H,0,0.876893,-0.164229,1.469359\C,0,-0.80999,-0.081763,0.163632\C,0,-1.687185,-0.566718,1.136928\C,0,-1.374525,0.387045,-1.031592\C,0,-3.057248,-0.577217,0.880019\H,0,-1.30058,-0.930174,2.087278\H,0,-0.725122,0.796212,-1.801909\C,0,-3.504587,-0.094397,-0.34965\H,0,-3.764296,-0.945787,1.617803\H,0,-4.567573,-0.086745,-0.586482\N,0,-2.686485,0.384734,-1.295515\\Version=ES64L-G16RevA.03\State=2-A\HF=-498.5318494\MP2=-499.2059702\RMSD=4.403e-09\PG=C01[X(C10H15N2)]\\

P-M2

GINC-NX360-M5-01-07\SP\ROB2PLYP-FC\GTMP2large\C10H15N2(2)\DSAKIC\19-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,3.860196,-0.389916,-0.49847\C,0,0.722201,0.016349,0.386485\C,0,1.424606,-1.186467,-0.284992\C,0,2.909569,-1.374008,0.099479\H,0,3.789026,-0.138314,-1.553944\H,0,4.775244,-0.114098,0.017184\H,0,0.877367,-2.09354,-0.003305\H,0,1.327635,-1.086395,-1.37422\H,0,3.006561,-1.375071,1.194389\H,0,3.200353,-2.393838,-0.217157\H,0,2.261672,1.193512,-0.223752\N,0,1.248647,1.276723,-0.135964\C,0,0.92393,2.43968,0.684005\H,0,-0.15666,2.617018,0.663845\H,0,1.226864,2.341634,1.74357\H,0,1.415078,3.324341,0.26621\H,0,0.897964,-0.074563,1.479395\C,0,-0.783562,-0.073107,0.167566\C,0,-1.625115,-0.662307,1.114413\C,0,-1.378331,0.388707,-1.015491\C,0,-2.988132,-0.775452,0.84557\H,0,-1.215835,-1.025733,2.055471\H,0,-0.757852,0.875218,-1.764563\C,0,-3.466183,-0.288008,-0.370782\H,0,-3.66742,-1.225599,1.563966\H,0,-4.524824,-0.359157,-0.616706\N,0,-2.684397,0.289242,-1.292191\\Version=ES64L-G16RevA.03\State=2-A\HF=-498.5649039\MP2=-499.2271518\RMSD=3.296e-09\PG=C01[X(C10H15N2)]\\



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.789551	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.454472	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.835797	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.504485	-	-	-
M2+	MIN_M2H+	-500.298773	-499.997286	-500.118262			
M2+ Nrad	MIN_M2+_Nrad	-499.661099	-499.353846		-57.95	-57.25	
M2+ Crad	TS_M2+_opt_fwd	-499.640562	-499.342635		-17.72	-17.12	
M2+Nrad		-499.661099	-499.353846		0.00	0.00	
R-M2+	TS_M2+_opt_rev	-499.658830	-499.351416		5.96	6.38	
TS-M2+	TS_M2+	-499.634883	-499.331177		68.83	59.52	
P-M2+	TS_M2+_opt_fwd	-499.647975	-499.348305		34.46	14.55	
M2+Crad		-499.647975	-499.348305		34.46	14.55	

M2+

1\1\GINC-NX360-M5-05-04\FOpt\RB3LYP\6-31G(d)\C10H17N2(1+)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,1\C,-1.1071176764,-0.5298080475,-1.1869659669\C,-0.5460453408,0.3802956434,-0.3028583845\C,-1.2388364396,0.6278874387,0.896055961\C,-2.434410
5715,-0.0329525263,1.1856885105\C,-2.9453384854,-0.9389878804,0.2719877125\H,-0.6651007385,-0.7828466985,-2.1437791161\H,-0.8265843603,1.361362
2458,1.5817676534\H,-2.9704710143,0.151244835,2.1098867079\H,-3.8649779803,-1.4943211638,0.4114139777\N,-2.2691077379,-1.1540198704,-0.87770482
82\C,0.7709903719,1.0805867586,-0.6016221304\H,0.9864361321,0.9601110981,-1.681197772\C,1.9290984034,0.4032323602,0.1719235306\H,1.7457544193,
0.5142408014,1.2493138008\H,2.8443790555,0.9634371625,-0.0468085935\C,2.1675318934,-1.0705639719,-0.1838378629\H,1.2861616849,-1.673723249,0.07
71026221\H,2.2993130227,-1.1666520087,-1.2712461628\C,3.3960212574,-1.6480716552,0.5281784398\H,3.2875007771,-1.5904415995,1.6172929232\H,3.54
58496073,-2.6991797127,0.2622925158\H,4.305288073,-1.1016759937,0.2537925975\N,0.6077012356,2.4839818547,-0.2097332353\H,-0.1502366064,2.88288
21739,-0.7617187084\H,-2.6536231918,-1.8140351494,-1.5494556023\C,1.7896789846,3.3405439269,-0.3795470479\H,1.4748806622,4.3792642673,-0.251796
0232\H,2.5324976589,3.1269910385,0.3925304043\H,2.2714646838,3.243331202,-1.3663729528\\Version=ES64L-G16RevC.01\State=1-
A\HF=-500.5750144\RMSD=7.635e-09\RMSF=4.518e-06\Dipole=-2.8677674,-1.0841295,-0.7386842\Quadrupole=10.3709574,-3.4901098,-6.8808476,10.7118431,
0.2265275,2.4539746\PG=C01[X(C10H17N2)]\

M2+ Nrad

1\1\GINC-NX360-M5-01-03\FOpt\UB3LYP\6-31G(d)\C10H16N2(1+,2)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,2\C,-1.0154654822,-0.6468272676,-1.0620378664\C,-0.5436352804,0.3978492134,-0.2806372795\C,-1.3493920174,0.8184019224,0.7918051258\C,-2.56640
42724,0.190603937,1.0656888701\C,-2.9871687688,-0.8523395031,0.2591851637\H,-0.4866385589,-1.0363024037,-1.9241589642\H,-1.0098314103,1.6602575
534,1.3861497198\H,-3.1904192402,0.5100840498,1.8926707335\H,-3.916833839,-1.3920666666,0.3927957581\N,-2.2026460657,-1.2316023167,-0.773674451
9\C,0.7908858095,1.071202462,-0.5722949303\H,1.0166045725,0.9631856171,-1.6478659414\C,1.9613197414,0.3880215566,0.2143654553\H,1.7539201353,0.
4763242474,1.288177463\H,2.8610752848,0.9822545732,0.0173919678\C,2.2320743632,-1.0741865966,-0.1631197484\H,1.3548958163,-1.6947849045,0.0682
328849\H,2.3933985645,-1.1483122706,-1.2479698859\C,3.4520419752,-1.640314986,0.5735851136\H,3.3124494887,-1.6041523158,1.6598942012\H,3.62718
1862,-2.6837167321,0.2931761103\H,4.3579691769,-1.0732705836,0.3327539079\N,0.6843458629,2.4557802451,-0.1833557995\H,-2.5221719007,-1.99001123
7,-1.3713644062\C,1.6699967156,3.3283392251,-0.770539666\H,1.1886285897,4.2793132438,-1.0293438139\H,2.4294032966,3.5730939827,-0.0101884381\H,
2.183725861,2.9236483049,-1.655218383\\Version=ES64L-G16RevC.01\State=2-
A\HF=-499.9226933\S2=0.753932\S2-1=0.\S2A=0.750012\RMSD=8.947e-09\RMSF=1.008e-05\Dipole=-2.3893228,-1.2996262,-0.5936273\Quadrupole=11.590887
2,-3.3075781,-8.2833092,11.6684356,-1.3996996,3.0270094\PG=C01[X(C10H16N2)]\

M2+ Crad

1\1\GINC-NX360-M5-03-06\FOpt\UB3LYP\6-31G(d)\C10H16N2(1+,2)\DSAKIC\25-Sep-2020\0\#optfreqb3lyp/6-31g(d)\nekaj\
\1,2\C,-0.8203183794,-0.9422130821,-0.7690360958\C,-0.4251098949,0.2820349864,-0.2409632837\C,-1.3606215685,0.9613227738,0.5543094752\C,-2.62374
92542,0.4231072673,0.8134644452\C,-2.9602933114,-0.8027243726,0.2670780491\H,-0.1724724644,-1.5510352964,-1.3908047752\H,-1.0973116636,1.930611
5101,0.9685106303\H,-3.3448431454,0.9481509201,1.4297361445\H,-3.9149632579,-1.2942476733,0.4091222555\N,-2.0497124739,-1.4400190285,-0.5028253
603\C,0.9770188724,0.8442919288,-0.5365707087\H,1.3133060991,0.3553127226,-1.4608350092\C,1.9758083021,0.469395218,0.5843086209\H,1.6857345591
,0.9841583897,1.5110674039\H,2.9394498219,0.8916490858,0.2789451612\C,2.127433124,-1.0359136515,0.8657625942\H,2.9061608704,-1.1438776547,1.642
1049611\H,1.2176075186,-1.4370528736,1.3362902116\C,2.4948422509,-1.8564648939,-0.3272810786\H,3.1609719816,-1.4517664299,-1.0855233146\H,2.387
3879838,-2.9371389514,-0.297485188\N,1.0268752844,2.2692852129,-0.7664748451\H,0.956753793,2.814603757,0.0871729667\H,-2.3027666037,-2.33861572
89,-0.9077719502\C,0.2349494711,2.8145570327,-1.8612506958\H,-0.8582408502,2.6945562642,-1.7562290666\H,0.4493653298,3.8822176874,-1.9550737611
\H,0.5365697952,2.33359387,-2.7986287465\\Version=ES64L-G16RevC.01\State=2-

A\HF=-499.9016403\S2=0.753645\S2-1=0.\S2A=0.750009\RMSD=6.992e-09\RMSF=2.230e-06\Dipole=-2.5527627,-1.227231,0.2237397\Quadrupole=7.0622853,1.6763988,-8.7386841,5.6956883,-1.4151909,3.6415477\PG=C01[X(C10H16N2)]\

R-M2+

1\1\GINC-NX360-M5-02-05\FOpt\UB3LYP\6-31G(d)\C10H16N2(1+,2)\DSAKIC\25-Sep-2020\0\#b3lyp/6-31G(d)optfreq\optircreverse\
\1,2\C,3.7191656267,-0.24161137,-0.8980796877\C,0.6215748509,0.0585298659,0.5627255535\C,1.3759465106,-1.082926295,-0.2034555554\C,2.8970037412,-1.1443782532,0.0289798065\H,3.582673417,-0.536225512,-1.9449566483\H,4.78650329,-0.3214432196,-0.6679848004\H,0.9133420692,-2.0250996829,0.1187174038\H,1.1650883808,-0.9757092003,-1.2748299415\H,3.121214441,-0.9251025903,1.0818931115\H,3.2114640289,-2.1835215584,-0.1262334943\H,3.4352279453,0.8123773826,-0.815873411\N,1.0799732606,1.3665346274,0.1530917602\H,0.7514399636,-0.1264394034,1.6425900735\C,-0.8643312591,-0.0514969588,0.2382302151\C,-1.7106009185,-0.9669368209,0.8800763369\C,-1.4222613665,0.7548945022,-0.7490627862\C,-3.061103433,-1.0667511704,0.5326257585\H,-1.3127842058,-1.6051587034,1.6646335897\H,-0.8404604488,1.5028685499,-1.2738335258\C,-3.5649496502,-0.2476553156,-0.4615620661\H,-3.7193033598,-1.7700942453,1.0298300814\H,-4.5956382797,-0.2543077574,-0.7944501165\N,-2.7301656695,0.6298356328,-1.0636475188\H,-3.1065826672,1.235134584,-1.7898079666\C,1.8841198591,2.0491333163,1.1359755131\H,2.3836693368,2.9085038199,0.6819559636\H,1.2260159441,2.4260466649,1.9396233558\H,2.6279255927,1.400259111,1.6217859956\Version=ES64L-G16RevC.01\State=2-
A\HF=-499.92049\S2=0.753916\S2-1=0.\S2A=0.750012\RMSD=5.422e-09\RMSF=3.088e-06\Dipole=-3.1963933,0.0031878,-0.2153189\Quadrupole=17.6630635,-9.0645787,-8.5984847,0.4842312,7.2446605,-3.2897995\PG=C01[X(C10H16N2)]\

TS-M2+

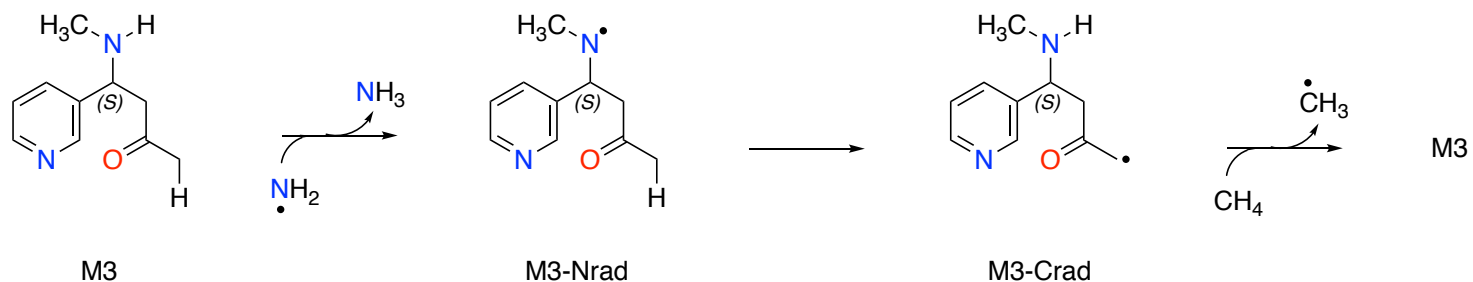
1\1\GINC-NX360-M5-05-04\FTS\UB3LYP\6-31G(d)\C10H16N2(1+,2)\DSAKIC\25-Sep-2020\0\#opt=(calcfc,ts,noeigentest)freqb3lyp/6-31g(d)\nekaj\
\1,2\C,-3.6031667924,-0.4965192027,-0.1107906169\C,-0.8080689416,0.2544887923,0.5427905899\C,-1.5345481279,0.7702394956,-0.7324174442\C,-3.050063361,0.8657226595,-0.4802847688\H,-3.7379828499,-1.1926027897,-0.9421007247\H,-4.4334795949,-0.5189336422,0.5955676833\H,-1.1198951106,1.7428368533,-1.0214719761\H,-1.3370539653,0.0735450249,-1.5579462044\H,-3.240734573,1.5885764058,0.3225906055\H,-3.5397075462,1.2610947692,-1.3812209034\H,-2.5311858478,-1.0219600157,0.5007434874\N,-1.3443874599,-1.0419590161,0.9515339486\H,-0.9257454099,1.0227855816,1.3272660343\C,0.6844917065,0.1196039375,0.2581740032\C,1.5693290134,1.2066607609,0.3050943363\C,1.2097835353,-1.119439962,-0.0933001546\C,2.9253927518,1.0462919515,0.044665716\H,1.1968280801,2.1881630216,0.5866027556\H,0.5905314985,-2.0084679955,-0.125579551\C,3.3957804466,-0.2061554925,-0.3467920679\H,3.6138495753,1.8826856197,0.0457503739\H,4.4278380392,-0.4238845378,-0.5930210673\N,2.5238153888,-1.2398416206,-0.3834298877\H,2.8754619062,-2.1603417405,-0.6369589258\C,-1.4576645197,-1.1978613292,2.4013853551\H,-1.9798557566,-2.1324703601,2.6225350572\H,-0.4539535339,-1.264417175,2.8454634062\H,-1.9842698111,-0.3686827238,2.8995785348\Version=ES64L-G16RevC.01\State=2-
A\HF=-499.8909727\S2=0.757043\S2-1=0.\S2A=0.750026\RMSD=7.022e-09\RMSF=4.544e-06\Dipole=2.8512955,-0.2001013,-0.4783729\Quadrupole=17.4309346,-5.1337246,-12.2972101,-3.6835468,-5.0437967,1.6984742\PG=C01[X(C10H16N2)]\

P-M2+

1\1\GINC-NX360-M5-01-10\FOpt\UB3LYP\6-31G(d)\C10H16N2(1+,2)\DSAKIC\25-Sep-2020\0\#b3lyp/6-31G(d)optfreq\optircforward\
\1,2\C,3.8823059484,-0.4914998556,-0.7400621768\C,0.8464367638,-0.0764726629,0.3990303359\C,1.4480156231,-1.2430607262,-0.4259627546\C,2.9481969182,-1.4997482073,-0.153802979\H,3.807649164,-0.235757652,-1.7947340566\H,4.8049363085,-0.2302218472,-0.2319765646\H,0.8868453533,-2.1559759476,-0.1924416414\H,1.2887440231,-1.0390671376,-1.4934293955\H,3.1138604579,-1.5932357927,0.9273302121\H,3.1794470458,-2.4950271629,-0.5738170673\H,2.3491250781,1.0754191524,-0.3323621191\N,1.3884381936,1.2110516749,-0.0141388377\H,1.045490874,-0.2893084251,1.4665867798\C,-0.6704375163,-0.0723493252,0.2233073186\C,-1.5268227153,-0.9122653535,0.9498394908\C,-1.2492353562,0.7670571845,-0.7218601536\C,-2.905924215,-0.9097514279,0.7207938405\H,-1.1121464722,-1.572254128,1.7075960005\H,-0.649322915,1.4591456657,-1.3021815397\C,-3.429760526,-0.0598839095,-0.2368888631\H,-3.5713389298,-1.5557757929,1.2821219252\H,-4.4830648024,0.0124763633,-0.4787493315\N,-2.5852562566,0.7460408425,-0.9205064747\H,-2.9759252129,1.37473

08656,-1.6186317736\C,1.3550289854,2.242059139,1.0280659751\H,1.8424343108,3.1453530808,0.6522902349\H,0.3174412626,2.5019260758,1.2702558717\
H,1.852139607,1.9388053095,1.9637627437\\Version=ES64L-G16RevC.01\State=2-
A\HF=-499.9092393\S2=0.753727\S2-1=0.\S2A=0.75001\RMSD=6.394e-09\RMSF=7.413e-06\Dipole=-2.8197652,0.1020062,-0.3530985\Quadrupole=18.1423799,
-8.528026,-9.6143539,-1.9209118,3.8850845,-4.4720529\PG=C01[X(C10H16N2)]\\

System M3



NAME	SYSTEM	H(kJ/mol)			Δ H(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.78955	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.45447	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.83579	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.50448	-	-	-
M3	Muniz_R2keton_TS_Ndown_eqMe_eqPy_neutM3	-573.962190	-573.660036				
M3-Nrad	Muniz_R2keton_TS_Ndown_axMe_axPy_rad_opt_rev	-573.318265	-573.010463		-41.54	-41.15	
M3-Crad	Muniz_R2keton_TS_Ndown_axMe_eqPy_rad_opt_fwd	-573.324904	-573.016917		-72.66	-47.40	
R-M3	Muniz_R2keton_TS_Ndown_axMe_axPy_rad_opt_rev	-573.318265	-573.010463		0.00	0.00	
	Muniz_R2keton_TS_Ndown_eqMe_axPy_rad_opt_rev	-573.311632	-573.008838		17.41	4.27	
	Muniz_R2keton_TS_Ndown_axMe_axPy_rad_opt_fwd	-573.310481	-573.006461		20.44	10.51	
TS-M3	Muniz_R2keton_TS_Ndown_axMe_axPy_rad	-573.294744	-572.989299		61.75	55.57	
	Muniz_R2keton_TS_Ndown_eqMe_eqPy_rad	-573.289498	-572.984273		75.53	68.76	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
	Muniz_R2keton_TS_Ndown_axMe_eqPy_rad	-573.288522	-572.983338		78.09	71.22	
P-M3	Muniz_R2keton_TS_Ndown_axMe_eqPy_rad_opt_fwd	-573.324904	-573.016917		-17.43	-16.94	
	Muniz_R2keton_TS_Ndown_eqMe_eqPy_rad_opt_rev	-573.324904	-573.016916		-17.43	-16.94	
	Muniz_R2keton_TS_Ndown_eqMe_eqPy_rad_opt_fwd	-573.319107	-573.014903		-2.21	-11.66	
M3-Crad	Muniz_R2keton_TS_Ndown_axMe_eqPy_rad_opt_fwd	-573.324904	-573.016917		-17.43	-16.94	
	Muniz_R2keton_TS_Ndown_eqMe_eqPy_CradM3	-573.315483	-573.012811		7.30	-6.16	

M3

GINC-SL250S-GEN8-03-03\SP\ROB2PLYP-FC\GTMP2large\C10H14N2O1\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \0,1\C,0,3.823527,-0.610324,-0.907359\C,0,0.463086,0.213184,0.257957\C,0,1.323597,-0.95827,-0.260094\C,0,2.780582,-0.769923,0.177444\H,0,3.785236,-1.44
 8783,-1.614259\H,0,0.959229,-1.897244,0.173208\H,0,1.237626,-1.04185,-1.35064\N,0,0.932831,1.44747,-0.38697\C,0,0.41239,2.67742,0.20809\H,0,-0.688239,
 2.745403,0.233876\H,0,0.780624,2.759408,1.236937\H,0,0.797268,3.535026,-0.352689\H,0,0.691008,0.313915,1.326042\C,0,-1.031878,-0.066535,0.119558\C,0,
 -1.854329,-0.232183,1.237666\C,0,-1.648098,-0.169666,-1.136071\C,0,-3.213366,-0.488995,1.060861\H,0,-1.431015,-0.16188,2.23763\H,0,-1.057937,-0.04687,-
 2.045507\C,0,-3.710068,-0.571301,-0.239468\H,0,-3.875241,-0.620113,1.912058\H,0,-4.765369,-0.770727,-0.418016\N,0,-2.947527,-0.414683,-1.330018\O,0,3.0
 60423,-0.740503,1.360782\H,0,4.820143,-0.538655,-0.466999\H,0,0.691171,1.423131,-1.376878\H,0,3.602324,0.303321,-1.473605\Version=ES64L-
 G16RevA.03\State=1-A\HF=-573.164321\MP2=-573.9031021\RMSD=8.120e-09\PG=C01[X(C10H14N2O1)]\

M3-Nrad

GINC-NX360-M5-05-05\SP\ROB2PLYP-FC\GTMP2large\C10H13N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \0,2\C,0,2.616158,1.559616,-0.851539\C,0,0.673356,-0.875005,0.583117\C,0,1.482062,0.345292,1.156563\C,0,1.551586,1.559413,0.226785\H,0,3.615245,1.518
 616,-0.397819\H,0,0.621242,-1.599214,1.415483\H,0,0.986193,0.666778,2.077323\H,0,2.490943,-0.006799,1.407489\H,0,2.510013,0.665487,-1.476641\N,0,1.38
 66,-1.417274,-0.557196\C,0,-0.753364,-0.489665,0.208888\C,0,-1.739177,-0.399959,1.195705\C,0,-1.135865,-0.212509,-1.109642\C,0,-3.032327,-0.029854,0.83
 7748\H,0,-1.496968,-0.618535,2.234204\H,0,-0.405658,-0.293484,-1.909944\C,0,-3.298298,0.23116,-0.507371\H,0,-3.819578,0.050415,1.581624\H,0,-4.298316,
 0.521651,-0.825877\N,0,-2.376148,0.139212,-1.471345\C,0,2.139453,-2.601486,-0.236612\H,0,1.452643,-3.440005,-0.025112\H,0,2.782116,-2.886214,-1.074743
 \H,0,2.75921,-2.475311,0.668405\H,0,2.527997,2.463096,-1.458245\O,0,0.772531,2.482242,0.370223\Version=ES64L-G16RevA.03\State=2-
 A\HF=-572.5120729\MP2=-573.238967\RMSD=4.164e-09\PG=C01[X(C10H13N2O1)]\

M3-Crad

GINC-SL230S-GEN8-02-06\SP\ROB2PLYP-FC\GTMP2large\C10H13N2O1(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \0,2\C,0,3.827201,-0.516035,-0.959467\C,0,0.511985,0.185578,0.254114\C,0,1.355057,-0.922216,-0.412327\C,0,2.817585,-0.801485,0.016047\H,0,4.858395,-0.4
 31802,-0.632776\H,0,0.985255,-1.901587,-0.087682\H,0,1.247635,-0.876129,-1.503379\N,0,0.978072,1.484437,-0.244628\C,0,0.448071,2.639633,0.476067\H,0,-
 0.652977,2.706091,0.494153\H,0,0.800991,2.605662,1.513122\H,0,0.840712,3.554472,0.02094\H,0,0.756439,0.15644,1.323479\C,0,-0.986387,-0.074505,0.1087

06\C,0,-1.782103,-0.415883,1.206116\C,0,-1.631314,0.01248,-1.133448\C,0,-3.143703,-0.652969,1.022389\H,0,-1.336044,-0.496047,2.19543\H,0,-1.06327,0.280306,-2.025615\C,0,-3.670181,-0.53848,-0.263789\H,0,-3.785194,-0.917951,1.857919\H,0,-4.728518,-0.716301,-0.447249\N,0,-2.933961,-0.209949,-1.333889\O,0,3.117372,-0.94796,1.212437\H,0,3.594778,-0.367077,-2.009073\H,0,0.756774,1.569473,-1.235599\\Version=ES64L-G16RevA.03\State=2-A\HF=-572.5117457\MP2=-573.2421998\RMSD=5.014e-09\PG=C01[X(C10H13N2O1)]\\

R-M3

GINC-NX360-M5-05-05\SP\ROB2PLYP-FC\GTMP2large\C10H13N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,2.616158,1.559616,-0.851539\C,0,0.673356,-0.875005,0.583117\C,0,1.482062,0.345292,1.156563\C,0,1.551586,1.559413,0.226785\H,0,3.615245,1.518616,-0.397819\H,0,0.621242,-1.599214,1.415483\H,0,0.986193,0.666778,2.077323\H,0,2.490943,-0.006799,1.407489\H,0,2.510013,0.665487,-1.476641\N,0,1.3866,-1.417274,-0.557196\C,0,-0.753364,-0.489665,0.208888\C,0,-1.739177,-0.399959,1.195705\C,0,-1.135865,-0.212509,-1.109642\C,0,-3.032327,-0.029854,0.837748\H,0,-1.496968,-0.618535,2.234204\H,0,-0.405658,-0.293484,-1.909944\C,0,-3.298298,0.23116,-0.507371\H,0,-3.819578,0.050415,1.581624\H,0,-4.298316,0.521651,-0.825877\N,0,-2.376148,0.139212,-1.471345\C,0,2.139453,-2.601486,-0.236612\H,0,1.452643,-3.440005,-0.025112\H,0,2.782116,-2.886214,-1.074743\H,0,2.75921,-2.475311,0.668405\H,0,2.527997,2.463096,-1.458245\O,0,0.772531,2.482242,0.370223\\Version=ES64L-G16RevA.03\State=2-A\HF=-572.5120729\MP2=-573.238967\RMSD=4.164e-09\PG=C01[X(C10H13N2O1)]\\

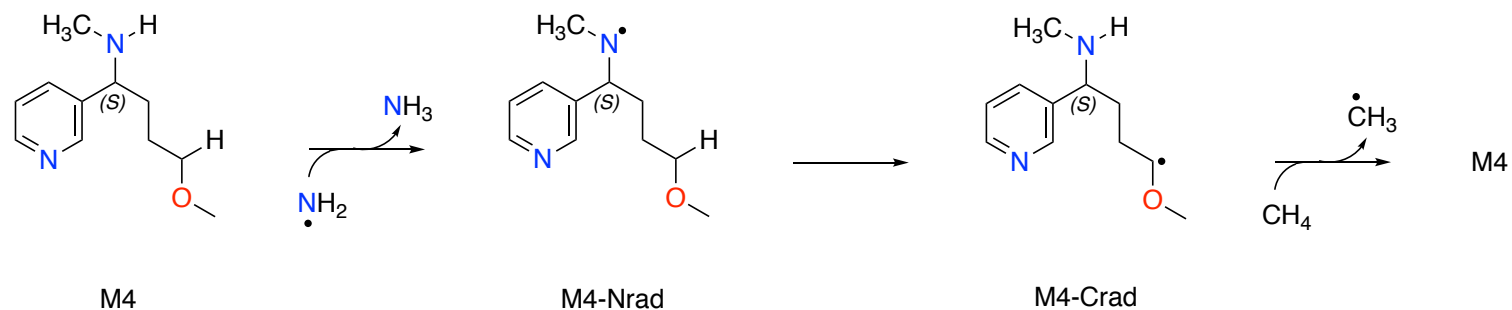
TS-M3

GINC-SL250S-GEN8-04-05\SP\ROB2PLYP-FC\GTMP2large\C10H13N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,3.263832,0.425295,-0.722931\C,0,0.490125,0.00659,0.309399\C,0,1.245035,-1.051928,-0.551563\C,0,2.732135,-0.87947,-0.261941\H,0,3.209534,0.612186,-1.798354\H,0,0.921171,-2.058404,-0.278107\H,0,1.018947,-0.872602,-1.609605\H,0,2.163051,1.178717,-0.395486\N,0,0.963274,1.348584,-0.056987\C,0,0.904049,2.301965,1.040552\H,0,-0.149942,2.505802,1.274655\H,0,1.384003,1.944607,1.966619\H,0,1.370941,3.242309,0.733596\H,0,0.718788,-0.224224,1.364981\C,0,-1.017912,-0.085194,0.130263\C,0,-1.821258,-0.73638,1.069936\C,0,-1.653226,0.453005,-0.998555\C,0,-3.192928,-0.83385,0.842942\H,0,-1.376841,-1.162607,1.966978\H,0,-1.064683,0.986358,-1.74199\C,0,-3.715191,-0.266353,-0.319449\H,0,-3.844826,-1.334166,1.553052\H,0,-4.782002,-0.321771,-0.530002\N,0,-2.967695,0.371355,-1.229766\O,0,3.357579,-1.6607,0.440735\H,0,4.194207,0.747736,-0.256859\\Version=ES64L-G16RevA.03\State=2-A\HF=-572.469828\MP2=-573.2126257\RMSD=6.081e-09\PG=C01[X(C10H13N2O1)]\\

P-M3

GINC-NX360-M5-03-10\SP\ROB2PLYP-FC\GTMP2large\C10H13N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,3.725137,-1.675149,-0.36099\C,0,0.410057,0.356027,0.209576\C,0,1.278863,-0.876683,-0.096838\C,0,2.760687,-0.637479,0.183017\H,0,3.387478,-2.692575,-0.130217\H,0,0.95528,-1.733425,0.51291\H,0,1.147007,-1.178138,-1.143492\H,0,3.768965,-1.593286,-1.454912\N,0,0.721989,1.388016,-0.773411\H,0,0.634427,0.679994,1.237411\C,0,-1.07785,0.026015,0.128267\C,0,-1.857211,-0.105493,1.280299\C,0,-1.716578,-0.167683,-1.106243\C,0,-3.206219,-0.436006,1.157858\H,0,-1.41222,0.048208,2.261136\H,0,-1.152118,-0.046094,-2.028207\C,0,-3.731403,-0.61687,-0.121325\H,0,-3.838557,-0.546391,2.034102\H,0,-4.780437,-0.875744,-0.25632\N,0,-3.008669,-0.484223,-1.241361\C,0,0.859022,2.694742,-0.182579\H,0,1.766357,2.718209,0.443595\H,0,0.946165,3.457578,-0.962311\H,0,0.010508,2.947711,0.475981\H,0,4.723004,-1.508764,0.049858\O,0,3.147985,0.328455,0.814703\\Version=ES64L-G16RevA.03\State=2-A\HF=-572.5198157\MP2=-573.2453619\RMSD=2.273e-09\PG=C01[X(C10H13N2O1)]\\

System M4



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.78955	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.45447	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.83579	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.50448	-	-	-
M4	Muniz_R2OMe_TS_Ndown_eqMe_eqPy_neutM4	-614.407351	-614.067930				
M4-Nrad	Muniz_R2OMe_TS_Ndown_eqMe_eqPy_NradM4	-613.768991	-613.424274		-56.15	-56.68	
M4-Crad	Muniz_R2OMe_TS_Ndown_eqMe_eqPy_CradM4	-613.765980	-613.427360		-61.94	-54.09	
M4-Nrad	Muniz_R2OMe_TS_Ndown_eqMe_eqPy_NradM4	-613.768991	-613.424274		0.00	0.00	
R-M4	Muniz_R2OMe_TS_Ndown_eqMe_axPy_rad_opt_fwd	-613.766447	-613.42207	-	6.68	5.79	
	Muniz_R2OMe_TS_Ndown_axMe_axPy_rad_opt_rev	-613.761019	-613.422046		20.93	5.85	
	Muniz_R2OMe_TS_Ndown_axMe_eqPy_rad_opt_fwd	-613.760373	-613.421605		22.63	7.01	
TS-M4	Muniz_R2OMe_TS_Ndown_eqMe_eqPy_rad	-613.749513	-613.407039		51.14	45.25	
	Muniz_R2OMe_TS_Ndown_axMe_axPy_rad	-613.745945	-613.404116		60.51	52.92	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
	Muniz_R2OMe_TS_Ndown_axMe_eqPy_rad	-613.743969	-613.402049		65.70	58.35	
P-M4	Muniz_R2OMe_TS_Ndown_eqMe_eqPy_rad_opt_fwd	-613.76598	-613.427359	-	7.91	-8.10	
	Muniz_R2OMe_TS_Ndown_eqMe_axPy_rad_opt_rev	-613.762649	-613.424612		16.65	-0.89	
M4-Crad	Muniz_R2OMe_TS_Ndown_eqMe_eqPy_CradM4	-613.765980	-613.427360		7.91	-8.10	

M4

GINC-SL230S-GEN8-02-01\SP\ROB2PLYP-FC\GTMP2large\C11H18N2O1\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \0,1\C,0,3.050551,-0.249041,-0.212036\C,0,-0.19814,0.116837,0.385145\C,0,0.59909,-1.107167,-0.117936\C,0,2.046507,-1.229577,0.387375\H,0,2.984009,-0.26
 313,-1.315895\H,0,0.052513,-2.006127,0.192055\H,0,0.582962,-1.116356,-1.218558\H,0,2.06878,-1.137023,1.481456\H,0,2.407258,-2.240439,0.15812\N,0,0.345
 331,1.353347,-0.188848\C,0,-0.239831,2.584576,0.336658\H,0,-1.333283,2.66453,0.216485\H,0,-0.014373,2.659886,1.407088\H,0,0.225099,3.441481,-0.161277
 \H,0,-0.04323,0.191086,1.471586\C,0,-1.699198,-0.084538,0.158132\C,0,-2.586334,-0.283896,1.219475\C,0,-2.252126,-0.087136,-1.13092\C,0,-3.942415,-0.477
 912,0.959159\H,0,-2.215963,-0.287474,2.242984\H,0,-1.610985,0.070467,-1.999144\C,0,-4.372071,-0.463936,-0.36724\H,0,-4.652743,-0.633306,1.76618\H,0,-5.
 422759,-0.612137,-0.611244\N,0,-3.547526,-0.270611,-1.405303\O,0,4.34636,-0.656923,0.202188\C,0,5.359907,0.205258,-0.260424\H,0,5.225277,1.234774,0.1
 10951\H,0,6.312629,-0.18305,0.110892\H,0,5.396845,0.242225,-1.362296\H,0,0.244834,1.330272,-1.20234\H,0,2.841967,0.779738,0.110184\Version=ES64L-
 G16RevA.03\State=1-A\HF=-613.5635706\MP2=-614.3655537\RMSD=2.456e-09\PG=C01[X(C11H18N2O1)]\

M4-Nrad

GINC-SL230S-GEN8-02-01\SP\ROB2PLYP-FC\GTMP2large\C11H17N2O1(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \0,2\C,0,2.973376,-0.333873,-0.269949\C,0,-0.216926,0.110568,0.458674\C,0,0.556879,-1.175216,0.09155\C,0,2.025024,-1.206845,0.545924\H,0,2.916083,-0.60
 5724,-1.338829\H,0,0.029547,-2.01897,0.553853\H,0,0.491821,-1.322604,-0.994318\H,0,2.098607,-0.918088,1.603579\H,0,2.39351,-2.238448,0.484849\N,0,0.28
 6003,1.249533,-0.299082\C,0,0.102908,2.504636,0.389033\H,0,-0.959577,2.681974,0.62675\H,0,0.643991,2.517631,1.3513\H,0,0.465115,3.331233,-0.229218\H,
 0,-0.111222,0.277542,1.546709\C,0,-1.710277,-0.046317,0.167377\C,0,-2.648453,-0.19302,1.192159\C,0,-2.190886,-0.060893,-1.151313\C,0,-3.993806,-0.3621
 26,0.867186\H,0,-2.328649,-0.179332,2.231937\H,0,-1.496951,0.071575,-1.978851\C,0,-4.35533,-0.368842,-0.479756\H,0,-4.746886,-0.482216,1.64068\H,0,-5.3
 96426,-0.497179,-0.771792\N,0,-3.47728,-0.218234,-1.47993\O,0,4.286313,-0.542252,0.223287\C,0,5.253377,0.217955,-0.465384\H,0,5.063029,1.300517,-0.377
 97\H,0,6.224522,-0.008013,-0.016152\H,0,5.288483,-0.037345,-1.537426\H,0,2.698116,0.730211,-0.201306\Version=ES64L-G16RevA.03\State=2-
 A\HF=-612.9181946\MP2=-613.7073747\RMSD=2.049e-09\PG=C01[X(C11H17N2O1)]\

M4-Crad

GINC-NX360-M5-05-03\SP\ROB2PLYP-FC\GTMP2large\C11H17N2O1(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \0,2\C,0,2.98246,-0.433504,-0.360288\C,0,-0.163584,-0.014881,0.458945\C,0,0.551827,-1.204013,-0.224424\C,0,2.016358,-1.427761,0.201257\H,0,2.943948,-0.
 180537,-1.424297\H,0,-0.014692,-2.112533,0.008798\H,0,0.489021,-1.070597,-1.312796\H,0,2.094672,-1.418765,1.297907\H,0,2.312943,-2.448101,-0.10522\N,
 0,0.406615,1.254301,0.007493\C,0,0.048788,2.394693,0.845226\H,0,-1.026079,2.590509,0.767928\H,0,0.28738,2.257701,1.916855\H,0,0.576277,3.284805,0.48
 714\H,0,-0.040046,-0.14866,1.554458\C,0,-1.658098,-0.07268,0.166781\C,0,-2.552778,-0.679161,1.051975\C,0,-2.18902,0.438152,-1.02652\C,0,-3.903012,-0.76
 0523,0.715359\H,0,-2.194329,-1.080662,1.998258\H,0,-1.526125,0.939148,-1.728283\C,0,-4.31518,-0.224635,-0.504657\H,0,-4.622479,-1.223287,1.384994\H,0,-

5.361863,-0.269887,-0.802518\N,0,-3.481725,0.369992,-1.367984\O,0,4.22647,-0.47894,0.197134\C,0,5.187778,0.382275,-0.398089\H,0,4.896529,1.434554,-0.284171\H,0,6.133179,0.206729,0.118993\H,0,5.309654,0.158206,-1.467123\H,0,1.42278,1.155076,-0.017941\\Version=ES64L-G16RevA.03\State=2-A\HF=-612.917233\MP2=-613.7112671\RMSD=6.006e-09\PG=C01[X(C11H17N2O1)]\\

R-M4

GINC-SL250S-GEN8-10-05\SP\ROB2PLYP-FC\GTMP2large\C11H17N2O1(2)\DSAKIC\21-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\0,2\C,0,-2.588684,0.083844,-0.207091\C,0,0.449814,-1.30448,-0.535578\C,0,-0.588636,-0.820071,-1.583207\C,0,-1.481934,0.375131,-1.217943\H,0,-3.157649,-0.813304,-0.512686\H,0,1.024451,-2.11508,-1.020734\H,0,-0.023614,-0.567771,-2.490322\H,0,-1.217549,-1.682707,-1.843112\H,0,-0.875991,1.214374,-0.85637\H,0,-1.971118,0.725429,-2.135772\H,0,-2.177624,-0.124681,0.79009\N,0,-0.217485,-1.792623,0.661565\C,0,1.465149,-0.21953,-0.168688\C,0,2.636443,-0.060396,-0.916607\C,0,1.267741,0.661155,0.905167\C,0,3.530835,0.953493,-0.5821\H,0,2.84486,-0.725768,-1.752062\H,0,0.380291,0.56435,1.526113\C,0,3.226893,1.773991,0.505147\H,0,4.447938,1.10115,-1.145107\H,0,3.903538,2.574818,0.79938\N,0,2.120298,1.635832,1.244013\C,0,0.465599,-2.910762,1.262193\H,0,0.454003,-3.783716,0.585834\H,0,1.527429,-2.683669,1.457724\H,0,-0.016799,-3.192978,2.202584\O,0,-3.443278,1.216731,-0.172558\C,0,-4.483626,1.083325,0.768142\H,0,-5.136149,0.223608,0.540231\H,0,-4.097191,0.95613,1.792925\H,0,-5.07986,1.999299,0.726095\\Version=ES64L-G16RevA.03\State=2-A\HF=-612.9158055\MP2=-613.7052963\RMSD=1.101e-09\PG=C01[X(C11H17N2O1)]\\

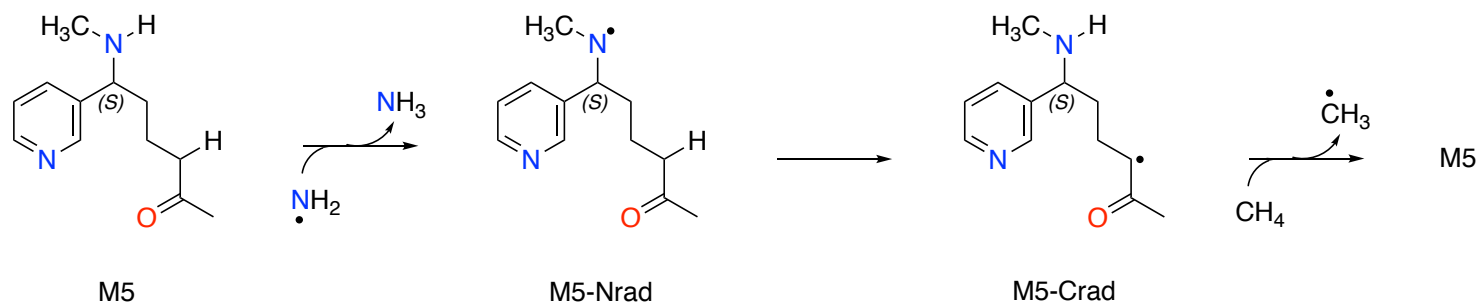
TS-M4

GINC-NX360-M5-01-03\SP\ROB2PLYP-FC\GTMP2large\C11H17N2O1(2)\DSAKIC\21-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\0,2\C,0,2.728788,-0.48054,-0.477527\C,0,-0.106814,-0.224668,0.374513\C,0,0.440188,-1.495322,-0.319945\C,0,1.936213,-1.688457,-0.01815\H,0,2.920312,-0.439983,-1.56187\H,0,-0.131694,-2.367282,0.016024\H,0,0.276397,-1.401874,-1.401643\H,0,2.083429,-1.794894,1.064585\H,0,2.308599,-2.612989,-0.482336\H,0,1.805514,0.472497,-0.340938\N,0,0.608795,0.945936,-0.1422\C,0,0.721301,2.017149,0.835954\H,0,-0.273306,2.448046,1.022704\H,0,1.127185,1.696984,1.812355\H,0,1.357592,2.814124,0.436077\H,0,0.057614,-0.352945,1.462625\C,0,-1.609047,-0.080579,0.156967\C,0,-2.529417,-0.527303,1.108493\C,0,-2.126255,0.474729,-1.022662\C,0,-3.894167,-0.417841,0.845911\H,0,-2.17981,-0.954369,2.04666\H,0,-1.440307,0.858403,-1.774218\C,0,-4.292699,0.142561,-0.367478\H,0,-4.633801,-0.753822,1.567177\H,0,-5.35001,0.244173,-0.608191\N,0,-3.432209,0.587456,-1.292371\O,0,3.872926,-0.290046,0.279884\C,0,4.726993,0.73492,-0.200454\H,0,4.231328,1.71555,-0.170197\H,0,5.601796,0.752433,0.453481\H,0,5.049145,0.53468,-1.233097\\Version=ES64L-G16RevA.03\State=2-A\HF=-612.8791271\MP2=-613.6849868\RMSD=7.758e-09\PG=C01[X(C11H17N2O1)]\\

P-M4

GINC-SL230S-GEN8-02-02\SP\ROB2PLYP-FC\GTMP2large\C11H17N2O1(2)\DSAKIC\21-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\0,2\C,0,2.982494,-0.433494,-0.36045\C,0,-0.163508,-0.015024,0.45875\C,0,0.551822,-1.204021,-0.224968\C,0,2.016326,-1.427968,0.200647\H,0,2.944148,-0.180304,-1.424416\H,0,-0.014713,-2.112592,0.007997\H,0,0.488999,-1.070227,-1.313289\H,0,2.094609,-1.419431,1.297304\H,0,2.312917,-2.448168,-0.106255\H,0,1.422852,1.155025,-0.017873\N,0,0.406678,1.254221,0.007437\C,0,0.048751,2.394555,0.845226\H,0,-1.026098,2.590409,0.76781\H,0,0.287201,2.257469,1.916873\H,0,0.576323,3.284678,0.48729\H,0,-0.039846,-0.149013,1.554216\C,0,-1.658044,-0.072739,0.166743\C,0,-2.552599,-0.679515,1.05188\C,0,-2.189138,0.438508,-1.02629\C,0,-3.902878,-0.760761,0.715437\H,0,-2.194006,-1.081316,1.997976\H,0,-1.526349,0.939721,-1.727999\C,0,-4.315224,-0.22448,-0.504354\H,0,-4.622252,-1.223745,1.385019\H,0,-5.361959,-0.26959,-0.802048\N,0,-3.4819,0.370453,-1.367585\O,0,4.226414,-0.479054,0.197154\C,0,5.187709,0.382603,-0.397441\H,0,4.896653,1.434811,-0.282375\H,0,6.133215,0.20639,0.119223\H,0,5.309276,0.15961,-1.466733\\Version=ES64L-G16RevA.03\State=2-A\HF=-612.9172327\MP2=-613.7112669\RMSD=6.019e-09\PG=C01[X(C11H17N2O1)]\\

System M5



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.78955	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.45447	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.83579	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.50448	-	-	-
M5	Muniz_R2acetyl_TS_Ndown_eqMe_eqPy_neutM5	-652.525868	-652.167755				
M5-Nrad	Muniz_R2acetyl_TS_Ndown_eqMe_eqPy_NradM5	-651.890502	-651.526390		-64.01	-62.70	
M5-Crad	Muniz_R2acetyl_TS_Ndown_eqMe_eqPy_CradM5	-651.894420	-651.535038		-87.99	-74.71	
M5-Nrad	Muniz_R2acetyl_TS_Ndown_eqMe_eqPy_NradM5	-651.890502	-651.526390		-0.00	-0.00	
R-M5	Muniz_R2acetyl_TS_Ndown_eqMe_eqPy_rad_opt_rev	-651.890501	-651.526389	-	0.00	0.00	
	Muniz_R2acetyl_TS_Ndown_eqMe_axPy_rad_opt_fwd	-651.888963	-651.525102		4.04	3.38	
	Muniz_R2acetyl_TS_Ndown_axMe_axPy_rad_opt_fwd	-651.886269	-651.523284		11.11	8.15	
	Muniz_R2acetyl_TS_Ndown_axMe_eqPy_rad_opt_rev	-651.885831	-651.522012		12.26	11.49	
TS-M5	Muniz_R2acetyl_TS_Ndown_eqMe_eqPy_rad	-651.869045	-651.507295		56.33	50.13	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
	Muniz_R2acetyl_TS_Ndown_axMe_eqPy_rad	-651.868832	-651.506831		56.89	51.35	
	Muniz_R2acetyl_TS_Ndown_axMe_axPy_rad	-651.867626	-651.506353		60.06	52.60	
	Muniz_R2acetyl_TS_Ndown_eqMe_axPy_rad	-651.860654	-651.499513		78.36	70.56	
P-M5	Muniz_R2acetyl_TS_Ndown_eqMe_eqPy_rad_opt_fwd	-651.889771	-651.530662	-	1.92	-11.22	
	Muniz_R2acetyl_TS_Ndown_axMe_eqPy_rad_opt_fwd	-651.889587	-651.529719		2.40	-8.74	
	Muniz_R2acetyl_TS_Ndown_eqMe_axPy_rad_opt_rev	-651.887473	-651.529025		7.95	-6.92	
	Muniz_R2acetyl_TS_Ndown_axMe_axPy_rad_opt_rev	-651.886843	-651.527499		9.60	-2.91	
M5-Crad	Muniz_R2acetyl_TS_Ndown_eqMe_eqPy_CradM5	-651.894420	-651.535038		-10.29	-22.71	

M5

GINC-SL230S-GEN8-02-02\SP\ROB2PLYP-FC\GTMP2large\C12H18N2O1\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\0,1\C,0,2.755475,-0.340426,-0.528749\C,0,-0.469754,0.27052,0.330687\C,0,0.365583,-1.024077,0.213587\C,0,1.854676,-0.897648,0.591647\H,0,2.669404,-0.959144,-1.428905\H,0,-0.101867,-1.767888,0.870585\H,0,0.271504,-1.428319,-0.805001\H,0,1.940796,-0.271608,1.48973\H,0,2.22084,-1.893934,0.873635\N,0,0.03198,1.302115,-0.585738\C,0,-0.608341,2.608839,-0.446745\H,0,-1.702277,2.603188,-0.583731\H,0,-0.398313,3.005957,0.553525\H,0,-0.172595,3.298611,-1.176408\H,0,-0.317898,0.668689,1.344967\C,0,-1.962602,-0.040926,0.191243\C,0,-2.83734,0.039715,1.278264\C,0,-2.518647,-0.433477,-1.035002\C,0,-4.185379,-0.270795,1.104198\H,0,-2.463861,0.343792,2.254433\H,0,-1.887238,-0.508116,-1.921243\C,0,-4.619544,-0.653053,-0.164622\H,0,-4.886391,-0.214558,1.93203\H,0,-5.664358,-0.903318,-0.340848\N,0,-3.806848,-0.734909,-1.226351\C,0,4.234295,-0.277101,-0.171723\O,0,5.079341,-0.818062,-0.861554\C,0,4.622561,0.501188,1.077905\H,0,4.093846,1.460038,1.133956\H,0,4.349721,-0.068898,1.975407\H,0,5.702114,0.665584,1.08394\H,0,-0.058294,0.976556,-1.546997\H,0,2.408306,0.670869,-0.776144\Version=ES64L-G16RevA.03\State=1-A\HF=-651.6195506\MP2=-652.4708015\RMSD=9.754e-09\PG=C01[X(C12H18N2O1)]\

M5-CH

GINC-SL230S-GEN8-02-01\SP\ROB2PLYP-FC\GTMP2large\C12H17N2O1(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\0,2\C,0,2.67647,-0.255173,-0.54042\C,0,-0.495978,0.037642,0.468444\C,0,0.290267,-1.148304,-0.134491\C,0,1.777079,-1.202739,0.258393\H,0,2.677513,-0.524402,-1.60729\H,0,-0.203268,-2.067094,0.206904\H,0,0.182374,-1.124335,-1.226788\H,0,1.891751,-0.990624,1.328676\H,0,2.143808,-2.227922,0.125459\N,0,-0.008875,1.310786,-0.049008\C,0,-0.205915,2.400325,0.876552\H,0,-1.259966,2.484558,1.189653\H,0,0.381767,2.245303,1.798398\H,0,0.10225,3.345732,0.420482\H,0,-0.388692,-0.00694,1.56791\C,0,-1.988644,-0.077298,0.15428\C,0,-2.920755,-0.435508,1.131348\C,0,-2.474107,0.161879,-1.140725\C,0,-4.265092,-0.554983,0.78103\H,0,-2.597133,-0.623106,2.152927\H,0,-1.785019,0.4635,-1.927014\C,0,-4.631761,-0.300539,-0.540252\H,0,-5.013538,-0.835286,1.516588\H,0,-5.672278,-0.382256,-0.850458\N,0,-3.75957,0.055863,-1.492303\C,0,4.115202,-0.211922,-0.045296\O,0,4.458017,-0.739379,0.997477\C,0,5.109745,0.533877,-0.921449\H,0,5.270386,-0.019397,-1.855988\H,0,4.727642,1.523457,-1.199489\H,0,6.062956,0.63519,-0.398362\H,0,2.275354,0.768571,-0.516717\Version=ES64L-G16RevA.03\State=2-A\HF=-650.9764868\MP2=-651.8146422\RMSD=2.287e-09\PG=C01[X(C12H17N2O1)]\

M5-NH

GINC-SL230S-GEN8-02-01\SP\ROB2PLYP-FC\GTMP2large\C12H17N2O1(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,2.776672,-1.057038,-0.306259\C,0,-0.138639,-0.224523,0.087141\C,0,0.311255,-1.68933,-0.078164\C,0,1.774302,-1.918682,0.380533\H,0,3.061481,-1.286592,-1.331066\H,0,-0.342954,-2.343871,0.510295\H,0,0.192401,-1.991335,-1.128316\H,0,1.836443,-1.729878,1.457601\H,0,2.01743,-2.977186,0.209358\N,0,0.518573,0.599115,-0.938388\C,0,0.477795,2.037597,-0.685876\H,0,-0.536942,2.443739,-0.537192\H,0,1.069938,2.253823,0.210136\H,0,0.935827,2.562577,-1.53038\H,0,0.245801,0.134455,1.050163\C,0,-1.659756,-0.084399,0.109692\C,0,-2.332458,0.463815,1.2056\C,0,-2.450694,-0.486114,-0.977562\C,0,-3.721655,0.582913,1.172309\H,0,-1.77089,0.791977,2.077861\H,0,-1.982214,-0.92165,-1.861281\C,0,-4.398606,0.146273,0.034486\H,0,-4.268787,1.006545,2.009616\H,0,-5.482882,0.222173,-0.028677\N,0,-3.782008,-0.382265,-1.031416\C,0,3.3404,0.109036,0.324936\O,0,2.982387,0.469895,1.45856\C,0,4.364117,0.918411,-0.458895\H,0,5.1256,0.276393,-0.916855\H,0,3.864492,1.462261,-1.270905\H,0,4.844438,1.640973,0.204425\H,0,0.119376,0.390725,-1.852281\\Version=ES64L-G16RevA.03\State=2-A\HF=-650.9796841\MP2=-651.8248536\RMSD=7.219e-09\PG=C01[X(C12H17N2O1)]\\

R-M5

GINC-SL250S-GEN8-01-03\SP\ROB2PLYP-FC\GTMP2large\C12H17N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,2.676378,-0.255709,-0.540834\C,0,-0.495894,0.037499,0.468417\C,0,0.290141,-1.148505,-0.134692\C,0,1.776976,-1.203173,0.258092\H,0,2.677895,-0.525413,-1.607581\H,0,-0.203526,-2.067243,0.206649\H,0,0.182158,-1.124426,-1.226978\H,0,1.891785,-0.991047,1.328347\H,0,2.143531,-2.228415,0.125143\H,0,2.274958,0.767933,-0.517695\N,0,-0.008603,1.310633,-0.048906\C,0,-0.205331,2.400039,0.876868\H,0,-1.259356,2.484449,1.190013\H,0,0.382333,2.244692,1.79867\H,0,0.103036,3.345465,0.420976\H,0,-0.388571,-0.007222,1.567869\C,0,-1.988572,-0.077215,0.154278\C,0,-2.920626,-0.435835,1.131251\C,0,-2.474108,0.162495,-1.1406\C,0,-4.264982,-0.555177,0.780957\H,0,-2.596953,-0.623828,2.15274\H,0,-1.785053,0.46442,-1.926801\C,0,-4.631723,-0.300217,-0.540204\H,0,-5.013384,-0.835776,1.516446\H,0,-5.672257,-0.381796,-0.850384\N,0,-3.759587,0.056602,-1.492152\C,0,4.114914,-0.211785,-0.045214\O,0,4.457491,-0.738289,0.998106\C,0,5.109548,0.533571,-0.921674\H,0,5.27073,-0.020502,-1.855642\H,0,4.727212,1.52276,-1.200758\H,0,6.062532,0.63569,-0.398337\\Version=ES64L-G16RevA.03\State=2-A\HF=-650.9764866\MP2=-651.8146422\RMSD=2.285e-09\PG=C01[X(C12H17N2O1)]\\

TS-M5

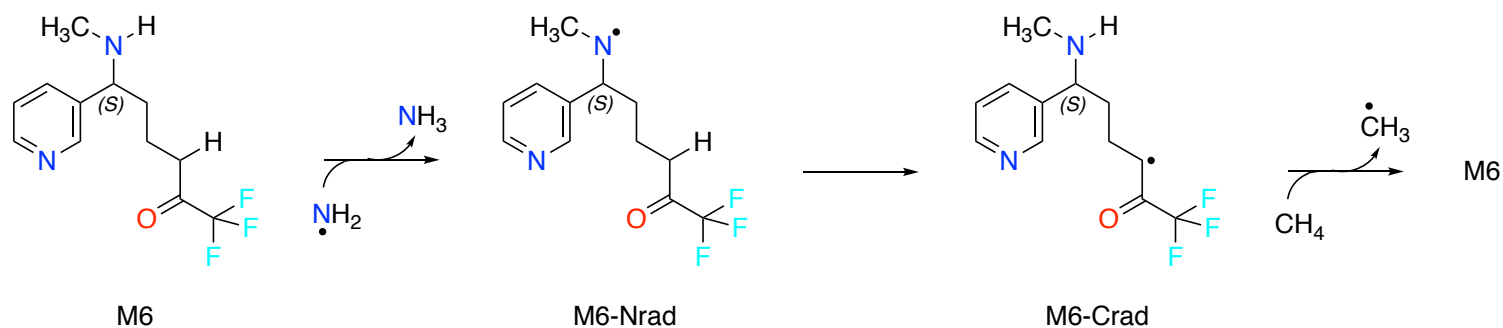
GINC-NX360-M5-03-08\SP\ROB2PLYP-FC\GTMP2large\C12H17N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,2.459162,-0.351171,-0.7994\C,0,-0.320822,-0.244552,0.275959\C,0,0.20769,-1.450863,-0.534141\C,0,1.728383,-1.609367,-0.347162\H,0,2.505582,-0.227097,-1.885236\H,0,-0.318853,-2.357094,-0.214997\H,0,-0.029673,-1.294835,-1.594139\H,0,1.935257,-1.817821,0.70995\H,0,2.080604,-2.48445,-0.911616\H,0,1.537508,0.549493,-0.542242\N,0,0.345503,0.973308,-0.192008\C,0,0.506312,1.984005,0.839981\H,0,-0.479176,2.41612,1.066811\H,0,0.919057,1.599226,1.788742\H,0,1.148732,2.788257,0.469535\H,0,-0.100789,-0.436215,1.34351\C,0,-1.833887,-0.100515,0.142285\C,0,-2.697486,-0.560552,1.139179\C,0,-2.414883,0.469412,-1.000185\C,0,-4.07477,-0.450112,0.954035\H,0,-2.296041,-0.999723,2.050356\H,0,-1.775191,0.86237,-1.787267\C,0,-4.540597,0.126167,-0.227565\H,0,-4.772425,-0.797681,1.71049\H,0,-5.609442,0.229937,-0.407664\N,0,-3.733327,0.584197,-1.193083\C,0,3.730437,0.099116,-0.169516\O,0,4.535715,0.769144,-0.80457\C,0,3.996626,-0.252225,1.28939\H,0,3.126874,-0.047638,1.925515\H,0,4.226707,-1.320487,1.392131\H,0,4.85332,0.325898,1.641117\\Version=ES64L-G16RevA.03\State=2-A\HF=-650.935544\MP2=-651.7905292\RMSD=9.859e-10\PG=C01[X(C12H17N2O1)]\\

P-M5

GINC-SL250S-GEN8-08-05\SP\ROB2PLYP-FC\GTMP2large\C12H17N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,2.753793,-0.44773,-0.881747\C,0,-0.304567,-0.071545,0.202602\C,0,0.27952,-1.13378,-0.757338\C,0,1.764031,-1.500709,-0.509262\H,0,2.662421,0.018266,-1.862309\H,0,-0.311559,-2.050019,-0.651763\H,0,0.142232,-0.786578,-1.789456\H,0,1.894868,-1.810308,0.53446\H,0,1.976467,-2.396816,-1.118586\H,0,1.203781,1.194348,-0.340366\N,0,0.210879,1.25729,-0.12364\C,0,0.007682,2.250597,0.927349\H,0,-1.063402,2.440762,1.051889\H,0,0.412002,1.951194,1.912242\H,0,0.483132,3.190298,0.630572\H,0,-0.02768,-0.374825,1.234535\C,0,-1.82726,-0.089586,0.126989\C,0,-2.593627,-0.823945,1.035412\C,0,-2.51568,0.591058,-0.887582\C,0,-3.979607,-0.858965,0.892426\H,0,-2.109115,-1.359778,1.849828\H,0,-1.954162,1.194034,-1.597458\C,0,-4.554842,-0.150026,-0.162297\H,0,-

4.602247,-1.41758,1.58539\H,0,-5.634188,-0.154357,-0.307115\N,0,-3.8451,0.568647,-1.041485\C,0,3.891387,-0.005033,-0.111056\O,0,4.637584,0.872435,-0.573907\C,0,4.16929,-0.612098,1.258541\H,0,3.335404,-0.441898,1.950715\H,0,4.320199,-1.696529,1.192889\H,0,5.070012,-0.150675,1.667442\\Version=ES64L-G16RevA.03\State=2-A\HF=-650.9754926\MP2=-651.8198406\RMSD=3.743e-09\PG=C01[X(C12H17N2O1)]\\

System M6



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.78955	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.45447	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.83579	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.50448	-	-	-
M6	Muniz_R2COCF3_TS_Ndown_eqMe_eqPy_neutM6	-950.256707	-949.876167				
M6-Nrad	Muniz_R2COCF3_TS_Ndown_eqMe_eqPy_NradM6	-949.618274	-949.232203		-55.96	-55.87	
M6-Crad	Muniz_R2COCF3_TS_Ndown_eqMe_eqPy_CradM6	-949.626643	-949.243657		-91.62	-75.25	
M6-Nrad	Muniz_R2COCF3_TS_Ndown_eqMe_eqPy_NradM6	-949.618274	-949.232203		0.00	0.00	
R-M6	Muniz_R2COCF3_TS_Ndown_eqMe_eqPy_rad_opt_rev	-949.618010	-949.231799	-	0.69	1.06	
	Muniz_R2COCF3_TS_Ndown_axMe_axPy_rad_opt_fwd	-949.616327	-949.230086		5.11	5.56	
	Muniz_R2COCF3_TS_Ndown_axMe_eqPy_rad_opt_fwd	-949.615537	-949.230030		7.19	5.71	
	Muniz_R2COCF3_TS_Ndown_eqMe_axPy_rad_opt_rev	-949.616325	-949.229917		5.12	6.00	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
TS-M6	Muniz_R2COCF3_TS_Ndown_eqMe_eqPy_rad	-949.602796	-949.217360		40.64	38.97	
	Muniz_R2COCF3_TS_Ndown_axMe_eqPy_rad	-949.600990	-949.216663		45.38	40.80	
	Muniz_R2COCF3_TS_Ndown_axMe_axPy_rad	-949.598926	-949.214006		50.80	47.78	
	Muniz_R2COCF3_TS_Ndown_eqMe_axPy_rad	-949.593815	-949.207879		64.22	63.86	
P-M6	Muniz_R2COCF3_TS_Ndown_eqMe_eqPy_rad_opt_fwd	-949.622566	-949.239930	-	-11.27	-20.29	
	Muniz_R2COCF3_TS_Ndown_axMe_eqPy_rad_opt_rev	-949.621564	-949.238989		-8.64	-17.82	
	Muniz_R2COCF3_TS_Ndown_eqMe_axPy_rad_opt_fwd	-949.621347	-949.237487		-8.07	-13.87	
	Muniz_R2COCF3_TS_Ndown_axMe_axPy_rad_opt_rev	-949.618720	-949.235643		-1.17	-9.03	
M6-Crad	Muniz_R2COCF3_TS_Ndown_eqMe_eqPy_CradM6	-949.626643	-949.243657		-21.97	-30.07	

M6

GINC-NX360-M5-05-03\SP\ROB2PLYP-FC\GTMP2large\C12H15F3N2O1\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \0,1\C,0,1.806476,-0.848693,-0.716551\C,0,-1.267942,0.204993,0.040125\C,0,-0.529462,-1.113485,0.363032\C,0,0.989292,-0.991859,0.587098\H,0,1.625114,-1.702359,-1.378032\H,0,-0.977397,-1.522946,1.276599\H,0,-0.735946,-1.851393,-0.426095\H,0,1.18627,-0.140027,1.247982\H,0,1.331884,-1.885538,1.123503\N,0,-0.834617,0.739491,-1.258985\C,0,-1.345144,2.074513,-1.569854\H,0,-2.444188,2.158893,-1.56157\H,0,-0.946906,2.788725,-0.839868\H,0,-0.982984,2.372862,-2.558589\H,0,-0.958894,0.947556,0.790034\C,0,-2.781569,0.025858,0.181329\C,0,-3.505992,0.646513,1.202851\C,0,-3.510303,-0.77764,-0.707774\C,0,-4.882057,0.441859,1.295195\H,0,-2.994817,1.285391,1.920607\H,0,-3.001182,-1.283695,-1.529142\C,0,-5.494915,-0.383233,0.352752\H,0,-5.468786,0.913747,2.078036\H,0,-6.567129,-0.567799,0.391502\N,0,-4.828434,-0.988177,-0.639432\C,0,3.30037,-0.775305,-0.517201\O,0,4.105142,-1.532656,-1.010369\C,0,3.836109,0.363324,0.394876\F,0,3.127829,1.501882,0.22498\F,0,5.121725,0.626521,0.15213\F,0,3.715326,-0.002091,1.692889\H,0,1.467906,0.059391,-1.230989\H,0,-1.105811,0.091373,-1.997365\\Version=ES64L-G16RevA.03\State=1-A\HF=-949.0776766\MP2=-950.1583149\RMSD=7.117e-09\PG=C01[X(C12H15F3N2O1)]\\

M6-Nrad

GINC-NX360-M5-02-11\SP\ROB2PLYP-FC\GTMP2large\C12H14F3N2O1(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \0,2\C,0,-1.740791,-1.111718,0.652251\C,0,1.237667,0.017508,-0.331156\C,0,0.651542,-1.412286,-0.271611\C,0,-0.856973,-1.483966,-0.565956\H,0,-1.369774,-0.191157,1.112345\H,0,1.187554,-2.016742,-1.013947\H,0,0.870564,-1.850285,0.710098\H,0,-1.09041,-0.821767,-1.409761\H,0,-1.125409,-2.497513,-0.884982\N,0,0.682781,0.853248,0.725421\C,0,0.469219,2.218731,0.310853\H,0,1.288514,2.616818,-0.30939\H,0,-0.450497,2.272489,-0.297941\H,0,0.330212,2.862017,1.185159\H,0,1.014807,0.432064,-1.331188\C,0,2.758865,-0.001746,-0.177579\C,0,3.607941,0.228974,-1.262591\C,0,3.356949,-0.264702,1.064511\C,0,4.988034,0.171247,-1.072729\H,0,3.194046,0.447625,-2.244674\H,0,2.731813,-0.425681,1.940306\C,0,5.470714,-0.108453,0.205477\H,0,5.675143,0.343259,-1.896102\H,0,6.542096,-0.160707,0.392192\N,0,4.677505,-0.32138,1.26366\C,0,-3.184614,-0.961888,0.237785\O,0,-3.977659,-1.867204,0.123088\C,0,-3.642341,0.487115

, -0.078127\F, 0, -3.627677, 1.224421, 1.052531\F, 0, -4.866534, 0.528846, -0.600888\F, 0, -2.78459, 1.073811, -0.954379\H, 0, -1.68746, -1.912453, 1.397455\
\Version=ES64L-G16RevA.03\State=2-A\HF=-948.4319823\MP2=-949.5000521\RMSE=4.461e-09\PG=C01[X(C12H14F3N2O1)]\

M6-Crad

GINC-NX360-M5-02-11\SP\ROB2PLYP-FC\GTMP2large\C12H14F3N2O1(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0, 2\C, 0, -1.823248, 1.523884, 0.011463\C, 0, 0.911674, 0.160072, 0.17292\C, 0, 0.489216, 1.353499, 1.050057\C, 0, -1.038792, 1.395373, 1.27652\H, 0, -1.651723, 2.40238
5, -0.605687\H, 0, 0.995383, 1.29527, 2.020636\H, 0, 0.823287, 2.289522, 0.580767\H, 0, -1.345771, 0.516927, 1.848958\H, 0, -1.258711, 2.269436, 1.909847\N, 0, 0.30711,
0.321197, -1.153154\C, 0, 0.271666, -0.874969, -1.990503\H, 0, 1.262322, -1.32226, -2.174033\H, 0, -0.364319, -1.624455, -1.509736\H, 0, -0.178921, -0.620147, -2.95411
9\H, 0, 0.460001, -0.743898, 0.600642\C, 0, 2.425214, -0.042147, 0.155655\C, 0, 3.013725, -1.217839, 0.630225\C, 0, 3.292239, 0.938354, -0.3492\C, 0, 4.400075, -1.36016
7, 0.585793\H, 0, 2.390347, -2.013901, 1.032376\H, 0, 2.891683, 1.876489, -0.735783\C, 0, 5.158381, -0.313483, 0.0627\H, 0, 4.883281, -2.263481, 0.946517\H, 0, 6.243299,
-0.386828, 0.011502\N, 0, 4.622397, 0.823338, -0.401454\C, 0, -2.85945, 0.678793, -0.476653\O, 0, -3.507225, 0.913745, -1.505458\C, 0, -3.192153, -0.617794, 0.300036\F
, 0, -2.098561, -1.427164, 0.40375\F, 0, -4.155283, -1.316707, -0.299809\F, 0, -3.594689, -0.348467, 1.566169\H, 0, 0.746613, 1.092817, -1.651041\Version=ES64L-
G16RevA.03\State=2-A\HF=-948.4362333\MP2=-949.5126147\RMSE=5.440e-09\PG=C01[X(C12H14F3N2O1)]\

R-M6

GINC-SL250S-GEN8-03-01\SP\ROB2PLYP-FC\GTMP2large\C12H14F3N2O1(2)\DSAKIC\21-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0, 2\C, 0, 1.734891, 1.188205, 0.53611\C, 0, -1.224753, -0.143607, -0.227126\C, 0, -0.590141, 1.222885, -0.572559\C, 0, 0.933237, 1.17242, -0.788092\H, 0, 1.633582, 2.161
146, 1.026415\H, 0, -1.067754, 1.582088, -1.492516\H, 0, -0.84035, 1.944702, 0.21482\H, 0, 1.183304, 0.281623, -1.376625\H, 0, 1.243592, 2.03366, -1.391862\H, 0, 1.3201
19, 0.427338, 1.20892\N, 0, -0.742413, -0.633164, 1.057926\C, 0, -0.626457, -2.070757, 1.102245\H, 0, -1.486789, -2.585821, 0.645161\H, 0, 0.270474, -2.382573, 0.53903
3\H, 0, -0.509934, -2.409155, 2.136223\H, 0, -0.975327, -0.848302, -1.041426\C, 0, -2.749479, -0.044851, -0.165374\C, 0, -3.560379, -0.575484, -1.171586\C, 0, -3.388923,
0.596921, 0.906484\C, 0, -4.9441, -0.431655, -1.078872\H, 0, -3.11411, -1.091492, -2.019029\H, 0, -2.795596, 1.003619, 1.722852\C, 0, -5.469222, 0.233998, 0.028513\H, 0,
-5.602021, -0.83017, -1.845658\H, 0, -6.544812, 0.364492, 0.135757\N, 0, -4.713682, 0.740667, 1.011658\C, 0, 3.211858, 0.9357, 0.359543\O, 0, 4.091206, 1.729907, 0.601
998\C, 0, 3.62639, -0.459077, -0.192988\F, 0, 2.79982, -1.434584, 0.255428\F, 0, 4.873791, -0.775119, 0.157273\F, 0, 3.552067, -0.455977, -1.544137\Version=ES64L-
G16RevA.03\State=2-A\HF=-948.431325\MP2=-949.4995164\RMSE=3.896e-09\PG=C01[X(C12H14F3N2O1)]\

TS-M6

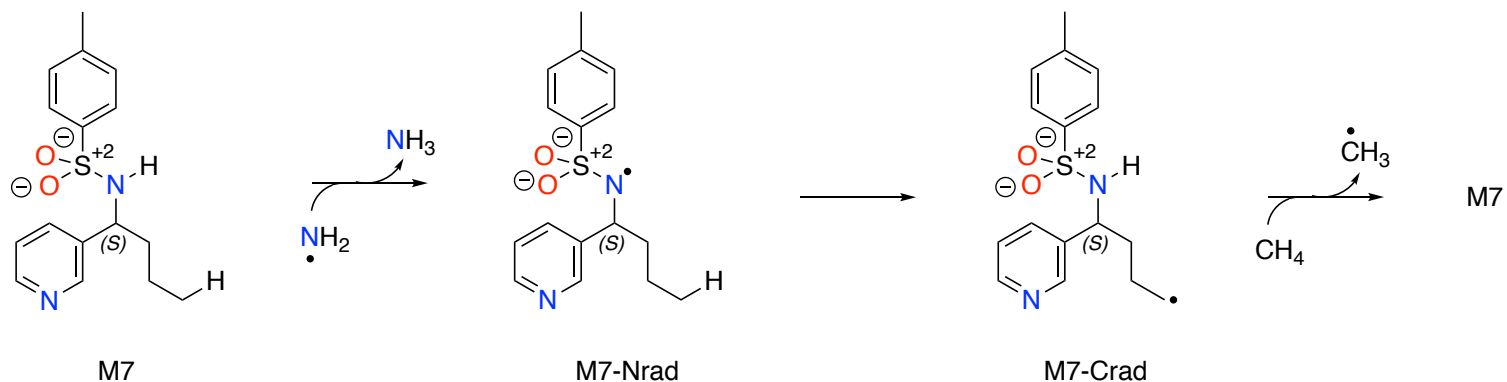
GINC-SL250S-GEN8-01-07\SP\ROB2PLYP-FC\GTMP2large\C12H14F3N2O1(2)\DSAKIC\21-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0, 2\C, 0, 1.625509, 1.243455, -0.583111\C, 0, -1.002465, -0.089625, -0.192306\C, 0, -0.561541, 0.460649, -1.567381\C, 0, 0.972246, 0.437233, -1.704785\H, 0, 1.583937, 2.
326529, -0.727556\H, 0, -1.024122, -0.136425, -2.360592\H, 0, -0.939235, 1.485655, -1.672276\H, 0, 1.314968, -0.600767, -1.695168\H, 0, 1.262043, 0.851686, -2.679594\
H, 0, 0.709243, 1.141967, 0.350485\N, 0, -0.447124, 0.771447, 0.856507\C, 0, -0.212553, 0.086989, 2.11793\H, 0, -1.185194, -0.174889, 2.558326\H, 0, 0.367894, -0.841819
, 2.015252\H, 0, 0.301495, 0.761049, 2.809265\H, 0, -0.622258, -1.122244, -0.098397\C, 0, -2.522048, -0.14344, -0.068274\C, 0, -3.217075, -1.349037, -0.189756\C, 0, -3.27
8454, 1.018836, 0.142713\C, 0, -4.609062, -1.344008, -0.114118\H, 0, -2.675027, -2.279999, -0.342362\H, 0, -2.773146, 1.974316, 0.266914\C, 0, -5.257824, -0.126141, 0.0
89223\H, 0, -5.179016, -2.263997, -0.205341\H, 0, -6.343759, -0.082835, 0.154599\N, 0, -4.613012, 1.040448, 0.220156\C, 0, 2.917633, 0.875878, 0.018667\O, 0, 3.69066, 1.
671912, 0.524556\C, 0, 3.304505, -0.627529, 0.064454\F, 0, 2.253364, -1.396537, 0.461079\F, 0, 4.314209, -0.850359, 0.904321\F, 0, 3.670718, -1.059366, -1.163865\
\Version=ES64L-G16RevA.03\State=2-A\HF=-948.3954294\MP2=-949.4798319\RMSE=5.390e-09\PG=C01[X(C12H14F3N2O1)]\

P-M6

GINC-SL250S-GEN8-02-03\SP\ROB2PLYP-FC\GTMP2large\C12H14F3N2O1(2)\DSAKIC\21-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0, 2\C, 0, 1.941204, 0.506461, -1.488186\C, 0, -0.938366, 0.056682, -0.11254\C, 0, -0.502638, -0.264231, -1.560219\C, 0, 1.000271, -0.625669, -1.719763\H, 0, 1.855968, 1.
379986, -2.133629\H, 0, -1.080201, -1.122185, -1.919704\H, 0, -0.763964, 0.585187, -2.204574\H, 0, 1.238904, -1.48188, -1.085136\H, 0, 1.139091, -0.957742, -2.761212\H

,0,0.377946,1.625955,-0.160918\N,0,-0.526418,1.412381,0.254764\C,0,-0.465078,1.644612,1.696371\H,0,-1.468385,1.542784,2.123076\H,0,0.205331,0.948272,
2.228935\H,0,-0.124333,2.667734,1.882149\H,0,-0.47026,-0.699685,0.546244\C,0,-2.449136,-0.099574,0.024208\C,0,-3.016428,-1.292442,0.48025\C,0,-3.32862
1,0.928304,-0.34377\C,0,-4.403583,-1.413539,0.537036\H,0,-2.377147,-2.116321,0.792688\H,0,-2.922704,1.880896,-0.676004\C,0,-5.180464,-0.327219,0.13351
7\H,0,-4.874047,-2.326081,0.891676\H,0,-6.26757,-0.384893,0.161961\N,0,-4.66278,0.829709,-0.298192\C,0,3.002129,0.605773,-0.534921\O,0,3.745232,1.5918
15,-0.461041\C,0,3.227178,-0.554855,0.463541\F,0,2.112275,-0.762188,1.213343\F,0,4.238859,-0.297949,1.289316\F,0,3.490543,-1.712864,-0.185589\
\Version=ES64L-G16RevA.03\State=2-A\HF=-948.4333018\MP2=-949.5083902\RMSD=3.543e-09\PG=C01[X(C12H14F3N2O1)]\

System M7



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.789551	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.454472	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.835797	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.504485	-	-	-
M7	Muniz_R1Tos_TS_Ndown_axMe_axPy_neutM7	-1279.459922	-1278.943403				
M7-Nrad	Muniz_R1Tos_TS_Ndown_eqMe_eqPy_rad_opt_rev	-1278.820302	-1278.293573		-52.84	-40.47	
M7-Crad	Muniz_R1Tos_TS_Ndown_axMe_eqPy_rad_opt_fwd	-1278.805075	-1278.289534	-	-26.55	-19.18	
R-M7	Muniz_R1Tos_TS_Ndown_eqMe_eqPy_rad_opt_rev	-1278.820302	-1278.293573		0.00	0.00	
	Muniz_R1Tos_TS_Ndown_eqMe_eqPy_rad	-1278.796475	-1278.275805		62.56	46.65	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
M7-Crad	Muniz_R1Tos_TS_Ndown_axMe_axPy_CradM7	-1278.808659	-1278.291794		30.57	4.67	
R-M7	Muniz_R1Tos_TS_Ndown_eqMe_eqPy_rad_opt_rev	-1278.820302	-1278.293573		0.00	0.00	
	Muniz_R1Tos_TS_Ndown_eqMe_axPy_rad_opt_rev	-1278.819252	-1278.292493		2.76	2.84	
	Muniz_R1Tos_TS_Ndown_axMe_axPy_rad_opt_fwd	-1278.819254	-1278.292490		2.75	2.84	
TS-M7	Muniz_R1Tos_TS_Ndown_eqMe_eqPy_rad	-1278.796475	-1278.275805		62.56	46.65	
	Muniz_R1Tos_TS_Ndown_axMe_axPy_rad	-1278.796431	-1278.275913		62.67	46.37	
	Muniz_R1Tos_TS_Ndown_eqMe_axPy_rad	-1278.789339	-1278.268628		81.29	65.49	
	Muniz_R1Tos_TS_Ndown_axMe_eqPy_rad	-1278.789004	-1278.267966		82.17	67.23	
P-M7	Muniz_R1Tos_TS_Ndown_axMe_eqPy_rad_opt_fwd	-1278.805075	-1278.289534	-	39.98	10.60	
	Muniz_R1Tos_TS_Ndown_eqMe_eqPy_rad_opt_fwd	-1278.810378	-1278.288516		26.06	13.28	
	Muniz_R1Tos_TS_Ndown_eqMe_axPy_rad_opt_fwd	-1278.806091	-1278.289036		37.31	11.91	
	Muniz_R1Tos_TS_Ndown_axMe_eqPy_rad_opt_rev	-1278.813252	-1278.286801		18.51	17.78	

M7

GINC-SL250S-GEN8-09-03\SP\ROB2PLYP-FC\GTMP2large\C16H20N2O2S1\ROOT\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
 \0,1\C,0,2.974306,-2.895667,0.346709\C,0,1.112691,-0.087512,0.571642\C,0,1.748619,-1.003038,1.650528\C,0,3.071763,-1.718197,1.325862\H,0,2.213797,-3.6
 144,0.671828\H,0,0.239995,0.387737,1.047219\H,0,1.907415,-0.355118,2.523982\H,0,0.99773,-1.744601,1.941544\H,0,3.812877,-0.992076,0.96675\H,0,3.46644
 9,-2.091929,2.280558\N,0,0.668412,-0.832427,-0.63449\C,0,2.036032,1.038705,0.135508\C,0,1.968353,2.288613,0.760517\C,0,2.999508,0.883486,-0.873053\C,
 0,2.840572,3.300685,0.36902\H,0,1.235097,2.465501,1.544494\H,0,3.097633,-0.068369,-1.391792\C,0,3.755734,3.031021,-0.649684\H,0,2.807972,4.280898,0.8
 35475\H,0,4.450825,3.798378,-0.98641\N,0,3.839934,1.8478,-1.267588\S,0,-0.766745,-1.72286,-0.629806\O,0,-0.692084,-2.665407,0.488386\O,0,-0.92898,-2.16
 0252,-2.017211\C,0,-2.098441,-0.571327,-0.262889\C,0,-2.544327,-0.417534,1.050857\C,0,-2.666465,0.173069,-1.301259\C,0,-3.560546,0.49909,1.322628\H,0,-
 2.116672,-1.02657,1.840206\C,0,-3.680073,1.081616,-1.01157\H,0,-2.331234,0.021669,-2.322406\C,0,-4.142859,1.260918,0.301756\H,0,-3.911594,0.616899,2.3
 44852\H,0,-4.126765,1.656763,-1.819105\C,0,-5.264227,2.228463,0.595904\H,0,-6.237933,1.789784,0.341523\H,0,-5.293328,2.499349,1.655811\H,0,-5.16267,3.
 149166,0.011067\H,0,3.934935,-3.420785,0.285605\H,0,0.69062,-0.271784,-1.483766\H,0,2.699028,-2.571436,-0.660256\\Version=ES64L-G16RevA.03\State=1-
 A\HF=-1278.1012502\MP2=-1279.3042374\RMSD=3.827e-09\PG=C01[X(C16H20N2O2S1)]\

M7-Nrad

GINC-SL250S-GEN8-05-03\SP\ROB2PLYP-FC\GTMP2large\C16H19N2O2S1(2)\DSAKIC\22-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,1.81253,3.688946,-1.13193\C,0,2.057092,0.576334,0.054113\C,0,2.977225,1.379736,-0.890955\C,0,3.029501,2.897064,-0.640483\H,0,1.632635,3.50874
5,-2.198987\H,0,3.98381,0.961442,-0.760972\H,0,2.68627,1.182205,-1.930068\H,0,3.184011,3.081833,0.432114\H,0,3.928102,3.279527,-1.142991\H,0,0.903512,
3.423874,-0.585547\N,0,0.647112,0.804584,-0.270683\H,0,2.290793,0.843794,1.093362\C,0,2.264684,-0.936413,-0.088643\C,0,2.598754,-1.725791,1.015017\C,
0,2.117781,-1.57806,-1.327218\C,0,2.811135,-3.090086,0.829378\H,0,2.68171,-1.277388,2.000771\H,0,1.825429,-1.00705,-2.206049\C,0,2.656602,-3.619869,-0.
452316\H,0,3.08258,-3.732404,1.661968\H,0,2.809489,-4.682764,-0.6325\N,0,2.309845,-2.8871,-1.518353\S,0,-0.366385,0.950357,1.094884\O,0,-0.481693,2.39
9954,1.327888\O,0,0.069517,0.06704,2.187795\C,0,-1.91255,0.336148,0.451079\C,0,-2.712837,1.174894,-0.32832\C,0,-2.300979,-0.97234,0.738991\C,0,-3.9152
35,0.684256,-0.827849\H,0,-2.399058,2.193715,-0.52896\C,0,-3.509518,-1.444174,0.230083\H,0,-1.667685,-1.60143,1.35508\C,0,-4.333034,-0.628389,-0.55751
8\H,0,-4.54302,1.330921,-1.435887\H,0,-3.818284,-2.462977,0.44989\C,0,-5.654293,-1.137206,-1.08163\H,0,-5.670942,-2.230198,-1.134576\H,0,-6.480604,-0.82
7208,-0.428345\H,0,-5.866863,-0.743439,-2.081198\H,0,1.977832,4.764433,-0.998263\\Version=ES64L-G16RevA.03\State=2-
A\HF=-1277.4486354\MP2=-1278.6405463\RMSD=2.732e-09\PG=C01[X(C16H19N2O2S1)]\\

M7-Crad

GINC-SL250S-GEN8-05-07\SP\ROB2PLYP-FC\GTMP2large\C16H19N2O2S1(2)\DSAKIC\22-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-4.345742,1.623727,-0.517346\C,0,-2.019612,-0.56876,-0.71301\C,0,-3.298214,-0.630424,0.150954\C,0,-4.491245,0.13786,-0.457701\H,0,-3.956647,2.1
72716,0.33629\H,0,-3.588169,-1.683923,0.250594\H,0,-3.08518,-0.255963,1.156577\H,0,-4.710339,-0.258392,-1.460038\H,0,-5.380271,-0.114482,0.150915\H,0,-
2.072053,1.474925,-1.133653\N,0,-1.395597,0.781587,-0.803798\H,0,-2.327774,-0.754856,-1.751866\C,0,-0.972093,-1.627793,-0.391048\C,0,-0.062132,-2.0215
27,-1.378877\C,0,-0.867218,-2.252888,0.857627\C,0,0.886167,-2.997463,-1.090002\H,0,-0.099147,-1.558892,-2.362458\H,0,-1.537075,-1.976112,1.666722\C,0,0
.893332,-3.553644,0.190343\H,0,1.602613,-3.324635,-1.837846\H,0,1.617507,-4.323174,0.454285\N,0,0.038391,-3.195115,1.154015\S,0,-0.617375,1.502798,0.5
25659\O,0,-0.990051,0.848154,1.788085\O,0,-0.848098,2.939554,0.326931\C,0,1.119783,1.167575,0.240573\C,0,1.813587,0.33408,1.11453\C,0,1.768979,1.791
607,-0.828404\C,0,3.175473,0.114184,0.90264\H,0,1.292802,-0.13463,1.941785\C,0,3.125997,1.559856,-1.024082\H,0,1.217623,2.450971,-1.49068\C,0,3.85141
8,0.72017,-0.162548\H,0,3.719166,-0.538949,1.580495\H,0,3.634916,2.041511,-1.855749\C,0,5.33086,0.500908,-0.371989\H,0,5.568309,0.354367,-1.431673\H,
0,5.909827,1.368351,-0.028955\H,0,5.689147,-0.372881,0.180899\H,0,-4.867658,2.197495,-1.277796\\Version=ES64L-G16RevA.03\State=2-
A\HF=-1277.4411138\MP2=-1278.6353152\RMSD=2.398e-09\PG=C01[X(C16H19N2O2S1)]\\

R-M7

GINC-SL250S-GEN8-05-03\SP\ROB2PLYP-FC\GTMP2large\C16H19N2O2S1(2)\DSAKIC\22-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,1.81253,3.688946,-1.13193\C,0,2.057092,0.576334,0.054113\C,0,2.977225,1.379736,-0.890955\C,0,3.029501,2.897064,-0.640483\H,0,1.632635,3.50874
5,-2.198987\H,0,3.98381,0.961442,-0.760972\H,0,2.68627,1.182205,-1.930068\H,0,3.184011,3.081833,0.432114\H,0,3.928102,3.279527,-1.142991\H,0,0.903512,
3.423874,-0.585547\N,0,0.647112,0.804584,-0.270683\H,0,2.290793,0.843794,1.093362\C,0,2.264684,-0.936413,-0.088643\C,0,2.598754,-1.725791,1.015017\C,
0,2.117781,-1.57806,-1.327218\C,0,2.811135,-3.090086,0.829378\H,0,2.68171,-1.277388,2.000771\H,0,1.825429,-1.00705,-2.206049\C,0,2.656602,-3.619869,-0.
452316\H,0,3.08258,-3.732404,1.661968\H,0,2.809489,-4.682764,-0.6325\N,0,2.309845,-2.8871,-1.518353\S,0,-0.366385,0.950357,1.094884\O,0,-0.481693,2.39
9954,1.327888\O,0,0.069517,0.06704,2.187795\C,0,-1.91255,0.336148,0.451079\C,0,-2.712837,1.174894,-0.32832\C,0,-2.300979,-0.97234,0.738991\C,0,-3.9152
35,0.684256,-0.827849\H,0,-2.399058,2.193715,-0.52896\C,0,-3.509518,-1.444174,0.230083\H,0,-1.667685,-1.60143,1.35508\C,0,-4.333034,-0.628389,-0.55751
8\H,0,-4.54302,1.330921,-1.435887\H,0,-3.818284,-2.462977,0.44989\C,0,-5.654293,-1.137206,-1.08163\H,0,-5.670942,-2.230198,-1.134576\H,0,-6.480604,-0.82
7208,-0.428345\H,0,-5.866863,-0.743439,-2.081198\H,0,1.977832,4.764433,-0.998263\\Version=ES64L-G16RevA.03\State=2-
A\HF=-1277.4486354\MP2=-1278.6405463\RMSD=2.732e-09\PG=C01[X(C16H19N2O2S1)]\\

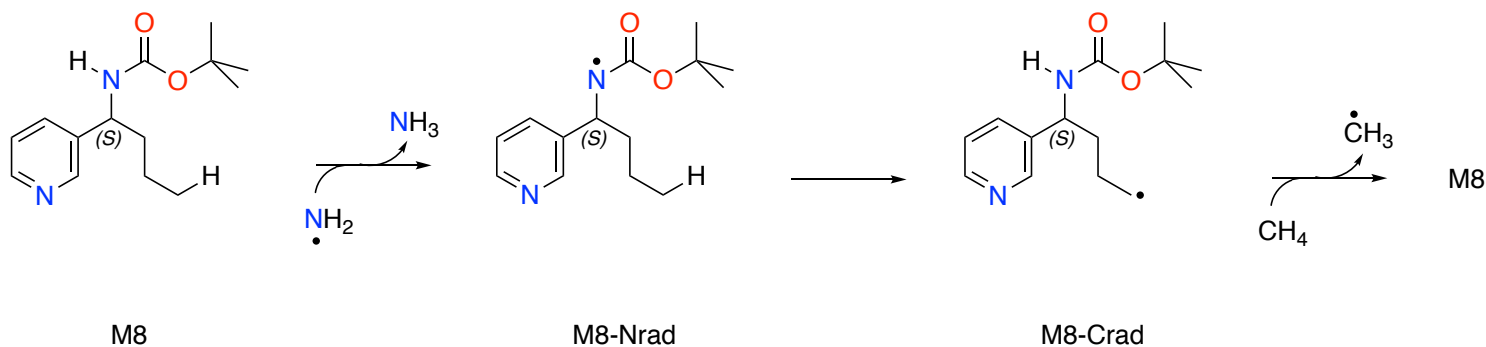
TS-M7

GINC-SL250S-GEN8-04-05\SP\ROB2PLYP-FC\GTMP2large\C16H19N2O2S1(2)\DSAKIC\21-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,0.385029,3.06537,-1.460611\C,0,1.942592,0.92287,-0.028095\C,0,2.554486,1.874307,-1.085848\C,0,1.842059,3.239117,-1.091661\H,0,0.180345,2.8606
49,-2.51444\H,0,3.621784,1.986807,-0.865745\H,0,2.479131,1.408723,-2.076975\H,0,1.925062,3.700344,-0.100102\H,0,2.347406,3.911161,-1.801434\H,0,0.165
887,1.864284,-0.904851\N,0,0.486574,0.788965,-0.298192\H,0,2.125509,1.366704,0.960001\C,0,2.609609,-0.44454,-0.065496\C,0,3.491214,-0.845343,0.939292
\C,0,2.390467,-1.336092,-1.124186\C,0,4.118798,-2.08592,0.838598\H,0,3.674336,-0.199659,1.794828\H,0,1.687577,-1.074026,-1.912935\C,0,3.83358,-2.88717
2,-0.266273\H,0,4.807206,-2.42926,1.60526\H,0,4.30416,-3.862801,-0.377761\N,0,2.981557,-2.530195,-1.236715\S,0,-0.46642,0.739839,1.117468\O,0,-0.76400
1,2.099702,1.596557\O,0,0.176788,-0.222778,2.02276\C,0,-1.979019,0.032513,0.475162\C,0,-3.138524,0.803703,0.452971\C,0,-1.985756,-1.296036,0.039884\C
,0,-4.320962,0.234794,-0.023207\H,0,-3.109688,1.828304,0.807715\C,0,-3.172483,-1.844187,-0.433347\H,0,-1.074867,-1.884878,0.071521\C,0,-4.357807,-1.090
404,-0.471749\H,0,-5.229041,0.832144,-0.0431\H,0,-3.182986,-2.875668,-0.777377\C,0,-5.641265,-1.709648,-0.971387\H,0,-5.491766,-2.218573,-1.930631\H,0,-
6.018264,-2.45991,-0.264592\H,0,-6.42449,-0.957427,-1.105376\H,0,-0.335913,3.738862,-0.997971\\Version=ES64L-G16RevA.03\State=2-
A\HF=-1277.4117333\MP2=-1278.6166647\RMSD=4.298e-09\PG=C01[X(C16H19N2O2S1)]\\

P-M7

GINC-SL250S-GEN8-05-07\SP\ROB2PLYP-FC\GTMP2large\C16H19N2O2S1(2)\DSAKIC\22-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-4.345742,1.623727,-0.517346\C,0,-2.019612,-0.56876,-0.71301\C,0,-3.298214,-0.630424,0.150954\C,0,-4.491245,0.13786,-0.457701\H,0,-3.956647,2.1
72716,0.33629\H,0,-3.588169,-1.683923,0.250594\H,0,-3.08518,-0.255963,1.156577\H,0,-4.710339,-0.258392,-1.460038\H,0,-5.380271,-0.114482,0.150915\H,0,-
2.072053,1.474925,-1.133653\N,0,-1.395597,0.781587,-0.803798\H,0,-2.327774,-0.754856,-1.751866\C,0,-0.972093,-1.627793,-0.391048\C,0,-0.062132,-2.0215
27,-1.378877\C,0,-0.867218,-2.252888,0.857627\C,0,0.886167,-2.997463,-1.090002\H,0,-0.099147,-1.558892,-2.362458\H,0,-1.537075,-1.976112,1.666722\C,0,0
.893332,-3.553644,0.190343\H,0,1.602613,-3.324635,-1.837846\H,0,1.617507,-4.323174,0.454285\N,0,0.038391,-3.195115,1.154015\S,0,-0.617375,1.502798,0.5
25659\O,0,-0.990051,0.848154,1.788085\O,0,-0.848098,2.939554,0.326931\C,0,1.119783,1.167575,0.240573\C,0,1.813587,0.33408,1.11453\C,0,1.768979,1.791
607,-0.828404\C,0,3.175473,0.114184,0.90264\H,0,1.292802,-0.13463,1.941785\C,0,3.125997,1.559856,-1.024082\H,0,1.217623,2.450971,-1.49068\C,0,3.85141
8,0.72017,-0.162548\H,0,3.719166,-0.538949,1.580495\H,0,3.634916,2.041511,-1.855749\C,0,5.33086,0.500908,-0.371989\H,0,5.568309,0.354367,-1.431673\H,
0,5.909827,1.368351,-0.028955\H,0,5.689147,-0.372881,0.180899\H,0,-4.867658,2.197495,-1.277796\\Version=ES64L-G16RevA.03\State=2-
A\HF=-1277.4411138\MP2=-1278.6353152\RMSD=2.398e-09\PG=C01[X(C16H19N2O2S1)]\\

System M8



NAME	SYSTEM	H(kJ/mol)			Δ H(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.78955	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.45447	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.83579	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.50448	-	-	-
M8	Muniz_R1Boc_TS_Ndown_eqR1_eqPy_neutM8	-806.355735	-805.927312				
M8-Nrad	Muniz_R1Boc_TS_Ndown_eqR1_eqPy_NradM8	-805.701073	-805.265255		-13.35	-8.37	
M8-Crad	Muniz_R1Boc_TS_Ndown_eqR1_eqPy_CradM8	-805.700566	-805.273790		-25.71	-20.09	
M8-Nrad	Muniz_R1Boc_TS_Ndown_eqR1_eqPy_NradM8	-805.701073	-805.265255		0.00	0.00	
R-M8	Muniz_R1Boc_TS_Ndown_axR1_axPy_rad_opt_rev	-805.698899	-805.263733	-	5.71	4.00	
	Muniz_R1Boc_TS_Ndown_eqR1_eqPy_rad_opt_rev	-805.698595	-805.2628		6.51	6.45	
	Muniz_R1Boc_TS_Ndown_axR1_eqPy_rad_opt_fwd	-805.69784	-805.262625		8.49	6.91	
	Muniz_R1Boc_TS_Ndown_eqR1_axPy_rad_opt_fwd	-805.696561	-805.2622		11.85	8.02	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
TS-M8	Muniz_R1Boc_TS_Ndown_eqR1_eqPy_rad	-805.680719	-805.249326		53.44	41.82	
	Muniz_R1Boc_TS_Ndown_axR1_axPy_rad	-805.680216	-805.248637		54.76	43.63	
	Muniz_R1Boc_TS_Ndown_eqR1_axPy_rad	-805.677257	-805.246715		62.53	48.68	
	Muniz_R1Boc_TS_Ndown_axR1_eqPy_rad	-805.673158	-805.242433		73.29	59.92	
P-M8	Muniz_R1Boc_TS_Ndown_eqR1_eqPy_rad_opt_fwd	-805.700566	-805.27379	-	1.33	-22.41	
	Muniz_R1Boc_TS_Ndown_eqR1_axPy_rad_opt_rev	-805.700335	-805.273705		1.94	-22.19	
	Muniz_R1Boc_TS_Ndown_axR1_axPy_rad_opt_fwd	-805.700335	-805.273705		1.94	-22.19	
	Muniz_R1Boc_TS_Ndown_axR1_eqPy_rad_opt_rev	-805.695414	-805.269249		14.86	-10.49	
M8-Crad	Muniz_R1Boc_TS_Ndown_eqR1_eqPy_CradM8	-805.700566	-805.273790		1.33	-22.41	

M8

GINC-SL230S-GEN8-02-05\SP\ROB2PLYP-FC\GTMP2large\C14H22N2O2\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\

\0,1\C,0,1.24505,-4.122994,0.000129\C,0,1.096412,-0.782431,-0.304485\C,0,2.297766,-1.755044,-0.342258\C,0,2.026987,-3.163209,-0.905846\H,0,1.728531,-4.221862,0.980929\H,0,1.20494,-5.123542,-0.445365\H,0,3.06781,-1.278425,-0.960274\H,0,2.73192,-1.825878,0.666952\H,0,1.510474,-3.06653,-1.871265\H,0,3.001896,-3.615356,-1.131727\N,0,0.129696,-1.210582,0.703416\H,0,0.592951,-0.827281,-1.276568\C,0,1.574827,0.653867,-0.101218\C,0,1.781841,1.502817,-1.191601\C,0,1.869383,1.166171,1.168449\C,0,2.266631,2.791139,-0.97562\H,0,1.558429,1.158665,-2.199676\H,0,1.705324,0.552524,2.053139\C,0,2.532093,3.189001,0.335053\H,0,2.430816,3.475629,-1.802916\H,0,2.913543,4.187273,0.543803\N,0,2.338585,2.398031,1.397533\C,0,-1.170702,-0.786543,0.818092\O,0,-1.887378,-1.090824,1.757496\O,0,-1.515622,-0.029035,-0.24882\C,0,-2.86012,0.561352,-0.355445\C,0,-3.915416,-0.546864,-0.431667\C,0,-3.105038,1.520228,0.814424\C,0,-2.77939,1.328768,-1.67776\H,0,-3.685636,-1.235569,-1.252422\H,0,-3.958341,-1.110266,0.501523\H,0,-4.899499,-0.104816,-0.624807\H,0,-2.307535,2.269593,0.864764\H,0,-4.056314,2.043964,0.666746\H,0,-3.14331,0.980589,1.761771\H,0,-3.730419,1.832915,-1.87899\H,0,-1.987362,2.083549,-1.637253\H,0,-2.566628,0.647637,-2.508514\H,0,0.45581,-1.724401,1.509389\H,0,0.216693,-3.789225,0.163232\\Version=ES64L-G16RevA.03\State=1-A\HF=-805.2549349\MP2=-806.2953467\RMSD=8.211e-09\PG=C01[X(C14H22N2O2)]\

M8-Nrad

GINC-SL230S-GEN8-02-05\SP\ROB2PLYP-FC\GTMP2large\C14H21N2O2(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\

\0,2\C,0,0.484642,3.981219,-0.408257\C,0,1.254336,0.913547,0.246609\C,0,2.202459,2.039306,-0.218432\C,0,1.786812,3.457366,0.207956\H,0,-0.383476,3.410551,-0.065323\H,0,0.323771,5.029205,-0.129096\H,0,3.195237,1.824201,0.197583\H,0,2.298121,1.984212,-1.310578\H,0,1.711188,3.491888,1.304325\H,0,2.608891,4.135676,-0.057987\N,0,0.046865,0.871798,-0.565932\H,0,0.989361,1.073718,1.302021\C,0,1.905608,-0.467205,0.129955\C,0,2.227283,-1.217458,1.263628\C,0,2.206377,-1.024701,-1.122316\C,0,2.845089,-2.456984,1.105102\H,0,2.001512,-0.833611,2.255839\H,0,1.951791,-0.483244,-2.03116\C,0,3.106642,-2.907968,-0.188763\H,0,3.114783,-3.062986,1.965161\H,0,3.585427,-3.872299,-0.351154\N,0,2.793731,-2.213376,-1.290362\C,0,-1.132448,0.570538,0.117216\O,0,-1

.47182,1.163784,1.13237\O,0,-1.833929,-0.348508,-0.552363\C,0,-3.168109,-0.792951,-0.091748\C,0,-3.058277,-1.420575,1.301265\C,0,-4.14234,0.388253,-0.12754\C,0,-3.541784,-1.845097,-1.137714\H,0,-2.309619,-2.22032,1.300794\H,0,-2.78356,-0.677278,2.051838\H,0,-4.022803,-1.859187,1.580185\H,0,-4.156429,0.839991,-1.125189\H,0,-5.153999,0.033694,0.099728\H,0,-3.866551,1.150838,0.602823\H,0,-4.529972,-2.260742,-0.914416\H,0,-3.568293,-1.402275,-2.13826\H,0,-2.813316,-2.662056,-1.142067\H,0,0.512009,3.925122,-1.502834\\Version=ES64L-G16RevA.03\State=2-A\HF=-804.5900655\MP2=-805.6192945\RMSD=3.141e-09\PG=C01[X(C14H21N2O2)]\\

M8-Crad

GINC-NX360-M5-05-01\SP\ROB2PLYP-FC\GTMP2large\C14H21N2O2(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\

\O,2\C,0,2.099004,-3.803324,0.251126\C,0,1.207685,-0.658622,-0.429101\C,0,2.569911,-1.387472,-0.466865\C,0,2.502453,-2.88426,-0.855468\H,0,2.624356,-3.768316,1.202913\H,0,1.442165,-4.648828,0.075144\H,0,3.196609,-0.854576,-1.190743\H,0,3.065443,-1.277573,0.507415\H,0,1.835951,-3.010847,-1.718567\H,0,3.508721,-3.170094,-1.212318\N,0,0.323788,-1.306225,0.537024\H,0,0.760388,-0.732249,-1.43051\C,0,1.41997,0.821015,-0.128913\C,0,1.537031,1.753389,-1.162014\C,0,1.562313,1.296643,1.180731\C,0,1.790977,3.0886,-0.853972\H,0,1.421715,1.437695,-2.197259\H,0,1.456532,0.608444,2.01728\C,0,1.92066,3.446363,0.488154\H,0,1.881124,3.837971,-1.635155\H,0,2.120227,4.479591,0.768236\N,0,1.807937,2.57339,1.497094\C,0,-1.041411,-1.162573,0.588744\O,0,-1.755654,-1.852155,1.298047\O,0,-1.444,-0.164931,-0.232782\C,0,-2.853004,0.258245,-0.278394\C,0,-3.730988,-0.890852,-0.785347\C,0,-3.291471,0.761745,1.100746\C,0,-2.821369,1.406304,-1.290827\H,0,-3.36285,-1.252803,-1.751998\H,0,-3.737347,-1.719852,-0.076387\H,0,-4.758035,-0.534745,-0.925384\H,0,-2.61684,1.551611,1.448635\H,0,-4.302033,1.180622,1.034863\H,0,-3.293507,-0.049121,1.830796\H,0,-3.824944,1.826976,-1.413908\H,0,-2.148849,2.200878,-0.95248\H,0,-2.473273,1.051733,-2.266824\H,0,0.649031,-2.161191,0.973716\\Version=ES64L-G16RevA.03\State=2-A\HF=-804.5962575\MP2=-805.626913\RMSD=2.938e-09\PG=C01[X(C14H21N2O2)]\\

R-M8

GINC-SL250S-GEN8-04-05\SP\ROB2PLYP-FC\GTMP2large\C14H21N2O2(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\

\O,2\C,0,-1.080224,3.193641,-0.584171\C,0,-0.717285,0.103606,0.533031\C,0,-0.881631,1.450661,1.327965\C,0,-1.711263,2.554714,0.657313\H,0,-0.079089,3.581765,-0.368243\H,0,-1.700823,4.022356,-0.944586\H,0,-0.194565,-0.57889,1.224632\H,0,-1.350786,1.177689,2.281781\H,0,0.121545,1.826192,1.563747\H,0,-2.706384,2.163196,0.410664\H,0,-1.874214,3.332896,1.415926\H,0,-0.973288,2.471758,-1.4\N,0,0.110256,0.285,-0.64064\C,0,-2.057806,-0.516691,0.171082\C,0,-2.823732,-1.151115,1.154327\C,0,-2.584633,-0.479271,-1.125947\C,0,-4.058723,-1.69678,0.814326\H,0,-2.454193,-1.223151,2.175709\H,0,-2.010476,-0.018837,-1.925291\C,0,-4.488618,-1.590029,-0.509279\H,0,-4.673929,-2.19856,1.555567\H,0,-5.449259,-2.003302,-0.813099\N,0,-3.771414,-0.997068,-1.469837\C,0,1.474387,0.477851,-0.405659\O,0,2.003062,1.568357,-0.518312\O,0,2.069987,-0.68916,-0.114939\C,0,3.542176,-0.797589,0.02861\C,0,4.219187,-0.383883,-1.280845\C,0,4.005798,0.044926,1.220419\C,0,3.73745,-2.290021,0.300651\H,0,3.822746,-0.969852,-2.116911\H,0,4.067443,0.67674,-1.488572\H,0,5.295495,-0.576687,-1.210639\H,0,3.462069,-0.243566,2.126846\H,0,5.073234,-0.128426,1.397036\H,0,3.849632,1.109149,1.036256\H,0,4.802153,-2.510287,0.430999\H,0,3.207659,-2.59102,1.210239\H,0,3.358235,-2.888377,-0.533658\\Version=ES64L-G16RevA.03\State=2-A\HF=-804.5881585\MP2=-805.6175748\RMSD=5.142e-09\PG=C01[X(C14H21N2O2)]\\

TS-M8

GINC-NX360-M5-03-08\SP\ROB2PLYP-FC\GTMP2large\C14H21N2O2(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\

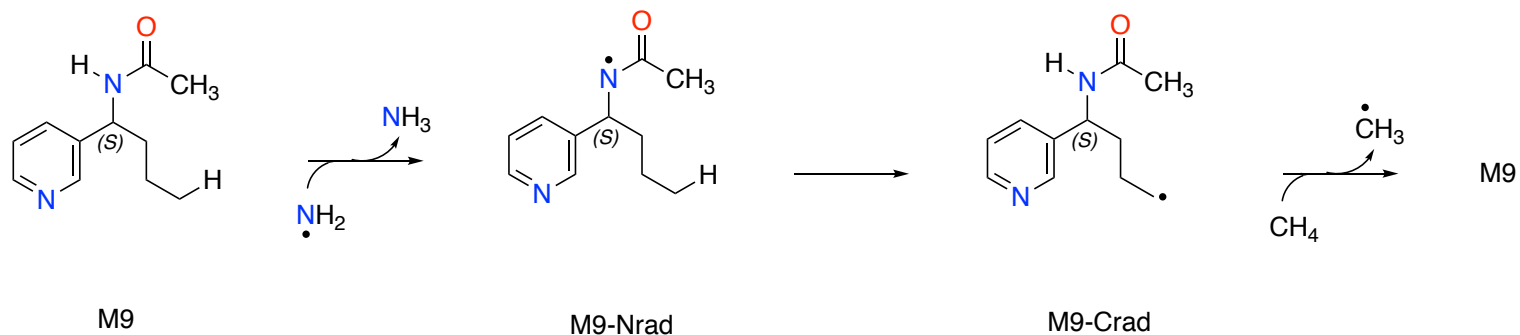
\O,2\C,0,-0.227385,3.762937,0.318989\C,0,-0.935671,0.949811,-0.458283\C,0,-1.901132,2.151414,-0.622188\C,0,-1.128746,3.462101,-0.862625\H,0,-0.732862,4.160266,1.203152\H,0,0.715436,4.270868,0.112336\H,0,-2.582969,1.937958,-1.452598\H,0,-2.514975,2.240768,0.283419\H,0,-0.533657,3.371157,-1.780542\H,0,-1.843089,4.281582,-1.029402\H,0,0.075388,2.57041,0.704573\N,0,0.013357,1.257381,0.615633\H,0,-0.411848,0.801085,-1.413257\C,0,-1.71485,-0.324082,-0.150077\C,0,-2.025222,-1.236056,-1.16054\C,0,-2.186976,-0.60583,1.138888\C,0,-2.788533,-2.361339,-0.853439\H,0,-1.66856,-1.069682,-2.174933\H,0,-1.943242,0.066111,1.958997\C,0,-3.213163,-2.535399,0.463571\H,0,-3.044664,-3.090921,-1.616361\H,0,-3.811369,-3.401859,0.741501\N,0,-2.920648,-1.679919,1.451494\C,0,1.323169,0.796454,0.563196\O,0,2.245488,1.3506,1.134926\O,0,1.402739,-0.35162,-0.15255\C,0,2.652769,-1.13306,-0.206309\C,0,3.749775,-0.315615,-

0.896251\C,0,3.053784,-1.573452,1.205098\C,0,2.252289,-2.33899,-1.059741\H,0,3.411693,0.018133,-1.88379\H,0,4.020656,0.557347,-0.300884\H,0,4.639681,-0.939933,-1.036066\H,0,2.229534,-2.113669,1.683283\H,0,3.915392,-2.248128,1.147338\H,0,3.320807,-0.715296,1.823833\H,0,3.10372,-3.018302,-1.173572\H,0,1.428744,-2.887059,-0.591376\H,0,1.930755,-2.018286,-2.056291\\Version=ES64L-G16RevA.03\State=2-A\HF=-804.5540842\MP2=-805.5975277\RMSD=2.799e-09\PG=C01[X(C14H21N2O2)]\\

P-M8

GINC-SL230S-GEN8-02-02\SP\ROB2PLYP-FC\GTMP2large\C14H21N2O2(2)\DSAKIC\20-Apr-2019\0\#\rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-2.098139,3.803772,0.251285\C,0,-1.207465,0.658814,-0.429216\C,0,-2.569472,1.388103,-0.467107\C,0,-2.501462,2.884901,-0.855509\H,0,-2.623498,3.768522,1.203061\H,0,-1.441554,4.649492,0.075395\H,0,-3.196207,0.855512,-1.191167\H,0,-3.065161,1.27822,0.507093\H,0,-1.834649,3.011389,-1.718387\H,0,-3.507535,3.171056,-1.212674\H,0,-0.648461,2.161322,0.973574\N,0,-0.323465,1.306256,0.53689\H,0,-0.760089,0.732253,-1.430612\C,0,-1.420249,-0.820725,-0.128962\C,0,-1.537474,-1.753118,-1.162022\C,0,-1.562919,-1.296244,1.180692\C,0,-1.791858,-3.088243,-0.853944\H,0,-1.421944,-1.437524,-2.197273\H,0,-1.457004,-0.608031,2.017216\C,0,-1.921774,-3.445904,0.48818\H,0,-1.88216,-3.837611,-1.635111\H,0,-2.121686,-4.479052,0.768307\N,0,-1.808928,-2.572895,1.497085\C,0,1.041649,1.162098,0.58895\O,0,1.755989,1.851653,1.298194\O,0,1.444009,0.163998,-0.232116\C,0,2.853067,-0.258824,-0.278369\C,0,3.730676,0.890396,-0.7857\C,0,3.292179,-0.762229,1.100613\C,0,2.821263,-1.406892,-1.290793\H,0,3.361954,1.252429,-1.752101\H,0,3.737448,1.719337,-0.076679\H,0,4.75764,0.534317,-0.926396\H,0,2.617941,-1.552351,1.44868\H,0,4.302885,-1.180712,1.034447\H,0,3.294096,0.048645,1.830655\H,0,3.824837,-1.827491,-1.414107\H,0,2.148889,-2.201508,-0.952255\H,0,2.472887,-1.052369,-2.266707\\Version=ES64L-G16RevA.03\State=2-A\HF=-804.5962591\MP2=-805.6269133\RMSD=2.940e-09\PG=C01[X(C14H21N2O2)]\\

System M9



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.7895	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.4544	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.8357	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.5044	-	-	-
M9	Muniz_R1acetyl_TS_Ndown_eqR1_eqPy_ver2_neutM9	-613.276890	-612.946594				
M9-Nrad	Muniz_R1acetyl_TS_Ndown_axR1_axPy_ver1_rad_opt_rev	-612.619704	-612.282337		-6.72	-2.59	
M9-Crad	Muniz_R1acetyl_TS_Ndown_eqR1_eqPy_ver2_CradM9	-612.621201	-612.293466		-24.34	-21.12	
R-M9	Muniz_R1acetyl_TS_Ndown_axR1_axPy_ver1_rad_opt_rev	-612.619704	-612.282337	-	0.00	0.00	
	Muniz_R1acetyl_TS_Ndown_eqR1_eqPy_ver2_rad_opt_rev	-612.619818	-612.281901		-0.30	1.14	
	Muniz_R1acetyl_TS_Ndown_eqR1_axPy_rad_opt_rev	-612.618876	-612.280579		2.17	4.62	
	Muniz_R1acetyl_TS_Ndown_eqR1_axPy_ver2_rad_opt_fwd	-612.618876	-612.280578		2.17	4.62	
TS-M9	Muniz_R1acetyl_TS_Ndown_eqR1_eqPy_ver2_rad	-612.603034	-612.27019		43.77	31.89	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
	Muniz_R1acetyl_TS_Ndown_axR1_axPy_ver1_rad	-612.602282	-612.269369		45.74	34.05	
	Muniz_R1acetyl_TS_Ndown_eqR1_axPy_ver2_rad	-612.598907	-612.266477		54.60	41.64	
	Muniz_R1acetyl_TS_Ndown_eqR1_eqPy_rad	-612.597546	-612.264794		58.18	46.06	
P-M9	Muniz_R1acetyl_TS_Ndown_eqR1_eqPy_ver2_rad_opt_fwd	-612.621202	-612.293467	-	-3.93	-29.22	
	Muniz_R1acetyl_TS_Ndown_eqR1_axPy_ver2_rad_opt_rev	-612.621364	-612.293392		-4.36	-29.02	
	Muniz_R1acetyl_TS_Ndown_axR1_axPy_ver1_rad_opt_fwd	-612.621364	-612.293392		-4.36	-29.02	
	Muniz_R1acetyl_TS_Ndown_eqR1_axPy_ver1_rad_opt_rev	-612.617023	-612.289115		7.04	-17.80	
M9-Crad	Muniz_R1acetyl_TS_Ndown_eqR1_eqPy_ver2_CradM9	-612.621201	-612.293466		-3.93	-29.22	

M9

GINC-SL230S-GEN8-02-02\SP\ROB2PLYP-FC\GTMP2large\C11H16N2O1\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\neka\

\O,1\C,0,-3.546372,-1.508779,0.169387\C,0,-0.400786,-0.448027,-0.344864\C,0,-0.975613,-1.85682,-0.103532\C,0,-2.39511,-2.107656,-0.648318\H,0,-3.510029,-1.85439,1.210877\H,0,-4.51335,-1.816697,-0.244652\H,0,-0.289982,-2.565047,-0.584424\H,0,-0.950364,-2.098104,0.969779\H,0,-2.450489,-1.744596,-1.683873\H,0,-2.538612,-3.194895,-0.702901\N,0,-1.07904,0.559633,0.481796\H,0,-0.622885,-0.153491,-1.37493\C,0,1.114493,-0.358346,-0.161848\C,0,1.862302,0.535802,-0.939007\C,0,1.812128,-1.108227,0.79353\C,0,3.236567,0.631168,-0.735094\H,0,1.359568,1.153246,-1.678042\H,0,1.285006,-1.821074,1.426061\C,0,3.822715,-0.16944,0.246387\H,0,3.844122,1.312091,-1.324331\H,0,4.894562,-0.121087,0.432948\N,0,3.131837,-1.027714,1.005715\C,0,-1.288045,1.840398,0.045123\O,0,-1.024946,2.202512,-1.097114\C,0,-1.887641,2.792311,1.069548\H,0,-2.758033,3.282347,0.624179\H,0,-2.189187,2.30581,2.002545\H,0,-1.154926,3.573317,1.298512\H,0,-1.18543,0.360696,1.46754\H,0,-3.517822,-0.415959,0.17718\Version=ES64L-G16RevA.03\State=1-A\HF=-612.4244377\MP2=-613.220293\RMSD=1.653e-09\PG=C01[X(C11H16N2O1)]\

M9-Nrad

GINC-NX360-M5-03-02\SP\ROB2PLYP-FC\GTMP2large\C11H15N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\neka\

\O,2\C,0,-1.540993,2.576141,0.542562\C,0,-0.331843,-0.285308,-0.650787\C,0,-0.681632,1.066342,-1.376224\C,0,-0.506015,2.356954,-0.564961\H,0,-2.559568,2.595534,0.1337\H,0,-1.37097,3.53116,1.052595\H,0,-0.494015,-1.063099,-1.413155\H,0,-0.031518,1.104528,-2.258832\H,0,-1.711322,0.987666,-1.749532\H,0,0.504541,2.38525,-0.138904\H,0,-0.559006,3.1958,-1.272366\H,0,-1.495312,1.781478,1.295672\N,0,-1.243538,-0.543714,0.434681\C,0,1.117002,-0.325912,-0.192548\C,0,2.135923,-0.58382,-1.115397\C,0,1.499854,-0.100701,1.135774\C,0,3.460967,-0.59421,-0.687454\H,0,1.892966,-0.783298,-2.157451\H,0,0.738312,0.076717,1.890734\C,0,3.724717,-0.345079,0.66027\H,0,4.272718,-0.796629,-1.380087\H,0,4.748337,-0.34344,1.031803\N,0,2.768823,-0.104197,1.564461\C,0,-2.438919,-1.184476,0.116194\O,0,-2.491215,-2.057413,-0.746485\C,0,-3.607819,-0.824565,1.00551\H,0,-3.409843,-1.166348,2.027787\H,0,-3.746584,0.26103,1.049042\H,0,-4.513452,-1.303864,0.629244\Version=ES64L-G16RevA.03\State=2-A\HF=-611.7556316\MP2=-612.5412742\RMSD=5.713e-09\PG=C01[X(C11H15N2O1)]\

M9-Crad

GINC-SL230S-GEN8-02-03\SP\ROB2PLYP-FC\GTMP2large\C11H15N2O1(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,3.335984,-1.7226,-0.540849\C,0,0.422478,-0.443263,0.474879\C,0,0.892426,-1.88784,0.206443\C,0,2.382387,-2.155805,0.524666\H,0,3.174692,-2.0367
55,-1.570127\H,0,4.312916,-1.319525,-0.292853\H,0,0.264939,-2.545731,0.818298\H,0,0.685145,-2.15756,-0.8384\H,0,2.645158,-1.69067,1.483573\H,0,2.49217,
-3.244357,0.682645\N,0,1.237987,0.516305,-0.267714\H,0,0.559844,-0.225194,1.541705\C,0,-1.062455,-0.288306,0.166951\C,0,-2.003309,-0.125165,1.184792\
C,0,-1.544054,-0.329974,-1.147838\C,0,-3.354548,-0.028603,0.856225\H,0,-1.677894,-0.05983,2.220326\H,0,-0.844639,-0.429219,-1.977664\C,0,-3.718065,-0.0
95242,-0.488309\H,0,-4.110379,0.105361,1.624651\H,0,-4.763996,-0.024243,-0.782759\N,0,-2.834515,-0.240147,-1.48506\C,0,1.327434,1.821061,0.141124\O,0,
0.667587,2.257165,1.076434\C,0,2.270391,2.698994,-0.668693\H,0,2.848666,3.321701,0.018799\H,0,2.954475,2.133817,-1.309903\H,0,1.676876,3.369078,-1.30
0335\H,0,1.925007,0.153159,-0.916353\\Version=ES64L-G16RevA.03\State=2-
A\HF=-611.7664273\MP2=-612.5520219\RMSD=2.786e-09\PG=C01[X(C11H15N2O1)]\\

R-M9

GINC-NX360-M5-03-02\SP\ROB2PLYP-FC\GTMP2large\C11H15N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-1.540993,2.576141,0.542562\C,0,-0.331843,-0.285308,-0.650787\C,0,-0.681632,1.066342,-1.376224\C,0,-0.506015,2.356954,-0.564961\H,0,-2.559568,
2.595534,0.1337\H,0,-1.37097,3.53116,1.052595\H,0,-0.494015,-1.063099,-1.413155\H,0,-0.031518,1.104528,-2.258832\H,0,-1.711322,0.987666,-1.749532\H,0,
0.504541,2.38525,-0.138904\H,0,-0.559006,3.1958,-1.272366\H,0,-1.495312,1.781478,1.295672\N,0,-1.243538,-0.543714,0.434681\C,0,1.117002,-0.325912,-0.1
92548\C,0,2.135923,-0.58382,-1.115397\C,0,1.499854,-0.100701,1.135774\C,0,3.460967,-0.59421,-0.687454\H,0,1.892966,-0.783298,-2.157451\H,0,0.738312,0.
076717,1.890734\C,0,3.724717,-0.345079,0.66027\H,0,4.272718,-0.796629,-1.380087\H,0,4.748337,-0.34344,1.031803\N,0,2.768823,-0.104197,1.564461\C,0,-2.
438919,-1.184476,0.116194\O,0,-2.491215,-2.057413,-0.746485\C,0,-3.607819,-0.824565,1.00551\H,0,-3.409843,-1.166348,2.027787\H,0,-3.746584,0.26103,1.0
49042\H,0,-4.513452,-1.303864,0.629244\\Version=ES64L-G16RevA.03\State=2-
A\HF=-611.7556316\MP2=-612.5412742\RMSD=5.713e-09\PG=C01[X(C11H15N2O1)]\\

TS-M9

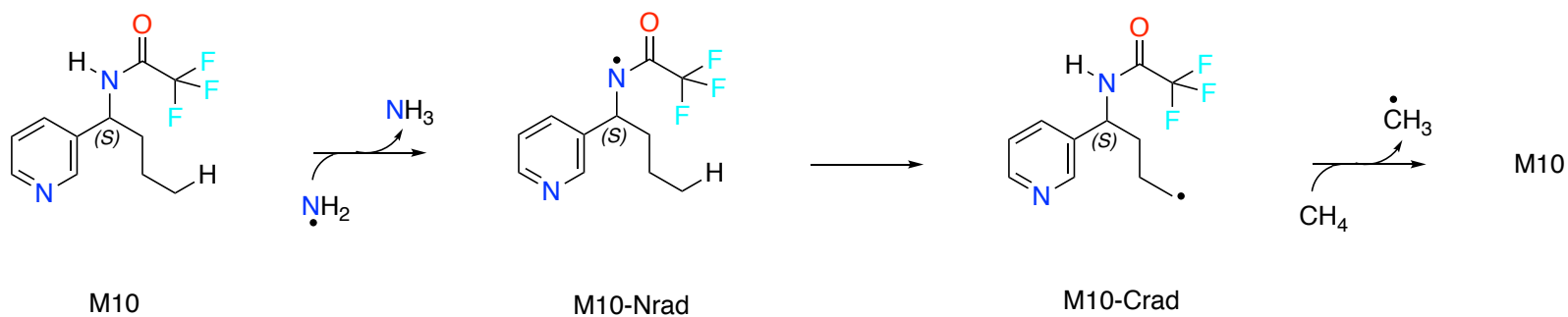
GINC-NX360-M5-04-06\SP\ROB2PLYP-FC\GTMP2large\C11H15N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,3.064117,-1.369187,-0.50533\C,0,0.369939,-0.481724,0.497661\C,0,0.766467,-1.964231,0.299657\C,0,2.277194,-2.173528,0.510468\H,0,3.061502,-1.77
0295,-1.522508\H,0,4.049936,-1.01486,-0.198736\H,0,0.185048,-2.573941,0.999731\H,0,0.487684,-2.286412,-0.711819\H,0,2.551039,-1.867683,1.528314\H,0,2.
515288,-3.244315,0.427054\H,0,2.283082,-0.324343,-0.626407\N,0,1.214325,0.364158,-0.354076\H,0,0.527605,-0.212579,1.551371\C,0,-1.102406,-0.252432,0.
177842\C,0,-2.013921,0.087828,1.178326\C,0,-1.598366,-0.38718,-1.125731\C,0,-3.358231,0.251208,0.847259\H,0,-1.671125,0.234639,2.199518\H,0,-0.916234,
-0.618503,-1.942349\C,0,-3.741372,0.076332,-0.481946\H,0,-4.092787,0.517469,1.601769\H,0,-4.78261,0.195792,-0.777501\N,0,-2.882986,-0.233539,-1.462877
\C,0,1.492879,1.643479,0.095472\O,0,0.846272,2.166729,0.998478\C,0,2.557607,2.392679,-0.683885\H,0,2.971318,3.184596,-0.05616\H,0,3.359684,1.736602,-
1.035677\H,0,2.097582,2.856199,-1.564514\\Version=ES64L-G16RevA.03\State=2-
A\HF=-611.7248433\MP2=-612.5238494\RMSD=2.069e-09\PG=C01[X(C11H15N2O1)]\\

P-M9

GINC-NX360-M5-01-09\SP\ROB2PLYP-FC\GTMP2large\C11H15N2O1(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-3.335826,-1.722659,0.541702\C,0,-0.422483,-0.443544,-0.474615\C,0,-0.892007,-1.888017,-0.20477\C,0,-2.381766,-2.156819,-0.523013\H,0,-3.174622
,-2.03522,1.571474\H,0,-4.312941,-1.320562,0.292835\H,0,-0.264171,-2.546358,-0.815785\H,0,-0.684785,-2.156501,0.840407\H,0,-2.644496,-1.692932,-1.48254
5\H,0,-2.491195,-3.245594,-0.679766\H,0,-1.925751,0.153511,0.915436\N,0,-1.238247,0.516389,0.267145\H,0,-0.559857,-0.226577,-1.54168\C,0,1.062416,-0.28
8066,-0.166798\C,0,2.003636,-0.128605,-1.18488\C,0,1.543613,-0.326003,1.14824\C,0,3.354831,-0.031772,-0.856239\H,0,1.678563,-0.066341,-2.220718\H,0,0.
843882,-0.422346,1.978134\C,0,3.717943,-0.094501,0.488601\H,0,4.11096,0.099421,-1.624849\H,0,4.763838,-0.023152,0.783103\N,0,2.834047,-0.235881,1.485

542\C,0,-1.327603,1.820933,-0.142498\O,0,-0.667373,2.256509,-1.077768\C,0,-2.270935,2.699274,0.666464\H,0,-2.848668,3.321869,-0.021581\H,0,-2.955541,2
.134383,1.307375\H,0,-1.677747,3.369433,1.298329\\Version=ES64L-G16RevA.03\State=2-
A\HF=-611.7664261\MP2=-612.5520221\RMSD=2.777e-09\PG=C01[X(C11H15N2O1)]\

System M10



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.78951	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.45441	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.83571	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.50441	-	-	-
M10	Muniz_R1COCF3_TS_Ndown_eqR1_eqPy_ver2_neutM10	-911.007989	-910.654728				
M10-Nrad	Muniz_R1COCF3_TS_Ndown_eqR1_eqPy_ver2_NradM10	-910.347191	-909.985816		2.76	9.63	
M10-Crad	Muniz_R1COCF3_TS_Ndown_eqR1_axPy_ver2_rad_opt_fwd	-910.352517	-910.002457		-24.91	-23.37	
M10-Nrad	Muniz_R1COCF3_TS_Ndown_eqR1_eqPy_ver2_NradM10	-910.347191	-909.985816		0.00	0.00	
R-M10	Muniz_R1COCF3_TS_Ndown_eqR1_eqPy_ver2_rad_opt_rev	-910.347191	-909.985816	-	0.00	0.00	
	Muniz_R1COCF3_TS_Ndown_axR1_axPy_ver1_rad_opt_rev	-910.345666	-909.985464		4.00	0.92	
	Muniz_R1COCF3_TS_Ndown_eqR1_axPy_ver2_rad_opt_rev	-910.344038	-909.983727		8.28	5.48	
	Muniz_R1COCF3_TS_Ndown_eqR1_axPy_rad_opt_rev	-910.341435	-909.982253		15.11	9.35	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
TS-M10	Muniz_R1COCF3_TS_Ndown_eqR1_eqPy_ver2_rad	-910.332782	-909.977597		37.83	21.58	
	Muniz_R1COCF3_TS_Ndown_axR1_axPy_ver1_rad	-910.332149	-909.977210		39.49	22.60	
	Muniz_R1COCF3_TS_Ndown_eqR1_axPy_ver2_rad	-910.329535	-909.974439		46.36	29.87	
	Muniz_R1COCF3_TS_Ndown_axR1_axPy_ver2_rad	-910.327357	-909.972123		52.07	35.95	
P-M10	Muniz_R1COCF3_TS_Ndown_eqR1_axPy_ver2_rad_opt_fwd	-910.352517	-910.002457	-	-13.98	-43.69	
	Muniz_R1COCF3_TS_Ndown_axR1_axPy_ver1_rad_opt_fwd	-910.352517	-910.002456		-13.98	-43.69	
	Muniz_R1COCF3_TS_Ndown_eqR1_eqPy_ver2_rad_opt_fwd	-910.352272	-910.002215		-13.34	-43.06	
	Muniz_R1COCF3_TS_Ndown_axR1_eqPy_ver2_rad_opt_fwd	-910.347825	-909.997304		-1.66	-30.16	
M10-Crad	Muniz_R1COCF3_TS_Ndown_eqR1_eqPy_ver2_CradM10	-910.352273	-910.002214		-13.34	-43.05	

M10
GINC-SL250S-GEN8-09-03\SP\ROB2PLYP-FC\GTMP2large\C11H13F3N2O1\ROOT\13-Oct-2019\0\#\rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,1\C,0,-1.963402,3.058119,-0.154149\C,0,0.571663,0.904936,0.430165\C,0,0.557046,2.385486,0.008512\C,0,-0.61332,3.226597,0.556904\H,0,-1.864708,3.240
796,-1.232168\H,0,-2.690397,3.780528,0.233609\H,0,1.498478,2.821811,0.363448\H,0,0.581887,2.466853,-1.088112\H,0,-0.731539,3.022219,1.62997\H,0,-0.31
7475,4.281102,0.483853\N,0,-0.546012,0.172937,-0.186875\H,0,0.375643,0.849544,1.505513\C,0,1.890387,0.180244,0.166219\C,0,2.260291,-0.902961,0.97426
2\C,0,2.754447,0.51977,-0.881531\C,0,3.448538,-1.576765,0.707541\H,0,1.613254,-1.211005,1.791602\H,0,2.521915,1.354182,-1.540837\C,0,4.231516,-1.1469
66,-0.365651\H,0,3.764973,-2.417593,1.317787\H,0,5.167287,-1.650106,-0.603955\N,0,3.899879,-0.118384,-1.153679\C,0,-1.286554,-0.731214,0.493271\O,0,-1.
130426,-1.06799,1.655972\C,0,-2.488865,-1.275597,-0.313656\F,0,-3.581181,-0.529373,-0.0507\F,0,-2.751586,-2.542014,0.008241\F,0,-2.269952,-1.213905,-1.65
2651\H,0,-0.709101,0.281146,-1.179365\H,0,-2.389887,2.060312,-0.020568\Version=ES64L-G16RevA.03\State=1-
A\HF=-909.8816358\MP2=-910.907421\RMSD=5.042e-09\PG=C01[X(C11H13F3N2O1)]\

M10-Nrad
GINC-SL250S-GEN8-09-03\SP\ROB2PLYP-FC\GTMP2large\C11H12F3N2O1(2)\ROOT\13-Oct-2019\0\#\rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-1.968554,3.04267,-0.263728\C,0,0.495532,0.943364,0.474785\C,0,0.527081,2.424195,0.04024\C,0,-0.671043,3.26042,0.521113\H,0,-1.831306,3.29147
9,-1.322774\H,0,-2.770796,3.678353,0.128137\H,0,1.452409,2.843503,0.454567\H,0,0.609449,2.485478,-1.051252\H,0,-0.84081,3.068117,1.590354\H,0,-0.3895
12,4.319283,0.449656\N,0,-0.522451,0.19497,-0.24117\H,0,0.334092,0.889513,1.559794\C,0,1.802412,0.202021,0.161009\C,0,2.423699,-0.581375,1.138311\C,0
,2.398933,0.258703,-1.107268\C,0,3.623347,-1.217508,0.829723\H,0,1.968657,-0.690776,2.118556\H,0,1.929611,0.823604,-1.909642\C,0,4.141191,-1.071984,-0
.458583\H,0,4.142172,-1.822581,1.567171\H,0,5.07157,-1.563337,-0.738084\N,0,3.545125,-0.353583,-1.418733\C,0,-1.19065,-0.768251,0.47107\O,0,-0.814224,-
1.282386,1.519497\C,0,-2.456409,-1.292868,-0.242267\F,0,-3.194826,-2.030693,0.592732\F,0,-2.117612,-2.050115,-1.300143\F,0,-3.216144,-0.269768,-0.687065
\H,0,-2.316443,2.005598,-0.21928\Version=ES64L-G16RevA.03\State=2-A\HF=-909.2074151\MP2=-910.2239731\RMSD=3.631e-09\PG=C01[X(C11H12F3N2O1)]\

M10-Crad

GINC-NX360-M5-02-09\SP\ROB2PLYP-FC\GTMP2large\C11H12F3N2O1(2)\DSAKIC\21-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-0.120564,3.103454,0.980116\C,0,0.540282,0.54599,-0.966253\C,0,0.852711,2.052006,-1.148603\C,0,1.094706,2.858764,0.145636\H,0,-1.035762,3.464
296,0.515235\H,0,-0.043463,3.201136,2.058837\H,0,0.377123,0.119208,-1.96134\H,0,1.748207,2.123351,-1.777141\H,0,0.030078,2.505008,-1.717178\H,0,1.876
037,2.3762,0.745247\H,0,1.520687,3.832668,-0.159996\H,0,-0.957425,1.008436,0.492952\N,0,-0.724502,0.366244,-0.256953\C,0,1.697202,-0.217509,-0.328625
\C,0,2.769756,-0.648339,-1.116606\C,0,1.763648,-0.495061,1.041893\C,0,3.837389,-1.311099,-0.517739\H,0,2.761699,-0.475658,-2.191049\H,0,0.944255,-0.20
4784,1.69701\C,0,3.79835,-1.522272,0.861626\H,0,4.679019,-1.665025,-1.105772\H,0,4.615388,-2.035487,1.365982\N,0,2.782848,-1.126767,1.63696\C,0,-1.605
738,-0.599679,-0.609318\O,0,-1.462073,-1.41451,-1.504335\C,0,-2.90886,-0.609512,0.224913\F,0,-3.079008,-1.803189,0.807736\F,0,-3.965238,-0.368652,-0.566
225\F,0,-2.904752,0.332946,1.204001\\Version=ES64L-G16RevA.03\State=2-
A\HF=-909.2243443\MP2=-910.2401745\RMSE=3.458e-09\PG=C01[X(C11H12F3N2O1)]\\

R-M10

GINC-NX360-M5-03-03\SP\ROB2PLYP-FC\GTMP2large\C11H12F3N2O1(2)\DSAKIC\21-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-1.968523,3.042842,-0.263816\C,0,0.495527,0.943405,0.474779\C,0,0.527103,2.424188,0.040268\C,0,-0.671018,3.260477,0.521065\H,0,-1.831212,3.29
1572,-1.322872\H,0,-2.770688,3.678657,0.127991\H,0,1.452405,2.843513,0.45465\H,0,0.609582,2.485537,-1.051218\H,0,-0.840842,3.068171,1.590297\H,0,-0.3
89419,4.319325,0.449639\H,0,-2.316559,2.005817,-0.219324\N,0,-0.522442,0.194931,-0.241213\H,0,0.33402,0.889515,1.559778\C,0,1.802371,0.202008,0.1610
41\C,0,2.423806,-0.581204,1.13838\C,0,2.398732,0.258501,-1.107339\C,0,3.623457,-1.21732,0.829738\H,0,1.968899,-0.690499,2.118699\H,0,1.929214,0.82320
9,-1.909738\C,0,4.141141,-1.071965,-0.458646\H,0,4.142408,-1.822249,1.567215\H,0,5.071516,-1.563303,-0.738184\N,0,3.544905,-0.353765,-1.418854\C,0,-1.1
90579,-0.768303,0.471054\O,0,-0.814044,-1.282509,1.519401\C,0,-2.456412,-1.292887,-0.242194\F,0,-3.195039,-2.030279,0.593009\F,0,-2.11771,-2.050581,-1.2
99791\F,0,-3.2159,-0.269785,-0.687401\\Version=ES64L-G16RevA.03\State=2-
A\HF=-909.2074157\MP2=-910.2239733\RMSE=3.618e-09\PG=C01[X(C11H12F3N2O1)]\\

TS-M10

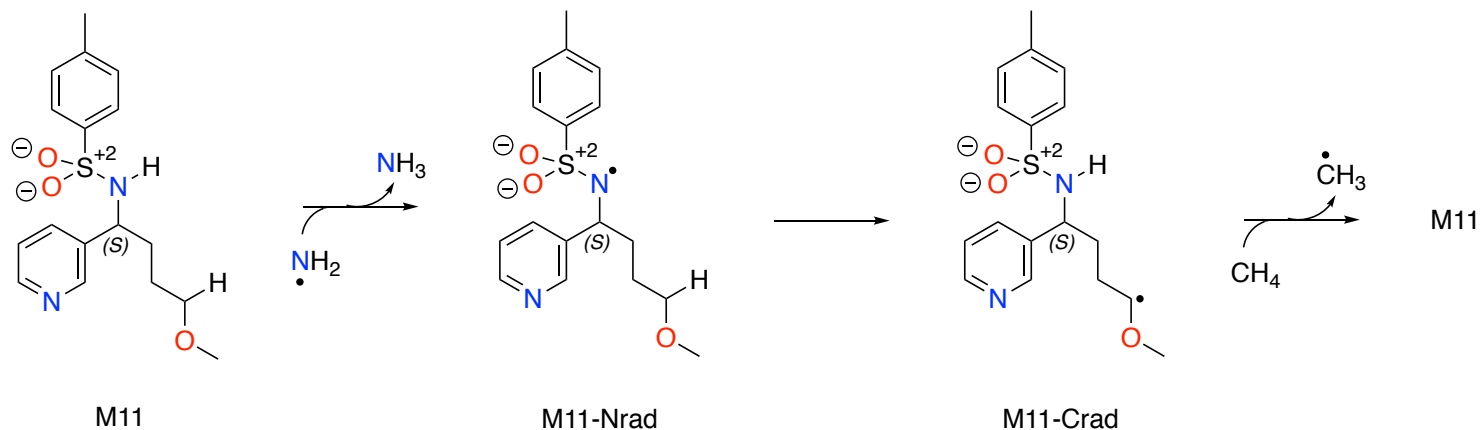
GINC-NX360-M5-04-06\SP\ROB2PLYP-FC\GTMP2large\C11H12F3N2O1(2)\DSAKIC\21-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,1.750287,2.626547,0.46302\C,0,-0.559046,0.974455,-0.522852\C,0,-0.685739,2.455636,-0.097805\C,0,0.623005,3.226394,-0.350722\H,0,1.727516,2.84
8133,1.533505\H,0,2.756286,2.683606,0.045146\H,0,-1.516843,2.901776,-0.654023\H,0,-0.947012,2.509793,0.966424\H,0,0.867728,3.196091,-1.419922\H,0,0.4
79758,4.28484,-0.087725\H,0,1.425074,1.380687,0.45553\N,0,0.613616,0.379747,0.134148\H,0,-0.424605,0.930751,-1.612502\C,0,-1.811582,0.178594,-0.17492
6\C,0,-2.621423,-0.361396,-1.175207\C,0,-2.201439,-0.029474,1.154771\C,0,-3.777839,-1.05067,-0.814058\H,0,-2.343094,-0.252566,-2.220403\H,0,-1.581459,0.
345276,1.967772\C,0,-4.076485,-1.182961,0.541649\H,0,-4.429615,-1.484126,-1.566835\H,0,-4.971104,-1.714888,0.861193\N,0,-3.305586,-0.688415,1.519288\
C,0,1.222258,-0.662897,-0.502159\O,0,0.753124,-1.287834,-1.443257\C,0,2.534987,-1.151061,0.152736\F,0,3.335674,-1.701706,-0.767625\F,0,2.268267,-2.0757
87,1.091795\F,0,3.217645,-0.14529,0.748848\\Version=ES64L-G16RevA.03\State=2-
A\HF=-909.1813402\MP2=-910.2101142\RMSE=5.812e-09\PG=C01[X(C11H12F3N2O1)]\\

P-M10

GINC-NX360-M5-02-09\SP\ROB2PLYP-FC\GTMP2large\C11H12F3N2O1(2)\DSAKIC\21-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-0.120564,3.103454,0.980116\C,0,0.540282,0.54599,-0.966253\C,0,0.852711,2.052006,-1.148603\C,0,1.094706,2.858764,0.145636\H,0,-1.035762,3.464
296,0.515235\H,0,-0.043463,3.201136,2.058837\H,0,0.377123,0.119208,-1.96134\H,0,1.748207,2.123351,-1.777141\H,0,0.030078,2.505008,-1.717178\H,0,1.876
037,2.3762,0.745247\H,0,1.520687,3.832668,-0.159996\H,0,-0.957425,1.008436,0.492952\N,0,-0.724502,0.366244,-0.256953\C,0,1.697202,-0.217509,-0.328625
\C,0,2.769756,-0.648339,-1.116606\C,0,1.763648,-0.495061,1.041893\C,0,3.837389,-1.311099,-0.517739\H,0,2.761699,-0.475658,-2.191049\H,0,0.944255,-0.20

4784,1.69701\C,0,3.79835,-1.522272,0.861626\H,0,4.679019,-1.665025,-1.105772\H,0,4.615388,-2.035487,1.365982\N,0,2.782848,-1.126767,1.63696\C,0,-1.605738,-0.599679,-0.609318\O,0,-1.462073,-1.41451,-1.504335\C,0,-2.90886,-0.609512,0.224913\F,0,-3.079008,-1.803189,0.807736\F,0,-3.965238,-0.368652,-0.566225\F,0,-2.904752,0.332946,1.204001\\Version=ES64L-G16RevA.03\State=2-A\HF=-909.2243443\MP2=-910.2401745\RMSD=3.458e-09\PG=C01[X(C11H12F3N2O1)]\\

System M11



NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.7895	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.4544	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.8357	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.5044	-	-	-
M11	Muniz_R1Tos_R2OMe_TS_Ndown_eqMe_axPy_neutM11	-1393.940204	-1393.380873				
M11-Nrad	Muniz_R1Tos_R2OMe_TS_Ndown_eqMe_eqPy_rad_opt_rev	-1393.298257	-1392.729297		-46.73	-35.89	
M11-Crad	Muniz_R1Tos_R2OMe_TS_Ndown_eqMe_eqPy_rad_opt_fwd	-1393.302296	-1392.742355		-71.03	-59.48	
R-M11	Muniz_R1Tos_R2OMe_TS_Ndown_eqMe_eqPy_rad_opt_rev	-1393.298257	-1392.729297	-	0.00	0.00	
	Muniz_R1Tos_R2OMe_TS_Ndown_eqMe_axPy_rad_opt_rev	-1393.297319	-1392.728240		2.46	2.78	
	Muniz_R1Tos_R2OMe_TS_Ndown_axMe_axPy_rad_opt_rev	-1393.297318	-1392.728235		2.47	2.79	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
TS-M11	Muniz_R1Tos_R2OMe_TS_Ndown_eqMe_axPy_rad	-1393.279158	-1392.714868		50.14	37.88	
	Muniz_R1Tos_R2OMe_TS_Ndown_axMe_eqPy_rad	-1393.278056	-1392.714717		53.04	38.28	
P-M11	Muniz_R1Tos_R2OMe_TS_Ndown_eqMe_eqPy_rad_opt_fwd	-1393.302296	-1392.742355	-	-10.60	-34.28	
	Muniz_R1Tos_R2OMe_TS_Ndown_axMe_axPy_rad_opt_fwd	-1393.300486	-1392.739987		-5.85	-28.07	
	Muniz_R1Tos_R2OMe_TS_Ndown_axMe_eqPy_rad_opt_fwd	-1393.297081	-1392.737779		3.09	-22.27	
M11-Crad	Muniz_R1Tos_R2OMe_TS_Ndown_eqMe_axPy_CradM11	-1393.297244	-1392.736524		2.66	-18.97	

M11
GINC-SL250S-GEN8-09-05\SP\ROB2PLYP-FC\GTMP2large\C17H22N2O3S1\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,1\C,0,-3.482109,0.968769,-0.723696\C,0,-1.392578,-0.679548,1.324313\C,0,-2.938077,-0.70192,1.188909\C,0,-3.567236,-0.460322,-0.192649\H,0,-3.821757,
1.686258,0.048106\H,0,-1.174431,-0.960881,2.362769\H,0,-3.255527,-1.692658,1.535657\H,0,-3.349195,0.014501,1.916063\H,0,-3.137297,-1.142944,-0.93418\
H,0,-4.632767,-0.711789,-0.123446\N,0,-0.889201,0.691757,1.079296\C,0,-0.713109,-1.702362,0.427574\C,0,-0.457482,-2.99068,0.907685\C,0,-0.353085,-1.433
597,-0.900488\C,0,0.115674,-3.937256,0.061823\H,0,-0.699117,-3.245436,1.937598\H,0,-0.502787,-0.437017,-1.308248\C,0,0.420378,-3.558631,-1.245996\H,0,
0.328547,-4.944282,0.40851\H,0,0.867002,-4.271286,-1.937789\N,0,0.198234,-2.329915,-1.727705\O,0,-4.314749,1.053415,-1.864883\C,0,-4.282159,2.325698,-
2.473707\H,0,-4.631298,3.116266,-1.789124\H,0,-3.268242,2.589904,-2.815864\H,0,-4.949293,2.286879,-3.338903\S,0,0.558821,1.170066,1.85786\O,0,0.87259
7,0.230797,2.942418\O,0,0.360955,2.601594,2.116318\C,0,1.819625,0.991251,0.602021\C,0,2.714454,-0.075264,0.670636\C,0,1.906987,1.94239,-0.417404\C,0,
3.699693,-0.19512,-0.308618\H,0,2.640691,-0.789734,1.482892\C,0,2.895467,1.804265,-1.386567\H,0,1.221216,2.782913,-0.438149\C,0,3.801446,0.732352,-1.3
53075\H,0,4.401366,-1.023814,-0.258419\H,0,2.970535,2.543274,-2.180473\C,0,4.846274,0.574442,-2.431198\H,0,5.208666,1.545639,-2.7844\H,0,5.706016,-0.0
02208,-2.075696\H,0,4.432914,0.045344,-3.299946\H,0,-1.568254,1.405098,1.342006\H,0,-2.446764,1.238772,-0.984079\Version=ES64L-G16RevA.03\State=1-
A\HF=-1392.4435201\MP2=-1393.7773393\RMSD=3.767e-09\PG=C01[X(C17H22N2O3S1)]\

M11-Nrad
GINC-SL250S-GEN8-04-05\SP\ROB2PLYP-FC\GTMP2large\C17H21N2O3S1(2)\DSAKIC\22-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-3.610908,-1.178846,-0.672846\C,0,-1.469298,1.181479,0.176716\C,0,-2.741312,1.257146,-0.69466\C,0,-3.864552,0.281718,-0.31175\H,0,-3.347027,-1.
267673,-1.74235\H,0,-3.120664,2.282297,-0.601154\H,0,-2.46385,1.120664,-1.747168\H,0,-4.074934,0.35074,0.763834\H,0,-4.782733,0.592862,-0.825335\H,0,-
2.77283,-1.595842,-0.095234\N,0,-0.699771,-0.021655,-0.14129\H,0,-1.752133,1.21762,1.237211\C,0,-0.518,2.356075,-0.082635\C,0,-0.112257,3.199671,0.9553
36\C,0,-0.018318,2.616866,-1.367226\C,0,0.725537,4.273733,0.662935\H,0,-0.443162,3.010348,1.972329\H,0,-0.283122,1.966076,-2.198073\C,0,1.147328,4.44
9869,-0.655736\H,0,1.051922,4.95683,1.441594\H,0,1.80677,5.275393,-0.918745\N,0,0.792843,3.638101,-1.660193\O,0,-4.801792,-1.89766,-0.398466\C,0,-4.66
2682,-3.28428,-0.618065\H,0,-3.88049,-3.722718,0.02174\H,0,-5.62287,-3.747898,-0.375047\H,0,-4.415108,-3.509459,-1.669004\S,0,0.06203,-0.759816,1.20321
2\O,0,-0.71334,-1.988455,1.437972\O,0,0.280178,0.192096,2.303964\C,0,1.644333,-1.19027,0.501084\C,0,1.746419,-2.319285,-0.31613\C,0,2.75812,-0.399553,
0.785601\C,0,2.985113,-2.648719,-0.856774\H,0,0.872205,-2.932338,-0.507408\C,0,3.990088,-0.747768,0.235351\H,0,2.657243,0.462563,1.435888\C,0,4.12296
3,-1.868683,-0.595469\H,0,3.073887,-3.529417,-1.487978\H,0,4.863608,-0.140495,0.458246\C,0,5.454344,-2.222047,-1.21301\H,0,6.286381,-1.791791,-0.64713

6\H,0,5.598277,-3.306643,-1.261308\H,0,5.522766,-1.839655,-2.240006\\Version=ES64L-G16RevA.03\State=2-
A\HF=-1391.790015\MP2=-1393.1120303\RMSD=2.291e-09\PG=C01[X(C17H21N2O3S1)]\\

M11-Crad

GINC-NX360-M5-02-09\SP\ROB2PLYP-FC\GTMP2large\C17H21N2O3S1(2)\DSAKIC\22-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\\nekaj\
\0,2\C,0,-4.032947,-0.077122,-0.848003\C,0,-1.281378,1.255628,0.220624\C,0,-2.431816,1.892527,-0.59598\C,0,-3.832412,1.307559,-0.313855\H,0,-3.946881,-
0.271696,-1.922456\H,0,-2.443554,2.961664,-0.356418\H,0,-2.195577,1.819288,-1.666036\H,0,-4.015186,1.284249,0.768166\H,0,-4.582226,2.000946,-0.734899\
H,0,-2.023931,-0.551689,-0.492059\N,0,-1.11754,-0.14974,-0.212825\H,0,-1.559977,1.291374,1.28261\C,0,0.005687,2.044985,0.045198\C,0,0.455087,2.917905,
1.038636\C,0,0.76316,1.968498,-1.132298\C,0,1.608178,3.669715,0.817148\H,0,-0.088629,3.000724,1.977276\H,0,0.463765,1.279344,-1.919308\C,0,2.274049,3
.519474,-0.398754\H,0,1.985727,4.353915,1.571546\H,0,3.175811,4.09264,-0.609251\N,0,1.869116,2.683507,-1.364246\O,0,-4.940791,-0.829716,-0.1733\C,0,-5
.043871,-2.184659,-0.60769\H,0,-4.110188,-2.721562,-0.403083\H,0,-5.861896,-2.632968,-0.041094\H,0,-5.271059,-2.236052,-1.681708\S,0,-0.440234,-1.26249
4,0.878651\O,0,-1.113441,-2.531048,0.563843\O,0,-0.452297,-0.711117,2.241048\C,0,1.271115,-1.399238,0.368583\C,0,1.584941,-2.123762,-0.783964\C,0,2.26
9809,-0.803925,1.136719\C,0,2.916134,-2.234014,-1.17215\H,0,0.797358,-2.603582,-1.355508\C,0,3.599109,-0.926598,0.732567\H,0,2.005135,-0.263451,2.038
662\C,0,3.942814,-1.633298,-0.426236\H,0,3.165755,-2.79985,-2.066505\H,0,4.381656,-0.466192,1.330478\C,0,5.380083,-1.732935,-0.877929\H,0,6.074129,-1.
561582,-0.049123\H,0,5.598334,-2.716572,-1.307696\H,0,5.599934,-0.984807,-1.650927\\Version=ES64L-G16RevA.03\State=2-
A\HF=-1391.7990642\MP2=-1393.1249039\RMSD=1.733e-09\PG=C01[X(C17H21N2O3S1)]\\

R-M11

GINC-SL250S-GEN8-04-05\SP\ROB2PLYP-FC\GTMP2large\C17H21N2O3S1(2)\DSAKIC\22-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\\nekaj\
\0,2\C,0,-3.610908,-1.178846,-0.672846\C,0,-1.469298,1.181479,0.176716\C,0,-2.741312,1.257146,-0.69466\C,0,-3.864552,0.281718,-0.31175\H,0,-3.347027,-1.
267673,-1.74235\H,0,-3.120664,2.282297,-0.601154\H,0,-2.46385,1.120664,-1.747168\H,0,-4.074934,0.35074,0.763834\H,0,-4.782733,0.592862,-0.825335\H,0,-
2.77283,-1.595842,-0.095234\N,0,-0.699771,-0.021655,-0.14129\H,0,-1.752133,1.21762,1.237211\C,0,-0.518,2.356075,-0.082635\C,0,-0.112257,3.199671,0.9553
36\C,0,-0.018318,2.616866,-1.367226\C,0,0.725537,4.273733,0.662935\H,0,-0.443162,3.010348,1.972329\H,0,-0.283122,1.966076,-2.198073\C,0,1.147328,4.44
9869,-0.655736\H,0,1.051922,4.95683,1.441594\H,0,1.80677,5.275393,-0.918745\N,0,0.792843,3.638101,-1.660193\O,0,-4.801792,-1.89766,-0.398466\C,0,-4.66
2682,-3.28428,-0.618065\H,0,-3.88049,-3.722718,0.02174\H,0,-5.62287,-3.747898,-0.375047\H,0,-4.415108,-3.509459,-1.669004\S,0,0.06203,-0.759816,1.20321
2\O,0,-0.71334,-1.988455,1.437972\O,0,0.280178,0.192096,2.303964\C,0,1.644333,-1.19027,0.501084\C,0,1.746419,-2.319285,-0.31613\C,0,2.75812,-0.399553,
0.785601\C,0,2.985113,-2.648719,-0.856774\H,0,0.872205,-2.932338,-0.507408\C,0,3.990088,-0.747768,0.235351\H,0,2.657243,0.462563,1.435888\C,0,4.12296
3,-1.868683,-0.595469\H,0,3.073887,-3.529417,-1.487978\H,0,4.863608,-0.140495,0.458246\C,0,5.454344,-2.222047,-1.21301\H,0,6.286381,-1.791791,-0.64713
6\H,0,5.598277,-3.306643,-1.261308\H,0,5.522766,-1.839655,-2.240006\\Version=ES64L-G16RevA.03\State=2-
A\HF=-1391.790015\MP2=-1393.1120303\RMSD=2.291e-09\PG=C01[X(C17H21N2O3S1)]\\

TS-M11

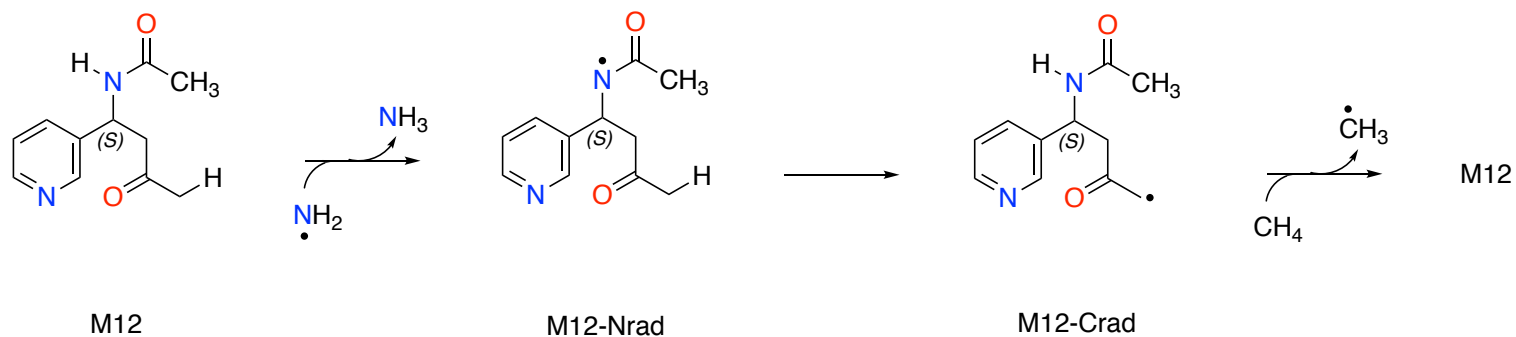
GINC-SL250S-GEN8-03-07\SP\ROB2PLYP-FC\GTMP2large\C17H21N2O3S1(2)\DSAKIC\22-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\\nekaj\
\0,2\C,0,-1.052678,2.497703,0.874188\C,0,-1.344822,-0.452587,1.333421\C,0,-1.769336,0.597105,2.398501\C,0,-2.143112,1.963157,1.789508\H,0,-0.232088,3.0
39054,1.372895\H,0,-1.031371,-1.351509,1.882422\H,0,-2.620726,0.204678,2.964895\H,0,-0.933324,0.713975,3.098745\H,0,-3.057904,1.871885,1.195353\H,0,-
2.353954,2.677006,2.59738\H,0,-0.450593,1.424762,0.532181\N,0,-0.124975,0.100924,0.720217\C,0,-2.5068,-0.864567,0.433074\C,0,-3.244606,-2.008332,0.754
479\C,0,-2.929434,-0.128424,-0.68416\C,0,-4.346258,-2.359474,-0.020269\H,0,-2.949741,-2.624888,1.601409\H,0,-2.384794,0.757096,-1.000934\C,0,-4.679016,
-1.54491,-1.102689\H,0,-4.930541,-3.247346,0.203515\H,0,-5.535066,-1.78345,-1.7322\N,0,-3.989162,-0.449183,-1.43696\O,0,-1.569708,3.171704,-0.206204\C,
0,-0.598177,3.722645,-1.09479\H,0,0.104493,4.371038,-0.55271\H,0,-0.051237,2.919822,-1.601808\H,0,-1.149865,4.31342,-1.828079\S,0,0.511152,-0.594441,-0
.673838\O,0,0.253252,0.280181,-1.831493\O,0,0.132593,-2.015597,-0.704966\C,0,2.274086,-0.507236,-0.335205\C,0,3.041053,0.504504,-0.908978\C,0,2.86224

4,-1.47265,0.485473\C,0,4.410099,0.555089,-0.643918\H,0,2.571459,1.22944,-1.56492\C,0,4.228644,-1.407594,0.739497\H,0,2.255918,-2.268204,0.905908\C,0,5.024537,-0.394712,0.18105\H,0,5.010921,1.342737,-1.092254\H,0,4.688841,-2.158498,1.377588\C,0,6.511416,-0.353876,0.442917\H,0,7.03927,-1.101845,-0.163148\H,0,6.935261,0.625143,0.198611\H,0,6.739408,-0.570791,1.492475\\Version=ES64L-G16RevA.03\\State=2-A\\HF=-1391.7522096\\MP2=-1393.092091\\RMSD=7.039e-09\\PG=C01[X(C17H21N2O3S1)]\\

P-M11

GINC-NX360-M5-02-09\SP\ROB2PLYP-FC\GTMP2large\C17H21N2O3S1(2)\DSAKIC\22-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\\nekaj\
\0,2\C,0,-4.032947,-0.077122,-0.848003\C,0,-1.281378,1.255628,0.220624\C,0,-2.431816,1.892527,-0.59598\C,0,-3.832412,1.307559,-0.313855\H,0,-3.946881,-0.271696,-1.922456\H,0,-2.443554,2.961664,-0.356418\H,0,-2.195577,1.819288,-1.666036\H,0,-4.015186,1.284249,0.768166\H,0,-4.582226,2.000946,-0.734899\H,0,-2.023931,-0.551689,-0.492059\N,0,-1.11754,-0.14974,-0.212825\H,0,-1.559977,1.291374,1.28261\C,0,0.005687,2.044985,0.045198\C,0,0.455087,2.917905,1.038636\C,0,0.76316,1.968498,-1.132298\C,0,1.608178,3.669715,0.817148\H,0,-0.088629,3.000724,1.977276\H,0,0.463765,1.279344,-1.919308\C,0,2.274049,3.519474,-0.398754\H,0,1.985727,4.353915,1.571546\H,0,3.175811,4.09264,-0.609251\N,0,1.869116,2.683507,-1.364246\O,0,-4.940791,-0.829716,-0.1733\C,0,-5.043871,-2.184659,-0.60769\H,0,-4.110188,-2.721562,-0.403083\H,0,-5.861896,-2.632968,-0.041094\H,0,-5.271059,-2.236052,-1.681708\S,0,-0.440234,-1.262494,0.878651\O,0,-1.113441,-2.531048,0.563843\O,0,-0.452297,-0.711117,2.241048\C,0,1.271115,-1.399238,0.368583\C,0,1.584941,-2.123762,-0.783964\C,0,2.269809,-0.803925,1.136719\C,0,2.916134,-2.234014,-1.17215\H,0,0.797358,-2.603582,-1.355508\C,0,3.599109,-0.926598,0.732567\H,0,2.005135,-0.263451,2.038662\C,0,3.942814,-1.633298,-0.426236\H,0,3.165755,-2.79985,-2.066505\H,0,4.381656,-0.466192,1.330478\C,0,5.380083,-1.732935,-0.877929\H,0,6.074129,-1.561582,-0.049123\H,0,5.598334,-2.716572,-1.307696\H,0,5.599934,-0.984807,-1.650927\\Version=ES64L-G16RevA.03\\State=2-A\\HF=-1391.7990642\\MP2=-1393.1249039\\RMSD=1.733e-09\\PG=C01[X(C17H21N2O3S1)]\\

System M12



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.7894	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.4544	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.8357	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.5044	-	-	-
M12	Muniz_R1acetyl_R2keton_TS_Ndown_eqMe_eqPy_neutM12	-687.308793	-686.972483				
M12-Nrad	Muniz_R1acetyl_R2keton_TS_Ndown_eqMe_eqPy_rad_opt_rev	-686.655003	-686.310351		-15.64	-8.17	
M12-Crad	Muniz_R1acetyl_R2keton_TS_Ndown_eqMe_eqPy_CradM12	-686.662024	-686.324919		-47.76	-35.73	
R-M12	Muniz_R1acetyl_R2keton_TS_Ndown_eqMe_eqPy_rad_opt_rev	-686.655003	-686.310351	-	0.00	0.00	
	Muniz_R1acetyl_R2keton_TS_Ndown_axMe_eqPy_rad_opt_fwd	-686.652963	-686.309251		5.36	2.89	
	Muniz_R1acetyl_R2keton_TS_Ndown_axMe_axPy_rad_opt_rev	-686.646681	-686.303026		21.85	19.23	
	Muniz_R1acetyl_R2keton_TS_Ndown_eqMe_axPy_rad_opt_fwd	-686.641997	-686.298960		34.15	29.91	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
TS-M12	Muniz_R1acetyl_R2keton_TS_Ndown_eqMe_eqPy_rad	-686.629631	-686.289841		66.61	53.85	
	Muniz_R1acetyl_R2keton_TS_Ndown_axMe_axPy_rad	-686.626814	-686.286993		74.01	61.33	
	Muniz_R1acetyl_R2keton_TS_Ndown_eqMe_axPy_rad	-686.620546	-686.281934		90.47	74.61	
	Muniz_R1acetyl_R2keton_TS_Ndown_axMe_eqPy_rad	-686.619699	-686.280212		92.69	79.13	
P-M12	Muniz_R1acetyl_R2keton_TS_Ndown_axMe_eqPy_rad_opt_rev	-686.662890	-686.326041	-	-20.71	-41.19	
	Muniz_R1acetyl_R2keton_TS_Ndown_axMe_axPy_rad_opt_fwd	-686.663018	-686.325648		-21.04	-40.16	
	Muniz_R1acetyl_R2keton_TS_Ndown_eqMe_eqPy_rad_opt_fwd	-686.662027	-686.324926		-18.44	-38.27	
	Muniz_R1acetyl_R2keton_TS_Ndown_eqMe_axPy_rad_opt_rev	-686.654437	-686.318048		1.49	-20.21	
M12-Crad	Muniz_R1acetyl_R2keton_TS_Ndown_eqMe_eqPy_CradM12	-686.662024	-686.324919		-18.43	-38.25	

M12
GINC-NX360-M5-01-11\SP\ROB2PLYP-FC\GTMP2large\C11H14N2O2\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,1\C,0,3.614742,-2.240851,-0.323748\C,0,0.31729,-0.191055,0.193107\C,0,1.166276,-1.418766,-0.157453\C,0,2.610745,-1.317715,0.342583\H,0,3.232502,-3.2
67412,-0.379853\H,0,0.730801,-2.313727,0.310221\H,0,1.166138,-1.62515,-1.236643\N,0,0.730645,0.943543,-0.640706\H,0,0.572036,0.109342,1.21218\C,0,-1.1
88695,-0.424004,0.118011\C,0,-2.048246,0.307096,0.949246\C,0,-1.780999,-1.318905,-0.781115\C,0,-3.422482,0.109119,0.847693\H,0,-1.631437,1.026361,1.6
48387\H,0,-1.163878,-1.916032,-1.451894\C,0,-3.897797,-0.813232,-0.086455\H,0,-4.115027,0.656833,1.480337\H,0,-4.96662,-0.993244,-0.191914\N,0,-3.1000
25,-1.520914,-0.894256\O,0,2.926999,-0.561039,1.237964\H,0,4.558354,-2.222954,0.225013\C,0,0.71719,2.231116,-0.168198\O,0,0.43558,2.50875,0.99106\C,0,
1.10204,3.301181,-1.179045\H,0,0.279259,4.017278,-1.268085\H,0,1.96945,3.84622,-0.794592\H,0,1.34336,2.908118,-2.171778\H,0,0.776917,0.800502,-1.6409
42\H,0,3.792793,-1.910125,-1.355652\Version=ES64L-G16RevA.03\State=1-A\HF=-686.364564\MP2=-687.2269499\RMSD=6.990e-09\PG=C01[X(C11H14N2O2)]\

M12-Nrad
GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C11H13N2O2(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-3.203869,-2.700203,-0.277166\C,0,-0.209573,-0.167016,-0.241229\C,0,-0.947935,-1.48257,0.054857\C,0,-2.444308,-1.388514,-0.218969\H,0,-2.909692
,-3.258175,-1.175582\H,0,-0.512496,-2.304479,-0.527718\H,0,-0.83337,-1.756449,1.112806\H,0,-2.962657,-3.333381,0.584931\N,0,-0.680526,0.832847,0.70716
3\H,0,-0.436596,0.140807,-1.27008\C,0,1.312541,-0.269279,-0.106238\C,0,2.118102,0.671606,-0.760135\C,0,1.959694,-1.250226,0.654819\C,0,3.501632,0.5768
48,-0.645404\H,0,1.650283,1.467868,-1.331946\H,0,1.387298,-2.003113,1.192399\C,0,4.037251,-0.449958,0.134149\H,0,4.154396,1.287107,-1.144463\H,0,5.11
5098,-0.551782,0.25094\N,0,3.288711,-1.352424,0.778076\O,0,-3.002593,-0.317809,-0.376153\H,0,-4.277766,-2.507359,-0.310754\C,0,-1.093497,2.048756,0.17
2893\O,0,-0.53985,2.536661,-0.811752\C,0,-2.18394,2.743811,0.949181\H,0,-1.897575,2.844912,2.001075\H,0,-2.377715,3.726429,0.514614\H,0,-3.093537,2.13
4317,0.909797\Version=ES64L-G16RevA.03\State=2-A\HF=-685.6991585\MP2=-686.5507612\RMSD=6.245e-09\PG=C01[X(C11H13N2O2)]\

M12-Crad

GINC-SL250S-GEN8-04-01\SP\ROB2PLYP-FC\GTMP2large\C11H13N2O2(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-3.593263,-2.080417,0.491172\C,0,-0.337644,-0.257728,-0.198261\C,0,-1.118814,-1.532457,0.15177\C,0,-2.577949,-1.462188,-0.311982\H,0,-3.371963,-2.569051,1.435342\H,0,-0.651166,-2.384685,-0.359593\H,0,-1.070688,-1.754997,1.22521\N,0,-0.819513,0.854833,0.629743\H,0,-0.603689,0.019709,-1.220872\C,0,1.178369,-0.405344,-0.115956\C,0,1.99861,0.362007,-0.954193\C,0,1.816536,-1.254481,0.796036\C,0,3.381429,0.242916,-0.845983\H,0,1.544961,1.047317,-1.664369\H,0,1.231699,-1.877483,1.472029\C,0,3.904221,-0.639195,0.101503\H,0,4.044444,0.820492,-1.483669\H,0,4.981059,-0.757491,0.212545\N,0,3.144393,-1.380519,0.9157\O,0,-2.87378,-0.909563,-1.381964\C,0,-0.862977,2.142437,0.157255\O,0,-0.596717,2.432021,-1.002577\C,0,-1.28499,3.19526,1.171503\H,0,-0.457848,3.897104,1.319947\H,0,-2.123183,3.76177,0.755821\H,0,-1.580413,2.782928,2.14147\H,0,-4.618369,-2.062803,0.136499\H,0,-0.856215,0.712469,1.630672\\Version=ES64L-G16RevA.03\State=2-A\HF=-685.7117086\MP2=-686.5658263\RMSD=2.049e-09\PG=C01[X(C11H13N2O2)]\\

R-M12

GINC-SL230S-GEN8-02-08\SP\ROB2PLYP-FC\GTMP2large\C11H13N2O2(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-3.203869,-2.700203,-0.277166\C,0,-0.209573,-0.167016,-0.241229\C,0,-0.947935,-1.48257,0.054857\C,0,-2.444308,-1.388514,-0.218969\H,0,-2.909692,-3.258175,-1.175582\H,0,-0.512496,-2.304479,-0.527718\H,0,-0.83337,-1.756449,1.112806\H,0,-2.962657,-3.333381,0.584931\N,0,-0.680526,0.832847,0.707163\H,0,-0.436596,0.140807,-1.27008\C,0,1.312541,-0.269279,-0.106238\C,0,2.118102,0.671606,-0.760135\C,0,1.959694,-1.250226,0.654819\C,0,3.501632,0.576848,-0.645404\H,0,1.650283,1.467868,-1.331946\H,0,1.387298,-2.003113,1.192399\C,0,4.037251,-0.449958,0.134149\H,0,4.154396,1.287107,-1.144463\H,0,5.115098,-0.551782,0.25094\N,0,3.288711,-1.352424,0.778076\O,0,-3.002593,-0.317809,-0.376153\H,0,-4.277766,-2.507359,-0.310754\C,0,-1.093497,2.048756,0.172893\O,0,-0.53985,2.536661,-0.811752\C,0,-2.18394,2.743811,0.949181\H,0,-1.897575,2.844912,2.001075\H,0,-2.377715,3.726429,0.514614\H,0,-3.093537,2.134317,0.909797\\Version=ES64L-G16RevA.03\State=2-A\HF=-685.6991585\MP2=-686.5507612\RMSD=6.245e-09\PG=C01[X(C11H13N2O2)]\\

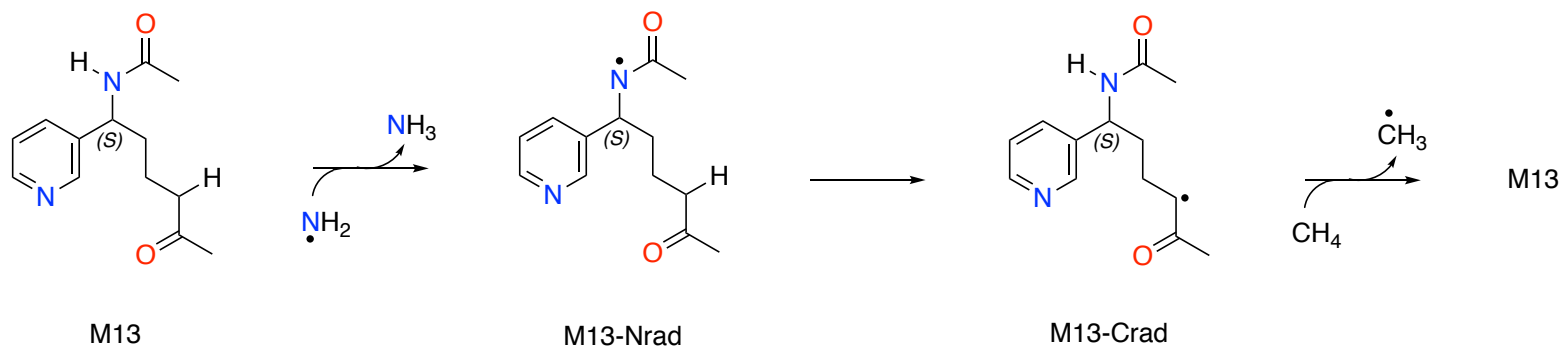
TS-M12

GINC-NX360-M5-01-09\SP\ROB2PLYP-FC\GTMP2large\C11H13N2O2(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,3.031325,-0.673933,-0.869224\C,0,0.28634,-0.355069,0.357524\C,0,0.888471,-1.727754,-0.066809\C,0,2.403762,-1.673166,0.050629\H,0,2.952195,-0.906281,-1.935166\H,0,0.49167,-2.516501,0.575868\H,0,0.602243,-1.939455,-1.104456\H,0,2.110313,0.261048,-0.786875\N,0,0.948259,0.717502,-0.405578\H,0,0.469387,-0.214698,1.430295\C,0,-1.216367,-0.306024,0.127147\C,0,-2.108043,-0.214343,1.197582\C,0,-1.759421,-0.361427,-1.163341\C,0,-3.477407,-0.209524,0.940442\H,0,-1.732183,-0.137659,2.214542\H,0,-1.099298,-0.40177,-2.028676\C,0,-3.905879,-0.283474,-0.385107\H,0,-4.198843,-0.140912,1.749232\H,0,-4.968227,-0.280189,-0.62337\N,0,-3.069263,-0.353668,-1.429026\O,0,3.038804,-2.291599,0.887136\H,0,4.017904,-0.322324,-0.567307\C,0,1.032637,1.965445,0.201132\O,0,0.326105,2.251971,1.161437\C,0,1.951977,2.961202,-0.476014\H,0,1.516906,3.272761,-1.432386\H,0,2.06579,3.836323,0.165638\H,0,2.935521,2.528252,-0.687458\\Version=ES64L-G16RevA.03\State=2-A\HF=-685.6574526\MP2=-686.5246048\RMSD=1.805e-09\PG=C01[X(C11H13N2O2)]\\

P-M12

GINC-NX360-M5-03-02\SP\ROB2PLYP-FC\GTMP2large\C11H13N2O2(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,3.321045,-1.925861,-1.166367\C,0,0.188651,-0.428355,0.511408\C,0,0.966121,-1.136127,-0.612338\C,0,2.361858,-1.564606,-0.159321\H,0,3.095853,-1.86159,-2.226553\H,0,0.412364,-2.037735,-0.910068\H,0,1.031318,-0.495997,-1.495652\H,0,1.119034,0.907447,1.862032\N,0,0.818892,0.846631,0.900498\H,0,0.298601,-1.057181,1.399222\C,0,-1.303325,-0.310106,0.223221\C,0,-2.221164,-1.011444,1.010397\C,0,-1.821199,0.462668,-0.830073\C,0,-3.583206,-0.920858,0.728364\H,0,-1.87193,-1.625263,1.838691\H,0,-1.145733,1.034233,-1.460833\C,0,-3.982366,-0.122859,-0.342397\H,0,-4.317718,-1.45451,1.324679\H,0,-5.037019,-0.026074,-0.596453\N,0,-3.126147,0.560853,-1.112154\H,0,4.302074,-2.268458,-0.854441\O,0,2.663062,-1.619208,1.044266\C,0,1.215023,1.84493,0.058672\O,0,1.008103,1.83765,-1.152949\C,0,1.943303,3.005003,0.724795\H,0,2.937205,3.099293,0.276423\H,0,1.398461,3.928522,0.506844\H,0,2.050502,2.90308,1.80901\\Version=ES64L-G16RevA.03\State=2-A\HF=-685.7132594\MP2=-686.5671706\RMSD=4.096e-09\PG=C01[X(C11H13N2O2)]\\

System M13



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.7895	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.4544 -	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.8357	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.5044 -	-	-	-
M13	Muniz_R1acetyl_R2acetyl_TS_Ndown_eqR1_axPy_neutM13	-765.869472	-765.478593				
M13-Nrad	Muniz_R1acetyl_R2acetyl_TS_Ndown_eqR1_axPy_NradM13	-765.215275	-764.816153		-14.57	-7.36	
M13-Crad	Muniz_R1acetyl_R2acetyl_TS_Ndown_eqR1_axPy_CradM13	-765.230332	-764.838006		-67.79	-54.05	
R-M13	Muniz_R1acetyl_R2acetyl_TS_Ndown_eqR1_eqPy_rad_opt_rev	-765.220668	-764.821285	-	0.00	0.00	
	Muniz_R1acetyl_R2acetyl_TS_Ndown_axR1_axPy_rad_opt_rev	-765.218324	-764.818421		6.15	7.52	
	Muniz_R1acetyl_R2acetyl_TS_Ndown_axR1_eqPy_rad_opt_rev	-765.216336	-764.817245		11.37	10.61	
TS-M13	Muniz_R1acetyl_R2acetyl_TS_Ndown_eqR1_axPy_TSM13	-765.201152	-764.805426		51.24	41.64	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
P-M13	Muniz_R1acetyl_R2acetyl_TS_Ndown_eqR1_eqPy_rad_opt_fwd	-765.239246	-764.846528	-	-48.78	-66.28	
	Muniz_R1acetyl_R2acetyl_TS_Ndown_eqR1_axPy_rad_opt_rev	-765.236565	-764.844095		-41.74	-59.89	
	Muniz_R1acetyl_R2acetyl_TS_Ndown_axR1_axPy_rad_opt_fwd	-765.236429	-764.842733		-41.38	-56.31	
	Muniz_R1acetyl_R2acetyl_TS_Ndown_axR1_eqPy_rad_opt_fwd	-765.234242	-764.841253		-35.64	-52.43	

M13
GINC-SL250S-GEN8-06-07\SP\ROB2PLYP-FC\GTMP2large\C13H18N2O2\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,1\C,0,-2.285987,0.424013,-0.05581\C,0,0.904104,0.518729,0.860278\C,0,-0.377087,0.365959,1.724625\C,0,-1.602339,-0.32914,1.103001\H,0,-2.471887,1.465
566,0.248906\H,0,1.690328,0.884085,1.529738\H,0,-0.098323,-0.205722,2.619159\H,0,-0.654907,1.367551,2.077388\H,0,-1.32302,-1.334013,0.762395\H,0,-2.33
1406,-0.470047,1.910641\N,0,0.785788,1.584312,-0.127129\C,0,1.377798,-0.807635,0.269771\C,0,1.777339,-1.849839,1.117337\C,0,1.449682,-1.055461,-1.105
822\C,0,2.20387,-3.056462,0.571717\H,0,1.765807,-1.713186,2.196555\H,0,1.1836,-0.274814,-1.814769\C,0,2.218929,-3.189803,-0.818259\H,0,2.524651,-3.876
487,1.207583\H,0,2.543373,-4.11988,-1.282147\N,0,1.853435,-2.210805,-1.650772\C,0,1.605342,2.686694,-0.111456\C,0,-3.619264,-0.177019,-0.501725\O,0,-3.
808788,-0.480652,-1.663892\C,0,-4.699715,-0.369208,0.551417\H,0,-4.478216,-1.257765,1.156418\H,0,-4.757026,0.48318,1.238204\H,0,-5.661858,-0.519745,0.
057627\C,0,1.353699,3.697258,-1.220265\H,0,0.454945,3.493378,-1.811108\H,0,1.273973,4.693384,-0.77631\H,0,2.21927,3.706797,-1.89092\O,0,2.484282,2.84
8542,0.724833\H,0,-1.658497,0.439369,-0.952587\H,0,0.062451,1.532165,-0.827846\\Version=ES64L-G16RevA.03\State=1-
A\HF=-764.8180775\MP2=-765.7934068\RMSD=5.554e-09\PG=C01[X(C13H18N2O2)]\\

M13-Nrad
GINC-SL250S-GEN8-06-03\SP\ROB2PLYP-FC\GTMP2large\C13H17N2O2(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-2.348201,-0.351342,0.263457\C,0,0.754427,0.947556,0.705742\C,0,-0.298416,0.324653,1.694024\C,0,-1.186451,-0.810836,1.167111\H,0,-2.949472,0.4
09427,0.772348\H,0,1.285175,1.707846,1.296579\H,0,0.293088,-0.049291,2.539983\H,0,-0.909903,1.151402,2.070467\H,0,-0.566977,-1.55101,0.646541\H,0,-1.
607771,-1.325821,2.041381\N,0,0.081914,1.553866,-0.420856\C,0,1.757378,-0.094535,0.223479\C,0,2.848619,-0.433434,1.030116\C,0,1.637323,-0.759032,-1.0
04183\C,0,3.741233,-1.410601,0.597653\H,0,2.998897,0.066359,1.984997\H,0,0.820812,-0.505832,-1.67569\C,0,3.514764,-2.01612,-0.639701\H,0,4.598355,-1.6
93692,1.201539\H,0,4.191203,-2.78407,-1.011378\N,0,2.487095,-1.699898,-1.435059\C,0,-0.181503,2.915238,-0.339652\C,0,-3.296215,-1.474838,-0.143961\O,0
,-4.488655,-1.411584,0.090888\C,0,-2.695985,-2.675299,-0.860435\H,0,-1.995818,-2.367272,-1.645831\H,0,-2.128426,-3.291561,-0.151258\H,0,-3.496643,-3.28
2537,-1.287665\C,0,-0.339867,3.617408,-1.667065\H,0,-1.273091,3.296305,-2.144472\H,0,-0.368657,4.697446,-1.51102\H,0,0.478718,3.354691,-2.345753\O,0,-
0.36867,3.463341,0.746446\H,0,-1.936575,0.102878,-0.64755\\Version=ES64L-G16RevA.03\State=2-
A\HF=-764.1516306\MP2=-765.1164301\RMSD=4.906e-09\PG=C01[X(C13H17N2O2)]\\

M13-Crad
GINC-SL250S-GEN8-06-03\SP\ROB2PLYP-FC\GTMP2large\C13H17N2O2(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,-2.53153,-0.176746,0.834234\C,0,0.638607,0.74867,1.030766\C,0,-0.328709,0.189453,2.107567\C,0,-1.418671,-0.791366,1.618857\H,0,-2.955269,0.763

778,1.185052\H,0,1.380972,1.33621,1.583537\H,0,0.279329,-0.332803,2.855283\H,0,-0.795934,1.041423,2.616742\H,0,-0.958227,-1.617549,1.066688\H,0,-1.857558,-1.247076,2.524629\N,0,-0.055762,1.66877,0.141935\C,0,1.394912,-0.370472,0.310297\C,0,2.40046,-1.085798,0.97238\C,0,1.116446,-0.742426,-1.010567\C,0,3.054361,-2.121898,0.312112\H,0,2.673625,-0.828882,1.994429\H,0,0.368334,-0.196611,-1.581325\C,0,2.676759,-2.416191,-0.999987\H,0,3.842453,-2.688871,0.798897\H,0,3.160475,-3.2239,-1.546698\N,0,1.728506,-1.742898,-1.659181\C,0,0.465326,2.759056,-0.524157\C,0,-3.211302,-0.754402,-0.3034\O,0,-4.170789,-0.148744,-0.804717\C,0,-2.756039,-2.093413,-0.866843\H,0,-1.711499,-2.059501,-1.199613\H,0,-2.831202,-2.887809,-0.113835\H,0,-3.392095,-2.347602,-1.716603\C,0,1.904407,3.13814,-0.207791\H,0,2.593283,2.305154,-0.386489\H,0,2.176546,3.976186,-0.850069\H,0,2.013178,3.44517,0.839605\O,0,-0.219512,3.391539,-1.313933\H,0,-1.003366,1.44357,-0.141124\\Version=ES64L-G16RevA.03\State=2-A\HF=-764.1700854\MP2=-765.1388312\RMSE=1.488e-09\PG=C01[X(C13H17N2O2)]\\

R-M13

GINC-NX360-M5-03-08\SP\ROB2PLYP-FC\GTMP2large\C13H17N2O2(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\0,2\C,0,2.670375,-0.415444,-0.327762\C,0,-0.482514,-0.246431,0.239614\C,0,0.301279,-1.468726,-0.287365\C,0,1.767574,-1.549222,0.163705\H,0,2.55841,-0.266859,-1.413045\H,0,-0.217621,-2.369105,0.065171\H,0,0.235645,-1.47649,-1.383117\H,0,1.811,-1.589149,1.26007\H,0,2.184998,-2.502152,-0.179968\H,0,2.391544,0.544107,0.126305\N,0,-0.172505,0.956522,-0.518219\H,0,-0.241686,-0.086172,1.300924\C,0,-1.996873,-0.439875,0.121814\C,0,-2.808793,-0.531302,1.255376\C,0,-2.621722,-0.530567,-1.131512\C,0,-4.178948,-0.729942,1.094359\H,0,-2.372777,-0.453819,2.248584\H,0,-2.028695,-0.446627,-2.040208\C,0,-4.690979,-0.813445,-0.200881\H,0,-4.83769,-0.813587,1.953712\H,0,-5.756763,-0.96339,-0.364744\N,0,-3.934685,-0.713254,-1.301691\C,0,-0.006287,2.143281,0.186507\O,0,0.710322,2.184847,1.183778\C,0,-0.643206,3.360218,-0.442939\H,0,-0.196232,3.546461,-1.425866\H,0,-1.714597,3.192928,-0.602169\H,0,-0.491154,4.227905,0.201953\C,0,4.149855,-0.660979,-0.047316\O,0,4.556901,-1.712345,0.411167\C,0,5.094241,0.486954,-0.36544\H,0,4.931589,0.8621,-1.38309\H,0,4.903057,1.324833,0.317403\H,0,6.129494,0.159005,-0.251056\\Version=ES64L-G16RevA.03\State=2-A\HF=-764.1580838\MP2=-765.1213673\RMSE=2.071e-09\PG=C01[X(C13H17N2O2)]\\

TS-M13

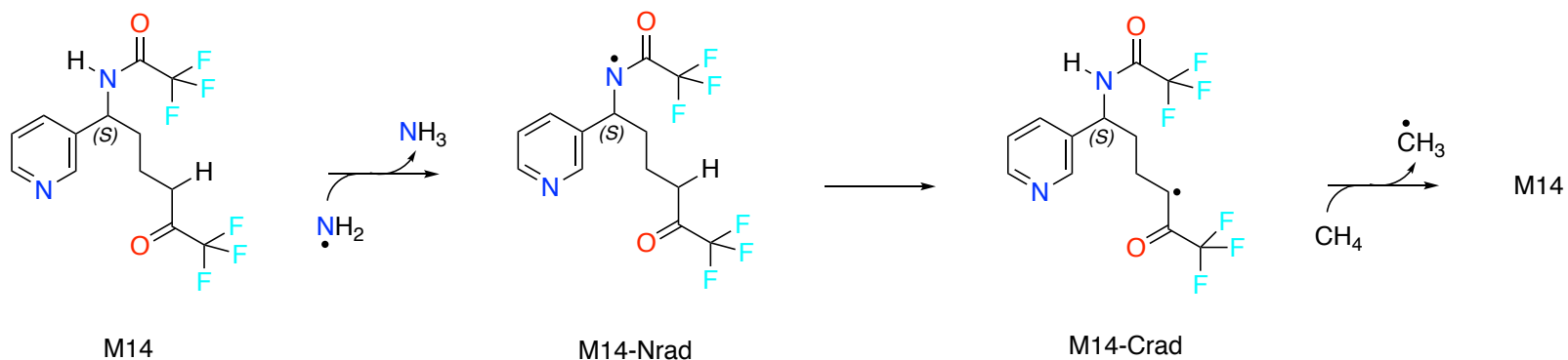
GINC-SL250S-GEN8-06-03\SP\ROB2PLYP-FC\GTMP2large\C13H17N2O2(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\0,2\C,0,-2.152571,-0.643955,0.852613\C,0,0.536924,0.659414,1.313852\C,0,-0.081235,-0.400963,2.268778\C,0,-1.013507,-1.387722,1.535064\H,0,-2.893129,-0.233994,1.547034\H,0,1.051397,1.394032,1.950352\H,0,0.727173,-0.947568,2.765459\H,0,-0.645542,0.13061,3.044784\H,0,-0.431295,-1.958773,0.804034\H,0,-1.407448,-2.111823,2.262329\H,0,-1.587168,0.415221,0.520829\N,0,-0.563652,1.361026,0.676316\C,0,1.58046,0.048478,0.382344\C,0,2.874689,-0.199254,0.851291\C,0,1.303323,-0.334274,-0.934574\C,0,3.804354,-0.809371,0.013449\H,0,3.154104,0.092446,1.861952\H,0,0.321734,-0.13757,-1.361514\C,0,3.406072,-1.161068,-1.277121\H,0,4.818255,-1.00555,0.349634\H,0,4.102848,-1.644685,-1.959622\N,0,2.177683,-0.929839,-1.753685\C,0,-0.394368,2.330359,-0.279707\C,0,-2.845251,-1.166311,-0.376599\O,0,-3.904709,-0.664835,-0.724257\C,0,-2.204361,-2.287343,-1.175803\H,0,-1.182892,-2.032852,-1.482048\H,0,-2.136691,-3.20038,-0.570842\H,0,-2.812406,-2.484758,-2.060406\C,0,-1.623399,2.721046,-1.074411\H,0,-1.343819,2.835609,-2.125655\H,0,-2.438944,1.998141,-0.986037\H,0,-1.979432,3.695889,-0.722744\O,0,0.684489,2.91027,-0.387119\\Version=ES64L-G16RevA.03\State=2-A\HF=-764.1187926\MP2=-765.1002239\RMSE=5.095e-09\PG=C01[X(C13H17N2O2)]\\

P-M13

GINC-SL230S-GEN8-02-02\SP\ROB2PLYP-FC\GTMP2large\C13H17N2O2(2)\DSAKIC\20-Apr-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\0,2\C,0,2.553276,-1.405155,-0.717193\C,0,-0.343245,-0.434357,-0.011279\C,0,0.010737,-1.770523,-0.707198\C,0,1.425298,-2.313325,-0.367691\H,0,2.855747,-1.304584,-1.758287\H,0,-0.721388,-2.527369,-0.404578\H,0,-0.108996,-1.64906,-1.793406\H,0,1.470317,-2.519181,0.706821\H,0,1.543929,-3.266883,-0.901221\H,0,0.564247,0.5832,-1.651759\N,0,0.379706,0.654879,-0.65803\H,0,0.016622,-0.5002,1.021273\C,0,-1.856741,-0.225481,0.025299\C,0,-2.626905,-0.797588,1.043747\C,0,-2.539254,0.500822,-0.957891\C,0,-4.009381,-0.63184,1.032653\H,0,-2.146276,-1.363053,1.840249\H,0,-1.983741,0.988287,-1.75673\C,0,-4.580958,0.103561,-0.007158\H,0,-4.632223,-1.057577,1.813907\H,0,-5.658622,0.251953,-0.052036\N,0,-3.867285,0.665824,-0.989052\C,0,0.885173,1.806996,-0.09673

8\O,0,1.526983,2.59359,-0.783935\C,0,0.643495,2.018953,1.38565\H,0,-0.401703,1.848978,1.664165\H,0,1.272176,1.331142,1.963893\H,0,0.924546,3.044408,1.628781\C,0,3.219057,-0.602796,0.284335\O,0,2.852979,-0.646841,1.47142\C,0,4.322775,0.341354,-0.156709\H,0,4.904232,-0.061321,-0.992894\H,0,3.870649,1.286799,-0.484794\H,0,4.98388,0.55183,0.68734\\Version=ES64L-G16RevA.03\State=2-A\HF=-764.17881\MP2=-765.147829\RMSD=2.369e-09\PG=C01[X(C13H17N2O2)]\

System M14



NAME	SYSTEM	H(kJ/mol)			ΔH(kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
1	NulC_rad	-39.804412	-39.773085	-39.789	0.00	0.00	0.00
1H	NulC_neut	-40.469373	-40.434258	-40.454	-	-	-
15	NH3_Nrad	-55.849865	-55.829037	-55.835	0.00	0.00	0.00
15H	NH3_neut	-56.509611	-56.494282	-56.504	-	-	-
M14	Muniz_R1COCF3_R2COCF3_TS_Ndown_axR1_axPy_neutM14	-1361.325344	-1360.888579				
M14-Nrad	Muniz_R1COCF3_R2COCF3_TS_Ndown_axR1_axPy_NradM14	-1360.672628			-18.46		a)
M14-Crad	Muniz_R1COCF3_R2COCF3_TS_Ndown_axR1_axPy_CradM14	-1360.695028	-1360.256312		-90.96	-75.89	b)
R-M14	Muniz_R1COCF3_R2COCF3_TS_Ndown_eqR1_eqPy_rad_opt_rev	-1360.673870	-1360.230650	-	0.00	0.00	
	Muniz_R1COCF3_R2COCF3_TS_Ndown_axR1_axPy_rad_opt_fwd	-1360.670177	-1360.227636		9.70	7.91	
TS-M14	Muniz_R1COCF3_R2COCF3_TS_Ndown_axR1_axPy_rad	-1360.659008	-1360.217682		39.02	34.05	
	Muniz_R1COCF3_R2COCF3_TS_Ndown_eqR1_eqPy_rad	-1360.659327	-1360.217488		38.18	34.56	

NAME	SYSTEM	H(kJ/mol)			ΔH (kJ/mol)		
		B3LYP	B2PLYP	G3B3	B3LYP	B2PLYP	G3B3
P-M14	Muniz_R1COCF3_R2COCF3_TS_Ndown_eqR1_axPy_rad_opt_fwd	-1360.699028	-1360.259166	-	-66.05	-74.86	
	Muniz_R1COCF3_R2COCF3_TS_Ndown_eqR1_eqPy_rad_opt_fwd	-1360.696335	-1360.256306	-	-58.98	-67.36	
	Muniz_R1COCF3_R2COCF3_TS_Ndown_axR1_axPy_rad_opt_rev	-1360.693177	-1360.253387	-	-50.69	-59.70	
	Muniz_R1COCF3_R2COCF3_TS_Ndown_axR1_eqPy_rad_opt_fwd	-1360.689574	-1360.250966	-	-41.23	-53.34	

M14
GINC-SL230S-GEN8-02-06\SP\ROB2PLYP-FC\GTMP2large\C13H12F6N2O2\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,1\C,0,1.877355,-0.057288,0.577482\C,0,-1.494859,0.232277,0.534465\C,0,-0.454485,0.206806,1.688336\C,0,0.945776,0.792833,1.448711\H,0,1.866145,-1.111298,0.892035\H,0,-2.415412,-0.173601,0.955248\H,0,-0.91181,0.76135,2.5181\H,0,-0.368678,-0.833941,2.022332\H,0,0.87586,1.805481,1.035043\H,0,1.426624,0.913731,2.425577\N,0,-1.132758,-0.637971,-0.597418\C,0,-1.82207,1.639621,0.052064\C,0,-2.941812,2.309895,0.556009\C,0,-1.033419,2.337532,-0.873175\C,0,-3.217058,3.606919,0.130629\H,0,-3.595252,1.816345,1.272137\H,0,-0.146437,1.876859,-1.3094\C,0,-2.358333,4.198094,-0.796629\H,0,-4.082672,4.146547,0.50273\H,0,-2.540545,5.209183,-1.155755\N,0,-1.282286,3.580299,-1.296955\C,0,-1.538253,-1.90127,-0.903562\O,0,-1.179385,-2.503079,-1.899302\C,0,-2.517312,-2.587602,0.084921\C,0,3.316719,0.412691,0.633399\O,0,3.740416,1.284552,1.354086\C,0,4.286916,-0.316065,-0.33405\F,0,5.545684,0.088553,-0.176313\F,0,4.230323,-1.649956,-0.127132\F,0,3.9132,-0.081449,-1.612149\F,0,-3.695844,-1.921563,0.140206\F,0,-2.013205,-2.617763,1.343799\F,0,-2.761264,-3.836892,-0.293558\H,0,1.582287,-0.079164,-0.479018\H,0,-0.538094,-0.254582,-1.32195\Version=ES64L-G16RevA.03\State=1-A\HF=-1359.7265239\MP2=-1361.1611136\RMSD=4.651e-09\PG=C01[X(C13H12F6N2O2)]\

M14-Nrad
GINC-SL230S-GEN8-02-05\SP\ROB2PLYP-FC\GTMP2large\C13H11F6N2O2(2)\SSHKUNNI\13-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,1.444857,0.813159,0.78599\C,0,-1.801388,-0.15612,1.01281\C,0,-0.838811,0.649751,1.973649\C,0,0.21318,1.551098,1.31856\H,0,1.920428,0.209063,1.57285\H,0,-2.443815,-0.750465,1.677369\H,0,-1.511487,1.263735,2.584663\H,0,-0.370719,-0.080455,2.643252\H,0,-0.238232,2.143132,0.514856\H,0,0.544864,2.280419,2.067249\N,0,-1.003217,-1.005076,0.170478\C,0,-2.665144,0.779615,0.175183\C,0,-3.809819,1.349644,0.741003\C,0,-2.364669,1.113929,-1.151227\C,0,-4.579841,2.227033,-0.017325\H,0,-4.097193,1.106364,1.762062\H,0,-1.501541,0.669701,-1.640407\C,0,-4.178471,2.499901,-1.326611\H,0,-5.474729,2.685426,0.392738\H,0,-4.754532,3.18097,-1.950591\N,0,-3.096956,1.954183,-1.892069\C,0,-0.751885,-2.275815,0.615824\O,0,-0.83226,-2.650808,1.781262\C,0,-0.176778,-3.19593,-0.480783\C,0,2.49499,1.752237,0.237239\O,0,2.406039,2.956882,0.202171\C,0,3.773703,1.06617,-0.313657\F,0,4.653789,1.952347,-0.777122\F,0,4.363402,0.343326,0.665499\F,0,3.447155,0.216883,-1.311723\F,0,1.08517,-2.820035,-0.770239\F,0,-0.909938,-3.107547,-1.604469\F,0,-0.162331,-4.467904,-0.075173\H,0,1.183173,0.098121,-0.005273\Version=ES64L-G16RevA.03\State=2-A\HF=-1359.0620593\MP2=-1360.4865011\RMSD=2.828e-09\PG=C01[X(C13H11F6N2O2)]\

M14-Crad
GINC-NX360-M5-03-05\SP\ROB2PLYP-FC\GTMP2large\C13H11F6N2O2(2)\SSHKUNNI\18-Oct-2019\0\#rob2plyp/gtmp2largemaxdisk=20gb\nekaj\
\0,2\C,0,1.697858,0.917371,1.364542\C,0,-1.39253,-0.212914,0.606576\C,0,-0.696226,0.205499,1.931189\C,0,0.346851,1.350956,1.818566\H,0,2.316895,0.339835,2.046008\H,0,-1.986747,-1.094935,0.845914\H,0,-1.479186,0.519546,2.631119\H,0,-0.22251,-0.685712,2.357603\H,0,-0.031604,2.149411,1.174138\H,0,0.464472,1.774958,2.825863\N,0,-0.425377,-0.607573,-0.422694\C,0,-2.369685,0.83902,0.092863\C,0,-3.720285,0.749995,0.448247\C,0,-1.992251,1.928173,-0.7068

94\C,0,-4.6137,1.723392,0.010293\H,0,-4.069946,-0.080361,1.058497\H,0,-0.959235,2.058043,-1.024374\C,0,-4.122905,2.764332,-0.778717\H,0,-5.66774,1.673655,0.266609\H,0,-4.788964,3.544812,-1.142537\N,0,-2.838918,2.872372,-1.135977\C,0,-0.001276,-1.847181,-0.79218\O,0,0.862279,-2.048719,-1.62623\C,0,-0.673899,-3.059165,-0.094449\C,0,2.231182,1.244625,0.079511\O,0,1.573679,1.767786,-0.831276\C,0,3.726581,0.948132,-0.164962\F,0,3.994742,0.830668,-1.464228\F,0,4.474203,1.954759,0.338767\F,0,4.104243,-0.189817,0.459567\F,0,-2.007752,-3.08587,-0.326774\F,0,-0.502377,-3.005276,1.252745\F,0,-0.151255,-4.199114,-0.53086\H,0,0.062457,0.133065,-0.918563\\Version=ES64L-G16RevA.03\State=2-A\HF=-1359.0872143\MP2=-1360.5159715\RMSE=2.954e-09\PG=C01[X(C13H11F6N2O2)]\\

R-M14

GINC-NX360-M5-04-08\SP\ROB2PLYP-FC\GTMP2large\C13H11F6N2O2(2)\DSAKIC\21-Apr-2019\0\\#rob2plyp/gtmp2largemaxdisk=20gb\\nekaj\0,2\C,0,2.026277,-0.991492,-0.140201\C,0,-1.151968,-0.96518,0.350179\C,0,-0.309413,-2.101642,-0.263802\C,0,1.141473,-2.18356,0.23452\H,0,1.95047,-0.748205,-1.209473\H,0,-0.810605,-3.045814,-0.018118\H,0,-0.334403,-2.006412,-1.356566\H,0,1.152008,-2.308916,1.324558\H,0,1.591997,-3.096325,-0.171539\H,0,1.727393,-0.076458,0.387717\N,0,-0.838972,0.320242,-0.247325\H,0,-0.983484,-0.921623,1.436167\C,0,-2.654571,-1.153898,0.111785\C,0,-3.538122,-1.346843,1.177099\C,0,-3.189165,-1.131574,-1.185602\C,0,-4.89076,-1.539125,0.905016\H,0,-3.171733,-1.353842,2.200819\H,0,-2.538248,-0.960232,-2.040624\C,0,-5.312001,-1.510037,-0.425718\H,0,-5.605523,-1.702049,1.705958\H,0,-6.362397,-1.649037,-0.674873\N,0,-4.484527,-1.307661,-1.458707\C,0,-0.704,1.405758,0.579125\O,0,-0.120428,1.387502,1.654539\C,0,-1.196235,2.730614,-0.044323\C,0,3.486209,-1.230919,0.176439\O,0,3.936401,-2.22567,0.694149\C,0,4.447155,-0.078345,-0.220737\F,0,4.062566,1.071779,0.373492\F,0,4.399082,0.11336,-1.558507\F,0,5.706796,-0.338534,0.1268\F,0,-0.317559,3.166474,-0.963965\F,0,-1.333045,3.667653,0.89805\F,0,-2.385399,2.54856,-0.648534\\Version=ES64L-G16RevA.03\State=2-A\HF=-1359.0657067\MP2=-1360.4887454\RMSE=3.341e-09\PG=C01[X(C13H11F6N2O2)]\\

TS-M14

GINC-NX360-M5-05-05\SP\ROB2PLYP-FC\GTMP2large\C13H11F6N2O2(2)\DSAKIC\21-Apr-2019\0\\#rob2plyp/gtmp2largemaxdisk=20gb\\nekaj\0,2\C,0,-1.508801,-0.142483,1.090384\C,0,1.448812,-0.030497,0.654542\C,0,0.813882,-0.171833,2.076742\C,0,-0.557004,-0.863505,2.025481\H,0,-1.880764,0.823868,1.442196\H,0,2.349539,0.581498,0.781085\H,0,1.498158,-0.734079,2.720435\H,0,0.722227,0.835277,2.502726\H,0,-0.452116,-1.902298,1.697367\H,0,-0.979409,-0.88987,3.039603\H,0,-0.750785,0.227805,0.163007\N,0,0.514876,0.682122,-0.209591\C,0,1.857921,-1.369343,0.056382\C,0,2.880728,-2.115243,0.654704\C,0,1.264494,-1.905033,-1.092661\C,0,3.248501,-3.337909,0.102304\H,0,3.392359,-1.739762,1.538794\H,0,0.484927,-1.350959,-1.608693\C,0,2.576631,-3.779095,-1.039749\H,0,4.040937,-3.936018,0.542124\H,0,2.834395,-4.731839,-1.499148\N,0,1.604532,-3.081519,-1.634732\C,0,0.413153,2.048737,-0.286429\O,0,-0.627587,2.667151,-0.397254\C,0,1.758644,2.835759,-0.299106\C,0,-2.563201,-0.965079,0.430693\O,0,-2.601267,-2.177329,0.446311\C,0,-3.64002,-0.165725,-0.343661\F,0,-4.541891,-0.970492,-0.904499\F,0,-4.278002,0.68028,0.49474\F,0,-3.050692,0.569469,-1.307309\F,0,2.711148,2.210861,-1.018979\F,0,2.216723,2.948031,0.974319\F,0,1.584165,4.057525,-0.791544\\Version=ES64L-G16RevA.03\State=2-A\HF=-1359.0314308\MP2=-1360.4704472\RMSE=4.207e-09\PG=C01[X(C13H11F6N2O2)]\\

P-M14

GINC-NX360-M5-03-08\SP\ROB2PLYP-FC\GTMP2large\C13H11F6N2O2(2)\DSAKIC\21-Apr-2019\0\\#rob2plyp/gtmp2largemaxdisk=20gb\\nekaj\0,2\C,0,-1.277586,-1.056665,1.744931\C,0,1.337012,0.87068,0.975945\C,0,0.973269,0.012744,2.220305\C,0,0.186294,-1.287135,1.929402\H,0,-1.782401,-0.450698,2.495668\H,0,1.61116,1.858726,1.357004\H,0,1.904859,-0.238304,2.739342\H,0,0.388006,0.64214,2.901504\H,0,0.630526,-1.845242,1.101774\H,0,0.295398,-1.934759,2.815568\H,0,-0.107275,0.425052,-0.564076\N,0,0.171112,1.111192,0.124493\C,0,2.52833,0.329465,0.198989\C,0,3.807451,0.826004,0.47757\C,0,2.438228,-0.676393,-0.773237\C,0,4.909286,0.310522,-0.198505\H,0,3.935455,1.61526,1.215246\H,0,1.477092,-1.103273,-1.049902\C,0,4.696211,-0.693271,-1.144428\H,0,5.910725,0.682672,-0.004305\H,0,5.531412,-1.121721,-1.69561\N,0,3.486211,-1.182224,-1.434708\C,0,-0.597647,2.217538,0.288136\O,0,-0.413038,3.099827,1.108576\C,0,-1.779683,2.321306,-0.70556\C,0,-2.166819,-1.559959,0.74805\O,0,-3.383829,-1.340127,0.768443\C,0,-1.604047,-2.389048,-0.429016\F,0,-2.023863,1.137222,-1.324398\F,0,-1.506439,3.230105,-1.655475\F,0,-2.891393,2.692808,-0.066319\F,0,-2.571607,-2.877688,-1.194808\F,0,-0.833971,-3.412

675,-0.001761\F,0,-0.808624,-1.59921,-1.218612\\Version=ES64L-G16RevA.03\\State=2-
A\\HF=-1359.0889491\\MP2=-1360.5185253\\RMSD=5.185e-09\\PG=C01[X(C13H11F6N2O2)]\\