

**Accurate Prediction of Enthalpies of Formation of Organic Azides by
Combining G4 Theory Calculation with Isodesmic Reaction Scheme**

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Supporting Information

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Table S1. G4 Energies and Cartesian Coordinates for the Lowest-Energy Conformers of Azido Compounds Optimized at the B3LYP/6-31G(2df,p) level

compound ^a	G4 enthalpy ^b	atom	x	y	z
1 HN ₃	-164.726051	N	-0.000468	0.000000	0.006650
		N	0.000547	0.000000	1.138776
		N	0.178791	0.000000	2.363736
		H	-0.718908	0.000000	2.848948
2 •N ₃	-164.084364	N	0.000000	0.000000	0.031415
		N	0.000000	0.000000	1.209999
		N	0.000000	0.000000	2.388586
3 CH ₃ N ₃	-203.992998	N	-0.225860	0.000000	0.168248
		N	-0.077129	0.000000	1.294862
		N	0.226866	0.000000	2.486189
		C	-0.900828	0.000000	3.434347
		H	-0.465994	0.000000	4.433299
		H	-1.525839	0.893188	3.319346
		H	-1.525839	-0.893188	3.319346
4 C ₆ H ₅ N ₃	-395.636405	C	1.397140	-0.021188	0.000000
		C	0.714003	1.190389	0.000000
		C	-0.684060	1.193383	0.000000
		C	-1.388192	-0.012615	0.000000
		C	-0.693430	-1.216127	0.000000
		C	0.700354	-1.227566	0.000000
		H	2.482064	-0.019122	0.000000
		H	1.262616	2.126387	0.000000
		N	-1.470323	2.375471	0.000000
		H	-2.471555	0.013420	0.000000
		H	-1.245548	-2.149942	0.000000
		H	1.239128	-2.168456	0.000000
		N	-0.892539	3.464023	0.000000
		N	-0.487527	4.524354	0.000000
5 C ₆ H ₅ CH ₂ N ₃	-434.908792	C	-0.075011	0.080071	-0.180592
		C	0.027769	0.303727	1.187726
		C	1.280061	0.319914	1.801411
		C	2.426091	0.111971	1.039959
		C	2.320385	-0.111712	-0.331504
		C	1.071065	-0.130505	-0.954163
		H	-1.050052	0.070591	-0.658334
		H	-0.868892	0.462411	1.777655
		H	1.359805	0.492576	2.869470
		H	3.403232	0.121761	1.511215
		H	3.216403	-0.278316	-0.922292

			C	0.957496	-0.344354	-2.444792
			H	1.872126	-0.803312	-2.839553
			H	0.121869	-1.003868	-2.684986
			N	0.660800	0.906340	-3.202371
			N	1.513604	1.789279	-3.118243
			N	2.227428	2.673215	-3.115073
6	1,4-NO ₂ -C ₆ H ₄ -N ₃	-600.090967	C	1.410422	-0.015115	0.000000
			C	0.722542	1.188146	0.000000
			C	-0.679231	1.189465	0.000000
			C	-1.385307	-0.019816	0.000000
			C	-0.699090	-1.222599	0.000000
			C	0.692885	-1.207040	0.000000
			H	2.491442	-0.048470	0.000000
			H	1.272178	2.122914	0.000000
			N	-1.464382	2.360839	0.000000
			H	-2.468135	0.005290	0.000000
			H	-1.217898	-2.171411	0.000000
			N	1.423120	-2.479754	0.000000
			O	2.647489	-2.431761	0.000000
			O	0.763427	-3.512091	0.000000
			N	-0.889105	3.455335	0.000000
			N	-0.497532	4.517975	0.000000
7	N≡CN ₃	-256.921325	N	-0.002252	0.000000	0.008164
			N	0.002560	0.000000	1.133737
			N	0.217397	0.000000	2.364222
			C	-0.833613	0.000000	3.199234
			N	-1.660198	0.000000	4.013501
8	N≡CCH ₂ N ₃	-296.206425	N	2.275869	-0.337588	-0.404957
			C	1.123205	-0.365908	-0.472273
			C	-0.343497	-0.400311	-0.534560
			N	-0.988468	0.619353	0.313107
			N	-0.834404	0.467814	1.531665
			N	-0.777986	0.449985	2.662482
			H	-0.689336	-1.411552	-0.285286
			H	-0.664081	-0.182240	-1.555034
9	CH ₃ N(NO ₂)CH ₂ N ₃	-503.026271	C	1.713999	1.426091	-0.489351
			H	1.591341	2.437043	-0.097415
			H	1.374706	1.398114	-1.530665
			H	2.764825	1.146055	-0.446937
			N	0.935533	0.534686	0.364099
			C	-0.363713	0.946079	0.854384
			H	-0.659679	0.279215	1.662881
			H	-0.240385	1.960011	1.235724
			N	-1.397278	1.024289	-0.198767

			N	-2.165226	0.057901	-0.280626
			N	-2.946999	-0.741334	-0.459343
			N	1.080428	-0.826510	0.103854
			O	0.242497	-1.575419	0.590621
			O	2.048179	-1.158064	-0.560538
10	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3$	-652.169989	C	-0.000236	-1.257502	-0.320094
			N	-0.947125	-2.140143	0.275909
			N	0.697368	-0.365662	0.770885
			N	-0.873311	-0.260269	-1.115040
			C	1.091692	-1.864555	-1.175828
			N	-0.490444	-3.145887	0.841574
			O	0.741725	-0.824922	1.892025
			O	1.186292	0.670148	0.368633
			O	-0.720395	-0.236162	-2.319939
			O	-1.649752	0.394984	-0.453847
			N	-0.231666	-4.099060	1.386898
			H	1.723768	-1.077223	-1.585954
			H	0.639391	-2.425281	-1.993891
			H	1.700391	-2.535567	-0.562934
11	$\text{C}(\text{NO}_2)_3\text{N}_3$	-817.311116	N	0.341188	0.207444	1.193320
			N	1.401429	-0.780811	-0.853250
			N	-0.800405	0.435601	-0.983365
			C	0.625802	0.440951	-0.325987
			N	1.398726	1.560765	-0.594859
			N	0.885470	2.682808	-0.391766
			N	0.588963	3.760321	-0.281627
			O	0.493287	-0.905904	1.630248
			O	-0.017324	1.214092	1.772380
			O	0.804378	-1.515563	-1.608970
			O	2.538696	-0.864444	-0.452377
			O	-0.935708	1.179887	-1.928802
			O	-1.613276	-0.299168	-0.472322
12	$\text{HOCH}_2\text{CH}_2\text{N}_3$	-318.469494	N	-0.459018	-0.771047	0.361204
			N	-0.457161	-0.652722	1.490611
			N	-0.399162	-0.641878	2.718580
			C	-0.918007	0.575760	3.387555
			C	-0.915477	0.294759	4.885295
			H	-0.282197	1.440378	3.155535
			H	-1.939860	0.785653	3.048623
			O	-1.757855	-0.785604	5.221255
			H	-1.456512	-1.542412	4.704855
			H	-1.297302	1.173327	5.414762
			H	0.120399	0.123785	5.217108
13	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3$	-357.731491	C	-5.189708	1.505406	0.094999

		H	-4.794375	1.946159	1.014323
		H	-4.799836	2.075131	-0.753144
		H	-6.279830	1.596617	0.103597
		C	-4.782654	0.046046	-0.009536
		H	-5.194401	-0.534898	0.832296
		H	-5.176609	-0.404187	-0.936098
		O	-3.368596	-0.026357	0.000298
		C	-2.862104	-1.336129	-0.071546
		H	-3.306068	-1.974676	0.709161
		H	-3.084249	-1.797385	-1.049819
		C	-1.353596	-1.262687	0.121426
		H	-0.916625	-2.252909	-0.021732
		H	-0.921694	-0.582019	-0.622525
		N	-0.975874	-0.854686	1.487672
		N	-1.116001	0.337368	1.764019
		N	-1.172417	1.401260	2.155609
14	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OC}_2\text{H}_5$		-471.054646		
		C	3.806187	-0.108404	0.216695
		H	4.638030	0.145100	-0.446924
		H	3.981871	-1.108317	0.622895
		H	3.797428	0.604564	1.045784
		C	2.503353	-0.058561	-0.556029
		H	2.488887	-0.769089	-1.387781
		H	2.304675	0.935535	-0.967992
		O	1.437291	-0.400478	0.360759
		C	0.200114	-0.408027	-0.155470
		O	-0.074492	-0.173265	-1.302522
		C	-0.818626	-0.723468	0.938368
		H	-0.456621	-1.556239	1.542239
		H	-0.883500	0.151101	1.601839
		N	-2.124661	-1.115336	0.418718
		N	-2.727275	-0.270327	-0.250162
		N	-3.407660	0.399905	-0.860288
15	azidocyclopentane		-359.918811		
		H	-0.902209	-0.012582	0.085118
		C	0.113928	0.071082	0.487245
		C	0.796167	1.397089	0.094681
		C	1.064801	-0.993247	-0.066310
		C	2.322876	1.108194	0.127519
		C	2.463693	-0.434471	0.252628
		N	0.057942	-0.118049	1.967158
		H	0.473915	1.661202	-0.918280
		H	0.496990	2.223573	0.745448
		H	0.877944	-1.979970	0.363564
		H	0.912021	-1.061515	-1.149513
		H	2.801360	1.481191	-0.782147
		H	2.807404	1.614510	0.965823
		H	2.736384	-0.704298	1.276641

		H	3.234439	-0.842173	-0.406250
		N	-0.664451	0.663850	2.578542
		N	-1.304085	1.330253	3.242379
16	azidocyclohexane		-399.205810		
		N	0.541498	0.822444	-0.471999
		N	1.578287	0.826766	0.186781
		C	-0.600475	0.070976	0.120021
		N	2.584362	0.904852	0.711422
		C	-1.856807	0.451472	-0.665349
		C	-0.358675	-1.445074	0.086485
		C	-3.084230	-0.314806	-0.150576
		C	-1.584670	-2.210579	0.607884
		C	-2.852472	-1.832264	-0.170741
		H	-0.723460	0.390177	1.166056
		H	-2.014363	1.532872	-0.602189
		H	-1.685137	0.218469	-1.724134
		H	-0.146586	-1.737541	-0.949801
		H	0.530119	-1.695587	0.677009
		H	-3.307520	0.004026	0.877031
		H	-3.960961	-0.052658	-0.752312
		H	-1.402089	-3.288703	0.545305
		H	-1.730302	-1.981987	1.672687
		H	-3.722079	-2.353800	0.243729
		H	-2.751740	-2.169457	-1.211408
17	1,2-diazidobenzene		-559.179969		
		C	0.011966	0.000000	-0.003672
		C	0.011966	0.000000	1.403672
		C	1.228031	0.000000	-0.690222
		C	1.228031	0.000000	2.090222
		C	2.432283	0.000000	0.003530
		C	2.432283	0.000000	1.396470
		N	-1.251672	0.000000	-0.635880
		N	-1.289915	0.000000	-1.867344
		N	-1.469822	0.000000	-2.987703
		N	-1.251672	0.000000	2.035880
		N	-1.289915	0.000000	3.267344
		N	-1.469822	0.000000	4.387703
		H	1.225068	0.000000	-1.775151
		H	1.225068	0.000000	3.175151
		H	3.367097	0.000000	-0.545350
		H	3.367097	0.000000	1.945350
18	1,3-diazidobenzene		-559.183703		
		C	0.828795	-0.541296	0.000000
		C	0.284475	-1.829340	0.000000
		C	-1.098620	-1.979683	0.000000
		C	-1.940724	-0.874905	0.000000
		C	-1.386015	0.407799	0.000000
		C	-0.001628	0.579273	0.000000

		N	2.220639	-0.271421	0.000000	
		N	3.001088	-1.226712	0.000000	
		N	3.823538	-2.007479	0.000000	
		H	0.931229	-2.699437	0.000000	
		H	-3.018119	-0.983809	0.000000	
		N	-2.306967	1.485040	0.000000	
		N	-1.862662	2.636081	0.000000	
		N	-1.590203	3.736818	0.000000	
		H	0.448272	1.565235	0.000000	
		H	-1.525521	-2.976745	0.000000	
19	1,4-diazidobenzene	-559.182802	C	-0.011749	0.000000	0.028336
			C	0.022333	0.000000	1.426971
			C	1.239371	0.000000	2.091471
			C	2.436620	0.000000	1.371664
			C	2.402538	0.000000	-0.026971
			C	1.185500	0.000000	-0.691471
			N	-1.203639	0.000000	-0.737716
			N	-2.284100	0.000000	-0.143832
			N	-3.338737	0.000000	0.275405
			H	-0.900258	0.000000	1.997579
			H	1.278298	0.000000	3.174386
			N	3.628510	0.000000	2.137716
			N	4.708971	0.000000	1.543832
			N	5.763608	0.000000	1.124595
			H	3.325129	0.000000	-0.597579
			H	1.146573	0.000000	-1.774386
20	1,3,5-triazidobenzene	-722.730680	C	-0.006346	0.000000	0.034737
			C	0.015592	0.000000	1.429487
			C	1.245692	0.000000	2.088128
			C	2.442612	0.000000	1.371754
			C	2.397961	0.000000	-0.022864
			C	1.179103	0.000000	-0.701241
			N	-1.198801	0.000000	-0.728447
			N	-2.277028	0.000000	-0.126612
			N	-3.328802	0.000000	0.295131
			H	-0.895901	0.000000	2.014380
			N	1.180983	0.000000	3.502416
			N	2.241301	0.000000	4.135270
			N	3.132428	0.000000	4.835261
			H	3.404890	0.000000	1.868683
			N	3.655125	0.000000	-0.673969
			N	3.673034	0.000000	-1.908658
			N	3.833681	0.000000	-3.030392
			H	1.128318	0.000000	-1.783063
21	4-azidopyridine	-411.680347	N	-0.000787	0.000000	-0.043154

			C	0.039017	0.000000	1.293172
			C	1.210120	0.000000	2.040283
			C	2.427683	0.000000	1.359681
			C	2.410051	0.000000	-0.037647
			C	1.175334	0.000000	-0.676251
			N	3.600460	0.000000	2.145783
			N	4.691260	0.000000	1.564545
			N	5.750988	0.000000	1.164771
			H	-0.922197	0.000000	1.801490
			H	1.190734	0.000000	3.123164
			H	3.327611	0.000000	-0.615313
			H	1.135131	0.000000	-1.763168
22	$(C_6H_5)_3CN_3$	-895.876224 ^c	N	1.907217	1.291912	2.886829
			N	1.086064	0.701661	2.369386
			N	0.158882	0.025285	1.934829
			C	0.000389	-0.035873	0.433964
			C	-0.378469	1.360809	-0.101516
			C	-0.043308	1.774522	-1.395139
			C	-1.154043	2.216957	0.688358
			C	-0.462094	3.012026	-1.879392
			H	0.557047	1.133811	-2.029761
			C	-1.567954	3.454402	0.206786
			H	-1.438671	1.906473	1.686784
			C	-1.222421	3.859203	-1.080030
			H	-0.185435	3.312506	-2.884700
			H	-2.164056	4.102614	0.840677
			H	-1.542982	4.825172	-1.455448
			C	1.314478	-0.592605	-0.143481
			C	2.426682	0.244168	-0.312904
			C	1.470911	-1.958862	-0.398062
			C	3.648859	-0.268318	-0.738403
			H	2.338655	1.306753	-0.120641
			C	2.692809	-2.470845	-0.825702
			H	0.632617	-2.630118	-0.260342
			C	3.786612	-1.628321	-1.000296
			H	4.493420	0.400867	-0.865023
			H	2.786701	-3.534017	-1.021303
			H	4.738018	-2.027525	-1.335575
			C	-1.190464	-0.980512	0.186803
			C	-1.666656	-1.156805	-1.117857
			C	-1.817011	-1.674269	1.222990
			C	-2.737373	-2.003547	-1.378405
			H	-1.199875	-0.624263	-1.938349
			C	-2.894997	-2.520099	0.961916
			H	-1.461085	-1.551504	2.237112
			C	-3.359902	-2.689425	-0.336909
			H	-3.088681	-2.123748	-2.397963

		H	-3.368408	-3.047189	1.783965
		H	-4.198963	-3.346922	-0.538469
23	$(\text{CH}_3\text{CH}_2)_3\text{CN}_3$		-439.669894		
		C	-0.029290	0.197496	0.000000
		C	-0.925584	0.131144	-1.258736
		H	-1.515030	-0.793055	-1.202079
		H	-1.654907	0.947338	-1.201831
		C	-0.925584	0.131144	1.258736
		H	-1.515030	-0.793055	1.202079
		H	-1.654907	0.947338	1.201831
		C	0.914738	1.416606	0.000000
		H	1.571893	1.334374	-0.871074
		H	1.571893	1.334374	0.871074
		C	-0.196037	0.183343	-2.604532
		H	0.583098	-0.581851	-2.665231
		H	-0.900746	0.012244	-3.423677
		H	0.276280	1.154995	-2.776502
		C	-0.196037	0.183343	2.604532
		H	0.276280	1.154995	2.776502
		H	-0.900746	0.012244	3.423677
		H	0.583098	-0.581851	2.665231
		C	0.224057	2.783407	0.000000
		H	-0.405628	2.927472	0.883625
		H	0.972727	3.581204	0.000000
		H	-0.405628	2.927472	-0.883625
		N	0.924441	-0.974284	0.000000
		N	0.421356	-2.093480	0.000000
		N	0.068414	-3.175618	0.000000
24	$(\text{CH}_3)_2(\text{C}_6\text{H}_5)\text{CN}_3$		-513.474479		
		C	-0.175324	-0.762661	-0.164209
		C	-1.697088	-0.665243	0.023356
		H	-2.000620	0.369670	0.195861
		H	-2.213343	-1.033471	-0.867910
		H	-2.004727	-1.263223	0.885255
		C	0.219081	-2.209369	-0.495472
		H	-0.269710	-2.512120	-1.424842
		H	1.300617	-2.313935	-0.623141
		H	-0.100947	-2.895810	0.292991
		C	0.542101	-0.194286	1.065645
		C	0.514080	1.187079	1.299482
		C	1.201233	-1.006518	1.991399
		C	1.122823	1.736551	2.421564
		H	0.020277	1.836012	0.584164
		C	1.810222	-0.457535	3.119351
		H	1.249347	-2.078533	1.843032
		C	1.773851	0.914555	3.339620
		H	1.091128	2.809881	2.577838
		H	2.317547	-1.109746	3.822742

			H	2.250906	1.341833	4.215199
			N	0.107080	0.099767	-1.370342
			N	1.288175	0.196255	-1.699230
			N	2.341150	0.360638	-2.093856
25	1-azidoadamantane	-553.967069	C	-0.390605	-0.426731	1.260065
			H	-0.613393	0.169371	2.152338
			H	-1.052087	-1.301881	1.280034
			C	1.085410	-0.875010	1.259239
			H	1.278305	-1.473976	2.156113
			C	-0.674023	0.416390	0.000000
			C	0.236174	1.655345	0.000000
			H	0.013103	2.268037	0.880839
			H	0.013103	2.268037	-0.880839
			C	1.995654	0.369540	1.258881
			H	3.049149	0.065207	1.279408
			H	1.818267	0.966715	2.161813
			C	1.712789	1.213351	0.000000
			H	2.351776	2.103119	0.000000
			C	1.995654	0.369540	-1.258881
			H	1.818267	0.966715	-2.161813
			H	3.049149	0.065207	-1.279408
			C	1.364318	-1.719079	0.000000
			H	0.734445	-2.617425	0.000000
			H	2.406289	-2.061377	0.000000
			C	-0.390605	-0.426731	-1.260065
			H	-1.052087	-1.301881	-1.280034
			H	-0.613393	0.169371	-2.152338
			C	1.085410	-0.875010	-1.259239
			H	1.278305	-1.473976	-2.156113
			N	-2.077176	0.933170	0.000000
			N	-2.970362	0.089898	0.000000
			N	-3.878306	-0.595908	0.000000
26	TAT	-770.903151	C	0.001887	1.287877	0.000000
			C	-1.116277	-0.642304	0.000000
			C	1.114390	-0.645572	0.000000
			N	0.059836	2.680794	0.000000
			N	-1.043239	3.264020	0.000000
			N	-1.948352	3.932120	0.000000
			N	-2.351553	-1.288577	0.000000
			N	-2.305105	-2.535481	0.000000
			N	-2.431140	-3.653382	0.000000
			N	2.291717	-1.392216	0.000000
			N	3.348344	-0.728538	0.000000
			N	4.379492	-0.278738	0.000000
			N	-1.191302	0.687671	0.000000
			N	0.000110	-1.375533	0.000000

		N	1.191192	0.687862	0.000000
27	TAH		-1103.215963 ^c		
		C	-1.399956	-0.118502	0.000000
		C	-1.498706	2.135387	0.000000
		C	0.597352	1.271648	0.000000
		C	2.598653	0.230224	0.000000
		C	0.802603	-1.153146	0.000000
		C	-1.099946	-2.365611	0.000000
		N	1.919120	1.375760	0.000000
		N	2.122974	-1.019106	0.000000
		N	-0.178916	2.348103	0.000000
		N	0.000000	0.000000	0.000000
		N	0.231883	-2.349887	0.000000
		N	-2.151003	0.974127	0.000000
		N	-1.944059	-1.328997	0.000000
		N	3.977930	0.404980	0.000000
		N	4.653759	-0.646825	0.000000
		N	5.399361	-1.487811	0.000000
		N	-2.339688	3.242499	0.000000
		N	-1.766713	4.353686	0.000000
		N	-1.638242	-3.647479	0.000000
		N	-2.887046	-3.706861	0.000000
		N	-3.988162	-3.932078	0.000000
		N	-1.411198	5.419889	0.000000
28	TAAT		-1321.860720 ^c		
		C	-0.709816	-3.782795	-0.685465
		C	-0.246704	-1.752574	0.103635
		C	-0.675300	3.535258	1.051179
		C	0.709816	3.782795	-0.685465
		C	0.246704	1.752574	0.103635
		N	0.514063	0.346861	0.060426
		N	-0.514063	-0.346861	0.060426
		N	0.572123	-2.202239	1.043816
		N	0.069930	-4.380121	0.212841
		N	-0.934510	-2.466224	-0.780107
		N	-0.572123	2.202239	1.043816
		N	0.934510	2.466224	-0.780107
		N	-0.069930	4.380121	0.212841
		N	1.509744	-4.042730	2.042987
		N	1.628829	-5.284894	2.063985
		N	1.838027	-6.380155	2.212452
		C	0.675300	-3.535258	1.051179
		N	-1.335557	-4.648240	-1.578759
		N	-2.074624	-4.105546	-2.425442
		N	-2.768583	-3.771148	-3.245182
		N	-1.509744	4.042730	2.042987
		N	-1.628829	5.284894	2.063985
		N	-1.838027	6.380155	2.212452

		N	1.335557	4.648240	-1.578759
		N	2.074624	4.105546	-2.425442
		N	2.768583	3.771148	-3.245182
29	DiAT				
			-623.297335		
		C	-1.198226	-0.414919	0.000000
		C	1.198226	0.414919	0.000000
		N	1.001389	-0.914448	0.000000
		N	-0.234062	-1.347761	0.000000
		N	0.234062	1.347761	0.000000
		N	-1.001389	0.914448	0.000000
		N	2.493903	0.918596	0.000000
		N	-2.493903	-0.918596	0.000000
		N	3.412635	0.076750	0.000000
		N	4.351448	-0.545857	0.000000
		N	-3.412635	-0.076750	0.000000
		N	-4.351448	0.545857	0.000000

^aThe compound's number according to Figure 1 is given for each molecule. ^bIn hartrees. ^cG4(MP2) energy.

Table S2. Enthalpies of Formation of Azido Compounds Calculated by Different Composite Methods (in kJ/mol)

compound ^a	G4	G4(MP2)	G3	G3(MP2)//B3LYP	W1U
1 HN ₃	289.0	291.5	297.5	294.8	293.3
2 •N ₃	445.5	449.0	450.0	452.5	450.4
3 CH ₃ N ₃	293.9	298.5	301.2	301.1	298.3
4 C ₆ H ₅ N ₃	409.5	410.0	417.8	410.4	410.1
5 C ₆ H ₅ CH ₂ N ₃	400.9	399.8	408.6	400.7	
6 1,4-NO ₂ -C ₆ H ₄ -N ₃	384.3	391.5	394.9	391.1	
7 N≡CN ₃	495.4	501.5	506.6	502.6	504.9
8 N≡CCH ₂ N ₃	453.3	457.8	463.0	459.0	
9 CH ₃ N(NO ₂)CH ₂ N ₃	330.5	343.8	341.6	346.2	
10 CH ₃ C(NO ₂) ₂ N ₃	246.0	264.1	259.1	264.3	
11 C(NO ₂) ₃ N ₃	337.8	362.0	356.2	361.7	
12 HOCH ₂ CH ₂ N ₃	112.5	116.4	117.6	117.3	
13 CH ₃ CH ₂ OCH ₂ CH ₂ N ₃	93.5	100.6	99.7	100.5	
14 N ₃ CH ₂ C(O)OC ₂ H ₅	-83.2	-74.9	-79.5	-77.0	
15 azidocyclopentane	256.5	259.8	260.9	261.1	
16 azidocyclohexane	208.0	211.9	212.8	213.1	
17 1,2-diazidobenzene	746.6	752.9	761.8	755.2	
18 1,3-diazidobenzene	736.7	742.9	752.1	745.3	
19 1,4-diazidobenzene	739.1	745.2	753.6	747.3	
20 1,3,5-triazidobenzene	1064.9	1077.6	1087.8	1081.7	
21 4-azidopyridine	463.8	466.9	473.0	467.6	
22 (C ₆ H ₅) ₃ CN ₃		592.6		589.3	
23 (CH ₃ CH ₂) ₃ CN ₃	126.1	131.7	130.0	133.3	
24 (CH ₃) ₂ (C ₆ H ₅)CN ₃	326.5	327.4	334.1	327.8	
25 1-azidoadamantane	170.1	174.6	175.6	175.1	
26 TAT	1120.8	1141.7	1150.7	1148.8	
27 TAH		1418.1		1422.4	
28 TAAT		1936.0		1948.0	
29 DiAT	1116.8	1130.1	1142.8	1139.7	

^aThe compound's number according to Figure 1 is given for each molecule.

Table S3. Experimental Enthalpies of Formations of Reference Compounds Used in Isodesmic Reaction Calculations and Their Comparison with Values Calculated by G4 Method from Atomization Reaction (in kJ/mol)

compound		$\Delta_f H_{298}^\circ$	reference	exp – calc
CHO	•C(O)H	42.5 ± 0.5	1	3.7
CH ₂ NO	•C(O)NH ₂	-15.1 ± 4.0	1	0.6
CH ₃	•CH ₃	146.7 ± 0.3	1	2.3
CH ₃ N ₂ O	•NHC(O)NH ₂	0.8 ± 12.6	1	0.2
CH ₃ O	•OCH ₃	-17.0 ± 4.0	1	-0.5
CH ₃ O	•CH ₂ OH	-17.0 ± 0.7	1	0.7
CH ₄ N	•NHCH ₃	184.1 ± 8.4	1	7.4
		177.2 ± 5.0 ^a	2	0.5
C ₂ H ₃ O	•C(O)CH ₃	-10.3 ± 1.8	1	3.0
C ₂ H ₃ O	•CH ₂ C(O)H	13.0 ± 2.0	1	0.5
C ₂ H ₅	•CH ₂ CH ₃	118.8 ± 1.3	1	-0.9
C ₂ H ₅ O	CH ₃ CH ₂ O•	-13.6 ± 3.3	1	2.7
C ₂ H ₅ O	•CH ₂ CH ₂ OH	-31.0 ± 7.0	1	-2.6
C ₂ H ₆ N	•N(CH ₃) ₂	158.2 ± 4.2	1	1.9
C ₃ H ₅ O	•C(O)CH ₂ CH ₃	-31.7 ± 3.4	1	3.7
C ₃ H ₇	•CH ₂ CH ₂ CH ₃	100.0 ± 2.0	1	-1.2
C ₃ H ₇	•CH(CH ₃) ₂	88.3 ± 3.0	1	0.5
C ₄ H ₉	•C(CH ₃) ₃	48.0 ± 3.0	1	-2.4
C ₆ H ₅	•C ₆ H ₅	339.7 ± 2.5	3	3.0
C ₇ H ₅ O	•C(O)C ₆ H ₅	116.3 ± 10.9	1	-0.5
C ₇ H ₇	•CH ₂ C ₆ H ₅	208.0 ± 1.7	1	0.1
H	•H	218.00 ± 0.01	4	0.0
N	•N	472.7 ± 0.4	4	0.0
NH ₂	•NH ₂	186.2 ± 1.0	1	0.1
NO ₂	•NO ₂	34.0 ± 0.1	1	4.6
H ₂	H ₂	0	4	1.4
N ₂	N ₂	0	4	0.1
O ₂	O ₂	0	4	-2.1
HNO ₂	HNO ₂	-78.5 ± 0.6	4	0.4
NH ₃	NH ₃	-45.9 ± 0.4	4	-3.4
CHN	HCN	132.0 ± 4.0	4	3.9
CHN ₃ O ₆	CH(NO ₂) ₃	23.8 ± 1.3	5	32.9
		-0.2 ± 2.1	6	-8.9
		8.6 ± 5.0 ^a	7	
CH ₂ N ₂ O ₄	CH ₂ (NO ₂) ₂	-38.5 ± 1.3	5	14.2 ^b
CH ₂ O	HC(O)H	-108.6 ± 0.5	6	3.5
CH ₂ O ₂	HC(O)OH	-378.7 ± 0.5	6	0.3
CH ₃ NO	HC(O)NH ₂	-188.6 ± 0.4	8	0.3
CH ₃ NO ₂	CH ₃ NO ₂	-74.5 ± 0.8	5	3.6
CH ₄	CH ₄	-74.4 ± 0.4	6	0.4
CH ₄ O	CH ₃ OH	-201.5 ± 0.2	6	-0.3
CH ₅ N	CH ₃ NH ₂	-23.4 ± 1.0	6	-3.8

CH ₆ N ₂	CH ₃ NHNH ₂	94.7 ± 0.7	6	-1.6
CN ₄ O ₈	C(NO ₂) ₄	82.4 ± 1.7	5	16.8 ^b
C ₂ H ₂	HCCH	228.2 ± 0.7	6	-0.2
C ₂ H ₂ N ₄	1,2,4,5-tetrazine	478.7 ± 5.0 ^c		
C ₂ H ₃ N	CH ₃ CN	74.0 ± 0.3	6	1.4
C ₂ H ₃ N ₃	1 <i>H</i> -1,2,4-triazole	192.7 ± 0.8	6	2.4
C ₂ H ₄	H ₂ C=CH ₂	52.5 ± 0.3	6	0.6
C ₂ H ₄ N ₂ O ₄	CH ₃ CH(NO ₂) ₂	-88.3 ± 0.8	9	13.5 ^b
C ₂ H ₄ N ₂ O ₄	CH ₂ (NO ₂)CH ₂ (NO ₂)	-96.7 ± 1.3	9	12.0 ^b
C ₂ H ₄ N ₄	5-methyl-1 <i>H</i> -tetrazole	280.7 ± 2.6	6	-2.8
C ₂ H ₄ O	CH ₃ C(O)H	-166.1 ± 0.5	6	-0.4
C ₂ H ₄ O ₂	CH ₃ C(O)OH	-432.8 ± 2.5	6	-2.3
C ₂ H ₄ O ₂	HC(O)OCH ₃	-357.4 ± 0.7	6	3.7
C ₂ H ₅ NO	CH ₃ C(O)NH ₂	-238.3 ± 0.8	6	-4.4
C ₂ H ₅ NO ₂	CH ₃ CH ₂ NO ₂	-102.5 ± 0.8	5	5.3
C ₂ H ₆	CH ₃ CH ₃	-83.8 ± 0.3	6	-0.3
C ₂ H ₆ N ₂	CH ₃ N=NCH ₃	152.7 ± 5.0 ^c		
C ₂ H ₆ N ₂ O ₂	CH ₃ N(NO ₂)CH ₃	-7.5 ± 2.1	10	1.8
C ₂ H ₆ O	CH ₃ CH ₂ OH	-235.2 ± 0.3	6	-2.0
C ₂ H ₆ O	CH ₃ OCH ₃	-184.1 ± 0.5	6	1.1
C ₂ H ₇ N	CH ₃ CH ₂ NH ₂	-47.5 ± 0.6	6	-1.0
C ₂ H ₇ N	NH(CH ₃) ₂	-18.8 ± 1.5	6	-2.9
C ₂ N ₂	NCCN	306.7 ± 0.8	6	2.6
C ₃ H ₃ N ₃	1,3,5-triazine	225.9 ± 0.8	6	2.8
C ₃ H ₃ N ₃ O ₃	1,3,5-triazine-2,4,6-trione (cyanuric acid)	-564.1 ± 1.5	11	1.1
C ₃ H ₄ N ₂	1 <i>H</i> -pyrazole	179.4 ± 0.8	6	3.1
C ₃ H ₅ N	CH ₃ CH ₂ CN	51.7 ± 0.7	6	-2.8
C ₃ H ₆	H ₂ C=CHCH ₃	20.0 ± 0.7	6	-0.2
C ₃ H ₆ N ₆ O ₆	1,3,5-trinitroperhydro-1,3,5-triazine (RDX)	195.0 ± 1.7	10	24.1
		176.0 ± 5.0 ^a		
C ₃ H ₆ O	CH ₃ C(O)CH ₃	-217.1 ± 0.7	6	-0.7
C ₃ H ₆ O ₂	CH ₃ C(O)OCH ₃	-413.3 ± 0.7	6	-2.4
C ₃ H ₇ NO ₂	CH ₃ CH ₂ CH ₂ NO ₂	-124.3 ± 1.3	9	5.1
C ₃ H ₈	CH ₃ CH ₂ CH ₃	-104.7 ± 0.5	6	-0.8
C ₃ H ₈ O	CH ₃ CH ₂ CH ₂ OH	-255.1 ± 0.4	6	-1.6
C ₃ H ₈ O	CH ₃ OCH ₂ CH ₃	-216.4 ± 0.6	6	1.7
C ₃ H ₉ N	N(CH ₃) ₃	-23.6 ± 1.3	6	1.9
C ₄ H ₄ N ₂ O ₂	uracil	-305.1 ± 2.5	36	-1.9
C ₄ H ₅ N	pyrrole	108.4 ± 0.6	6	0.0
C ₄ H ₆	1,3-butadiene	110.0 ± 1.1	6	-1.0
C ₄ H ₆ N ₂ O ₂	5,6-dihydrouracil	-377.2 ± 1.6	36	-0.8
C ₄ H ₈	cyclobutane	27.7 ± 1.1	6	-0.8
C ₄ H ₈ N ₄ O ₄	1,4-dinitropiperazine	49.8 ± 2.1	10	-1.7
C ₄ H ₈ O ₂	CH ₃ C(O)OCH ₂ CH ₃	-443.6 ± 0.5	6	0.7
C ₄ H ₉ NO ₂	CH ₃ CH ₂ CH ₂ CH ₂ NO ₂	-144.8 ± 0.8	12	5.4 ^b
C ₄ H ₉ NO ₂	(CH ₃) ₃ CNO ₂	-177.1 ± 3.3	6	4.1
C ₄ H ₁₀	CH ₃ CH ₂ CH ₂ CH ₃	-125.7 ± 0.6	6	-0.7
C ₄ H ₁₀	CH(CH ₃) ₃	-134.2 ± 0.6	6	-0.7

C ₄ H ₁₀ O	CH ₃ OCH ₂ CH ₂ CH ₃	-238.1 ± 0.7	6	0.5
C ₄ H ₁₀ O	CH ₃ CH ₂ OCH ₂ CH ₃	-252.1 ± 0.7	6	-1.1
C ₅ H ₅ N	pyridine	140.4 ± 0.7	6	1.3
C ₅ H ₇ N	N-methylpyrrole	103.1 ± 0.5	6	1.5
C ₅ H ₁₀	cyclopentane	-76.4 ± 0.7	6	-3.9
C ₅ H ₁₀ O ₂	CH ₃ CH ₂ C(O)OCH ₂ CH ₃	-463.4 ± 0.7	6	2.4
C ₅ H ₁₁ N	piperidine	-47.2 ± 0.6	6	0.2
C ₅ H ₁₂	CH ₃ CH ₂ CH ₂ CH ₂ CH ₃	-146.9 ± 0.8	6	-0.9
C ₅ H ₁₂	C(CH ₃) ₄	-168.0 ± 0.8	6	-0.9
C ₅ H ₁₂ O	CH ₃ OCH ₂ CH ₂ CH ₂ CH ₃	-258.1 ± 1.2	6	0.8
C ₅ H ₁₂ O	CH ₃ CH ₂ OCH ₂ CH ₂ CH ₃	-272.0 ± 1.1	6	0.1
C ₆ H ₃ N ₇	tri- <i>s</i> -triazine (1,3,4,6,7,9,9b-heptaazaphenalene)	514.0 ± 6.0 ^c		
C ₆ H ₄ ClNO ₂	1,4-Cl-C ₆ H ₄ -NO ₂	39.7 ± 2.6	13	12.2 ^b
C ₆ H ₄ N ₂ O ₄	1,2-O ₂ N-C ₆ H ₄ -NO ₂	93.7 ± 1.2	14	19.2 ^b
C ₆ H ₄ N ₂ O ₄	1,3-O ₂ N-C ₆ H ₄ -NO ₂	54.0 ± 1.7	6	11.2 ^b
C ₆ H ₄ N ₂ O ₄	1,4-O ₂ N-C ₆ H ₄ -NO ₂	55.6 ± 0.8	14	12.5 ^b
C ₆ H ₅ Cl	C ₆ H ₅ Cl	52.0 ± 1.3	6	1.7
C ₆ H ₅ NO ₂	C ₆ H ₅ NO ₂	67.5 ± 0.5	6	11.0
		63.0 ± 2.0 ^a	7	
C ₆ H ₆ N ₂ O ₂	1,4-NO ₂ -C ₆ H ₄ -NH ₂	55.2 ± 1.8	37	2.0
C ₆ H ₆	C ₆ H ₆	82.9 ± 0.9	15	-0.7
C ₆ H ₆ N ₂ O	4-pyridinecarboxamide	-34.1 ± 2.1	16	5.0
C ₆ H ₆ O	C ₆ H ₅ OH	-96.4 ± 0.9	6	-4.4
C ₆ H ₇ N	C ₆ H ₅ NH ₂	87.1 ± 1.1	6	-0.5
C ₆ H ₇ N	4-methylpyridine	104.0 ± 0.9	6	1.7
C ₆ H ₈	trans-1,3,5-hexatriene	168.0 ± 3.0	6	1.9
C ₆ H ₉ N ₃ O ₃	trimethyl cyanurate	-387.9 ± 1.5	17	6.5 ^b
C ₆ H ₁₁ NO ₂	nitrocyclohexane	-159.3 ± 0.7	14	5.1 ^b
C ₆ H ₁₂	cyclohexane	-123.3 ± 0.8	6	-2.2
C ₆ H ₁₂	methylcyclopentane	-106.2 ± 0.7	6	-2.3
C ₆ H ₁₃ N	aminocyclohexane	-104.9 ± 1.3	18	-2.1
C ₆ H ₁₄	CH ₃ (CH ₂) ₄ CH ₃	-166.9 ± 0.8	6	0.5
C ₆ H ₁₄ O	CH ₃ CH ₂ CH ₂ OCH ₂ CH ₂ CH ₃	-293.0 ± 0.8	6	-0.3
C ₆ H ₁₄ O	(CH ₃) ₂ CHOCH(CH ₃) ₂	-319.2 ± 1.4	6	2.3
C ₇ H ₅ N	C ₆ H ₅ CN	215.7 ± 2.1	6	2.2
C ₇ H ₆ O	C ₆ H ₅ C(O)H	-36.7 ± 2.8	6	2.0
C ₇ H ₆ O ₂	C ₆ H ₅ C(O)OH	-294.0 ± 2.2	6	2.9
C ₇ H ₇ NO	C ₆ H ₅ C(O)NH ₂	-99.0 ± 1.2	19,20	-0.1
C ₇ H ₇ NO ₂	1,4-O ₂ N-C ₆ H ₄ -CH ₃	31.0 ± 3.8	6	10.0 ^b
C ₇ H ₈	C ₆ H ₅ CH ₃	50.1 ± 1.1	15	-0.1
C ₇ H ₈ O	C ₆ H ₅ OCH ₃	-67.9 ± 0.8	6	3.4
C ₇ H ₈ O	1,4-CH ₃ -C ₆ H ₄ -OH	-125.3 ± 1.6	6	-1.9
C ₇ H ₉ N	1,4-CH ₃ -C ₆ H ₄ -NH ₂	57.0 ± 1.3	21	0.2
C ₇ H ₁₄	methylcyclohexane	-154.6 ± 1.0	6	-1.0
C ₇ H ₁₆	(C ₂ H ₅) ₃ CH	-189.5 ± 1.1	6	-1.7
C ₇ H ₁₆	(C ₂ H ₅) ₂ C(CH ₃) ₂	-201.0 ± 1.1	6	1.5
C ₇ H ₁₇ N	(C ₂ H ₅) ₃ CNH ₂	-177.3 ± 5.0 ^c		
C ₈ H ₆ N ₂ O ₂	5-nitroindole	136.9 ± 2.1	22	11.1 ^b

C ₈ H ₇ N	indole	164.3 ± 1.3	23	4.1
C ₈ H ₇ NO ₃	1,4-O ₂ N-C ₆ H ₄ -C(O)CH ₃	148.0 ± 1.4	6	7.2 ^b
C ₈ H ₈	C ₆ H ₅ CH=CH ₂	148.0 ± 1.4	6	0.4
C ₈ H ₈	1,3,5,7-cyclooctatetraene	295.9 ± 1.7	6	-2.8
C ₈ H ₈ O	C ₆ H ₅ C(O)CH ₃	-86.7 ± 1.5	6	-2.0
C ₈ H ₈ O ₂	C ₆ H ₅ C(O)OCH ₃	-287.9 ± 2.4	6	-9.2
		-269.3 ± 5.1	24	9.4
		-276.7 ± 4 ^a		
C ₈ H ₈ O ₂	CH ₃ C(O)OC ₆ H ₅	-279.7 ± 1.2	6	-4.9
C ₈ H ₉ NO	C ₆ H ₅ NHC(O)CH ₃	-109.2 ± 2.2	25	-0.7
C ₈ H ₁₀	1,2-CH ₃ -C ₆ H ₄ -CH ₃	19.1 ± 1.0	6	2.7
C ₈ H ₁₀	1,3-CH ₃ -C ₆ H ₄ -CH ₃	17.3 ± 0.3	6	0.3
C ₈ H ₁₀	1,4-CH ₃ -C ₆ H ₄ -CH ₃	18.1 ± 1.0	6	0.2
C ₈ H ₁₀	C ₆ H ₅ CH ₂ CH ₃	29.9 ± 0.4	26	1.2
C ₈ H ₁₀ N ₂ O ₂	1,4-O ₂ N-C ₆ H ₄ -N(CH ₃) ₂	62.8 ± 2.6	27	2.0
C ₈ H ₁₁ N	C ₆ H ₅ N(CH ₃) ₂	100.5 ± 3.2	6	1.3
C ₈ H ₁₆	cyclooctane	-124.4 ± 1.0	6	-2.6
C ₈ H ₁₈	(C ₂ H ₅) ₃ C(CH ₃)	-214.8 ± 1.4	6	4.9
C ₉ H ₁₂	C ₆ H ₅ CH(CH ₃) ₂	4.0 ± 1.0	6	3.4
C ₉ H ₁₂	1,3,5-trimethylbenzene	-15.9 ± 1.3	6	0.5
C ₉ H ₁₃ N	C ₆ H ₅ (CH ₃) ₂ CNH ₂	22.1 ± 1.5	28	3.5
C ₉ H ₂₀	(C ₂ H ₅) ₄ C	-233.3 ± 1.7	6	3.6
C ₁₀ H ₈ N ₂ O ₂	1-(4-nitrophenyl)pyrrole	205.5 ± 2.5	29	8.1 ^b
C ₁₀ H ₁₄	C ₆ H ₅ C(CH ₃) ₂	-23.0 ± 1.5	6	4.4
C ₁₀ H ₁₆	adamantane	-132.3 ± 2.2	30	7.2
C ₁₀ H ₁₇ N	1-aminoadamantane	-133.8 ± 2.4	31	4.1
C ₁₁ H ₁₇ NO	1-adamantylcarboxamide	-319.0 ± 2.5	32	10.6
C ₁₁ H ₁₈	1-methyladamantane	-174.9 ± 2.1	33	10.4
C ₁₂ H ₁₀	C ₆ H ₅ -C ₆ H ₅	180.3 ± 3.3	15	5.1
C ₁₂ H ₁₀ N ₂	C ₆ H ₅ -N=N-C ₆ H ₅	405.5 ± 1.3	34	2.3
C ₁₃ H ₁₂	C ₆ H ₅ CH ₂ C ₆ H ₅	164.7 ± 0.7	35	3.6
C ₁₉ H ₁₆	(C ₆ H ₅) ₃ CH	271.2 ± 1.4	6	23.7 ^d

^aValue calculated from isodesmic reactions is recommended as more reliable. ^bIsodesmic reaction calculations support the experimental value. ^cThe G4 value is used when experimental data are not available. ^dG4(MP2) value. Isodesmic reaction calculations predict a somewhat lower value of enthalpy of formation (266.7 kJ·mol⁻¹) compared with experiment; experimental value is used in this work.

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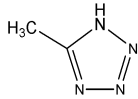
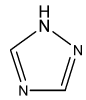

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Table S4. Enthalpies of Formation of Gaseous Azido Compounds Calculated from Isogyric, Isodesmic, and Other Balanced Reactions Using G4 Energies (in kJ/mol)^a

No	reaction	$\Delta_r H^\circ{}^b$	$\Delta_f H^\circ{}_{298}$
HN₃ (1)^c			
1	HN ₃ + •CH ₂ CH ₃ → N ₂ + •N(CH ₃) ₂	-252.5	291.9
2	HN ₃ + •CH ₃ → •NHCH ₃ + N ₂	-256.8	294.2
3	HN ₃ + •C(O)NH ₂ → N ₂ + •NHC(O)NH ₂	-272.9	288.8
4	HN ₃ + H• → •NH ₂ + N ₂	-321.0	289.2
5	HN ₃ + O ₂ → HNO ₂ + N ₂	-369.6	291.1
6	HN ₃ + CH ₃ CH ₂ NH ₂ → C ₂ H ₄ N ₄ + 2 H ₂	41.6	286.6
			
7	HN ₃ + CH ₃ CH ₂ NH ₂ + 2 H ₂ → 2 CH ₃ NHNH ₂	-52.3	289.2
8	HN ₃ + CH ₃ NH ₂ → CH ₂ N ₄ + 2 H ₂	61.0	296.9
9	HN ₃ + H ₂ C=CH ₂ → C ₂ H ₃ N ₃ + H ₂	-152.0	292.2
			
10	HN ₃ + 2 HCCH → C ₃ H ₄ N ₂ + HCN	-443.8	298.8
			
	average:		291.2
•N₃ (2)			
1	•N ₃ + C ₆ H ₅ C(O)H → •C(O)C ₆ H ₅ + HN₃	-0.9	446.4
2	•N ₃ + C ₆ H ₅ CH ₃ → •CH ₂ C ₆ H ₅ + HN₃	1.3	449.1
3	•N ₃ + CH ₃ C(O)H → •C(O)CH ₃ + HN₃	-3.3	451.6
4	•N ₃ + CH ₃ CH ₂ C(O)H → •C(O)CH ₂ CH ₃ + HN₃	-3.8	450.2
5	•N ₃ + H ₂ CO → •C(O)H + HN₃	-5.6	449.2
6	•N ₃ + NH(CH ₃) ₂ → •N(CH ₃) ₂ + HN₃	15.8	453.7
7	•N ₃ + HC(O)NH ₂ → •C(O)NH ₂ + HN₃	16.7	449.5
8	•N ₃ + CH ₃ C(O)H → •CH ₂ C(O)H + HN₃	22.6	449.0
9	•N ₃ + CH ₃ OH → •CH ₂ OH + HN₃	27.1	449.9
10	•N ₃ + CH(CH ₃) ₃ → •C(CH ₃) ₃ + HN₃	27.4	447.3

11	$\bullet\text{N}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \bullet\text{CH}(\text{CH}_3)_2 + \text{HN}_3$	35.0	450.2
12	$\bullet\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \bullet\text{CH}_2\text{CH}_3 + \text{HN}_3$	46.8	448.3
13	$\bullet\text{N}_3 + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \bullet\text{CH}_2\text{CH}_2\text{OH} + \text{HN}_3$	48.6	448.1
14	$\bullet\text{N}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \bullet\text{CH}_2\text{CH}_2\text{CH}_3 + \text{HN}_3$	48.6	448.6
15	$\bullet\text{N}_3 + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \bullet\text{OCH}_2\text{CH}_3 + \text{HN}_3$	60.7	453.4
16	$\bullet\text{N}_3 + \text{CH}_3\text{OH} \rightarrow \bullet\text{OCH}_3 + \text{HN}_3$	62.2	448.8
17	$\bullet\text{N}_3 + \text{CH}_4 \rightarrow \bullet\text{CH}_3 + \text{HN}_3$	62.7	450.9
18	$\bullet\text{N}_3 + \text{H}_2 \rightarrow \bullet\text{H} + \text{HN}_3$	62.9	447.6
19	$\bullet\text{N}_3 + \text{NH}_2\text{C}(\text{O})\text{NH}_2 \rightarrow \bullet\text{NHC}(\text{O})\text{NH}_2 + \text{HN}_3$	76.1	452.7
20	$\bullet\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \bullet\text{C}_6\text{H}_5 + \text{HN}_3$	96.6	452.7

average: 449.9

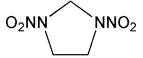
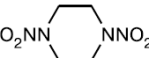

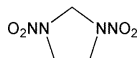
CH₃N₃ (3)

1	$\text{CH}_3\text{N}_3 + \bullet\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{OCH}_3 + \bullet\text{N}_3$	-16.0	298.9
2	$\text{CH}_3\text{N}_3 + \bullet\text{CH}_2\text{C}_6\text{H}_5 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 + \bullet\text{N}_3$	-28.3	300.2
3	$\text{CH}_3\text{N}_3 + \bullet\text{N}(\text{CH}_3)_2 \rightarrow \text{N}(\text{CH}_3)_3 + \bullet\text{N}_3$	-30.3	298.5
4	$\text{CH}_3\text{N}_3 + \bullet\text{NO}_2 \rightarrow \text{CH}_3\text{NO}_2 + \bullet\text{N}_3$	44.1	297.4
5	$\text{CH}_3\text{N}_3 + \bullet\text{CH}_2\text{C}(\text{O})\text{H} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{H} + \bullet\text{N}_3$	-49.0	300.4
6	$\text{CH}_3\text{N}_3 + \bullet\text{C}(\text{O})\text{C}_6\text{H}_5 \rightarrow \text{C}_6\text{H}_5\text{C}(\text{O})\text{CH}_3 + \bullet\text{N}_3$	-50.0	297.0
7	$\text{CH}_3\text{N}_3 + \bullet\text{OCH}_3 \rightarrow \text{CH}_3\text{OCH}_3 + \bullet\text{N}_3$	-51.2	300.1
8	$\text{CH}_3\text{N}_3 + \bullet\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_3 + \bullet\text{N}_3$	-51.2	298.4
9	$\text{CH}_3\text{N}_3 + \bullet\text{C}(\text{O})\text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{CH}_3 + \bullet\text{N}_3$	-51.6	294.8
10	$\text{CH}_3\text{N}_3 + \bullet\text{C}(\text{O})\text{H} \rightarrow \text{CH}_3\text{C}(\text{O})\text{H} + \bullet\text{N}_3$	-53.8	295.2
11	$\text{CH}_3\text{N}_3 + \bullet\text{C}(\text{O})\text{NH}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{NH}_2 + \bullet\text{N}_3$	-66.7	293.5
12	$\text{CH}_3\text{N}_3 + \bullet\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}(\text{CH}_3)_3 + \bullet\text{N}_3$	-69.4	297.2
13	$\text{CH}_3\text{N}_3 + \bullet\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \bullet\text{N}_3$	-72.1	298.6
14	$\text{CH}_3\text{N}_3 + \bullet\text{CH}_2\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} + \bullet\text{N}_3$	-73.6	299.5
15	$\text{CH}_3\text{N}_3 + \bullet\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \bullet\text{N}_3$	-74.6	298.9
16	$\text{CH}_3\text{N}_3 + \bullet\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3 + \bullet\text{N}_3$	-76.5	296.0
17	$\text{CH}_3\text{N}_3 + \bullet\text{NHC}(\text{O})\text{NH}_2 \rightarrow \text{CH}_3\text{NHC}(\text{O})\text{NH}_2 + \bullet\text{N}_3$	-76.8	297.0
18	$\text{CH}_3\text{N}_3 + \bullet\text{C}_6\text{H}_5 \rightarrow \text{C}_6\text{H}_5\text{CH}_3 + \bullet\text{N}_3$	-135.0	295.4
19	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{NH}_2 \rightarrow \text{NH}(\text{CH}_3)_2 + \text{HN}_3$	-1.3	298.4
20	$\text{CH}_3\text{N}_3 + \text{HCl} \rightarrow \text{CH}_3\text{Cl} + \text{HN}_3$	4.0	298.9
21	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_3 + \text{HN}_3$	9.5	301.8
22	$\text{CH}_3\text{N}_3 + \text{NH}_2\text{NH}_2 \rightarrow \text{CH}_3\text{NHNH}_2 + \text{HN}_3$	-10.0	302.0
23	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{OCH}_3 + \text{HN}_3$	11.0	298.9

24	$\text{CH}_3\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_3 + \text{HN}_3$	-13.7	296.8
25	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{COOH} \rightarrow \text{CH}_3\text{COOCH}_3 + \text{HN}_3$	14.0	298.0
26	$\text{CH}_3\text{N}_3 + \text{HN}(\text{CH}_3)_2 \rightarrow \text{N}(\text{CH}_3)_3 + \text{HN}_3$	-14.5	302.2
27	$\text{CH}_3\text{N}_3 + \text{C}_6\text{H}_5\text{OH} \rightarrow \text{C}_6\text{H}_5\text{OCH}_3 + \text{HN}_3$	15.8	305.2
28	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{CH}_2\text{NH}_2 \rightarrow \text{N}(\text{CH}_3)_3 + \text{HN}_3$	17.0	299.4
29	$\text{CH}_3\text{N}_3 + \text{NH}_3 \rightarrow \text{CH}_3\text{NH}_2 + \text{HN}_3$	18.0	297.1
30	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{CN} \rightarrow \text{CH}_3\text{CH}_2\text{CN} + \text{HN}_3$	-23.0	293.2
31	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{HN}_3$	-25.3	296.9
32	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{NH}_2 + \text{HN}_3$	-25.7	295.6
33	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{HN}_3$	-26.0	297.5
34	$\text{CH}_3\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 + \text{HN}_3$	-27.0	299.3
35	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{NH}_2 + \text{HN}_3$	-32.7	301.1
36	$\text{CH}_3\text{N}_3 + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{OH} + \text{HN}_3$	33.9	298.9
37	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}(\text{CH}_3)_3 + \text{HN}_3$	-34.5	297.5
38	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{NO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{NO}_2 + \text{HN}_3$	-34.7	299.2
39	$\text{CH}_3\text{N}_3 + \text{C}_5\text{H}_{10}$ (cyclopentane) $\rightarrow \text{C}_5\text{H}_9\text{CH}_3$ (methylcyclopentane) + HN_3	-36.3	299.0
40	$\text{CH}_3\text{N}_3 + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{HN}_3$	-36.7	296.7
41	$\text{CH}_3\text{N}_3 + \text{C}_6\text{H}_{12}$ (cyclohexane) $\rightarrow \text{C}_5\text{H}_9\text{CH}_3$ (methylcyclohexane) + HN_3	-37.4	298.6
42	$\text{CH}_3\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{C}_6\text{H}_5\text{CH}_3 + \text{HN}_3$	-38.4	298.1
43	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{CH}_2\text{OCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{HN}_3$	-38.6	295.4
44	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{OCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_3 + \text{HN}_3$	-38.8	299.0
45	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_3\text{CH}(\text{NH}_2)\text{CH}_3 + \text{HN}_3$	-41.4	297.8
46	$\text{CH}_3\text{N}_3 + \text{C}_6\text{H}_5\text{C}(\text{O})\text{H} \rightarrow \text{C}_6\text{H}_5\text{C}(\text{O})\text{CH}_3 + \text{HN}_3$	-50.9	293.4
47	$\text{CH}_3\text{N}_3 + \text{CH}_3\text{C}(\text{O})\text{H} \rightarrow \text{CH}_3\text{C}(\text{O})\text{CH}_3 + \text{HN}_3$	-54.8	296.3
48	$\text{CH}_3\text{N}_3 + \text{HC}(\text{O})\text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OH} + \text{HN}_3$	-56.5	294.9
49	$\text{CH}_3\text{N}_3 + \text{HC}(\text{O})\text{H} \rightarrow \text{CH}_3\text{C}(\text{O})\text{H} + \text{HN}_3$	-59.8	294.8
50	$\text{CH}_3\text{N}_3 + \text{HCN} \rightarrow \text{CH}_3\text{CN} + \text{HN}_3$	-60.5	295.0
		average:	297.9
$\text{C}_6\text{H}_5\text{N}_3$ (4)			
1	$\text{C}_6\text{H}_5\text{N}_3 + \bullet\text{CH}_2\text{C}_6\text{H}_5 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{C}_6\text{H}_5 + \bullet\text{N}_3$	-11.9	417.6
2	$\text{C}_6\text{H}_5\text{N}_3 + \bullet\text{N}(\text{CH}_3)_2 \rightarrow \text{C}_6\text{H}_5\text{N}(\text{CH}_3)_2 + \bullet\text{N}_3$	-21.1	413.4
3	$\text{C}_6\text{H}_5\text{N}_3 + \bullet\text{C}(\text{O})\text{H} \rightarrow \text{C}_6\text{H}_5\text{C}(\text{O})\text{H} + \bullet\text{N}_3$	-41.6	412.4
4	$\text{C}_6\text{H}_5\text{N}_3 + \bullet\text{C}(\text{O})\text{NH}_2 \rightarrow \text{C}_6\text{H}_5\text{C}(\text{O})\text{NH}_2 + \bullet\text{N}_3$	-47.2	413.3
5	$\text{C}_6\text{H}_5\text{N}_3 + \bullet\text{CH}(\text{CH}_3)_2 \rightarrow \text{C}_6\text{H}_5\text{CH}(\text{CH}_3)_2 + \bullet\text{N}_3$	-51.0	417.0
6	$\text{C}_6\text{H}_5\text{N}_3 + \bullet\text{OCH}_3 \rightarrow \text{C}_6\text{H}_5\text{OCH}_3 + \bullet\text{N}_3$	-52.8	417.9

7	$C_6H_5N_3 + \bullet CH_2CH_3 \rightarrow C_6H_5CH_2CH_3 + \bullet N_3$	-55.6	416.7
8	$C_6H_5N_3 + \bullet CH_3 \rightarrow C_6H_5CH_3 + \bullet N_3$	-58.3	411.7
9	$C_6H_5N_3 + \bullet NO_2 \rightarrow C_6H_5NO_2 + \bullet N_3$	63.1	415.9
10	$C_6H_5N_3 + CH_4 \rightarrow C_6H_5CH_3 + HN_3$	4.4	413.0
11	$C_6H_5N_3 + NH_2C(O)CH_3 \rightarrow C_6H_5NHC(O)CH_3 + HN_3$	4.9	416.7
12	$C_6H_5N_3 + CH_3CH_3 \rightarrow C_6H_5CH_2CH_3 + HN_3$	-8.9	415.1
13	$C_6H_5N_3 + NH_3 \rightarrow C_6H_5NH_2 + HN_3$	9.7	415.9
14	$C_6H_5N_3 + C_6H_5CH_3 \rightarrow C_6H_5CH_2C_6H_5 + HN_3$	-10.6	417.7
15	$C_6H_5N_3 + CH_3CH_2CH_3 \rightarrow C_6H_5CH(CH_3)_2 + HN_3$	-16.0	417.2
16	$C_6H_5N_3 + H_2C=CH_2 \rightarrow C_6H_5CH=CH_2 + HN_3$	16.4	412.8
17	$C_6H_5N_3 + CH_3CH_3 \rightarrow 1,4-CH_3-C_6H_4-CH_3 + HN_3$	-19.0	413.4
18	$C_6H_5N_3 + HC(O)NH_2 \rightarrow C_6H_5C(O)NH_2 + HN_3$	-30.5	412.9
19	$C_6H_5N_3 + HCN \rightarrow C_6H_5CN + HN_3$	-35.2	411.4
20	$C_6H_5N_3 + HC(O)OH \rightarrow C_6H_5C(O)OH + HN_3$	-38.4	415.6
21	$C_6H_5N_3 + CH_3C(O)H \rightarrow C_6H_5C(O)CH_3 + HN_3$	-38.6	410.5
22	$C_6H_5N_3 + CH_3OH \rightarrow 1,4-CH_3-C_6H_4-OH + HN_3$	-42.7	411.4
23	$C_6H_5N_3 + CH_3NH_2 \rightarrow H_2NC_6H_4CH_3 + HN_3$	-44.0	416.9
24	$C_6H_5N_3 + HC(O)H \rightarrow C_6H_5C(O)H + HN_3$	-47.5	411.9
25	$C_6H_5N_3 + CH_3OH \rightarrow C_6H_5OH + CH_3N_3$	-6.4	409.5
26	$C_6H_5N_3 + CH_3NH_2 \rightarrow C_6H_5NH_2 + CH_3N_3$	-8.3	416.8
27	$C_6H_5N_3 + N(CH_3)_3 \rightarrow C_6H_5N(CH_3)_2 + CH_3N_3$	9.1	413.0
28	$C_6H_5N_3 + CH_3C(O)H \rightarrow C_6H_5C(O)H + CH_3N_3$	12.2	415.2
29	$C_6H_5N_3 + CH_3C(O)CH_3 \rightarrow C_6H_5C(O)CH_3 + CH_3N_3$	16.2	412.2
30	$C_6H_5N_3 + H_2C=CHCH_3 \rightarrow C_6H_5CH=CH_2 + CH_3N_3$	16.4	414.1
31	$C_6H_5N_3 + CH_3CH_2C_6H_5 \rightarrow C_6H_5CH_2C_6H_5 + CH_3N_3$	16.4	416.3
32	$C_6H_5N_3 + CH_3CH_2CH_3 \rightarrow C_6H_5CH_2CH_3 + CH_3N_3$	16.5	416.1
33	$C_6H_5N_3 + CH_3C(O)OH \rightarrow C_6H_5C(O)OH + CH_3N_3$	18.1	418.7
34	$C_6H_5N_3 + CH_3CH_3 \rightarrow C_6H_5CH_3 + CH_3N_3$	18.2	414.1
35	$C_6H_5N_3 + CH(CH_3)_3 \rightarrow C_6H_5CH(CH_3)_2 + CH_3N_3$	18.5	417.7
36	$C_6H_5N_3 + CH_3NO_2 \rightarrow C_6H_5NO_2 + CH_3N_3$	19.0	416.5
37	$C_6H_5N_3 + CH_4 \rightarrow C_6H_6 + CH_3N_3$	42.8	412.2
38	$C_6H_5N_3 + CH_3NHCH_3 \rightarrow 1,4-CH_3-C_6H_4-NH_2 + CH_3N_3$	-42.8	416.6
	average:	414.7	

CH₃N(NO₂)CH₂N₃ (9)

1	$\text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3 + \cdot\text{H} \rightarrow \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_3 + \cdot\text{N}_3$	-112.3	336.8
2	$2 \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow (\text{CH}_2\text{CH}_2\text{CH}_2)(\text{NNO}_2)_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + 2 \text{HN}_3$	1.5	333.2
			
3	$2 \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3 \rightarrow (\text{CH}_2\text{CH}_2)_2(\text{NNO}_2)_2 + 2 \text{HN}_3$	-29.0	331.9
			
4	$\text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3 + 2 \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_2\text{NO}_2 + \text{CH}_3\text{CH}_2\text{NH}_2 + \text{HN}_3$	-47.2	338.5
5	$\text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3 + \text{H}_2 \rightarrow \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_3 + \text{HN}_3$	-49.4	334.4
6	$\text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3 + 2 \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{NO}_2 + \text{N}(\text{CH}_3)_3 + \text{CH}_3\text{N}_3$	-2.8	342.3
7	$\text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_3 + \text{CH}_3\text{N}_3$	28.9	336.0
8	$2 \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3 + \text{H}_2\text{C}=\text{CH}_2 \rightarrow (\text{CH}_2\text{CH}_2)_2(\text{NNO}_2)_2 + 2 \text{CH}_3\text{N}_3$	-73.6	333.4
			
9	$2 \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3 + \text{C}_5\text{H}_{10} \text{ (cyclopentane)} \rightarrow (\text{CH}_2\text{CH}_2\text{CH}_2)(\text{NNO}_2)_2 + \text{C}_4\text{H}_8 \text{ (cyclobutane)} + 2 \text{CH}_3\text{N}_3$	132.8	335.5
			
10	$\text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	-13.9	338.5
	average:		336.1

C₆H₅CH₂N₃ (5)

1	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \cdot\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 + \cdot\text{N}_3$	-71.0	404.2
2	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \cdot\text{H} \rightarrow \text{C}_6\text{H}_5\text{CH}_3 + \cdot\text{N}_3$	-122.5	404.6
3	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \cdot\text{H} \rightarrow \cdot\text{CH}_2\text{C}_6\text{H}_5 + \text{HN}_3$	-121.2	403.7
4	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \text{CH}_4 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 + \text{HN}_3$	-8.3	405.1
5	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}(\text{CH}_3)_2 + \text{HN}_3$	-27.0	407.3
6	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \text{H}_2 \rightarrow \text{C}_6\text{H}_5\text{CH}_3 + \text{HN}_3$	-59.6	402.2
7	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \cdot\text{CH}_3 \rightarrow \cdot\text{CH}_2\text{C}_6\text{H}_5 + \text{CH}_3\text{N}_3$	-42.7	402.0
8	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}(\text{CH}_3)_2 + \text{CH}_3\text{N}_3$	-1.7	408.4
9	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{C}_6\text{H}_5 + \text{CH}_3\text{N}_3$	3.7	408.9
10	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	5.4	406.3
11	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \text{H}_2\text{C}=\text{CH}_2 \rightarrow \text{C}_6\text{H}_5\text{CH}=\text{CH}_2 + \text{CH}_3\text{N}_3$	-10.6	404.1
12	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \text{CH}_4 \rightarrow \text{C}_6\text{H}_5\text{CH}_3 + \text{CH}_3\text{N}_3$	18.7	403.8
13	$\text{C}_6\text{H}_5\text{CH}_2\text{N}_3 + \text{H}_2 \rightarrow \text{C}_6\text{H}_6 + \text{CH}_3\text{N}_3$	-21.2	402.1

14	$C_6H_5CH_2N_3 + CH_3CH_3 \rightarrow CH_3CH_2CH_3 + C_6H_5N_3$	-11.0	405.1
15	$C_6H_5CH_2N_3 + CH_3CH_2CH_3 \rightarrow CH_3CH_2CH_2CH_3 + C_6H_5N_3$	-11.7	405.7
16	$C_6H_5CH_2N_3 + C_6H_5CH_3 \rightarrow C_6H_5CH_2CH_3 + C_6H_5N_3$	-12.7	407.5
17	$C_6H_5CH_2N_3 + C_6H_5CH_2CH_3 \rightarrow C_6H_5CH(CH_3)_2 + C_6H_5N_3$	-18.2	407.3
18	$C_6H_5CH_2N_3 + H_2C=CH_2 \rightarrow CH_3CH=CH_2 + C_6H_5N_3$	-22.4	404.9
19	$C_6H_5CH_2N_3 + CH_3OCH_2CH_3 \rightarrow CH_3CH_2OCH_2CH_3 + C_6H_5N_3$	-24.4	403.7
20	$C_6H_5CH_2N_3 + HC(O)NH_2 \rightarrow CH_3C(O)NH_2 + C_6H_5N_3$	-35.7	401.3
21	$C_6H_5CH_2N_3 + CH_3C(O)H \rightarrow CH_3C(O)CH_3 + C_6H_5N_3$	-40.6	404.6
22	$C_6H_5CH_2N_3 + HC(O)H \rightarrow CH_3C(O)H + C_6H_5N_3$	-45.1	402.6
23	$C_6H_5CH_2N_3 + CH_3N(NO_2)CH_3 \rightarrow C_6H_5CH_3 + CH_3N(NO_2)CH_2N_3$	-10.2	403.8
	average:		404.7
NCN₃ (7)			
1	$NCN_3 + \bullet CH_3 \rightarrow CH_3CN + \bullet N_3$	-121.8	499.1
2	$NCN_3 + \bullet H \rightarrow HCN + \bullet N_3$	-139.8	503.8
3	$NCN_3 + \bullet C_6H_5 \rightarrow C_6H_5CN + \bullet N_3$	-173.2	499.2
4	$NCN_3 + CH_3CN \rightarrow NCCH_2CN + HN_3$	-26.3	497.5
5	$NCN_3 + HCN \rightarrow NCCN + HN_3$	-30.4	497.6
6	$NCN_3 + CH_4 \rightarrow CH_3CN + HN_3$	-59.1	500.0
7	$NCN_3 + C_6H_6 \rightarrow C_6H_5CN + HN_3$	-76.6	501.9
8	$NCN_3 + CH_4 \rightarrow HCN + CH_3N_3$	1.4	503.0
9	$NCN_3 + CH_3CN \rightarrow NCCN + CH_3N_3$	30.1	500.6
10	$NCN_3 + C_6H_5CH_3 \rightarrow C_6H_5CN + CH_3N_3$	-38.2	501.8
11	$NCN_3 + CH_3CH_3 \rightarrow CH_3CN + CH_3N_3$	-45.3	501.1
12	$NCN_3 + C_6H_5CN \rightarrow NCCN + C_6H_5N_3$	4.8	501.2
13	$NCN_3 + C_6H_6 \rightarrow HCN + C_6H_5N_3$	-41.4	505.5
14	$NCN_3 + 2 C_6H_5CH_3 \rightarrow C_6H_5CN + CH_3CH_3 + C_6H_5N_3$	-56.4	503.1
15	$NCN_3 + C_6H_5CH_3 \rightarrow CH_3CN + C_6H_5N_3$	-63.5	502.4
16	$NCN_3 + C_6H_5CH_2CH_3 \rightarrow CH_3CN + C_6H_5CH_2N_3$	-50.8	499.9
	average:		501.1
1,4-NO₂-C₆H₄-N₃ (6)			
1	$1,4-NO_2-C_6H_4-N_3 + \bullet NO_2 \rightarrow 1,4-NO_2-C_6H_4-NO_2 + \bullet N_3$	74.9	396.7
2	$1,4-NO_2-C_6H_4-N_3 + \bullet H \rightarrow C_6H_5NO_2 + \bullet N_3$	-100.2	395.2
3	$1,4-NO_2-C_6H_4-N_3 + NH_3 \rightarrow 1,4-O_2N-C_6H_4-NH_2 + HN_3$	0.5	393.2
4	$1,4-NO_2-C_6H_4-N_3 + C_4H_5N(\text{pyrrole}) \rightarrow NO_2-C_6H_4-C_4H_4N [1-(4\text{-nitrophenyl})\text{pyrrole}] + HN_3$	-6.2	395.8
5	$1,4-NO_2-C_6H_4-N_3 + NH(CH_3)_2 \rightarrow 1,4-NO_2-C_6H_4-N(CH_3)_2 + HN_3$	-18.5	392.6

6	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_3\text{C(O)H} \rightarrow 1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-C(O)CH}_3 + \text{HN}_3$	-35.0	394.5
7	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{N(CH}_3)_3 \rightarrow 1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N(CH}_3)_2 + \text{CH}_3\text{N}_3$	-4.0	388.4
8	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_4\text{H}_4\text{N-CH}_3(\text{methylpyrrole}) \rightarrow \text{NO}_2\text{-C}_6\text{H}_4\text{-C}_4\text{H}_4\text{N [1-(4-nitrophenyl)pyrrole]} + \text{CH}_3\text{N}_3$	5.5	393.9
9	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{CH}_3 \rightarrow 1,4\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + \text{CH}_3\text{NO}_2 + \text{CH}_3\text{N}_3$	16.6	392.6
10	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_3\text{NH}_2 \rightarrow 1,4\text{-O}_2\text{N-C}_6\text{H}_4\text{-NH}_2 + \text{CH}_3\text{N}_3$	-17.5	394.1
11	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_3\text{C(O)CH}_3 \rightarrow 1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-C(O)CH}_3 + \text{CH}_3\text{N}_3$	19.8	396.2
12	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_3\text{NO}_2 \rightarrow 1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-NO}_2 + \text{CH}_3\text{N}_3$	30.8	397.3
13	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_4 \rightarrow \text{C}_6\text{H}_6 + \text{CH}_3\text{NO}_2 + \text{CH}_3\text{N}_3$	64.8	390.4
14	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \cdot\text{H} \rightarrow \cdot\text{NO}_2 + \text{C}_6\text{H}_5\text{N}_3$	-163.4	394.3
15	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{C}_6\text{H}_5\text{NO}_2 + \text{C}_6\text{H}_5\text{N}_3$	-1.8	396.9
16	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_5\text{Cl} \rightarrow 1,4\text{-Cl-C}_6\text{H}_4\text{-NO}_2 + \text{C}_6\text{H}_5\text{N}_3$	2.5	400.2
17	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_5\text{C(O)CH}_3 \rightarrow 1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-C(O)CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	3.6	399.0
18	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_8\text{H}_7\text{N}(\text{indole}) \rightarrow \text{C}_8\text{H}_6\text{N}_2\text{O}_2 (5\text{-nitroindole}) + \text{C}_6\text{H}_5\text{N}_3$	-9.1	396.7
19	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_5\text{NH}_2 \rightarrow 1,4\text{-O}_2\text{N-C}_6\text{H}_4\text{-NH}_2 + \text{C}_6\text{H}_5\text{N}_3$	-9.2	392.3
20	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_5\text{N(CH}_3)_2 \rightarrow 1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N(CH}_3)_2 + \text{C}_6\text{H}_5\text{N}_3$	-13.1	390.4
21	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \cdot\text{CH}_3 \rightarrow \cdot\text{NO}_2 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	-99.1	391.4
22	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{NH}_2 \rightarrow 1,4\text{-O}_2\text{N-C}_6\text{H}_4\text{-NH}_2 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	-18.0	390.4
23	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{NO}_2 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	22.3	395.6
24	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{HCN} \rightarrow \text{C}_6\text{H}_5\text{NO}_2 + \text{NCN}_3$	39.6	392.4
25	$1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3 + \text{N(CH}_3)_3 \rightarrow \text{C}_6\text{H}_5\text{CH}_3 + \text{CH}_3\text{N(NO}_2)\text{CH}_2\text{N}_3$	21.9	387.8
		average:	393.9

HOCH₂CH₂N₃ (12)

1	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \cdot\text{H} \rightarrow \text{CH}_3\text{CH}_2\text{OH} + \cdot\text{N}_3$	-116.6	113.4
2	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \cdot\text{H} \rightarrow \text{CH}_3\text{CH}_2\text{O}\cdot + \text{HN}_3$	-55.9	116.8
3	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \cdot\text{H} \rightarrow \cdot\text{CH}_2\text{CH}_2\text{OH} + \text{HN}_3$	-68.0	111.5
4	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} + \text{HN}_3$	-0.4	112.2
5	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{HN}_3$	9.1	115.1
6	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_3 + \text{HN}_3$	34.1	116.4
7	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} + \text{CH}_3\text{N}_3$	13.4	113.3
8	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_2\text{OH} + \text{CH}_3\text{N}_3$	24.6	112.6
9	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{C}_6\text{H}_5\text{OCH}_3 + \text{CH}_3\text{N}_3$	28.4	118.8
10	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	34.5	116.1
11	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_3 + \text{CH}_3\text{N}_3$	47.8	117.6
12	$\text{HOCH}_2\text{CH}_2\text{N}_3 + 2 \text{CH}_4 \rightarrow \text{CH}_3\text{OH} + \text{CH}_3\text{CH}_3 + \text{CH}_3\text{N}_3$	48.1	113.4
13	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} + \text{C}_6\text{H}_5\text{N}_3$	-4.8	114.6

14	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	18.0	115.0
15	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{CH}_3\text{CH}_2\text{OH} + \text{C}_6\text{H}_5\text{N}_3$	-18.2	115.4
16	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_3 + \text{C}_6\text{H}_5\text{N}_3$	29.6	118.9
17	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{CH}_3\text{OH} + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	4.7	116.2
18	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OH} + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	5.9	113.4
19	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CN} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} + \text{NCN}_3$	58.7	113.2
20	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{NO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{OH} + \text{1,4-NO}_2\text{-C}_6\text{H}_4\text{-N}_3$	-16.4	112.2
21	$\text{HOCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OH} + \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3$	-4.3	112.6
	average:		114.7
CH₃C(NO₂)₂N₃ (10)			
1	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \cdot\text{H} \rightarrow \text{CH}_3\text{CH}(\text{NO}_2)_2 + \cdot\text{N}_3$	-120.3	264.0
2	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \cdot\text{H} \rightarrow \text{CH}_2(\text{NO}_2)\text{CH}_2(\text{NO}_2) + \cdot\text{N}_3$	-127.2	262.5
3	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + 3 \cdot\text{H} \rightarrow \cdot\text{CH}_2\text{CH}_3 + 2 \cdot\text{NO}_2 + \text{HN}_3$	-432.5	257.7
4	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{H}_2 \rightarrow \text{CH}_3\text{CH}(\text{NO}_2)_2 + \text{HN}_3$	-57.3	261.5
5	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{H}_2 \rightarrow \text{CH}_2(\text{NO}_2)_2 + \text{CH}_3\text{N}_3$	-3.3	262.8
6	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + 2 \text{CH}_4 \rightarrow \text{CH}_3\text{NO}_2 + \text{CH}_3\text{CH}_2\text{NO}_2 + \text{CH}_3\text{N}_3$	11.6	258.2
7	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_2(\text{NO}_2)\text{CH}_2(\text{NO}_2) + \text{CH}_3\text{N}_3$	14.1	261.6
8	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}(\text{NO}_2)_2 + \text{CH}_3\text{N}_3$	21.0	263.1
9	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + 2 \text{C}_6\text{H}_6 \rightarrow \text{1,4-NO}_2\text{-C}_6\text{H}_4\text{-NO}_2 + \text{C}_6\text{H}_5\text{CH}_3 + \text{CH}_3\text{N}_3$	-26.0	263.9
10	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{CH}_3\text{CH}(\text{NO}_2)_2 + \text{C}_6\text{H}_5\text{N}_3$	-21.8	265.9
11	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{CH}_2(\text{NO}_2)\text{CH}_2(\text{NO}_2) + \text{C}_6\text{H}_5\text{N}_3$	-28.7	264.4
12	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + 2 \text{C}_6\text{H}_6 \rightarrow \text{1,4-NO}_2\text{-C}_6\text{H}_4\text{-NO}_2 + \text{CH}_3\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	-44.1	265.1
13	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + 3 \text{C}_6\text{H}_6 \rightarrow 2 \text{C}_6\text{H}_5\text{NO}_2 + \text{CH}_3\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	-57.7	267.1
14	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{CH}_2(\text{NO}_2)\text{CH}_2(\text{NO}_2) + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	-4.6	262.8
15	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{CH}_2(\text{NO}_2)_2 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	17.9	265.7
16	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NO}_2 + \text{1,4-NO}_2\text{-C}_6\text{H}_4\text{-N}_3$	-41.3	261.5
17	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{NO}_2 + \text{1,4-NO}_2\text{-C}_6\text{H}_4\text{-N}_3$	-41.7	261.3
18	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{C}_2\text{H}_5\text{NO}_2 + \text{1,4-NO}_2\text{-C}_6\text{H}_4\text{-N}_3$	-53.1	262.0
19	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_2(\text{NO}_2)_2 + \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3$	20.8	263.3
20	$\text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3 + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\text{NO}_2 + \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3$	26.1	258.8
	average:		262.7
C(NO₂)₃N₃ (11)			
1	$\text{C}(\text{NO}_2)_3\text{N}_3 + \cdot\text{H} \rightarrow \text{CH}(\text{NO}_2)_3 + \cdot\text{N}_3$	-119.4	360.0
2	$\text{C}(\text{NO}_2)_3\text{N}_3 + \cdot\text{NO}_2 \rightarrow \text{C}(\text{NO}_2)_4 + \cdot\text{N}_3$	143.9	354.6
3	$\text{C}(\text{NO}_2)_3\text{N}_3 + 2 \cdot\text{H} \rightarrow \text{CH}_2(\text{NO}_2)_2 + \cdot\text{NO}_2 + \cdot\text{N}_3$	-351.7	361.1

4	$C(NO_2)_3N_3 + 4 \cdot H \rightarrow CH_4 + 3 \cdot NO_2 + \cdot N_3$	-751.0	356.5
5	$C(NO_2)_3N_3 + H_2 \rightarrow CH(NO_2)_3 + HN_3$	-56.5	357.6
6	$C(NO_2)_3N_3 + HNO_2 \rightarrow C(NO_2)_4 + HN_3$	96.4	357.0
7	$C(NO_2)_3N_3 + CH_4 + H_2 \rightarrow CH_2(NO_2)_2 + CH_3NO_2 + HN_3$	-103.4	357.3
8	$C(NO_2)_3N_3 + CH_4 \rightarrow CH(NO_2)_3 + CH_3N_3$	21.8	359.2
9	$C(NO_2)_3N_3 + 2 CH_4 \rightarrow CH_2(NO_2)_2 + CH_3NO_2 + CH_3N_3$	-25.1	358.9
10	$C(NO_2)_3N_3 + 3 CH_4 \rightarrow 3 CH_3NO_2 + CH_3N_3$	-53.8	351.5
11	$C(NO_2)_3N_3 + CH_3CH_3 + CH_4 \rightarrow CH_3CH(NO_2)_2 + CH_3NO_2 + CH_3N_3$	-65.4	358.8
12	$C(NO_2)_3N_3 + CH_3CH_3 + CH_4 \rightarrow CH_2(NO_2)CH_2(NO_2) + CH_3NO_2 + CH_3N_3$	-72.3	357.3
13	$C(NO_2)_3N_3 + CH_3NO_2 \rightarrow C(NO_2)_4 + CH_3N_3$	99.8	355.1
14	$C(NO_2)_3N_3 + 4 CH_3CH_3 \rightarrow 3 CH_3NO_2 + C(CH_3)_4 + CH_3N_3$	-110.9	352.6
15	$C(NO_2)_3N_3 + 3 CH_3CH_3 \rightarrow (CH_3)_3CNO_2 + 2 CH_3NO_2 + CH_3N_3$	-130.5	353.8
16	$C(NO_2)_3N_3 + C_6H_6 \rightarrow CH(NO_2)_3 + C_6H_5N_3$	-21.0	361.7
17	$C(NO_2)_3N_3 + C_6H_5NO_2 \rightarrow C(NO_2)_4 + C_6H_5N_3$	80.7	353.7
18	$C(NO_2)_3N_3 + C_6H_5CH_3 + H_2 \rightarrow CH_2(NO_2)_2 + CH_3NO_2 + C_6H_5N_3$	-107.8	359.7
19	$C(NO_2)_3N_3 + 4 C_6H_5CH_3 \rightarrow 3 C_6H_5NO_2 + C(CH_3)_4 + C_6H_5N_3$	-126.4	360.4
20	$C(NO_2)_3N_3 + 2 C_6H_6 \rightarrow 1,4-NO_2-C_6H_4-NO_2 + CH_3NO_2 + C_6H_5N_3$	-130.5	360.8
21	$C(NO_2)_3N_3 + HCN \rightarrow CH(NO_2)_3 + NCN_3$	20.4	357.2
22	$C(NO_2)_3N_3 + CH_3CN + CH_3NO_2 \rightarrow C(NO_2)_4 + CH_3CH_3 + NCN_3$	145.1	355.0
23	$C(NO_2)_3N_3 + 2 C_6H_5CH_3 \rightarrow 1,4-NO_2-C_6H_4-NO_2 + CH_3CH_2NO_2 + C_6H_5CH_2N_3$	-102.8	360.7
24	$C(NO_2)_3N_3 + CH_3CH_3 \rightarrow CH_3NO_2 + CH_3C(NO_2)_2N_3$	-86.4	358.7
25	$C(NO_2)_3N_3 + CH_3CH_2CH_2CH_3 + N(CH_3)_3 \rightarrow C(CH_3)_4 + CH_2(NO_2)_2 + CH_3N(NO_2)CH_2N_3$	-76.6	355.4
26	$C(NO_2)_3N_3 + CH_3N(NO_2)CH_3 + CH_3CH_2NO_2 \rightarrow C(NO_2)_4 + CH_3CH_3 + CH_3N(NO_2)CH_2N_3$	91.9	352.7
		average:	357.2
C₅H₉-N₃ azidocyclopentane (15)			
1	$C_5H_9-N_3 + \cdot H \rightarrow C_5H_{10} \text{ (cyclopentane)} + \cdot N_3$	-100.4	256.0
2	$C_5H_9-N_3 + CH_4 \rightarrow C_5H_9-CH_3 \text{ (methylcyclopentane)} + HN_3$	4.5	256.2
3	$C_5H_9-N_3 + H_2 \rightarrow C_5H_{10} \text{ (cyclopentane)} + HN_3$	-37.5	253.6
4	$C_5H_9-N_3 + CH_3CH_3 \rightarrow C_5H_9-CH_3 \text{ (methylcyclopentane)} + CH_3N_3$	18.2	257.4
5	$C_5H_9-N_3 + CH_4 \rightarrow C_5H_{10} \text{ (cyclopentane)} + CH_3N_3$	40.8	255.2
6	$C_5H_9-N_3 + HCN \rightarrow C_5H_{10} \text{ (cyclopentane)} + NCN_3$	39.4	253.2
7	$C_5H_9-N_3 + CH_3CN \rightarrow C_6H_{12} \text{ (cyclohexane)} + NCN_3$	46.3	257.4
8	$C_5H_9-N_3 + C_6H_5CH_3 \rightarrow C_5H_9-CH_3 \text{ (methylcyclopentane)} + C_6H_5N_3$	0.1	258.6
9	$C_5H_9-N_3 + C_6H_6 \rightarrow C_5H_{10} \text{ (cyclopentane)} + C_6H_5N_3$	-2.0	258.0
10	$C_5H_9-N_3 + C_6H_5NO_2 \rightarrow C_5H_{10} \text{ (cyclopentane)} + 1,4-NO_2-C_6H_4-N_3$	-0.2	254.8

11	$C_5H_9-N_3 + 1,4-NO_2-C_6H_4-CH_3 \rightarrow C_5H_9-CH_3$ (methylcyclopentane) + $1,4-NO_2-C_6H_4-N_3$	4.0	252.8
12	$C_5H_9-N_3 + C_6H_5CH_3 \rightarrow C_5H_{10}$ (cyclopentane) + $C_6H_5CH_2N_3$	22.1	256.4
13	$C_5H_9-N_3 + 1,4-CH_3-C_6H_4-CH_3 \rightarrow C_5H_9-CH_3$ (methylcyclopentane) + $C_6H_5CH_2N_3$	23.0	257.7
14	$C_5H_9-N_3 + CH(NO_2)_2CH_3 \rightarrow C_5H_{10}$ (cyclopentane) + $CH_3C(NO_2)_2N_3$	19.8	255.1
15	$C_5H_9-N_3 + CH_3CH_2CH_2OH \rightarrow C_5H_9-CH_3$ (methylcyclopentane) + $HOCH_2CH_2N_3$	4.9	259.0
16	$C_5H_9-N_3 + CH_3CH_2OH \rightarrow C_5H_{10}$ (cyclopentane) + $HOCH_2CH_2N_3$	16.2	257.6
		average:	256.2
$C_6H_{11}-N_3$ azidocyclohexane (16)			
1	$C_6H_{11}-N_3 + \bullet H \rightarrow C_6H_{12}$ (cyclohexane) + $\bullet N_3$	-101.3	210.0
2	$C_6H_{11}-N_3 + CH_4 \rightarrow C_6H_{11}-CH_3$ (methylcyclohexane) + HN_3	2.5	209.8
3	$C_6H_{11}-N_3 + H_2 \rightarrow C_6H_{12}$ (cyclohexane) + HN_3	-38.4	207.6
4	$C_6H_{11}-N_3 + CH_3NO_2 \rightarrow C_6H_{11}-NO_2$ (nitrocyclohexane) + CH_3N_3	-0.1	213.3
5	$C_6H_{11}-N_3 + CH_3CH_3 \rightarrow C_6H_{11}-CH_3$ (methylcyclohexane) + CH_3N_3	16.2	211.0
6	$C_6H_{11}-N_3 + CH_4 \rightarrow C_6H_{12}$ (cyclohexane) + CH_3N_3	39.9	209.2
7	$C_6H_{11}-N_3 + HCN \rightarrow C_6H_{12}$ (cyclohexane) + NCN_3	38.5	207.2
8	$C_6H_{11}-N_3 + CH_3CN \rightarrow C_7H_{14}$ (cycloheptane) + NCN_3	99.9	209.0
9	$C_6H_{11}-N_3 + C_6H_5CH_3 \rightarrow C_6H_{11}-CH_3$ (methylcyclohexane) + $C_6H_5N_3$	-1.9	212.2
10	$C_6H_{11}-N_3 + C_6H_6 \rightarrow C_6H_{12}$ (cyclohexane) + $C_6H_5N_3$	-2.9	212.0
11	$C_6H_{11}-N_3 + C_6H_5NO_2 \rightarrow C_6H_{11}-NO_2$ (nitrocyclohexane) + $C_6H_5N_3$	-19.1	211.8
12	$C_6H_{11}-N_3 + C_6H_5NO_2 \rightarrow C_6H_{12}$ (cyclohexane) + $1,4-NO_2-C_6H_4-N_3$	-1.1	208.8
13	$C_6H_{11}-N_3 + 1,4-NO_2-C_6H_4-CH_3 \rightarrow C_6H_{11}-CH_3$ (methylcyclohexane) + $1,4-NO_2-C_6H_4-N_3$	2.0	206.4
14	$C_6H_{11}-N_3 + 1,4-NO_2-C_6H_4-CH_3 \rightarrow C_6H_{11}-NO_2$ (nitrocyclohexane) + $C_6H_5CH_2N_3$	7.1	207.6
15	$C_6H_{11}-N_3 + 1,4-CH_3-C_6H_4-CH_3 \rightarrow C_6H_{11}-CH_3$ (methylcyclohexane) + $C_6H_5CH_2N_3$	21.0	211.3
16	$C_6H_{11}-N_3 + C_6H_5CH_3 \rightarrow C_6H_{12}$ (cyclohexane) + $C_6H_5CH_2N_3$	21.2	210.4
17	$C_6H_{11}-N_3 + CH(NO_2)_2CH_3 \rightarrow C_6H_{12}$ (cyclohexane) + $CH_3C(NO_2)_2N_3$	19.0	209.0
18	$C_6H_{11}-N_3 + CH_3CH_2CH_2OH \rightarrow C_6H_{11}-CH_3$ (methylcyclohexane) + $HOCH_2CH_2N_3$	2.9	212.6
19	$C_6H_{11}-N_3 + CH_3CH_2OH \rightarrow C_6H_{12}$ (cyclohexane) + $HOCH_2CH_2N_3$	15.3	211.6
20	$C_6H_{11}-N_3 + C_5H_{10}$ (cyclopentane) $\rightarrow C_6H_{12}$ (cyclohexane) + $C_5H_9-N_3$ (azidocyclopentane)	-0.8	209.9
21	$C_6H_{11}-N_3 + C_5H_9-CH_3$ (methylcyclopentane) $\rightarrow C_6H_{11}-CH_3$ (methylcyclohexane) + $C_5H_9-N_3$ (azidocyclopentane)	-2.0	209.6
		average:	210.0
$1,2-N_3-C_6H_4-N_3$ 1,2-diazidobenzene (17)			
1	$1,2-N_3-C_6H_4-N_3 + 2 \bullet H \rightarrow C_6H_6 + 2 \bullet N_3$	-208.0	754.9
2	$1,2-N_3-C_6H_4-N_3 + 2 CH_4 \rightarrow 1,2-CH_3-C_6H_4-CH_3 + 2 HN_3$	-2.7	755.6
3	$1,2-N_3-C_6H_4-N_3 + 2 H_2 \rightarrow C_6H_6 + 2 HN_3$	-82.2	750.1
4	$1,2-N_3-C_6H_4-N_3 + 2 CH_3CH_3 \rightarrow 1,2-CH_3-C_6H_4-CH_3 + 2 CH_3N_3$	24.8	757.9

5	$1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_4 \rightarrow \text{C}_6\text{H}_6 + 2 \text{CH}_3\text{N}_3$	74.4	753.3
6	$1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_6 \rightarrow 2 \text{C}_6\text{H}_5\text{N}_3$	-11.2	758.3
7	$1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{C}_6\text{H}_5\text{CH}_3 \rightarrow 1,2\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{C}_6\text{H}_5\text{N}_3$	-11.5	760.4
8	$1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{N}_3 + \text{C}_6\text{H}_5\text{N}_3$	31.6	755.8
9	$1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{H}_2 \rightarrow \text{HN}_3 + \text{C}_6\text{H}_5\text{N}_3$	-46.7	754.2
10	$1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow 1,2\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	13.9	755.4
11	$1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_4 \rightarrow \text{HN}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	17.4	754.5
12	$1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow 2 \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	25.7	754.4
13	$1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	31.1	755.7
14	$1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} \rightarrow 1,2\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{HOCH}_2\text{CH}_2\text{N}_3$	-1.9	761.2
15	$1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{C}_6\text{H}_6 + 2 \text{HOCH}_2\text{CH}_2\text{N}_3$	25.3	758.0
16	$1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{CN} \rightarrow 1,2\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{NCN}_3$	115.4	757.7
		average:	756.1
1,3-N₃-C₆H₄-N₃ 1,3-diazidobenzene (18)			
1	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \cdot\text{H} \rightarrow \text{C}_6\text{H}_6 + 2 \cdot\text{N}_3$	-198.2	745.1
2	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_4 \rightarrow 1,3\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{HN}_3$	7.7	743.4
3	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{H}_2 \rightarrow \text{C}_6\text{H}_6 + 2 \text{HN}_3$	-72.4	740.3
4	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{CH}_3 \rightarrow 1,3\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{CH}_3\text{N}_3$	35.2	745.7
5	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{NO}_2 \rightarrow 1,3\text{-NO}_2\text{-C}_6\text{H}_4\text{-NO}_2 + 2 \text{CH}_3\text{N}_3$	49.8	749.2
6	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_4 \rightarrow \text{C}_6\text{H}_6 + 2 \text{CH}_3\text{N}_3$	84.2	743.5
7	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{C}_6\text{H}_5\text{CH}_3 \rightarrow 1,3\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{C}_6\text{H}_5\text{N}_3$	-1.1	748.2
8	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_6 \rightarrow 2 \text{C}_6\text{H}_5\text{N}_3$	-1.4	748.5
9	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{H}_2 \rightarrow \text{HN}_3 + \text{C}_6\text{H}_5\text{N}_3$	-36.9	744.4
10	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{N}_3 + \text{C}_6\text{H}_5\text{N}_3$	41.4	746.0
11	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow 1,3\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	24.3	743.2
12	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_4 \rightarrow \text{HN}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	27.2	746.2
13	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow 2 \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	35.5	744.6
14	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	40.9	745.9
15	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} \rightarrow 1,3\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{HOCH}_2\text{CH}_2\text{N}_3$	8.5	749.0
16	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{C}_6\text{H}_6 + 2 \text{HOCH}_2\text{CH}_2\text{N}_3$	35.1	748.2
17	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{CN} \rightarrow 1,3\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{NCN}_3$	125.9	745.4
18	$1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 \rightarrow 1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3$	9.8	746.2
		average:	745.7
1,4-N₃-C₆H₄-N₃ 1,4-diazidobenzene (19)			
1	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \cdot\text{H} \rightarrow \text{C}_6\text{H}_6 + 2 \cdot\text{N}_3$	-200.6	747.5

2	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_4 \rightarrow 1,4\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{HN}_3$	6.3	745.6
3	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{H}_2 \rightarrow \text{C}_6\text{H}_6 + 2 \text{HN}_3$	-74.7	742.6
4	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{CH}_3 \rightarrow 1,4\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{CH}_3\text{N}_3$	33.8	747.9
5	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{NO}_2 \rightarrow 1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-NO}_2 + 2 \text{CH}_3\text{N}_3$	47.9	752.7
6	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_4 \rightarrow \text{C}_6\text{H}_6 + 2 \text{CH}_3\text{N}_3$	81.9	745.8
7	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{C}_6\text{H}_5\text{CH}_3 \rightarrow 1,4\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{C}_6\text{H}_5\text{N}_3$	-2.6	750.5
8	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_6 \rightarrow 2 \text{C}_6\text{H}_5\text{N}_3$	-3.7	750.8
9	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{N}_3 + \text{C}_6\text{H}_5\text{N}_3$	39.1	748.3
10	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{H}_2 \rightarrow \text{HN}_3 + \text{C}_6\text{H}_5\text{N}_3$	-39.2	746.7
11	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow 1,4\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	22.9	745.4
12	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_4 \rightarrow \text{HN}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	24.8	747.1
13	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow 2 \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	33.1	747.0
14	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	38.5	748.3
15	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} \rightarrow 1,4\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{HOCH}_2\text{CH}_2\text{N}_3$	7.0	751.3
16	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{C}_6\text{H}_6 + 2 \text{HOCH}_2\text{CH}_2\text{N}_3$	32.7	750.6
17	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 + 2 \text{CH}_3\text{CN} \rightarrow 1,4\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 + 2 \text{NCN}_3$	124.4	747.7
18	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 \rightarrow 1,2\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3$	7.4	748.6
19	$1,4\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3 \rightarrow 1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3$	-2.4	748.4
		average:	748.0
C₆H₃(N₃)₃ 1,3,5-triazidobenzene (20)			
1	$\text{C}_6\text{H}_3(\text{N}_3)_3 + 3 \bullet\text{H} \rightarrow \text{C}_6\text{H}_6 + 3 \bullet\text{N}_3$	-298.8	1077.7
2	$\text{C}_6\text{H}_3(\text{N}_3)_3 + 3 \text{CH}_4 \rightarrow \text{C}_6\text{H}_3(\text{CH}_3)_3$ (1,3,5-trimethylbenzene) + 3 HN₃	10.1	1074.7
3	$\text{C}_6\text{H}_3(\text{N}_3)_3 + 3 \text{H}_2 \rightarrow \text{C}_6\text{H}_6 + 3 \text{HN}_3$	-110.1	1070.5
4	$\text{C}_6\text{H}_3(\text{N}_3)_3 + 3 \text{CH}_3\text{CH}_3 \rightarrow \text{C}_6\text{H}_3(\text{CH}_3)_3 + 3 \text{CH}_3\text{N}_3$	51.3	1078.2
5	$\text{C}_6\text{H}_3(\text{N}_3)_3 + 3 \text{CH}_4 \rightarrow \text{C}_6\text{H}_6 + 3 \text{CH}_3\text{N}_3$	124.8	1075.3
6	$\text{C}_6\text{H}_3(\text{N}_3)_3 + 3 \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{C}_6\text{H}_3(\text{CH}_3)_3 + 3 \text{C}_6\text{H}_5\text{N}_3$	-3.2	1082.0
7	$\text{C}_6\text{H}_3(\text{N}_3)_3 + 2 \text{C}_6\text{H}_6 \rightarrow 3 \text{C}_6\text{H}_5\text{N}_3$	-3.6	1082.8
8	$\text{C}_6\text{H}_3(\text{N}_3)_3 + 2 \text{H}_2 \rightarrow 2 \text{HN}_3 + \text{C}_6\text{H}_5\text{N}_3$	-74.6	1074.6
9	$\text{C}_6\text{H}_3(\text{N}_3)_3 + 2 \text{CH}_4 \rightarrow 2 \text{CH}_3\text{N}_3 + \text{C}_6\text{H}_5\text{N}_3$	82.0	1077.8
10	$\text{C}_6\text{H}_3(\text{N}_3)_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow 3 \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	57.4	1077.6
11	$\text{C}_6\text{H}_3(\text{N}_3)_3 + \text{C}_6\text{H}_6 \rightarrow \text{C}_6\text{H}_5\text{N}_3 + 1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3$	-2.2	1079.3
12	$\text{C}_6\text{H}_3(\text{N}_3)_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{N}_3 + 1,3\text{-N}_3\text{-C}_6\text{H}_4\text{-N}_3$	40.6	1077.8
		average:	1077.4
C₅H₄N-N₃ 4-azidopyridine (21)			
1	$\text{C}_5\text{H}_4\text{N-N}_3 + \bullet\text{H} \rightarrow \text{C}_5\text{H}_5\text{N}$ (pyridine) + •N₃	-97.2	469.6

2	$C_5H_4N-N_3 + CH_4 \rightarrow C_5H_4N-CH_3$ (4-methylpyridine) + HN_3	2.3	468.6
3	$C_5H_4N-N_3 + NH_2C(O)H \rightarrow C_5H_4N-C(O)NH_2$ (4-pyridinecarboxamide) + HN_3	-25.0	472.2
4	$C_5H_4N-N_3 + H_2 \rightarrow C_5H_5N$ (pyridine) + HN_3	-34.2	467.1
5	$C_5H_4N-N_3 + CH_3CH_3 \rightarrow C_5H_4N-CH_3$ (4-methylpyridine) + CH_3N_3	16.0	469.8
6	$C_5H_4N-N_3 + CH_3C(O)NH_2 \rightarrow C_5H_4N-C(O)NH_2$ (4-pyridinecarboxamide) + CH_3N_3	25.0	477.2
7	$C_5H_4N-N_3 + CH_4 \rightarrow C_5H_5N$ (pyridine) + CH_3N_3	44.1	468.7
8	$C_5H_4N-N_3 + C_6H_6 \rightarrow C_5H_5N$ (pyridine) + $C_6H_5N_3$	1.3	471.2
9	$C_5H_4N-N_3 + C_6H_5CH_3 \rightarrow C_5H_4N-CH_3$ (4-methylpyridine) + $C_6H_5N_3$	-2.1	471.0
10	$C_5H_4N-N_3 + C_6H_5C(O)NH_2 \rightarrow C_5H_4N-C(O)NH_2$ (4-pyridinecarboxamide) + $C_6H_5N_3$	5.5	474.4
11	$C_5H_4N-N_3 + C_6H_5CH_2CH_3 \rightarrow C_5H_4N-CH_3$ (4-methylpyridine) + $C_6H_5CH_2N_3$	10.6	468.5
12	$C_5H_4N-N_3 + C_6H_5CH_3 \rightarrow C_5H_5N$ (pyridine) + $C_6H_5CH_2N_3$	25.4	469.9
13	$C_5H_4N-N_3 + CH_3CH_2CH_2OH \rightarrow C_5H_4N-CH_3$ (4-methylpyridine) + $HOCH_2CH_2N_3$	2.7	471.4
14	$C_5H_4N-N_3 + CH_3CH_2OH \rightarrow C_5H_5N$ (pyridine) + $HOCH_2CH_2N_3$	19.5	471.1
15	$C_5H_4N-N_3 + HCN \rightarrow C_5H_5N$ (pyridine) + NCN_3	42.6	466.8
16	$C_5H_4N-N_3 + CH_3CN \rightarrow C_5H_4N-CH_3$ (4-methylpyridine) + NCN_3	61.4	469.6
17	$C_5H_4N-N_3 + C_5H_9-CH_3$ (methylcyclopentane) $\rightarrow C_5H_4N-CH_3$ (4-methylpyridine) + $C_5H_9-N_3$ (azidocyclopentane)	-2.2	468.4
18	$C_5H_4N-N_3 + C_5H_{10}$ (cyclopentane) $\rightarrow C_5H_5N$ (pyridine) + $C_5H_9-N_3$ (azidocyclopentane)	3.3	469.5
19	$C_5H_4N-N_3 + C_6H_{11}-CH_3$ (methylcyclohexane) $\rightarrow C_5H_4N-CH_3$ (4-methylpyridine) + $C_6H_{11}-N_3$ (azidocyclohexane)	-0.2	468.8
20	$C_5H_4N-N_3 + C_6H_{12}$ (cyclohexane) $\rightarrow C_5H_5N$ (pyridine) + $C_6H_{11}-N_3$ (azidocyclohexane)	4.1	469.6
21	$C_5H_4N-N_3 + C_6H_5N_3 \rightarrow C_5H_5N$ (pyridine) + $1,4-N_3-C_6H_4-N_3$	5.0	469.4
		average:	470.1
(C₆H₅)₃CN₃ (22)^c			
1	$(C_6H_5)_3CN_3 + \bullet H \rightarrow (C_6H_5)_3CH + \bullet N_3$	-114.1	617.3
2	$(C_6H_5)_3CN_3 + 3 CH_3CH_3 + CH_4 \rightarrow 3 C_6H_5CH_3 + C(CH_3)_4 + HN_3$	-9.2	609.8
3	$(C_6H_5)_3CN_3 + 2 CH_3CH_3 + 2 CH_4 \rightarrow 3 C_6H_5CH_3 + CH(CH_3)_3 + HN_3$	15.6	609.4
4	$(C_6H_5)_3CN_3 + 2 CH_3CH_3 + CH_4 \rightarrow C_6H_5-C_6H_5 + C_6H_5CH_3 + C(CH_3)_4 + HN_3$	-17.1	614.0
5	$(C_6H_5)_3CN_3 + H_2 + CH_4 \rightarrow C_6H_5CH_2C_6H_5 + C_6H_5CH_3 + HN_3$	-27.0	607.7
6	$(C_6H_5)_3CN_3 + H_2 \rightarrow (C_6H_5)_3CH + HN_3$	-49.4	613.1
7	$(C_6H_5)_3CN_3 + 4 CH_3CH_3 \rightarrow 3 C_6H_5CH_3 + C(CH_3)_4 + CH_3N_3$	6.8	608.7
8	$(C_6H_5)_3CN_3 + 2 CH_3CH_3 + C_6H_6 \rightarrow 2 C_6H_5C_6H_5 + CH(CH_3)_3 + CH_3N_3$	-8.2	617.3
9	$(C_6H_5)_3CN_3 + 3 CH_3CH_3 \rightarrow 3 C_6H_5CH_2CH_3 + CH_3N_3$	25.0	614.1
10	$(C_6H_5)_3CN_3 + CH_4 \rightarrow (C_6H_5)_3CH + CH_3N_3$	27.1	616.5
11	$(C_6H_5)_3CN_3 + 3 CH_4 \rightarrow 3 C_6H_5CH_3 + CH_3N_3$	64.0	607.5
12	$(C_6H_5)_3CN_3 + 3 CH_3CH_3 + C_6H_6 \rightarrow 3 C_6H_5CH_3 + CH(CH_3)_3 + C_6H_5N_3$	-9.4	609.0
13	$(C_6H_5)_3CN_3 + 3 CH_3CH_3 \rightarrow 2 C_6H_5CH_3 + C(CH_3)_4 + C_6H_5N_3$	-10.1	608.7

14	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{C}_6\text{H}_6 \rightarrow (\text{C}_6\text{H}_5)_3\text{CH} + \text{C}_6\text{H}_5\text{N}_3$	-13.7	617.0
15	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + 2 \text{CH}_3\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{-C}_6\text{H}_5 + \text{C}(\text{CH}_3)_4 + \text{C}_6\text{H}_5\text{N}_3$	-18.0	612.9
16	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{H}_2 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{C}_6\text{H}_5 + \text{C}_6\text{H}_5\text{N}_3$	-27.9	606.6
17	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + 2 \text{CH}_3\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow 2 \text{C}_6\text{H}_5\text{CH}_3 + \text{C}(\text{CH}_3)_4 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	0.4	609.1
18	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{C}_6\text{H}_6 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow (\text{C}_6\text{H}_5)_3\text{CH} + \text{CH}_3\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	-3.2	617.4
19	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{H}_2 \rightarrow \text{C}_6\text{H}_5\text{C}_6\text{H}_5 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	-22.5	607.8
20	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{CH}_4 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{C}_6\text{H}_5 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	31.5	611.6
21	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{HCN} \rightarrow (\text{C}_6\text{H}_5)_3\text{CH} + \text{NCN}_3$	28.1	612.1
22	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{CH}_3\text{CN} + \text{H}_2 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{C}_6\text{H}_5 + \text{C}_6\text{H}_5\text{CH}_3 + \text{NCN}_3$	35.2	605.6
23	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{CH}_3\text{CN} + 3 \text{CH}_3\text{CH}_3 \rightarrow \text{C}(\text{CH}_3)_4 + 3 \text{C}_6\text{H}_5\text{CH}_3 + \text{NCN}_3$	53.0	607.7
24	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + 3 \text{CH}_3\text{NO}_2 \rightarrow 2 \text{C}_6\text{H}_5\text{CH}_3 + \text{C}_6\text{H}_5\text{NO}_2 + \text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3$	37.1	612.6
25	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{CH}_3(\text{CH}_2)_2\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{-C}_6\text{H}_5 + \text{C}_6\text{H}_6 + \text{C}_5\text{H}_9\text{-N}_3$ (azidocyclopentane)	39.1	605.8
26	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{CH}_3(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{C}_6\text{H}_5 + \text{C}_6\text{H}_6 + \text{C}_5\text{H}_9\text{-N}_3$ (azidocyclopentane)	44.7	604.8
27	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{C}(\text{CH}_3)_4 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{C}_6\text{H}_5 + \text{C}_6\text{H}_6 + \text{C}_5\text{H}_9\text{-N}_3$ (azidocyclopentane)	65.9	604.7
28	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{CH}_3(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{-C}_6\text{H}_5 + \text{C}_6\text{H}_6 + \text{C}_6\text{H}_{11}\text{-N}_3$ (azidocyclohexane)	12.4	607.7
29	$(\text{C}_6\text{H}_5)_3\text{CN}_3 + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{C}_6\text{H}_5 + \text{C}_6\text{H}_6 + \text{C}_6\text{H}_{11}\text{-N}_3$ (azidocyclohexane)	18.2	605.3
	average:		610.4
NCCH₂N₃ (8)			
1	$\text{NCCH}_2\text{N}_3 + \bullet\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CN} + \bullet\text{N}_3$	-97.2	452.2
2	$\text{NCCH}_2\text{N}_3 + \bullet\text{H} \rightarrow \text{CH}_3\text{CN} + \bullet\text{N}_3$	-152.6	458.6
3	$\text{NCCH}_2\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_2\text{CN} + \text{HN}_3$	-34.4	453.0
4	$\text{NCCH}_2\text{N}_3 + \text{C}_6\text{H}_6 + \text{CH}_4 \rightarrow \text{C}_6\text{H}_5\text{CN} + \text{CH}_3\text{CH}_3 + \text{HN}_3$	-42.6	458.5
5	$\text{NCCH}_2\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CN} + \text{CH}_3\text{N}_3$	-11.4	457.8
6	$\text{NCCH}_2\text{N}_3 + \text{HCN} \rightarrow \text{NCCN} + \text{CH}_3\text{N}_3$	17.2	455.5
7	$\text{NCCH}_2\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CN} + \text{CH}_3\text{N}_3$	-20.7	454.2
8	$\text{NCCH}_2\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{C}_6\text{H}_5\text{CN} + \text{CH}_3\text{N}_3$	-28.9	459.7
9	$\text{NCCH}_2\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{NCN}_3$	22.3	457.8
10	$\text{NCCH}_2\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_3 + \text{NCN}_3$	33.9	457.7
11	$\text{NCCH}_2\text{N}_3 + 2 \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CN} + \text{CH}_3\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	-34.0	459.8
12	$\text{NCCH}_2\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{CH}_3\text{CN} + \text{C}_6\text{H}_5\text{N}_3$	-54.2	460.3
13	$\text{NCCH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CN} + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	-26.1	452.9
14	$\text{NCCH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{CH}_3\text{CN} + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	-30.1	459.0
15	$\text{NCCH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CN} \rightarrow \text{NCCN} + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	38.1	457.9
16	$\text{NCCH}_2\text{N}_3 + \text{CH}_3\text{NO}_2 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{HCN} + \text{CH}_3\text{CH}_2\text{CH}_3 + \text{1,4-NO}_2\text{-C}_6\text{H}_4\text{-N}_3$	-16.4	462.1
17	$\text{NCCH}_2\text{N}_3 + \text{CH}_3\text{NO}_2 + \text{1,4-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CN} + \text{CH}_3\text{CH}_3 + \text{1,4-NO}_2\text{-C}_6\text{H}_4\text{-N}_3$	-37.4	455.7

18	$\text{NCCH}_2\text{N}_3 + \text{CH}_3\text{NO}_2 + 1,4\text{-CH}_3\text{-C}_6\text{H}_4\text{-CH}_3 \rightarrow \text{CH}_3\text{CN} + \text{CH}_3\text{CH}_2\text{CH}_3 + 1,4\text{-NO}_2\text{-C}_6\text{H}_4\text{-N}_3$	-39.6	459.3
19	$\text{NCCH}_2\text{N}_3 + \text{CH}_3\text{OH} \rightarrow \text{HCN} + \text{HOCH}_2\text{CH}_2\text{N}_3$	-12.7	461.2
20	$\text{NCCH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{CN} + \text{HOCH}_2\text{CH}_2\text{N}_3$	-34.1	455.9
21	$\text{NCCH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CN} + \text{HOCH}_2\text{CH}_2\text{N}_3$	-36.0	460.2
22	$\text{NCCH}_2\text{N}_3 + \text{C}_5\text{H}_9\text{-CH}_3 \text{ (methylcyclopentane)} \rightarrow \text{CH}_3\text{CH}_2\text{CN} + \text{C}_5\text{H}_9\text{-N}_3 \text{ (azidocyclopentane)}$	-38.9	452.8
23	$\text{NCCH}_2\text{N}_3 + \text{C}_5\text{H}_{10} \text{ (cyclopentane)} \rightarrow \text{CH}_3\text{CN} + \text{C}_5\text{H}_9\text{-N}_3 \text{ (azidocyclopentane)}$	-52.2	458.6
24	$\text{NCCH}_2\text{N}_3 + \text{C}_6\text{H}_{11}\text{-CH}_3 \text{ (methylcyclohexane)} \rightarrow \text{CH}_3\text{CH}_2\text{CN} + \text{C}_6\text{H}_{11}\text{-N}_3 \text{ (azidocyclohexane)}$	-36.9	453.2
25	$\text{NCCH}_2\text{N}_3 + \text{C}_6\text{H}_{12} \text{ (cyclohexane)} \rightarrow \text{CH}_3\text{CN} + \text{C}_6\text{H}_{11}\text{-N}_3 \text{ (azidocyclohexane)}$	-51.3	458.6
26	$\text{NCCH}_2\text{N}_3 + \text{CH}_2(\text{NO}_2)_2 \rightarrow \text{HCN} + \text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3$	-25.9	459.4
27	$\text{NCCH}_2\text{N}_3 + \text{CH}_3\text{CH}(\text{NO}_2)_2 \rightarrow \text{CH}_3\text{CN} + \text{CH}_3\text{C}(\text{NO}_2)_2\text{N}_3$	-32.4	457.7
28	$\text{NCCH}_2\text{N}_3 + \text{C}(\text{NO}_2)_4 + \text{CH}_4 \rightarrow \text{CH}_3\text{CN} + \text{CH}_3\text{NO}_2 + \text{C}(\text{NO}_2)_3\text{N}_3$	-111.2	459.7
29	$\text{NCCH}_2\text{N}_3 + \text{C}(\text{NO}_2)_4 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CN} + \text{CH}_3\text{NO}_2 + \text{C}(\text{NO}_2)_3\text{N}_3$	-120.5	456.1
		average:	457.4
$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{H}_5$ (14)			
1	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \bullet\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \bullet\text{N}_3$	-81.6	-78.5
2	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \bullet\text{H} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \bullet\text{N}_3$	-133.6	-78.0
3	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_4 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OCH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{HN}_3$	-6.0	-82.3
4	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + 3 \text{CH}_4 \rightarrow \text{HC}(\text{O})\text{OH} + 2 \text{CH}_3\text{CH}_2\text{CH}_3 + \text{HN}_3$	9.6	-82.0
5	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{HN}_3$	-18.9	-77.6
6	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{HN}_3$	-18.3	-79.4
7	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_6 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OC}_6\text{H}_5 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{HN}_3$	-27.7	-84.3
8	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_6 + \text{CH}_3\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{C}(\text{O})\text{OCH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{HN}_3$	-31.5	-77.4
9	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + 2 \text{CH}_4 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{HN}_3$	-33.8	-83.4
10	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + 2 \text{CH}_4 \rightarrow \text{HC}(\text{O})\text{OCH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{HN}_3$	35.7	-77.5
11	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	-5.1	-76.5
12	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	7.6	-78.8
13	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + 2 \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OCH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	7.7	-81.1
14	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_3 + \text{CH}_4 \rightarrow \text{C}_6\text{H}_5\text{C}(\text{O})\text{OCH}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	19.1	-78.2
15	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_4 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	-20.0	-82.3
16	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + 2 \text{CH}_4 \rightarrow \text{HC}(\text{O})\text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	22.7	-80.3
17	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OC}_6\text{H}_5 + \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	23.0	-85.1
18	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_4 + \text{CH}_3\text{CH}_3 \rightarrow \text{HC}(\text{O})\text{OCH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	49.4	-76.3
19	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{HCN} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{NCN}_3$	6.2	-80.8
20	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_3\text{CN} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{NCN}_3$	40.2	-76.6
21	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CN} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{NCCH}_2\text{N}_3$	15.6	-73.7

22	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{CH}_3\text{CN} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{NCCH}_2\text{N}_3$	19.0	-79.6
23	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	-23.3	-75.2
24	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + 2 \text{C}_6\text{H}_6 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OC}_6\text{H}_5 + \text{CH}_3\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	-32.9	-81.4
25	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_6 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	-35.2	-76.3
26	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + 2 \text{C}_6\text{H}_6 \rightarrow \text{C}_6\text{H}_5\text{C}(\text{O})\text{OCH}_3 + \text{CH}_3\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	-36.8	-74.6
27	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	-10.5	-77.8
28	$\text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	-11.1	-77.6
		average:	-79.0
CH₃CH₂OCH₂CH₂N₃ (13)			
1	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \bullet\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \bullet\text{N}_3$	-62.1	100.3
2	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \bullet\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \bullet\text{N}_3$	-66.1	97.4
3	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \bullet\text{H} \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \bullet\text{N}_3$	-118.8	98.7
4	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{HN}_3$	-3.3	98.2
5	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{HN}_3$	-15.4	98.7
6	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow (\text{CH}_3)_2\text{CHOCH}(\text{CH}_3)_2 + \text{HN}_3$	-42.5	99.6
7	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	10.0	99.7
8	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	10.4	99.4
9	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow (\text{CH}_3)_2\text{CHOCH}(\text{CH}_3)_2 + \text{CH}_3\text{N}_3$	-17.1	100.6
10	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	22.4	97.9
11	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	23.3	100.4
12	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	5.1	101.7
13	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	-6.5	98.6
14	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	-7.8	100.7
15	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{N}_3$	-20.4	100.7
16	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow (\text{CH}_3)_2\text{CHOCH}(\text{CH}_3)_2 + \text{C}_6\text{H}_5\text{N}_3$	-33.6	99.5
17	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	3.7	99.1
18	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_6 \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	3.9	102.1
19	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	5.0	98.1
20	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	17.8	99.2
21	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{CN} \rightarrow (\text{CH}_3)_2\text{CHOCH}(\text{CH}_3)_2 + \text{NCN}_3$	25.9	104.2
22	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{CN} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{NCN}_3$	53.0	103.3
23	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CN} \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{NCN}_3$	55.7	99.3
24	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CN} \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{NCN}_3$	68.6	100.3
25	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{NO}_2 \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{1,4-NO}_2\text{-C}_6\text{H}_4\text{-N}_3$	-5.4	98.3
26	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_5\text{NO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{1,4-NO}_2\text{-C}_6\text{H}_4\text{-N}_3$	-18.6	97.5

27	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3$	-6.5	97.9
28	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_3 \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}(\text{NO}_2)\text{CH}_2\text{N}_3$	6.7	98.7
29	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_5\text{H}_4\text{N}-\text{CH}_3$ (4-methylpyridine) $\rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{C}_5\text{H}_4\text{N}-\text{N}_3$ (4-azidopyridine)	-5.6	99.6
30	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_5\text{H}_4\text{N}-\text{CH}_3$ (4-methylpyridine) $\rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{C}_5\text{H}_4\text{N}-\text{N}_3$ (4-azidopyridine)	7.2	100.7
31	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_5\text{H}_5\text{N}$ (pyridine) $\rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{C}_5\text{H}_4\text{N}-\text{N}_3$ (4-azidopyridine)	-8.4	99.9
32	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_5\text{H}_5\text{N}$ (pyridine) $\rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{C}_5\text{H}_4\text{N}-\text{N}_3$ (4-azidopyridine)	-21.7	99.2
33	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_5\text{H}_9-\text{CH}_3$ (methylcyclopentane) $\rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{C}_5\text{H}_9-\text{N}_3$ (azidocyclopentane)	5.0	99.1
34	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_5\text{H}_{10}$ (cyclopentane) $\rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{C}_5\text{H}_9-\text{N}_3$ (azidocyclopentane)	-5.2	99.5
35	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_5\text{H}_9-\text{CH}_3$ (methylcyclopentane) $\rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{C}_5\text{H}_9-\text{N}_3$ (azidocyclopentane)	-7.8	98.0
36	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_5\text{H}_{10}$ (cyclopentane) $\rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{C}_5\text{H}_9-\text{N}_3$ (azidocyclopentane)	-18.4	98.7
37	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_{12}$ (cyclohexane) $\rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_{11}-\text{N}_3$ (azidocyclohexane)	-4.3	99.5
38	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_{11}-\text{CH}_3$ (methylcyclohexane) $\rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_{11}-\text{N}_3$ (azidocyclohexane)	-5.8	98.4
39	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_{11}-\text{CH}_3$ (methylcyclohexane) $\rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_{11}-\text{N}_3$ (azidocyclohexane)	7.0	99.5
40	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{C}_6\text{H}_{12}$ (cyclohexane) $\rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{C}_6\text{H}_{11}-\text{N}_3$ (azidocyclohexane)	-17.5	98.7
41	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3$	14.7	97.8
42	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{C}(\text{O})\text{OCH}_3 \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_3 + \text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3$	15.8	102.1
43	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{N}_3\text{CH}_2\text{C}(\text{O})\text{OCH}_2\text{CH}_3$	28.0	98.5
44	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_3 + \text{HOCH}_2\text{CH}_2\text{N}_3$	-0.8	100.9
45	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{HOCH}_2\text{CH}_2\text{N}_3$	-2.2	100.3
46	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{HOCH}_2\text{CH}_2\text{N}_3$	-3.0	101.1
47	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{HOCH}_2\text{CH}_2\text{N}_3$	9.9	102.1
48	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_3 + \text{HOCH}_2\text{CH}_2\text{N}_3$	11.0	101.1
49	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{HOCH}_2\text{CH}_2\text{N}_3$	-12.1	96.8
50	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{N}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{HOCH}_2\text{CH}_2\text{N}_3$	-24.3	97.4
	average:		99.6
(CH₃CH₂)₃CN₃ (23)			
1	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \bullet\text{C}_2\text{H}_5 \rightarrow (\text{C}_2\text{H}_5)_4\text{C} + \bullet\text{N}_3$	-37.2	135.1
2	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \bullet\text{CH}_3 \rightarrow (\text{C}_2\text{H}_5)_3\text{C}(\text{CH}_3) + \bullet\text{N}_3$	-44.8	133.3
3	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \bullet\text{H} \rightarrow (\text{C}_2\text{H}_5)_3\text{CH} + \bullet\text{N}_3$	-86.4	128.9
4	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \bullet\text{H} \rightarrow (\text{C}_2\text{H}_5)_2\text{C}(\text{CH}_3)_2 + \bullet\text{N}_3$	-101.1	132.1
5	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{CH}_3\text{CH}_3 \rightarrow (\text{C}_2\text{H}_5)_4\text{C} + \text{HN}_3$	9.6	133.4
6	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{CH}_4 \rightarrow (\text{C}_2\text{H}_5)_3\text{C}(\text{CH}_3) + \text{HN}_3$	17.9	134.2
7	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{H}_2 \rightarrow (\text{C}_2\text{H}_5)_3\text{CH} + \text{HN}_3$	-23.5	126.5
8	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{H}_2 \rightarrow (\text{C}_2\text{H}_5)_2\text{C}(\text{CH}_3)_2 + \text{HN}_3$	-38.2	129.7
9	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{CH}_3\text{CH}_3 \rightarrow (\text{C}_2\text{H}_5)_3\text{C}(\text{CH}_3) + \text{CH}_3\text{N}_3$	31.7	135.3

10	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow (\text{C}_2\text{H}_5)_4\text{C} + \text{CH}_3\text{N}_3$	34.9	134.5
11	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{CH}_4 \rightarrow (\text{C}_2\text{H}_5)_2\text{C}(\text{CH}_3)_2 + \text{CH}_3\text{N}_3$	40.1	131.3
12	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{CH}_4 \rightarrow (\text{C}_2\text{H}_5)_3\text{CH} + \text{CH}_3\text{N}_3$	54.8	128.1
13	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{C}_6\text{H}_6 \rightarrow (\text{C}_2\text{H}_5)_2\text{C}(\text{CH}_3)_2 + \text{C}_6\text{H}_5\text{N}_3$	-2.7	133.8
14	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{C}_6\text{H}_6 \rightarrow (\text{C}_2\text{H}_5)_3\text{CH} + \text{C}_6\text{H}_5\text{N}_3$	12.0	130.6
15	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow (\text{C}_2\text{H}_5)_3\text{C}(\text{CH}_3) + \text{C}_6\text{H}_5\text{N}_3$	13.5	136.6
16	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow (\text{C}_2\text{H}_5)_4\text{C} + \text{C}_6\text{H}_5\text{N}_3$	18.4	133.4
17	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow (\text{C}_2\text{H}_5)_2\text{C}(\text{CH}_3)_2 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	21.4	132.5
18	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow (\text{C}_2\text{H}_5)_3\text{C}(\text{CH}_3) + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	26.2	134.1
19	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow (\text{C}_2\text{H}_5)_3\text{CH} + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	36.1	129.3
20	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{C}_6\text{H}_5\text{CH}(\text{CH}_3)_2 \rightarrow (\text{C}_2\text{H}_5)_4\text{C} + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	36.6	131.1
21 ^c	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + 3 \text{C}_6\text{H}_5\text{CH}_3 \rightarrow 3 \text{CH}_3\text{CH}_2\text{CH}_3 + (\text{C}_6\text{H}_5)_3\text{CN}_3$	13.7	131.9
22 ^c	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + 3 \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow 3 \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + (\text{C}_6\text{H}_5)_3\text{CN}_3$	15.9	127.3
23 ^c	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + 3 \text{C}_6\text{H}_6 \rightarrow 3 \text{CH}_3\text{CH}_3 + (\text{C}_6\text{H}_5)_3\text{CN}_3$	-23.3	133.2
24	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{C}_2\text{H}_5\text{OC}_2\text{H}_5 \rightarrow (\text{C}_2\text{H}_5)_2\text{C}(\text{CH}_3)_2 + \text{C}_2\text{H}_5\text{OCH}_2\text{CH}_2\text{N}_3$	17.7	133.4
25	$(\text{C}_2\text{H}_5)_3\text{CN}_3 + \text{C}_2\text{H}_5\text{OC}_2\text{H}_5 \rightarrow (\text{C}_2\text{H}_5)_3\text{CH} + \text{C}_2\text{H}_5\text{OCH}_2\text{CH}_2\text{N}_3$	32.4	130.2
		average:	132.0

(CH₃)₂(C₆H₅)CN₃ (24)

1	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \cdot\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{C}(\text{CH}_3)_3 + \cdot\text{N}_3$	-53.0	333.3
2	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \cdot\text{H} \rightarrow \text{C}_6\text{H}_5\text{CH}(\text{CH}_3)_2 + \cdot\text{N}_3$	-98.5	334.5
3	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{CH}_4 + \text{CH}_3\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}_3 + \text{C}(\text{CH}_3)_4 + \text{HN}_3$	3.9	328.9
4	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{CH}_4 \rightarrow \text{C}_6\text{H}_5\text{C}(\text{CH}_3)_3 + \text{HN}_3$	9.8	334.1
5	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{H}_2 + \text{CH}_4 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_3 + \text{HN}_3$	-16.9	329.9
6	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{H}_2 \rightarrow \text{C}_6\text{H}_5\text{CH}(\text{CH}_3)_2 + \text{HN}_3$	-35.6	332.1
7	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{H}_2 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 + \text{CH}_3\text{N}_3$	-3.1	331.0
8	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + 2 \text{CH}_3\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}_3 + \text{C}(\text{CH}_3)_4 + \text{CH}_3\text{N}_3$	17.6	330.1
9	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{C}(\text{CH}_3)_3 + \text{CH}_3\text{N}_3$	23.5	335.3
10	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{CH}_4 \rightarrow \text{C}_6\text{H}_5\text{CH}(\text{CH}_3)_2 + \text{CH}_3\text{N}_3$	42.7	333.7
11	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{C}_6\text{H}_6 \rightarrow \text{C}_6\text{H}_5\text{CH}(\text{CH}_3)_2 + \text{C}_6\text{H}_5\text{N}_3$	-0.1	336.2
12	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{C}(\text{CH}_3)_4 + \text{C}_6\text{H}_5\text{N}_3$	-0.6	331.4
13	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{C}(\text{CH}_3)_3 + \text{C}_6\text{H}_5\text{N}_3$	5.3	336.6
14	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{CH}_4 \rightarrow \text{CH}(\text{CH}_3)_3 + \text{C}_6\text{H}_5\text{N}_3$	24.2	331.0
15	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{C}(\text{CH}_3)_4 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	10.5	331.2
16	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{C}_6\text{H}_6 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	18.1	333.9

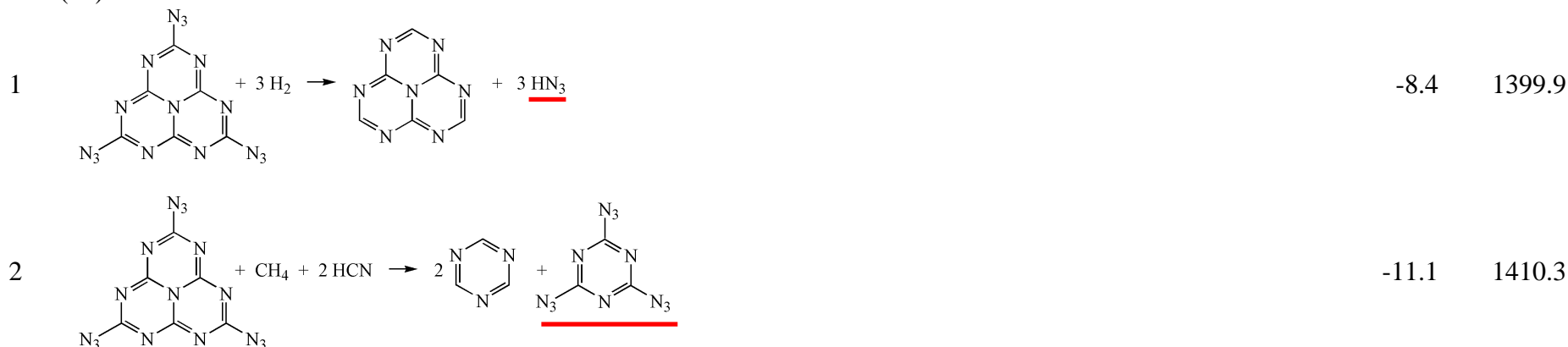
17	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{C}(\text{CH}_3)_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	18.1	334.0
18	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}(\text{CH}_3)_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	23.7	330.9
19	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}(\text{CH}_3)_2 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	24.0	334.9
20	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	32.2	330.9
21	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{N}_3$	44.4	330.3
22 ^c	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + \text{C}_6\text{H}_5\text{C}(\text{CH}_3)_3 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{C}(\text{CH}_3)_4 + \text{CH}_3\text{CH}_3 + (\text{C}_6\text{H}_5)_3\text{CN}_3$	1.9	329.2
23 ^c	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + 2 \text{C}_6\text{H}_5\text{CH}_3 \rightarrow 2 \text{CH}_3\text{CH}_3 + (\text{C}_6\text{H}_5)_3\text{CN}_3$	8.5	333.7
24 ^c	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + 2 \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow 2 \text{CH}_3\text{CH}_2\text{CH}_3 + (\text{C}_6\text{H}_5)_3\text{CN}_3$	11.1	329.7
25 ^c	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + 2 \text{C}_6\text{H}_6 \rightarrow 2 \text{CH}_4 + (\text{C}_6\text{H}_5)_3\text{CN}_3$	-39.5	334.9
26	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + (\text{C}_2\text{H}_5)_3\text{C}(\text{CH}_3) \rightarrow \text{C}_6\text{H}_5\text{C}(\text{CH}_3)_3 + (\text{C}_2\text{H}_5)_3\text{CN}_3$	1.9	333.1
27	$(\text{C}_6\text{H}_5)(\text{CH}_3)_2\text{CN}_3 + (\text{C}_2\text{H}_5)_3\text{CH} \rightarrow \text{C}_6\text{H}_5\text{CH}(\text{CH}_3)_2 + (\text{C}_2\text{H}_5)_3\text{CN}_3$	-12.1	337.6
	average:		332.7

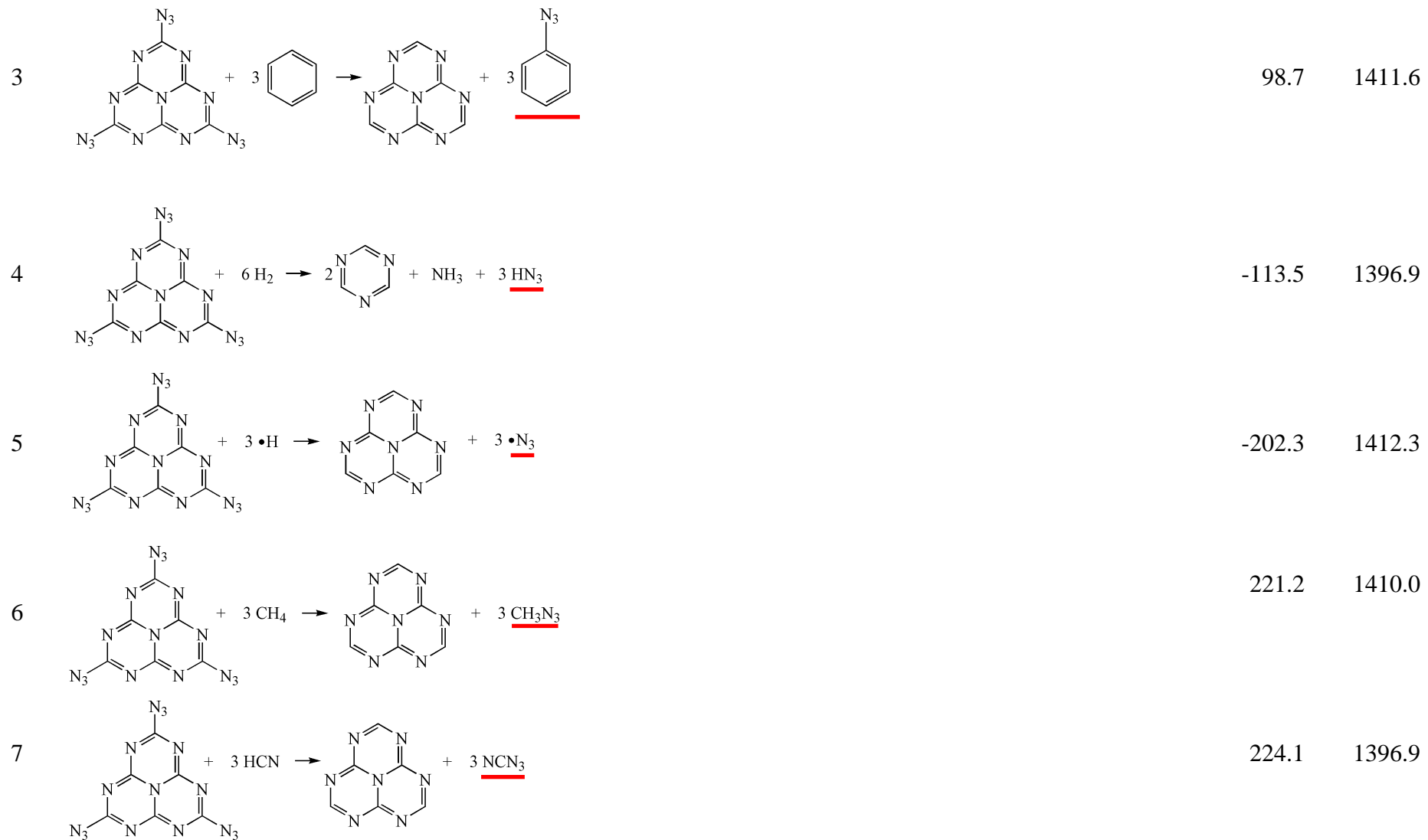
1-azidoadamantane (25)

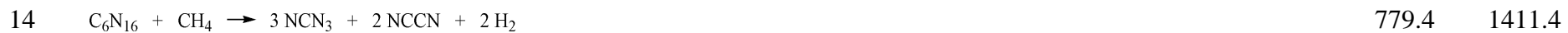
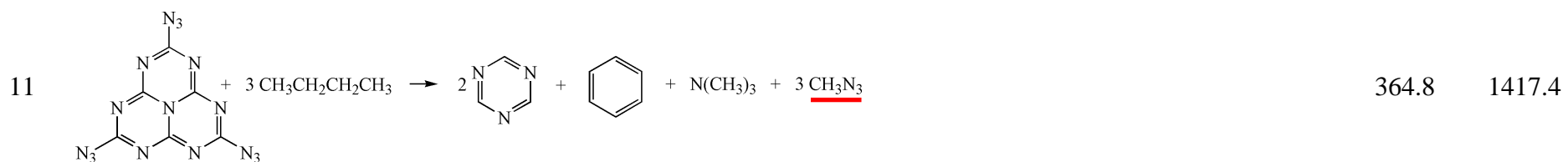
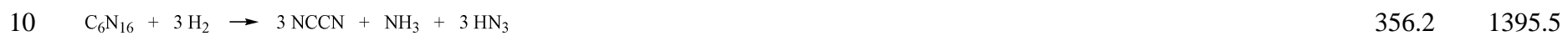
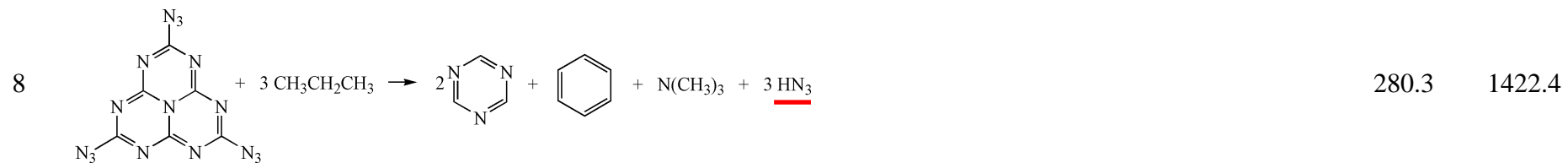
1	1-azidoadamantane + $\bullet\text{C}(\text{O})\text{NH}_2 \rightarrow$ 1-adamantylcarboxamide + $\bullet\text{N}_3$	-38.6	184.7
2	1-azidoadamantane + $\bullet\text{NH}_2 \rightarrow$ 1-aminoadamantane + $\bullet\text{N}_3$	-48.7	178.7
3	1-azidoadamantane + $\bullet\text{CH}_3 \rightarrow$ 1-methyladamantane + $\bullet\text{N}_3$	-54.4	182.8
4	1-azidoadamantane + $\bullet\text{H} \rightarrow$ adamantane + $\bullet\text{N}_3$	-82.2	181.9
5	1-azidoadamantane + $\text{CH}_4 \rightarrow$ 1-methyladamantane + HN_3	8.3	183.7
6	1-azidoadamantane + $\text{H}_2 \rightarrow$ adamantane + HN_3	-19.3	179.5
7	1-azidoadamantane + $\text{HC}(\text{O})\text{NH}_2 \rightarrow$ 1-adamantylcarboxamide + HN_3	-21.9	184.3
8	1-azidoadamantane + $\text{NH}_3 \rightarrow$ 1-aminoadamantane + HN_3	23.5	181.2
9	1-azidoadamantane + $\text{CH}_3\text{NH}_2 \rightarrow$ 1-aminoadamantane + CH_3N_3	5.5	182.1
10	1-azidoadamantane + $\text{CH}_3\text{CH}_3 \rightarrow$ 1-methyladamantane + CH_3N_3	22.0	184.9
11	1-azidoadamantane + $\text{CH}_3\text{C}(\text{O})\text{NH}_2 \rightarrow$ 1-adamantylcarboxamide + CH_3N_3	28.1	189.2
12	1-azidoadamantane + $\text{CH}_4 \rightarrow$ adamantane + CH_3N_3	59.0	181.1
13	1-azidoadamantane + $\text{C}_6\text{H}_5\text{CH}_3 \rightarrow$ 1-methyladamantane + $\text{C}_6\text{H}_5\text{N}_3$	3.9	186.1
14	1-azidoadamantane + $\text{C}_6\text{H}_5\text{C}(\text{O})\text{NH}_2 \rightarrow$ 1-adamantylcarboxamide + $\text{C}_6\text{H}_5\text{N}_3$	8.6	186.4
15	1-azidoadamantane + $\text{C}_6\text{H}_5\text{NH}_2 \rightarrow$ 1-aminoadamantane + $\text{C}_6\text{H}_5\text{N}_3$	13.8	180.3
16	1-azidoadamantane + $\text{C}_6\text{H}_6 \rightarrow$ adamantane + $\text{C}_6\text{H}_5\text{N}_3$	16.2	183.6
17	1-azidoadamantane + $\text{C}_6\text{H}_{11}\text{-NH}_2$ (aminocyclohexane) \rightarrow 1-aminoadamantane + $\text{C}_6\text{H}_{11}\text{-N}_3$ (azidocyclohexane)	2.5	178.6
18	1-azidoadamantane + C_6H_{12} (cyclohexane) \rightarrow adamantane + $\text{C}_6\text{H}_{11}\text{-N}_3$ (azidocyclohexane)	19.1	181.9
	average:		182.8

TAT (26)

1	$C_3N_3(N_3)_3 + 3 \cdot H \rightarrow C_3H_3N_3$ (1,3,5-triazine) + 3 $\cdot N_3$	-215.3	1137.2
2	$C_3N_3(N_3)_3 + 3 H_2 \rightarrow C_3H_3N_3$ (1,3,5-triazine) + 3 HN_3	-26.6	1130.0
3	$C_3N_3(N_3)_3 + 3 CH_3OH \rightarrow C_3N_3(OCH_3)_3$ (trimethyl cyanurate) + 3 HN_3	-45.9	1140.0
4	$C_3N_3(N_3)_3 + 3 H_2 \rightarrow 3 HCN + 3 \mathbf{HN_3}$	139.7	1133.8
5	$C_3N_3(N_3)_3 + 3 CH_4 \rightarrow 3 CH_3CN + 3 \mathbf{HN_3}$	193.2	1129.5
6	$C_3N_3(N_3)_3 + 3 CH_3OCH_3 \rightarrow C_3N_3(OCH_3)_3$ (trimethyl cyanurate) + 3 $\mathbf{CH_3N_3}$	-79.1	1137.5
7	$C_3N_3(N_3)_3 + 3 CH_3OH \rightarrow C_3H_3N_3O_3$ (cyanuric acid) + 3 $\mathbf{CH_3N_3}$	-200.5	1134.9
8	$C_3N_3(N_3)_3 + 3 CH_4 \rightarrow C_3H_3N_3$ (1,3,5-triazine) + 3 $\mathbf{CH_3N_3}$	208.3	1134.8
9	$C_3N_3(N_3)_3 + 3 CH_4 \rightarrow 3 HCN + 3 \mathbf{CH_3N_3}$	374.6	1138.6
10	$C_3N_3(N_3)_3 + 3 C_6H_5OCH_3 \rightarrow C_3N_3(OCH_3)_3$ (trimethyl cyanurate) + 3 $\mathbf{C_6H_5N_3}$	-74.3	1135.1
11	$C_3N_3(N_3)_3 + 3 C_6H_6 \rightarrow C_3H_3N_3$ (1,3,5-triazine) + 3 $\mathbf{C_6H_5N_3}$	79.9	1143.2
12	$C_3N_3(N_3)_3 + 3 C_6H_5CH_3 \rightarrow 3 CH_3CN + 3 \mathbf{C_6H_5N_3}$	179.9	1136.8
13	$C_3N_3(N_3)_3 + 3 C_6H_6 \rightarrow 3 HCN + 3 \mathbf{C_6H_5N_3}$	246.2	1146.1
14	$C_3N_3(N_3)_3 \rightarrow 3 \mathbf{NCN_3}$	370.4	1133.8
15	$C_3N_3(N_3)_3 + 2 C_6H_6 \rightarrow 3 \mathbf{C_5H_4N-N_3}$ (4-azidopyridine)	103.2	1141.6
16	$C_3N_3(N_3)_3 + 2 C_6H_6 \rightarrow C_3H_3N_3$ (1,3,5-triazine) + $\mathbf{C_6H_5N_3}$ + $\mathbf{1,3-N_3-C_6H_4-N_3}$	81.3	1139.4
17	$C_3N_3(N_3)_3 + C_6H_6 \rightarrow C_3H_3N_3$ (1,3,5-triazine) + $\mathbf{C_6H_3(N_3)_3}$ (1,3,5-triazidobenzene)	83.5	1136.8
	average:		1137.0

TAH (27)^c






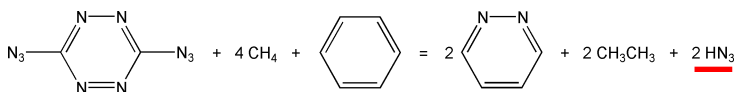
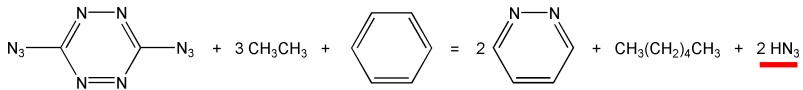
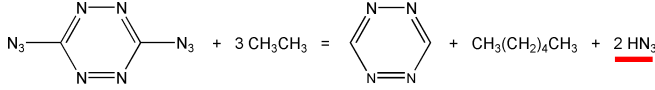
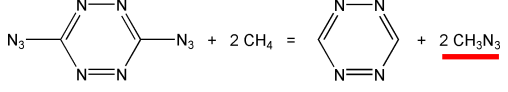
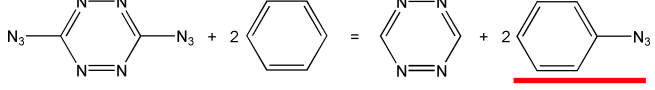
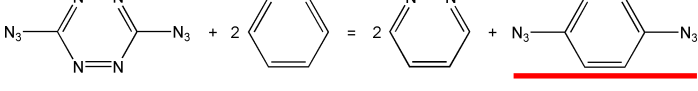
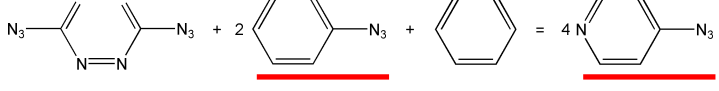
average of isodesmic (3, 6, 7, and 9) reactions: 1410.6

average of all reactions: 1408.7

TAAT (28): see Table 4

DiAT (29)



2		66.4	1122.3
3		17.7	1125.5
4		23.2	1125.1
5		99.3	1124.3
6		13.7	1129.3
7		11.9	1126.9
8		-164.5	1125.1
	average:	1125.0	

^aExperimental enthalpies of formation of all species used in isodesmic reactions are given in Table S2. The compounds are arranged in order of their position in Table 2. Reference azido compounds are given in red color. ^bThe values of enthalpies of reaction ($\Delta_r H^\circ$) are given together with enthalpies of formation ($\Delta_f H_{298}^\circ$) for each isodesmic reaction. ^cG4(MP2) energies are used in isodesmic reaction calculations. ^dThe compound's number according to Figure 1 is given in parentheses for each molecule.

Table S5. Comparison of Experimental Enthalpies of Hydrogenation with Those Calculated by G4 Method (in kJ/mol)^a

hydrogenation reaction	$\Delta_f H_{298}^\circ$ (exp)		$\Delta_{\text{hyd}} H_{298}^\circ$		
	(1)	(2)	exp	G4	Δ^b
benzene + 3 H ₂ → cyclohexane	82.9	-123.3	-206.2	-204.7	-1.5
H ₂ C=CH-CH=CH ₂ + 2 H ₂ → CH ₃ CH ₂ CH ₂ CH ₃	110.0	-125.7	-235.7	-236.0	0.3
H ₂ C=CH-CH=CH-CH=CH ₂ + 3 H ₂ → CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	168.0	-166.9	-334.9	-333.5	-1.4
1,3,5,7-cyclooctatetraene + 4 H ₂ → cyclooctane	295.9	-124.4	-420.3	-420.5	0.2
pyridine + 3 H ₂ → piperidine	140.4	-47.2	-187.6	-186.5	-1.1
uracil + H ₂ → 5,6-dihydrouracil	-301.5	-377.2	-75.7	-76.8	1.1
C ₆ H ₅ NO ₂ + 3 H ₂ → C ₆ H ₁₁ NO ₂	63.0	-159.3	-222.3	-220.9	-1.4
HN ₃ + H ₂ → NH ₃ + N ₂	292.5 ^c	-45.9	-339.9	-331.5	-6.9
CH ₃ N ₃ + H ₂ → CH ₃ NH ₂ + N ₂	298 ^c	-23.4	-321.4	-313.5	-7.9
O ₂ N-C ₆ H ₄ -N ₃ + H ₂ → O ₂ N-C ₆ H ₄ -NH ₂ + N ₂	389.7	55.2	-334.5	-331.1	-3.4
1-azidoadamantane + H ₂ → 1-aminoadamantane + N ₂			-336.0	-308.0	-28.0
(C ₂ H ₅) ₃ CN ₃ + H ₂ → (C ₂ H ₅) ₃ CNH ₂ + N ₂			-337.2	-303.4	-33.9
(C ₆ H ₅)(CH ₃) ₂ CN ₃ + H ₂ → (C ₆ H ₅)(CH ₃) ₂ CNH ₂ + N ₂			-344.3	-307.9	-36.4

^a For all compounds with the exception of the last three, the experimental enthalpies of hydrogenation were determined as the difference between experimental enthalpies of formation for compound (1) and product of its hydrogenation (2); the references for experimental data are given in Table S3. For the last three compounds, the enthalpies of hydrogenation were measured directly (see text and ref 43). ^bDifference between experimental and calculated enthalpy of hydrogenation. ^cValues accepted in this work (see text).