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The Gaussian G4 enthalpy of formation of propargylamine and propargyloxy derivatives of triazido-*s*-triazine

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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	G4 enthalpy, hartree	Atom	x	y	z
2a 2,4-diazido-6-propynyloxy-1,3,5-triazine	-797.941152	C	0.31279100	1.28977700	-0.17929700
		C	1.39455600	-0.64374200	0.04029900
		C	-0.79054900	-0.63377700	-0.40711900
		N	-0.85520000	0.69605900	-0.41942600
		N	0.30120300	-1.36913600	-0.18751900
		N	1.47758400	0.68742900	0.06258300
		N	2.60422000	-1.29646000	0.28703700
		N	2.55346200	-2.54194200	0.27352800
		N	2.66904700	-3.66132400	0.29435100
		N	0.26121400	2.68498800	-0.19331700
		N	1.34230700	3.26399300	0.03123900
		N	2.23240300	3.92756300	0.21590400
		O	-1.88747600	-1.34644700	-0.64325000
		C	-3.13238900	-0.63820600	-0.83467100
		C	-3.75397100	-0.26504700	0.42733000
		C	-4.28568600	0.03072700	1.46235500
		H	-3.75835200	-1.35022900	-1.37808000
		H	-2.96200200	0.24300000	-1.45736200
		H	-4.75202800	0.30222900	2.37738700
2b 2-azido-4,6-bis(propynyloxy)-1,3,5-triazine	-824.978078	O	2.49731300	-1.40602700	-0.58287400
		N	-1.20890000	2.84033700	0.01039300
		N	-0.08759700	2.37538400	-0.26509800
		N	1.24281600	0.51566400	-0.43735600
		N	0.37707700	-1.64257300	0.08109300
		N	-2.15966000	3.40551500	0.22380000
		N	-1.01281300	0.27779600	0.27315600
		C	-0.77212900	-1.03378000	0.35082100
		C	1.34045000	-0.80994200	-0.30253900
		C	0.04058900	0.98834600	-0.13229600
		C	3.61832900	-0.57791800	-0.95632100
		C	4.29576700	-0.00808100	0.19980700
		C	4.87513300	0.45147900	1.14573200
		H	5.38183400	0.86682800	1.98177400
		H	3.28521200	0.21082300	-1.63480600
		H	4.28231800	-1.25998500	-1.49332500
		O	-1.74679500	-1.85181400	0.74492700
		C	-3.04546100	-1.28597200	1.01193900
		C	-3.81059100	-1.04357300	-0.20338300
		C	-4.45948500	-0.85857800	-1.19656900

		H	-5.03116500	-0.68793600	-2.07545800
		H	-3.53829100	-2.03941300	1.63150600
		H	-2.93612300	-0.36434000	1.58883100
2c 2,4,6-tripropargyloxy-1,3,5-triazine	-852.016557	O	-1.54624100	-1.96089400	1.00070900
		N	-0.93634700	0.00754400	-0.01719600
		N	0.60106200	-1.75582800	0.40451200
		N	1.33553300	0.24952500	-0.65373200
		C	1.52188800	-0.97076000	-0.15336700
		C	-0.60323000	-1.20293800	0.43773900
		C	0.08012600	0.67594700	-0.55199900
		C	-2.88269600	-1.42963000	1.07371400
		C	-3.60609200	-1.54317100	-0.18656000
		C	-4.22253400	-1.64855100	-1.21195800
		H	-4.76587400	-1.74191000	-2.11988300
		H	-2.84967400	-0.38799500	1.40344000
		H	-3.36540700	-2.03494300	1.84530300
		O	2.73806100	-1.51534000	-0.20388500
		C	3.81531700	-0.72143200	-0.73889500
		C	4.37604800	0.19102100	0.24838700
		C	4.86133300	0.93236200	1.05872300
		H	5.28214900	1.59660100	1.77265800
		H	4.56136000	-1.45905700	-1.04578900
		H	3.46884700	-0.17104200	-1.61674800
		O	-0.13289000	1.89139800	-1.05938200
		C	-1.46984800	2.42381200	-0.98298700
		H	-1.48182700	3.21612600	-1.73582000
		H	-2.19088000	1.65111500	-1.26214100
		C	-1.78688600	2.96660700	0.33168300
		C	-2.05645200	3.43562400	1.40394700
		H	-2.29370200	3.84775300	2.35378200
3a 4,6-diazido-*N*-(prop-2-yn-1-yl)-1,3,5-triazine-2-amine	-778.164296	C	0.96501400	1.18757300	-0.08110700
		C	1.16391800	-1.02646000	0.01586900
		C	-0.84837900	-0.09751200	-0.32974000
		N	-0.34379500	1.14678200	-0.29045800
		N	-0.13277500	-1.23136100	-0.18083800
		N	1.79089800	0.14874500	0.07955700
		N	2.00932500	-2.13168900	0.18145000
		N	1.45480300	-3.24393500	0.12650200
		N	1.09796300	-4.31235400	0.10127200
		N	1.49917500	2.48029600	-0.03218700
		N	2.72751700	2.54590700	0.16397500
		N	3.81805100	2.76944700	0.33345200
		C	-3.12850800	0.83846400	-0.65456000
		C	-4.24895300	0.68141600	0.26897400
		C	-5.17931400	0.53041000	1.01331500
		H	-3.50658100	0.90495000	-1.68378000
		H	-2.58278900	1.76414600	-0.45469400
		H	-5.99853600	0.41188600	1.67900700
		N	-2.17043300	-0.25229500	-0.54190900
		H	-2.50985700	-1.20114600	-0.52273300

3b 6-azido-N^2,N^4-bis(prop-2-yn-1-yl)-1,3,5-triazine-2,4-diamine	-785.255229	N	-1.22063800	3.18163100	0.02537000
		N	-0.09510000	2.71627600	-0.21738500
		N	1.22993200	0.85490600	-0.38146900
		N	0.32299000	-1.31828300	0.04200500
		N	-2.17869000	3.74496600	0.21716500
		N	-1.06446000	0.61767900	0.21504000
		C	-0.84549800	-0.70967500	0.27961300
		C	1.32139400	-0.48598000	-0.28265800
		C	0.01730000	1.31726000	-0.11908800
		C	3.74843200	-0.33285700	-0.80878300
		C	4.79871300	-0.64362000	0.15963700
		C	5.66423800	-0.92532200	0.94362500
		H	6.42954200	-1.15750100	1.64242700
		H	3.49786400	0.73072500	-0.78225200
		H	4.10975100	-0.55423500	-1.82220900
		C	-3.25121700	-1.06962700	0.80875700
		C	-4.17516300	-1.71605900	-0.12217800
		C	-4.93003100	-2.27248300	-0.87293300
		H	-5.60123100	-2.74947500	-1.54372400
		H	-3.57793400	-1.26233300	1.83954800
		H	-3.25635000	0.01410900	0.66843400
		N	2.51751400	-1.06106400	-0.54696800
		H	2.56051300	-2.05726200	-0.40193600
		N	-1.87816300	-1.51226400	0.62981100
		H	-1.68486700	-2.50078300	0.59877200
3c N^2,N^4,N^6-tri(prop-2-yn-1-yl)-1,3,5-triazine-2,4,6-triamine	-792.428922	N	-1.25444700	0.78599500	0.23559900
		N	-0.72993700	-1.53560600	-0.00870800
		N	0.95503000	0.12038100	-0.35728100
		C	0.51768900	-1.15247800	-0.30681400
		C	-1.56908800	-0.52428500	0.25206300
		C	0.01190700	1.01601000	-0.07509900
		C	-3.92485000	0.07504400	0.78306200
		C	-5.03340100	-0.13480600	-0.14676500
		C	-5.95087800	-0.33173500	-0.89682000
		H	-6.75944000	-0.48971500	-1.56703700
		H	-3.50209900	1.07594700	0.66402500
		H	-4.29522300	0.00159800	1.81457600
		C	2.81808000	-1.95170100	-0.82303700
		C	3.64257400	-2.66427100	0.15197200
		C	4.31128300	-3.27504600	0.94118000
		H	4.90888900	-3.80040800	1.64463800
		H	3.08531200	-2.28074000	-1.83631400
		H	3.00590600	-0.87621700	-0.77554200
		N	-2.83780600	-0.86765500	0.57414600
		H	-3.04855900	-1.85119800	0.51481500
		N	1.39497600	-2.14243700	-0.59583600
		H	1.04123300	-3.07878700	-0.47916700
		N	0.39096500	2.31123900	-0.10972100
		C	1.38343000	2.88955800	0.77518600
		H	0.94226500	3.69036600	1.33104500

		H	1.73895300	2.13988000	1.45082300
		C	2.52786300	3.42085600	0.04061300
		C	3.46466900	3.89334500	-0.54175000
		H	4.29459900	4.29463100	-1.06499600
		H	-0.03896000	2.90827900	-0.78700000
4a 4,6-diazido-*N*-methyl-*N*-(prop-2-yn-1-yl)-1,3,5-triazine-2-amine	-817.351359	C	-1.13594500	-1.20039400	-0.12251200
		C	-1.30087900	1.00521500	0.06861100
		C	0.70802000	0.06657100	-0.31727100
		N	0.17058100	-1.17009300	-0.32414100
		N	-0.00176500	1.19730300	-0.12326600
		N	-1.94914900	-0.15748700	0.08526900
		N	-2.12475600	2.12028800	0.28205500
		N	-1.54805100	3.22173300	0.27299600
		N	-1.16752700	4.28242900	0.29185800
		N	-1.69119800	-2.48607000	-0.13510500
		N	-2.92066500	-2.54140800	0.05492100
		N	-4.01526800	-2.75556200	0.21114500
		C	2.87716000	-1.00812600	-0.70734600
		C	3.76598200	-1.25079900	0.42961900
		C	4.50164200	-1.44116900	1.36005900
		H	3.47576100	-0.87606500	-1.61863600
		H	2.21660500	-1.86262600	-0.85952800
		H	5.14680200	-1.62310900	2.18405100
		N	2.04096300	0.17847200	-0.52891100
		C	2.73043200	1.45974200	-0.50975700
		H	3.48009500	1.46959700	0.28866200
		H	3.24109600	1.62357500	-1.46638800
		H	2.00901100	2.25515700	-0.34432800
4b 6-azido-N^2,N^4-dimethyl-N^2,N^4-di(prop-2-yn-1-yl)-1,3,5-triazine-2,4-diamine	-863.862886	N	1.32229600	3.36678600	-0.05300100
		N	0.19032000	2.92157900	0.19462900
		N	-1.16221900	1.08331600	0.37613600
		N	-0.29113500	-1.10001400	-0.03047800
		N	2.28942100	3.91274400	-0.25123300
		N	1.12443900	0.80527700	-0.22226900
		C	0.89105300	-0.52280900	-0.28017300
		C	-1.28349700	-0.25897500	0.29224700
		C	0.05551500	1.52194400	0.10770300
		C	-3.65047100	0.07456600	0.85180800
		C	-4.63307200	0.08369100	-0.23417400
		C	-5.44206800	0.07926300	-1.12257300
		H	-6.15595300	0.09084500	-1.90878700
		H	-3.27263400	1.08289300	1.02585200
		H	-4.13336300	-0.27131400	1.77590300
		C	3.27441000	-0.77460500	-0.81156600
		C	4.17205300	-1.09180800	0.30183800
		C	4.90537600	-1.36534900	1.21348400
		H	5.55677100	-1.59311300	2.02081200
		H	3.69489700	-1.17543500	-1.74351100
		H	3.18260100	0.30628600	-0.92303800
		N	-2.50502200	-0.78807500	0.57583700

		N	1.93304700	-1.32359500	-0.63730600
		C	-2.77437900	-2.21279700	0.48761500
		H	-3.41659700	-2.43626200	-0.37250700
		H	-1.83455300	-2.74882800	0.38813900
		H	-3.29050700	-2.54548700	1.39599300
		C	1.81664500	-2.77135200	-0.67915300
		H	2.31923300	-3.23258100	0.17967800
		H	0.76530400	-3.04593100	-0.67255500
		H	2.28738500	-3.14781600	-1.59452300
4-azido-*N*-(prop-2-yn-1-yl)-6-(prop-2-yn-1-yloxy)-1,3,5-triazineo-2-amine	-805.117075	N	-0.61597800	3.17778800	-0.12788000
		N	0.41311800	2.52112900	-0.36221400
		N	1.41060900	0.45874200	-0.46047100
		N	0.17322900	-1.51321200	0.04120200
		N	-1.46268400	3.90060500	0.04910100
		N	-0.87801400	0.62847300	0.16943500
		C	-0.88067200	-0.71400300	0.27511000
		C	1.27196600	-0.86257800	-0.31311200
		C	0.29287000	1.13160400	-0.20534400
		C	3.57929500	-1.02892000	-0.88105800
		C	4.31205300	-0.60261900	0.30360500
		C	4.93464200	-0.26499100	1.27327700
		H	5.48029700	0.04487000	2.13018100
		H	3.41044200	-0.18364300	-1.55200600
		H	4.13137300	-1.80832200	-1.41279900
		C	-3.29816200	-0.66802400	0.86702600
		C	-4.34569500	-1.18743500	-0.01033000
		C	-5.20634500	-1.63797200	-0.71669400
		H	-5.96865000	-2.02291400	-1.34826500
		H	-3.61073100	-0.77669900	1.91425100
		H	-3.13840000	0.39828600	0.68981900
		N	-2.01977100	-1.32940900	0.65888000
		H	-1.98203300	-2.33679100	0.66875600
		O	2.32180400	-1.65174600	-0.55264700
4-azido-*N*-methyl-*N*-(prop-2-yn-1-yl)-6-(prop-2-yn-1-yloxy)-1,3,5-triazine-2-amine	-844.388422	N	-0.47635400	3.29245700	0.04076600
		N	0.55081300	2.64803200	-0.23122400
		N	1.54360500	0.59299600	-0.45726100
		N	0.29715800	-1.39699800	-0.06476400
		N	-1.32146400	4.00542100	0.26096300
		N	-0.74490600	0.73072300	0.17975800
		C	-0.76271200	-0.62052200	0.21433600
		C	1.39717700	-0.73161300	-0.38416100
		C	0.42527200	1.25086800	-0.16037800
		C	3.70255700	-0.88134700	-0.96505200
		C	4.44182200	-0.52979700	0.24004800
		C	5.06991900	-0.25411900	1.22564800
		H	5.62041300	0.00159700	2.09717700
		H	3.53760900	0.00276800	-1.58499800
		H	4.24818700	-1.63179400	-1.54317800
		C	-3.13056000	-0.45158500	0.83728100
		C	-4.13092200	-0.56088600	-0.22642400

		C	-4.95297500	-0.66116000	-1.09675600
		H	-5.67986100	-0.73733300	-1.86745900
		H	-3.56326500	-0.80475900	1.78283800
		H	-2.83855200	0.59044100	0.97182300
		N	-1.92364100	-1.22776000	0.56590700
		O	2.44206100	-1.51393100	-0.66938300
		C	-2.06411400	-2.67586100	0.58954800
		H	-2.80955000	-2.99504400	-0.14729000
		H	-1.10388200	-3.13035900	0.36023500
		H	-2.39685200	-3.00202600	1.58236200
s-triazine	-280.229253	N	1.35314100	0.22686800	-0.00000500
		N	-0.48009600	-1.28524700	0.00001300
		N	-0.87306300	1.05836600	-0.00003000
		C	-1.27373300	-0.21361500	0.00001400
		C	0.82189000	-0.99624600	-0.00000900
		C	0.45186900	1.20987600	0.00001500
		H	0.83235900	2.22899700	0.00006700
		H	-2.34655600	-0.39365400	-0.00000100
		H	1.51417500	-1.83534600	-0.00003000