Supplementary Material (ESI) for *PCCP*

Supplementary Information for the Manuscript

Ab initio quantum chemical computations of substituent effects on triaziridine strain energy and heat of formation.

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Coordinates of Primary Computed Structures

Optimized M06/DZV(2d,p) structures

Trans-triaziridine cs

N	7.0	0.7884282119	-0.3063933409	0.0000000000
N	7.0	-0.3249179371	0.2704044047	0.7257613666
N	7.0	-0.3249179371	0.2704044047	-0.7257613666
H	1.0	1.4876410290	0.4429404635	0.0000000000
H	1.0	-0.8505766834	-0.5517929660	1.0439121616
H	1.0	-0.8505766834	-0.5517929660	-1.0439121616

TOTAL ENERGY = -165.8650763984
ZPE: 0.047845

cis-triaziridine c3v

N	7.0	-0.4196681997	0.7268866442	-0.2314781129
N	7.0	-0.4196681997	-0.7268866442	-0.2314781129
N	7.0	0.8393363994	0.0000000000	-0.2314781129
H	1.0	-0.5997294195	1.0387618254	0.7314781129
H	1.0	-0.5997294195	-1.0387618254	0.7314781129
H	1.0	1.1994588391	0.0000000000	0.7314781129

TOTAL ENERGY = -165.8494756160
ZPE: 0.046381

flat-triaziridine d3h

N	7.0	-0.4011038603	0.6947322651	0.0000000000
N	7.0	-0.4011038603	-0.6947322651	0.0000000000
N	7.0	0.8022077206	0.0000000000	0.0000000000
H	1.0	-0.8986167877	1.5564499328	0.0000000000
H	1.0	-0.8986167877	-1.5564499328	0.0000000000
H	1.0	1.7972335754	0.0000000000	0.0000000000

TOTAL ENERGY = -165.6583979862
ZPE: 0.041419

CH3-cis-triaziridine - absolute minimum

N	7.0	-0.6970497457	0.0808635184	0.6988786861
N	7.0	-1.6195278928	-0.7558748896	-0.0272397042
N	7.0	-1.7189096344	0.6961981329	-0.1090262800
C	6.0	0.6031047529	0.0397091486	0.0375366521
H	1.0	-2.3301569057	-1.0044816131	0.6685011261
H	1.0	-1.2977273023	0.8961688037	-1.0286112480
H	1.0	0.5096558880	-0.1660723038	-1.0401288788
H	1.0	1.1027377616	0.9994851995	0.1980093814
H	1.0	1.2012692706	-0.7491767284	0.5007405458

TOTAL ENERGY = -205.1509325722
ZPE: 0.074900

CH3-trans-triaziridine - 2nd minimum

N	7.0	0.1898008847	0.0000493795	-0.5584896083
N	7.0	-0.8031361771	0.7291675935	0.1948911321
N	7.0	-0.8031020577	-0.7292567130	0.1947585947
C	6.0	1.4425832487	0.0000016652	0.1958240510
H	1.0	-1.4700309322	1.0424375688	-0.5200138821
H	1.0	-1.4699965125	-1.0424050282	-0.5202017054
H	1.0	2.0092636290	0.8905154819	-0.0889108945
H	1.0	2.0092093682	-0.8905289257	-0.0889734179
H	1.0	1.2612876748	-0.0000326478	1.2764181765

TOTAL ENERGY = -205.1492781917
ZPE: 0.074598

all-cis-CH3-triaziridine - 3rd minimum

N	7.0	0.8631714737	-0.7347943725	0.1548455103
N	7.0	-0.1341679418	-0.0000020574	-0.5737674047
N	7.0	0.8632637139	0.7347451672	0.1548830996
C	6.0	-1.4389383915	-0.0000423063	0.0663336930
H	1.0	0.4271442542	-1.0216340181	1.0475084439
H	1.0	0.4270285446	1.0217639817	1.0473868855
H	1.0	-1.9908205986	0.8883078252	-0.2539178003
H	1.0	-1.3598926173	-0.0000986946	1.1723417982
H	1.0	-1.9909791201	-0.8882382802	-0.2540336891

TOTAL ENERGY = -205.1378503552
ZPE: 0.073981

CF3-cis-triaziridine - absolute minimum

N	7.0	-0.7301655298	0.1412058017	0.6825984281
N	7.0	-1.6308755613	-0.7613875412	0.0177627402
N	7.0	-1.7691768328	0.6748712853	-0.1567756894
C	6.0	0.5734360161	0.0520534486	0.0571743233
H	1.0	-2.3147005330	-0.9930678094	0.7450084382
H	1.0	-1.3683782421	0.8279359058	-1.0918037897
F	9.0	0.5522240883	-0.0531500345	-1.2681536376
F	9.0	1.2452348387	1.1459374440	0.3639634053
F	9.0	1.1957979482	-0.9975792321	0.5488860620

TOTAL ENERGY = -502.8893117796
ZPE: 0.053213

CF3-trans-triaziridine - 2nd minimum

N	7.0	0.7195602552	-0.0001491014	0.7091507016
N	7.0	1.6916543791	0.7279826655	-0.0594869115
N	7.0	1.6917512292	-0.7277387757	-0.0598768132
C	6.0	-0.5554901699	-0.0000397675	0.0096701180
H	1.0	2.3546081072	1.0559333546	0.6521866600
H	1.0	2.3547514547	-1.0559908984	0.6516160208
F	9.0	-0.4782105495	0.0002332663	-1.3021013304
F	9.0	-1.2155807806	-1.0772206000	0.3952549065
F	9.0	-1.2156486164	1.0769366387	0.3957048262

TOTAL ENERGY = -502.8867008923
ZPE: 0.052703

all-cis-CF3-triaziridine - 3rd minimum

N	7.0	1.7315515600	-0.7313044639	0.1132379752
N	7.0	0.7606157186	-0.0003193498	-0.6577926236
N	7.0	1.7314650176	0.7312452655	0.1128867817
C	6.0	-0.5663475332	-0.0001386635	-0.0947228892
H	1.0	1.2715901828	-1.0280059270	0.9869286461
H	1.0	1.2712579388	1.0286047348	0.9862103737
F	9.0	-1.1987953884	1.0770102735	-0.5063093011
F	9.0	-0.6012255278	-0.0005612133	1.2499892350
F	9.0	-1.1994613277	-1.0765340224	-0.5071682598

TOTAL ENERGY = -502.8760399979
ZPE: 0.052210

O^--cis-triaziridine - absolute minimum

N	7.0	0.2254198190	-0.1615257107	0.5978718332
N	7.0	-0.8949521843	0.7891759576	0.1553234069
N	7.0	-0.9668857450	-0.5788646242	-0.3717405221
O	8.0	1.3071261748	0.0350374868	-0.0487208489
H	1.0	-0.3876012171	1.2580369224	-0.6114455716
H	1.0	-1.6222980435	-1.0137923823	0.2926472942

TOTAL ENERGY = -240.4466363351
ZPE: 0.036467

O^--trans-triaziridine - 2nd minimum

N	7.0	-0.3227907673	0.0000333332	-0.5123129130
N	7.0	0.9694826955	0.7297157357	0.1222663440
N	7.0	0.9693969659	-0.7298020964	0.1222943277
O	8.0	-1.3088697833	0.0001125406	0.2534146257
H	1.0	1.4567137524	1.0240721973	-0.7365102409
H	1.0	1.4566175091	-1.0242029377	-0.7364785488

TOTAL ENERGY = -240.4354045283
ZPE: 0.034951

all-cis-O^--triaziridine - 3rd minimum

N	7.0	0.9619890247	-0.7393163847	0.1488014686
N	7.0	-0.1556658462	-0.0000523267	-0.5721881700
N	7.0	0.9620666821	0.7393058834	0.1489255701
O	8.0	-1.2475663232	0.0000111993	0.1405734948
H	1.0	0.4251486500	-0.9906593025	0.9957835538
H	1.0	0.4250843348	0.9907163485	0.9957629211

TOTAL ENERGY = -240.4470762758
ZPE: 0.036709

BH2-cis-triaziridine - absolute minimum

N	7.0	0.2152547516	-0.0017885248	-0.1174947521
N	7.0	-1.0333333321	-0.5966633470	-0.3218132893
N	7.0	-0.8923998473	0.8311096955	0.0672768278
B	5.0	1.5852767997	-0.1390118265	-0.1042038587
H	1.0	-1.2834118282	-1.0519274461	0.5652977815
H	1.0	-1.0319463918	1.3249100141	-0.8234464615
H	1.0	2.2309109920	0.8381615309	0.0973330816

H	1.0	2.0297246391	-1.2246844041	-0.2937964305

TOTAL ENERGY = -191.3167146983
ZPE: 0.058843

BH2-trans and all-cis-BH2 same structure - 2nd minimum

N	7.0	-0.2973422267	-0.0403851758	0.0390412346
N	7.0	0.8712824236	-0.7820685699	-0.1662013882
N	7.0	0.8848544510	0.7047159853	-0.0348811144
B	5.0	-1.6755299826	-0.0248937553	0.0131104048
H	1.0	1.1243221878	-1.1678545392	0.7548003719
H	1.0	1.1439171547	0.9174390266	0.9390856977
H	1.0	-2.2110282121	1.0305854481	0.1174810160
H	1.0	-2.2322027715	-1.0712561760	-0.0699801075

TOTAL ENERGY = -191.3090894148
ZPE: 0.058418

OH-cis-triaziridine - absolute minimum

N	7.0	-0.1702631091	-0.1724959204	-0.5435668969
N	7.0	0.8627168356	-0.6798395715	0.3032519065
N	7.0	0.8393718648	0.7373116052	-0.0483150939
O	8.0	-1.3109515890	-0.0887820749	0.2799876867
H	1.0	1.5394612189	-1.0918237854	-0.3472225779
H	1.0	0.4083237487	1.1607527846	0.7842409545
H	1.0	-2.0215880614	0.0111777982	-0.3664830682

TOTAL ENERGY = -241.0383893477
ZPE: 0.051095

OH-trans-triaziridine - 2nd minimum

N	7.0	0.1756915763	-0.0068054950	0.5418010989
N	7.0	-0.8286813662	-0.7278832135	-0.1931037397
N	7.0	-0.8202059771	0.7309163588	-0.1876282487
O	8.0	1.3364482077	-0.0102668844	-0.2339502977
H	1.0	-1.4661612592	-1.0624556522	0.5391974291
H	1.0	-1.4539758430	1.0672904071	0.5470597305
H	1.0	2.0272737943	-0.0187417054	0.4400702498

TOTAL ENERGY = -241.0314587704
ZPE: 0.050583

all-cis-OH-triaziridine - 3rd minimum

N	7.0	-0.8684178902	0.7345307200	0.1002408052
N	7.0	0.1606467487	0.0019071580	-0.5891372151
N	7.0	-0.8661325521	-0.7352263725	0.0989334184
O	8.0	1.3135586032	0.0029046947	0.2438590696
H	1.0	-0.4131755189	1.0409566879	0.9711949069
H	1.0	-0.4099852904	-1.0420031043	0.9692553383
H	1.0	2.0373023349	0.0037984322	-0.3958934384

TOTAL ENERGY = -241.0295320965
ZPE: 0.050224

F-cis-triaziridine - absolute minimum

N	7.0	0.0982202591	-0.1498862770	0.6368174286
N	7.0	-0.8592452508	0.8025082982	0.1517163335
N	7.0	-0.8785860454	-0.5800661321	-0.3105980084
F	9.0	1.2724387668	0.0037898026	-0.1140375314
H	1.0	-0.3792825696	1.2928019647	-0.6135403632
H	1.0	-1.5927363561	-1.0410800068	0.2635777325

TOTAL ENERGY = -265.0500355786
ZPE: 0.038337

F-trans-triaziridine - 2nd minimum

N	7.0	-0.1714156440	0.0000881577	-0.5630710809
N	7.0	0.8782815236	0.7274850416	0.0834121401
N	7.0	0.8781434653	-0.7275091106	0.0834359928
O	9.0	-1.2393946848	0.0000041197	0.3148383797
H	1.0	1.4375650780	1.0798336464	-0.7029883293
H	1.0	1.4373706342	-1.0799730821	-0.7029535077

TOTAL ENERGY = -265.0445030899
ZPE: 0.038301

all-cis-F-triaziridine - 3rd minimum

N	7.0	0.9232869627	-0.7312654692	0.1492380139
N	7.0	-0.0579965356	-0.0000294195	-0.5996051023
N	7.0	0.9233257260	0.7312901820	0.1492593998
F	9.0	-1.2431783842	0.0000152636	0.2002156782
H	1.0	0.4128249308	-1.0598193978	0.9792788873
H	1.0	0.4127938222	1.0598142583	0.9792719614

TOTAL ENERGY = -265.0402648148

ZPE: 0.037500

F-triaziridine c2-TransitionState M06/DZV(2d,p)

N	7.0	0.0000000000	0.0000000000	0.0903050520
N	7.0	-0.7033603569	-0.3654554756	-1.0260386624
N	7.0	0.7033603569	0.3654554756	-1.0260386624
F	9.0	0.0000000000	0.0000000000	1.4258153708
H	1.0	-1.3147245001	0.4355646212	-1.2785665490
H	1.0	1.3147245001	-0.4355646212	-1.2785665490

TOTAL ENERGY = -264.9238561804
ZPE: 0.036888

F-triaziridine cs-TransitionState M06/DZV(2d,p)

N	7.0	-0.0680872649	-0.9114953801	-0.7974323949
N	7.0	-0.0680872649	-0.9114953801	0.7974323949
N	7.0	-0.0488358314	0.1945307395	0.0000000000
H	1.0	0.9280793002	-1.1498088076	-1.0230636283
H	1.0	0.9280793002	-1.1498088076	1.0230636283
F	9.0	-0.0700502393	1.5289556360	0.0000000000

TOTAL ENERGY = -264.9184195337
ZPE: 0.036075

CN-cis-triaziridine - absolute minimum

N	7.0	-0.2778651976	-0.1277899787	0.5929457909
N	7.0	-1.1519915545	-0.6479031914	-0.4451613464
N	7.0	-1.2165116740	0.7535547063	-0.0857202781
C	6.0	1.0102637791	-0.0377127414	0.1384018707
H	1.0	-1.9120717546	-1.0747585264	0.0967495032
H	1.0	-0.7018141551	1.2181775334	-0.8469326181
N	7.0	2.1395442629	0.0531133912	-0.1298960373

TOTAL ENERGY = -258.0391304584
ZPE: 0.045466

CN-trans-triaziridine - 2nd minimum

N	7.0	-0.2912151261	-0.0002115912	-0.5989728123
N	7.0	-1.2020237240	0.7252023855	0.2707537364

N	7.0	-1.2022084208	-0.7251885563	0.2708673409
C	6.0	0.9842128230	0.0000019700	-0.0924289796
N	7.0	2.1095548087	0.0001608328	0.1995021416
H	1.0	-1.9247101554	1.0520202516	-0.3831877469
H	1.0	-1.9248831259	-1.0519826630	-0.3831312162

TOTAL ENERGY = -258.0354801835
ZPE: 0.045440

all-cis-CN-triaziridine - 3rd minimum

N	7.0	-1.2089165478	-0.7945946332	-0.1874056328
N	7.0	-0.2985026722	-0.0091832423	0.6376689951
N	7.0	-1.3326671670	0.6516191172	-0.1482898609
C	6.0	0.9503773782	0.1088421553	0.0973969324
H	1.0	-0.6933786996	-1.0431708225	-1.0451268877
H	1.0	-0.8758076389	1.0323528477	-0.9908783466
N	7.0	2.0474795514	0.2112329620	-0.2849253806

TOTAL ENERGY = -258.0274351962
ZPE: 0.045048

CN-triaziridine c2-TransitionState M06/DZV(2d,p)

N	0.0000000000	0.0000000000	0.0341272252
N	-0.6659965197	-0.3469987583	-1.1424380072
N	0.6659965197	0.3469987583	-1.1424380072
C	0.0000000000	0.0000000000	1.3294008275
N	0.0000000000	0.0000000000	2.5017362495
H	-1.3149630940	0.4301779593	-1.3367391439
H	1.3149630940	-0.4301779593	-1.3367391439

TOTAL ENERGY = -258.0089207717
ZPE: 0.044947

CN-triaziridine cs-TransitionState M06/DZV(2d,p)

N	7.0	-0.0822253185	-1.3381816257	-0.7548458166
N	7.0	-0.0822253185	-1.3381816257	0.7548458166
N	7.0	-0.0789279769	-0.1647798007	0.0000000000
H	1.0	0.8996316593	-1.4987050378	-1.0364766474
H	1.0	0.8996316593	-1.4987050378	1.0364766474
C	6.0	-0.0357300758	1.1304442077	0.0000000000
N	7.0	0.0118533710	2.3017069201	0.0000000000

TOTAL ENERGY = -258.0012542438
ZPE: 0.044527

O$^-$-triaziridine c2-TransitionState M06/DZV(2d,p)

N	7.0	0.0000000000	0.0000000000	0.1189590997
N	7.0	-0.6916161417	-0.3483986617	-1.0311460150
N	7.0	0.6916161417	0.3483986617	-1.0311460150
O	8.0	0.0000000000	0.0000000000	1.3475438297
H	1.0	-1.3346113755	0.4295218168	-1.2486504497
H	1.0	1.3346113755	-0.4295218168	-1.2486504497

TOTAL ENERGY = -240.3643451145
ZPE: 0.037454

O$^-$-triaziridine cs-TransitionState M06/DZV(2d,p)

N	7.0	-0.0860804716	-0.8560913849	-0.7731619651
N	7.0	-0.0860804716	-0.8560913849	0.7731619651
N	7.0	0.0057190445	0.2724471845	0.0000000000
H	1.0	0.9307836948	-1.2119942216	-0.9729546300
H	1.0	0.9307836948	-1.2119942216	0.9729546300
O	8.0	-0.1053334908	1.5956430284	0.0000000000

TOTAL ENERGY = -240.3367738467

ZERO POINT ENERGY: 0.031920

Cl, cs_min

N	1.3228374847	-0.1559205759	-0.7289862069
N	1.3228374847	-0.1559205759	0.7289862069
N	0.3935278247	0.6683370226	0.0000000000
H	0.7890977048	-0.9701878235	-1.0609520976
H	0.7890977048	-0.9701878235	1.0609520976
CL	-1.2458282038	-0.0986002238	0.0000000000

TOTAL ENERGY = -625.3911612111
ZPE 0.036406

Cl, cs_ts

N	7.0	1.4373842380	0.0663257925	-0.7737280132
N	7.0	1.4373842380	0.0663257925	0.7737280132
N	7.0	0.2911553632	0.0247320484	0.0000000000
H	1.0	1.6699141252	-0.9184559354	-1.0196880903
H	1.0	1.6699141252	-0.9184559354	1.0196880903
CL	17.0	-1.3498920894	-0.0042317627	0.0000000000

TOTAL ENERGY = -625.3092096390
ZPE: 0.035869

Cl, tr_c1min

N	0.9079418595	-0.1455917785	0.0269697670
N	-0.3706003929	-0.8118754594	-0.1510940882
N	-0.3108231668	0.6177553554	-0.0026855012
H	1.2802493749	-0.0398568847	-0.9242224029
H	-0.5686690399	-1.2020824030	0.7789716451
CL	-0.6700986349	1.1174615536	1.6720605801

TOTAL ENERGY = -625.4005848228
ZPE: 0.036996

Cl, tr_c2ts

N	7.0	0.7626215077	0.0918849785	1.4450390456
N	7.0	-0.7626215077	-0.0918849785	1.4450390456
N	7.0	0.0000000000	0.0000000000	0.2898488690
H	1.0	1.0736580037	-0.8686601813	1.6716126297
H	1.0	-1.0736580037	0.8686601813	1.6716126297
CL	17.0	0.0000000000	0.0000000000	-1.3507722196

TOTAL ENERGY = -625.3155960319
ZPE: 0.036235

CCH, cs_c1min

N	7.0	1.2459995812	-0.1922254254	-0.7286993147
N	7.0	1.2459995812	-0.1922254254	0.7286993147
N	7.0	0.2966159536	0.6394360820	0.0000000000
H	1.0	0.7185589319	-1.0249878211	-1.0320703009
H	1.0	0.7185589319	-1.0249878211	1.0320703009
C	6.0	-0.9757051204	0.1414062130	0.0000000000
C	6.0	-2.1309436051	-0.2203844621	0.0000000000
H	1.0	-3.1492442545	-0.5362113400	0.0000000000

TOTAL ENERGY = -241.9327964817
ZPE: 0.055410

CCH, cs_ts

N	7.0	1.3713047140	0.0552249637	-0.7567436964
N	7.0	1.3713047140	0.0552249637	0.7567436964
N	7.0	0.1995393292	0.0494668749	0.0000000000
H	1.0	1.5384256516	-0.9280536560	-1.0324729716
H	1.0	1.5384256516	-0.9280536560	1.0324729716
C	6.0	-1.0960246377	0.0170550017	0.0000000000
C	6.0	-2.3105827960	-0.0565803720	0.0000000000
H	1.0	-3.3724526267	-0.0003741200	0.0000000000

TOTAL ENERGY = -241.9052673578
ZPE: 0.054396

CCH, tr_c1min

N	7.0	0.7575424877	-0.1783994105	-0.8412258487
N	7.0	-0.6622086336	-0.4730394549	-0.7716942093
N	7.0	-0.0762997735	0.5080884760	0.1317337285
H	1.0	0.8232959834	0.5052013188	-1.6039772829
H	1.0	-0.6843168512	-1.3630709258	-0.2541812088
C	6.0	0.1504896385	0.0441125132	1.3992727328
C	6.0	0.2860913298	-0.2622425381	2.5606722957
H	1.0	0.4234058191	-0.5438777008	3.5793997927

TOTAL ENERGY = -241.9433530712
ZPE: 0.055900

CCH, tr_c2ts

N	7.0	0.7467361875	0.0934591477	1.3736681197
N	7.0	-0.7467361875	-0.0934591477	1.3736681197
N	7.0	0.0000000000	0.0000000000	0.1978483711
H	1.0	1.0811838599	-0.8614321084	1.5730384888
H	1.0	-1.0811838599	0.8614321084	1.5730384888
C	6.0	0.0000000000	0.0000000000	-1.0978320015
C	6.0	0.0000000000	0.0000000000	-2.3141523904
H	1.0	0.0000000000	0.0000000000	-3.3771471962

TOTAL ENERGY = -241.9125497254
ZPE: 0.054599

NO2, cis_csmin

N	7.0	0.8379403213	-0.2800573638	0.1795127109
N	7.0	-0.5065684394	-0.6274125448	-0.2383955512
N	7.0	-0.1943495739	0.7263893596	0.0366956112
H	1.0	1.3746666659	-0.2010921351	-0.6910353004
H	1.0	-0.9344745778	-1.0057495840	0.6224311235
N	7.0	-0.5142579017	1.0667867102	1.5141190512
O	8.0	-0.2015616222	2.1812545177	1.8028345166

O	8.0	-1.0630101144	0.2211396910	2.1738378380

TOTAL ENERGY = -370.3081075980
ZPE: 0.049538

NO2, cis_csts

N	7.0	1.6294600405	0.0577091505	-0.7727899928
N	7.0	1.6294600405	0.0577091505	0.7727899928
N	7.0	0.4880314139	0.0449726640	0.0000000000
H	1.0	1.8008208429	-0.9225954052	-1.0566085228
H	1.0	1.8008208429	-0.9225954052	1.0566085228
N	7.0	-0.8634681526	0.0063798475	0.0000000000
O	8.0	-1.3800175139	-0.0120800011	-1.0990722473
O	8.0	-1.3800175139	-0.0120800011	1.0990722473

TOTAL ENERGY = -370.2437461919
ZPE: 0.048384

NO2, tr_c1min

N	7.0	0.8379403213	-0.2800573638	0.1795127109
N	7.0	-0.5065684394	-0.6274125448	-0.2383955512
N	7.0	-0.1943495739	0.7263893596	0.0366956112
H	1.0	1.3746666659	-0.2010921350	-0.6910353004
H	1.0	-0.9344745778	-1.0057495840	0.6224311235
N	7.0	-0.5142579017	1.0667867102	1.5141190512
O	8.0	-0.2015616221	2.1812545176	1.8028345167
O	8.0	-1.0630101145	0.2211396910	2.1738378380

TOTAL ENERGY = -370.3081075980
ZPE: 0.049538

NO2, tr_c2ts

N	7.0	0.7618748514	0.0948017261	1.6309875323
N	7.0	-0.7618748514	-0.0948017261	1.6309875323
N	7.0	0.0000000000	0.0000000000	0.4862648374
H	1.0	1.1016788540	-0.8571231618	1.8376103847
H	1.0	-1.1016788540	0.8571231618	1.8376103847
N	7.0	0.0000000000	0.0000000000	-0.8640537874
O	8.0	1.0991978320	-0.0027328337	-1.3817684420
O	8.0	-1.0991978320	0.0027328337	-1.3817684420

TOTAL ENERGY = -370.2516317732
ZPE: 0.048834

NH2_cis_csmin

N	7.0	0.8264723235	0.0259659862	0.0101868061

N	7.0	-0.4383010802	-0.6998222190	0.0104283582
N	7.0	-0.4225619249	0.7366790408	-0.1544474053
H	1.0	1.1976632862	-0.0535109944	-0.9502423321
H	1.0	-0.5558909657	-1.0625487006	-0.9491953848
N	7.0	-0.5832314387	1.0160025007	-1.5714243292
H	1.0	-1.5906192017	1.1417586304	-1.6909997592
H	1.0	-0.2009665894	1.9567639986	-1.6881804184

TOTAL ENERGY = -221.1671813312
ZPE: 0.063926

NH2_cis_csts

N	7.0	0.8796201807	-0.0953214732	-0.7307634156
N	7.0	0.8796201807	-0.0953214732	0.7307634156
N	7.0	-0.1805182358	0.5822446454	0.0000000000
H	1.0	0.4902013021	-1.0074158130	-1.0175578825
H	1.0	0.4902013021	-1.0074158130	1.0175578825
N	7.0	-1.4249892120	-0.1377206508	0.0000000000
H	1.0	-1.4996777589	-0.7179747111	-0.8328144698
H	1.0	-1.4996777589	-0.7179747111	0.8328144698

TOTAL ENERGY = -221.1482114704
ZPE: 0.062176

NH2_cis_csts new

N	7.0	1.6395245898	-0.2215126358	-0.8403600503
N	7.0	1.6707915522	0.2369623827	0.6413243680
N	7.0	0.5011779405	0.0307842080	-0.0741450605
H	1.0	1.8243150850	-1.2435674337	-0.7799859397
H	1.0	1.8678916522	-0.6407845548	1.1638564932
N	7.0	-0.8158590645	0.0784463368	-0.0049544285
H	1.0	-1.2534269382	0.8072700968	-0.5646578981
H	1.0	-1.3002048170	-0.8164284001	-0.0628274839

TOTAL ENERGY = -221.1003752065

ZPE: 0.062264

NH2_tr_c1min

N	7.0	0.8306795458	0.0853357588	0.0315117471
N	7.0	-0.2249459221	-0.9225441653	-0.0072624698
N	7.0	-0.5500216475	0.4765459296	0.1545229066
H	1.0	1.0654328201	0.2413321136	-0.9539766547
H	1.0	-0.2168094014	-1.3045696687	0.9485628696
N	7.0	-0.8069827044	0.7724100038	1.5253461013
H	1.0	0.0959053262	0.9262923588	1.9777510532

H	1.0	-1.3082707187	1.6564563201	1.5235444466

TOTAL ENERGY = -221.1773462357
ZPE: 0.063852

NH2_tr_c2ts

N	7.0	0.7652541939	0.0944743652	0.9402402561
N	7.0	-0.7652541939	-0.0944743652	0.9402402561
N	7.0	0.0000000000	0.0000000000	-0.2248587079
H	1.0	1.0771887867	-0.8628178389	1.1731012838
H	1.0	-1.0771887867	0.8628178389	1.1731012838
N	7.0	0.0000000000	0.0000000000	-1.5247493022
H	1.0	-0.0475806742	0.8712167520	-2.0412025348
H	1.0	0.0475806742	-0.8712167520	-2.0412025348

TOTAL ENERGY = -221.1055688851
ZPE: 0.061854

Trans-triaziridine at B3LYP/dzv(2d,p):

N	7.0	0.0000203471	0.8391698400	-0.0956998934
N	7.0	0.7348734129	-0.4196356819	0.0802569556
N	7.0	-0.7348925387	-0.4196008290	0.0802575279
H	1.0	0.0000309150	1.2488387313	0.8443905342
H	1.0	1.0540046916	-0.6414065894	-0.8706055596
H	1.0	-1.0540377305	-0.6413552972	-0.8706054319

TOTAL ENERGY = -165.8762720938

Cis-triaziridine at B3LYP/dzv(2d,p)

N	7.0	0.8462449711	0.0772309406	0.0808061320
N	7.0	-0.3562388005	-0.7714798939	0.0808048748
N	7.0	-0.4900097421	0.6942464271	0.0808044672
H	1.0	1.2090510901	0.1103477430	-0.8815768515
H	1.0	-0.5089443999	-1.1022273724	-0.8816376290
H	1.0	-0.7000634844	0.9918932095	-0.8816269657

TOTAL ENERGY = -165.8613367694

Flat-triaziridine at B3LYP/dzv(2d,p)

N	7.0	0.7297001698	0.3521558553	0.0000000000
N	7.0	-0.6698100984	0.4557820878	0.0000000000
N	7.0	-0.0598383454	-0.8079381157	0.0000000000
H	1.0	1.6273646723	0.7849086597	0.0000000000
H	1.0	-1.4940275193	1.0159986384	0.0000000000

H	1.0	-0.1335429768	-1.8017447226	0.0000000000

TOTAL ENERGY = -165.6660080512

MONO-SUBSTITUTED TRIAZIRIDINES:

CH3-cis-triaziridine with B3LYP/dzv(2d,p) – absolute minimum of the PES

N	7.0	-0.5761496400	1.2068056336	0.1086466053
N	7.0	0.0202653206	0.0015974352	-0.3789683165
N	7.0	-0.5820856362	-1.2031093550	0.1029631675
C	6.0	1.4290182367	-0.0023722985	0.0058536507
H	1.0	-1.4881859657	1.2946132176	-0.3364589751
H	1.0	-0.7419502114	1.1306907720	1.1225587460
H	1.0	-1.4910326219	-1.2882648687	-0.3488840877
H	1.0	-0.7549338711	-1.1283892000	1.1157439793
H	1.0	1.5636195215	-0.0061620041	1.1049671523
H	1.0	1.9008130499	-0.8974299475	-0.4050520686
H	1.0	1.9042324321	0.8935102654	-0.3993581274

TOTAL ENERGY = -206.4278486941

CH3-trans-triaziridine with B3LYP/dzv(2d,p) – 2nd minimum of the PES

N	7.0	0.1932310925	-0.0000064107	-0.5531319263
N	7.0	-0.8211364233	0.7386878268	0.1957649786
N	7.0	-0.8211645118	-0.7386852989	0.1957507538
C	6.0	1.4525885678	-0.0000342992	0.2011985807
H	1.0	-1.4781284849	1.0551392027	-0.5277189037
H	1.0	-1.4781606628	-1.0551069827	-0.5277207247
H	1.0	2.0170427693	0.8916845963	-0.0910217503
H	1.0	2.0171570062	-0.8915645634	-0.0912433775
H	1.0	1.2844497728	-0.0001656967	1.2834248154

TOTAL ENERGY = -205.1665784367

All-cis-CH3-triaziridine with B3LYP/dzv(2d,p) – 3rd minimum of the PES

N	7.0	0.8743304908	-0.7453823585	0.1548891899
N	7.0	-0.1396944996	0.0000023161	-0.5720884253
N	7.0	0.8743389632	0.7453790477	0.1548654833
C	6.0	-1.4538227424	-0.0000007461	0.0679812117
H	1.0	0.4518022918	-1.0343230276	1.0524347256
H	1.0	0.4517932427	1.0343298795	1.0524516478
H	1.0	-2.0019237415	0.8895833005	-0.2609532876
H	1.0	-1.3890831620	-0.0000066454	1.1729644328

H	1.0	-2.0019315259	-0.8895745212	-0.2609644417

TOTAL ENERGY = -205.1549312558

CF3-cis-triaziridine with B3LYP/dzv(2d,p) – absolute minimum of the PES

N	7.0	-0.7270363442	0.1330318198	0.6842436864
N	7.0	-1.6517355694	-0.7692140635	0.0138934286
N	7.0	-1.7794491304	0.6881877607	-0.1556243170
C	6.0	0.5817709086	0.0489818302	0.0601370778
H	1.0	-2.3322393559	-0.9986838663	0.7460330318
H	1.0	-1.3850017122	0.8401777391	-1.0935117694
F	9.0	0.5659847984	-0.0636221851	-1.2812925485
F	9.0	1.2560570766	1.1610124876	0.3638969070
F	9.0	1.2250455208	-1.0030522543	0.5608847838

TOTAL ENERGY = -502.8947726183

CF3-trans-triaziridine with B3LYP/dzv(2d,p) – 2nd minimum of the PES

N	7.0	0.7180557706	0.0000083820	0.7055870448
N	7.0	1.7122945556	0.7363587756	-0.0615900633
N	7.0	1.7122575669	-0.7363077924	-0.0616688530
C	6.0	-0.5626276325	0.0000022898	0.0093970201
H	1.0	2.3653820756	1.0674975701	0.6588220602
H	1.0	2.3653104908	-1.0675677171	0.6587072117
F	9.0	-0.4956892427	0.0005109110	-1.3188202347
F	9.0	-1.2335709966	-1.0877402206	0.4004422546
F	9.0	-1.2340172787	1.0871845836	0.4012417378

TOTAL ENERGY = -502.8921571220

All-cis-CF3-triaziridine with B3LYP/dzv(2d,p) – 3rd minimum of the PES

N	7.0	1.7448497538	-0.7404061198	0.1162889097
N	7.0	0.7585091382	-0.0000015625	-0.6598696528
N	7.0	1.7448442644	0.7404062226	0.1163021699
C	6.0	-0.5741220636	0.0000112064	-0.1000857386
H	1.0	1.2899503851	-1.0384650956	0.9918092349
H	1.0	1.2899560222	1.0384606749	0.9918065475
F	9.0	-1.2190415178	1.0867239096	-0.5174172608
F	9.0	-0.6152406868	-0.0000161926	1.2618717323
F	9.0	-1.2190546548	-1.0867164091	-0.5174460042

TOTAL ENERGY = -502.8822273664

O^--cis-triaziridine with B3LYP/dzv(2d,p) – absolute minimum of the PES

N	7.0	0.8252603381	-0.5748597403	-0.2455590341
N	7.0	-0.4737655392	-0.2526905174	0.4778629626
N	7.0	1.1024573370	0.8266255261	0.0511414752
H	1.0	1.3464428207	-1.0616381058	0.4946966432
O	8.0	-1.4256706022	-0.1471945061	-0.3224015628
H	1.0	0.6280449801	1.2750702812	-0.7445689473

TOTAL ENERGY = -240.4652572702

O^--trans-triaziridine with B3LYP/dzv(2d,p) – 2nd minimum of the PES

N	7.0	-0.4753466398	0.0001536978	0.5012955254
N	7.0	0.9539972115	-0.7269487185	-0.1308536767
N	7.0	0.9522403261	0.7265308439	-0.1301502783
O	8.0	-1.4312374831	0.0002480354	-0.2832475523
H	1.0	1.3863950722	-1.0373658876	0.7524086558
H	1.0	1.3855293639	1.0374507952	0.7524937681

TOTAL ENERGY = -240.4550184232

All-cis-O^--triaziridine with B3LYP/dzv(2d,p) – 3rd minimum of the PES

N	7.0	0.9120126906	-0.7459649451	0.1528989973
N	7.0	-0.2665355152	0.0000234577	-0.5783608762
N	7.0	0.9118988971	0.7459380977	0.1528940426
O	8.0	-1.3485368873	0.0000161193	0.1436878119
H	1.0	0.3932514850	-1.0096219281	1.0044284047
H	1.0	0.3932727336	1.0096146144	1.0043982217

TOTAL ENERGY = -240.4620080484

BH2-cis-triaziridine with B3LYP/dzv(2d,p) – absolute minimum of the PES

N	7.0	0.2184884117	-0.0014485558	-0.1168031974
N	7.0	-1.0342392953	-0.6121368235	-0.3235503240
N	7.0	-0.8915977035	0.8461115381	0.0683931015
B	5.0	1.5888232434	-0.1390362696	-0.1034353690
H	1.0	-1.2894677906	-1.0611784341	0.5661540658
H	1.0	-1.0371333709	1.3348730840	-0.8251771718
H	1.0	2.2344071502	0.8407837045	0.0952797672
H	1.0	2.0307951379	-1.2278625516	-0.2917079734

TOTAL ENERGY = -191.3283260302

BH2-trans-triaziridine with B3LYP/dzv(2d,p) – 2nd minimum of the PES

Same structure of all-cis-BH2 – see the article draft

All-cis-BH2-triaziridine with B3LYP/dzv(2d,p) – 2nd minimum of the PES

N	7.0	-0.3017228872	-0.0411111229	0.0499502293
N	7.0	0.8687521037	-0.7972134734	-0.1667916044
N	7.0	0.8830549004	0.7191650830	-0.0327144245
B	5.0	-1.6800211449	-0.0244488988	0.0121145574
H	1.0	1.1354971850	-1.1803496096	0.7526235033
H	1.0	1.1548593482	0.9299128019	0.9392822094
H	1.0	-2.2161628549	1.0331922619	0.1125963922
H	1.0	-2.2359836262	-1.0728647983	-0.0746047478

TOTAL ENERGY = -191.3210192534

OH-cis-triaziridine with B3LYP/dzv(2d,p) – absolute minimum of the PES

N	7.0	-0.1715681683	-0.1747963599	-0.5451407941
N	7.0	0.8722812526	-0.6886204684	0.3054861131
N	7.0	0.8437997464	0.7512112397	-0.0496575069
O	8.0	-1.3327360497	-0.1008834775	0.2834271545
H	1.0	1.5487533403	-1.0983291882	-0.3480442597
H	1.0	0.4221838297	1.1714995744	0.7887882229
H	1.0	-2.0356430426	0.0162195157	-0.3729660191

TOTAL ENERGY = -241.0518753522

OH-trans-triaziridine with B3LYP/dzv(2d,p) – 2nd minimum of the PES

N	7.0	0.1769849959	-0.0013299321	0.5434658580
N	7.0	-0.8359417833	-0.7389653917	-0.1927935392
N	7.0	-0.8314036941	0.7407049565	-0.1895301774
O	8.0	1.3546916033	0.0018922410	-0.2388717301
H	1.0	-1.4703499994	-1.0761846824	0.5425769365
H	1.0	-1.4646745242	1.0797702378	0.5456405721
H	1.0	2.0410825347	-0.0338336137	0.4429583023

TOTAL ENERGY = -241.0453101296

All-cis-OH-triaziridine with B3LYP/dzv(2d,p) – 3rd minimum of the PES

N	7.0	-0.8739854418	0.7463325156	0.1014701730
N	7.0	0.1604263886	0.0004615657	-0.5917947231
N	7.0	-0.8730180900	-0.7466322518	0.1006220026

O	8.0	1.3366691836	-0.0001728206	0.2454078529
H	1.0	-0.4249604263	1.0533688024	0.9752919541
H	1.0	-0.4241486161	-1.0543570150	0.9742763834
H	1.0	2.0528134371	0.0078674196	-0.4068207580

TOTAL ENERGY = -241.0434316034

F-cis-triaziridine with B3LYP/dzv(2d,p) – absolute minimum of the PES

N	7.0	0.0975374035	-0.1492642572	0.6430644207
N	7.0	-0.8616664240	0.8151426324	0.1535811310
N	7.0	-0.8842195330	-0.5910934237	-0.3121151617
F	9.0	1.2984128672	-0.0007702517	-0.1162473049
H	1.0	-0.3871003354	1.3025226104	-0.6168920678
H	1.0	-1.6021551744	-1.0484696607	0.2625445743

TOTAL ENERGY = -265.0628992461

F-trans-triaziridine with B3LYP/dzv(2d,p) – 2nd minimum of the PES

N	7.0	-0.1723787693	0.0001195302	-0.5675087127
N	7.0	0.8838554239	0.7383422326	0.0822478063
N	7.0	0.8837029206	-0.7384184845	0.0821795484
O	9.0	-1.2624737893	0.0000834185	0.3235024715
H	1.0	1.4439097718	1.0939123228	-0.7039027382
H	1.0	1.4439348146	-1.0941102469	-0.7038447806

TOTAL ENERGY = -265.0573310686

All-cis-F-triaziridine with B3LYP/dzv(2d,p) – 3rd minimum of the PES

N	7.0	0.9280614029	-0.7428688150	0.1505790465
N	7.0	-0.0536945917	-0.0000030800	-0.6060131893
N	7.0	0.9280477920	0.7428760794	0.1505976535
F	9.0	-1.2697042759	-0.0000015417	0.1991511907
H	1.0	0.4191673383	-1.0723370658	0.9816813268
H	1.0	0.4191788564	1.0723398405	0.9816628102

TOTAL ENERGY = -265.0539803872

CN-cis-triaziridine with B3LYP/dzv(2d,p) – minimum of the PES

N	7.0	-0.2648538231	-0.1300788786	0.5889374395
N	7.0	-1.1670883719	-0.6543698453	-0.4518491967
N	7.0	-1.2250980029	0.7647567957	-0.0857760815

C	6.0	1.0251600978	-0.0410013812	0.1365450015
H	1.0	-1.9192519298	-1.0809051310	0.1025049186
H	1.0	-0.7194333858	1.2284047786	-0.8533550936
N	7.0	2.1601191220	0.0498748548	-0.1166201028

TOTAL ENERGY = -258.0606734452

CN-trans-triaziridine with B3LYP/dzv(2d,p) – 2nd minimum of the PES

N	7.0	-0.2801567919	-0.0000015829	-0.5913149673
N	7.0	-1.2187169155	0.7336761768	0.2772895253
N	7.0	-1.2186969951	-0.7336622165	0.2773141111
C	6.0	0.9961548260	-0.0000013918	-0.0872844156
N	7.0	2.1280764070	-0.0000030484	0.1878886636
H	1.0	-1.9289589983	1.0621829391	-0.3902433442
H	1.0	-1.9289744527	-1.0621882469	-0.3902471089

TOTAL ENERGY = -258.0571986019

All-cis-CN-triaziridine with B3LYP/dzv(2d,p) – 3rd minimum of the PES

N	7.0	-1.2178477240	-0.8040040220	-0.1878571852
N	7.0	-0.2818976098	-0.0088980907	0.6331901295
N	7.0	-1.3419895735	0.6602513200	-0.1482100716
C	6.0	0.9699219022	0.1117366887	0.0969507941
H	1.0	-0.7188876467	-1.0578919803	-1.0539711044
H	1.0	-0.8968763066	1.0406817900	-0.9971625593
N	7.0	2.0761611625	0.2152226786	-0.2645001842

TOTAL ENERGY = -258.0492733710

CN-triaziridine c2-TransitionState B3LYP/DZV(2d,p)

N	7.0	0.0000000000	0.0000000000	0.0370179340
N	7.0	0.6824058042	0.3498154588	-1.1441244482
C	6.0	0.0000000000	0.0000000000	1.3339229340
N	7.0	0.0000000000	0.0000000000	2.5086581341
H	1.0	1.3238667945	-0.4338696102	-1.3422200529

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
N	7.0	0.0000000000	0.0000000000	0.0370179340
N	7.0	-0.6824058042	-0.3498154588	-1.1441244482
N	7.0	0.6824058042	0.3498154588	-1.1441244482
C	6.0	0.0000000000	0.0000000000	1.3339229340

N	7.0	0.0000000000	0.0000000000	2.5086581341
H	1.0	-1.3238667945	0.4338696102	-1.3422200529
H	1.0	1.3238667945	-0.4338696102	-1.3422200529

TOTAL ENERGY = -258.0289375294
ZPE: 0.044176

F-triaziridine c2-TransitionState B3LYP/DZV(2d,p)

N	7.0	0.0000000000	0.0000000000	0.0829053804
N	7.0	0.7309039856	0.3739352445	-1.0243284489
F	9.0	0.0000000000	0.0000000000	1.4435900038
H	1.0	1.3255777921	-0.4380433930	-1.2854642432

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
N	7.0	0.0000000000	0.0000000000	0.0829053804
N	7.0	-0.7309039856	-0.3739352445	-1.0243284489
N	7.0	0.7309039856	0.3739352445	-1.0243284489
F	9.0	0.0000000000	0.0000000000	1.4435900038
H	1.0	-1.3255777921	0.4380433930	-1.2854642432
H	1.0	1.3255777921	-0.4380433930	-1.2854642432

TOTAL ENERGY = -264.9389051354
ZPE: 0.035863

O$^-$-triaziridine c2-TransitionState B3LYP/DZV(2d,p)

N	7.0	0.0000000000	0.0000000000	0.1184040198
N	7.0	0.7098394360	0.3539296882	-1.0336206257
O	8.0	0.0000000000	0.0000000000	1.3596828330
H	1.0	1.3452728272	-0.4312012812	-1.2519678007

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
N	7.0	0.0000000000	0.0000000000	0.1184040198
N	7.0	-0.7098394360	-0.3539296882	-1.0336206257
N	7.0	0.7098394360	0.3539296882	-1.0336206257
O	8.0	0.0000000000	0.0000000000	1.3596828330
H	1.0	-1.3452728272	0.4312012812	-1.2519678007
H	1.0	1.3452728272	-0.4312012812	-1.2519678007

TOTAL ENERGY = -240.3842915891
ZPE: 0.036691

CN-triaziridine cs-TransitionState B3LYP/DZV(2d,p)

N	7.0	0.6671025528	-0.7688441758	0.0000000000
N	7.0	-0.3922276449	-0.0477787112	0.7350939583
C	6.0	1.8789733582	-0.1360562953	0.0000000000
N	7.0	2.9584168067	0.3110766091	0.0000000000
H	1.0	0.0149812860	0.8446906423	1.0533724673

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
N	7.0	0.6671025528	-0.7688441758	0.0000000000
N	7.0	-0.3922276449	-0.0477787112	-0.7350939583
N	7.0	-0.3922276449	-0.0477787112	0.7350939583
C	6.0	1.8789733582	-0.1360562953	0.0000000000
N	7.0	2.9584168067	0.3110766091	0.0000000000
H	1.0	0.0149812860	0.8446906423	-1.0533724673
H	1.0	0.0149812860	0.8446906423	1.0533724673

TOTAL ENERGY = -258.0492733102
ZPE: 0.043990

F-triaziridine cs-TransitionState B3LYP/DZV(2d,p)

N	7.0	1.1042492883	0.4372209409	0.0000000000
N	7.0	0.0062450203	-0.1390734379	0.7383357779
F	9.0	2.1311965344	-0.5257976596	0.0000000000
H	1.0	-0.4989679317	0.6833617972	1.0939474976

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
N	7.0	1.1042492883	0.4372209409	0.0000000000
N	7.0	0.0062450203	-0.1390734379	-0.7383357779
N	7.0	0.0062450203	-0.1390734379	0.7383357779
F	9.0	2.1311965344	-0.5257976596	0.0000000000
H	1.0	-0.4989679317	0.6833617972	-1.0939474976
H	1.0	-0.4989679317	0.6833617972	1.0939474976

TOTAL ENERGY = -265.0573310683

ZPE: 0.037474

O^--triaziridine cs-TransitionState B3LYP/DZV(2d,p)

N	7.0	1.3243970937	0.3750969367	0.0000000000
N	7.0	-0.1351737444	-0.1814345188	0.7267169060
O	8.0	2.2381698933	-0.4580833407	0.0000000000
H	1.0	-0.5211097491	0.7229277208	1.0374949673

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
N	7.0	1.3243970937	0.3750969367	0.0000000000
N	7.0	-0.1351737444	-0.1814345188	-0.7267169060
N	7.0	-0.1351737444	-0.1814345188	0.7267169060
O	8.0	2.2381698933	-0.4580833407	0.0000000000
H	1.0	-0.5211097491	0.7229277208	-1.0374949673
H	1.0	-0.5211097491	0.7229277208	1.0374949673

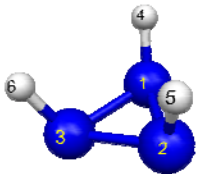
TOTAL ENERGY = -240.4550183140

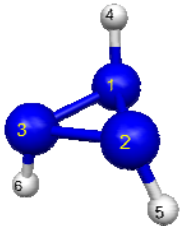
ZPE: 0.032526

Basis Set	ΔE (kcal/mol)	cis N-N (Å)	ΔSCF (eV)	Breathing Mode (cm-1)
DZV(d)	12.221	1.423	0.375	1405.53
DZV(2d)	10.717	1.424	0.376	1363.58
DZV(2d,p)	10.412	1.425	0.374	1362.71
DZV+ (2d,p)	10.688	1.425	0.394	1359.97
DZV++(2d,p)	10.707	1.425	0.394	1359.44
DZV(2df,p)	10.398	1.420	0.373	1372.71
DZV(2df,2p)	10.305	1.420		
DZV(3d)	10.335	1.422	0.362	1384.47
DZV(3d,p)	10.238	1.421	0.373	1384.76
TZV(d)	12.481	1.420	0.374	1382.88
TZV(2d)	11.054	1.424	0.363	1366.49
TZV(2d,p)	10.800	1.425	0.374	1364.08
TZV(2df,p)	10.830	1.419		
TZV(3d,p)	10.287	1.421	0.374	1365.55
aug-cc-pVDZ	10.680	1.423		
aug-cc-pVTZ	10.369	1.419		
aug-cc-pVQZ	10.358	1.418		
aug-cc-pV5Z	10.358	1.418		
RHF/DZV(2d,p)	10.412	1.425	0.374	1362.71
B3LYP/DZV(2d,p)		1.472		
M06/DZV(2d,p)	9.79	1.454		
MP2/DZV(2d,p)	10.0	1.489		
Expt[1]		1.49	0.3528 ± 0.0004	

[1] Kim, Y., Seff K., J Am Chem Soc (1977) vol. 99 (21) pp. 7057-7059

Principal geometry results for triaziridine system using different wavefunction types, with distances in Angstrom and angles in degrees.





(Z)-triaziridine			
	HF	MP2	DFT
r (N-N)	1.425	1.489	1.472
r (N-H)	1.005	1.028	1.029
α (N-N-H)	109.4	106.6	107.9
δ (Nplane-H)	101.7	99.9	100.7
Experimaental N-N dist. [XXX]		1.49	

(E)-triaziridine			
	HF	MP2	DFT
r (N-N)	1.419	1.486	1.468
r (N-N')	1.424	1.487	1.470
r (N-H)	1.004	1.026	1.027
r (N'-H)	1.002	1.025	1.025
α (N-N-N')	60.2	60.0	60.1
α (N1-N2-N3)	59.9	60.0	60.0
α (N1-N2-H5)	105.5	106.8	108.1
α (N2-N1-H4)	105.9	101.9	103.5
δ (Nplane-H5)	104.2	102.7	103.4
δ (Nplane-H4)	99.5	97.0	98.0

[XXX]: Kim, Y., Seff K., J Am Chem Soc (1977) vol. 99 (21) pp. 7057-7059

Calculated ionization energies for (E)-triaziridine and the lowest N_3H_3 potential energy surface minimum (E)-triazene.

Molecule	Calculated Ionization Potential (DZV(2d,p))		
	HF	MP2	B3LYP
(E)-triazene	0.3476	0.8895	0.3579
(E)-triaziridine	0.3744	0.9329	0.3947
Experiment[S2]	0.4163±0.004 kcal/mol (9.6±0.1 eV)		

[S2] Foner, S.N., Hudson, R. L., . J Chem Phys (1958) vol. 29 (2) pp. 442-443 (experiment showed an isomer of N3H3, but not which isomer). Since triazene should be the most stable they assigned the value to it. The same value is also reported on the NIST chemistry book as the only experimental data on triazene.

PES relative energes using DZV(2d,p)

Structure	**HF**	**MP2**	**B3LYP**	**M06**
(E)-triazene	0.0	0.0	0.0	
(Z)-triazene	6.3	5.2	4.7	
(Z,Z)-azimine	29.1	13.0	16.2	
(E,Z)-azimine	30.3	14.8	15.8	
(E,E)-azimine	37.3	21.7	24.0	
(E)-triaziridine, C_s	45.8	40.9	43.3	
(Z)-triaziridne, C_{3v}	56.2	50.9	52.7	
Flat-triazirdine, D_{3h}	184.8	188.0	175.3