Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for:

Quantum chemical investigation of the thermal denitrogenation of 1-pyrazoline

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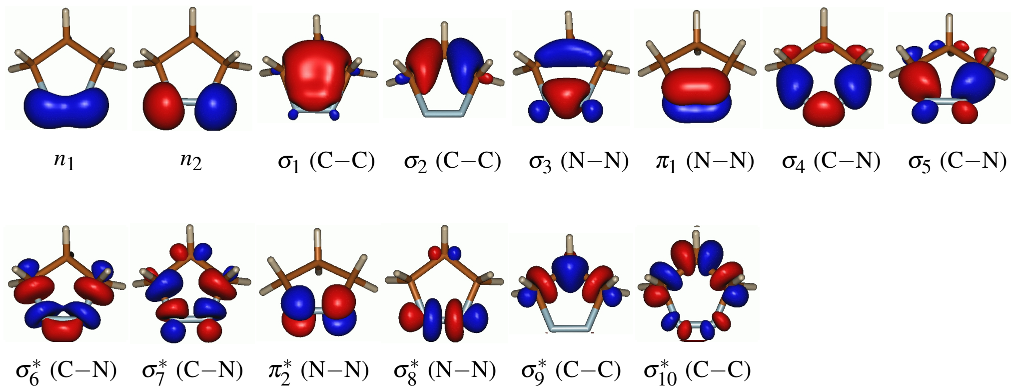

Figure S1: Orbitals used in the active space for CASSCF calculations.

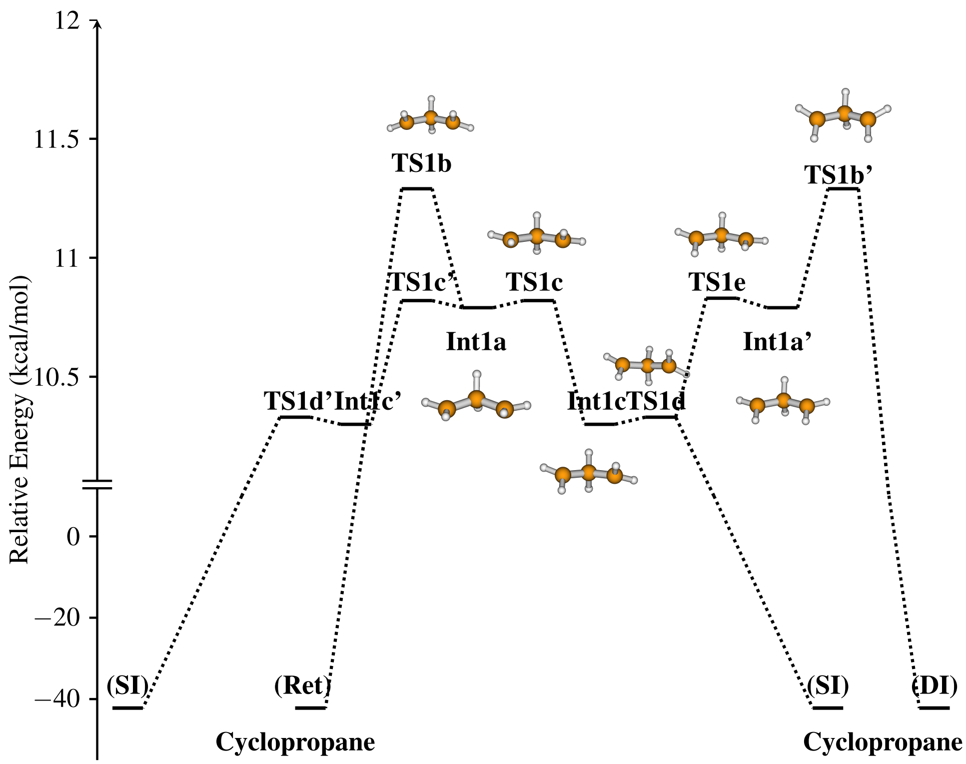

Figure S2: Potential energy profile for conrotatory and disrotatory closure of **Int1a** to cyclopropane obtained at CASSCF(4,4)/6-31+G* level of theory. The stationary points include N_2 kept at a distance of 10 Å from the rest of the molecule. The energies are relative to the reactant.

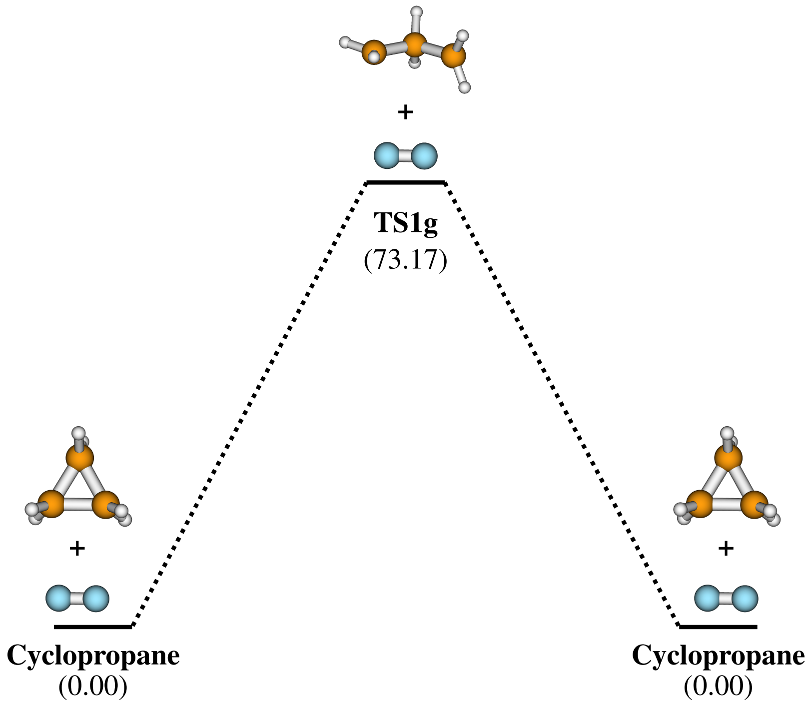

Figure S3: Potential energy profile for cis-trans isomerization of cyclopropane via **TS1g**.

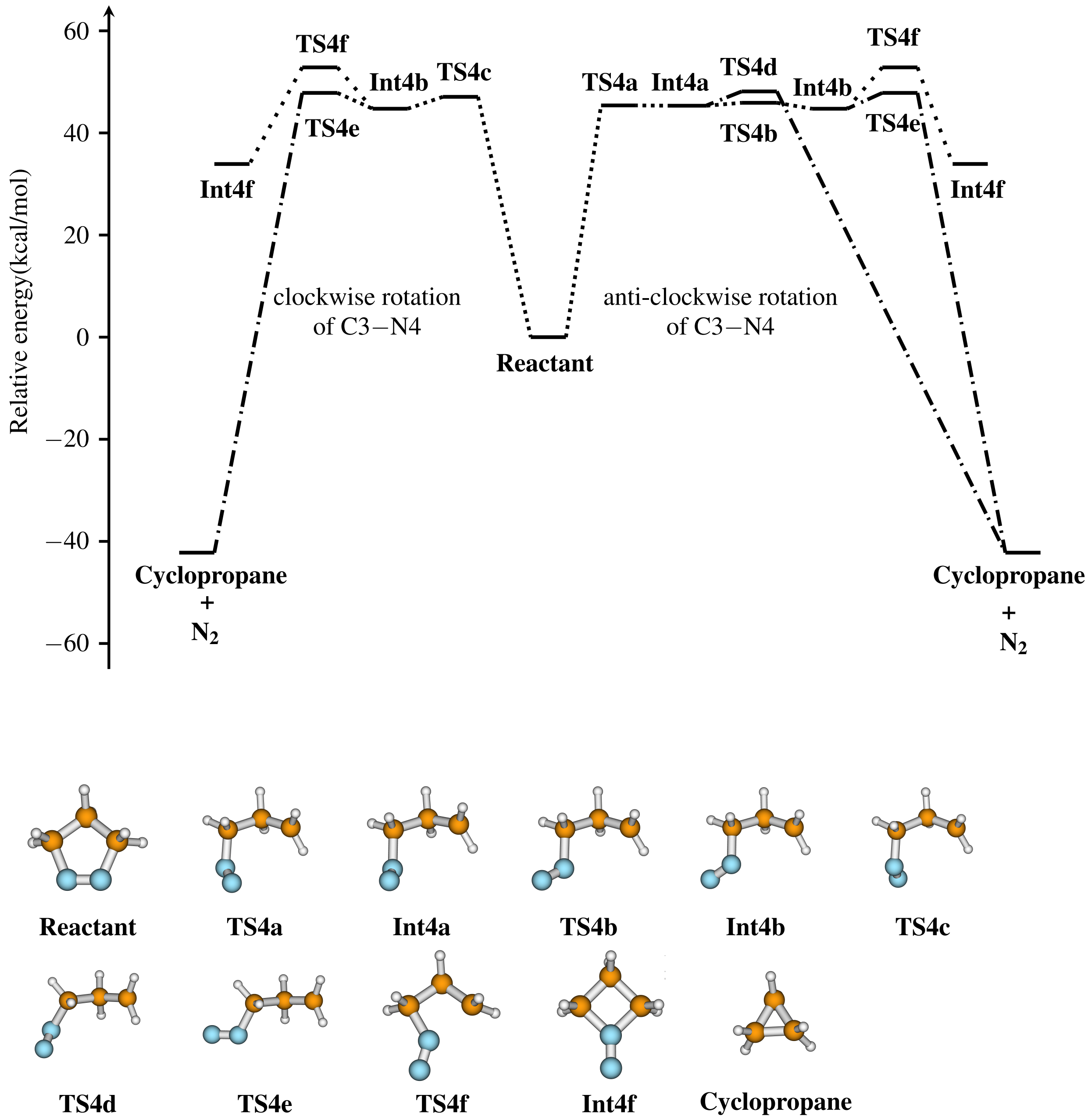

Figure S4: Potential energy profile and the stationary point structures for the asynchronous stepwise elimination of N_2 through perpendicular-like diazenyl intermediates at CASSCF(4,4)/6-31+G* level.

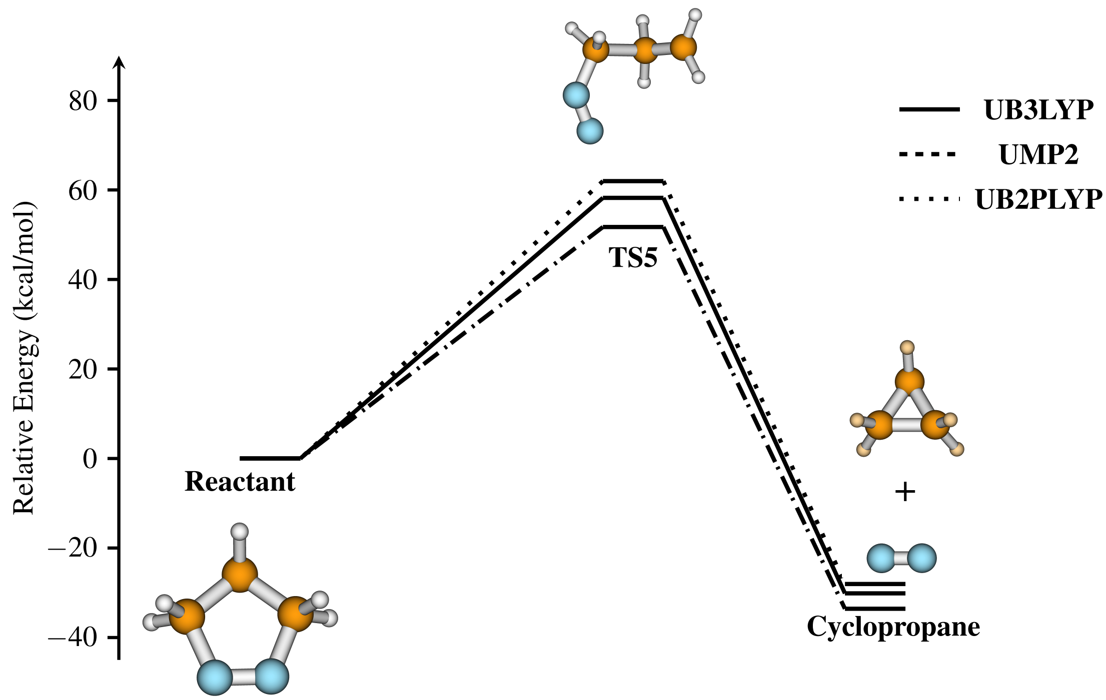

Figure S5: Asynchronous concerted denitrogenation paths obtained using DFT and MP2 methods.

Table S1: Geometrical parameters for synchronous denitrogenation path obtained at different CASSCF active space and 6-31+G* basis set[a]

Structure	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5	ϕ_6	θ	d_1	d_2
CASSCF(4,4)									
REACTANT	-17.74	12.04	-98.21	136.33	98.21	-136.33	101.59	1.51	1.51
TS1a	-40.78	22.19	-61.98	155.97	61.98	-155.97	113.86	2.08	2.08
SO1	0.00	0.00	-110.11	110.11	110.11	-110.11	118.40	2.10	2.10
Int1a	–	–	-27.19	176.04	27.19	-176.04	115.17	–	–
CASSCF(6,6)									
REACTANT	-20.04	13.49	-95.68	138.63	95.68	-138.63	101.68	1.52	1.52
TS1a	-39.81	21.84	-63.72	155.12	63.72	-155.12	113.48	2.05	2.05
SO1	0.00	0.00	-110.11	110.11	110.11	-110.11	117.98	2.07	2.07
Int1a	–	–	-27.17	176.09	27.19	-176.04	115.17	–	–
CASSCF(10,8)									
REACTANT	-19.73	13.24	-95.85	138.21	95.85	-138.21	102.04	1.53	1.53
TS1a	-39.71	21.64	-63.66	155.57	63.66	-155.57	114.06	2.05	2.05
SO1	0.00	0.00	-110.10	110.10	110.10	-110.10	118.22	2.08	2.08
Int1a	–	–	-27.17	176.09	27.17	-176.09	115.17	–	–
CASSCF(12,10)									
REACTANT	-20.40	13.59	-95.19	138.85	95.19	-138.85	102.38	1.53	1.53
TS1a	-40.16	21.73	-63.11	156.06	63.11	-156.06	114.33	2.06	2.06
SO1	0.00	0.00	-110.08	110.08	110.08	-110.08	118.89	2.09	2.09
Int1a	–	–	-27.16	176.09	27.16	-176.09	115.16	–	–
CASSCF(12,12)									
REACTANT	-17.68	12.01	-98.40	136.00	98.40	-136.00	101.24	1.52	1.52
TS1a	-40.71	22.17	-62.12	155.86	62.12	-155.86	113.87	2.08	2.08
SO1	0.00	0.00	-109.82	109.82	109.82	-109.82	118.87	2.11	2.11
Int1a	–	–	-25.71	175.53	25.71	-175.53	113.69	–	–

[a] Distances are in Å and angles are in degrees.

Table S2: Relative energies (kcal/mol) of stationary points along the conrotatory and disrotatory closure paths of **Int1a** to cyclopropane obtained at CASSCF(4,4)/6-31+G* level of theory[a]

Structure	**Int1a/ Int1a'**	**TS1b/ TS1b'**	**TS1c/ TS1c'**	**Int1c/ Int1c'**	**TS1d/ TS1d'**	**TS1e/ TS1e'**
without ZPE	10.79	11.29	10.82	10.30	10.33	10.83
with ZPE	1.0	1.47	0.77	0.70	0.61	0.86

[a] Energies are with respect to reactant.

Table S3: Geometrical parameters for synchronous denitrogenation path obtained at CASSCF(4,4)/6-31+G* level of theory[a]

Structure	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5	ϕ_6	θ	d_1	d_2
CASSCF(4,4)									
Int1a	–	–	-27.19	176.04	27.19	-176.04	115.17	–	–
TS1b	–	–	-46.46	152.50	47.46	-152.50	110.99	–	–
TS1c	–	–	-35.57	168.22	6.32	171.08	115.14	–	–
Int1c	–	–	-39.95	161.96	-39.83	161.96	113.96	–	–
TS1d	–	–	-46.67	152.65	-46.17	152.89	113.49	–	–
TS1e	–	–	6.35	171.12	-35.54	168.23	115.16	–	–
Int1a'	–	–	27.19	-176.04	-27.19	176.04	115.17	–	–
TS1b'	–	–	46.46	-152.50	-47.46	152.50	111.0	–	–
TS1g	–	–	-72.50	14.93	84.45	173.41	114.20	–	–
Cp	–	–	-107.64	107.64	-107.64	107.64	61.24	–	–

[a] Distances are in Å and angles are in degrees.

Table S4: Geometrical parameters for asynchronous denitrogenation path (Planar-like intermediate) obtained at CASSCF(n,m) levels using 6-31+G* basis set[a]

Structure	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5	ϕ_6	θ	d_1	d_2
CASSCF(4,4)									
TS3a	-70.28	97.31	-56.83	140.53	173.65	50.38	113.85	3.30	1.54
Int3a	-67.11	125.98	-44.61	157.10	177.43	54.33	113.89	3.63	1.54
TS3b	-61.46	171.17	-46.00	155.03	-179.29	-57.42	113.64	4.02	1.55
Int3b	-59.35	-132.59	-50.74	147.66	179.11	55.60	113.39	4.07	1.53
TS3c	-62.59	-54.36	-46.39	155.20	177.63	55.31	113.99	3.52	1.55
TS3d	-66.14	146.95	-40.09	163.39	-178.83	50.51	114.67	3.90	1.75
TS3e	-123.22	124.94	-51.36	150.77	121.42	-2.51	113.27	4.23	1.54
TS3f	-60.21	-142.12	-42.61	160.63	-177.88	51.03	114.74	4.15	1.75
TS3g	-118.57	-125.68	-52.76	147.29	120.39	-3.61	113.40	4.64	1.54
CASSCF(10,8)									
TS3a	-68.39	113.89	-49.96	151.30	176.13	51.09	114.23	3.41	1.59
Int3b	-54.38	-141.49	-51.01	150.91	-174.73	59.29	112.86	4.03	1.59
TS3c	-63.02	-53.38	-47.86	154.32	178.65	53.76	114.30	3.54	1.61
TS3f	-54.69	-145.66	-46.84	157.32	-173.37	57.31	113.75	4.06	1.68
TS3g	-119.43	-128.96	-52.58	148.04	119.92	-4.15	113.44	4.69	1.55
CASSCF(12,10)									
TS3a	-68.61	103.98	-49.81	151.63	176.13	50.79	114.24	3.43	1.60
Int3b	-57.29	-135.38	-51.58	147.93	-178.41	57.23	112.98	4.08	1.57
TS3c	-63.05	-53.80	-46.93	155.53	178.78	53.44	114.34	3.56	1.63
TS3f	-54.51	-145.12	-47.22	156.90	-173.30	57.56	113.68	4.08	1.68
TS3g	-122.00	-129.22	-54.05	146.79	117.74	-7.06	113.58	4.71	1.54
CASSCF(12,12)									
TS3a	-68.61	103.98	-49.81	151.63	176.13	50.79	114.24	3.43	1.60
Int3b	-57.29	-135.38	-51.58	147.93	-178.41	57.23	112.98	4.08	1.57
TS3c	-63.05	-53.80	-46.93	155.53	178.78	53.44	114.34	3.56	1.63
TS3f	-54.51	-145.12	-47.22	156.90	-173.30	57.56	113.68	4.08	1.68
TS3g	-122.00	-129.22	-54.05	146.79	117.74	-7.06	113.58	4.71	1.54

[a] Distances are in Å and angles are in degrees.

Table S5: Geometrical parameters for asynchronous denitrogenation path (perpendicular-like intermediate) obtained at CASSCF(n,m) levels using 6-31+G* basis set[a]

Structure	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5	ϕ_6	θ	d_1	d_2
CASSCF(4,4)									
TS4a	-69.65	99.58	-71.50	93.61	174.30	51.06	114.26	3.33	1.53
Int4a	-68.05	119.85	-72.29	90.29	176.47	53.30	114.33	3.58	1.53
TS4b	-63.16	171.47	-67.29	95.85	178.99	55.84	114.11	4.05	1.54
Int4b	-59.95	-131.51	-61.76	103.01	178.41	55.01	113.76	4.09	1.53
TS4c	-63.70	-53.69	-73.05	89.32	176.63	54.29	114.56	3.53	1.54
TS4d	-118.64	124.21	-81.26	78.37	126.03	1.99	113.13	4.18	1.55
TS4e	-113.04	-128.99	-77.59	80.17	125.99	1.83	113.08	4.62	1.55
TS4f	-19.86	162.84	-86.75	127.55	-138.01	91.83	101.36	3.09	1.52
Int4f	0.00	180.00	-113.27	113.28	113.27	-113.28	90.62	2.50	1.52
CASSCF(10,8)									
TS4a	-64.79	152.46	-67.32	96.61	179.29	54.36	114.31	3.95	1.59
Int3b	-54.39	-141.02	-50.82	151.14	-174.75	59.30	112.87	4.03	1.59
TS4c	-64.67	-53.70	-69.77	94.99	176.75	52.48	114.77	3.57	1.59
TS4f	-21.87	162.87	-83.95	131.88	-139.85	88.93	102.80	3.17	1.55
Int4f	0.00	180.00	-112.64	112.61	112.64	-112.61	92.37	2.55	1.57
CASSCF(12,10)									
TS4a	-65.44	150.49	-71.21	91.07	179.11	54.01	114.29	3.95	1.59
Int3b	-55.13	-137.82	-56.97	142.26	-175.36	57.77	113.05	4.05	1.61
TS4c	-64.89	-54.13	-69.60	95.16	176.67	51.97	114.79	3.59	1.60
TS4e	-113.59	-130.89	-79.02	78.91	125.09	2.11	113.28	4.66	1.52
TS4f	-22.19	-162.63	-83.35	132.47	-140.16	88.42	103.09	3.19	1.56
CASSCF(12,12)									
TS4a	-64.61	161.09	-70.91	95.13	179.71	53.96	114.08	4.05	1.61
Int4b	-59.14	-132.70	-63.96	105.63	-179.98	54.37	113.55	4.15	1.59
TS4c	-64.48	-52.66	-73.76	92.93	177.30	51.71	114.48	3.58	1.63
TS4e	-110.34	-127.78	-78.25	82.01	128.52	4.30	112.41	4.65	1.55
TS4f	-17.61	-164.37	-90.39	125.67	-135.52	94.31	100.97	3.14	1.51

[a] Distances are in Å and angles are in degrees.

Table S6: Energies (kcal/mol) of the stationary point structures with respect to cyclopropane obtained for the propene formation pathways at the CASSCF(4,4)/6-31+G* and CASSCF(6,6)/6-31+G* levels of theory[a]

Method	**TS1h**	**TS2a**	**Int2a**	**TS2b**	
CASSCF(4,4)	73.06 (67.11)	76.97 (73.68)	60.31 (57.00)	70.97 (66.49)	
CASSCF(6,6)	71.90 (65.62)	77.33 (74.15)	61.96 (58.61)	70.30 (65.88)	
CCSD(T)/TZ2P[b]	70.0 (64.2)	69.7 (66.6)	69.2 (66.5)	68.8 (64.2)	
MkCCSD(T)/cc-pV5Z[c]			72.59		
E_a (expt)[d]					64-66

[a]Numbers in the parentheses are zero point energy corrected values.
[b]Values are taken from *Chem. Commun*, **1999**, 1515-1516.
[c]Values are taken from *Mol. Phys.*, **2017**, 1-12.
[d]Values are taken from *J. Am. Chem. Soc.*, **1934**, 56, 399, *Proc. R. Soc. London.*, **1953**, 217, 563, *J. Chem. Phys.*, **1958**, 28, 504, *J. Am. Chem. Soc.*, **1960**, 82, 5996, *J. Chem. Soc.*, **1961**, 609, *Can. J. Chem.*, **1982**, 60, 916, *Phys. Chem.*, **1990**, 94, 1414

Table S7: Energetics of denitrogenation of 1-pyrazoline at CASSCF(4,4) with different basis sets[a]

Structure	6-31+G*	6-311+G*	cc-pVDZ	aug-cc-pVDZ	cc-pVTZ
TS1a	40.04	39.50	37.98	39.98	38.89
Int1a	10.79	9.18	8.7	10.80	7.90
TS3a	45.47	45.09	44.76	45.82	45.35
Int3a	45.24	44.81	44.43	45.39	45.02
TS3b	45.72	45.24	45.06	45.93	45.54
Int3b	44.71	44.25	43.98	44.97	44.51
TS3c	47.07	46.58	46.21	47.25	46.83
TS3d	47.56	46.80	46.46		46.30
TS3e	48.63	48.23	48.10	49.00	48.48
TS3f	47.13	46.30	45.95	47.13	46.30
TS3g	48.51	48.11	47.99	48.85	48.35
TS4a	45.40	45.05	44.72	45.78	45.33
Int4a	45.33	44.95	44.67	45.76	45.30
TS4b	45.90	45.47	45.36	46.24	45.87
Int4b	44.74	44.33	44.13	45.08	44.65
TS4c	47.08	46.64	46.26	47.31	46.89
TS4d	48.13	47.71	47.69	48.51	48.00
TS4e	47.84	47.40	47.37	48.17	47.70
TS4f	52.84	52.19	52.57	53.73	52.56
Int4f	33.92	33.65	35.80	35.71	35.08
TS5	48.21	47.77	47.45	48.44	47.90

[a] Energies are with respect to reactant.

Sample input file for CASSCF calculation of Reactant in Gaussian 09

1. The initial orbitals were choosen from a HF orbital calculation.

```
%chk=reactant.chk
# RHF/6-31+G* pop=full gfprint gfinput

xxxxxxx

0 1
N      0.056333     -1.117680      0.605127
N      0.056333     -1.117680     -0.605127
C     -0.094863      0.269143     -1.183589
C      0.112021      1.212155      0.000000
C     -0.094863      0.269143      1.183589
H      0.622453      0.379476      1.985095
H     -1.090569      0.318327      1.610838
H     -0.583060      2.041984      0.000000
H      1.117584      1.617017      0.000000
H      0.622453      0.379476     -1.985095
H     -1.090569      0.318327     -1.610838
```

2. The second step involves reading the HF orbitals, rotation of orbitals followed by the CASSCF calculation.

```
%chk=reactant.chk
# CASSCF(4,4)/6-31+G* guess=(read,alter) scf=(maxcycle=200) pop=full gfprint gfinput

xxxxxxx

0 1
```

N	0.056333	-1.117680	0.605127
N	0.056333	-1.117680	-0.605127
C	-0.094863	0.269143	-1.183589
C	0.112021	1.212155	0.000000
C	-0.094863	0.269143	1.183589
H	0.622453	0.379476	1.985095
H	-1.090569	0.318327	1.610838
H	-0.583060	2.041984	0.000000
H	1.117584	1.617017	0.000000
H	0.622453	0.379476	-1.985095
H	-1.090569	0.318327	-1.610838

13 18
37 20
50 21

XYZ coordinates of all the stationary point structures along the different paths for the thermal denitrogenation of 1-pyrazoline obtained at the CASSCF(4,4)/6-31+G* level of theory are given below.

Reactant

N	0.056333	-1.117680	0.605127
N	0.056333	-1.117680	-0.605127
C	-0.094863	0.269143	-1.183589
C	0.112021	1.212155	0.000000
C	-0.094863	0.269143	1.183589
H	0.622453	0.379476	1.985095
H	-1.090569	0.318327	1.610838
H	-0.583060	2.041984	0.000000
H	1.117584	1.617017	0.000000
H	0.622453	0.379476	-1.985095
H	-1.090569	0.318327	-1.610838

TS1a

N	0.096360	-1.408443	0.563894

N	0.096360	-1.408443	-0.563894
C	-0.194627	0.536902	-1.253272
C	0.273916	1.205036	0.000000
C	-0.194627	0.536902	1.253272
H	0.382795	0.685420	2.150314
H	-1.259216	0.492986	1.421812
H	-0.129448	2.221165	0.000000
H	1.354867	1.292481	0.000000
H	0.382795	0.685420	-2.150314
H	-1.259216	0.492986	-1.421812

Int1a

N	3.773431	7.055425	-0.104123
N	4.775303	6.638239	-0.019458
C	0.169857	-1.623339	-1.268310
C	-0.619995	-1.781402	0.000011
C	0.169721	-1.623471	1.268434
H	-0.346228	-1.660634	2.210807
H	1.221686	-1.846276	1.281393
H	-1.090693	-2.769148	-0.000065
H	-1.447268	-1.074058	0.000002
H	-0.345991	-1.660423	-2.210741
H	1.221824	-1.846143	-1.281177

TS3a

C	0.002841	0.002590	-0.002364
C	0.000627	-0.005189	1.496147
C	1.395732	0.024929	2.115694
N	2.094359	-1.324591	1.868272
N	2.826322	-1.403004	0.972439
H	0.495373	0.798487	-0.531051
H	1.344503	0.129545	3.190115
H	2.007410	0.815634	1.698910
H	-0.536175	-0.870252	1.870724
H	-0.695159	-0.598565	-0.552599
H	-0.525982	0.873674	1.870017

Int3a

C	-0.825834	0.119074	-1.283677
C	-0.785313	0.131253	0.215244
C	0.623512	0.142478	0.794242
N	1.316141	-1.193036	0.477248
N	2.344900	-1.169195	-0.057305
H	-0.178980	0.773371	-1.840913
H	0.597450	0.196266	1.874434
H	1.224224	0.955734	0.404854
H	-1.325016	-0.723194	0.610220
H	-1.697708	-0.252175	-1.789015
H	-1.293373	1.019421	0.594669

TS3b

C	-0.892900	0.147135	-1.290116
C	-0.793679	0.140134	0.204348
C	0.635346	0.135367	0.719857
N	1.342474	-1.151442	0.225198
N	2.483022	-1.252167	0.390755
H	-0.280364	0.820106	-1.863823
H	0.672673	0.117982	1.801311
H	1.207882	0.979410	0.356828
H	-1.321316	-0.718769	0.606211
H	-1.771466	-0.242256	-1.769048
H	-1.281670	1.024497	0.618480

Int3b

C	1.287207	-0.921900	0.098232
C	0.610402	0.321367	-0.387023
C	-0.720429	0.592687	0.300604
N	-1.652633	-0.601124	0.046628
N	-2.739033	-0.405071	-0.300966
H	1.423116	-1.079748	1.152960
H	-1.190872	1.503389	-0.049870
H	-0.608062	0.633596	1.376751

H	0.456916	0.270257	-1.460249
H	1.890815	-1.505937	-0.569822
H	1.242573	1.192484	-0.207247

TS3c

C	-0.319647	0.835211	1.443117
C	0.353351	1.045901	0.119184
C	-0.229291	0.206992	-1.013008
N	-0.077360	-1.317900	-0.777710
N	0.971928	-1.754991	-0.562627
H	-1.393698	0.828333	1.500035
H	0.256164	0.418769	-1.957037
H	-1.292291	0.363642	-1.122595
H	1.417067	0.854650	0.205178
H	0.217369	1.036155	2.351000
H	0.252732	2.089249	-0.185535

TS3d

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.499038
C	1.373545	0.000000	2.129840
N	2.109492	-1.538036	1.719235
N	3.233946	-1.528391	1.571631
H	0.713954	0.601120	-0.535185
H	1.357803	-0.020097	3.209163
H	2.049368	0.755314	1.755423
H	-0.562129	-0.851557	1.869328
H	-0.898624	-0.268045	-0.524262
H	-0.521075	0.888754	1.863356

TS3e

C	2.094547	-0.584933	0.080946
C	1.077833	0.418322	-0.378668
C	-0.168358	0.477610	0.522324
N	-1.432975	0.209994	-0.325822

N	-2.142978	-0.645031	0.003045
H	2.431816	-0.572345	1.102317
H	-0.326688	1.464034	0.934854
H	-0.135082	-0.247022	1.324899
H	0.770582	0.188071	-1.392123
H	2.736361	-1.061484	-0.636404
H	1.530552	1.408009	-0.421717

TS3f

C	1.844356	-0.762057	0.119387
C	1.187786	0.494708	-0.359014
C	-0.109723	0.835318	0.335488
N	-1.185458	-0.517235	0.021777
N	-2.275366	-0.272315	-0.163919
H	1.886749	-0.974611	1.172880
H	-0.601263	1.723137	-0.035042
H	-0.054269	0.829554	1.414181
H	1.023327	0.443803	-1.431186
H	2.575228	-1.243042	-0.503810
H	1.861476	1.340196	-0.197194

TS3g

C	2.081839	-0.586958	0.076916
C	1.091230	0.444401	-0.374299
C	-0.162045	0.518666	0.515782
N	-1.414481	0.176508	-0.325834
N	-2.289602	0.936086	-0.334427
H	2.428698	-0.584548	1.095099
H	-0.305321	1.493470	0.963318
H	-0.149608	-0.234634	1.290684
H	0.788053	0.233782	-1.393255
H	2.682676	-1.109418	-0.643388
H	1.559898	1.427391	-0.395280

TS4a

C	1.588108	-0.886034	0.082006
C	1.155609	0.511863	-0.239859
C	-0.205751	0.899738	0.345014
N	-1.311284	0.121503	-0.382287
N	-1.744743	-0.824058	0.131168
H	1.891081	-1.136200	1.082226
H	-0.421155	1.944300	0.166707
H	-0.266931	0.686565	1.405059
H	1.128535	0.662462	-1.314396
H	1.382341	-1.695594	-0.591474
H	1.880458	1.217177	0.160673

INT4a

C	1.175032	-1.016319	-0.012088
C	0.715030	0.379473	-0.310266
C	-0.663642	0.723504	0.257206
N	-1.732551	-0.092165	-0.480576
N	-2.395611	-0.819521	0.133941
H	1.478058	-1.277758	0.985567
H	-0.911341	1.758876	0.062338
H	-0.733395	0.523747	1.319569
H	0.698801	0.548300	-1.382123
H	0.950912	-1.820610	-0.686756
H	1.418706	1.092472	0.113187

TS4b

C	1.748169	-0.877920	0.058448
C	1.224727	0.497190	-0.226130
C	-0.164533	0.765467	0.344016
N	-1.176537	-0.191257	-0.326811
N	-2.254773	-0.229531	0.094261
H	1.986540	-1.160456	1.068219
H	-0.494939	1.774468	0.130000
H	-0.212366	0.592684	1.411507
H	1.200549	0.672062	-1.296713
H	1.639702	-1.664260	-0.663307

H	1.895136	1.240202	0.201997

Int4b

C	-1.365706	-0.789733	-0.346305
C	-0.604154	0.130309	0.556228
C	0.673172	0.688169	-0.069358
N	1.593253	-0.483476	-0.428947
N	2.705687	-0.436787	-0.108294
H	-1.756507	-0.421116	-1.277450
H	1.192740	1.372536	0.591845
H	0.467042	1.179482	-1.011884
H	-0.354460	-0.372681	1.484746
H	-1.327311	-1.852754	-0.210172
H	-1.223757	0.986051	0.819592

TS4c

C	-1.765913	-0.687313	-0.263839
C	-0.999138	0.302034	0.561444
C	0.174737	0.963903	-0.166183
N	1.274126	-0.044312	-0.569732
N	1.733064	-0.737040	0.235992
H	-2.414518	-0.340392	-1.047629
H	0.655407	1.709635	0.455400
H	-0.133763	1.423857	-1.093089
H	-0.630929	-0.169398	1.466379
H	-1.477535	-1.721137	-0.282871
H	-1.663594	1.105761	0.871050

TS4d

C	-2.273870	-0.314396	-0.123263
C	-1.043793	0.240332	0.528502
C	0.133820	0.421356	-0.453744
N	1.327439	-0.464121	-0.000254
N	1.762909	-1.225494	-0.755126
H	-2.933298	0.337496	-0.666991

H	0.524035	1.429759	-0.435837
H	-0.120950	0.151858	-1.469837
H	-0.722035	-0.409443	1.335403
H	-2.340556	-1.365931	-0.336871
H	-1.276475	1.199674	0.978598

TS4e

C	2.141287	-0.495905	0.016116
C	1.119756	0.527283	-0.375530
C	-0.140269	0.495589	0.514736
N	-1.360125	0.025153	-0.331650
N	-2.314338	0.679178	-0.295268
H	2.770034	-0.320354	0.870822
H	-0.374811	1.459485	0.949296
H	-0.066551	-0.243240	1.300335
H	0.819168	0.376209	-1.406620
H	2.021254	-1.516947	-0.298529
H	1.557758	1.518542	-0.318723

TS4f

N	1.767658	0.462844	-1.242893
C	-0.531559	-1.357366	-0.243730
C	0.436346	0.512566	0.806974
N	0.935598	0.081907	-0.563174
C	-0.341241	-0.763351	1.133854
H	-0.239115	-2.378184	-0.421156
H	1.262534	0.776026	1.455404
H	0.250247	-1.420075	1.761857
H	-1.269868	-0.551977	1.654169
H	-0.196460	1.377086	0.649487
H	-1.389072	-1.034202	-0.811479

Int4f

N	1.160171	0.749776	-1.884488
C	-0.333638	-0.829982	-0.639051

C	0.416421	0.883554	0.504470
N	0.569744	0.368165	-0.925386
C	-0.496942	-0.321193	0.807254
H	0.199138	-1.761825	-0.767407
H	1.368647	0.909870	1.015568
H	-0.107138	-0.993794	1.559469
H	-1.511331	-0.052386	1.069784
H	-0.047796	1.859697	0.521345
H	-1.217275	-0.811882	-1.261558

TS5

C	-0.005726	-0.010854	-0.000771
C	-0.006502	0.013634	1.493111
C	1.413434	0.029161	2.103671
N	1.829533	-1.252922	2.881058
N	1.176350	-2.203295	2.877787
H	0.073080	0.906296	-0.555608
H	1.545333	0.822124	2.827033
H	2.189794	0.126395	1.357509
H	-0.546005	-0.844283	1.880215
H	0.231729	-0.920885	-0.522002
H	-0.531611	0.898295	1.838064

Product (Cyclopropane + N_2)

C	-0.112995	-0.755181	2.953453
C	0.058683	-0.006316	4.240194
C	0.047051	0.763044	2.954143
N	0.546910	-0.083140	-5.778833
N	-0.528950	0.078972	-5.744139
H	-1.083635	-1.161641	2.728197
H	0.710252	-1.350701	2.598889
H	-0.794224	0.083299	4.890486
H	0.995066	-0.105261	4.761498
H	-0.817477	1.363170	2.729347
H	0.976415	1.174131	2.600045

Product (Propene + N_2)

N	4.319689	-0.191458	0.675065
N	4.151179	-0.565056	1.683535
C	-5.651992	-1.224741	0.168244
C	-5.591870	0.143622	-0.454407
C	-5.389823	1.286313	0.218230
H	-5.357120	2.236304	-0.284915
H	-5.252611	1.298662	1.286375
H	-6.611128	-1.697553	-0.025097
H	-5.723826	0.186473	-1.524355
H	-4.885290	-1.874023	-0.245931
H	-5.509714	-1.178110	1.242730