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TS1-1	G3(MP2)		
n	-0.037572	0.568778	1.07638
n	0.037572	-0.568778	1.07638
c	-0.12621	1.809794	-0.79797
c	0.12621	-1.809794	-0.79797
h	0	2.812602	-0.40957
h	0	-2.812602	-0.40957
h	0.726307	1.313001	-1.25119
h	-0.726307	-1.313001	-1.25119
h	-1.120056	1.482716	-1.08605
h	1.120056	-1.482716	-1.08605

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TS1-2	G3(MP2)		
n	0	0.569605	0.00000
n	0	-0.569605	0.00000
c	-2.144944	1.263144	0.00000
c	2.144944	-1.263144	0.00000
h	-2.671898	0.314589	0.00000
h	-2.077611	1.815401	0.93056
h	-2.077611	1.815401	-0.93056
h	2.671898	-0.314589	0.00000
h	2.077611	-1.815401	0.93056
h	2.077611	-1.815401	-0.93056

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TS1-3	B3LYP/6-31G(d)		
7	0.193033	-1.230543	-0.000077
7	1.043241	-0.436842	0.000069
6	-1.728481	0.245440	-0.000027
6	0.927205	0.970662	-0.000106
1	-2.169051	1.248835	-0.003556
1	-2.023010	-0.291637	0.900637
1	-2.024205	-0.298218	-0.896319
1	-0.366138	0.905586	-0.000390

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2-1	G3		
n	0.542018	0.247433	-0.024401
n	-0.461825	-0.580161	-0.05598
c	1.844717	-0.039364	0.042727
c	-1.730833	0.119013	0.031253
h	2.134686	-1.078071	0.081301
h	2.539548	0.778361	-0.054536
h	0.32973	1.258045	-0.057682
h	-1.668313	1.170358	-0.300963
h	-2.456828	-0.391328	-0.606318
h	-2.123485	0.113838	1.05699

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n	-0.428418	0.439774	-0.257281
n	0.612985	-0.453189	-0.138439
c	-1.699807	-0.153438	0.130298
c	1.778165	0.028852	0.116718
h	-1.748984	-0.433344	1.190845
h	-1.853434	-1.047105	-0.474309
h	-2.494163	0.56364	-0.08818
h	1.969086	1.09324	0.289774
h	2.6139	-0.660116	0.14363
h	-0.248525	1.325106	0.226178

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2-3	G3		
n	-0.652768	-0.541393	0
n	0.633051	-0.783663	-0.000001
c	-1.376641	0.58885	-0.000001
c	1.370597	0.459148	0
h	-0.891823	1.549539	-0.000001
h	-2.449815	0.48157	0.000005
h	-1.193062	-1.406424	0.000002
h	1.138064	1.072604	-0.887005
h	1.138062	1.072602	0.887008
h	2.432864	0.21751	0.000001

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2-4	G3		
n	0.809775	-0.626165	0.05547
n	-0.544018	-0.672852	-0.156623
c	1.413198	0.512632	-0.008936
c	-1.354339	0.515128	0.045732
h	0.933224	1.47276	-0.193707
h	2.48999	0.493244	0.112187
h	-0.904608	-1.498262	0.306752
h	-1.111966	1.035864	0.984389
h	-1.219306	1.215808	-0.782162
h	-2.400789	0.207151	0.059831

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TS3-1	G3		
7	0.494226	0.291344	-0.136539
7	-0.451754	-0.544447	-0.024434
6	1.807101	-0.055319	0.053801
6	-1.745597	0.123749	0.022257
1	2.085452	-1.093891	0.224430
1	2.516259	0.648367	-0.363522
1	1.014465	0.960172	0.692151
1	-1.691836	1.164238	-0.320629
1	-2.447961	-0.428695	-0.607762
1	-2.142709	0.110944	1.045799

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7	0.474274	0.290456	0.109585
7	-0.363358	-0.720847	0.233031
6	1.246322	0.334070	-1.134323
6	-1.378167	-0.125491	0.970074
1	2.166099	0.893493	-0.961327
1	1.459470	-0.694958	-1.432682
1	0.665614	0.820130	-1.923872
1	-1.999125	0.525472	0.354481
1	-1.943420	-0.765446	1.644804
1	-0.333981	0.982573	0.905785
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TS3-3 G3

7	-0.286566	0.669154	-0.457627
7	-0.110834	-0.507698	-0.852646
6	-0.046670	1.265455	0.732114
6	0.287086	-1.400889	0.226602
1	0.251886	0.737597	1.634702
1	-0.492206	2.248336	0.826401
1	0.388402	1.637933	-0.568071
1	1.284582	-1.144605	0.624348
1	-0.413842	-1.384531	1.078444
1	0.320485	-2.412316	-0.176208
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TS3-4 G3

7	0.756769	-0.566847	0.132881
7	-0.631268	-0.734456	0.212685
6	1.405279	0.552530	-0.102823
6	-1.376086	0.474678	-0.085612
1	0.917596	1.521137	-0.106690
1	2.477782	0.476902	-0.223620
1	0.263190	-1.418410	-0.500138
1	-1.236429	1.208297	0.719827
1	-1.043842	0.945778	-1.026387
1	-2.431956	0.212170	-0.151341
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TS3-5 G3

7	0.463166	0.564691	-0.133209
7	-0.591569	-0.411105	-0.079561
6	1.713784	-0.137928	0.141972
6	-1.809424	0.075983	0.110749
1	1.698932	-1.187683	-0.182142
1	1.904527	-0.128108	1.221735
1	2.524893	0.396373	-0.357081
1	-1.943466	1.097786	0.447514
1	-2.649182	-0.577100	-0.077433
1	-0.063043	-0.304700	-1.079534
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n	-0.384009	0.542537	-0.07141
n	0.795687	-0.081603	0.61907
c	-1.555482	-0.343197	-0.07018
c	1.603232	-0.146402	-0.39875
h	-1.817184	-0.60303	0.95589
h	-1.273746	-1.243724	-0.61584
h	-2.392168	0.152234	-0.56523
h	0.32903	0.548365	-1.03318
h	2.569019	-0.595829	-0.12051
h	-0.583194	1.453045	0.35879

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TS5-1	G3		
7	-0.753888	0.049992	-0.676437
7	-0.758005	0.047966	0.672458
6	0.417830	-0.099448	-1.306467
6	0.409784	-0.105687	1.308381
1	1.193287	-0.803578	-0.990175
1	1.232441	0.957555	-0.431096
1	0.395616	0.128478	-2.368408
1	1.184675	-0.810357	0.992060
1	1.229113	0.956118	0.442655
1	0.382434	0.116886	2.371333

Rate Constant by RRKM Calculation

1atm	k_1 (s^{-1}) for CH ₄ Elimination	k_1 (s^{-1}) for Stepwise C—N homolysis
500K	1.15E-07	1.20E-01
600K	4.10E-04	5.80E+01
700K	1.40E-01	3.47E+03
800K	1.05E+01	5.55E+04
900K	2.74E+02	3.70E+05
1000K	3.31E+03	1.35E+06
1500K	1.46E+06	1.83E+07
2000K	7.51E+06	2.40E+07
2500K	1.24E+07	5.59E+07
3000K	1.22E+07	6.08E+07
3500K	7.71E+06	2.56E+07