

Supporting Information

Development and validation of a parameter-free model chemistry for the computation of reliable reaction rates

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Extended Table of results for the HTBH38/08 dataset

Table 1: Theoretical values of the barrier heights for the forward and reverse reactions in the HTBH38/08 and NHTBH38/08 datasets, obtained at different levels of theory. All values (not including zero-point energy and spin-orbit corrections) are in kcal mol⁻¹.

Reaction	forward/reverse barrier height		jChS/QCISD ^e				"best" ^f
	revDSD ^a	CCSD(T)/revDSD ^b	CCSD(T)/QCISD ^c	jChS/revDSD ^d	jChS/QCISD ^e		
c1	H [•] + HCl → H ₂ + Cl [•]	1.27/7.54	5.63/9.07	5.90/9.34	4.97/7.80	5.57/7.95	5.49/7.42 ^g
c2	OH [•] + H ₂ → H ₂ O + H [•]	5.88/20.92	6.04/20.92	5.97/20.84	5.47/21.76	5.38/21.69	5.10/21.20
c3	CH ₃ [•] + H ₂ → CH ₄ + H [•]	11.32/14.36	12.30/14.99	12.29/14.97	11.96/14.64	11.95/14.64	12.10/15.30
c4	H [•] + H ₂ → H ₂ + H [•]	8.96/8.96	10.02/10.02	10.01/10.01	9.58/9.58	9.58/9.58	9.60/9.60
c5	OH [•] + NH ₃ → H ₂ O + NH ₂ [•]	4.67/14.37	4.21/14.29	4.18/14.27	3.93/14.41	3.35/13.85	3.20/12.70
c6	HCl + CH ₃ [•] → Cl [•] + CH ₄	1.09/10.40	2.27/8.39	2.27/8.39	1.69/6.35	1.70/6.77	1.70/7.90
c7	OH [•] + C ₂ H ₆ → H ₂ O + C ₂ H ₅ [•]	4.47/19.97	4.17/19.71	4.03/19.57	3.80/20.91	3.64/20.75	3.40/19.90
c8	F [•] + H ₂ → HF + H [•]	2.77/32.22	2.26/32.76	2.26/32.75	1.69/33.90	1.77/34.00	1.80/33.40
c9	³ O + CH ₄ → OH [•] + CH ₃ [•]	14.60/8.24	15.33/8.42	15.36/8.45	14.55/9.63	14.65/9.62	13.70/8.10
c10	H [•] + PH ₃ → PH ₂ [•] + H ₂	2.61/24.50	3.33/25.90	3.30/25.88	2.85/25.09	2.82/25.05	3.10/23.20
c11	O + HCl → OH [•] + Cl [•]	7.60/10.56	11.67/10.89	11.61/10.81	10.59/10.34	10.63/10.66	9.80/10.40
c12	NH ₂ [•] + CH ₃ [•] → CH ₄ + NH	8.94/21.97	8.69/22.99	8.69/23.01	9.49/22.09	9.50/22.11	8.00/22.40
c13	NH ₂ [•] + C ₂ H ₅ → NH + C ₂ H ₅	9.28/18.81	9.01/19.98	9.43/20.40	9.97/19.08	10.39/19.51	7.50/18.30
c14	NH ₂ [•] + C ₂ H ₆ → NH ₃ + C ₂ H ₅ [•]	11.62/17.43	11.85/17.31	11.83/17.28	11.24/17.85	11.18/17.80	10.40/17.40
c15	NH ₂ [•] + CH ₄ → NH ₃ + CH ₃ [•]	14.11/46.42	14.47/16.59	14.47/16.58	13.82/16.94	13.80/16.92	14.50/17.80
c16	s-trans cis-C ₃ H ₈ → same	39.42/39.42	39.87/39.87	39.87/39.87	39.66/39.66	39.63/39.63	38.40/38.40
c17	H [•] + FH → HF + H [•]	40.68/40.68	42.64/42.64	42.64/42.64	41.99/41.99	42.02/42.02	42.18/42.18
c18	H [•] + FCH ₃ → HF + CH ₃ [•]	30.97/55.29	30.51/57.43	30.47/57.40	30.31/57.54	30.31/57.54	30.38/57.02
c19	H [•] + F ₂ → HF + F [•]	9.32/111.60	5.07/108.93	1.85/105.78	2.38/106.07 ^h	1.49/105.25	2.59/105.77 ⁱ
c20	F ⁻ + CH ₃ F → FCH ₃ + F ⁻	-0.71/-0.71	-0.02/-0.02	-0.04/-0.04	-0.70/-0.70	-0.71/-0.71	-0.34/-0.34
c21	F ⁻ ...CH ₃ F → FCH ₃ ...F ⁻	12.72/12.72	13.53/13.53	13.50/13.50	13.21/13.21	13.20/13.20	13.38/13.38
c22	Cl ⁻ + CH ₃ Cl → ClCH ₃ + Cl ⁻	1.86/1.86	3.11/3.11	3.12/3.12	2.27/2.27	2.33/2.33	3.10/3.10
c23	F ⁻ + CH ₃ Cl → FCH ₃ + Cl ⁻	-12.48/19.02	-11.73/20.09	-11.73/20.08	-12.32/19.29	-12.31/19.31	-12.54/20.11
c24	OH ⁻ ...CH ₃ F → HOCH ₃ ...F ⁻	10.42/47.21	11.18/47.80	11.15/47.76	11.14/47.38	11.14/47.38	10.96/47.20
c25	H [•] + CO → HCO [•]	3.52/23.65	3.74/22.52	3.71/22.50	3.22/22.87	3.19/22.82	3.17/22.68
c26	CH ₃ [•] + C ₂ H ₄ → CH ₃ CH ₂ CH ₂ [•]	7.91/35.57	6.74/32.64	6.61/32.51	6.37/32.77	6.35/32.74	6.85/32.97
	MUE	1.27/2.18 (0.89/2.25)	0.73/0.71 (0.61/0.60)	0.64/0.63 (0.61/0.63)	0.70/0.88 (0.50/0.58)	0.52/0.66 (0.50/0.59)	-
	RMSD	1.91/5.84 (1.02/6.49)	0.99/1.05 (0.82/0.89)	0.85/0.90 (0.84/0.93)	1.04/1.23 (0.74/0.73)	0.80/0.80 (0.81/0.74)	-

^arevDSD-PBEP86-D3(BJ)/jun-cc-pV(T+d)Z;^bCCSD(T)/

jun-cc-pV(T+d)Z//revDSD-PBEP86-D3(BJ)/jun-cc-pV(T+d)Z;^cCCSD(T)/jun-cc-pV(T+d)Z//QCISD/MG3;^djChS on

revDSD-PBEP86-D3(BJ)/jun-cc-pV(T+d)Z optimized geometry;^ejChS on QCISD/MG3 optimized geometry;^fZheng *et al.* *J. Chem. Theory Comput.* 2009, 5, 808–821; ^gCBS-CVH result (this work); the original values were 5.49/7.42; ^hjChS geometry;

the values at the rev-DSD geometry are: 4.46/108.14; ⁱCBS-CVH result (this work): the original values were 2.27/105.80

XYZ geometries

rev-DSD geometries from Table 1

N₂O

3

N	0.00000000	0.00000000	-1.20449800
N	0.00000000	0.00000000	-0.06931700
O	0.00000000	0.00000000	1.11458800

OH

2

O	0.00000000	0.00000000	0.10796800
H	0.00000000	0.00000000	-0.86374100

N₂

2

N	0.00000000	0.00000000	0.55106900
N	0.00000000	0.00000000	-0.55106900

HCl

2

Cl	0.00000000	0.00000000	0.07091900
H	0.00000000	0.00000000	-1.20561900

CH₃

4

C	0.00000000	0.00000000	0.00000100
H	0.00000000	0.00000000	1.07836500
H	0.00000000	0.93388900	-0.53918400
H	0.00000000	-0.93388900	-0.53918400

FCI

2

F	0.00000000	0.00000000	-1.06890300
Cl	0.00000000	0.00000000	0.56589000

CH₃F

5

C	-0.11963200	0.23669900	0.57744300
F	0.14156200	-0.28008900	-0.68329500
H	-0.41636400	-0.58026000	1.23539400
H	0.78523800	0.71418400	0.95372800
H	-0.92513700	0.96668400	0.49587700

Cl⁻...CH₃Cl

6

Cl	0.00021800	2.37466100	0.00000000
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C	0.00000000	0.55243500	0.00000000
H	1.02753300	0.21197500	0.00000000
H	-0.51382900	0.21215200	0.88990200
H	-0.51382900	0.21215200	-0.88990200
Cl	-0.00021000	-2.60706600	0.00000000

F⁻...CH₃Cl

6

Cl	0.00000000	0.00000000	1.62730400
C	0.00000000	0.00000000	-0.22587400
H	0.00000000	1.02932800	-0.55203400
H	0.89142400	-0.51466400	-0.55203400
H	-0.89142400	-0.51466400	-0.55203400
F	0.00000000	0.00000000	-2.73920200

FCH₃...Cl⁻

6

F	0.00011000	2.64364200	0.00000000
C	0.00000000	1.22601700	0.00000000
H	1.02766800	0.87517100	0.00000000
H	-0.51387800	0.87528800	0.89000800
H	-0.51387800	0.87528800	-0.89000800
Cl	-0.00005300	-1.98674300	0.00000000

OH⁻

2

O	0.00000000	0.00000000	0.10741400
H	0.00000000	0.00000000	-0.85931500

HOCH₃

6

C	-0.04671600	0.66506200	0.00000000
O	-0.04671600	-0.75718100	0.00000000
H	-1.08963800	0.97778100	0.00000000
H	0.86530900	-1.05817500	0.00000000
H	0.43917800	1.07373600	0.89160500
H	0.43917800	1.07373600	-0.89160500

HN₂

3

N	-0.06194600	0.65702500	0.00000000
N	-0.06194600	-0.51361200	0.00000000
H	0.86725100	-1.00388900	0.00000000

C₂H₄

6

C	0.00000000	0.00000000	0.66586300
C	0.00000000	0.00000000	-0.66586300

H	0.00000000	0.92390200	1.23192700
H	0.00000000	-0.92390200	1.23192700
H	0.00000000	0.92390200	-1.23192700
H	0.00000000	-0.92390200	-1.23192700

C₂H₅

7

C	0.79370900	0.00000000	-0.02223600
C	-0.69434100	0.00000000	-0.00075100
H	-1.10385100	0.88509600	-0.49249500
H	1.34818600	-0.92501100	0.04802900
H	-1.08488000	0.00000400	1.02685000
H	-1.10385100	-0.88510000	-0.49248700
H	1.34818600	0.92501100	0.04802900

HCN

3

C	0.00000000	0.00000000	-0.50248700
N	0.00000000	0.00000000	0.65497200
H	0.00000000	0.00000000	-1.56988000

HNC

3

C	0.00000000	0.00000000	-0.74075100
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N	0.00000000	0.00000000	0.43090100
H	0.00000000	0.00000000	1.42820500

CH₄

5

H	0.00000000	0.00000000	1.08935100
C	0.00000000	0.00000000	0.00000100
H	0.00000000	1.02704900	-0.36311900
H	0.88945000	-0.51352400	-0.36311900
H	-0.88945000	-0.51352400	-0.36311900

H₂O

3

H	0.00000000	0.75969600	-0.47089100
O	0.00000000	0.00000000	0.11772300
H	0.00000000	-0.75969600	-0.47089100

H₂

2

H	0.00000000	0.00000000	0.37111100
H	0.00000000	0.00000000	-0.37111100

H₂S

3

S	0.00000000	0.00000000	0.10283900
H	0.00000000	0.96667600	-0.82271600
H	0.00000000	-0.96667600	-0.82271600

HS

2

S	0.00000000	0.00000000	0.07895200
H	0.00000000	0.00000000	-1.26323400

TS a1

4

H	-0.28672400	-1.90580400	0.00000000
O	-0.84331200	-0.64877200	0.00000000
N	0.00000000	0.25005100	0.00000000
N	1.00474500	0.76366000	0.00000000

TS a2

3

H	0.00000000	0.00000000	1.47241200
Cl	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	-1.47241200

TS a3

6

Cl	-0.01883600	-0.16267900	-1.42378200
F	0.00423300	0.03653300	0.31971100
C	0.03087500	0.26668400	2.33406700
H	0.46724300	1.25305400	2.32376700
H	-1.03483100	0.16734500	2.46768800
H	0.66444700	-0.58375300	2.53103100

TS a4

6

Cl	0.00223800	0.07207200	2.31171800
C	0.00004200	0.00000200	0.00000000
H	1.07057500	0.03261400	-0.00205800
H	-0.50693500	-0.94296300	0.02989200
H	-0.56350400	0.91035700	-0.02783400
Cl	-0.00226100	-0.07207300	-2.31171800

TS a5

6

F	-0.00000600	2.53726300	0.00000000
C	0.00000000	0.48884500	0.00000000
H	1.06442400	0.61446100	0.00000000
H	-0.53221200	0.61445500	0.92181900
H	-0.53221200	0.61445500	-0.92181900

C1	0.00000300	-1.62422400	0.00000000
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TS a6

7

F	1.85894200	-0.01120900	0.00000000
C	0.09868900	0.00683800	0.00000000
H	0.03897700	1.07773800	-0.00000200
H	0.03933100	-0.52279000	-0.93079900
H	0.03933100	-0.52278700	0.93080100
O	-1.90573700	0.10540100	0.00000000
H	-2.19435100	-0.81551500	0.00000000

TS a7

3

N	0.08169700	-0.64381200	0.00000000
N	0.08169700	0.47395400	0.00000000
H	-1.14375200	1.18900300	0.00000000

TS a8

7

C	0.56786200	0.00000000	-0.21084400
C	-0.74556700	0.00000000	0.03764800
H	1.44928100	-0.00000200	1.50772900
H	1.10461300	-0.92212500	-0.39688400

H	1.10461200	0.92212600	-0.39688200
H	-1.29613900	0.92392700	0.16260900
H	-1.29613900	-0.92392700	0.16260700

TS a9

3

C	0.08061200	0.61925400	0.00000000
N	0.08061200	-0.56884400	0.00000000
H	-1.04796200	0.26638400	0.00000000

TS a10

7

C	1.21493800	-0.00887100	0.00002100
O	-1.30325700	0.10924900	0.00000400
H	0.01803300	0.12353700	0.00018100
H	1.47468900	-0.53859200	0.91255000
H	1.47250600	-0.56262700	-0.89876100
H	1.59400300	1.01016400	-0.01409000
H	-1.42280200	-0.85324600	-0.00003900

TS a11

3

H	0.66994500	-0.41203400	0.00000000
O	0.00000000	0.28747500	0.00000000
H	-0.66994500	-1.88776200	0.00000000

TS a12

4

H	1.26507000	-0.21794900	0.00000000
S	0.00000000	0.22302700	0.00000000
H	-0.49484900	-1.11057200	0.00000000
H	-0.77022100	-2.23991800	0.00000000

rev-DSD geometries from Table 2

HF

2

F	0.00000000	0.00000000	0.09210800
H	0.00000000	0.00000000	-0.82896800

F₂

2

F	0.00000000	0.00000000	0.70105300
F	0.00000000	0.00000000	-0.70105300

F⁻...CH₃F

6

F	-0.00025200	1.85774300	0.00000000
C	0.00000000	0.42346500	0.00000000

H	1.02703500	0.07809000	0.00000000
H	-0.51342300	0.07780600	0.88938100
H	-0.51342300	0.07780600	-0.88938100
F	0.00023100	-2.16602000	0.00000000

CH₃Cl

5

C	0.00000000	-1.12712700	0.00000000
Cl	0.00000000	0.65728000	0.00000000
H	1.03070500	-1.47033300	0.00000000
H	-0.51535200	-1.47033500	0.89261600
H	-0.51535200	-1.47033500	-0.89261600

OH⁻...CH₃F

7

F	-1.91031200	-0.06570700	0.00000400
C	-0.49045200	0.09360600	-0.00000500
H	-0.07922800	-0.37683200	0.88573100
H	-0.07923300	-0.37693100	-0.88569100
H	-0.27063400	1.15670800	-0.00006500
O	2.18342400	-0.07592400	-0.00000300
H	3.09722800	0.23417100	0.00004500

HOCH₃...F⁻

7

C	-1.30881600	-0.38528200	0.00000000
O	-0.47349300	0.72499800	0.00000000
H	-2.36139800	-0.06245400	-0.00001500
H	-1.16521500	-1.03114400	-0.88476000
H	-1.16523600	-1.03112900	0.88477400
H	0.52803100	0.35447000	0.00000100
F	1.75607300	-0.19089300	0.00000000

CO

2

O	0.00000000	0.00000000	0.48547300
C	0.00000000	0.00000000	-0.64729700

HCO

3

H	-0.85895000	1.22445300	0.00000000
C	0.06135400	0.58622500	0.00000000
O	0.06135400	-0.59272500	0.00000000

CH₃CH₂CH₂

10

C	1.20801100	-0.28741000	0.00006100
C	-0.06699700	0.57684200	-0.00006100

C	-1.31352300	-0.23961300	-0.00001100
H	1.24057100	-0.92923200	0.88298600
H	1.24059800	-0.92943600	-0.88271600
H	2.10233700	0.34062600	0.00000000
H	-0.04842000	1.22813100	-0.87902300
H	-0.04847400	1.22832900	0.87875100
H	-1.72595200	-0.61836100	0.92552200
H	-1.72560200	-0.61896800	-0.92545300

TS NHT1

3

H	0.00000000	0.00000000	1.13917200
F	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	-1.13917200

TS NHT2

6

H	-0.58871400	-0.83945800	1.70578700
F	-0.22493300	-0.32073100	0.65173200
C	0.26709400	0.38085000	-0.77389300
H	-0.52726100	1.08632400	-0.97600700
H	1.21871800	0.81869900	-0.50511600
H	0.31908900	-0.46408500	-1.44689100

TS NHT3

3

H	0.00000000	0.00000000	-2.15146300
F	0.00000000	0.00000000	-0.58150700
F	0.00000000	0.00000000	0.82055800CH3CH2CH2

TS NHT4

6

F	0.00146400	0.05174800	1.83052400
C	0.00000000	0.00000300	0.00000000
H	0.01227600	-1.07142600	0.03027900
H	-0.93439200	0.52511100	-0.01409800
H	0.92211700	0.54632400	-0.01618200
F	-0.00146400	-0.05175000	-1.83052400

TS NHT5 same as TS NHT4

TS NHT6 same as TS a4

TS NHT7 same as TS a5

TS NHT8 same as TS a6

TS NHT9

3

H	-1.55294800	1.39709400	0.00000000
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C	0.11092500	0.54987900	0.00000000
O	0.11092500	-0.58704600	0.00000000

TS NHT10

10

C	-0.47567100	0.64170500	0.00000000
C	-1.37852700	-0.36149500	0.00000000
H	-0.22646300	1.15659100	-0.91922400
H	-0.22646300	1.15659100	0.91922400
H	-1.72825800	-0.80471700	0.92392800
H	-1.72825800	-0.80471700	-0.92392800
C	1.61125700	-0.24084300	0.00000000
H	2.18972000	0.67457000	-0.00000100
H	1.58868000	-0.80726300	-0.92055800
H	1.58868100	-0.80726100	0.92055900

rev-DSD geometries from Table 3

NH₃

4

N	0.00000000	0.00000000	0.11448400
H	0.00000000	0.93911400	-0.26712900
H	0.81329700	-0.46955700	-0.26712900
H	-0.81329700	-0.46955700	-0.26712900

NH₂

3

N	0.00000000	0.00000000	0.14168900
H	0.00000000	0.80311100	-0.49591000
H	0.00000000	-0.80311100	-0.49591000

C₂H₆

8

C	-0.04827700	-0.18287700	-0.73954500
C	0.04827700	0.18287700	0.73954500
H	1.08142200	0.14022000	1.09087900
H	0.32210000	-1.19391600	-0.92193700
H	-0.53946000	-0.50125800	1.35531200
H	-0.32209500	1.19391700	0.92193600
H	-1.08142300	-0.14022600	-1.09087700
H	0.53945600	0.50126200	-1.35531200

PH₃

4

P	0.00000000	0.00000000	0.12703000
H	0.00000000	1.19265400	-0.63515200
H	1.03286900	-0.59632700	-0.63515200
H	-1.03286900	-0.59632700	-0.63515200

PH₂

3

P	0.00000000	0.00000000	0.11591300
H	0.00000000	1.02116400	-0.86935100
H	0.00000000	-1.02116400	-0.86935100

NH

2

N	0.00000000	0.00000000	0.12948000
H	0.00000000	0.00000000	-0.90636200

TS HT1

3

H	0.00000000	0.00000000	-2.21052500
H	0.00000000	0.00000000	-1.22601200
Cl	0.00000000	0.00000000	0.20214900

TS HT2

4

O	0.30472300	-0.10771900	-0.00001100
H	0.42755600	0.85550300	0.00003000
H	-1.04029200	-0.11694900	0.00001500
H	-1.82504600	0.12319700	0.00004100

TS HT3

6

C	0.00000000	0.26867500	0.00000000
H	1.05620400	0.51471000	0.00000000
H	-0.52810300	0.51470700	0.91470000
H	-0.52810300	0.51470700	-0.91470000
H	0.00000100	-1.13209900	0.00000000
H	0.00000100	-2.02407300	0.00000000

TS HT4

3

H	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	0.92695800
H	0.00000000	0.00000000	-0.92695800

TS HT5

6

N	-1.15209900	-0.05370300	-0.09360700
O	1.18186400	-0.08933100	-0.01417400
H	-1.26785000	-0.46768800	0.82852200
H	-1.31832100	0.94522700	0.00824800
H	-0.08940900	-0.20128300	-0.38389300
H	1.28535900	0.81431200	0.31576300

TS HT6

6

C	0.27345300	0.53814400	1.71911200
H	1.18480100	1.11418200	1.61229600
H	0.36219700	-0.41711300	2.22249500
H	-0.63382700	1.10001000	1.90601700
H	0.06285700	0.12370200	0.39516800
Cl	-0.15392600	-0.30292000	-0.96768500

TS HT7

10

C	1.47328000	-0.44609800	0.02563600
C	0.47467600	0.69211600	-0.02785600
O	-1.87944100	-0.31389300	-0.05246800
H	1.31244600	-1.06992600	0.90604800
H	1.39457600	-1.08058000	-0.85839200
H	2.49526300	-0.05792800	0.07022600
H	0.47764800	1.31793300	0.86494500
H	0.55504300	1.30827400	-0.92361200
H	-0.60420500	0.21557900	-0.08961400
H	-2.28297800	0.40169000	0.46346300

TS HT8

3

H	0.25006300	-1.14652900	0.00000000
F	0.00000000	0.32045700	0.00000000
H	-0.25006300	-1.73758100	0.00000000

TS HT9

6

C	0.00070000	0.02702100	-1.04395900
H	0.02709100	1.09726200	-1.20666900
H	-0.93520300	-0.47795800	-1.24809300
H	0.91059400	-0.52346500	-1.24803300
H	-0.00011900	-0.00460100	0.17787000
O	-0.00082000	-0.03167000	1.22358500

TS HT10

5

P	0.21701600	0.00000000	-0.11225000
H	0.26709200	1.03090500	0.85756000
H	0.26710300	-1.03090000	0.85756600
H	-1.25861200	-0.00000600	-0.13528400
H	-2.53082800	0.00000000	0.10390800

TS HT11

3

Cl	0.01825000	-0.81940600	0.00000000
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H	-0.45624300	0.54463300	0.00000000
O	0.01825000	1.67315800	0.00000000

TS HT12

7

C	-1.19384500	-0.01136400	0.00000000
N	1.39551200	0.13004100	0.00000000
H	-1.41734100	-0.55411600	0.91283500
H	-1.41733800	-0.55424000	-0.91276200
H	-1.51925300	1.02403300	-0.00007100
H	0.18284400	0.13055300	-0.00000200
H	1.56556800	-0.88833300	0.00000000

TS HT13

10

C	-1.39822200	-0.44485300	0.00000700
C	-0.42981900	0.71044700	-0.00000700
N	1.92687300	-0.37397900	-0.00001200
H	-1.26525300	-1.07213000	-0.88327800
H	-1.26525600	-1.07210700	0.88330800
H	-2.43389900	-0.08725300	0.00000000
H	-0.42060700	1.31739800	-0.90360100
H	-0.42060400	1.31741800	0.90357300
H	0.79556000	0.12926300	-0.00001100
H	2.49019000	0.49170600	0.00009600

TS HT14

11

C	-1.48924100	-0.44549000	-0.00002400
C	-0.50065600	0.69814200	0.00003400
N	1.86779000	-0.34239400	-0.00005300
H	-1.36205900	-1.07527800	-0.88238900
H	-1.36204600	-1.07538100	0.88226600
H	-2.51959400	-0.07454500	0.00000700
H	-0.51794200	1.31445400	-0.89830500
H	-0.51792100	1.31434700	0.89844600
H	0.65349300	0.14703500	-0.00003100
H	2.24555100	0.16537200	-0.80475500
H	2.24536700	0.16484100	0.80507100

TS HT15

8

C	-1.25631100	0.00000000	0.01233800
N	1.31177600	0.00000000	-0.13801200
H	-1.58551200	0.90751000	-0.48687700
H	-1.45412000	-0.00006900	1.08014300
H	-1.58552500	-0.90744000	-0.48699700
H	0.03417400	-0.00000100	-0.15929300
H	1.47320600	0.80546000	0.47253900
H	1.47320700	-0.80545900	0.47254000

TS HT16

13

C	-1.30158100	-0.90607500	-0.02048200
C	-1.20775300	0.50665300	-0.01259500
C	0.00000000	1.18410000	0.15328400
C	1.20775300	0.50665300	-0.01259500
C	1.30158100	-0.90607400	-0.02048200
H	2.17093600	-1.32925400	-0.52016100
H	1.03576900	-1.45554500	0.87644200
H	2.03901900	1.08789900	-0.40199500
H	-0.00000100	2.26603000	0.08622200
H	-2.03901900	1.08789700	-0.40199500
H	-2.17093400	-1.32925600	-0.52016100
H	0.00000000	-1.18376800	-0.51757100
H	-1.03576700	-1.45554500	0.87644200

jChS geometries from Table 4

HCl

2

H	0.00000000	0.00000000	0.00000000
Cl	0.00000000	0.00000000	1.27415090

H₂

2

H	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	0.74097310

OH

2

O	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	0.96809910

NH₃

4

N	-0.00000322	0.11355682	-0.00000557
H	-0.46818172	-0.26495985	0.81102387
H	-0.46825389	-0.26497806	-0.81098485
H	0.93645813	-0.26495985	-0.00000000

H₂O

3

O	0.00000000	0.00000000	-0.11712295
H	-0.75600683	0.00000000	0.46849179
H	0.75600683	0.00000000	0.46849179

NH₂

3

N	0.00000000	0.00000000	-0.14126973
H	-0.80120657	0.00000000	0.49444406
H	0.80120657	0.00000000	0.49444406

CH₄

5

C	0.00000000	0.00000000	0.00000000
H	-0.00000000	-0.00000000	1.08556369
H	-0.00000000	-1.02347927	-0.36185456
H	-0.88635904	0.51173963	-0.36185456
H	0.88635904	0.51173963	-0.36185456

CH₃

4

C	0.00000000	0.00000000	-0.00000000
H	0.00000000	1.07554100	0.00000000
H	0.93144583	-0.53777050	0.00000000
H	-0.93144583	-0.53777050	0.00000000

PH₃

4

P	0.00000000	0.00000000	-0.12746980
H	0.00000000	1.18641086	0.63734902

H	-1.02746195	-0.59320543	0.63734902
H	1.02746195	-0.59320543	0.63734902

PH₂

3

P	0.00000000	-0.00000000	-0.11573335
H	-1.01728832	0.00000000	0.86800012
H	1.01728832	0.00000000	0.86800012

NH

2

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.03484400

TS HT1

3

H	0.00000000	0.00000000	-2.21125700
H	0.00000000	0.00000000	-1.22280300
Cl	0.00000000	0.00000000	0.20200400

TS HT5

6

N	-1.14133900	-0.05189400	-0.09534500
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H	-1.26271400	-0.48497400	0.81430000
H	-1.30792100	0.94205900	0.02696700
H	-0.05845900	-0.19831900	-0.38949500
O	1.17013500	-0.08908700	-0.01122900
H	1.25738400	0.81718500	0.30547300

TS HT9

6

C	0.00034300	-1.13919300	0.00000000
H	0.00874600	0.14688000	0.00000000
O	0.00034300	1.35985100	0.00000000
H	-1.05392000	-1.38394200	0.00000000
H	0.52018500	-1.40329300	0.91109300
H	0.52018500	-1.40329300	-0.91109300

TS HT10

5

P	0.00000000	0.24569100	0.00000000
H	0.70361700	-1.04668400	0.00000000
H	1.05247100	-2.29895300	0.00000000
H	-0.87804400	-0.16986600	1.02573000
H	-0.87804400	-0.16986600	-1.02573000

TS HT11

3

C1	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.43913970
O	0.86437469	0.00000000	2.32106356

TS HT12

7

C	0.05344200	-1.19631300	0.00000000
H	0.12640200	0.19798400	0.00000000
N	0.05344200	1.40089400	0.00000000
H	1.10298000	-1.45851400	0.00000000
H	-0.97157100	1.50765300	0.00000000
H	-0.47628100	-1.43775300	0.91173100
H	-0.47628100	-1.43775300	-0.91173100

rev-DSD geometries from Table 5

BHPERI R1

10

H	-0.88933800	1.23994800	-1.14081100
C	0.00000000	0.78409000	-0.69990000
C	0.00000000	-0.78409000	-0.69990000
C	0.00000000	0.67117100	0.81343900
C	0.00000000	-0.67117100	0.81343900
H	0.88933800	-1.23994800	-1.14081100
H	0.00000000	-1.41595200	1.60038800

H	0.88933800	1.23994800	-1.14081100
H	-0.88933800	-1.23994800	-1.14081100
H	0.00000000	1.41595200	1.60038800

TS b1

10

H	1.27301700	-1.44172100	-1.10516200
C	0.40152100	-0.99226500	-0.62626700
C	-0.40152100	0.99226500	-0.62626700
C	0.40152100	-0.55817900	0.73335500
C	-0.40152100	0.55817900	0.73335500
H	-1.27301700	1.44172100	-1.10516200
H	-0.98738100	0.98632400	1.53989800
H	-0.54430000	-1.25769500	-1.07726700
H	0.54430000	1.25769500	-1.07726700
H	0.98738100	-0.98632400	1.53989800

BHPERI P1

10

C	1.84275400	-0.11077100	-0.00000200
C	0.60637600	0.40386500	0.00000200
C	-0.60637600	-0.40386500	0.00000200
H	0.47352100	1.48270500	0.00000300
H	-0.47352100	-1.48270500	0.00000300
C	-1.84275400	0.11077100	-0.00000100

H	-2.00274600	1.18355400	-0.00000500
H	2.71995900	0.52340700	-0.00000200
H	2.00274600	-1.18355400	-0.00000500
H	-2.71995900	-0.52340700	-0.00000300

CRBH R1

8

C	1.06711200	-0.35628800	0.02744700
C	-1.09659400	-0.25354600	0.11379200
O	-0.55726500	1.03239300	-0.12511300
N	0.85640800	0.90121500	0.06249000
H	-1.42013700	-0.35532400	1.15741100
H	-1.90077400	-0.45361100	-0.59085000
H	2.04476800	-0.80751600	0.07410000
O	-0.01046200	-1.16152500	-0.11557800

TS b2

8

C	1.18878600	0.17279700	0.05659200
C	-1.51142200	-0.57461900	0.26464800
O	-1.25146200	0.43616900	-0.37077200
N	0.38323900	1.16845800	0.14877800
H	-0.93220400	-0.86617200	1.14376100
H	-2.35815000	-1.19375600	-0.05146800
H	2.01938400	0.91887600	0.38734900

0	1.31697700	-1.01457100	-0.18529400
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CRBH P1

4

0	1.21281500	0.01229700	-0.00000100
H	-1.82074500	0.63530400	-0.00000100
N	-1.16405800	-0.12648800	-0.00000100
C	0.04443900	0.02529000	0.00000200

CRBH R4

8

C	-0.01983800	1.20834800	0.09805900
C	-0.10581400	-1.20379700	0.19680500
0	-1.30456200	-0.56346400	-0.21620800
N	-1.23817300	0.82239400	0.03382200
S	1.23627200	0.00058400	-0.08428700
H	-0.15266800	-1.45043300	1.26166300
H	0.02883100	-2.09373700	-0.41349000
H	0.20111100	2.25847600	0.22415200

TS b3

8

C	0.53610600	0.90733200	0.04937200
C	-1.17508300	-1.06840300	0.22993200

O	-1.71371100	-0.08553300	-0.29173300
N	-0.55374900	1.50338000	0.08660300
S	1.40328000	-0.48420800	-0.06686400
H	-0.93805200	-1.09060800	1.29857800
H	-1.06856700	-2.00061500	-0.33789800
H	0.97392800	1.96558000	0.16097000

CRBH P4

4

H	-2.43180800	0.57139700	0.00000000
N	-1.69356100	-0.11046100	0.00000000
C	-0.49322700	0.01458800	0.00000100
S	1.07788100	0.00714400	0.00000000

CH₂O

4

C	-0.53090900	0.00000000	0.00000000
O	0.67628200	0.00000000	0.00000000
H	-1.11240200	-0.93854600	0.00000100
H	-1.11240000	0.93854700	0.00000100

CADBH R1

3

N	0.00000000	0.00000000	-1.20449800
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N	0.00000000	0.00000000	-0.06931700
O	0.00000000	0.00000000	1.11458800

TS b4

9

C	0.77409400	-1.15620000	0.00000000
C	-0.61241800	-1.25132500	0.00000000
O	-1.12824800	0.72531500	0.00000000
N	0.00000000	1.22488000	0.00000000
N	1.10163000	0.80273100	0.00000000
H	1.32112000	-1.33253200	0.91714300
H	1.32112000	-1.33253200	-0.91714300
H	-1.14886100	-1.44279000	0.91946700
H	-1.14886100	-1.44279000	-0.91946700

CADBH P1

9

C	0.43426000	1.10542700	-0.05649000
C	1.15240000	-0.23361800	0.06657300
O	0.08660700	-1.19324400	-0.07101100
N	-1.14111300	-0.48722200	0.02056000
N	-0.99428000	0.72864100	0.04830900
H	0.66903000	1.81700600	0.73261700
H	0.56868900	1.59516200	-1.02221900
H	1.62235200	-0.37242400	1.04180500

H	1.87485500	-0.41457900	-0.72669800
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CADBH R4

4

C	0.00000000	0.00000000	-1.18283000
H	0.00000000	0.00000000	-2.24409100
N	0.00000000	0.00000000	-0.01763800
O	0.00000000	0.00000000	1.18306700

TS b5

10

C	0.71356300	-1.31978900	0.00000000
C	-0.65459700	-1.37172200	0.00000000
O	-1.16503100	0.90438300	0.00000000
N	0.00000000	1.25943500	0.00000000
C	1.12682200	0.79168800	0.00000000
H	1.26165900	-1.48377800	0.92045500
H	1.26165900	-1.48377800	-0.92045500
H	-1.21240700	-1.45882600	0.92243900
H	-1.21240700	-1.45882600	-0.92243900
H	2.10701500	1.23303400	0.00000000

CADBH P4

10

C	0.31041400	1.18534400	-0.09470600
C	1.17022200	-0.05889600	0.11507200
O	0.27740200	-1.17556100	-0.11390100
N	-1.04141900	-0.72276400	0.02739700
C	-1.04605600	0.55487300	0.05849900
H	0.50331700	1.96699700	0.63963100
H	0.41560900	1.61933800	-1.09339200
H	1.53745000	-0.12207800	1.14348800
H	2.00055700	-0.15759100	-0.58125100
H	-1.99369400	1.06924500	0.13776400

C₂H₄

6

H	0.00000000	0.92390300	1.23192600
C	0.00000000	0.00000000	0.66586300
C	0.00000000	0.00000000	-0.66586300
H	0.00000000	-0.92390300	-1.23192600
H	0.00000000	-0.92390300	1.23192600
H	0.00000000	0.92390300	-1.23192600

PXBH R1

16

H	-0.56885700	1.70111300	0.00005300
H	1.70111300	0.56885700	-0.00005300
H	1.94101600	-2.07980100	-0.81088800

H	-1.94101600	2.07980100	-0.81088800
H	2.07980100	1.94101600	0.81088800
H	0.56885700	-1.70111300	0.00005300
H	-1.70111300	-0.56885700	-0.00005300
H	-2.07980100	-1.94101600	0.81088800
N	1.58545400	1.58545400	-0.00010100
N	-1.58545400	1.58545400	0.00010100
N	1.58545400	-1.58545400	0.00010100
N	-1.58545400	-1.58545400	-0.00010100
H	1.94092700	-2.07964000	0.81122700
H	2.07964000	1.94092700	-0.81122700
H	-1.94092700	2.07964000	0.81122700
H	-2.07964000	-1.94092700	-0.81122700

TS b6

16

H	1.41516600	0.30742700	0.00000000
H	0.47203800	-1.45181800	0.00000000
H	-1.51896900	0.15313700	0.00000000
H	0.00000000	1.44815700	0.00000000
H	1.49446500	1.85390800	0.82111800
H	1.97444700	-1.68834100	-0.81211100
H	-1.54631000	-1.91818800	0.80075200
H	-2.06887200	1.57118200	-0.81211300
N	1.12021200	1.38964800	0.00000000
N	-1.14883700	-1.42513900	0.00000000

N	1.56138300	-1.24047300	0.00000000
N	-1.54357200	1.26253200	0.00000000
H	-2.06887200	1.57118200	0.81211300
H	-1.54631000	-1.91818800	-0.80075200
H	1.97444700	-1.68834100	0.81211100
H	1.49446500	1.85390800	-0.82111800

BHDIV R2

12

C	-0.35454300	-0.48817800	2.24342900
C	0.35454300	0.48817800	2.24342900
C	1.37619600	2.27050400	-1.30902500
C	0.35454300	1.75015600	-0.93233700
C	-1.37619600	-2.27050400	-1.30902500
C	-0.35454300	-1.75015600	-0.93233700
H	-0.97732600	-1.35114500	2.23026800
H	0.97732600	1.35114500	2.23026800
H	2.27389600	2.73099500	-1.64712300
H	-0.54125600	1.28282900	-0.59555000
H	-2.27389600	-2.73099500	-1.64712300
H	0.54125600	-1.28282900	-0.59555000

TS b7

12

C	0.28006900	1.73863800	0.00110500
---	------------	------------	------------

C	1.34718200	1.12805100	-0.09165800
C	1.36868900	-1.10193700	0.09280100
C	0.31387200	-1.73300600	-0.00330500
C	-1.64928900	-0.62459300	-0.09502000
C	-1.66085700	0.59283900	0.09607500
H	-0.30584400	2.62717000	0.02683200
H	2.40181000	1.08012700	-0.23080200
H	2.42187700	-1.03358000	0.23427900
H	-0.25469000	-2.63261800	-0.03267500
H	-2.11586300	-1.56605900	-0.26576700
H	-2.14528400	1.52500700	0.26814400

BHDIV P2

12

C	-0.35454300	-0.48817800	2.24342900
C	0.35454300	0.48817800	2.24342900
C	1.37619600	2.27050400	-1.30902500
C	0.35454300	1.75015600	-0.93233700
C	-1.37619600	-2.27050400	-1.30902500
C	-0.35454300	-1.75015600	-0.93233700
H	-0.97732600	-1.35114500	2.23026800
H	0.97732600	1.35114500	2.23026800
H	2.27389600	2.73099500	-1.64712300
H	-0.54125600	1.28282900	-0.59555000
H	-2.27389600	-2.73099500	-1.64712300
H	0.54125600	-1.28282900	-0.59555000

MESS input files

H[•] + CO

jChS

```
!*****
!           GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]          50 100 200 300 500 700 1000 1500 2000 2500 3000 3500 4000
PressureList[atm]          0.5 1
!
!
EnergyStepOverTemperature   .2
ExcessEnergyOverTemperature 30
ModelEnergyLimit [kcal/mol] 400
!
CalculationMethod          direct
!
WellCutoff                 20
ChemicalEigenvalueMax      0.2
!
ReductionMethod            diagonalization
!
AtomDistanceMin[bohr]      1.3
!!
RateOutput                 jChS.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!           MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation
  Exponential
    Factor[1/cm]           260
    Power                   0.875
    ExponentCutoff         10
  End
!
  CollisionFrequency
  LennardJones
    Epsilons[K]            90.58 617.0
    Sigmas[angstrom]       3.54 5.62
    Masses[amu]            39.948 69.0
  End
!
```

```

!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS
!*****

Bimolecular REACS
Fragment REACT1
RRHO
Geometry[angstrom]      2
C          0.00000000    0.00000000   -0.64729900
O          0.00000000    0.00000000    0.48547400
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies [1/cm]      1
2159.29
ZeroEnergy[kcal/mol]    0.
ElectronicLevels [1/cm]      1
  0      1
!*****
End
!*****
Fragment REACT2
Atom
Name H
ElectronicLevels [1/cm]      1
  0      2
!*****
End
!*****
GroundEnergy[kcal/mol] 0.0
End
Well HCO
Species
RRHO ! well
Geometry[angstrom]      3
H          -0.85891600    1.22453100    0.00000000
C          0.06135100    0.58622300    0.00000000
O          0.06135100   -0.59273400    0.00000000
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies [1/cm]      3
1118.88
1898.84
2722.82
ZeroEnergy[kcal/mol]   -14.72
ElectronicLevels [1/cm]      1
  0.0000000000000000    2.0000000000000000
End
End
!*****

```

```

Barrier TS REACS HCO
RRHO      !
Geometry[angstrom]      3
H          -1.55075700    1.39879200    0.00000000
C          0.11076800    0.54977800    0.00000000
O          0.11076800   -0.58718200    0.00000000

Core RigidRotor
      SymmetryFactor  1
End

Tunneling Eckart
ImaginaryFrequency[1/cm]  786.26
WellDepth[kcal/mol]      3.67
WellDepth[kcal/mol]      18.39
End

Frequencies[1/cm]        2
387.45
2116.64
ZeroEnergy[kcal/mol]     3.67
ElectronicLevels[1/cm]   1
0.000000000000000000    2.000000000000000000
End
End

```

CBS-CVH

```

!*****
!          GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]  50 100 200 300 500 700 1000 1500 2000 2500 3000 3500 4000
PressureList[atm]           0.5 1
!
!
EnergyStepOverTemperature      .2
ExcessEnergyOverTemperature    30
ModelEnergyLimit[kcal/mol]     400
!
CalculationMethod              direct
!
WellCutoff                     20
ChemicalEigenvalueMax          0.2
!
ReductionMethod                diagonalization
!
AtomDistanceMin[bohr]          1.3
!!
RateOutput                     HEATlike.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

!*****
!           MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation
    Exponential
      Factor[1/cm]           260
      Power                   0.875
      ExponentCutoff         10
    End
!
  CollisionFrequency
    LennardJones
      Epsilons[K]            90.58  617.0
      Sigmas[angstrom]       3.54   5.62
      Masses[amu]            39.948  69.0
    End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS
!*****

Bimolecular REACS
Fragment REACT1
RRHO
Geometry[angstrom]         2
C          0.00000000    0.00000000   -0.64729900
O          0.00000000    0.00000000    0.48547400

Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies[1/cm]        1
2159.29
  ZeroEnergy[kcal/mol]     0.
  ElectronicLevels[1/cm]   1
  0          1
!*****
End
!*****
Fragment REACT2
Atom
Name H
ElectronicLevels[1/cm]    1
  0          2
!*****
End
!*****

```

```

GroundEnergy[kcal/mol] 0.0
End
Well HCO
Species
RRHO ! well
Geometry[angstrom] 3
H -0.85891600 1.22453100 0.00000000
C 0.06135100 0.58622300 0.00000000
O 0.06135100 -0.59273400 0.00000000
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 3
1118.88
1898.84
2722.82
ZeroEnergy[kcal/mol] -14.64
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
End
!*****
Barrier TS REACS HCO
RRHO !
Geometry[angstrom] 3
H -1.55075700 1.39879200 0.00000000
C 0.11076800 0.54977800 0.00000000
O 0.11076800 -0.58718200 0.00000000
Core RigidRotor
SymmetryFactor 1
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 786.26
WellDepth[kcal/mol] 3.70
WellDepth[kcal/mol] 18.34
End
Frequencies[1/cm] 2
387.45
2116.64
ZeroEnergy[kcal/mol] 3.70
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
End

```

CBS-QB3

```

!*****
! GLOBAL SECTION
!*****

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K] 50 100 200 300 500 700 1000 1500 2000 2500 3000 3500 4000
PressureList[atm]          0.5 1
!
!
EnergyStepOverTemperature      .2
ExcessEnergyOverTemperature    30
ModelEnergyLimit[kcal/mol]     400

CalculationMethod              direct

WellCutoff                     20
ChemicalEigenvalueMax          0.2

ReductionMethod                 diagonalization
AtomDistanceMin[bohr]          1.3
!!
RateOutput                      CBSQB3.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!
!           MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation
    Exponential
      Factor[1/cm]              260
      Power                     0.875
      ExponentCutoff            10
    End
!
  CollisionFrequency
    LennardJones
      Epsilons[K]               90.58 617.0
      Sigmas[angstrom]          3.54 5.62
      Masses[amu]               39.948 69.0
    End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!
! REACTANTS
!*****

Bimolecular REACS
Fragment REACT1

```

```

RRHO
Geometry[angstrom]      2
C      0.000000   0.000000  -0.439519
O      0.000000   0.000000   0.687439
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies [1/cm]      1
2220.1880
ZeroEnergy[kcal/mol]    0.
ElectronicLevels[1/cm]      1
0      1
!*****
End
!*****
Fragment REACT2
Atom
Name H
ElectronicLevels[1/cm]      1
0      2
!*****
End
!*****
GroundEnergy[kcal/mol]  0.0
End
Well HCO
Species
RRHO ! well
Geometry[angstrom]      3
H     -0.004524   0.000000  -0.010121
C     -0.012232  -0.000000   1.117494
O     0.956706   0.000000   1.780877
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies [1/cm]      3
1111.0094
1940.9807
2618.5897
ZeroEnergy[kcal/mol]    -14.42
ElectronicLevels[1/cm]      1
0.0000000000000000    2.0000000000000000
End
End
!*****
Barrier TS REACS HCO
RRHO !
Geometry[angstrom]      3
H     -1.673385   1.508927   0.000000
C     0.201286   0.486214   0.000000
O     0.168499  -0.642581   0.000000
Core RigidRotor
SymmetryFactor  1
End
Tunneling Eckart

```



```

ImaginaryFrequency[1/cm]  401.8416
WellDepth[kcal/mol]      3.18
WellDepth[kcal/mol]      17.60
End
Frequencies[1/cm]        2
255.3456
2190.6226
ZeroEnergy[kcal/mol]     3.18
ElectronicLevels[1/cm]   1
0.0000000000000000      2.0000000000000000
End
End

```

BHPERI1

jChS

```

!*****
!          GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]  200 225 250 275 300 325  350 375 400 425  450 475 500 525 550 575 600 625 650 675 700 750 800 850 900 950 1000 1200 1400 1600 1800 2000
PressureList[atm]          0.5 1 10 100
!
!
EnergyStepOverTemperature      .2
ExcessEnergyOverTemperature    30
ModelEnergyLimit[kcal/mol]     400
!
CalculationMethod              direct
!
WellCutoff                     20
ChemicalEigenvalueMax          0.2
!
ReductionMethod                diagonalization
!
AtomDistanceMin[bohr]          1.3
!!
RateOutput                     jChS.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!          MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

!
!
Model
!
EnergyRelaxation
  Exponential
    Factor [1/cm]          260
    Power                  0.875
    ExponentCutoff         10
  End
!
CollisionFrequency
  LennardJones
    Epsilons [K]          90.58  617.0
    Sigmas [angstrom]     3.54   5.62
    Masses [amu]          39.948  69.0
  End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS
!*****
Well PROD_OPEN
Species
RRHO   ! well
Geometry [angstrom]      10
H       0.09014100  -2.59586800  -0.43089500
C      -0.11062500  -1.53355200  -0.49117800
C       0.11062500   1.53355200  -0.49117800
C       0.11062500  -0.72689500   0.55277800
C      -0.11062500   0.72689500   0.55277800
H      -0.09014100   2.59586800  -0.43089500
H      -0.46064100   1.16147500   1.48541400
H      -0.51010600  -1.15189600  -1.42411600
H       0.51010600   1.15189600  -1.42411600
H       0.46064100  -1.16147500   1.48541400
Core RigidRotor
SymmetryFactor  2.0000000000000000
End
  Frequencies [1/cm]      24
170.10
272.90
467.36
620.96
756.62
891.37
947.55
948.99
1015.80
1035.56
1068.60
1106.93
1311.72

```

```

1342.25
1443.83
1474.01
1680.75
1687.83
3148.39
3152.66
3156.81
3167.66
3245.09
3246.62
  ZeroEnergy[kcal/mol]    -9.41
  ElectronicLevels[1/cm]          1
  0.0000000000000000      1.0000000000000000
End
End

Well REAC_CLOSE
Species
RRHO      ! well
Geometry[angstrom]      10
H          -0.88924800    1.24031000   -1.14101400
C          0.00000000    0.78411900   -0.69986400
C          0.00000000   -0.78411900   -0.69986400
C          0.00000000    0.67116200    0.81344400
C          0.00000000   -0.67116200    0.81344400
H          0.88924800   -1.24031000   -1.14101400
H          0.00000000   -1.41596600    1.60054700
H          0.88924800    1.24031000   -1.14101400
H          -0.88924800   -1.24031000   -1.14101400
H          0.00000000    1.41596600    1.60054700
Core RigidRotor
SymmetryFactor  2.0000000000000000
End
  Frequencies[1/cm]      24
314.78
649.95
862.03
872.09
902.35
908.73
938.80
1007.03
1041.49
1107.07
1140.87
1182.60
1224.13
1245.15
1330.27
1476.24
1497.72
1618.65
3056.87
3062.55
3101.07

```

```

3115.22
3183.69
3215.37
  ZeroEnergy[kcal/mol]    0.
  ElectronicLevels[1/cm]          1
    0.0000000000000000    1.0000000000000000
End
End
!*****
Barrier TS REAC_CLOSE PROD_OPEN
RRHO      !
Geometry[angstrom]      10
H          1.27409200  -1.44251600  -1.10412100
C          0.40274700  -0.99171600  -0.62582600
C         -0.40274700   0.99171600  -0.62582600
C          0.40274700  -0.55749800   0.73298600
C         -0.40274700   0.55749800   0.73298600
H         -1.27409200   1.44251600  -1.10412100
H         -0.99058900   0.98389500   1.53917500
H         -0.54267000  -1.25670400  -1.07801000
H          0.54267000   1.25670400  -1.07801000
H          0.99058900  -0.98389500   1.53917500
Core RigidRotor
      SymmetryFactor  2
End
Tunneling Eckart
  ImaginaryFrequency[1/cm]  772.41
  WellDepth[kcal/mol]    33.16
  WellDepth[kcal/mol]    42.56
End
  Frequencies[1/cm]      23
  468.21
651.10
686.76
736.38
889.19
896.86
925.61
954.15
1013.63
1035.60
1126.18
1171.08
1248.29
1390.19
1520.16
1527.47
1539.91
3096.35
3096.48
3169.26
3189.54
3226.30
3226.71
  ZeroEnergy[kcal/mol]    33.16
  ElectronicLevels[1/cm]          1

```

```

0.0000000000000000      1.0000000000000000
End
End

```

W3lite-F12

```

!*****
!          GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]   200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 750 800 850 900 950 1000 1200 1400 1600 1800 2000
PressureList[atm]           0.5 1 10 100
!
!
EnergyStepOverTemperature      .2
ExcessEnergyOverTemperature    30
ModelEnergyLimit[kcal/mol]     400
!
CalculationMethod              direct
!
WellCutoff                     20
ChemicalEigenvalueMax          0.2
!
ReductionMethod                diagonalization
!
AtomDistanceMin[bohr]         1.3
!!
RateOutput                     Karton.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!          MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
EnergyRelaxation
  Exponential
    Factor[1/cm]               260
    Power                       0.875
    ExponentCutoff              10
  End
!
CollisionFrequency
  LennardJones

```

```

Epsilon[K]          90.58  617.0
Sigma[angstrom]     3.54   5.62
Masses[amu]         39.948 69.0

End

!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS
!*****

Well PROD_OPEN

Species
RRHO   ! well
Geometry[angstrom]    10
H       0.09014100  -2.59586800  -0.43089500
C      -0.11062500  -1.53355200  -0.49117800
C       0.11062500   1.53355200  -0.49117800
C       0.11062500  -0.72689500   0.55277800
C      -0.11062500   0.72689500   0.55277800
H      -0.09014100   2.59586800  -0.43089500
H      -0.46064100   1.16147500   1.48541400
H      -0.51010600  -1.15189600  -1.42411600
H       0.51010600   1.15189600  -1.42411600
H       0.46064100  -1.16147500   1.48541400

Core RigidRotor
SymmetryFactor  2.0000000000000000

End

Frequencies[1/cm]    24
170.10
272.90
467.36
620.96
756.62
891.37
947.55
948.99
1015.80
1035.56
1068.60
1106.93
1311.72
1342.25
1443.83
1474.01
1680.75
1687.83
3148.39
3152.66
3156.81
3167.66
3245.09
3246.62

ZeroEnergy[kcal/mol]  0.

ElectronicLevels[1/cm]  1

```

```

0.0000000000000000    1.0000000000000000
End
End

Well REAC_CLOSE
Species
RRHO      ! well
Geometry[angstrom]      10
H          -0.88681500   1.24201700  -1.14058200
C          0.00000000   0.78467600  -0.69862500
C          0.00000000  -0.78467600  -0.69862500
C          0.00000000   0.66758300   0.81245700
C          0.00000000  -0.66758300   0.81245700
H          0.88681500  -1.24201700  -1.14058200
H          0.00000000  -1.41114900   1.59816800
H          0.88681500   1.24201700  -1.14058200
H          -0.88681500  -1.24201700  -1.14058200
H          0.00000000   1.41114900   1.59816800

Core RigidRotor
SymmetryFactor  2.0000000000000000
End

Frequencies[1/cm]      24
314.78
649.95
862.03
872.09
902.35
908.73
938.80
1007.03
1041.49
1107.07
1140.87
1182.60
1224.13
1245.15
1330.27
1476.24
1497.72
1618.65
3056.87
3062.55
3101.07
3115.22
3183.69
3215.37

ZeroEnergy[kcal/mol]   0.
ElectronicLevels[1/cm]      1
0.0000000000000000    1.0000000000000000

End
End
!*****
Barrier TS REAC_CLOSE PROD_OPEN
RRHO      !
Geometry[angstrom]      10
H          1.25355500  -1.44515000  -1.10420900

```

```

C          0.38407400  -0.99466100  -0.62685100
C         -0.38407400   0.99466100  -0.62685100
C          0.38407400  -0.56603600   0.73361200
C         -0.38407400   0.56603600   0.73361200
H         -1.25355500   1.44515000  -1.10420900
H         -0.95204700   1.01049400   1.54226800
H         -0.55574500  -1.27074700  -1.07862800
H          0.55574500   1.27074700  -1.07862800
H          0.95204700  -1.01049400   1.54226800

```

Core RigidRotor

SymmetryFactor 2

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 772.41

WellDepth[kcal/mol] 33.20

WellDepth[kcal/mol] 33.20

End

Frequencies[1/cm] 23

468.21

651.10

686.76

736.38

889.19

896.86

925.61

954.15

1013.63

1035.60

1126.18

1171.08

1248.29

1390.19

1520.16

1527.47

1539.91

3096.35

3096.48

3169.26

3189.54

3226.30

3226.71

ZeroEnergy[kcal/mol] 33.20

ElectronicLevels[1/cm] 1

0.0000000000000000 1.0000000000000000

End

End

CBS-QB3

!*****


```

!           GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]      200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 750 800 850 900 950 1000 1200 1400 1600 1800 2000
PressureList[atm]       0.5 1 10 100
!
!
EnergyStepOverTemperature      .2
ExcessEnergyOverTemperature    30
ModelEnergyLimit[kcal/mol]     400
!
CalculationMethod              direct
!
WellCutoff                     20
ChemicalEigenvalueMax         0.2
!
ReductionMethod                diagonalization
!
AtomDistanceMin[bohr]         1.3
!!
RateOutput                     CBSQB3.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!           MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation
    Exponential
      Factor[1/cm]             260
      Power                    0.875
      ExponentCutoff           10
    End
!
  CollisionFrequency
    LennardJones
      Epsilons[K]              90.58 617.0
      Sigmas[angstrom]         3.54 5.62
      Masses[amu]              39.948 69.0
    End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS
!*****
Well REAC_OPEN

```

```

Species
RRHO      ! well
Geometry[angstrom]      10
H          0.08687000 -2.60781500 -0.41351600
C          -0.09972500 -1.54300300 -0.48926600
C          0.09972500  1.54300300 -0.48926600
C          0.09972500 -0.72766100  0.54889400
C          -0.09972500  0.72766100  0.54889400
H          -0.08687000  2.60781500 -0.41351600
H          -0.41569100  1.15953600  1.49655400
H          -0.46881200 -1.17501500 -1.44080700
H          0.46881200  1.17501500 -1.44080700
H          0.41569100 -1.15953600  1.49655400

Core RigidRotor
SymmetryFactor  2.0000000000000000
End

Frequencies [1/cm]      24
162.53 274.81 473.28 619.75 757.49 883.62
943.63 945.02 1018.93 1033.03 1068.72 1105.98
1311.61 1343.79 1437.80 1463.52 1673.74 1695.09
3118.16 3128.83 3133.92 3139.64 3217.68 3219.63

ZeroEnergy[kcal/mol]    0.
ElectronicLevels[1/cm]  1
0.0000000000000000    1.0000000000000000

End
End

```

```

Well PROD_CLOSE
Species
RRHO      ! well
Geometry[angstrom]      10
H          -0.88863500  1.24565400 -1.14339500
C          0.00000000  0.78638500 -0.70000000
C          0.00000000 -0.78638500 -0.70000000
C          0.00000000  0.66864600  0.81426400
C          0.00000000 -0.66864600  0.81426400
H          0.88863500 -1.24565400 -1.14339500
H          0.00000000 -1.41442700  1.60121000
H          0.88863500  1.24565400 -1.14339500
H          -0.88863500 -1.24565400 -1.14339500
H          0.00000000  1.41442700  1.60121000

Core RigidRotor
SymmetryFactor  2.0000000000000000
End

Frequencies [1/cm]      24
323.85 650.74 865.67 868.08 886.30 897.37
940.68 997.79 1039.73 1099.04 1129.89 1169.32
1214.61 1235.80 1317.40 1469.09 1488.90 1635.56
3027.58 3033.12 3063.30 3077.99 3162.14 3193.97

ZeroEnergy[kcal/mol]    9.76
ElectronicLevels[1/cm]  1
0.0000000000000000    1.0000000000000000

End
End

!*****
Barrier TS REAC_OPEN PROD_CLOSE

```

```

RRHO      !
Geometry[angstrom]      10
H          1.26136400   -1.45280700   -1.10161500
C          0.39035400   -0.99502000   -0.62651600
C         -0.39035400    0.99502000   -0.62651600
C          0.39035400   -0.56452900    0.73348100
C         -0.39035400    0.56452900    0.73348100
H         -1.26136400    1.45280700   -1.10161500
H         -0.96838000    1.00190500    1.54234100
H         -0.55034900   -1.27028000   -1.08251700
H          0.55034900    1.27028000   -1.08251700
H          0.96838000   -1.00190500    1.54234100

Core RigidRotor
      SymmetryFactor  2

End

Tunneling Eckart
ImaginaryFrequency[1/cm]  736.27
WellDepth[kcal/mol]      41.79
WellDepth[kcal/mol]      32.03

End

Frequencies[1/cm]        23
471.50 650.21 699.95 742.79 892.64 898.73
930.18 957.37 1013.46 1030.91 1122.30 1164.77
1244.74 1384.76 1512.78 1519.63 1543.75 3069.37
3069.63 3139.20 3159.86 3205.60 3206.58

ZeroEnergy[kcal/mol]      41.79

ElectronicLevels[1/cm]          1
0.0000000000000000  1.0000000000000000

End

End

```

CRBH4

jChS

```

!*****
!          GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]      200 225 250 275 300 325  350 375 400 425  450 475 500 525 550 575  600 625 650 675 700 750 800 850 900 950 1000 1200 1400 1600 1800 2000
PressureList[atm]              0.5 1 10 100
!
!
EnergyStepOverTemperature      .2
ExcessEnergyOverTemperature    30
ModelEnergyLimit[kcal/mol]     400

```

```

!
CalculationMethod          direct
!
WellCutoff                 20
ChemicalEigenvalueMax     0.2
!
ReductionMethod           diagonalization
!
AtomDistanceMin[bohr]    1.3
!!
RateOutput                 jChS.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!           MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation
    Exponential
      Factor[1/cm]         260
      Power                 0.875
      ExponentCutoff       10
    End
!
  CollisionFrequency
    LennardJones
      Epsilons[K]          90.58  617.0
      Sigmas [angstrom]    3.54   5.62
      Masses [amu]         39.948 69.0
    End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS
!*****
Well REAC_CLOSE
Species
RRHO      ! well
Geometry[angstrom]      8
C          -0.02003100   1.20888100   0.09746300
C          -0.10577400  -1.20488100   0.19540400
O          -1.30542900  -0.56334400  -0.21480400
N          -1.23844900   0.82283300   0.03373200
S          1.23690200   0.00076400  -0.08372100
H          -0.15182500  -1.45533700   1.25953400
H          0.02811200  -2.09328300  -0.41762100
H          0.20068500   2.25932500   0.22272800
Core RigidRotor

```

```

SymmetryFactor 1.0000000000000000
End
Frequencies [1/cm] 18
200.42
482.41
524.75
678.99
784.64
837.75
842.42
891.51
981.53
996.21
1214.28
1233.98
1338.13
1500.31
1584.01
3042.71
3158.81
3246.18
ZeroEnergy[kcal/mol] 0.
ElectronicLevels [1/cm] 1
0.0000000000000000 1.0000000000000000
End
End

```

Well PROD_OPEN

Species

RRHO ! well

```

Geometry[angstrom] 8
C -0.02003100 1.20888100 0.09746300
C -0.10577400 -1.20488100 0.19540400
O -1.30542900 -0.56334400 -0.21480400
N -1.23844900 0.82283300 0.03373200
S 1.23690200 0.00076400 -0.08372100
H -0.15182500 -1.45533700 1.25953400
H 0.02811200 -2.09328300 -0.41762100
H 0.20068500 2.25932500 0.22272800

```

Core RigidRotor

SymmetryFactor 1.0000000000000000

End

```

Frequencies [1/cm] 18
200.42
482.41
524.75
678.99
784.64
837.75
842.42
891.51
981.53
996.21
1214.28
1233.98
1338.13

```

```

1500.31
1584.01
3042.71
3158.81
3246.18
ZeroEnergy[kcal/mol]    0.
ElectronicLevels[1/cm]          1
0.0000000000000000    1.0000000000000000
End
End
!*****
Barrier TS REAC_CLOSE PROD_OPEN
RRHO      !
Geometry[angstrom]      8
C          0.53937900    0.90635200    0.04997800
C          -1.18561800   -1.06690900    0.22990500
O          -1.71476700   -0.07944500   -0.29278100
N          -0.55193700    1.50114300    0.08705600
S          1.40708400   -0.48628900   -0.06684700
H          -0.94611600   -1.08967800    1.29798200
H          -1.08921000   -2.00070800   -0.33725500
H          0.98111600    1.96190800    0.16239100
Core RigidRotor
SymmetryFactor  1
End
Tunneling Eckart
ImaginaryFrequency[1/cm]  713.47
WellDepth[kcal/mol]    42.06
WellDepth[kcal/mol]    42.06
End
Frequencies[1/cm]      17
149.17
210.79
349.28
468.32
499.70
581.09
615.17
648.09
816.47
1110.21
1238.50
1481.70
1635.27
1763.29
2705.60
3016.87
3109.01
ZeroEnergy[kcal/mol]    42.06
ElectronicLevels[1/cm]          1
0.0000000000000000    1.0000000000000000
End
End

```

W3lite-F12

```
!*****
!           GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]  200 225 250 275 300 325  350 375 400 425  450 475 500 525 550 575 600 625 650 675 700 750 800 850 900 950 1000 1200 1400 1600 1800 2000
PressureList[atm]           0.5 1 10 100
!
!
EnergyStepOverTemperature      .2
ExcessEnergyOverTemperature    30
ModelEnergyLimit [kcal/mol]    400
!
CalculationMethod              direct
!
WellCutoff                     20
ChemicalEigenvalueMax          0.2
!
ReductionMethod                diagonalization
AtomDistanceMin[bohr]          1.3
!!
RateOutput                     Karton.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!           MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation
    Exponential
      Factor [1/cm]             260
      Power                     0.875
      ExponentCutoff            10
    End
!
  CollisionFrequency
    LennardJones
      Epsilons[K]               90.58  617.0
      Sigmas [angstrom]         3.54    5.62
      Masses [amu]              39.948  69.0
    End
!
!*****
!
```

```

!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS
!*****

Well REAC_CLOSE

Species
RRHO      ! well

Geometry[angstrom]      8
C -0.0211260 1.2143720 0.0861400
C -0.1086300 -1.2218440 0.1704460
O -1.3154940 -0.5575770 -0.1896810
N -1.2315760 0.8329400 0.0324420
S 1.2396090 0.0010990 -0.0736110
H -0.1370880 -1.5274350 1.2190290
H 0.0170930 -2.0785540 -0.4853320
H 0.2097690 2.2632700 0.1949200

Core RigidRotor
SymmetryFactor 1.0000000000000000

End

Frequencies [1/cm]      18
200.42
482.41
524.75
678.99
784.64
837.75
842.42
891.51
981.53
996.21
1214.28
1233.98
1338.13
1500.31
1584.01
3042.71
3158.81
3246.18

ZeroEnergy[kcal/mol]    0.

ElectronicLevels[1/cm]      1
0.0000000000000000      1.0000000000000000

End
End

```

```

Well PROD_OPEN

Species
RRHO      ! well

Geometry[angstrom]      8
C -0.0211260 1.2143720 0.0861400
C -0.1086300 -1.2218440 0.1704460
O -1.3154940 -0.5575770 -0.1896810
N -1.2315760 0.8329400 0.0324420
S 1.2396090 0.0010990 -0.0736110
H -0.1370880 -1.5274350 1.2190290
H 0.0170930 -2.0785540 -0.4853320

```



```

H 0.2097690 2.2632700 0.1949200
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies [1/cm] 18
200.42
482.41
524.75
678.99
784.64
837.75
842.42
891.51
981.53
996.21
1214.28
1233.98
1338.13
1500.31
1584.01
3042.71
3158.81
3246.18
ZeroEnergy[kcal/mol] 0.
ElectronicLevels[1/cm] 1
0.0000000000000000 1.0000000000000000
End
End
!*****
Barrier TS REAC_CLOSE PROD_OPEN
RRHO !
Geometry[angstrom] 8
C 0.6112370 0.8781110 0.0482300
C -1.3356260 -1.0194430 0.2278640
O -1.7615960 0.0024910 -0.2939760
N -0.4252580 1.5553560 0.0890100
S 1.4144820 -0.5569100 -0.0651010
H -1.0756240 -1.0632920 1.2908480
H -1.3035850 -1.9597990 -0.3387530
H 1.1634070 1.8742220 0.1616990
Core RigidRotor
SymmetryFactor 1
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 713.47
WellDepth[kcal/mol] 40.40
WellDepth[kcal/mol] 40.40
End
Frequencies [1/cm] 17
149.17
210.79
349.28
468.32
499.70
581.09
615.17

```

```

648.09
816.47
1110.21
1238.50
1481.70
1635.27
1763.29
2705.60
3016.87
3109.01
  ZeroEnergy[kcal/mol]    40.40
  ElectronicLevels[1/cm]                1
  0.0000000000000000    1.0000000000000000
  End
End

```

CBS-QB3

```

!*****
!          GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]  200 225 250 275 300 325  350 375 400 425  450 475 500 525 550 575 600 625 650 675 700 750 800 850 900 950 1000 1200 1400 1600 1800 2000
PressureList[atm]          0.5 1 10 100
!
!
EnergyStepOverTemperature      .2
ExcessEnergyOverTemperature    30
ModelEnergyLimit [kcal/mol]    400
!
CalculationMethod              direct
!
WellCutoff                     20
ChemicalEigenvalueMax          0.2
!
ReductionMethod                diagonalization
!
AtomDistanceMin[bohr]         1.3
!!
RateOutput                     CBSQB3.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!          MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!

```

```

!
Model
!
EnergyRelaxation
  Exponential
    Factor[1/cm]          260
    Power                 0.875
    ExponentCutoff        10
  End
!
CollisionFrequency
  LennardJones
    Epsilons[K]          90.58 617.0
    Sigmas[angstrom]     3.54 5.62
    Masses[amu]          39.948 69.0
  End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS
!*****
Well REAC_CLOSE
Species
RRHO ! well
Geometry[angstrom]      8
C      -0.02928800  1.21849000  0.08546900
C      -0.10614600 -1.22508200  0.16950700
O      -1.31591700 -0.56038300 -0.18814800
N      -1.23878600  0.82698400  0.03157200
S      1.24518900  0.00477200 -0.07300900
H      -0.13019700 -1.53357800  1.21944500
H      0.01958900 -2.07884900 -0.49316700
H      0.19901900  2.26980600  0.19619700
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies[1/cm]      18
168.97
479.75
521.55
645.50
763.59
825.51
830.77
890.45
960.90
971.36
1199.34
1228.19
1333.46
1495.04
1615.51
3022.61

```

3137.17
 3224.14
 ZeroEnergy[kcal/mol] 0.
 ElectronicLevels[1/cm] 1
 0.0000000000000000 1.0000000000000000
 End
 End

Well PROD_OPEN
 Species
 RRHO ! well
 Geometry[angstrom] 8
 C -0.02928800 1.21849000 0.08546900
 C -0.10614600 -1.22508200 0.16950700
 O -1.31591700 -0.56038300 -0.18814800
 N -1.23878600 0.82698400 0.03157200
 S 1.24518900 0.00477200 -0.07300900
 H -0.13019700 -1.53357800 1.21944500
 H 0.01958900 -2.07884900 -0.49316700
 H 0.19901900 2.26980600 0.19619700
 Core RigidRotor
 SymmetryFactor 1.0000000000000000
 End

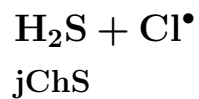
Frequencies[1/cm] 18
 168.97
 479.75
 521.55
 645.50
 763.59
 825.51
 830.77
 890.45
 960.90
 971.36
 1199.34
 1228.19
 1333.46
 1495.04
 1615.51
 3022.61
 3137.17
 3224.14

ZeroEnergy[kcal/mol] 0.
 ElectronicLevels[1/cm] 1
 0.0000000000000000 1.0000000000000000
 End
 End
 !*****
 Barrier TS REAC_CLOSE PROD_OPEN
 RRHO !
 Geometry[angstrom] 8
 C 0.62540400 0.86937200 0.05343600
 C -1.40090400 -1.00407800 0.23980900
 O -1.77069800 0.02065800 -0.31383200
 N -0.41894900 1.54383800 0.09299400
 S 1.44466900 -0.56454400 -0.06828200

```

H          -1.09770700  -1.02370500  1.29457800
H          -1.44615500  -1.96860400  -0.29007000
H          1.18038200   1.86112200   0.18824100
Core RigidRotor
      SymmetryFactor  1
End
Tunneling Eckart
ImaginaryFrequency[1/cm]  477.57
WellDepth[kcal/mol]  40.96
WellDepth[kcal/mol]  40.96
End
Frequencies[1/cm]  17
132.98
183.66
289.22
409.57
456.92
495.68
602.17
629.43
795.76
1133.67
1239.93
1498.06
1690.59
1724.18
2719.43
2965.64
3055.29
ZeroEnergy[kcal/mol]  40.96
ElectronicLevels[1/cm]  1
0.0000000000000000  1.0000000000000000
End
End

```



```

!*****
!          GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]          200 225 250 275 300 325 350 375 400 425 430 450 475 500 600 700 800 900 1000
PressureList[atm]          0.5 1
!

```

```

!
EnergyStepOverTemperature      .2
ExcessEnergyOverTemperature    30
ModelEnergyLimit [kcal/mol]    400
!
CalculationMethod              direct
!
WellCutoff                     20
ChemicalEigenvalueMax         0.2
!
ReductionMethod                diagonalization
!
AtomDistanceMin[bohr]         1.3
!!
RateOutput                     junchs.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!           MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation
    Exponential
      Factor [1/cm]             260
      Power                     0.875
      ExponentCutoff            10
    End
!
  CollisionFrequency
    LennardJones
      Epsilons [K]              90.58  617.0
      Sigmas [angstrom]         3.54   5.62
      Masses [amu]              39.948  69.0
    End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS
!*****

Bimolecular REACS
Fragment REACT1
RRHO
Geometry[angstrom]            3
S      0.00000000  0.00000000  0.10283933
H      0.00000000  0.96667700 -0.82271467
H      0.00000000 -0.96667700 -0.82271467

```

```

Core RigidRotor
SymmetryFactor 2.0000000000000000
End
  Frequencies [1/cm]      3
  1217.90 2736.90 2751.70
ZeroEnergy [kJ/mol]      0.
ElectronicLevels [1/cm]      1
  0      1
!*****
End
!*****
Fragment REACT2
Atom
Name Cl
ElectronicLevels [1/cm]      2
  0      4
  881.00 2
!*****
End
!*****
GroundEnergy [kJ/mol] 0.0
End
Bimolecular PRODS
Fragment PROD1
RRHO
Geometry [angstrom]      2
  H      0.00000000  0.00000000 -1.26323400
  S      0.00000000  0.00000000  0.07895200
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
  Frequencies [1/cm]      1
  2719.97
ZeroEnergy [kJ/mol]      0.
ElectronicLevels [1/cm]      2
  0.0000000000000000  2.0000000000000000
  376.95999999999998  2.0000000000000000
!*****
End
!*****
Fragment PROD2
RRHO
Geometry [angstrom]      2
  H      0.00000000  0.00000000 -1.20561900
  Cl     0.00000000  0.00000000  0.07091900
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
  Frequencies [1/cm]      1
  3006.52
ZeroEnergy [kJ/mol]      0.
ElectronicLevels [1/cm]      1
  0.0000000000000000  1.0000000000000000
!*****

```

```

End
GroundEnergy[kJ/mol]   -53.18
End
!*****
Well WR
Species
RRHO   ! well
Geometry[angstrom]    4
  H      0.86853200  -1.21794200  0.97069800
  S     -0.05263800  -1.26295000  0.00000000
  H      0.86853200  -1.21794200 -0.97069800
  Cl    -0.05263800  1.33194700  0.00000000
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
  Frequencies[1/cm]    6
  235.51 361.29 394.61 1211.09 2735.17 2749.91
ZeroEnergy[kJ/mol]   -38.35
ElectronicLevels[1/cm] 1
  0.0000000000000000  2.0000000000000000
End
End
!*****
Well WP
Species
RRHO   ! well
Geometry[angstrom]    4
  S     -1.89837200  -0.07864900 -0.00000300
  H     -1.96120000  1.26293700 -0.00000900
  H      0.58255000  -0.07505800  0.00001500
  Cl    1.86780000  0.00414800  0.00000200
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
  Frequencies[1/cm]    6
  92.55 144.41 254.63 397.12 2715.09 2844.57
ZeroEnergy[kJ/mol]   -61.64
ElectronicLevels[1/cm] 1
  0.0000000000000000  2.0000000000000000
End
End
!*****
Barrier B1 REACS WR
RRHO
  Stoichiometry H2S1Cl1
  Core PhaseSpaceTheory
    FragmentGeometry[angstrom] 3
  S      0.00000000  0.00000000  0.10283933
  H      0.00000000  0.96667700 -0.82271467
  H      0.00000000 -0.96667700 -0.82271467
    FragmentGeometry[angstrom] 1
  Cl     0. 0. 0.
  SymmetryFactor 2.0000000000000000
    PotentialPrefactor[au] 230.
!    PotentialPrefactor[au] 10.
    PotentialPowerExponent 6

```



```

End
Frequencies[1/cm]      3
1217.89 2735.01 2750.20
ZeroEnergy[kJ/mol]    0.
ElectronicLevels[1/cm]  2
0.0000000000000000  4.0000000000000000
881.00000000000000  2.0000000000000000
End
!*****
Barrier B3 WP PRODS
RRHO
Stoichiometry H2SiCl1
Core PhaseSpaceTheory
FragmentGeometry[angstrom]  2
H      0.00000000  0.00000000 -1.26323400
S      0.00000000  0.00000000  0.07895200
FragmentGeometry[angstrom]  2
H      0.00000000  0.00000000 -1.20561900
Cl     0.00000000  0.00000000  0.07091900
SymmetryFactor  2.0000000000000000
PotentialPrefactor[au]  230.
PotentialPowerExponent  6
End
Frequencies[1/cm]      2
2719.96 3006.51
ZeroEnergy[kJ/mol]    -53.18
ElectronicLevels[1/cm]  2
0.0000000000000000  2.0000000000000000
376.95999999999998  2.0000000000000000
End
!*****
Barrier B2 WR WP
RRHO  !
Geometry[angstrom]    4
Cl     1.40626100  0.00424200 -0.01712600
H      -0.08527300 -0.19676000  0.61791700
S      -1.40388600 -0.07129300 -0.02507700
H      -1.35899500  1.26533600  0.07445500
Core RigidRotor
SymmetryFactor  0.5000000000000000
End
Tunneling Eckart
ImaginaryFrequency[1/cm]  759.25
WellDepth[kJ/mol]  29.03
WellDepth[kJ/mol]  52.32
End
Frequencies[1/cm]      5
232.63 422.36 1013.96 1427.75 2728.71
ZeroEnergy[kJ/mol]    -9.32
ElectronicLevels[1/cm]  1
0.0000000000000000  2.0000000000000000
End
End

```

CBS-CVH

```
!*****
!           GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]           200 225 250 275 300 325 350 375 400 425 430 450 475 500 600 700 800 900 1000
PressureList[atm]            0.5 1
!
!
EnergyStepOverTemperature    .2
ExcessEnergyOverTemperature  30
ModelEnergyLimit [kcal/mol]  400
!
CalculationMethod            direct
!
WellCutoff                    20
ChemicalEigenvalueMax        0.2
!
ReductionMethod               diagonalization
!
AtomDistanceMin[bohr]        1.3
!!
RateOutput                    heatlike.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!           MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation
    Exponential
      Factor[1/cm]            260
      Power                    0.875
      ExponentCutoff           10
    End
!
  CollisionFrequency
    LennardJones
      Epsilons[K]              90.58  617.0
      Sigmas [angstrom]        3.54    5.62
      Masses [amu]              39.948 69.0
    End
!
!*****
!
```

```

!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS
!*****

Bimolecular REACS
Fragment REACT1
RRHO
Geometry[angstrom]      3
S      0.00000000  0.00000000  0.10283933
H      0.00000000  0.96667700 -0.82271467
H      0.00000000 -0.96667700 -0.82271467

Core RigidRotor
SymmetryFactor  2.0000000000000000
End

  Frequencies [1/cm]      3
  1217.90 2736.90 2751.70
ZeroEnergy[kJ/mol]      0.
ElectronicLevels [1/cm]      1
  0      1
!*****
End
!*****
Fragment REACT2
Atom
Name Cl
ElectronicLevels [1/cm]      2
  0      4
  881.00 2
!*****
End
!*****
GroundEnergy[kJ/mol] 0.0
End

Bimolecular PRODS
Fragment PROD1
RRHO
Geometry[angstrom]      2
H      0.00000000  0.00000000 -1.26323400
S      0.00000000  0.00000000  0.07895200

Core RigidRotor
SymmetryFactor  1.0000000000000000
End

  Frequencies [1/cm]      1
  2719.97
ZeroEnergy[kJ/mol]      0.
ElectronicLevels [1/cm]      2
  0.0000000000000000  2.0000000000000000
  376.9599999999998  2.0000000000000000
!*****
End
!*****
Fragment PROD2

```

```

RRHO
Geometry[angstrom]      2
  H      0.00000000    0.00000000   -1.20561900
  Cl     0.00000000    0.00000000    0.07091900
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies [1/cm]    1
  3006.52
ZeroEnergy[kJ/mol]      0.
ElectronicLevels[1/cm]  1
  0.0000000000000000    1.0000000000000000

```

!*****

```

End
GroundEnergy[kJ/mol]  -51.383
End

```

!*****

```

Well WR
Species
RRHO ! well
Geometry[angstrom]    4
  H      0.86853200   -1.21794200    0.97069800
  S     -0.05263800   -1.26295000    0.00000000
  H      0.86853200   -1.21794200   -0.97069800
  Cl    -0.05263800    1.33194700    0.00000000
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies [1/cm]    6
  235.51 361.29 394.61 1211.09 2735.17 2749.91
ZeroEnergy[kJ/mol]    -39.68
ElectronicLevels[1/cm]  1
  0.0000000000000000    2.0000000000000000

```

End

End

!*****

```

Well WP
Species
RRHO ! well
Geometry[angstrom]    4
  S     -1.89837200   -0.07864900   -0.00000300
  H     -1.96120000    1.26293700   -0.00000900
  H      0.58255000   -0.07505800    0.00001500
  Cl     1.86780000    0.00414800    0.00000200
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies[1/cm]    6
  92.55 144.41 254.63 397.12 2715.09 2844.57
ZeroEnergy[kJ/mol]    -61.47
ElectronicLevels[1/cm]  1
  0.0000000000000000    2.0000000000000000

```

End

End

!*****

```

Barrier B1 REACS WR
RRHO
Stoichiometry H2S1Cl1
Core PhaseSpaceTheory
FragmentGeometry[angstrom] 3
S 0.00000000 0.00000000 0.10283933
H 0.00000000 0.96667700 -0.82271467
H 0.00000000 -0.96667700 -0.82271467
FragmentGeometry[angstrom] 1
Cl 0. 0. 0.
SymmetryFactor 2.0000000000000000
PotentialPrefactor[au] 230.
! PotentialPrefactor[au] 10.
PotentialPowerExponent 6
End
Frequencies[1/cm] 3
1217.89 2735.01 2750.20
ZeroEnergy[kJ/mol] 0.
ElectronicLevels[1/cm] 2
0.0000000000000000 4.0000000000000000
881.00000000000000 2.0000000000000000
End
!*****
Barrier B3 WP PRODS
RRHO
Stoichiometry H2S1Cl1
Core PhaseSpaceTheory
FragmentGeometry[angstrom] 2
H 0.00000000 0.00000000 -1.26323400
S 0.00000000 0.00000000 0.07895200
FragmentGeometry[angstrom] 2
H 0.00000000 0.00000000 -1.20561900
Cl 0.00000000 0.00000000 0.07091900
SymmetryFactor 2.0000000000000000
PotentialPrefactor[au] 230.
PotentialPowerExponent 6
End
Frequencies[1/cm] 2
2719.96 3006.51
ZeroEnergy[kJ/mol] -51.38
ElectronicLevels[1/cm] 2
0.0000000000000000 2.0000000000000000
376.95999999999998 2.0000000000000000
End
!*****
Barrier B2 WR WP
RRHO !
Geometry[angstrom] 4
Cl 1.40626100 0.00424200 -0.01712600
H -0.08527300 -0.19676000 0.61791700
S -1.40388600 -0.07129300 -0.02507700
H -1.35899500 1.26533600 0.07445500
Core RigidRotor
SymmetryFactor 0.5000000000000000
End
Tunneling Eckart

```

```

ImaginaryFrequency[1/cm]      759.25
WellDepth[kJ/mol]             30.37
WellDepth[kJ/mol]             52.16
End
Frequencies[1/cm]              5
232.63 422.36 1013.96 1427.75 2728.71
ZeroEnergy[kJ/mol]            -9.31
ElectronicLevels[1/cm]                1
0.0000000000000000          2.0000000000000000
End
End

```

CBS-QB3

```

|*****
!           GLOBAL SECTION
|*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]             200 225 250 275 300 325 350 375 400 425 430 450 475 500 600 700 800 900 1000
PressureList[atm]              0.5 1
!
!
EnergyStepOverTemperature      .2
ExcessEnergyOverTemperature    30
ModelEnergyLimit[kcal/mol]     400
!
CalculationMethod              direct
!
WellCutoff                     20
ChemicalEigenvalueMax          0.2
!
ReductionMethod                diagonalization
!
AtomDistanceMin[bohr]         1.3
!!
RateOutput                     qb3.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
|*****
!           MODEL SECTION
|*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
EnergyRelaxation
Exponential

```

```

Factor[1/cm]          260
Power                 0.875
ExponentCutoff       10
End
!
CollisionFrequency
  LennardJones
    Epsilons[K]       90.58  617.0
    Sigmas [angstrom] 3.54   5.62
    Masses [amu]      39.948 69.0
  End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS
!*****

Bimolecular REACS
Fragment REACT1
RRHO
Geometry[angstrom]    3
H      0.00000000    0.97117900  -0.82531100
S      0.00000000    0.00000000   0.10316400
H      0.00000000   -0.97117900  -0.82531100
Core RigidRotor
SymmetryFactor 2.0000000000000000
End
  Frequencies [1/cm]    3
  1213.82 2676.31 2690.23
  ZeroEnergy[kJ/mol]    0.
  ElectronicLevels [1/cm] 1
  0      1
!*****
End
!*****
Fragment REACT2
Atom
Name Cl
ElectronicLevels [1/cm] 2
  0      4
  881.00 2
!*****
End
!*****
GroundEnergy[kJ/mol] 0.0
End
Bimolecular PRODS
Fragment PROD1
RRHO
Geometry[angstrom]    2
H      0.00000000    0.00000000  -1.26857400

```

```

S          0.00000000  0.00000000  0.07928600
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies [1/cm]      1
  2659.89
ZeroEnergy [kJ/mol]      0.
ElectronicLevels [1/cm]      2
  0.0000000000000000      2.0000000000000000
  376.95999999999998      2.0000000000000000
!*****
End
!*****
Fragment PROD2
RRHO
Geometry [angstrom]      2
  H          0.00000000  0.00000000  -1.21155800
  Cl         0.00000000  0.00000000  0.07126800
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies [1/cm]      1
  2936.93
ZeroEnergy [kJ/mol]      0.
ElectronicLevels [1/cm]      1
  0.0000000000000000      1.0000000000000000
!*****
End
GroundEnergy [kJ/mol]  -59.25
End
!*****
Well WR
Species
RRHO ! well
Geometry [angstrom]      4
  H          0.87236400  -1.25413500  0.97382500
  S          -0.05287100  -1.30634600  0.00000000
  H          0.87236400  -1.25413500  -0.97382500
  Cl         -0.05287100  1.37704700  0.00000000
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies [1/cm]      6
  215.04 338.57 371.63 1210.51 2677.85 2691.64
ZeroEnergy [kJ/mol]      -42.68
ElectronicLevels [1/cm]      1
  0.0000000000000000      2.0000000000000000
End
End
!*****
Well WP
Species
RRHO ! well
Geometry [angstrom]      4
  S          1.88505200  -0.08051500  0.00020300

```



```

H          2.01586800   1.26180900   0.00006400
H          -0.56242200  -0.05095100   0.00032000
Cl         -1.85966300   0.00455200  -0.00021400

Core RigidRotor
SymmetryFactor  1.0000000000000000
End

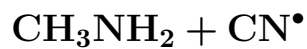
Frequencies[1/cm]      6
93.81 170.86 281.81 435.99 2656.40 2710.28
ZeroEnergy[kJ/mol]      -62.50
ElectronicLevels[1/cm]      1
0.0000000000000000    2.0000000000000000
End
End
!*****
Barrier B1 REACS WR
RRHO
Stoichiometry H2S1Cl1
Core PhaseSpaceTheory
FragmentGeometry[angstrom]      3
H          0.00000000   0.97117900  -0.82531100
S          0.00000000   0.00000000   0.10316400
H          0.00000000  -0.97117900  -0.82531100
FragmentGeometry[angstrom]      1
Cl         0. 0. 0.
SymmetryFactor  2.0000000000000000
PotentialPrefactor[au] 230.
! PotentialPrefactor[au] 10.
PotentialPowerExponent 6
End
Frequencies[1/cm]      3
1213.82 2676.31 2690.23
ZeroEnergy[kJ/mol]      0.
ElectronicLevels[1/cm]      2
0.0000000000000000    4.0000000000000000
881.00000000000000    2.0000000000000000
End
!*****
Barrier B3 WP PRODS
RRHO
Stoichiometry H2S1Cl1
Core PhaseSpaceTheory
FragmentGeometry[angstrom]      2
H          0.00000000   0.00000000  -1.26857400
S          0.00000000   0.00000000   0.07928600
FragmentGeometry[angstrom]      2
H          0.00000000   0.00000000  -1.21155800
Cl         0.00000000   0.00000000   0.07126800
SymmetryFactor  2.0000000000000000
PotentialPrefactor[au] 230.
PotentialPowerExponent 6
End
Frequencies[1/cm]      2
2659.89 2936.93
ZeroEnergy[kJ/mol]      -59.25
ElectronicLevels[1/cm]      2
0.0000000000000000    2.0000000000000000

```

```

376.9599999999998      2.0000000000000000
End
!*****
Barrier E2 WR WP
RRHO      !
Geometry[angstrom]      4
  C1      1.46141200    0.00420700   -0.01507200
  H      -0.04359800   -0.14801900    0.52866300
  S      -1.45887600   -0.07462900   -0.01976900
  H      -1.45838600    1.27056300    0.04385800
Core RigidRotor
  SymmetryFactor 0.5000000000000000
End
Tunneling Eckart
  ImaginaryFrequency[1/cm] 1016.86
  WellDepth[kJ/mol] 27.77
  WellDepth[kJ/mol] 47.58
End
  Frequencies[1/cm] 5
  211.63 409.67 979.18 1162.65 2669.09
  ZeroEnergy[kJ/mol] -14.92
  ElectronicLevels[1/cm] 1
  0.0000000000000000 2.0000000000000000
End
End

```



CN attack to the CH₃ moiety
jChS

```

!*****
!      GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]      30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 220 240 260 280 300 350 400 450 500
PressureList[atm]      1.e-8
!
!
EnergyStepOverTemperature      .2
ExcessEnergyOverTemperature      30
ModelEnergyLimit[kcal/mol]      400
!
CalculationMethod      low-eigenvalue
!
WellCutoff      20

```

```

ChemicalEigenvalueMax          0.2
!
ReductionMethod                 diagonalization
AtomDistanceMin[bohr]         1.3
!!
RateOutput                     fc01_ChS.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!           MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
EnergyRelaxation
  Exponential
    Factor [1/cm]              260
    Power                      0.875
    ExponentCutoff             10
  End
!
CollisionFrequency
  LennardJones
    Epsilons[K]                127.697  1382.375
    Sigmas [angstrom]          3.462   4.046
    Masses [amu]               39.948  70.07
  End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS - CH3NH2 + CN
!*****
Bimolecular REACS
Fragment CH3NH2
RRHO
Geometry [angstrom]           7
C          -0.74064000   0.00000000   0.01360800
H          -1.12725000  -0.87638300  -0.50253800
H          -1.14607300   0.00000000   1.03050000
H          -1.12725000   0.87638400  -0.50253700
N           0.72026000   0.00000000  -0.07006200
H           1.10585300   0.81199300   0.39300800
H           1.10585300  -0.81199300   0.39300800
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies [1/cm]           15
300.20
834.61
978.18

```

```

1064.10
1178.30
1354.60
1472.48
1517.20
1536.05
1672.27
3006.41
3092.76
3129.63
3519.95
3601.33
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000      1.0000000000000000
!*****
End
!*****
Fragment CN
RRHO
Geometry[angstrom]          2
C          0.00000000      0.00000000      -0.63181100
N          0.00000000      0.00000000      0.54143400
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]          1
2076.80
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
!*****
End
!*****
GroundEnergy[kJ/mol] 0.0
End
!*****
! PRODUCT P1 - CH2NH2 + HCN
!*****
Bimolecular P1
Fragment CH2NH2
RRHO
Geometry[angstrom]          6
C          0.73716300      0.05207300      0.00000000
H          1.24098000      -0.16233200      0.92778800
H          1.24098000      -0.16233200      -0.92778800
N          -0.65004100      -0.05946900      0.00000000
H          -1.11367100      0.26546000      0.83278100
H          -1.11367100      0.26546000      -0.83278100
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]          12
455.87
608.48
672.66

```

```

941.68
1228.92
1332.81
1494.17
1661.62
3175.68
3289.29
3563.85
3668.18
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
!*****
End
!*****
Fragment HCN
RRHO
Geometry[angstrom]         3
C          0.00000000    0.00000000   -0.55868200
H          0.00000000    0.00000000   -1.62356200
N          0.00000000    0.00000000    0.59561500
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]         4
747.43
747.43
2124.86
3444.80
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000      1.0000000000000000
!*****
End
!*****
GroundEnergy[kJ/mol] -141.40
End
!*****
! PRODUCT P2 - AAN + H
!*****
Bimolecular P2
Fragment AAN
RRHO
Geometry[angstrom]         8
N          -1.57103400   -0.47328200   -0.06614300
H          -1.48750500   -1.09302700    0.72899000
H          -2.51570100   -0.11296900   -0.07859300
C          -0.61799900    0.62930100    0.03134800
H          -0.75621900    1.28659100   -0.82625400
H          -0.71181000    1.24606600    0.93131000
C          0.75714200    0.12420400   -0.00760700
N          1.84557000   -0.26792000   -0.00857200
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]         18

```

```

200.35
247.71
372.97
569.46
821.26
878.29
1011.17
1090.52
1198.39
1316.21
1430.00
1511.75
1668.36
2294.29
3014.18
3099.75
3522.30
3610.24

ZeroEnergy[kJ/mol]          0.
ElectronicLevels[i/cm]      1
0.0000000000000000        1.0000000000000000
!*****
End
!*****
Fragment HYDROGEN
Atom
Name H
ElectronicLevels[i/cm]      1
0.0000000000000000        2.0000000000000000
!*****
End
GroundEnergy[kJ/mol]       -84.10
End

Well FC01
Species
RRHO ! transition state
Geometry[angstrom]        9
C          -1.75961900    0.70751200    0.00000200
N          -1.94559400   -0.66454800    0.00000100
H          -1.96563500    1.22008800   -0.92616900
H          -1.96559300    1.22008100    0.92618500
H           0.53087300    0.59788100   -0.00001100
H          -1.70666100   -1.16502300   -0.83939700
H          -1.70662200   -1.16502800    0.83938500
C           1.54268600    0.22600200   -0.00000600
N           2.62188500   -0.18638800    0.00000300

Core RigidRotor
SymmetryFactor  1.0000000000000000
End

Frequencies[i/cm]        21
40.34 71.38 136.95 149.68 185.17
511.30 575.14 729.22 848.06 861.82
943.55 1246.23 1328.18 1493.79 1665.76
2104.04 3165.10 3238.70 3277.59 3579.46
3687.37

```

```

ZeroEnergy[kJ/mol]          -155.30
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
End
End
!*****
Well RI
Species
RRHO ! transition state
Geometry[angstrom]         9
C          -0.81668500   -0.17355500   0.35900500
N          -1.83377000   -0.09517100  -0.34924000
C          0.47780400    0.59647500    0.08989800
H          0.69617500    1.20943200    0.96394100
N          1.62364600   -0.25534900  -0.18366100
H          1.83966100   -0.85986400    0.59799600
H          0.31432000    1.26303800   -0.75239800
H          1.45881200   -0.84041500  -0.99214800
H          -0.80481900   -0.85607000   1.21949000

Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm]         21
111.64
295.78
361.91
429.13
781.88
814.81
917.98
961.28
1098.84
1131.21
1254.02
1353.86
1386.79
1495.95
1670.85
1726.45
2985.23
3076.44
3139.85
3519.41
3606.32
ZeroEnergy[kJ/mol]          -177.40
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
End
End
Barrier L1 REACS FC01
RRHO
Stoichiometry C2N2H5
Core PhaseSpaceTheory
FragmentGeometry[angstrom]  7
C          -0.74064000   0.00000000   0.01360800
H          -1.12725000  -0.87638300  -0.50253800

```

```

H          -1.14607300   0.00000000   1.03050000
H          -1.12725000   0.87638400  -0.50253700
N           0.72026000   0.00000000  -0.07006200
H           1.10585300   0.81199300   0.39300800
H           1.10585300  -0.81199300   0.39300800

  FragmentGeometry [angstrom]          2
  C           0.00000000   0.00000000  -0.63181100
  N           0.00000000   0.00000000   0.54143400
SymmetryFactor  1.0000000000000000
  PotentialPrefactor [au]           64.2
  PotentialPowerExponent  6

End

Frequencies [1/cm]    16
  300.20
  834.61
  978.18
 1064.10
1178.30
1354.60
1472.48
1517.20
1536.05
1672.27
2076.80
3006.41
3092.76
3129.63
3519.95
3601.33

ZeroEnergy [kJ/mol]      0.00
ElectronicLevels [1/cm]      1
  0.0000000000000000    2.0000000000000000

End

Barrier TS0 FC01 RI
RRHO
  Geometry [angstrom]      9
  C           0.00000000  -1.09720900   0.00000000
  N           1.35452600  -0.84778800   0.00000000
  C          -1.11626800   0.70603600   0.00000000
  N          -0.47146700   1.69048500   0.00000000
  H          -0.39627600  -1.51179700  -0.91690600
  H          -0.39627600  -1.51179700   0.91690600
  H          -2.09283800   0.25152700   0.00000000
  H           1.70079300  -0.38988800  -0.82932000
  H           1.70079300  -0.38988800   0.82932000

Core RigidRotor
  SymmetryFactor  1.0

End

Tunneling Eckart
  ImaginaryFrequency [1/cm] 439.55
  WellDepth [kJ/mol]   43.6
  WellDepth [kJ/mol]   65.7

End

Frequencies [1/cm]    20
68.52 174.51 303.62 417.15 639.48
733.00 765.24 810.83 989.56 1002.28

```



```

1250.86 1360.71 1504.14 1679.45 1971.74
3132.64 3236.08 3238.57 3555.29 3650.56
ZeroEnergy[kJ/mol] -111.70
ElectronicLevels[1/cm] 1
  0 2
End
!*****
Barrier TS1 RI P1
RRHO
Geometry[angstrom] 9
C -0.37637500 -1.15785300 0.00000000
N -1.50393100 -1.48970200 0.00000000
C 0.00000000 0.94119800 0.00000000
H -0.52635600 1.16094400 0.91597600
N 1.34770700 1.24412200 0.00000000
H 1.86810200 1.06171100 0.84146500
H -0.52635600 1.16094400 -0.91597600
H 1.86810200 1.06171100 -0.84146500
H 0.66832000 -1.42632400 0.00000000
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 410.85
WellDepth[kJ/mol] 69.3
WellDepth[kJ/mol] 33.3
End
Frequencies[1/cm] 20
47.12 198.55 350.87 369.37 533.13
629.46 765.47 840.02 981.05 983.13
1231.41 1337.86 1496.14 1669.51 1977.54
3160.36 3212.85 3268.30 3580.86 3689.26
ZeroEnergy[kJ/mol] -108.10
ElectronicLevels[1/cm] 1
  0 2
End
!*****
Barrier TS2 RI P2
RRHO
Geometry[angstrom] 9
C -0.73927000 -0.02404700 0.00004600
N -1.85483100 -0.37639800 0.00001400
C 0.59330900 0.60138700 0.00002100
H 0.65490000 1.24835300 0.87485500
N 1.73184700 -0.30796900 -0.00002000
H 1.71082400 -0.90752400 0.81447000
H -2.99472100 0.64481000 -0.00036300
H 0.65486100 1.24837800 -0.87480000
H 1.71079000 -0.90749300 -0.81453100
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1219.30
WellDepth[kJ/mol] 120.1
WellDepth[kJ/mol] 26.8

```

```

End
Frequencies[1/cm]      20
10.91
182.81
263.95
415.59
441.95
649.53
825.77
890.51
918.53
1105.48
1194.16
1365.77
1391.15
1474.75
1676.62
2189.59
3070.93
3113.30
3522.03
3605.56
ZeroEnergy[kJ/mol]    -57.30
ElectronicLevels[1/cm]      1
  0      2
End
End

```

CBS-CVH

```

!*****
!          GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]      30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 220 240 260 280 300 350 400 450 500
PressureList[atm]       1.e-8
!
!
EnergyStepOverTemperature      .2
ExcessEnergyOverTemperature    30
ModelEnergyLimit[kcal/mol]     400
!
CalculationMethod              low-eigenvalue
!
WellCutoff                     20
ChemicalEigenvalueMax          0.2
!
ReductionMethod                 diagonalization
!
AtomDistanceMin[bohr]          1.3
!!
RateOutput                      fc01_HEATlike.out
!
!

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!           MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation
    Exponential
      Factor[1/cm]           260
      Power                   0.875
      ExponentCutoff         10
    End
!
  CollisionFrequency
    LennardJones
      Epsilons[K]            127.697  1382.375
      Sigmas[angstrom]       3.462    4.046
      Masses[amu]             39.948  70.07
    End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS - CH3NH2 + CN
!*****
Bimolecular REACS
Fragment CH3NH2
RRHO
Geometry[angstrom]         7
C          -0.74064000    0.00000000    0.01360800
H          -1.12725000   -0.87638300   -0.50253800
H          -1.14607300    0.00000000    1.03050000
H          -1.12725000    0.87638400   -0.50253700
N           0.72026000    0.00000000   -0.07006200
H           1.10585300    0.81199300    0.39300800
H           1.10585300   -0.81199300    0.39300800
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies[1/cm]        15
  300.20
  834.61
  978.18
  1064.10
  1178.30
  1354.60
  1472.48
  1517.20
  1536.05
  1672.27
  3006.41

```

```

3092.76
3129.63
3519.95
3601.33
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000        1.0000000000000000
!*****
End
!*****
Fragment CN
RRHO
Geometry[angstrom]         2
C          0.00000000    0.00000000   -0.63181100
N          0.00000000    0.00000000    0.54143400
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]         1
2076.80
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000        2.0000000000000000
!*****
End
!*****
GroundEnergy[kJ/mol] 0.0
End
!*****
! PRODUCT P1 - CH2NH2 + HCN
!*****
Bimolecular P1
Fragment CH2NH2
RRHO
Geometry[angstrom]         6
C          0.73716300    0.05207300    0.00000000
H          1.24098000   -0.16233200    0.92778800
H          1.24098000   -0.16233200   -0.92778800
N          -0.65004100   -0.05946900    0.00000000
H          -1.11367100    0.26546000    0.83278100
H          -1.11367100    0.26546000   -0.83278100
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]         12
455.87
608.48
672.66
941.68
1228.92
1332.81
1494.17
1661.62
3175.68
3289.29
3563.85

```

```

3668.18
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
!*****
End
!*****
Fragment HCN
RRHO
Geometry[angstrom]         3
C          0.00000000    0.00000000   -0.55868200
H          0.00000000    0.00000000   -1.62356200
N          0.00000000    0.00000000    0.59561500
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]         4
747.43
747.43
2124.86
3444.80
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000      1.0000000000000000
!*****
End
!*****
GroundEnergy[kJ/mol] -140.20
End
!*****
! PRODUCT P2 - AAN + H
!*****
Bimolecular P2
Fragment AAN
RRHO
Geometry[angstrom]         8
N          -1.57103400   -0.47328200   -0.06614300
H          -1.48750500   -1.09302700    0.72899000
H          -2.51570100   -0.11296900   -0.07859300
C          -0.61799900    0.62930100    0.03134800
H          -0.75621900    1.28659100   -0.82625400
H          -0.71181000    1.24606600    0.93131000
C          0.75714200    0.12420400   -0.00760700
N          1.84557000   -0.26792000   -0.00857200
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]         18
200.35
247.71
372.97
569.46
821.26
878.29
1011.17
1090.52

```

```

1198.39
1316.21
1430.00
1511.75
1668.36
2294.29
3014.18
3099.75
3522.30
3610.24
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000        1.0000000000000000
!*****
End
!*****
Fragment HYDROGEN
Atom
Name H
ElectronicLevels[1/cm]      1
0.0000000000000000        2.0000000000000000
!*****
End
GroundEnergy[kJ/mol]       -82.80
End
Well FC01
Species
RRHO ! transition state
Geometry[angstrom]         9
C      -1.75961900   0.70751200   0.00000200
N      -1.94559400  -0.66454800   0.00000100
H      -1.96563500   1.22008800  -0.92616900
H      -1.96559300   1.22008100   0.92618500
H       0.53087300   0.59788100  -0.00001100
H      -1.70666100  -1.16502300  -0.83939700
H      -1.70662200  -1.16502800   0.83938500
C       1.54268600   0.22600200  -0.00000600
N       2.62188500  -0.18638800   0.00000300
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]         21
40.34 71.38 136.95 149.68 185.17
511.30 575.14 729.22 848.06 861.82
943.55 1246.23 1328.18 1493.79 1665.76
2104.04 3165.10 3238.70 3277.59 3579.46
3687.37
ZeroEnergy[kJ/mol]          -153.50
ElectronicLevels[1/cm]      1
0.0000000000000000        2.0000000000000000
End
End
!*****
Well RI
Species
RRHO ! transition state

```

```

Geometry[angstrom]          9
C      -0.81668500  -0.17355500  0.35900500
N      -1.83377000  -0.09517100  -0.34924000
C      0.47780400   0.59647500  0.08989800
H      0.69617500   1.20943200  0.96394100
N      1.62364600  -0.25534900  -0.18366100
H      1.83966100  -0.85986400  0.59799600
H      0.31432000   1.26303800  -0.75239800
H      1.45881200  -0.84041500  -0.99214800
H      -0.80481900  -0.85607000  1.21949000

Core RigidRotor
SymmetryFactor  1.0000000000000000
End

Frequencies[1/cm]          21
111.64
295.78
361.91
429.13
781.88
814.81
917.98
961.28
1098.84
1131.21
1254.02
1353.86
1386.79
1495.95
1670.85
1726.45
2985.23
3076.44
3139.85
3519.41
3606.32

ZeroEnergy[kJ/mol]        -176.90

ElectronicLevels[1/cm]          1
0.0000000000000000  2.0000000000000000

End

End

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

Barrier L1 REACS FC01
RRHO
Stoichiometry C2N2H5
Core PhaseSpaceTheory
FragmentGeometry[angstrom]      7
C      -0.74064000  0.00000000  0.01360800
H      -1.12725000  -0.87638300  -0.50253800
H      -1.14607300  0.00000000  1.03050000
H      -1.12725000  0.87638400  -0.50253700
N      0.72026000  0.00000000  -0.07006200
H      1.10585300  0.81199300  0.39300800
H      1.10585300  -0.81199300  0.39300800

FragmentGeometry[angstrom]      2
C      0.00000000  0.00000000  -0.63181100
N      0.00000000  0.00000000  0.54143400

```

```

SymmetryFactor      1.0000000000000000
PotentialPrefactor[au]  64.2
PotentialPowerExponent  6
End
Frequencies[1/cm]    16
300.20
834.61
978.18
1064.10
1178.30
1354.60
1472.48
1517.20
1536.05
1672.27
2076.80
3006.41
3092.76
3129.63
3519.95
3601.33
ZeroEnergy[kJ/mol]   0.00
ElectronicLevels[1/cm]  1
0.0000000000000000  2.0000000000000000
End
!*****
Barrier TS0 FC01 RI
RRHO
Geometry[angstrom]  9
C      0.00000000  -1.09720900  0.00000000
N      1.35452600  -0.84778800  0.00000000
C     -1.11626800   0.70603600  0.00000000
N     -0.47146700   1.69048500  0.00000000
H     -0.39627600  -1.51179700  -0.91690600
H     -0.39627600  -1.51179700   0.91690600
H     -2.09283800   0.25152700  0.00000000
H      1.70079300  -0.38988800  -0.82932000
H      1.70079300  -0.38988800   0.82932000
Core RigidRotor
SymmetryFactor      1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm]  439.55
WellDepth[kJ/mol]        41.6
WellDepth[kJ/mol]        65.0
End
Frequencies[1/cm]    20
68.52 174.51 303.62 417.15 639.48
733.00 765.24 810.83 989.56 1002.28
1250.86 1360.71 1504.14 1679.45 1971.74
3132.64 3236.08 3238.57 3555.29 3650.56
ZeroEnergy[kJ/mol]   -111.90
ElectronicLevels[1/cm]  1
0      2
End
!*****

```



```

Barrier TS1 RI P1
RRHO
  Geometry [angstrom]      9
  C      -0.37637500  -1.15785300  0.00000000
  N      -1.50393100  -1.48970200  0.00000000
  C      0.00000000    0.94119800  0.00000000
  H      -0.52635600  1.16094400  0.91597600
  N      1.34770700   1.24412200  0.00000000
  H      1.86810200   1.06171100  0.84146500
  H      -0.52635600  1.16094400 -0.91597600
  H      1.86810200   1.06171100 -0.84146500
  H      0.66832000  -1.42632400  0.00000000
Core RigidRotor
  SymmetryFactor  1.0
End
Tunneling Eckart
  ImaginaryFrequency [1/cm]  410.85
  WellDepth [kJ/mol]      68.6
  WellDepth [kJ/mol]      31.9
End
Frequencies [1/cm]      20
47.12 198.55 350.87 369.37 533.13
629.46 765.47 840.02 981.05 983.13
1231.41 1337.86 1496.14 1669.51 1977.54
3160.36 3212.85 3268.30 3580.86 3689.26
ZeroEnergy [kJ/mol] -108.10
  ElectronicLevels [1/cm]      1
    0      2

```

End

!*****

```

Barrier TS2 RI P2
RRHO
  Geometry [angstrom]      9
  C      -0.73927000  -0.02404700  0.00004600
  N      -1.85483100  -0.37639800  0.00001400
  C      0.59330900    0.60138700  0.00002100
  H      0.65490000   1.24835300  0.87485500
  N      1.73184700  -0.30796900 -0.00002000
  H      1.71082400  -0.90752400  0.81447000
  H      -2.99472100  0.64481000 -0.00036300
  H      0.65486100   1.24837800 -0.87480000
  H      1.71079000  -0.90749300 -0.81453100
Core RigidRotor
  SymmetryFactor  1.0
End
Tunneling Eckart
  ImaginaryFrequency [1/cm]  1219.30
  WellDepth [kJ/mol]      120.10
  WellDepth [kJ/mol]      26.00
End
Frequencies [1/cm]      20
10.91
182.81
263.95
415.59
441.95

```

```

649.53
825.77
890.51
918.53
1105.48
1194.16
1365.77
1391.15
1474.75
1676.62
2189.59
3070.93
3113.30
3522.03
3605.56
ZeroEnergy[kJ/mol] -56.80
ElectronicLevels[1/cm] 1
0 2
End
End

```

CBS-QB3

```

!*****
! GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K] 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 220 240 260 280 300 350 400 450 500
PressureList[atm] 1.e-8
!
!
EnergyStepOverTemperature .2
ExcessEnergyOverTemperature 30
ModelEnergyLimit[kcal/mol] 400
!
CalculationMethod low-eigenvalue
!
WellCutoff 20
ChemicalEigenvalueMax 0.2
!
ReductionMethod diagonalization
AtomDistanceMin[bohr] 1.3
!!
RateOutput fc01_CBSQB3.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model

```

```

!
EnergyRelaxation
  Exponential
    Factor[1/cm]          260
    Power                 0.875
    ExponentCutoff       10
  End
!
CollisionFrequency
  LennardJones
    Epsilons[K]          127.697  1382.375
    Sigmas[angstrom]    3.462  4.046
    Masses[amu]         39.948  70.07
  End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS - CH3NH2 + CN
!*****
Bimolecular REACS
Fragment CH3NH2
RRHO
Geometry[angstrom]      7
C      0.05052800  0.70535200  0.00000000
H      0.59223700  1.06563400 -0.87850300
H     -0.94333700  1.18056700  0.00000000
H      0.59223700  1.06563400  0.87850300
N      0.05052800 -0.76080300  0.00000000
H     -0.44900100 -1.10916200  0.81210100
H     -0.44900100 -1.10916200 -0.81210100
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies[1/cm]    15
316.27
851.39
979.67
1056.00
1170.62
1352.24
1461.12
1496.80
1518.88
1668.86
2947.98
3051.48
3086.76
3488.87
3562.98
ZeroEnergy[kJ/mol]    0.
ElectronicLevels[1/cm]  1
0.0000000000000000  1.0000000000000000
!*****

```

```

End
!*****
Fragment CN
RRHO
Geometry[angstrom]      2
C      0.00000000  0.00000000  -0.62766800
N      0.00000000  0.00000000   0.53800100
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies [1/cm]      1
  2152.08
ZeroEnergy[kJ/mol]      0.
ElectronicLevels[1/cm]      1
  0.0000000000000000  2.0000000000000000
!*****
End
!*****
GroundEnergy[kJ/mol] 0.0
End
!*****
! PRODUCT P1 - CH2NH2 + HCN
!*****
Bimolecular P1
Fragment CH2NH2
RRHO
Geometry[angstrom]      6
C      0.01156800  0.73376100  0.00000000
H      0.29512000  1.21317300  0.92862900
H      0.29512000  1.21317300 -0.92862900
N      0.01156800 -0.66370000  0.00000000
H      -0.37031000 -1.09150700  0.83280600
H      -0.37031000 -1.09150700 -0.83280600
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies [1/cm]      12
456.57
634.33
718.25
945.40
1221.52
1327.71
1477.69
1655.79
3127.77
3235.58
3530.33
3629.03
ZeroEnergy[kJ/mol]      0.
ElectronicLevels[1/cm]      1
  0.0000000000000000  2.0000000000000000
!*****
End
!*****
Fragment HCN

```

```

RRHO
Geometry[angstrom]      3
C      0.00000000  0.00000000 -0.49814100
H      0.00000000  0.00000000 -1.56440500
N      0.00000000  0.00000000  0.65046400

Core RigidRotor
SymmetryFactor  1.0000000000000000
End

Frequencies[1/cm]      4
785.56
785.56
2200.47
3457.47

ZeroEnergy[kJ/mol]      0.
ElectronicLevels[1/cm]      1
0.0000000000000000  1.0000000000000000
!*****
End
!*****
GroundEnergy[kJ/mol] -140.86
End
!*****
! PRODUCT P2 - AAN + H
!*****
Bimolecular P2
Fragment AAN
RRHO
Geometry[angstrom]      8
N      -1.48498600 -0.48890600 -0.11390600
H      -1.45790900 -1.10714600  0.69034800
H      -2.42302700 -0.10779600 -0.17350900
C      -0.52292900  0.60257600  0.04826100
H      -0.64995500  1.30621000 -0.77974700
H      -0.61951800  1.18427500  0.97839000
C      0.85402500  0.09840800 -0.00847600
N      1.93696200 -0.29415800 -0.02240700

Core RigidRotor
SymmetryFactor  1.0000000000000000
End

Frequencies[1/cm]      18
208.33
247.34
384.37
575.08
822.17
875.77
999.57
1082.24
1195.93
1313.31
1421.78
1492.19
1664.62
2365.29
2959.46
3061.83

```

```

3502.01
3583.99
ZeroEnergy [kJ/mol]          0.
ElectronicLevels [1/cm]      1
0.000000000000000000      1.000000000000000000
!*****
End
!*****
Fragment HYDROGEN
Atom
Name H
ElectronicLevels [1/cm]      1
0.000000000000000000      2.000000000000000000
!*****
End
GroundEnergy [kJ/mol]       -85.55
End
!*****
Well FC01
Species
RRHO ! transition state
Geometry [angstrom]         9
C          -1.55252900   0.68848400   0.00000700
N          -2.15266700  -0.56470500   0.00001000
H          -1.62056800   1.24692800  -0.92650100
H          -1.62057600   1.24693700   0.92650900
H          0.73366900    0.35009000   0.00000200
H          -2.05433600  -1.11687100  -0.83979300
H          -2.05434500  -1.11686300   0.83982000
C          1.78462000    0.09203600  -0.00000600
N          2.89889700   -0.19148700  -0.00001600
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies [1/cm]         21
27.76
86.45
117.58
157.89
192.92
518.78
616.91
775.47
890.37
902.06
950.71
1239.85
1323.73
1479.00
1659.86
2170.61
3119.15
3211.56
3225.90
3553.56
3655.27

```

```

ZeroEnergy[kJ/mol]          -153.30
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
End
End
!*****
Well RI
Species
RRHO ! transition state
Geometry[angstrom]         9
C          -0.82498100  -0.17560100  0.35612500
N          -1.84233100  -0.09200500  -0.34956600
C           0.48411900   0.59567200  0.09332400
H           0.70097200   1.20639300  0.97490100
N           1.63189700  -0.25472300  -0.18405100
H           1.83523500  -0.87435200  0.59344800
H           0.32059100   1.27170300  -0.74654200
H           1.46555600  -0.83254100  -1.00134800
H           -0.80414300  -0.86453800  1.21816300
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm]         21
108.91
313.96
358.17
427.84
769.98
822.12
912.75
928.74
1096.05
1125.66
1245.90
1342.55
1382.17
1479.10
1668.53
1717.76
2937.10
3044.11
3107.73
3498.34
3579.19
ZeroEnergy[kJ/mol]          -180.90
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
End
End
!*****
Barrier L1 REACS FC01
RRHO
Stoichiometry C2N2H5
Core PhaseSpaceTheory
FragmentGeometry[angstrom] 7
C           0.05052800  0.70535200  0.00000000

```

```

H          0.59223700   1.06563400  -0.87850300
H          -0.94333700   1.18056700   0.00000000
H          0.59223700   1.06563400   0.87850300
N          0.05052800  -0.76080300   0.00000000
H          -0.44900100  -1.10916200   0.81210100
H          -0.44900100  -1.10916200  -0.81210100
  FragmentGeometry[angstrom]      2
C          0.00000000   0.00000000  -0.62766800
N          0.00000000   0.00000000   0.53800100
SymmetryFactor  1.0000000000000000
  PotentialPrefactor[au]      94.4
  PotentialPowerExponent  6
End
Frequencies[1/cm]      16
316.27
851.39
979.67
1056.00
1170.62
1352.24
1461.12
1496.80
1518.88
1668.86
2152.08
2947.98
3051.48
3086.76
3488.87
3562.98
ZeroEnergy[kJ/mol]      0.00
ElectronicLevels[1/cm]      1
  0.0000000000000000      2.0000000000000000
End
Barrier TSO FC01 RI
RRHO
  Geometry[angstrom]      9
C          0.00000000   1.13383200   0.00000000
N          1.35605500   0.87199700   0.00000000
C          -1.13064900  -0.75223200   0.00000000
N          -0.45504300  -1.71237700   0.00000000
H          -0.39615700   1.55087000   0.92022400
H          -0.39615700   1.55087000  -0.92022400
H          -2.11415300  -0.30942200   0.00000000
H          1.69163900   0.40036800   0.83024300
H          1.69163900   0.40036800  -0.83024300
Core RigidRotor
  SymmetryFactor  1.0
End
Tunneling Eckart
  ImaginaryFrequency[1/cm]  367.27
  WellDepth[kJ/mol]      36.0
  WellDepth[kJ/mol]      63.6
End
Frequencies[1/cm]      20
62.30

```



```

160.79
286.91
397.00
620.62
753.71
754.32
776.79
943.39
993.56
1243.97
1352.35
1489.97
1672.67
1976.26
3106.77
3207.91
3240.18
3531.68
3621.98
ZeroEnergy[kJ/mol] -117.32
ElectronicLevels[1/cm] 1
0 2
End
!*****
Barrier TS1 RI P1
RRHO
Geometry[angstrom] 9
C -0.38083300 -1.19919900 0.00000000
N -1.50353400 -1.53720700 0.00000000
C 0.00000000 0.97709500 0.00000000
H -0.52965100 1.19378200 0.91914200
N 1.35088200 1.28243600 0.00000000
H 1.87045500 1.08368200 0.84246500
H -0.52965100 1.19378200 -0.91914200
H 1.87045500 1.08368200 -0.84246500
H 0.67195300 -1.43890100 0.00000000
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 339.79
WellDepth[kJ/mol] 67.2
WellDepth[kJ/mol] 27.2
End
Frequencies[1/cm] 20
47.13
175.78
335.20
352.64
559.08
609.78
754.45
790.32
934.94
972.71
1227.71

```

```

1328.82
1481.76
1662.58
1982.61
3134.67
3216.22
3239.94
3557.74
3660.87
ZeroEnergy[kJ/mol] -113.71
ElectronicLevels[1/cm] 1
0 2
End
!*****
Barrier TS2 RI P2
RRHO
Geometry[angstrom] 9
C -0.74374200 0.00743800 0.00000800
N -1.83837200 -0.39316500 0.00000500
C 0.60087800 0.61071200 0.00000300
H 0.67763900 1.26156500 0.87618400
N 1.72634900 -0.32216400 -0.00000600
H 1.68399000 -0.92523900 0.81537600
H -3.08189000 0.62574800 -0.00005100
H 0.67762900 1.26157000 -0.87617400
H 1.68397700 -0.92523800 -0.81538900
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 952.55
WellDepth[kJ/mol] 123.9
WellDepth[kJ/mol] 28.6
End
Frequencies[1/cm] 20
26.79
176.11
276.40
417.37
425.02
615.91
829.35
889.62
911.65
1096.45
1192.55
1358.22
1385.83
1457.88
1673.45
2210.83
3040.62
3076.78
3498.74
3576.03
ZeroEnergy[kJ/mol] -57.00

```

```

ElectronicLevels[1/cm]          1
    0      2
End
End

```

CN attack to the NH₂ moiety jChS

```

!*****
!          GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]              30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 220 240 260 280 300 350 400 450 500
PressureList[atm]               1.e-8

!
!
EnergyStepOverTemperature       .2
ExcessEnergyOverTemperature     30
ModelEnergyLimit[kcal/mol]      400
!
CalculationMethod               low-eigenvalue
!
WellCutoff                      20
ChemicalEigenvalueMax           0.2
!
ReductionMethod                 diagonalization
!
AtomDistanceMin[bohr]          1.3
!!
RateOutput                      ic01_ChS.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!          MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation
    Exponential
      Factor[1/cm]              260
      Power                     0.875
      ExponentCutoff            10
    End
!
  CollisionFrequency

```

```

LennardJones
  Epsilons[K]          127.697  1382.375
  Sigmas[angstrom]    3.462   4.046
  Masses[amu]         39.948  70.07
End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS - CH3NH2 + CN
!*****

Bimolecular REACS
Fragment CH3NH2
RRHO
Geometry[angstrom]    7
C          -0.74064000  0.00000000  0.01360800
H          -1.12725000 -0.87638300 -0.50253800
H          -1.14607300  0.00000000  1.03050000
H          -1.12725000  0.87638400 -0.50253700
N           0.72026000  0.00000000 -0.07006200
H           1.10585300  0.81199300  0.39300800
H           1.10585300 -0.81199300  0.39300800

Core RigidRotor
SymmetryFactor  1.0000000000000000
End

  Frequencies[1/cm]    15
  300.20
  834.61
  978.18
  1064.10
  1178.30
  1354.60
  1472.48
  1517.20
  1536.05
  1672.27
  3006.41
  3092.76
  3129.63
  3519.95
  3601.33

ZeroEnergy[kJ/mol]    0.
ElectronicLevels[1/cm]  1
  0.0000000000000000  1.0000000000000000
!*****
End
!*****
Fragment CN
RRHO
Geometry[angstrom]    2
C          0.00000000  0.00000000 -0.63181100
N          0.00000000  0.00000000  0.54143400

Core RigidRotor
SymmetryFactor  1.0000000000000000

```

```

End
  Frequencies [1/cm]      1
  2076.80
ZeroEnergy [kJ/mol]      0.
ElectronicLevels [1/cm]      1
  0.0000000000000000      2.0000000000000000
!*****
End
!*****
GroundEnergy [kJ/mol] 0.0
End
Bimolecular P3
Fragment CH3NH
RRHO
Geometry [angstrom]      6
  C      -0.69085600      0.00887000      0.00000000
  H      -1.05474600      0.55868200      0.87622200
  H      -1.05474500      0.55864600      -0.87624400
  H      -1.13400600      -0.98338300      0.00002000
  N      0.74594800      -0.08039400      0.00000000
  H      1.10494300      0.87746000      0.00000000
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
  Frequencies [1/cm]      12
255.66
958.87
1010.57
1053.99
1343.98
1410.00
1498.21
1500.11
2985.70
3026.18
3127.98
3420.26
  ZeroEnergy [kJ/mol]      0.
  ElectronicLevels [1/cm]      1
  0.0000000000000000      2.0000000000000000
!*****
End
!*****
Fragment HCN
RRHO
Geometry [angstrom]      3
  C      0.00000000      0.00000000      -0.55868200
  H      0.00000000      0.00000000      -1.62356200
  N      0.00000000      0.00000000      0.59561500
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
  Frequencies [1/cm]      4
  747.43
  747.43
  2124.86

```

```

3444.80
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000      1.0000000000000000
!*****
End
!*****
GroundEnergy[kJ/mol] -111.90
End
!*****
! PRODUCT P4 - CH3NHCN + H
!*****
Bimolecular P4
Fragment CH3NHCN
RRHO
Geometry[angstrom]         8
C          1.53244100    -0.37898500    0.02157500
N          0.43209200    0.58397800   -0.10011300
C          -0.81909400    0.11839600   -0.00760600
N          -1.90285100   -0.30468800    0.02081700
H          2.45946800    0.13032500   -0.22343000
H          1.60598600   -0.80817300    1.02109600
H          1.37601000   -1.17815600   -0.69645000
H          0.57376600    1.46450200    0.37003800
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm]         18
158.52
218.91
423.84
536.28
640.38
932.04
1152.59
1162.17
1204.99
1471.04
1475.34
1512.01
1535.38
2280.77
3055.05
3135.64
3169.35
3599.36
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000      1.0000000000000000
!*****
End
!*****
Fragment HYDROGEN
Atom
Name H
ElectronicLevels[1/cm]      1

```

```

0.0000000000000000    2.0000000000000000
!*****
End
GroundEnergy[kJ/mol] -58.00
End
!*****
! PRODUCT P5 - NH2CN + CH3
!*****
Bimolecular P5
Fragment NH2CN
RRHO
Geometry[angstrom]      5
N          -0.08716600   -1.12179000   0.00000000
C           0.00000000    0.21953600   0.00000000
N           0.01641700    1.38102100   0.00000000
H           0.24762200   -1.56591400   0.84100100
H           0.24762200   -1.56591400  -0.84100100

Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]      9
404.14
486.58
594.16
1083.11
1204.01
1643.46
2300.28
3564.12
3659.42
ZeroEnergy[kJ/mol]      0.
ElectronicLevels[1/cm]  1
0.0000000000000000    1.0000000000000000
!*****
End
!*****
Fragment CH3
RRHO
Geometry[angstrom]      4
H           0.00000000    1.07590000   0.00000000
C           0.00000000    0.00000000   0.00000000
H          -0.93175700   -0.53795000   0.00000000
H           0.93175700   -0.53795000   0.00000000

Core RigidRotor
SymmetryFactor  6.0
End
Frequencies[1/cm]      6
526.96
1426.53
1426.53
3138.66
3319.82
3319.82
ZeroEnergy[kJ/mol]      0.
ElectronicLevels[1/cm]  1
0.0000000000000000    2.0000000000000000

```

```

!*****
End
!*****
GroundEnergy[kJ/mol] -142.70
End
!*****
Well IC
Species
RRHO ! transition state
Geometry[angstrom] 9
C 0.29460700 -1.50040600 0.00000000
N -0.86441000 -0.61200300 0.00000000
C -0.18734900 1.31574300 0.00000000
N 0.92703100 1.68660400 0.00000000
H 0.00000000 -2.54992400 0.00000000
H 0.89462600 -1.28692000 -0.87827200
H 0.89462600 -1.28692000 0.87827200
H -1.43557700 -0.64523300 -0.83215800
H -1.43557700 -0.64523300 0.83215800
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 21
24.78
132.03
172.11
264.31
436.02
536.71
839.50
962.22
1049.53
1155.95
1321.96
1469.63
1510.06
1514.86
1651.20
2066.50
3060.30
3148.70
3181.49
3541.98
3642.59
ZeroEnergy[kJ/mol] -65.60
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
End
!*****
Well FC02
Species
RRHO ! transition state
Geometry[angstrom] 9
C 1.66001200 0.06662700 -0.00000400
N 2.79086200 -0.17012900 0.00000300

```



```

C          -2.42608800  -0.48814000  0.00000100
N          -1.45407200  0.57096900  -0.00000200
H          -3.08074200  -0.41850500  0.87608300
H          -3.08076300  -0.41848500  -0.87606400
H          -1.93627100  -1.45772100  -0.00001700
H           0.60167200  0.28371700  -0.00000900
H          -1.95618900  1.46047500  0.00002200

```

Core RigidRotor

SymmetryFactor 1.0000000000000000

End

Frequencies[1/cm] 21

37.26

71.02

153.41

155.12

188.95

342.93

918.96

927.71

967.71

1016.71

1068.77

1344.50

1409.88

1494.32

1504.55

2104.21

2994.20

3037.06

3136.97

3219.83

3442.82

ZeroEnergy[kJ/mol] -134.10

ElectronicLevels[1/cm] 1

0.0000000000000000 2.0000000000000000

End

End

Barrier L2 REACS IC

RRHO

Stoichiometry C2N2H5

Core PhaseSpaceTheory

FragmentGeometry[angstrom] 7

C -0.74064000 0.00000000 0.01360800

H -1.12725000 -0.87638300 -0.50253800

H -1.14607300 0.00000000 1.03050000

H -1.12725000 0.87638400 -0.50253700

N 0.72026000 0.00000000 -0.07006200

H 1.10585300 0.81199300 0.39300800

H 1.10585300 -0.81199300 0.39300800

FragmentGeometry[angstrom] 2

C 0.00000000 0.00000000 -0.63181100

N 0.00000000 0.00000000 0.54143400

SymmetryFactor 1.0000000000000000

PotentialPrefactor[au] 94.4

PotentialPowerExponent 6

End

```

Frequencies[1/cm]      16
300.20
834.61
978.18
1064.10
1178.30
1354.60
1472.48
1517.20
1536.05
1672.27
2076.80
3006.41
3092.76
3129.63
3519.95
3601.33
ZeroEnergy[kJ/mol]    0.00
ElectronicLevels[1/cm]      1
0.0000000000000000    2.0000000000000000
End
Barrier L4 FC02 P3
RRHO
Stoichiometry C2N2H5
Core PhaseSpaceTheory
FragmentGeometry[angstrom]      6
  C      -0.69085600   0.00887000   0.00000000
H      -1.05474600   0.55868200   0.87622200
H      -1.05474500   0.55864600  -0.87624400
H      -1.13400600  -0.98338300   0.00002000
N       0.74594800  -0.08039400   0.00000000
H       1.10494300   0.87746000   0.00000000
FragmentGeometry[angstrom]      3
  C       0.00000000   0.00000000  -0.55868200
H       0.00000000   0.00000000  -1.62356200
N       0.00000000   0.00000000   0.59561500
SymmetryFactor      1.0000000000000000
PotentialPrefactor[au]      3703.38
PotentialPowerExponent      6
End
Frequencies[1/cm]      16
255.66
747.43
747.43
958.87
1010.57
1053.99
1343.98
1410.00
1498.21
1500.11
2124.86
2985.70
3026.18
3127.98
3420.26

```

```

3444.80
ZeroEnergy[kJ/mol]      -111.90
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
End
!*****
Barrier TS3 IC FC02
RRHO
Geometry[angstrom]      9
C      -1.33741800      0.19176100      0.17890200
N      -2.34945200      -0.30513400      -0.12626400
C      1.70239700      -0.56940300      0.00091500
N      1.07127000      0.73480900      0.02464900
H      1.23907200      -1.25220200      -0.71168700
H      2.74469900      -0.43572600      -0.28906700
H      1.66084400      -1.00657900      0.99315100
H      0.12879500      0.79015700      0.53223000
H      0.98398500      1.16247500      -0.89221900
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 535.14
WellDepth[kJ/mol]      30.2
WellDepth[kJ/mol]      98.7
End
Frequencies[1/cm]      20
77.52
103.17
147.98
227.06
350.41
713.50
973.18
1052.64
1105.93
1315.92
1452.23
1489.76
1514.96
1583.50
2126.15
2478.08
3049.19
3107.07
3166.10
3535.45
ZeroEnergy[kJ/mol] -35.40
ElectronicLevels[1/cm]      1
0      2
End
!*****
Barrier TS4 IC P4
RRHO
Geometry[angstrom]      9
C      1.52806200      -0.43812800      0.02657200

```

N	0.41957900	0.56413300	-0.02968000
C	-0.84204700	-0.01160500	-0.20031800
N	-1.94366900	-0.25912100	0.11660800
H	2.44466700	0.10873900	0.22491700
H	1.31521500	-1.11200800	0.84889100
H	1.58828300	-0.98581600	-0.90655900
H	0.61920500	1.31471200	1.04264900
H	0.58516800	1.23768500	-0.77592400

Core RigidRotor

SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1434.92

WellDepth[kJ/mol] 89.5

WellDepth[kJ/mol] 81.9

End

Frequencies[1/cm] 20

174.82

199.88

382.91

537.21

705.43

789.04

893.61

1082.33

1092.11

1172.72

1214.86

1412.44

1452.21

1503.22

1517.79

2155.85

3091.68

3184.78

3196.63

3455.44

ZeroEnergy[kJ/mol] 23.90

ElectronicLevels[1/cm] 1

0 2

End

!*****

Barrier TS5 IC P5

RRHO

Geometry[angstrom] 9

C	-1.74878000	0.21620800	0.00000000
N	0.00000000	0.78377900	0.00000000
C	1.11650200	-0.14313300	0.00000000
N	1.36926600	-1.29687500	0.00000000
H	-2.34597400	1.11780000	0.00000000
H	-1.80704600	-0.36970000	-0.90503900
H	-1.80704600	-0.36970000	0.90503900
H	0.08443400	1.38741300	-0.81741300
H	0.08443400	1.38741300	0.81741300

Core RigidRotor

SymmetryFactor 1.0

```

End
Tunneling   Eckart
  ImaginaryFrequency[1/cm]  791.49
  WellDepth[kJ/mol]        87.0
  WellDepth[kJ/mol]        164.1
End
Frequencies[1/cm]          20
86.08
151.75
242.52
502.17
577.01
656.91
863.11
874.81
1114.14
1144.58
1214.79
1448.80
1460.47
1601.47
2054.94
3113.24
3252.34
3260.97
3419.62
3507.47
ZeroEnergy[kJ/mol]  21.40
  ElectronicLevels[1/cm]          1
    0      2
End
End

```

CBS-CVH

```

!*****
!          GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]          30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 220 240 260 280 300 350 400 450 500
PressureList[atm]           1.e-8
!
!
EnergyStepOverTemperature   .2
ExcessEnergyOverTemperature 30
ModelEnergyLimit[kcal/mol]  400
!
CalculationMethod           low-eigenvalue
!
WellCutoff                  20
ChemicalEigenvalueMax       0.2
!
ReductionMethod             diagonalization

```

```

AtomDistanceMin[bohr]          1.3
!!
RateOutput                      ic01_HEATlike.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!           MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation
    Exponential
      Factor[1/cm]              260
      Power                     0.875
      ExponentCutoff            10
    End
!
  CollisionFrequency
    LennardJones
      Epsilons[K]               127.697  1382.375
      Sigmas[angstrom]          3.462   4.046
      Masses[amu]                39.948  70.07
    End
!
!*****
!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS - CH3NH2 + CN
!*****
Bimolecular REACS
Fragment CH3NH2
RRHO
Geometry[angstrom]             7
C          -0.74064000  0.00000000  0.01360800
H          -1.12725000 -0.87638300 -0.50253800
H          -1.14607300  0.00000000  1.03050000
H          -1.12725000  0.87638400 -0.50253700
N           0.72026000  0.00000000 -0.07006200
H           1.10585300  0.81199300  0.39300800
H           1.10585300 -0.81199300  0.39300800
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
  Frequencies[1/cm]            15
  300.20
  834.61
  978.18
  1064.10
  1178.30
  1354.60

```

```

1472.48
1517.20
1536.05
1672.27
3006.41
3092.76
3129.63
3519.95
3601.33
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000      1.0000000000000000
!*****
End
!*****
Fragment CN
RRHO
Geometry[angstrom]         2
C          0.00000000    0.00000000   -0.63181100
N          0.00000000    0.00000000    0.54143400
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]         1
2076.80
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
!*****
End
!*****
GroundEnergy[kJ/mol] 0.0
End
!*****
! PRODUCT P3 - CH3NH + HCN
!*****
Bimolecular P3
Fragment CH3NH
RRHO
Geometry[angstrom]         6
C          -0.69085600    0.00887000    0.00000000
H          -1.05474600    0.55868200    0.87622200
H          -1.05474500    0.55864600   -0.87624400
H          -1.13400600   -0.98338300    0.00002000
N           0.74594800   -0.08039400    0.00000000
H           1.10494300    0.87746000    0.00000000
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]         12
255.66
958.87
1010.57
1053.99
1343.98
1410.00

```

```

1498.21
1500.11
2985.70
3026.18
3127.98
3420.26
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000        2.0000000000000000
!*****
End
!*****
Fragment HCN
RRHO
Geometry[angstrom]         3
C          0.00000000    0.00000000   -0.55868200
H          0.00000000    0.00000000   -1.62356200
N          0.00000000    0.00000000    0.59561500
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]         4
747.43
747.43
2124.86
3444.80
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000        1.0000000000000000
!*****
End
!*****
GroundEnergy[kJ/mol] -110.70
End
!*****
! PRODUCT P4 - CH3NHCN + H
!*****
Bimolecular P4
Fragment CH3NHCN
RRHO
Geometry[angstrom]         8
C          1.53244100   -0.37898500    0.02157500
N          0.43209200    0.58397800   -0.10011300
C          -0.81909400    0.11839600   -0.00760600
N          -1.90285100   -0.30468800    0.02081700
H          2.45946800    0.13032500   -0.22343000
H          1.60598600   -0.80817300    1.02109600
H          1.37601000   -1.17815600   -0.69645000
H          0.57376600    1.46450200    0.37003800
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]         18
158.52
218.91
423.84

```



```

536.28
640.38
932.04
1152.59
1162.17
1204.99
1471.04
1475.34
1512.01
1535.38
2280.77
3055.05
3135.64
3169.35
3599.36
ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]      1
0.0000000000000000        1.0000000000000000
!*****
End
!*****
Fragment HYDROGEN
Atom
Name H
ElectronicLevels[1/cm]      1
0.0000000000000000        2.0000000000000000
!*****
End
GroundEnergy[kJ/mol] -56.70
End
!*****
! PRODUCT P5 - NH2CN + CH3
!*****
Bimolecular P5
Fragment NH2CN
RRHO
Geometry[angstrom]          5
N          -0.08716600  -1.12179000  0.00000000
C           0.00000000   0.21953600  0.00000000
N           0.01641700   1.38102100  0.00000000
H           0.24762200  -1.56591400  0.84100100
H           0.24762200  -1.56591400 -0.84100100
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]          9
404.14
486.58
594.16
1083.11
1204.01
1643.46
2300.28
3564.12
3659.42
ZeroEnergy[kJ/mol]          0.

```

```

ElectronicLevels[1/cm]          1
0.0000000000000000          1.0000000000000000
!*****

End

!*****

Fragment CH3
RRHO
Geometry[angstrom]          4
  H          0.00000000    1.07590000    0.00000000
  C          0.00000000    0.00000000    0.00000000
  H         -0.93175700   -0.53795000    0.00000000
  H          0.93175700   -0.53795000    0.00000000

Core RigidRotor
SymmetryFactor    6.0
End

  Frequencies[1/cm]          6
  526.96
  1426.53
  1426.53
  3138.66
  3319.82
  3319.82

ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]          1
0.0000000000000000          2.0000000000000000
!*****

End

!*****

GroundEnergy[kJ/mol] -140.40
End

!*****

Well IC
Species
RRHO ! transition state
Geometry[angstrom]          9
  C          0.29460700   -1.50040600    0.00000000
  N         -0.86441000   -0.61200300    0.00000000
  C         -0.18734900    1.31574300    0.00000000
  N          0.92703100    1.68660400    0.00000000
  H          0.00000000   -2.54992400    0.00000000
  H          0.89462600   -1.28692000   -0.87827200
  H          0.89462600   -1.28692000    0.87827200
  H         -1.43557700   -0.64523300   -0.83215800
  H         -1.43557700   -0.64523300    0.83215800

Core RigidRotor
SymmetryFactor    1.0000000000000000
End

  Frequencies[1/cm]          21
  24.78
  132.03
  172.11
  264.31
  436.02
  536.71
  839.50
  962.22

```

```

1049.53
1155.95
1321.96
1469.63
1510.06
1514.86
1651.20
2066.50
3060.30
3148.70
3181.49
3541.98
3642.59
ZeroEnergy[kJ/mol]      -63.60
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
End
End
!*****
Well FC02
Species
RRHO ! transition state
Geometry[angstrom]      9
C      1.66001200      0.06662700      -0.00000400
N      2.79086200      -0.17012900      0.00000300
C      -2.42608800      -0.48814000      0.00000100
N      -1.45407200      0.57096900      -0.00000200
H      -3.08074200      -0.41850500      0.87608300
H      -3.08076300      -0.41848500      -0.87606400
H      -1.93627100      -1.45772100      -0.00001700
H      0.60167200      0.28371700      -0.00000900
H      -1.95618900      1.46047500      0.00002200
Core RigidRotor
SymmetryFactor      1.0000000000000000
End
Frequencies[1/cm]      21
37.26
71.02
153.41
155.12
188.95
342.93
918.96
927.71
967.71
1016.71
1068.77
1344.50
1409.88
1494.32
1504.55
2104.21
2994.20
3037.06
3136.97
3219.83

```

```

3442.82
ZeroEnergy[kJ/mol]      -133.00
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
End
End
!*****
Barrier L2 REACS IC
RRHO
Stoichiometry C2N2H5
Core PhaseSpaceTheory
FragmentGeometry[angstrom]      7
C      -0.74064000  0.00000000  0.01360800
H      -1.12725000 -0.87638300 -0.50253800
H      -1.14607300  0.00000000  1.03050000
H      -1.12725000  0.87638400 -0.50253700
N      0.72026000  0.00000000 -0.07006200
H      1.10585300  0.81199300  0.39300800
H      1.10585300 -0.81199300  0.39300800
FragmentGeometry[angstrom]      2
C      0.00000000  0.00000000 -0.63181100
N      0.00000000  0.00000000  0.54143400
SymmetryFactor 1.0000000000000000
PotentialPrefactor[au]      94.4
PotentialPowerExponent 6
End
Frequencies[1/cm]      16
300.20
834.61
978.18
1064.10
1178.30
1354.60
1472.48
1517.20
1536.05
1672.27
2076.80
3006.41
3092.76
3129.63
3519.95
3601.33
ZeroEnergy[kJ/mol]      0.00
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
End
Barrier L4 FC02 P3
RRHO
Stoichiometry C2N2H5
Core PhaseSpaceTheory
FragmentGeometry[angstrom]      6
C      -0.69085600  0.00887000  0.00000000
H      -1.05474600  0.55868200  0.87622200
H      -1.05474500  0.55864600 -0.87624400
H      -1.13400600 -0.98338300  0.00002000

```

```

N          0.74594800  -0.08039400  0.00000000
H          1.10494300  0.87746000  0.00000000
  FragmentGeometry[angstrom]          3
    C          0.00000000  0.00000000  -0.55868200
    H          0.00000000  0.00000000  -1.62356200
    N          0.00000000  0.00000000  0.59561500
SymmetryFactor  1.0000000000000000
  PotentialPrefactor[au]          3703.38
  PotentialPowerExponent  6
End
Frequencies[1/cm]  16
255.66
747.43
747.43
958.87
1010.57
1053.99
1343.98
1410.00
1498.21
1500.11
2124.86
2985.70
3026.18
3127.98
3420.26
3444.80
ZeroEnergy[kJ/mol]          -110.70
ElectronicLevels[1/cm]          1
0.0000000000000000  2.0000000000000000
End
!*****
Barrier TS3 IC FC02
RRHO
  Geometry[angstrom]          9
    C          -1.33741800  0.19176100  0.17890200
    N          -2.34945200  -0.30513400  -0.12626400
    C          1.70239700  -0.56940300  0.00091500
    N          1.07127000  0.73480900  0.02464900
    H          1.23907200  -1.25220200  -0.71168700
    H          2.74469900  -0.43572600  -0.28906700
    H          1.66084400  -1.00657900  0.99315100
    H          0.12879500  0.79015700  0.53223000
    H          0.98398500  1.16247500  -0.89221900
Core RigidRotor
  SymmetryFactor  1.0
End
Tunneling Eckart
  ImaginaryFrequency[1/cm]  535.14
  WellDepth[kJ/mol]  27.2
  WellDepth[kJ/mol]  96.6
End
Frequencies[1/cm]  20
  77.52
  103.17
  147.98

```

```

227.06
350.41
713.50
973.18
1052.64
1105.93
1315.92
1452.23
1489.76
1514.96
1583.50
2126.15
2478.08
3049.19
3107.07
3166.10
3535.45
ZeroEnergy[kJ/mol] -36.40
ElectronicLevels[1/cm] 1
0 2
End
!*****
Barrier TS4 IC P4
RRHO
Geometry[angstrom] 9
C 1.52806200 -0.43812800 0.02657200
N 0.41957900 0.56413300 -0.02968000
C -0.84204700 -0.01160500 -0.20031800
N -1.94366900 -0.25912100 0.11660800
H 2.44466700 0.10873900 0.22491700
H 1.31521500 -1.11200800 0.84889100
H 1.58828300 -0.98581600 -0.90655900
H 0.61920500 1.31471200 1.04264900
H 0.58516800 1.23768500 -0.77592400
Core RigidRotor
SymmetryFactor 1.0
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1434.92
WellDepth[kJ/mol] 87.6
WellDepth[kJ/mol] 80.7
End
Frequencies[1/cm] 20
174.82
199.88
382.91
537.21
705.43
789.04
893.61
1082.33
1092.11
1172.72
1214.86
1412.44
1452.21

```

```

1503.22
1517.79
2155.85
3091.68
3184.78
3196.63
3455.44
ZeroEnergy[kJ/mol] 24.00
  ElectronicLevels[1/cm]          1
    0      2
End
!*****
Barrier TS5 IC P5
RRHO
  Geometry[angstrom]      9
  C      -1.74878000   0.21620800   0.00000000
  N      0.00000000   0.78377900   0.00000000
  C      1.11650200  -0.14313300   0.00000000
  N      1.36926600  -1.29687500   0.00000000
  H      -2.34597400   1.11780000   0.00000000
  H      -1.80704600  -0.36970000  -0.90503900
  H      -1.80704600  -0.36970000   0.90503900
  H      0.08443400   1.38741300  -0.81741300
  H      0.08443400   1.38741300   0.81741300
Core RigidRotor
  SymmetryFactor 1.0
End
Tunneling Eckart
  ImaginaryFrequency[1/cm] 791.49
  WellDepth[kJ/mol]      86.5
  WellDepth[kJ/mol]     163.3
End
Frequencies[1/cm]      20
86.08
151.75
242.52
502.17
577.01
656.91
863.11
874.81
1114.14
1144.58
1214.79
1448.80
1460.47
1601.47
2054.94
3113.24
3252.34
3260.97
3419.62
3507.47
ZeroEnergy[kJ/mol] 22.90
  ElectronicLevels[1/cm]          1
    0      2

```

End
End

CBS-QB3

```
!*****
!           GLOBAL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]           30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 220 240 260 280 300 350 400 450 500
PressureList[atm]            1.e-8
!
!
EnergyStepOverTemperature    .2
ExcessEnergyOverTemperature  30
ModelEnergyLimit [kcal/mol]  400
!
CalculationMethod            low-eigenvalue
!
WellCutoff                   20
ChemicalEigenvalueMax        0.2
!
ReductionMethod              diagonalization
!
AtomDistanceMin[bohr]        1.3
!!
RateOutput                   ic01_CBSQB3.out
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
!           MODEL SECTION
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
  EnergyRelaxation
  Exponential
    Factor [1/cm]             260
    Power                     0.875
    ExponentCutoff            10
  End
!
  CollisionFrequency
  LennardJones
    Epsilons[K]               127.697  1382.375
    Sigmas [angstrom]         3.462    4.046
    Masses [amu]              39.948  70.07
  End
!
!*****
```



```

!
!*****
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*****
! REACTANTS - CH3NH2 + CN
!*****

Bimolecular REACS
Fragment CH3NH2
RRHO
Geometry[angstrom]          7
C          0.05052800   0.70535200   0.00000000
H          0.59223700   1.06563400  -0.87850300
H         -0.94333700   1.18056700   0.00000000
H          0.59223700   1.06563400   0.87850300
N          0.05052800  -0.76080300   0.00000000
H         -0.44900100  -1.10916200   0.81210100
H         -0.44900100  -1.10916200  -0.81210100

Core RigidRotor
SymmetryFactor  1.0000000000000000
End

Frequencies[1/cm]          15
316.27
851.39
979.67
1056.00
1170.62
1352.24
1461.12
1496.80
1518.88
1668.86
2947.98
3051.48
3086.76
3488.87
3562.98

ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]          1
0.0000000000000000   1.0000000000000000
!*****
End
!*****

Fragment CN
RRHO
Geometry[angstrom]          2
C          0.00000000   0.00000000  -0.62766800
N          0.00000000   0.00000000   0.53800100

Core RigidRotor
SymmetryFactor  1.0000000000000000
End

Frequencies[1/cm]          1
2152.08

ZeroEnergy[kJ/mol]          0.
ElectronicLevels[1/cm]          1
0.0000000000000000   2.0000000000000000
!*****

```

```

End
!*****
GroundEnergy[kJ/mol] 0.0
End
!*****
! PRODUCT P3 - CH3NH + HCN
!*****
Bimolecular P3
Fragment CH3NH
RRHO
Geometry[angstrom]      6
C          -0.62788900   -0.01188200   0.00000000
H          -0.97212900   -0.58181800  -0.87879400
H          -0.97212600   -0.58178500   0.87881800
H          -1.12710100   0.95935900  -0.00001700
N          0.80507200    0.15292000  -0.00000200
H          1.20318700   -0.79490500   0.00000700
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies [1/cm]      12
256.20
949.26
1008.25
1042.84
1341.71
1394.87
1479.27
1486.82
2939.89
2972.35
3082.63
3370.22
ZeroEnergy[kJ/mol]      0.
ElectronicLevels [1/cm]      1
0.0000000000000000      2.0000000000000000
!*****
End
!*****
Fragment HCN
RRHO
Geometry[angstrom]      3
C          0.00000000    0.00000000  -0.49814100
H          0.00000000    0.00000000  -1.56440500
N          0.00000000    0.00000000   0.65046400
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies [1/cm]      4
785.56
785.56
2200.47
3457.47
ZeroEnergy[kJ/mol]      0.
ElectronicLevels [1/cm]      1
0.0000000000000000      1.0000000000000000

```

```

!*****
End
!*****
GroundEnergy[kJ/mol] -113.03
End
!*****
! PRODUCT P4 - CH3NHCN + H
!*****
Bimolecular P4
Fragment CH3NHCN
RRHO
Geometry[angstrom]      8
C          1.54537800    -0.37046500    0.02081200
N          0.42494100    0.57313700   -0.09318200
C          -0.82589600    0.11111900   -0.00754900
N          -1.90883200   -0.30115300    0.02014500
H          2.46023400    0.14566000   -0.27121100
H          1.66201800   -0.77180700    1.03325800
H          1.38190500   -1.19686900   -0.67061600
H          0.56618800    1.47520500    0.34025300
Core RigidRotor
SymmetryFactor  1.0000000000000000
End
Frequencies[1/cm]      18
150.70
223.65
412.21
542.28
636.06
929.71
1140.20
1161.77
1203.81
1463.06
1469.04
1494.25
1521.31
2342.83
3018.44
3099.67
3134.52
3585.82
ZeroEnergy[kJ/mol]      0.
ElectronicLevels[1/cm]      1
0.0000000000000000      1.0000000000000000
!*****
End
!*****
Fragment HYDROGEN
Atom
Name H
ElectronicLevels[1/cm]      1
0.0000000000000000      2.0000000000000000
!*****
End
GroundEnergy[kJ/mol] -63.09

```

```

End
!*****
! PRODUCT P5 - NH2CN + CH3
!*****
Bimolecular P5
Fragment NH2CN
RRHO
Geometry[angstrom]      5
N          -0.09084700   -1.11782700   0.00000000
C          0.00000000    0.22085100   0.00000000
N          0.02567200    1.37768600   0.00000000
H          0.22811300   -1.57206300   0.84494500
H          0.22811300   -1.57206300  -0.84494500

Core RigidRotor
SymmetryFactor  1.0000000000000000
End

Frequencies[1/cm]      9
415.74
491.92
572.53
1096.32
1197.75
1636.02
2361.64
3550.73
3641.60

ZeroEnergy[kJ/mol]      0.
ElectronicLevels[1/cm]  1
0.0000000000000000    1.0000000000000000
!*****
End
!*****
Fragment CH3
RRHO
Geometry[angstrom]      4
H          0.00000000    1.08045600   0.00000000
C          0.00000000    0.00000000   0.00000000
H          0.93570200   -0.54022800   0.00000000
H          -0.93570200  -0.54022800   0.00000000

Core RigidRotor
SymmetryFactor  6.0
End

Frequencies[1/cm]      6
505.11
1403.09
1403.09
3103.65
3282.67
3282.67

ZeroEnergy[kJ/mol]      0.
ElectronicLevels[1/cm]  1
0.0000000000000000    2.0000000000000000
!*****
End
!*****
GroundEnergy[kJ/mol] -138.33

```

```

End
!*****
Well IC
Species
RRHO ! transition state
Geometry[angstrom] 9
C 1.40985800 0.68350600 0.00000000
N 0.00000000 1.07029000 0.00000000
C -1.18538600 -0.65684100 0.00000000
N -0.85538900 -1.77768800 0.00000000
H 2.07361500 1.55497200 0.00000000
H 1.60558700 0.07397300 0.88102200
H 1.60558700 0.07397300 -0.88102200
H -0.32195000 1.54443700 0.83450600
H -0.32195000 1.54443700 -0.83450600
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 21
12.91
106.76
164.75
232.66
406.04
526.42
814.73
960.00
1044.02
1141.45
1313.03
1456.10
1493.90
1497.40
1646.27
2118.95
3020.96
3114.27
3148.60
3535.84
3632.78
ZeroEnergy[kJ/mol] -69.14
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
End
!*****
Well FC02
Species
RRHO ! transition state
Geometry[angstrom] 9
C 1.83345300 0.03434200 -0.00000200
N 2.96465600 -0.17257200 -0.00001300
C -2.33316100 -0.42244100 0.00001300
N -1.27398200 0.55184600 -0.00000200
H -2.98601300 -0.30103800 0.87882600
H -2.98600700 -0.30107300 -0.87881000

```

```

H          -1.92733300  -1.43508900  0.00003500
H          0.76705300   0.22778900  0.00000800
H          -1.70417000   1.48309400 -0.00002200
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Frequencies[1/cm] 21
48.73
71.19
156.70
157.47
202.19
351.47
940.25
959.26
966.32
1014.49
1064.32
1337.14
1394.35
1475.49
1490.33
2172.03
2953.03
2988.37
3099.85
3209.15
3407.51
ZeroEnergy[kJ/mol] -135.36
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
End
!*****
Barrier L2 REACS IC
RRHO
Stoichiometry C2N2H5
Core PhaseSpaceTheory
FragmentGeometry[angstrom] 7
C          0.05052800  0.70535200  0.00000000
H          0.59223700  1.06563400 -0.87850300
H          -0.94333700  1.18056700  0.00000000
H          0.59223700  1.06563400  0.87850300
N          0.05052800 -0.76080300  0.00000000
H          -0.44900100 -1.10916200  0.81210100
H          -0.44900100 -1.10916200 -0.81210100
FragmentGeometry[angstrom] 2
C          0.00000000  0.00000000 -0.62766800
N          0.00000000  0.00000000  0.53800100
SymmetryFactor 1.0000000000000000
PotentialPrefactor[au] 94.4
PotentialPowerExponent 6
End
Frequencies[1/cm] 16
316.27
851.39

```

```

979.67
1056.00
1170.62
1352.24
1461.12
1496.80
1518.88
1668.86
2152.08
2947.98
3051.48
3086.76
3488.87
3562.98
ZeroEnergy[kJ/mol]          0.00
ElectronicLevels[1/cm]      1
0.000000000000000000      2.000000000000000000
End
Barrier L4 FC02 P3
RRHO
Stoichiometry C2N2H5
Core PhaseSpaceTheory
FragmentGeometry[angstrom]  6
C          -0.62788900  -0.01188200  0.00000000
H          -0.97212900  -0.58181800  -0.87879400
H          -0.97212600  -0.58178500  0.87881800
H          -1.12710100  0.95935900  -0.00001700
N          0.80507200   0.15292000  -0.00000200
H          1.20318700  -0.79490500  0.00000700
FragmentGeometry[angstrom]  3
C          0.00000000   0.00000000  -0.49814100
H          0.00000000   0.00000000  -1.56440500
N          0.00000000   0.00000000  0.65046400
SymmetryFactor 1.0000000000000000
PotentialPrefactor[au]      3703.38
PotentialPowerExponent 6
End
Frequencies[1/cm] 16
256.20
785.56
785.56
949.26
1008.25
1042.84
1341.71
1394.87
1479.27
1486.82
2200.47
2939.89
2972.35
3082.63
3370.22
3457.47
ZeroEnergy[kJ/mol]          -113.03
ElectronicLevels[1/cm]      1

```

```

0.0000000000000000      2.0000000000000000
End
!*****
Barrier TS3 IC FC02
RRHO
  Geometry[angstrom]      9
C      -1.38528600    0.15805100    0.14934700
N      -2.42905700   -0.28650200   -0.10902500
C      1.76902700   -0.55603500   -0.00472200
N      1.09189200    0.72566900    0.03119700
H      1.28510700   -1.27251300   -0.67686700
H      2.79231900   -0.39866000   -0.35838500
H      1.79985800   -0.97739900    0.99933600
H      0.20713800    0.78922000    0.58673900
H      0.97328400    1.17308900   -0.87377400
Core RigidRotor
  SymmetryFactor  1.0
End
Tunneling Eckart
  ImaginaryFrequency[1/cm]  299.22
  WellDepth[kJ/mol]        40.7
  WellDepth[kJ/mol]        176.1
End
  Frequencies[1/cm]        20
75.03
102.52
143.38
211.48
300.00
689.54
961.21
1050.33
1099.16
1305.23
1441.69
1474.45
1501.09
1608.46
2198.72
2952.25
3018.71
3073.48
3133.36
3546.51
  ZeroEnergy[kJ/mol]  -28.43
  ElectronicLevels[1/cm]      1
    0      2
End
!*****
Barrier TS4 IC P4
RRHO
  Geometry[angstrom]      9
C      1.54138300   -0.42609200    0.03378800
N      0.41103500    0.55615300   -0.03357600
C      -0.84677200   -0.04590900   -0.21448800
N      -1.95011000   -0.24089900    0.12901500

```


H	2.44972500	0.13919700	0.24123400
H	1.33736900	-1.10840100	0.85650700
H	1.62127700	-0.97638600	-0.90109900
H	0.62553400	1.35670000	1.01721700
H	0.57195000	1.21412100	-0.79772700

Core RigidRotor
SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm]	1231.85
WellDepth[kJ/mol]	94.2
WellDepth[kJ/mol]	88.2

End

Frequencies[1/cm] 20

171.48
202.59
389.15
543.78
750.62
804.85
903.73
1077.20
1102.87
1164.16
1228.20
1410.27
1440.53
1487.75
1504.63
2148.03
3064.99
3152.23
3165.33
3450.08

ZeroEnergy[kJ/mol] 25.08

ElectronicLevels[1/cm]	1
0	2

End

!*****

Barrier TS5 IC P5

RRHO

Geometry[angstrom] 9

C	1.76544900	0.23959900	0.00000000
N	0.00000000	0.76894900	0.00000000
C	-1.14942100	-0.14605200	0.00000000
N	-1.36655600	-1.30739400	0.00000000
H	2.35933700	1.14832400	0.00000000
H	1.84066500	-0.34872300	0.90647500
H	1.84066500	-0.34872300	-0.90647500
H	-0.08547300	1.37847400	0.81581400
H	-0.08547300	1.37847400	-0.81581400

Core RigidRotor

SymmetryFactor 1.0

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 746.35

```
WellDepth[kJ/mol]      84.2
WellDepth[kJ/mol]      153.4
End
Frequencies[1/cm]      20
83.72
147.85
236.40
508.19
574.54
635.53
845.04
873.70
1115.58
1164.31
1220.66
1436.81
1448.91
1594.80
2027.05
3088.27
3222.09
3234.43
3418.60
3499.22
ZeroEnergy[kJ/mol]    15.07
ElectronicLevels[1/cm]      1
0      2
End
End
```