

Annexure A

A.1 POTENTIAL ENERGY PROFILE HFCO

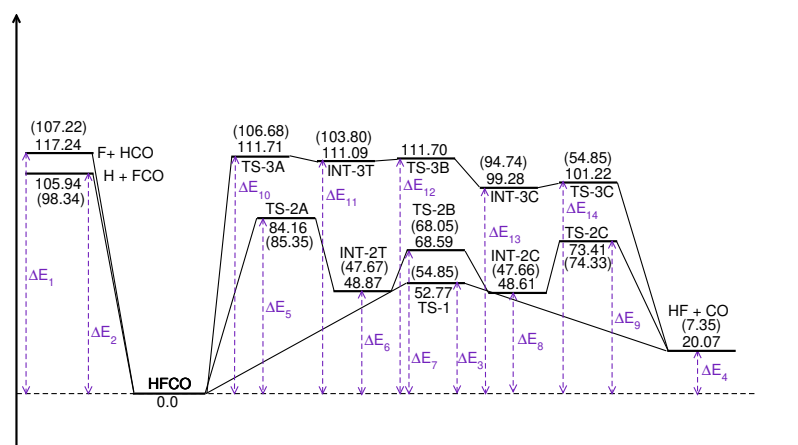


Figure A.1 : Dissociation energy profile of HFCO computed using B3LYP/6-31G*/ECP level of theory. The given energies are in units of kcal/mol and without zero point energy corrections. The numbers in bracket are CCSD(T)/6-31G*/ECP single point energies computed using MP2/6-31G*/ECP optimized geometries.

HCICO

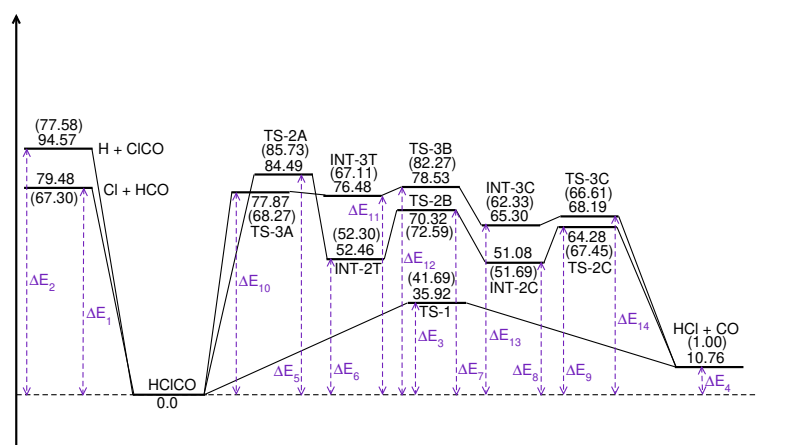


Figure A.2 : Dissociation energy profile of HCICO computed using B3LYP/6-31G*/ECP level of theory. The given energies are in units of kcal/mol and without zero point energy corrections. The numbers in bracket are CCSD(T)/6-31G*/ECP single point energies computed using MP2/6-31G*/ECP optimized geometries.

HBrCO

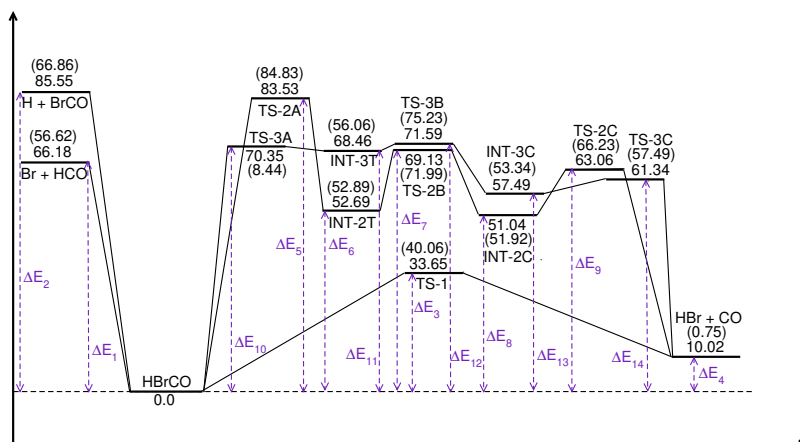


Figure A.3. : Dissociation energy profile of HBrCO computed using B₃LYP/6-31G*/ECP level of theory. The given energies are in units of kcal/mol and without zero point energy corrections. The numbers in bracket are CCSD(T)/6-31G*/ECP single point energies computed using MP2/6-31G*/ECP optimized geometries.

HICO

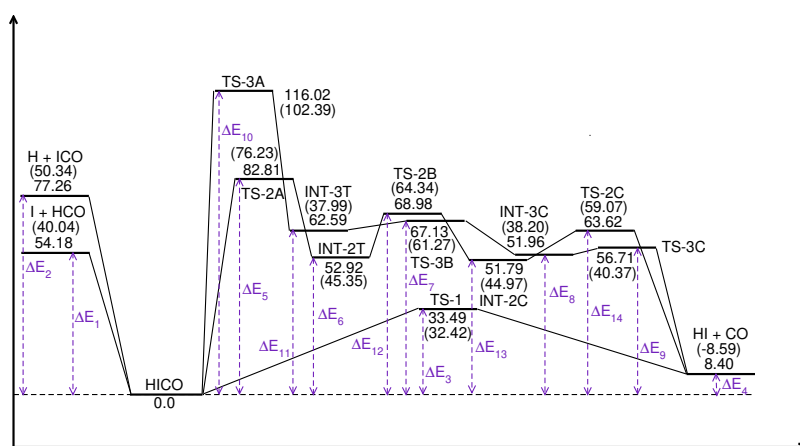


Figure A.4. : Dissociation energy profile of HICO computed using B₃LYP/6-31G*/ECP level of theory. The given energies are in units of kcal/mol and without zero point energy corrections. The numbers in bracket are CCSD(T)/6-31G*/ECP single point energies computed using MP2/6-31G*/ECP optimized geometries.

A.2 TRAJECTORY SNAPSHOTS

A.2.1 HFCO

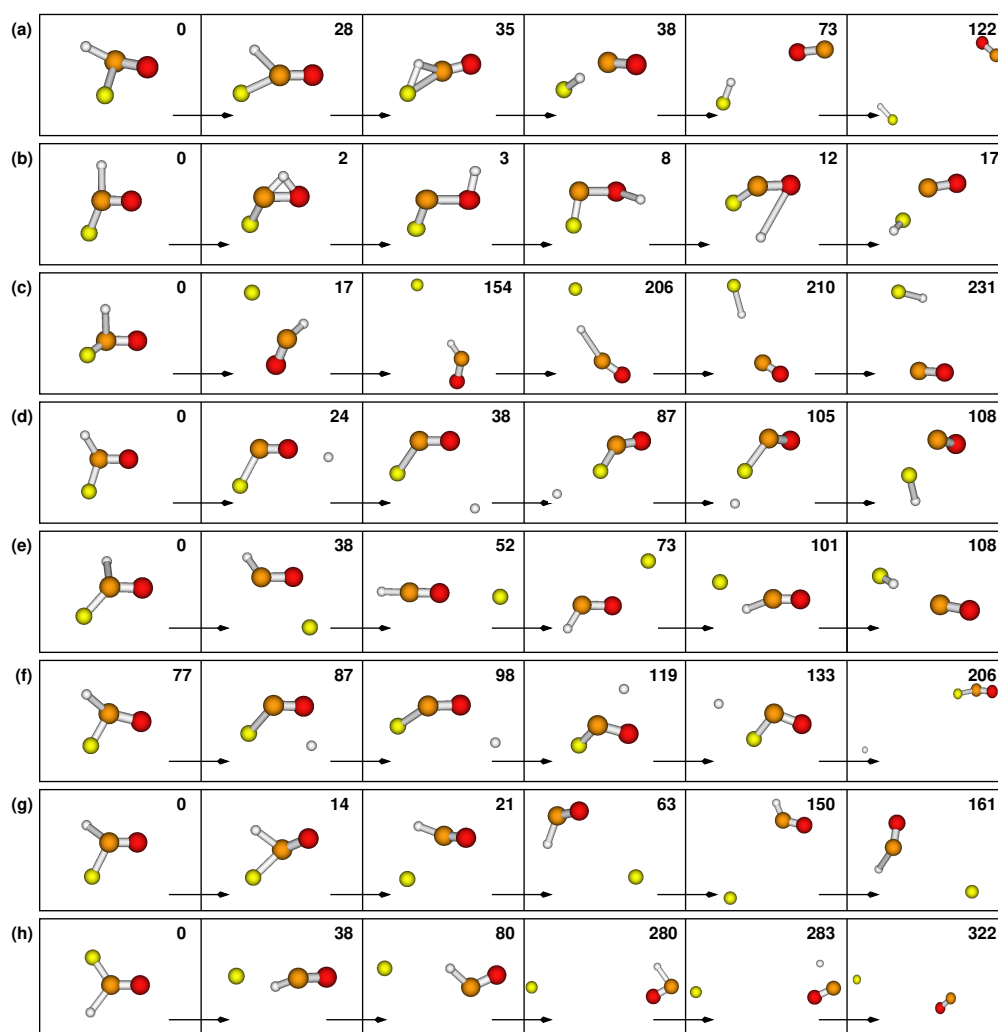


Figure A.5. : Snapshots of HFCO Trajectories. The numbers inside the frames are time in fs at which the snapshot was taken.

Descriptions of the trajectories:

- (a) $\text{HFCO} \rightarrow \text{HF} + \text{CO}$ (concerted)
- (b) $\text{HFCO} \rightarrow \text{HOCF} \rightarrow \text{HF} + \text{CO}$ (1,2-H shift)
- (c) $\text{HFCO} \rightarrow \text{F} + \text{HCO} \rightarrow \text{HF} + \text{CO}$ (radical recombination)
- (d) $\text{HFCO} \rightarrow \text{H} + \text{FCO} \rightarrow \text{HF} + \text{CO}$ (H roaming)
- (e) $\text{HFCO} \rightarrow \text{F} + \text{HCO} \rightarrow \text{HF} + \text{CO}$ (F roaming)
- (f) $\text{HFCO} \rightarrow \text{H} + \text{FCO}$ (radical path)
- (g) $\text{HFCO} \rightarrow \text{F} + \text{HCO}$ (radical path)
- (h) $\text{HFCO} \rightarrow \text{F} + \text{HCO} \rightarrow \text{F} + \text{H} + \text{CO}$

A.2.2 HCICO

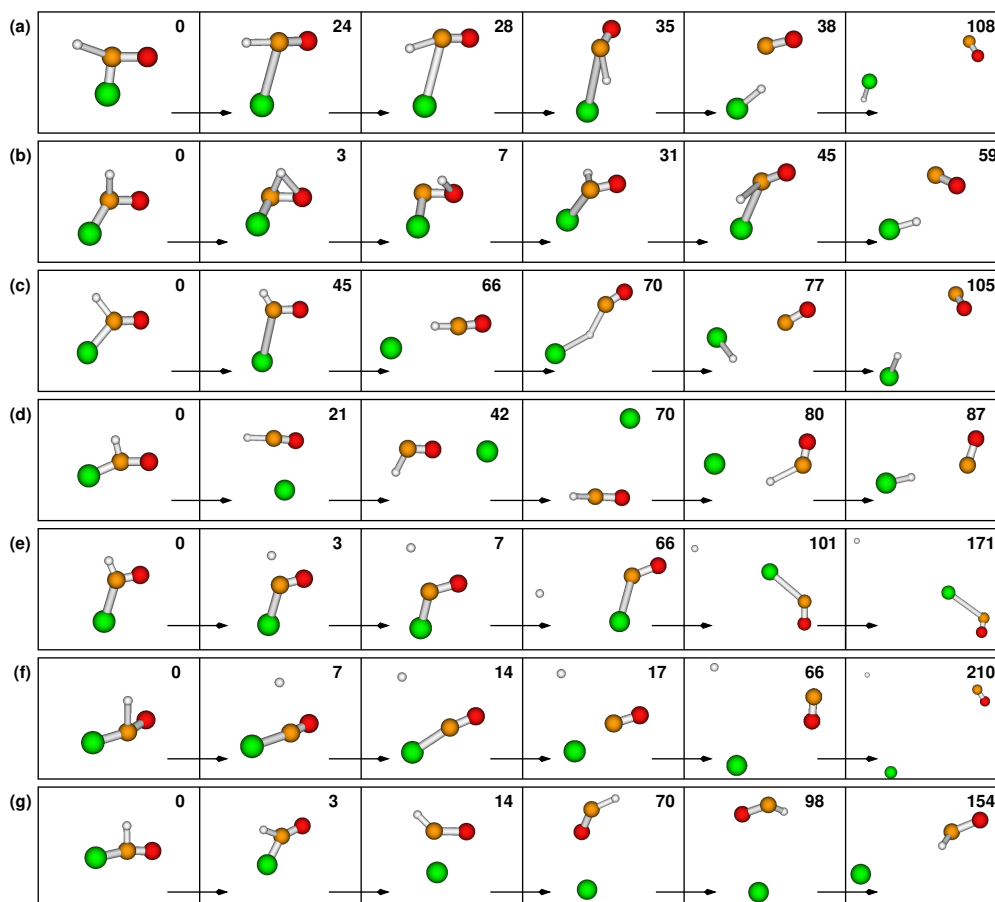


Figure A.6. : Snapshots of HCICO Trajectories. The numbers inside the frames are time in fs at which the snapshot was taken.

Descriptions of the trajectories:

- (a) $\text{HCICO} \rightarrow \text{HCl} + \text{CO}$ (concerted)
- (b) $\text{HCICO} \rightarrow \text{HOCCl} \rightarrow \text{HCICO} \rightarrow \text{HCl} + \text{CO}$ (1,2-H-shift and recross)
- (c) $\text{HCICO} \rightarrow \text{Cl} + \text{HCO} \rightarrow \text{HCl} + \text{CO}$ (radical recombination)
- (d) $\text{HCICO} \rightarrow \text{Cl} + \text{HCO} \rightarrow \text{HCl} + \text{CO}$ (Cl roaming)
- (e) $\text{HCICO} \rightarrow \text{H} + \text{ClCO}$ (radical pathway)
- (f) $\text{HCICO} \rightarrow \text{H} + \text{ClCO} \rightarrow \text{H} + \text{Cl} + \text{CO}$
- (g) $\text{HCICO} \rightarrow \text{Cl} + \text{HCO}$ (radical pathway)

A.2.3 HBrCO

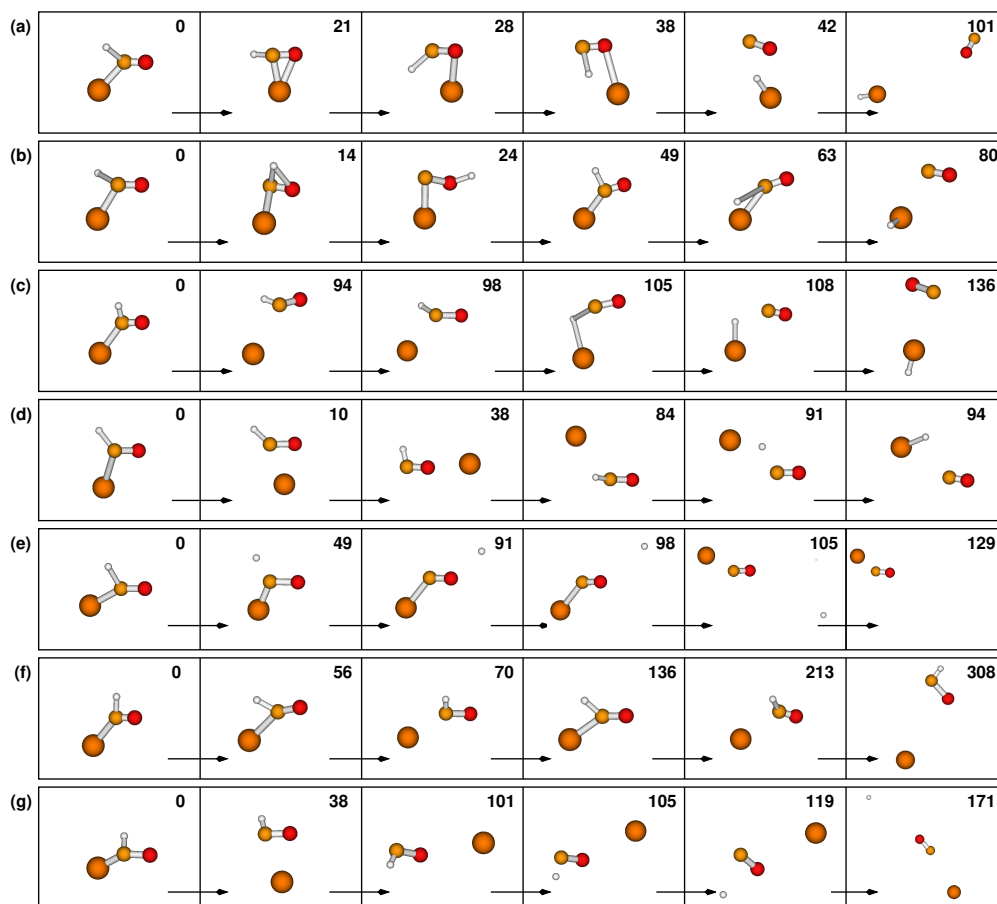


Figure A.7. : Snapshots of HBrCO Trajectories. The numbers inside the frames are time in fs at which the snapshot was taken.

Descriptions of the trajectories:

- (a) $\text{HBrCO} \rightarrow \text{HBr} + \text{CO}$ (concerted)
- (b) $\text{HBrCO} \rightarrow \text{HOBr} \rightarrow \text{HBrCO} \rightarrow \text{HBr} + \text{CO}$ (1,2-H-shift and recross)
- (c) $\text{HBrCO} \rightarrow \text{Br} + \text{HCO} \rightarrow \text{HBr} + \text{CO}$ (radical recombination)
- (d) $\text{HBrCO} \rightarrow \text{Br} + \text{HCO} \rightarrow \text{HBr} + \text{CO}$ (Br roaming)
- (e) $\text{HBrCO} \rightarrow \text{H} + \text{BrCO} \rightarrow \text{H} + \text{Br} + \text{CO}$
- (f) $\text{HBrCO} \rightarrow \text{Br} + \text{HCO}$ (radical pathway)
- (g) $\text{HBrCO} \rightarrow \text{Br} + \text{HCO} \rightarrow \text{Br} + \text{H} + \text{CO}$

A.2.4 HICO

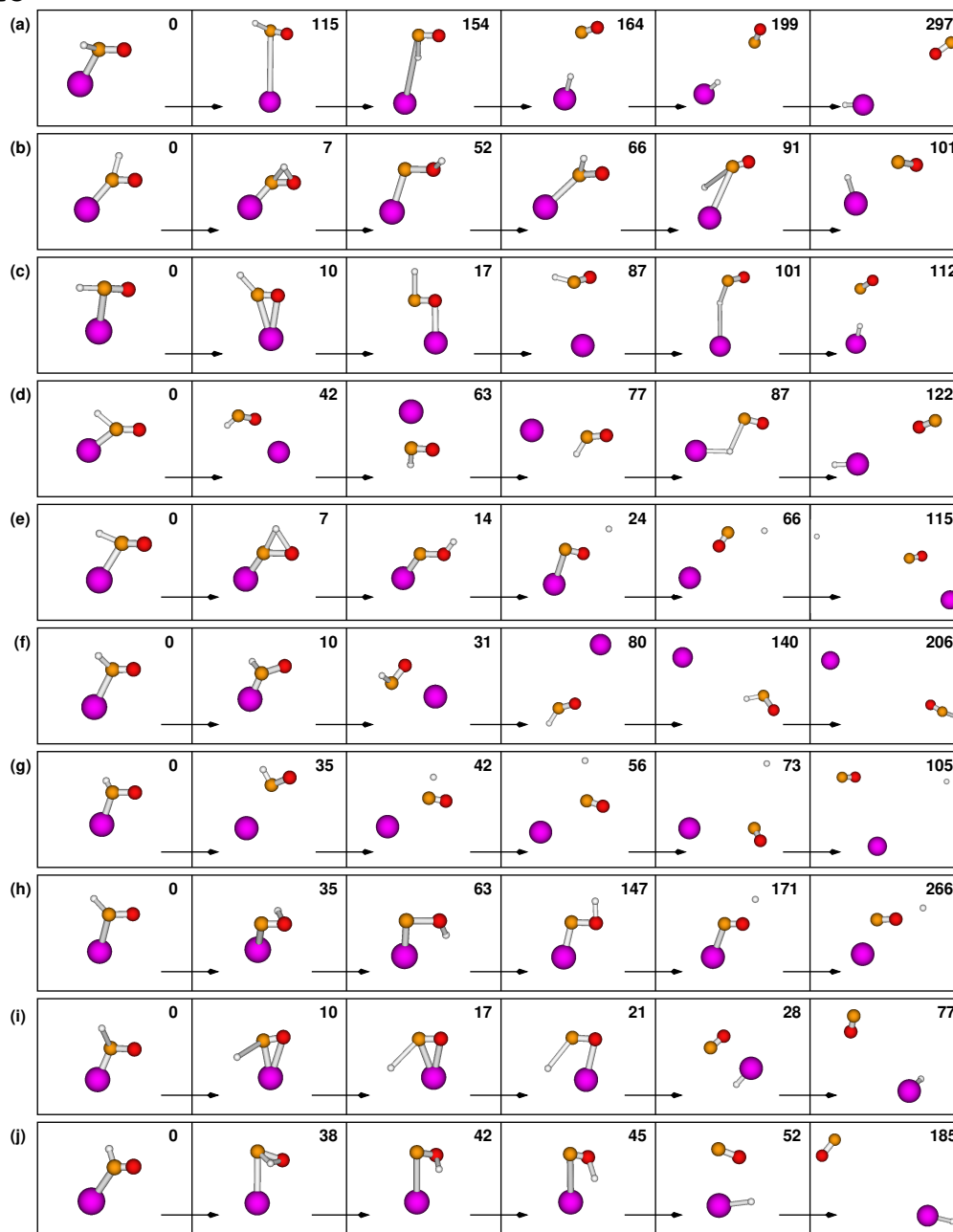


Figure A.8. : Snapshots of HICO Trajectories. The numbers inside the frames are time in fs at which the snapshot was taken.

Descriptions of the trajectories:

- (a) $\text{HICO} \rightarrow \text{HI} + \text{CO}$ (concerted)
- (b) $\text{HICO} \rightarrow \text{HOCl} \rightarrow \text{HICO} \rightarrow \text{HI} + \text{CO}$ (1,2-H-shift and recross)
- (c) $\text{HICO} \rightarrow \text{I} + \text{HCO} \rightarrow \text{HI} + \text{CO}$ (radical recombination)
- (d) $\text{HICO} \rightarrow \text{I} + \text{HCO} \rightarrow \text{HI} + \text{CO}$ (I roaming)
- (e) $\text{HICO} \rightarrow \text{HOCl} \rightarrow \text{H} + \text{ICO} \rightarrow \text{H} + \text{I} + \text{CO}$

- (f) $\text{HICO} \rightarrow \text{I} + \text{HCO}$ (radical pathway)
- (g) $\text{HICO} \rightarrow \text{I} + \text{HCO} \rightarrow \text{I} + \text{H} + \text{CO}$
- (h) $\text{HICO} \rightarrow \text{H} + \text{ICO} \rightarrow \text{H} + \text{I} + \text{CO}$
- (i) $\text{HICO} \rightarrow \text{HCOI} \rightarrow \text{HI} + \text{CO}$ (1,2-I-shift)
- (j) $\text{HICO} \rightarrow \text{HOCl} \rightarrow \text{HI} + \text{CO}$ (1,2-H-shift)

Table A.1. : Total calculated energy (in kcal/mol) for species in HFCO system

Theory	HFCO	HF+CO	INT-2T	INT-2C	INT-3T	INT-3C	F+HCO	H+FCO	Ref.
B3LYP/6-31G* (ECP)	0.0	20.07	48.87	48.61	111.09	99.28	117.24	105.94	p
MP2/6-31G* (ECP)	0.0	8.21	52.35	52.62	107.60	96.49	112.44	98.51	p
CCSD(T)/ 6-31G* (ECP)// MP2/ 6-31G* (ECP)	0.0	7.35	47.67	47.66	103.80	94.74	107.22	98.34	p
UHF/ 6-31G(d)	0.0	4.4	43.6	44.5	149.1	146.2	84.9	86.3	[Francisco and Zhao, 1992]
UMP2/ 6-31G(d)	0.0	10.6	51.6	51.8	120.5	109.7	125.4	98.2	[Francisco and Zhao, 1992]
UMP2/ 6-311(d,p)	0.0	0.0	47.5	48.8	117.9	106.6	121.9	102.6	[Francisco and Zhao, 1992]
UMP4SDTQ/ 6-311++G(d,p)	0.0	-4.5	44.1	46.3	99.9	90	116.2	104.1	[Francisco and Zhao, 1992]
PMP4SDTQ/ 6-311++G(d,p)	0.0	-4.5	44.1	46.3	99.9	90	114.4	102.4	[Francisco and Zhao, 1992]
PMP4SDTQ + ZPE	0.0	-9.0	43.6	45.4	97.8	88.2	109.5	94.4	[Francisco and Zhao, 1992]
HF/3-21G*	0.0	-0.08	36.54						[Okuno, 1999]
HF/3-21G* + ZPE	0.0	-5.05	35.44						[Okuno, 1999]
MP2/cc-pVQZ	0.0	2.68	46.93						[Okuno, 1999]
MP2/cc-pVQZ + ZPE	0.0	-1.49	46.62						[Okuno, 1999]
HF/3-21G	0.0	10.6							[Kamiya and Morokuma, 1991]
HF/6-31G*	0.0	4.4							[Kamiya and Morokuma, 1991]
HF/6-31G* + ZPE	0.0	-0.4							[Kamiya and Morokuma, 1991]
MP2/6-31G*	0.0	10.6							[Kamiya and Morokuma, 1991]
MP2/6-31G* + ZPE	0.0	6.1							[Kamiya and Morokuma, 1991]
HF/6-311G*// MP2/6-31G*	0.0	-3.8							[Kamiya and Morokuma, 1991]
MP2/6-311G**// MP2/6-31G*	0.0	0.0							[Kamiya and Morokuma, 1991]
MP3/6-311G**// MP2/6-31G*	0.0	-0.5							[Kamiya and Morokuma, 1991]
MP4(DQ)/ 6-311G**// MP2/6-31G*	0.0	-2.4							[Kamiya and Morokuma, 1991]
MP4(SDQ)/ 6-311G**// MP2/6-31G*	0.0	-2.2							[Kamiya and Morokuma, 1991]
MP4(SDTQ)/ 6-311G**// MP2/6-31G*	0.0	-1.7							[Kamiya and Morokuma, 1991]
MP4(SDTQ)/ 6-311G**// MP2/6-31G* + ZPE	0.0	-6.3							[Kamiya and Morokuma, 1991]

Theory	HFCO	HF+CO	INT-2T	INT-2C	INT-3T	INT-3C	F+HCO	H+FCO	Ref.
CI-SD/6-31G**// HF/4-31G	0.0	-1							[Kamiya and Morokuma, 1991]
CI-SD/6-31G**// HF/4-31G + ZPE	0.0	-4							[Kamiya and Morokuma, 1991]
DZ + P SCF// DZ + P SCF	0.0		39.4	41.2					[Goddard and Schaefer, 1990]
DZ + P CISD// DZ + P CISD	0.0		42.4	43.6					[Goddard and Schaefer, 1990]
DZ + P CCSD// DZ + P CCSD	0.0		42.2	43.1					[Goddard and Schaefer, 1990]
DZ + P CCSD// DZ + P CCSD	0.0		42.5	43.4					[Goddard and Schaefer, 1990]
DZ + P CCSDT-1// DZ + P CCSD	0.0		42.7	43.4					[Goddard and Schaefer, 1990]
TZ + 2P CCSD// DZ + P CCSD	0.0		42.7	43.7					[Goddard and Schaefer, 1990]
CASSCF	0.0						109.8	101	[Fang and Liu, 2001b]

	TS-1	TS-2A	TS-2B	TS-2C	TS-3A	TS-3B	TS-3C	Ref.
B3LYP/6-31G* (ECP)	52.77	84.16	68.59	73.41	111.71	111.70	101.22	p
MP2/6-31G* (ECP)	53.01	85.95	73.79	77.69	108.88	108.88	53.01	p
CCSD(T)/6-31G* (ECP)// MP2/6-31G* (ECP)	54.85	85.35	68.05	74.33	106.68	106.69	54.85	p
UHF/6-31G(d)	72.1	100.6	63.4	82.1	162.5		148.2	[Francisco and Zhao, 1992]
UMP2/6-31G(d)	57.9	86.1	73.4	75.7	121.4	124.5	111.6	[Francisco and Zhao, 1992]
UMP2/6-311(d,p)	53.8	81.6	69.5	73.3	118.9		108.7	[Francisco and Zhao, 1992]
UMP4SDTQ/6-311++G(d,p)	46.9	79	65.1	69.2	102	103	92.8	[Francisco and Zhao, 1992]
PMP4SDTQ/6-311++G(d,p)	46.9	79	65.1	69.2	102	103	92.8	[Francisco and Zhao, 1992]
PMP4SDTQ + ZPE	43.2	74.9	62.6	65	99.3	99.8	90.1	[Francisco and Zhao, 1992]
HF/3-21G*	56.96	101.73						[Okuno, 1999]
HF/3-21G* + ZPE	53.34	96.63						[Okuno, 1999]
MP2/cc-pVQZ	50.75	79.63						[Okuno, 1999]
MP2/cc-pVQZ + ZPE	47.3	75.69						[Okuno, 1999]
HF/3-21G	69.3							[Kamiya and Morokuma, 1991]
HF/6-31G*	72.1							[Kamiya and Morokuma, 1991]
HF/6-31G* + ZPE	68.2							[Kamiya and Morokuma, 1991]
MP2/6-31G*	57.9							[Kamiya and Morokuma, 1991]
MP2/6-31G* + ZPE	54.2							[Kamiya and Morokuma, 1991]
HF/6-311G**//MP2/6-31G*	68.1							[Kamiya and Morokuma, 1991]
MP2/6-311G**//MP2/6-31G*	53.7							[Kamiya and Morokuma, 1991]
MP3/6-311G**//MP2/6-31G*	62.1							[Kamiya and Morokuma, 1991]
MP4(DQ)/6-311G**//MP2/6-31G*	60							[Kamiya and Morokuma, 1991]
MP4(SDQ)/6-311G**//MP2/6-31G*	56.1							[Kamiya and Morokuma, 1991]
MP4(SDTQ)/6-311G**//MP2/6-31G*	50.6							[Kamiya and Morokuma, 1991]
MP4(SDTQ)/6-311G**// MP2/6-31G* + ZPE	46.9							[Kamiya and Morokuma, 1991]
CI-SD/6-31G**//HF/4-31G	61							[Kamiya and Morokuma, 1991]
CI-SD/6-31G**//HF/4-31G + ZPE	58							[Kamiya and Morokuma, 1991]
DZ + P SCF//DZ + P SCF	67.6	95.2	58.5					[Goddard and Schaefer, 1990]
DZ + P CISD//DZ + P CISD	60.9	86.9	62.7					[Goddard and Schaefer, 1990]
TZ + 2P CISD//TZ + 2P CISD	58.4							[Goddard and Schaefer, 1990]
DZ + P CCSD//DZ + P CCSD	57.7	83.3	62.4					[Goddard and Schaefer, 1990]
DZ + P CCSD//DZ + P CCSD	57.9	83.5	62.7					[Goddard and Schaefer, 1990]
DZ + P CCSDT-1//DZ + P CCSD	53.2	80.2	62.9					[Goddard and Schaefer, 1990]
TZ + 2P CCSD//DZ + P CCSD	55	84.6						[Goddard and Schaefer, 1990]
MP4/VTZ/SPF5	44.5							[Wei and Wyatt, 1993]
MP4/VTZ/SPF6	44.4							[Wei and Wyatt, 1993]
MP4/VTZ/MBE	45.7							[Wei and Wyatt, 1993]
MP2/6-31G*	46.9							[Wei and Wyatt, 1993]
CCSD/DZ+P	47							[Wei and Wyatt, 1993]
MP2/6-31G(d)	43.2							[Wei and Wyatt, 1993]

Table A.2. : Total calculated energy (in kcal/mol) for species in HCICO system

Theory	HCICO	HCl+CO	INT-2T	INT-2C	INT-3T	INT-3C	Cl+HCO	H+ClCO	Ref.
B3LYP/6-31G* (ECP)	0.0	10.76	52.46	51.08	76.48	65.30	79.48	94.57	p
MP2/6-31G* (ECP)	0.0	2.60	57.79	57.71	79.53	67.99	67.78	75.91	p
CCSD(T)/6-31G* (ECP)// MP2/6-31G* (ECP)	0.0	1.00	52.30	51.69	67.11	62.33	67.30	77.58	p
UHF/6-31G(d)	0.0	-10.2	46.8	48	106.7		54	76.7	[Francisco and Zhao, 1992]
UMP2/6-31G(d)	0.0	2	55.9	56.5	85.8	73.4	82.2	88.9	[Francisco and Zhao, 1992]
UMP2/6-311(d,p)	0.0	-5.9	51.8	53.4	85.3	72.7	82	93.1	[Francisco and Zhao, 1992]
UMP4SDTQ/6-311++G(d,p)	0.0	-5.9	48.3	50.6	82	71.9	80.2	93.8	[Francisco and Zhao, 1992]
PMP4SDTQ/6-311++G(d,p)	0.0	-5.9	48.3	50.6	82	71.9	78.5	91.7	[Francisco and Zhao, 1992]
PMP4SDTQ+ZPE	0.0	-10.8	48	50	80.3	70.6	74.4	83.8	[Francisco and Zhao, 1992]
MP2/cc-pVTZ	0.0						94.5	93.9	[Fang and Liu, 2001a]
CAS-MP2/cc-pVTZ	0.0						90	95.4	[Fang and Liu, 2001a]
	TS-1	TS-2A	TS-2B	TS-2C	TS-3A	TS-3B	TS-3C		Ref.
B3LYP/6-31G* (ECP)	35.92	84.49	70.32	64.28	77.87	78.53	68.19		p
MP2/6-31G* (ECP)	41.40	87.21	79.79	74.20	82.18	84.91	72.36		p
CCSD(T)/6-31G* (ECP)// MP2/6-31G* (ECP)	41.69	85.73	72.59	67.45	68.27	82.27	66.61		p
UHF/6-31G(d)	45.2	99.5	67.9	69.4	116.2				[Francisco and Zhao, 1992]
UMP2/6-31G(d)	45.8	86.2	79.1	77.5	88	89.1	77.7		[Francisco and Zhao, 1992]
UMP2/6-311(d,p)	40.1	82.5	75.3	69.7	87.1		76.9		a
UMP4SDTQ/6-311++G(d,p)	41.1	80	70.7	67.5	84.4	86.9	75.7		[Francisco and Zhao, 1992]
PMP4SDTQ/6-311++G(d,p)	41.1	80	70.7	67.5	84.4	86.9	75.7		[Francisco and Zhao, 1992]
PMP4SDTQ+ZPE	37.8	76	68.3	62.9	81.9	83.8	73.2		[Francisco and Zhao, 1992]

Table A.3. : Total calculated energy (in kcal/mol) for species in HBrCO system

Theory	HBrCO	HBr+CO	INT-2T	INT-2C	INT-3T	INT-3C	Br+HCO	H+BrCO	Ref.
B3LYP/6-31G* (ECP)	0.0	10.02	52.69	51.04	68.46	57.49	66.18	85.55	p
MP2/6-31G* (ECP)	0.0	2.77	58.76	58.27	70.78	59.59	56.73	64.80	p
CCSD(T)/6-31G* (ECP)// MP2/6-31G* (ECP)	0.0	0.75	52.89	51.92	56.06	53.34	56.62	66.86	p
UHF/962(d)/6-311G(d,p)	0.0	-16.2					41.4		[Zhao and Francisco, 1992]
UMP2/962(d)/6-311G(d,p)+ZPE	0.0	-4.8					69.8		[Zhao and Francisco, 1992]
UMP4SDTQ/962(d)/6-311G(d,p)// UMP2/962(d)/6-311G(d,p)	0.0	-8.0					65.8		[Zhao and Francisco, 1992]
PMP4SDTQ+ZPE	0.0	-12.8					62.4		[Zhao and Francisco, 1992]
	TS-1	TS-2A	TS-2B	TS-2C	TS-3A	TS-3B	TS-3C		Ref.
B3LYP/6-31G* (ECP)	33.65	83.53	69.13	63.06	70.35	71.59	61.34		p
MP2/6-31G* (ECP)	39.67	86.70	79.62	73.24	73.90		65.46		p
CCSD(T)/6-31G* (ECP)// MP2/6-31G* (ECP)	40.06	84.83	71.99	66.23		75.23	57.49		p
UMP2/962(d)/6-311G(d,p)+ZPE	35.3								[Zhao and Francisco, 1992]
UMP2/962(d)/6-311G(d,p)+ZPE	34.3								[Zhao and Francisco, 1992]
UMP4SDTQ/962(d)/6-311G(d,p)// UMP2/962(d)/6-311G(d,p)	33.7								[Zhao and Francisco, 1992]
PMP4SDTQ+ZPE	31								[Zhao and Francisco, 1992]

Table A.4. : Total calculated energy (in kcal/mol) for species in HICO system

Theory	HICO	HI+CO	INT-2T	INT-2C	INT-3T	INT-3C	I+HCO	H+ICO	Ref.
B3LYP/6-31G* (ECP)	0.0	8.40	52.92	51.79	62.59	51.96	54.18	77.26	p
MP2/6-31G* (ECP)	0.0	1.74	59.42	59.45	63.42	53.02	47.97	56.06	p
CCSD(T)/6-31G* (ECP)// MP2/6-31G* (ECP)	0.0	-8.59	45.35	44.97	37.99	38.20	40.04	50.34	p
B3LYP/6-31G*	0.0	7.34	52.26	51.09	65.06	53.97			[Lin <i>et al.</i> , 1999]
CCSD(T)/6-31G **//B3LYP/6-31G*	0.0	-3.51	49.40	48.33	55.07	49.40			[Lin <i>et al.</i> , 1999]
CCSD(T)/6-31G **//B3LYP/6-31G* + ZPE	0.0	-7.14	48.92	47.61	53.22	48.07			[Lin <i>et al.</i> , 1999]
	TS-1	TS-2A	TS-2B	TS-2C	TS-3A	TS-3B	TS-3C		Ref.
B3LYP/6-31G* (ECP)	33.49	82.81	68.98	63.62	116.02	67.13	56.71		p
MP2/6-31G* (ECP)	39.90	86.30	80.21	74.41	116.63	74.89	60.04		p
CCSD(T)/6-31G* (ECP)// MP2/6-31G* (ECP)	32.42	76.23	64.34	59.07	102.39	61.27	40.37		p
B3LYP/6-31G*	33.44	82.87	69.21	62.90	111.20	68.72	58.27		[Lin <i>et al.</i> , 1999]
CCSD(T)/6-31G **//B3LYP/6-31G*	35.03	81.53	68.00	61.26	108.30	71.19	54.51		[Lin <i>et al.</i> , 1999]
CCSD(T)/6-31G **//B3LYP/6-31G* + ZPE	32.34	77.68	65.93	56.98	105.20	68.94	52.47		[Lin <i>et al.</i> , 1999]

p- present work

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