Supporting Information for:
“Pressure dependent isotopic fractionation in the photolysis of Formaldehyde-d2”

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Contains energies, vibrational frequencies and geometries used in theoretical analysis

Energy conversion factors from Hartree (E_h) to other energy units

Unit	scale
Eh	1
kcal / mol	627.509608
kJ / mol	2625.5002
eV	27.211399
cm-1	219474.63

Energy

All energies in Hartree (E_h)

Absolute energies

	uccsd(t)/avqz	uccsd(t)/av5z	scf/avqz	scf/av5z
H2CO	-114.37238228	-114.3816325	-113.921066	-113.922794
H2—CO_M	-114.23437417	-114.243494	-113.759924	-113.761614
H2	-1.17386745	-1.174252084	-1.13346039	-1.13359776
CO	-113.19037099	-113.1992746	-112.788548	-112.790166
Products	-114.36423844	-114.3735267	-113.922008	-113.923764

correlation energies / extrapolated energies

	uccsd(t)/avqz	uccsd(t)/av5z	extrapolate2	uccsd(t)/cbs2
H2CO	-0.451316	-0.458839	-0.466731	-114.389525
H2—CO_M	-0.474450	-0.481880	-0.489674	-114.251289
H2	-0.040407	-0.040654	-0.040914	-1.174512
CO	-0.401823	-0.409109	-0.416752	-113.206918
Products	-0.442230	-0.449763	-0.457666	-114.381430

Relative energies (relative to H2CO)

	uccsd(t)/avqz	uccsd(t)/av5z	scf/avqz	scf/av5z	uccsd(t)/cbs2
H2CO	0.000000	0.000000	0.000000	0.000000	0.000000
H2—CO_M	0.138008	0.138138	0.161142	0.161179	0.138236
Products	0.008144	0.008106	-0.000942	-0.000970	0.008095

Vibrations

All vibrational energies in cm-1 uccsd(t)/avqz

	H2CO	HDCO	D2CO
1	1185.9100	1041.81	950.3900
2	1268.3000	1074.64	1000.0700
3	1533.1200	1424.33	1118.6500
4	1774.8000	1750.13	1720.7400
5	2933.8900	2186.48	2134.8600
6	3005.5400	2972.21	2244.7300
ZPE	5850.7800	5224.8000	4584.7200

	H2—CO_M	HD—CO_M	DH—CO_M	D2—CO_M
i	1833.3000	1477.1600	1768.8300	1405.1200
1	786.2000	684.26	606.7900	602.5300
2	873.7500	774.33	866.5600	675.0700
3	1287.4200	1254.16	993.3900	960.2200
4	1850.8200	1727.96	1840.9500	1731.4500
5	3143.8900	2406.3	3140.8000	2400.6300
ZPE	3971.0400	3423.5050	3724.2450	3184.9500

	H2	HD	D2
1	4399.6600	3810.7100	3112.2300
ZPE	2199.8300	1905.3550	1556.1150

	CO
1	2160.0000
ZPE	1080.0000

Formaldehyde

uccsd(t)/avqz, coordinates in atomic units (bohr)

	x	y	z
C	0.000000005	0	1.142491338
H	1.772360251	0	2.236695816
H	-1.77236038	0	2.236695643
O	0.000000005	0	-1.13950359

TS_M

uccsd(t)/avqz, coordinates in atomic units (bohr)

	x	y	z
C	0	-0.32940298	-1.02710317
O	0	0.108019487	1.137441011
H	0	2.342473478	-2.72747583
H	0	-0.13181397	-3.0881854

CO

uccsd(t)/avqz, coordinates in atomic units (bohr)

	x	y	z
C	0	0	-1.22170597
O	0	0	0.917153794

H2

uccsd(t)/avqz, coordinates in atomic units (bohr)

	x	y	z
H	0	0	-0.70111239
H	0	0	0.70111239