

Supporting information for

The dissociation of glycolate — astrochemical and prebiotic relevance.

Anton Simakov^a, Glenn B. S. Miller^a, Osamu Sekiguchi^a, Arne J. C.

Bunkan^a, Mark Hoffmann^b and Einar Uggerud^{a,*}

^a*Mass Spectrometry Laboratory and Centre for Theoretical and
Computational Chemistry (CTCC), Department of Chemistry, University of
Oslo, P. O. Box 1033 Blindern, N-0315 Oslo (Norway), and ^bDepartment of
Chemistry, University of North Dakota, Abbott Hall Room 236, 151 Cornell
Street Stop 9024, Grand Forks, ND 58202-9024, U.S.A*

E-mail: einar.uggerud@kjemi.uio.no

Accurate determination of the thresholds by applying the program L-CID developed by Chen and co-workers (Narancic, S. ; Bach, A; and Chen, P. , *J. Phys. Chem. A*. **111**(30), 7006(2007)) was pursued but was hampered by the complexity of the dissociation reactions (L-CID is most reliable for one or two fragmentation reactions).

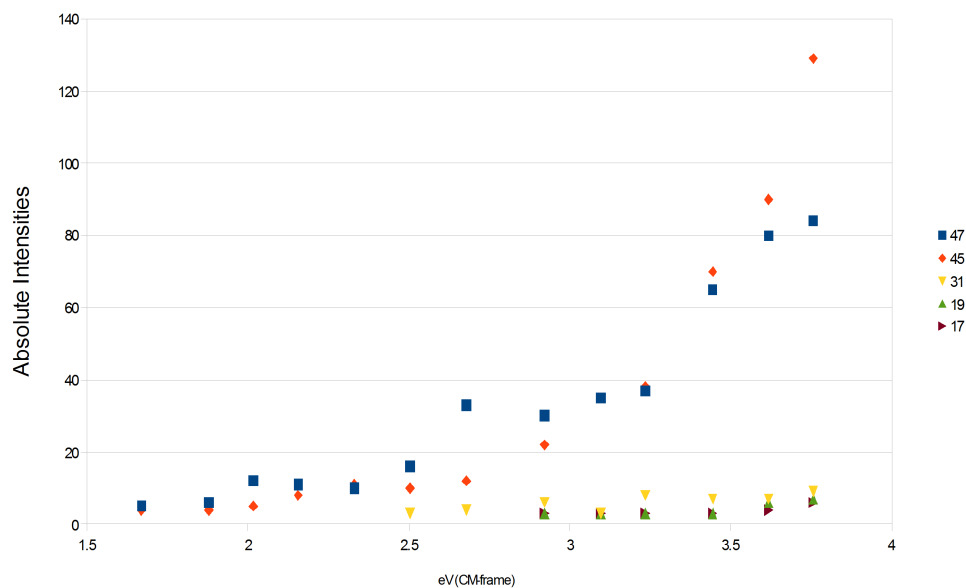


Fig. S1 Energy-resolved CID cross section (arbitrary intensity units) for the various dissociation routes. The experimental data were obtained under near single collision conditions $p = 3.6 \times 10^{-5}$ mbar.

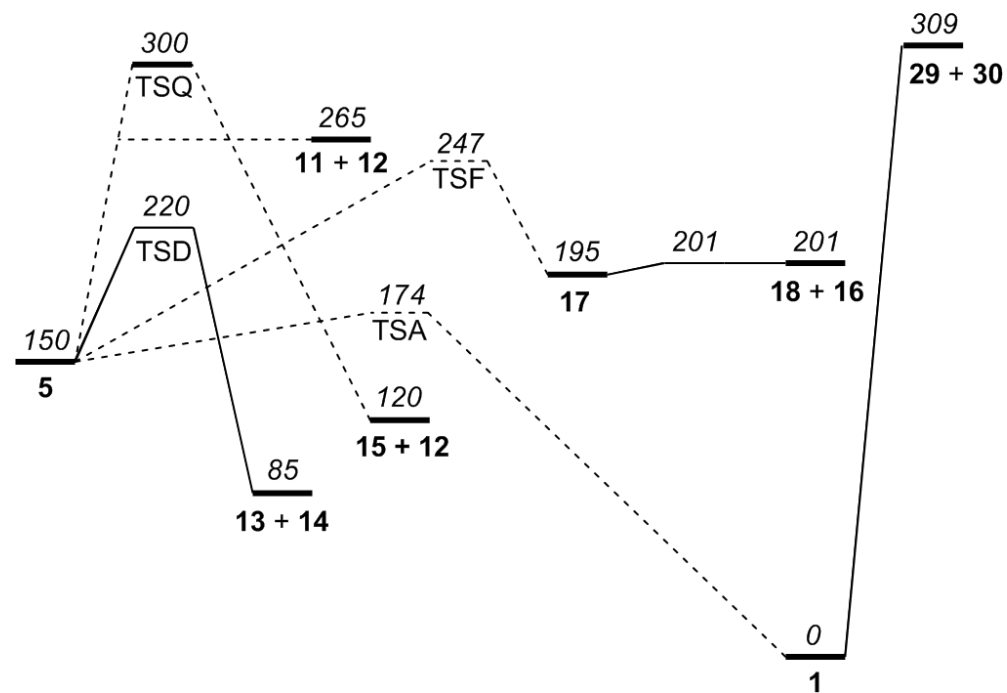
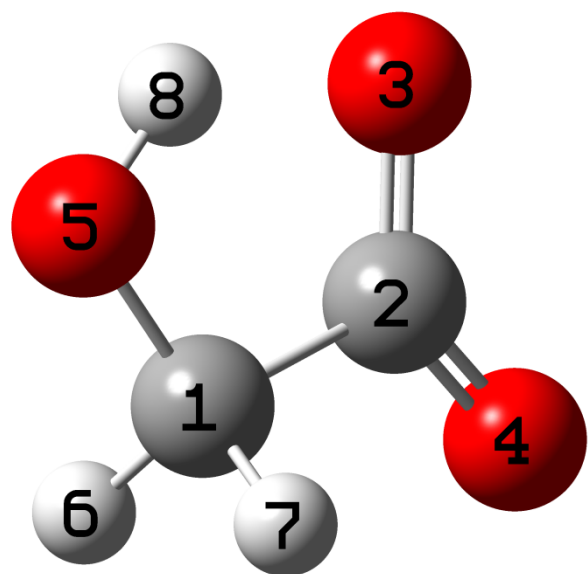


Fig. S2 Simplified energy diagram used for the kinetic simulations.

Cartesian coordinates of key structures

1



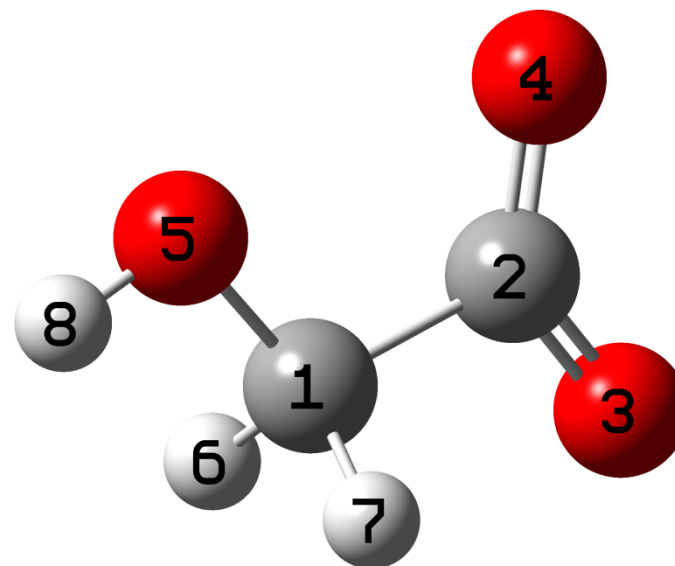
Cartesian coordinates

C	-0.73463	-0.73732	0.00000
C	0.00000	0.64858	0.00000
O	1.25834	0.52650	0.00000
O	-0.70446	1.67031	0.00000
O	0.21652	-1.78062	0.00000
H	-1.39319	-0.79056	0.88456
H	-1.39319	-0.79056	-0.88456
H	1.03093	-1.21598	0.00000

G4

G4(0 K)	-303.645753 (Hartree/Particle)
G4 Enthalpy	-303.640143 (Hartree/Particle)

2



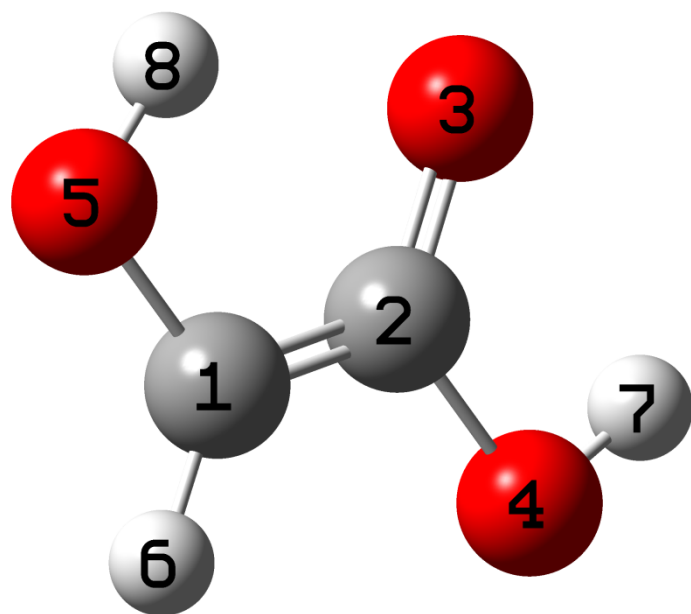
Cartesian coordinates

C	-0.69310	-0.66203	0.00001
C	0.69318	0.07707	-0.00000
O	1.64649	-0.73579	0.00000
O	0.67753	1.31983	-0.00001
O	-1.81945	0.22674	0.00000
H	-0.71739	-1.32131	-0.88468
H	-0.71739	-1.32130	0.88470
H	-2.60230	-0.33388	0.00001

G4

G4(0 K)	-303.624470 (Hartree/Particle)
G4 Enthalpy	-303.618188 (Hartree/Particle)

3



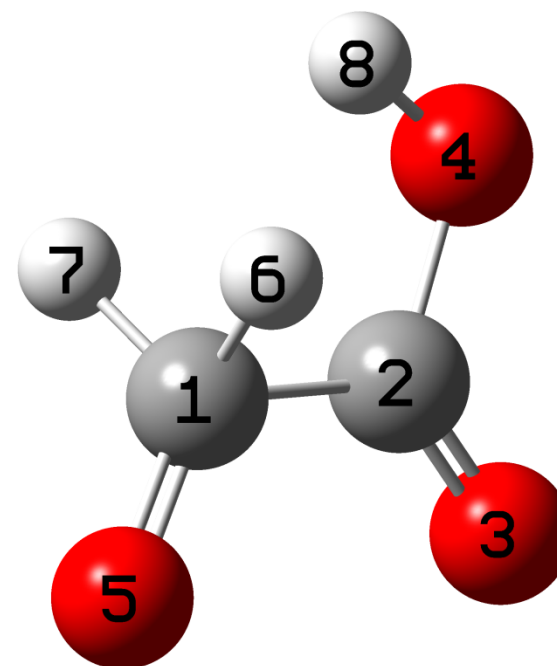
Cartesian coordinates

C	0.70106	-0.71888	-0.00003
C	-0.42845	0.03274	0.00000
O	-0.49508	1.30487	-0.00001
O	-1.67215	-0.66193	0.00002
O	1.94702	-0.02679	-0.00001
H	0.77402	-1.79545	0.00004
H	-2.27156	0.09439	0.00002
H	1.62350	0.88869	0.00002

G4

G4(0 K)	-303.591317 (Hartree/Particle)
G4 Enthalpy	-303.584742 (Hartree/Particle)

4



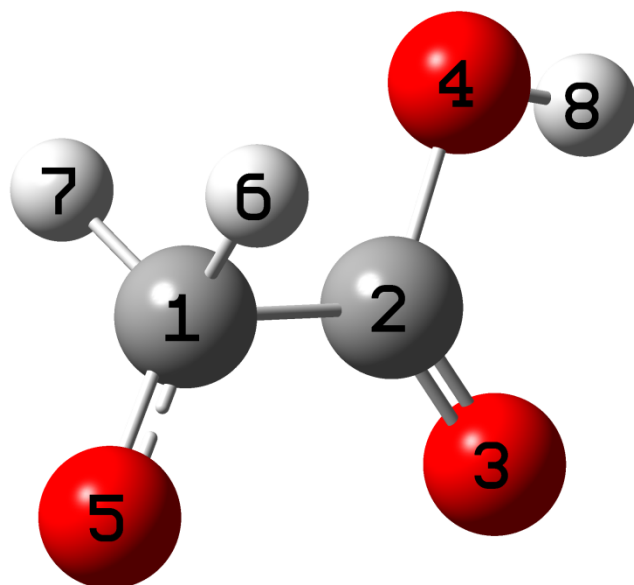
Cartesian coordinates

C	0.89711	-0.54624	0.00000
C	-0.49504	0.17614	0.00001
O	-0.74012	1.35392	0.00000
O	-1.56506	-0.71626	-0.00000
O	1.96788	0.16061	-0.00001
H	0.71849	-1.28677	0.88554
H	0.71848	-1.28678	-0.88553
H	-1.15105	-1.59203	-0.00001

G4

G4(0 K)	-303.588736 (Hartree/Particle)
G4 Enthalpy	-303.582482 (Hartree/Particle)

5



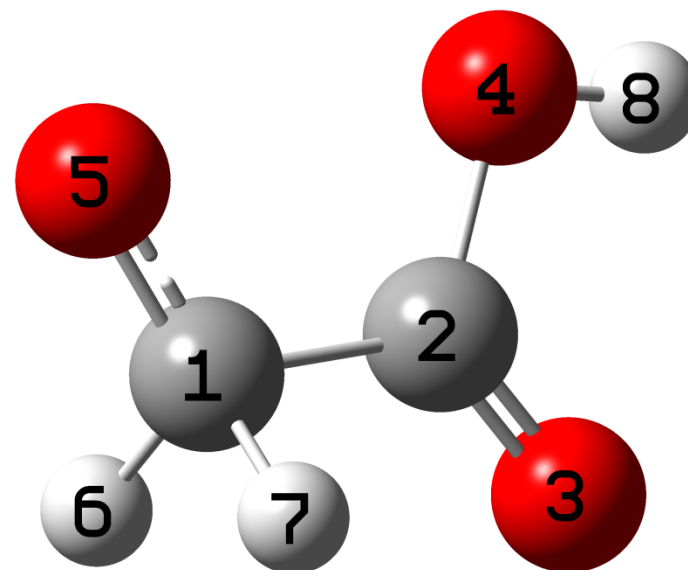
Cartesian coordinates

C	-0.31596	-1.05486	0.00000
C	0.00000	0.47887	0.00000
O	1.07234	1.03978	0.00000
O	-1.15324	1.26425	0.00000
O	0.68432	-1.87013	0.00000
H	-1.06487	-1.09086	0.87811
H	-1.06487	-1.09086	-0.87811
H	-0.80190	2.16652	0.00000

G4

G4(0 K)	-303.588568 (Hartree/Particle)
G4 Enthalpy	-303.582435 (Hartree/Particle)

6



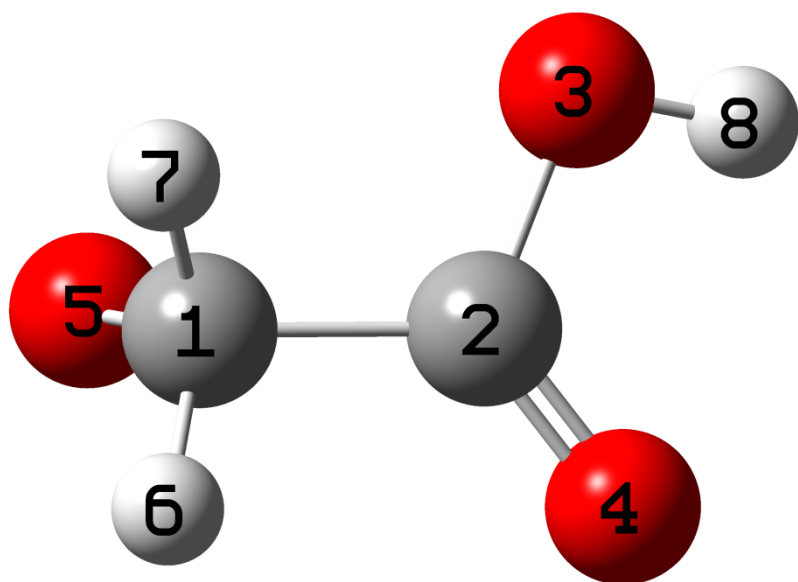
Cartesian coordinates

C	-0.95595	-0.59860	0.00000
C	0.54074	-0.12286	0.00000
O	1.54406	-0.81737	0.00000
O	0.68300	1.23925	-0.00000
O	-1.89785	0.28622	-0.00000
H	-0.89401	-1.34562	-0.87726
H	-0.89401	-1.34561	0.87727
H	1.64558	1.35526	-0.00000

G4

G4(0 K)	-303.588329 (Hartree/Particle)
G4 Enthalpy	-303.582192 (Hartree/Particle)

7



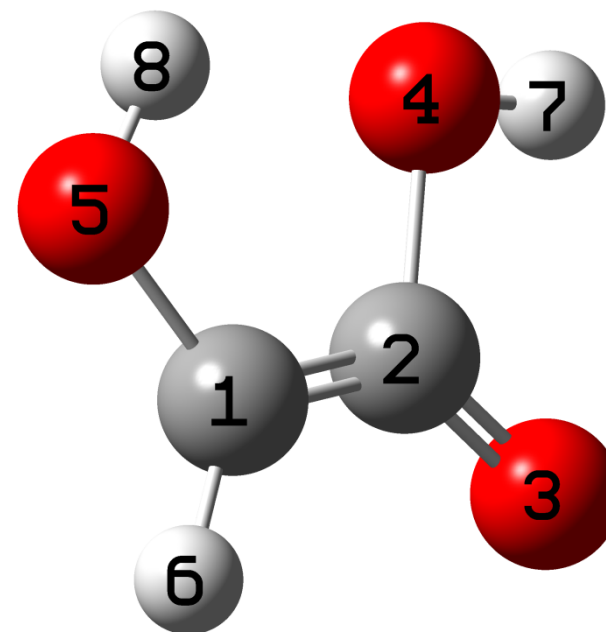
Cartesian coordinates

C	-1.02296	-0.12455	0.52776
C	0.47011	-0.14551	0.15047
O	1.00563	1.12055	0.01857
O	1.15155	-1.09833	-0.18691
O	-1.68331	0.12378	-0.59137
H	-1.19990	-1.12671	1.03746
H	-1.13117	0.62529	1.38357
H	1.85724	0.95390	-0.41268

G4

G4(0 K)	-303.588283 (Hartree/Particle)
G4 Enthalpy	-303.582237 (Hartree/Particle)

8



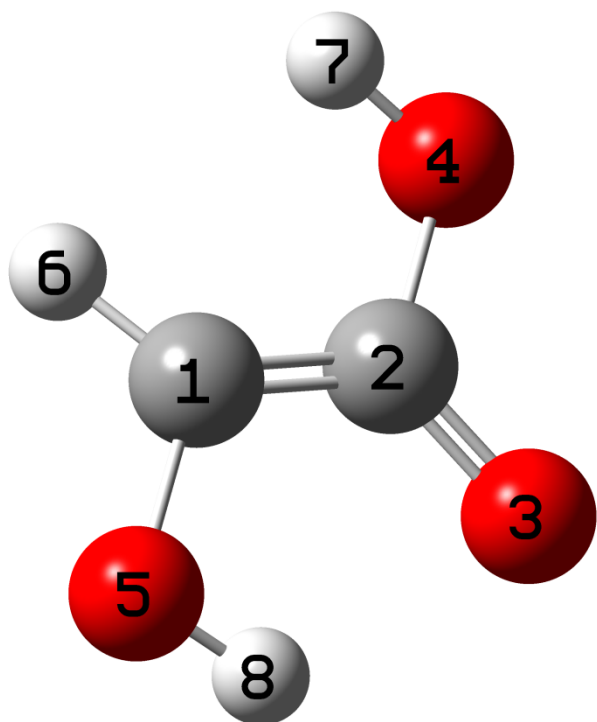
Cartesian coordinates

C	-0.70469	-0.74957	-0.00000
C	0.53604	-0.19013	0.00000
O	1.70131	-0.66347	0.00000
O	0.46110	1.26841	-0.00001
O	-1.90550	0.02677	0.00000
H	-0.87865	-1.81536	0.00000
H	1.40358	1.47052	0.00001
H	-1.56836	0.92937	0.00002

G4

G4(0 K)	-303.586926 (Hartree/Particle)
G4 Enthalpy	-303.580045 (Hartree/Particle)

9



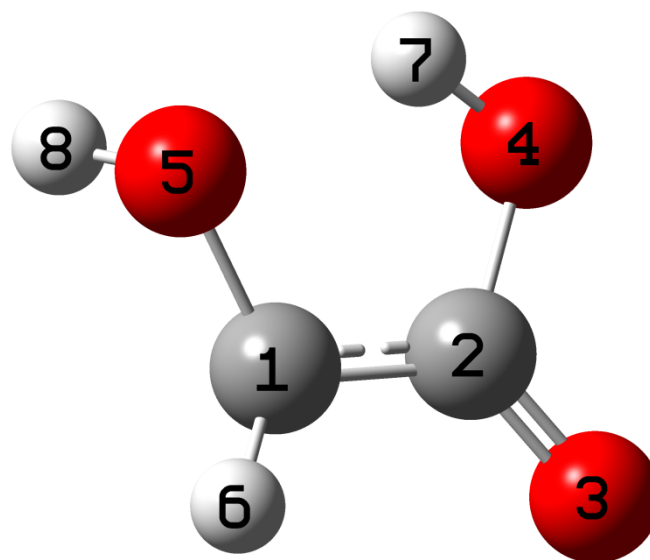
Cartesian coordinates

C	-0.63845	-0.73447	-0.08422
C	0.44395	0.10840	-0.00628
O	0.41098	1.36357	-0.00559
O	1.74173	-0.48654	0.03036
O	-1.92104	-0.10960	0.01310
H	-0.63334	-1.77154	0.23961
H	1.59008	-1.42809	-0.11034
H	-1.64313	0.81662	0.11076

G4

G4(0 K)	-303.585104 (Hartree/Particle)
G4 Enthalpy	-303.578671 (Hartree/Particle)

10



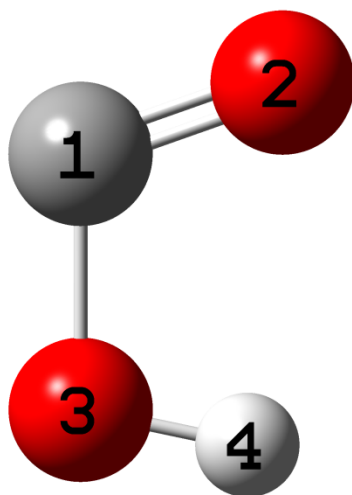
Cartesian coordinates

C	0.60908	-0.78619	0.09814
C	-0.61081	-0.11597	0.01020
O	-1.76294	-0.57182	-0.01257
O	-0.48235	1.30109	0.00864
O	1.81927	-0.00866	-0.13147
H	0.69083	-1.82393	-0.21327
H	0.47594	1.42154	-0.07882
H	2.25174	0.05041	0.72524

G4

G4(0 K)	-303.583494 (Hartree/Particle)
G4 Enthalpy	-303.577371 (Hartree/Particle)

11



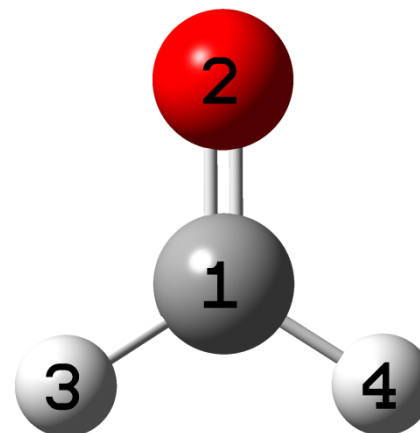
Cartesian coordinates

C	0.00000	0.62822	0.00000
O	1.11425	0.09414	0.00000
O	-1.04968	-0.41117	0.00000
H	-0.51660	-1.23301	0.00000

G4

G4(0 K)	-189.091687 (Hartree/Particle)
G4 Enthalpy	-189.087445 (Hartree/Particle)

12



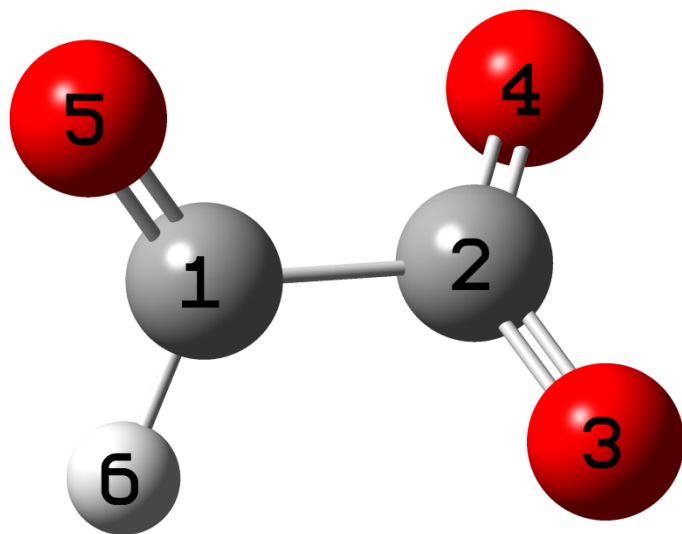
Cartesian coordinates

C	-0.00000	-0.52541	0.00000
O	-0.00000	0.67455	0.00000
H	0.00000	-1.12195	0.93711
H	0.00000	-1.12195	-0.93711

G4

G4(0 K)	-114.453193 (Hartree/Particle)
G4 Enthalpy	-114.449379 (Hartree/Particle)

13



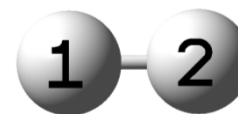
Cartesian coordinates

C	0.88240	-0.29257	0.30823
C	-0.60357	0.03563	0.03456
O	-1.22073	-1.03512	-0.18132
O	-0.97378	1.22013	0.05464
O	1.86005	0.14764	-0.26328
H	1.00262	-1.11968	1.06299

G4

G4(0 K)	-302.445337 (Hartree/Particle)
G4 Enthalpy	-302.439566 (Hartree/Particle)

14



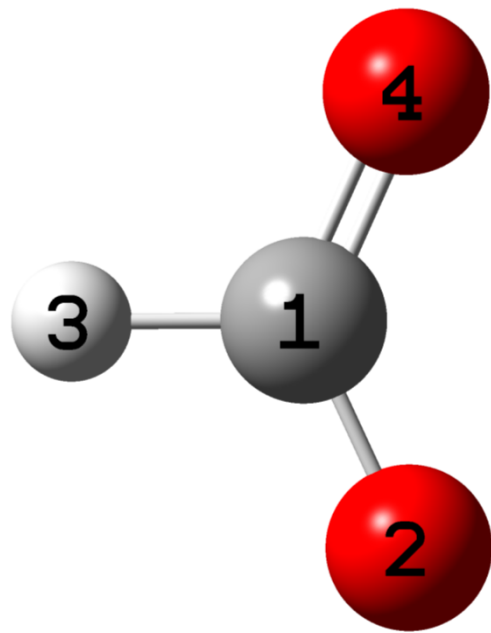
Cartesian coordinates

H	0.00000	0.00000	0.37140
H	0.00000	0.00000	-0.37140

G4

G4(0 K)	-1.168020 (Hartree/Particle)
G4 Enthalpy	-1.164715 (Hartree/Particle)

15



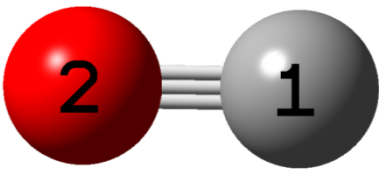
Cartesian coordinates

C	0.00000	0.30901	0.00000
O	0.00000	-0.20736	1.13654
O	0.00000	-0.20736	-1.13654
H	-0.00001	1.46372	0.00000

G4

G4(0 K)	-189.147027 (Hartree/Particle)
G4 Enthalpy	-189.143108 (Hartree/Particle)

16



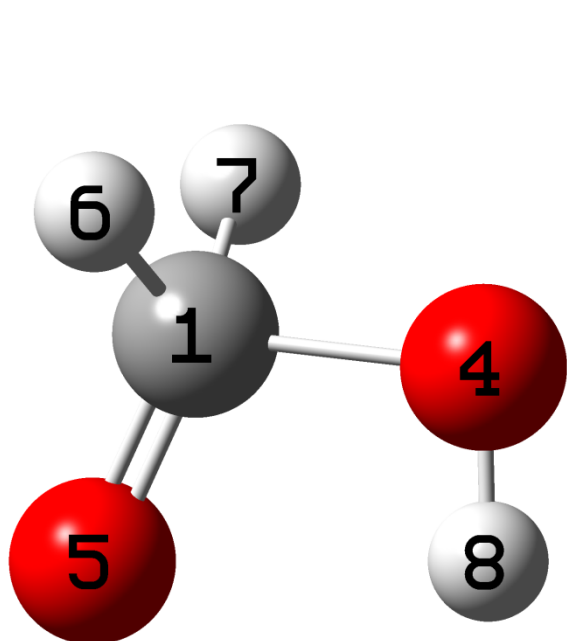
Cartesian coordinates

C	0.00000	0.00000	-0.64624
O	0.00000	0.00000	0.48468

G4

G4(0 K)	-113.289425 (Hartree/Particle)
G4 Enthalpy	-113.286120 (Hartree/Particle)

17



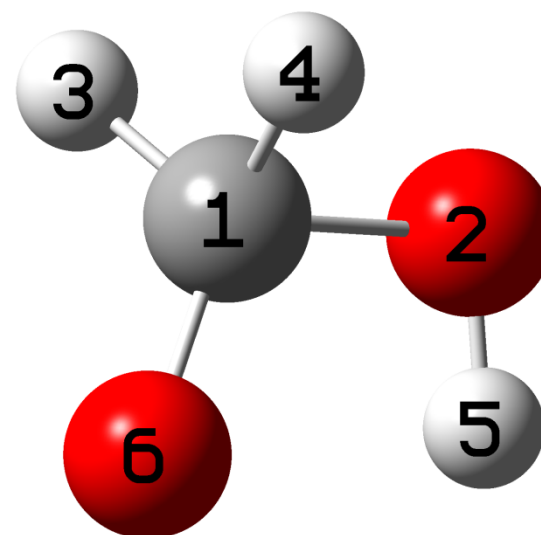
Cartesian coordinates

C	1.33230	-0.31971	0.40573
C	-1.98187	0.37136	-0.46365
O	-2.28461	-0.56987	0.10758
O	0.27162	0.83898	0.34677
O	2.12400	-0.29230	-0.59743
H	1.76771	-0.13106	1.43963
H	0.65053	-1.21956	0.53091
H	0.59107	1.22626	-0.47830

G4

G4(0 K)	-303.570996 (Hartree/Particle)
G4 Enthalpy	-303.562885 (Hartree/Particle)

18



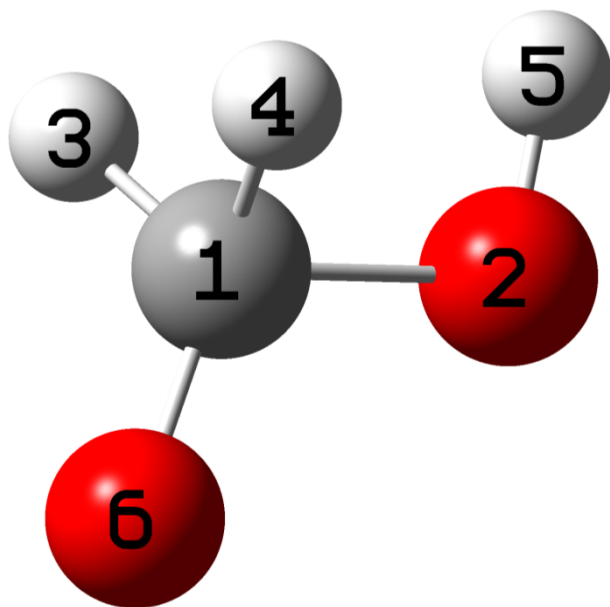
Cartesian coordinates

C	0.00000	0.52489	0.00000
O	-1.06356	-0.56819	0.00000
H	-0.31305	1.15814	0.90118
H	-0.31305	1.15814	-0.90118
H	-0.43847	-1.30409	0.00000
O	1.19663	0.04800	0.00000

G4

G4(0 K)	-190.279661 (Hartree/Particle)
G4 Enthalpy	-190.274983 (Hartree/Particle)

19



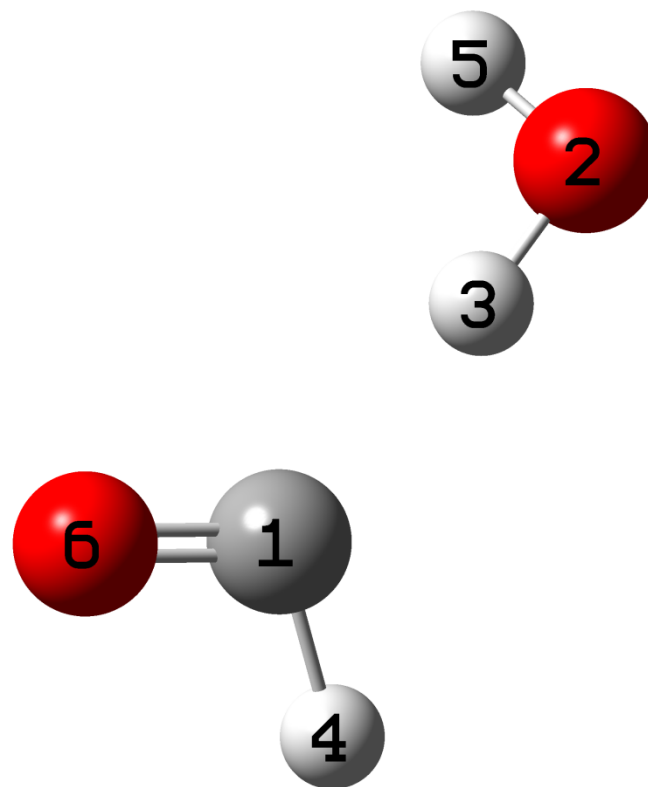
Cartesian coordinates

C	0.19419	0.43835	0.00000
O	-1.14169	-0.33966	0.00000
H	0.05013	1.14178	0.90623
H	0.05013	1.14183	-0.90620
H	-1.81643	0.35304	-0.00004
O	1.21057	-0.31868	-0.00001

G4

G4(0 K)	-190.270400 (Hartree/Particle)
G4 Enthalpy	-190.265533 (Hartree/Particle)

20



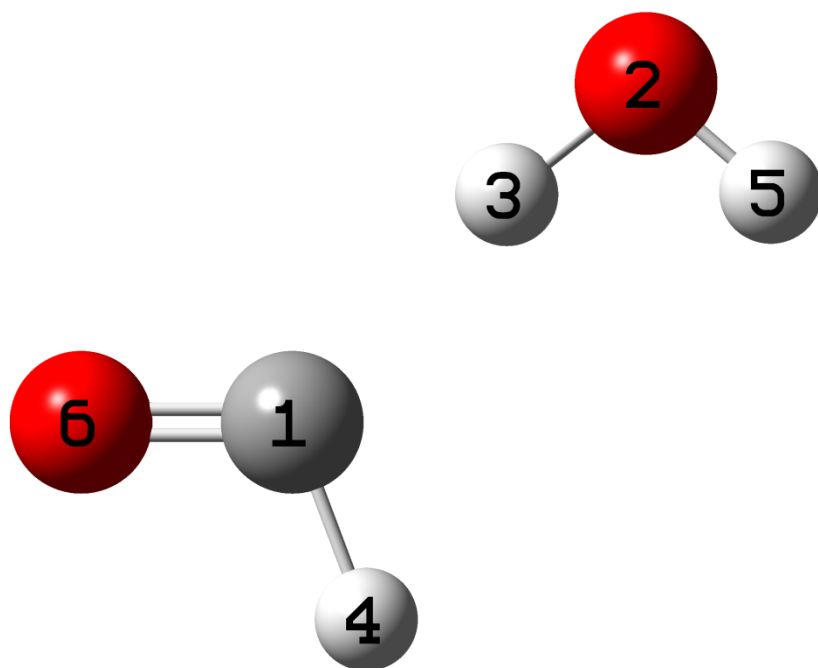
Cartesian coordinates

C	-0.77147	0.40648	0.01971
O	2.04064	-0.02900	-0.07642
H	1.01760	0.15745	-0.09996
H	-1.19192	1.53612	0.18978
H	2.07568	-0.68977	0.62304
O	-1.69971	-0.40134	-0.02747

G4

G4(0 K)	-190.249790 (Hartree/Particle)
G4 Enthalpy	-190.243404 (Hartree/Particle)

21



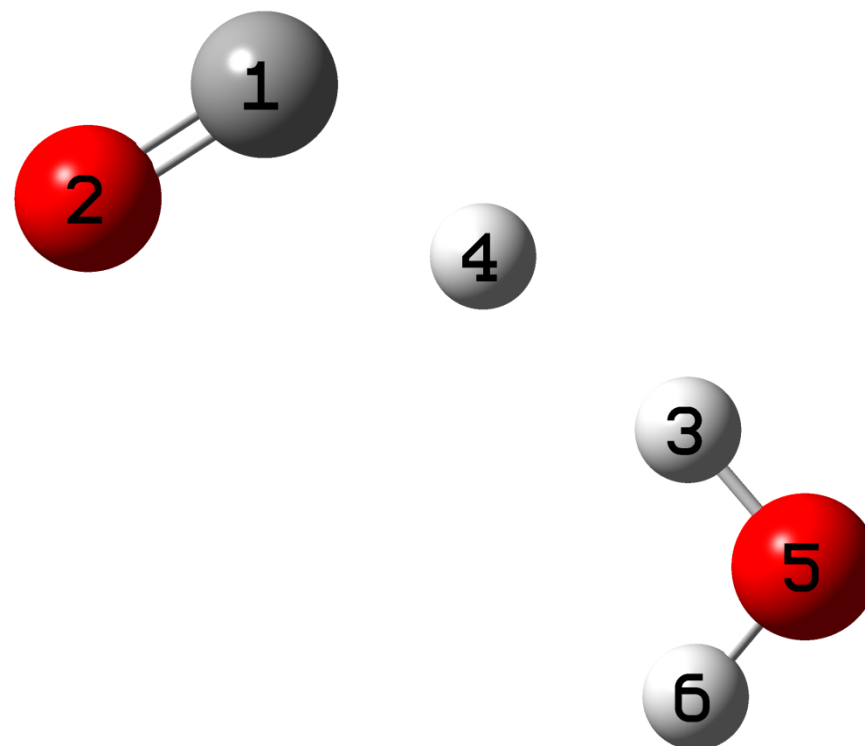
Cartesian coordinates

C	0.00000	0.82251	0.00000
O	-0.66705	-1.95233	0.00000
H	-0.33400	-0.96883	0.00000
H	-0.98170	1.55282	0.00000
H	-1.61962	-1.81428	0.00000
O	1.03397	1.48923	0.00000

G4

G4(0 K)	-190.249613	(Hartree/Particle)
G4 Enthalpy	-190.243987	(Hartree/Particle)

22



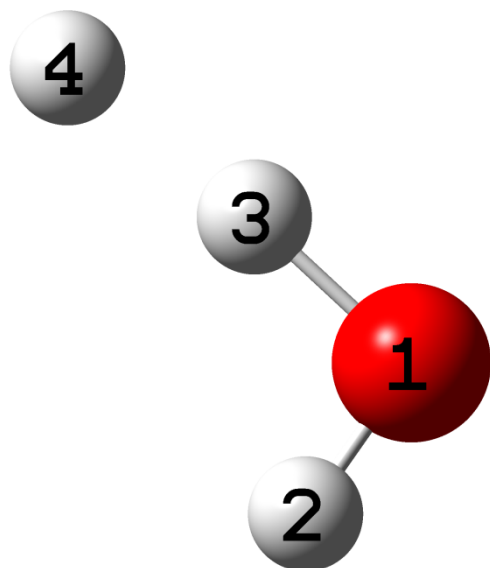
Cartesian coordinates

C	1.48100	0.62773	-0.00008
O	1.96282	-0.45904	0.00003
H	-1.58521	0.29729	-0.00002
H	-0.08179	0.48767	-0.00005
O	-2.55960	0.00856	0.00003
H	-2.44471	-0.94751	0.00012

G4

G4(0 K)	-190.237063	(Hartree/Particle)
G4 Enthalpy	-190.230148	(Hartree/Particle)

23



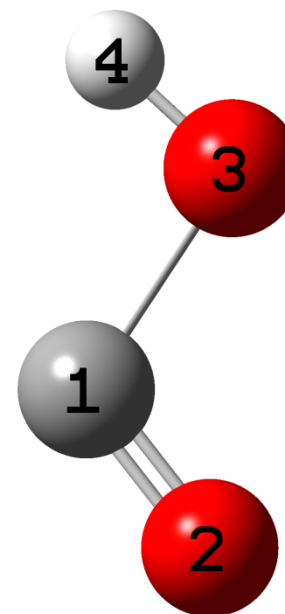
Cartesian coordinates

O	0.00000	0.31828	0.00000
H	0.95150	0.16217	0.00000
H	-0.33432	-0.74781	0.00000
H	-0.61718	-1.96056	0.00000

G4

G4(0 K)	-76.945080 (Hartree/Particle)
G4 Enthalpy	-76.941073 (Hartree/Particle)

24



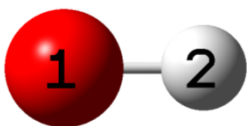
Cartesian coordinates

C	0.24895	0.56207	0.00000
O	1.15891	-0.23723	0.00000
O	-1.12821	-0.24648	0.00000
H	-1.73930	0.49720	0.00000

G4

G4(0 K)	-189.089398 (Hartree/Particle)
G4 Enthalpy	-189.084871 (Hartree/Particle)

25



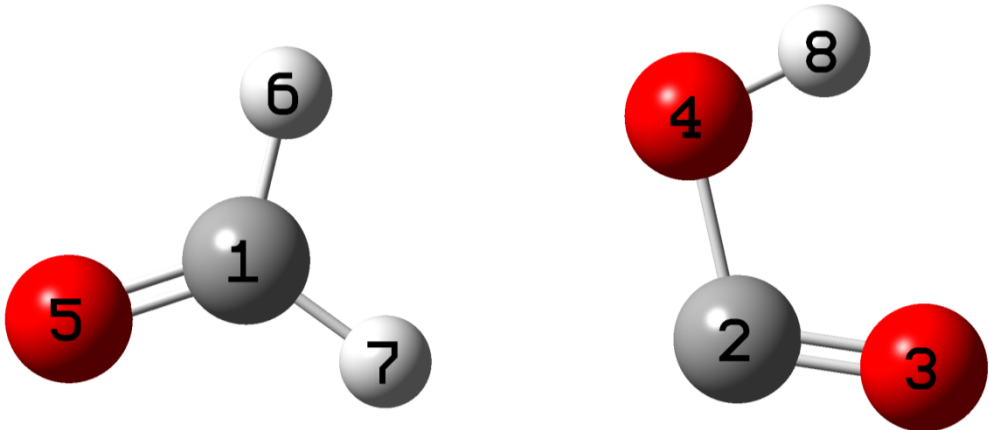
Cartesian coordinates

O	0.00000	0.00000	0.10861
H	0.00000	0.00000	-0.86889

G4

G4(0 K)	-75.778357	(Hartree/Particle)
G4 Enthalpy	-75.775052	(Hartree/Particle)

26



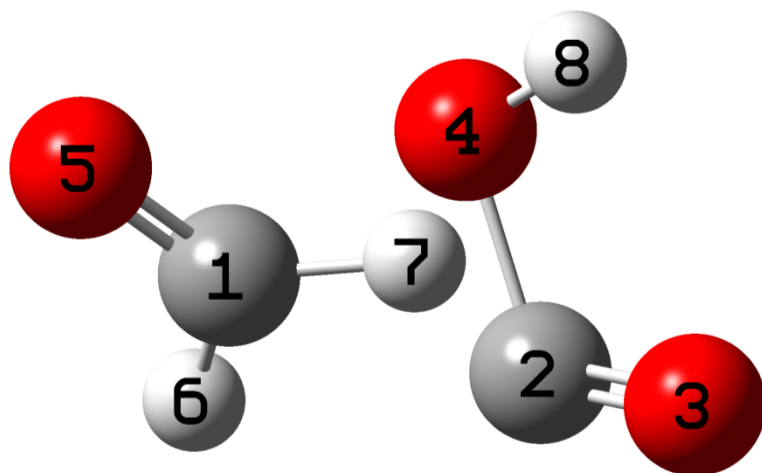
Cartesian coordinates

C	-1.87356	0.06123	0.00002
C	1.31745	-0.44828	-0.00003
O	2.52958	-0.63278	0.00002
O	1.00086	0.99424	-0.00002
O	-3.02566	-0.31733	-0.00001
H	-1.61439	1.14556	0.00010
H	-0.96964	-0.59400	-0.00002
H	1.88249	1.41767	0.00003

G4

G4(0 K)	-303.561388	(Hartree/Particle)
G4 Enthalpy	-303.552751	(Hartree/Particle)

27



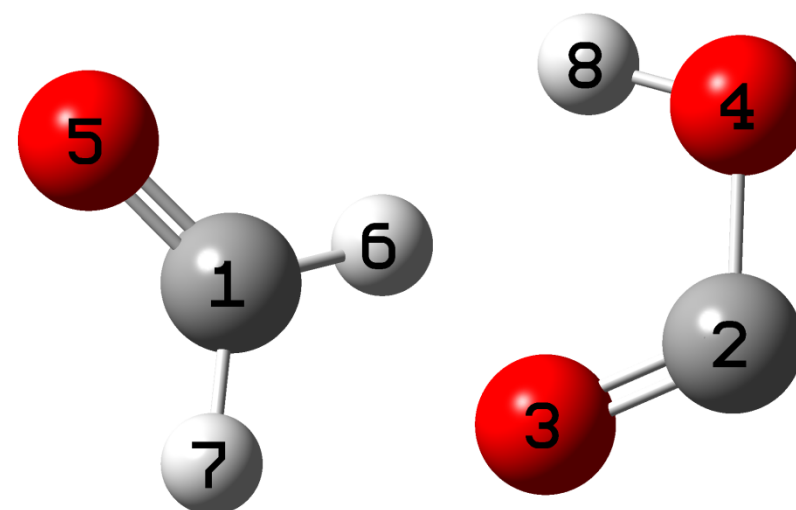
Cartesian coordinates

C	1.42906	-0.36394	0.10433
C	-1.51680	-0.01077	0.56580
O	-1.69622	-0.90041	-0.26698
O	-0.89585	1.16585	-0.08750
O	2.55511	0.04597	-0.06717
H	0.92717	-0.38606	1.09188
H	0.79181	-0.76617	-0.70740
H	-0.89692	0.90924	-1.03203

G4

G4(0 K)	-303.559257 (Hartree/Particle)
G4 Enthalpy	-303.551198 (Hartree/Particle)

28



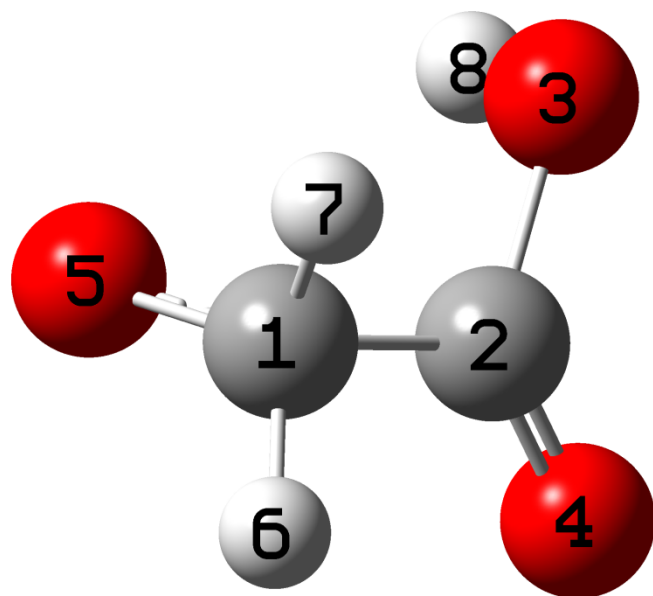
Cartesian coordinates

C	1.61818	-0.26835	0.34677
C	-1.82210	-0.40174	-0.03544
O	-0.72330	-0.97067	-0.16759
O	-1.68874	1.00385	0.05939
O	2.32783	0.48500	-0.29634
H	1.08258	0.05015	1.26043
H	1.54083	-1.34753	0.13705
H	-0.72613	1.17244	-0.02913

G4

G4(0 K)	-303.556474 (Hartree/Particle)
G4 Enthalpy	-303.548598 (Hartree/Particle)

TSA



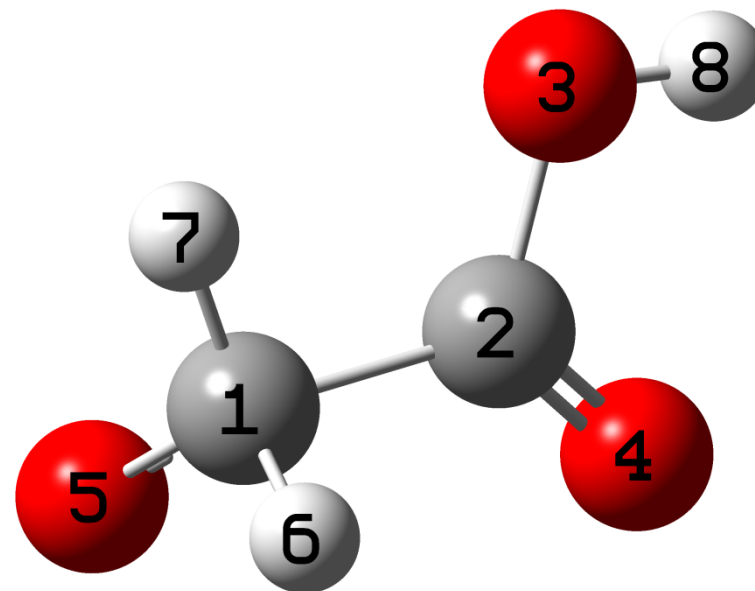
Cartesian coordinates

C	-0.99696	-0.27068	0.53234
C	0.47384	-0.18080	0.17050
O	0.92823	1.16456	0.15270
O	1.19635	-1.05351	-0.26185
O	-1.54142	0.17515	-0.60973
H	-1.21144	-1.34027	0.82923
H	-1.19679	0.32960	1.47411
H	0.88162	1.42992	-0.76933

G4

G4(0 K)	-303.579653 (Hartree/Particle)
G4 Enthalpy	-303.573927 (Hartree/Particle)

TSB



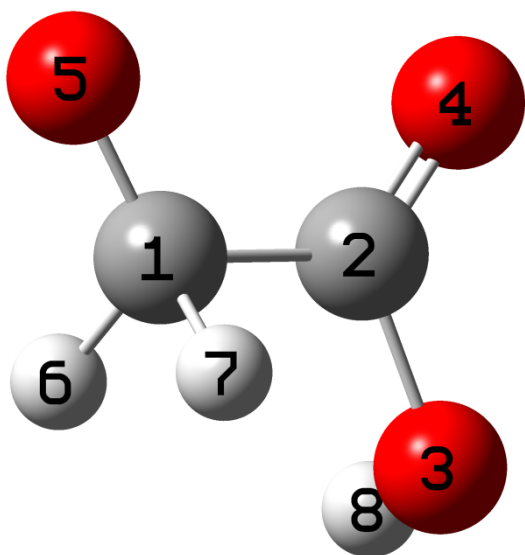
Cartesian coordinates

C	0.98920	-0.40714	0.37322
C	-0.46727	0.10822	0.11106
O	-1.37014	-0.90158	-0.18865
O	-0.85976	1.25449	0.06561
O	1.86580	0.14318	-0.42339
H	1.09474	-0.21633	1.50905
H	0.87483	-1.54123	0.34365
H	-2.18840	-0.41765	-0.38687

G4

G4(0 K)	-303.586337 (Hartree/Particle)
G4 Enthalpy	-303.581033 (Hartree/Particle)

TSC



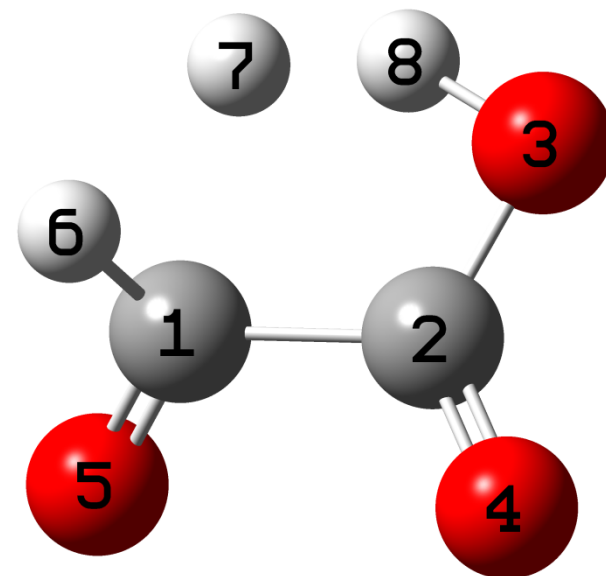
Cartesian coordinates

C	0.90385	-0.57138	-0.02690
C	-0.45992	0.17453	-0.02292
O	-1.58671	-0.73047	-0.09017
O	-0.68259	1.35289	0.00310
O	1.99105	0.11527	0.03689
H	0.67246	-1.34249	0.81242
H	0.72362	-1.26355	-0.93234
H	-1.83369	-0.91440	0.82030

G4

G4(0 K)	-303.575639 (Hartree/Particle)
G4 Enthalpy	-303.569754 (Hartree/Particle)

TSD



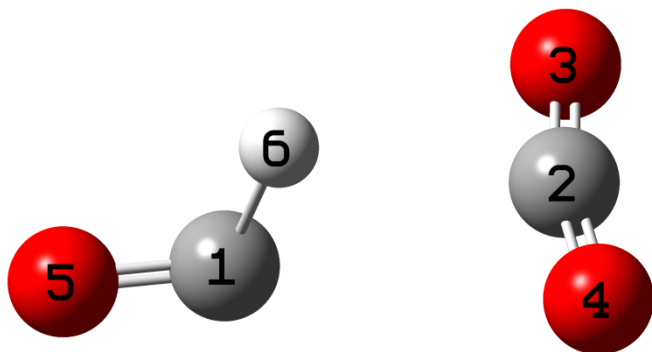
Cartesian coordinates

C	0.90902	-0.31272	0.29877
C	-0.55880	0.15202	0.02202
O	-1.40298	-0.84070	-0.12918
O	-0.85185	1.33622	0.03489
O	1.88633	0.16440	-0.27482
H	0.99414	-0.68502	1.35336
H	0.46463	-1.98410	-0.15333
H	-0.61201	-1.64612	-0.17194

G4

G4(0 K)	-303.561460 (Hartree/Particle)
G4 Enthalpy	-303.555690 (Hartree/Particle)

TSE



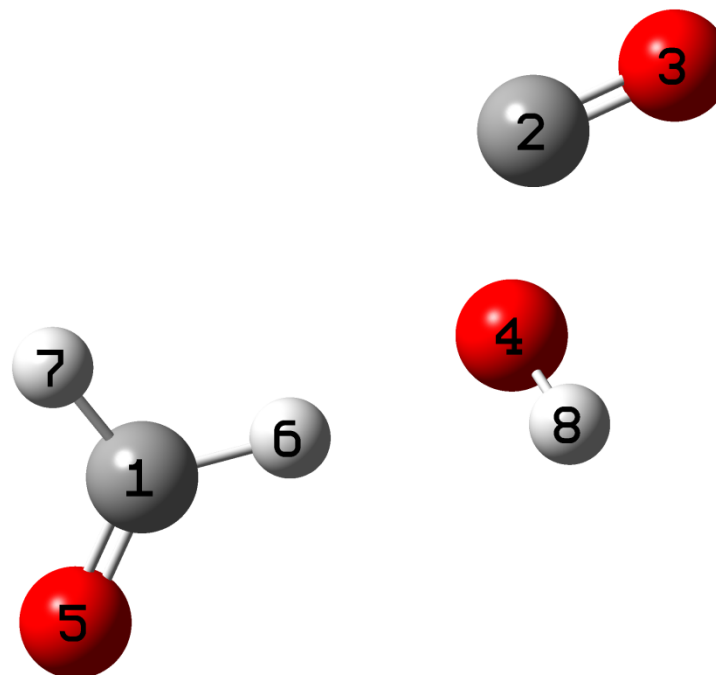
Cartesian coordinates

C	-0.09147	-1.38429	0.00000
C	-0.05212	1.25062	0.00000
O	-0.09147	1.37942	1.16298
O	-0.09147	1.37942	-1.16298
O	0.15493	-2.57291	0.00000
H	1.08555	-0.68528	0.00000

G4

G4(0 K)	-302.370009	(Hartree/Particle)
G4 Enthalpy	-302.363542	(Hartree/Particle)

TSF



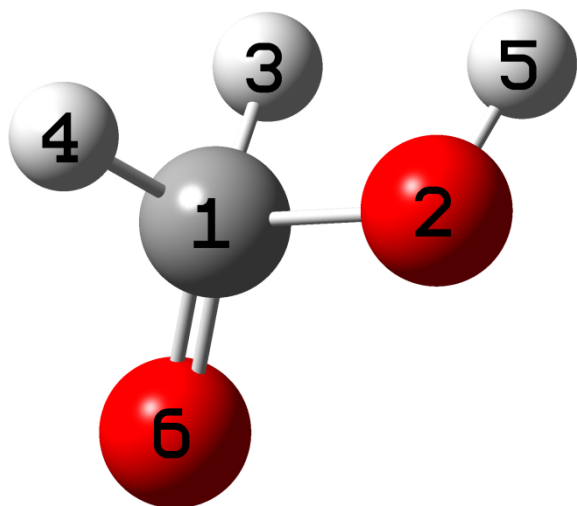
Cartesian coordinates

C	2.10809	-0.36150	-0.13318
C	-2.00868	-0.62322	0.19341
O	-3.02536	-0.10980	-0.05260
O	-0.57850	0.79893	-0.15178
O	3.21816	0.05595	0.13034
H	1.14878	0.24122	-0.18008
H	1.96866	-1.46342	-0.32755
H	-0.62833	1.16981	0.73861

G4

G4(0 K)	-303.551713	(Hartree/Particle)
G4 Enthalpy	-303.542931	(Hartree/Particle)

TSG



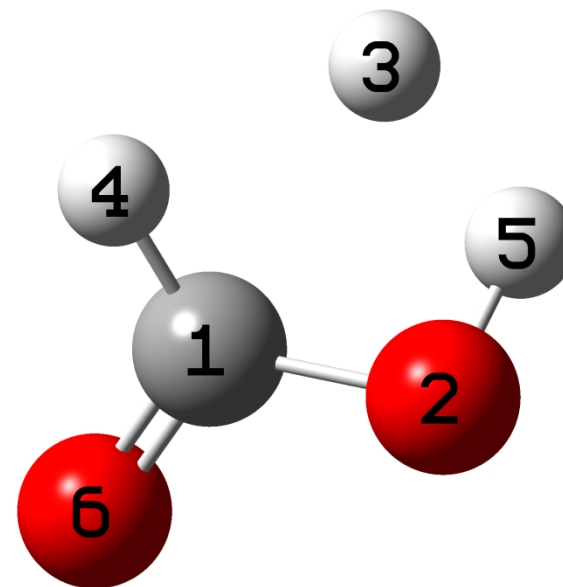
Cartesian coordinates

C	-0.20539	0.43695	0.03435
O	1.16713	-0.30646	0.06841
H	-0.02124	1.17553	-0.84037
H	-0.11571	1.09692	0.96659
H	1.71821	0.20304	-0.53514
O	-1.21074	-0.33068	-0.04306

G4

G4(0 K)	-190.270795 (Hartree/Particle)
G4 Enthalpy	-190.266548 (Hartree/Particle)

TSH



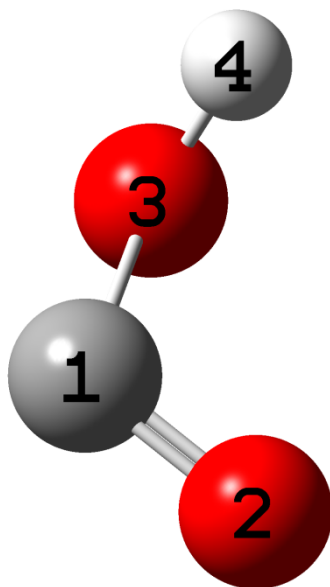
Cartesian coordinates

C	-0.14788	0.27758	0.20587
O	1.05350	-0.41088	0.00331
H	0.73831	1.78994	-0.81370
H	-0.07852	1.01221	1.02310
H	1.53706	0.37402	-0.34663
O	-1.21720	-0.19433	-0.14056

G4

G4(0 K)	-190.234156 (Hartree/Particle)
G4 Enthalpy	-190.229743 (Hartree/Particle)

TSI



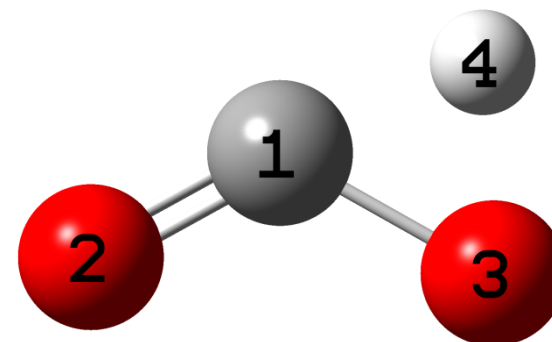
Cartesian coordinates

C	-0.37661	0.59330	0.02296
O	-1.15901	-0.30317	-0.00533
O	1.26486	-0.11196	-0.11566
H	1.41280	-0.23884	0.83016

G4

G4(0 K)	-189.079708 (Hartree/Particle)
G4 Enthalpy	-189.075182 (Hartree/Particle)

TSJ



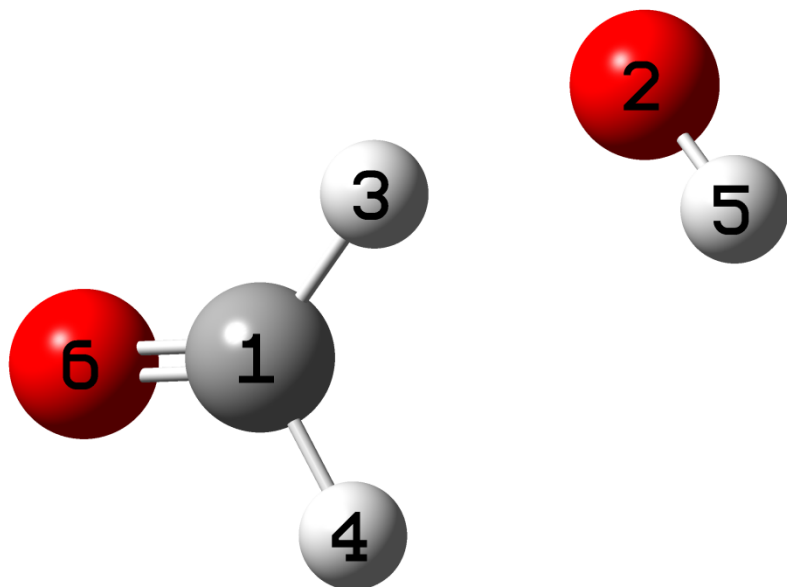
Cartesian coordinates

C	-0.09839	0.42175	-0.00002
O	-1.17417	-0.17087	0.00001
O	1.11611	-0.26256	0.00000
H	1.05487	0.93691	0.00006

G4

G4(0 K)	-189.045390 (Hartree/Particle)
G4 Enthalpy	-189.041238 (Hartree/Particle)

TSK



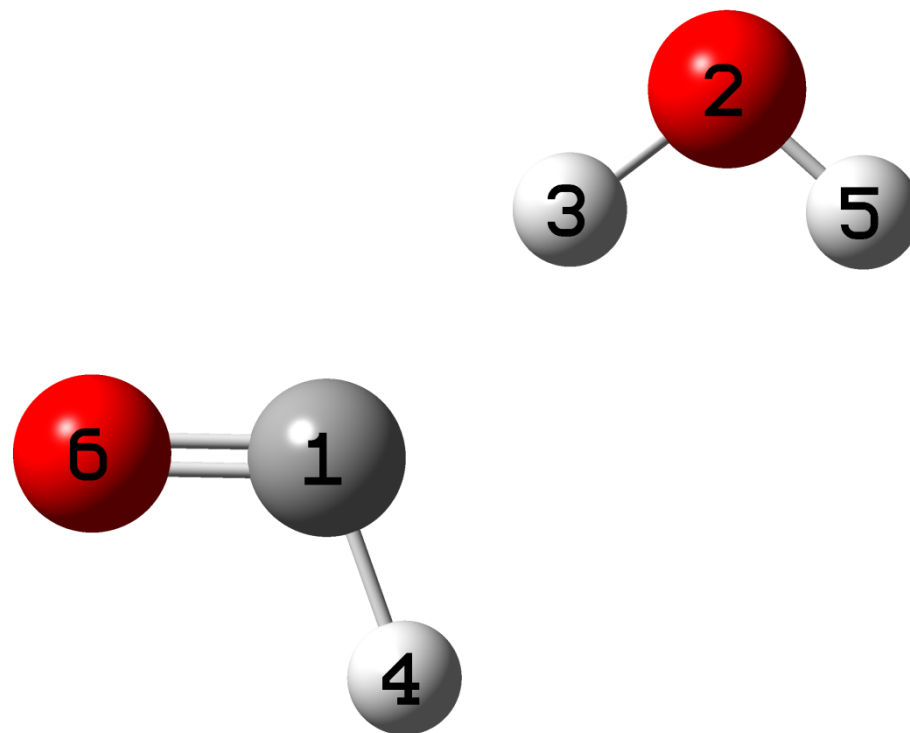
Cartesian coordinates

C	0.64542	0.36381	0.14040
O	-1.88939	-0.22526	-0.03324
H	-0.36631	0.04042	0.56408
H	0.59601	1.40278	-0.32621
H	-2.09313	0.70931	-0.18466
O	1.63825	-0.31666	-0.07871

G4

G4(0 K)	-190.251612	(Hartree/Particle)
G4 Enthalpy	-190.246129	(Hartree/Particle)

TSL



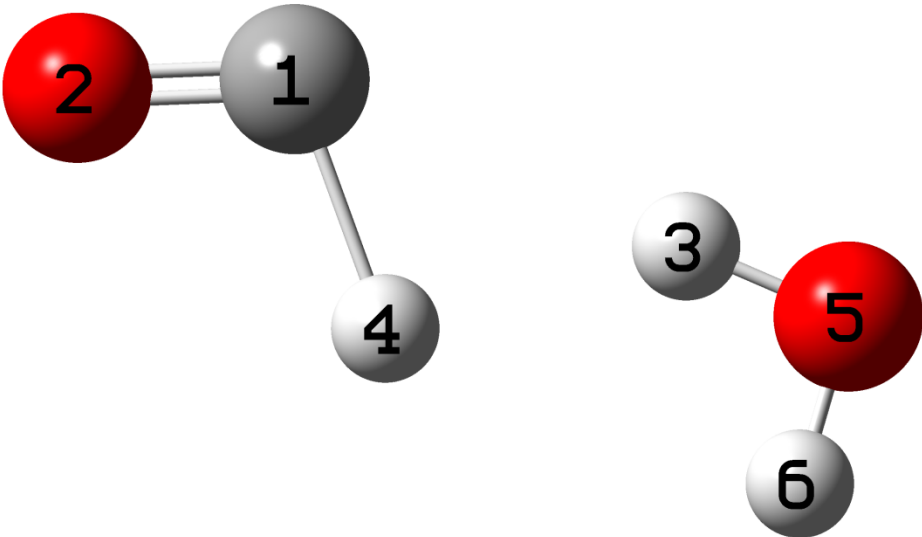
Cartesian coordinates

C	0.74954	0.33853	-0.00000
O	-2.05381	-0.19581	-0.00000
H	-1.02039	-0.09448	-0.00000
H	1.01081	1.53387	-0.00000
H	-2.32013	0.72913	0.00001
O	1.78287	-0.32916	0.00000

G4

G4(0 K)	-190.249614	(Hartree/Particle)
G4 Enthalpy	-190.243988	(Hartree/Particle)

TSM



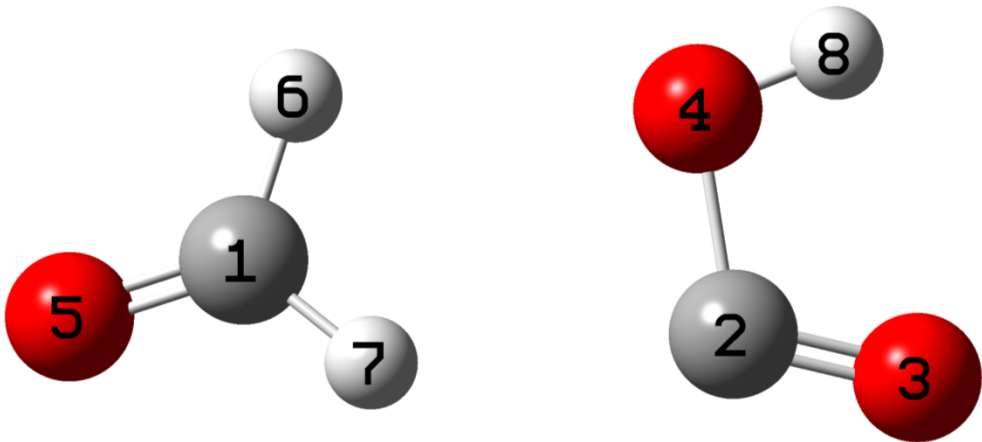
Cartesian coordinates

C	-0.99059	-0.26291	0.00000
O	-2.08733	0.23613	0.00000
H	1.37059	-0.22718	0.00000
H	0.00000	0.82316	0.00000
O	2.35212	-0.20724	0.00000
H	2.45468	0.75032	0.00000

G4

G4(0 K)	-190.237019	(Hartree/Particle)
G4 Enthalpy	-190.230277	(Hartree/Particle)

TSN



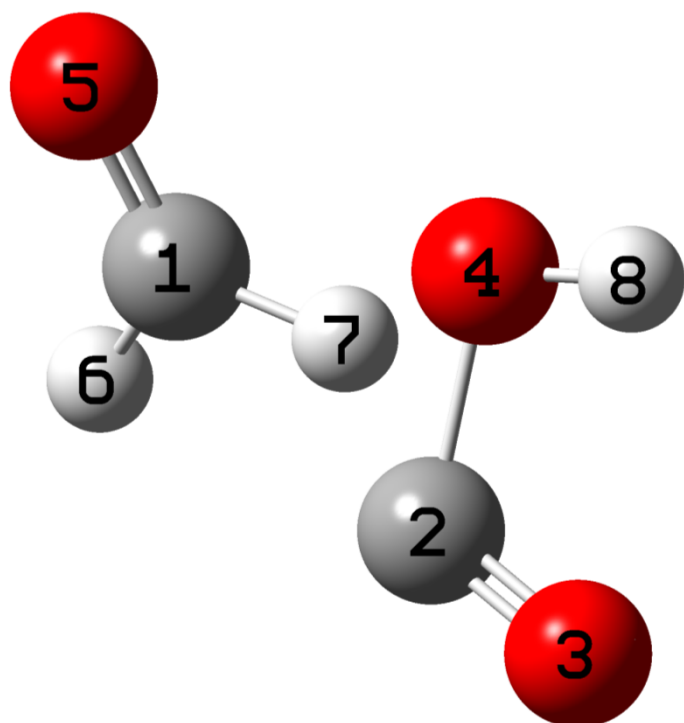
Cartesian coordinates

C	-1.86734	0.05994	0.15434
C	1.27733	-0.41641	0.09660
O	2.45894	-0.69476	-0.07794
O	1.04912	1.02930	-0.00535
O	-2.98547	-0.30467	-0.14682
H	-1.53311	1.11224	0.01485
H	-1.04851	-0.59902	0.51462
H	1.94094	1.38665	-0.19431

G4

G4(0 K)	-303.561159	(Hartree/Particle)
G4 Enthalpy	-303.553181	(Hartree/Particle)

TSO



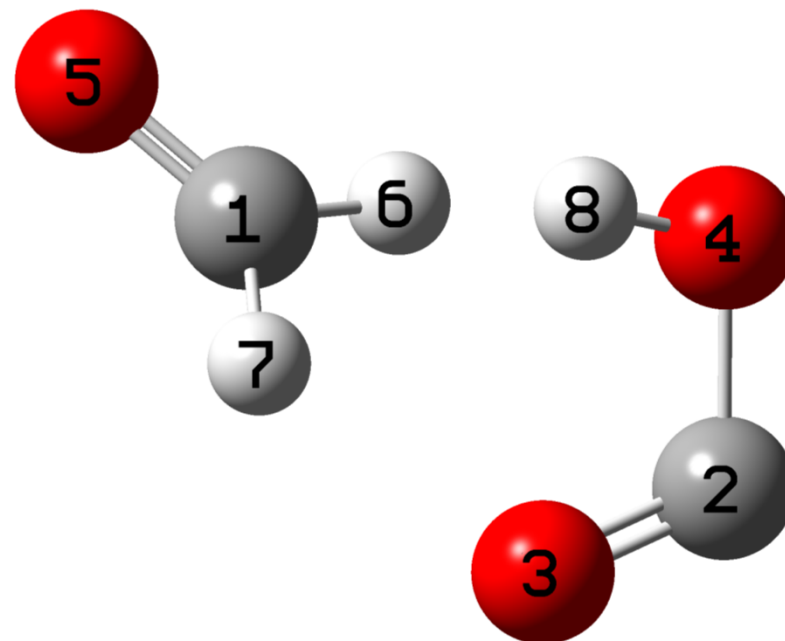
Cartesian coordinates

C	1.47981	-0.43411	0.02256
C	-1.47521	-0.03273	0.59606
O	-2.03517	-0.69330	-0.27096
O	-0.68798	1.07691	-0.05004
O	2.60316	0.01508	-0.02878
H	0.92459	-0.60962	0.96276
H	0.91366	-0.73982	-0.88044
H	-0.90594	0.96096	-0.99578

G4

G4(0 K)	-303.558803 (Hartree/Particle)
G4 Enthalpy	-303.551517 (Hartree/Particle)

TSP



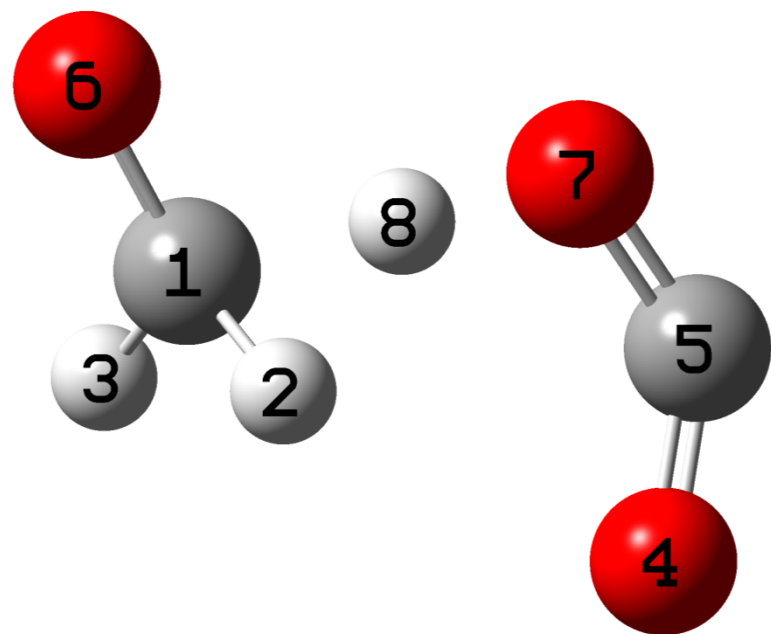
Cartesian coordinates

C	1.55406	-0.14655	0.26748
C	-1.82773	-0.07320	0.39579
O	-1.39842	-1.06368	-0.20837
O	-1.22826	1.14533	-0.13077
O	2.67285	0.03336	-0.16730
H	1.15518	0.43173	1.12725
H	0.82426	-0.86054	-0.15701
H	-0.70677	0.82721	-0.89829

G4

G4(0 K)	-303.558961 (Hartree/Particle)
G4 Enthalpy	-303.551342 (Hartree/Particle)

TSQ



Cartesian coordinates

C	1.54830	-0.52727	0.00000
H	1.24963	-1.09253	-0.91909
H	1.24963	-1.09252	0.91911
O	-2.07858	-0.80197	-0.00000
C	-1.80543	0.38133	0.00000
O	2.59588	0.17436	-0.00000
O	-0.67734	0.97561	0.00000
H	0.32380	0.27670	0.00000

G4

G4(0 K)	-303.531094 (Hartree/Particle)
G4 Enthalpy	-303.524012 (Hartree/Particle)