Supporting Information Available:

* Cartesian coordinates and absolute energies of the stationary points and conical intersections of formaldehyde (H_2CO) optimized at the CAS-SCF(10,9)/6-31G* level.

* Cartesian coordinates of the branching plane vectors of the conical intersections of formaldehyde (H_2CO) optimized at the CAS-SCF(10,9)/6-31G* level.

* Full citation of Gaussian.

* MEP movies (to open with Quicktime), starting from four different points, and leading to the molecular products in S0:
      a) from S0 TS ("CH2O_MEP_from_S0TS.mpg");
      b) from CsCoIn ("CH2O_MEP_from_CsCoIn.mpg");
      c) from C1CoIn ("CH2O_MEP_from_C1CoIn.mpg");
      d) from a point midway along the CoIn intersection seam
("CH2O_MEP_from_midCoIn.mpg").

* Seam-MEP movie (to open with Quicktime) within the intersection space, connecting CsCoIn to C1CoIn ("CH2O_Seam_MEP.mpg").

* Branching Space vectors animations (to open with Quicktime):
      1) CsCoIn Gradient Difference ("CsCoIn_GD_animation.mpg");
      2) CsCoIn Derivative Coupling ("CsCoIn_DC_animation.mpg");
      3) C1CoIn Gradient Difference ("C1CoIn_GD_animation.mpg");
      4) C1CoIn Derivative Coupling ("C1CoIn_DC_animation.mpg").

Absolute energies of the stationary points and conical intersections of formaldehyde (H$_2$CO) optimized at the CAS-SCF(10,9)/6-31G* level. Values are given in Eh.

Structure		Energy
S$_0$ minimum	S$_1$ (FC)	-113.83138
	S$_0$	-113.99620
S$_0$ TS	S$_0$	-113.85603
S$_1$ minimum	S$_1$	-113.85525
	S$_0$	-113.93950
C$_1$ S$_1$ TS*	S$_1$	-113.81139
	S$_0$	-113.86700
C$_1$ S$_1$/S$_0$ CI*	S$_1$	-113.82506
	S$_0$	-113.82519
C$_s$ S$_1$/S$_0$ CI*	S$_1$	-113.76542
	S$_0$	-113.76554

* State-averaged calculations without CP-MCSCF corrections.

Cartesian coordinates (XYZ) for the CAS-SCF/6-31G* optimized structures. Values are given in Å.

S₀ minimum

6	0.000000	0.000000	-0.529712
8	0.000000	0.000000	0.681346
1	0.000000	0.938994	-1.136246
1	0.000000	-0.938994	-1.136246

S₀ TS

6	0.118436	0.485251	0.000000
8	0.118436	-0.695473	0.000000
1	-1.532134	1.115548	0.000000
1	-0.125975	1.536725	0.000000

S₁ minimum

6	0.045377	0.624000	0.000000
8	0.045377	-0.736630	0.000000
1	-0.317642	1.074521	0.942892
1	-0.317642	1.074521	-0.942892

C₁ S₁ TS

6	-0.486401	-0.188598	-0.149585
8	0.695072	0.057634	0.046670
1	-1.312513	1.205768	0.051559
1	-1.329661	-0.535250	0.472593

C₁ S₁/S₀ CI

6	-0.419241	-0.277467	-0.116455
8	0.696955	0.119339	0.039608
1	-1.693121	1.204109	-0.025346
1	-1.367074	-0.494016	0.407213

Cₛ S₁/S₀ CI

6	-0.124422	0.575044	0.000000
8	-0.124422	-0.680093	0.000000
1	0.870957	0.995238	0.519380
1	0.870957	0.995238	-0.519380

Cartesian coordinates (XYZ) for the branching plane vectors of the CAS-SCF(10,9)/6-31G* optimized C_1 S_1/S_0 CI and C_s S_1/S_0 CI. Values are given in Å.

C_1 S_1/S_0 CI

Derivative Coupling

6	0.0003047243	-0.0022193923	0.0298395934
8	0.0063249382	0.0047690791	-0.0132925433
1	0.0062864938	-0.0131357573	0.0062023095
1	-0.0129161562	0.0105860706	-0.0227493596

Unscaled Gradient Difference

6	-0.0850783711	0.0978267325	0.0400034388
8	0.0276372647	-0.0246765943	-0.0034711891
1	0.0248678616	-0.0135569800	-0.0268049798
1	0.0325732448	-0.0595931582	-0.0097272699

C_s S_1/S_0 CI

Derivative Coupling

6	0.0000000000	0.0000000000	-0.0011857772
8	0.0000000000	0.0000000000	0.0008678821
1	0.0058657689	0.0018077785	0.0001589475
1	-0.0058657689	-0.0018077785	0.0001589476

Unscaled Gradient Difference

6	0.0296881636	-0.0016151043	0.0000000000
8	-0.0083385274	-0.0031949321	0.0000000000
1	-0.0106748181	0.0024050182	0.0298012381
1	-0.0106748181	0.0024050182	-0.0298012381

Full citation of Gaussian (Ref. 4 in the paper)

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