Supporting Information for:

The Spin-Flip Variant of the Algebraic-Diagrammatic Construction Yields the Correct Topology of S_1/S_0 Conical Intersections

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This Supporting Information contains the Cartesian coordinates of the S_1/S_0 minimum-energy conical intersections (MECIs) of formaldinium optimized with SF-ADC(3) and MS-CASPT2. Furthermore, the **g**- and **h**-branching-plane (BP) vectors computed with MS-CASPT2 are given. Finally, Figure S1 shows the comparison of the MS-CASPT2 and SA-CASSCF potential-energy surfaces in the vicinity of the MS-CASPT2 conical intersection (CI).

1 Optimized MECI Geometries

SF-ADC(3)

N	-0.1697626689	0.1925911828	-0.6551511781
C	0.0230029223	-0.1851916098	0.6476384164
H	1.0300113837	-0.3539783866	1.0427473323
H	0.0240243541	1.1624120661	-0.9317780337
H	-0.0711642873	-0.4956149524	-1.4055465490
H	-0.8361132846	-0.3202191225	1.3020905512

MS-CASPT2

N	-0.1836936768	0.1965191003	-0.6551516027
C	0.0223735596	-0.1854558274	0.6472534499
H	1.0291912204	-0.3512839629	1.0364654438
H	0.0286097799	1.1608087027	-0.9312859307
H	-0.0619078946	-0.4947139467	-1.4025060316
H	-0.8345729886	-0.3258740658	1.3052246712

2 BP Vectors Computed with MS-CASPT2

g-vector:

N	-0.0412208198	-0.0113463748	0.0255276889
C	0.0130098109	0.0163451544	-0.0546852101
H	-0.0041200107	-0.0233144178	0.0034093415
H	-0.0070033530	-0.0047742828	0.0054937220
H	0.0366953855	0.0061377647	0.0113994128
H	0.0026389871	0.0169521563	0.0088550450

h-vector:

N	-0.0029544797	0.0151611395	0.0069964973
C	0.0010036384	-0.0022915006	-0.0061839804
H	0.0027762183	0.0556222852	0.0167682757
H	0.0584057068	-0.0144640664	0.0004080740
H	-0.0567298952	-0.0053710627	-0.0045157840
H	-0.0025011886	-0.0486567950	-0.0134730827

3 Additional Figures

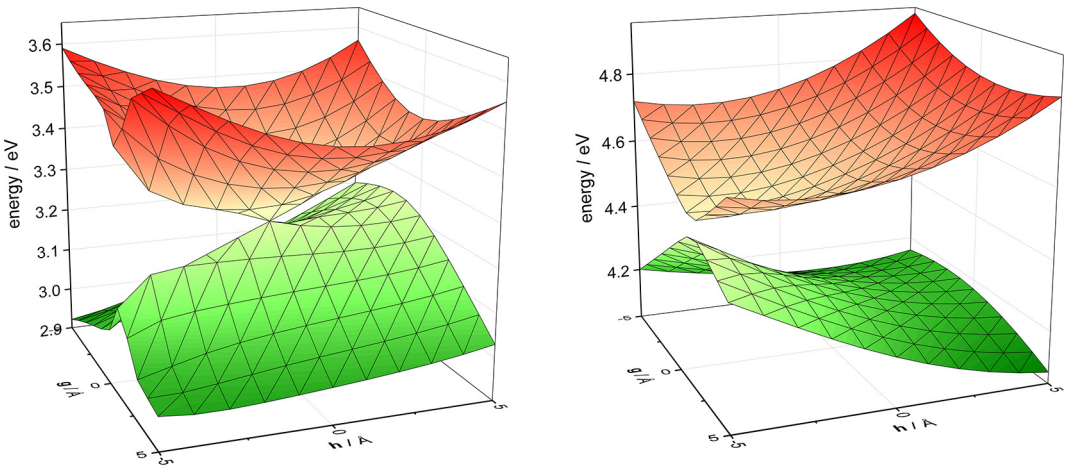

Figure S1: 2D plot of the S_1 and S_0 PESs along the BP spanned by the orthonormalized MS-CASPT2 BP vectors in the vicinity of the MS-CASPT2 MECI of formaldinium. The 2D grids were computed with MS-CASPT2 (left) and with SA2-CASSCF(2,2) (right). The MS-CASPT2 PESs exhibit a ridge of discontinuities in a region of the BP where the SA2-CASSCF PESs converge toward the CASSCF CI.