Supporting Information: The 3s Rydberg state as a doorway state in the ultrafast dynamics of 1,1-Difluoroethylene

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1 MECI optimized geometries

Table 1: Absolute (given in Hartree) and relative (given in eV) SA(11)-CAS(2,6)PT2 energies and state characters of the optimized MECIs.

	$E_{abs}(S_0)$	$E_{abs}(S_1)$	$E_{rel}(S_0)$	$E_{rel}(S_1)$	character (S_0)	character (S_1)
CI_1	-276.2181	-276.2171	6.44	6.47	$\pi\pi$	$\pi\pi^*$
CI_2	-276.2606	-276.2605	5.29	5.29	$\pi\pi$	$\pi\pi^*$
CI_3	-276.2547	-276.2544	5.45	5.46	$\pi\pi$	$\pi\pi^*$
CI_4	-276.3196	-276.3192	3.68	3.69	$\pi\pi$	$\pi\pi^*$
CI_5	-276.3093	-276.3085	3.96	3.98	$\pi\pi$	$\pi\pi^*$
CI_a	-276.2073	-276.2071	6.74	6.74	π-3s	$\pi\pi^*$

In the following, the coordinates of the optimized MECIs are listed in the xyz-format in Ångströms.

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CI_1
  C   0.10159185672908      0.59124106923943     -0.31787663699201
  C   0.07080961384080      0.02659675604750      1.68177903050885
  H   1.04633722341898      0.05518315479232      2.20616014222336
  H   -0.64653148873821     -0.59975132234163      2.25096006491009
  F   -1.17252950845987      0.16936093395398     -0.65759996692368
  F   0.86403405220923      -0.53365319769160     -0.68820693372663
6
CI_2
  C   -0.10363949715912     -0.70299124344654      0.00863505360807
  C   0.02671220107902      0.15659200515217      1.29728567030134
  H   0.54054067152593      -0.22056301397574     2.16928841306125
  H   -0.32355236384549      1.20296595790263      1.43563325327245
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  F   -1.10389167689232      0.06873084888086     -0.63519334312863
  F   1.03616166529198       0.34985944548662     -0.41572004711449
6
CI_3
  C   0.43215203007952      -0.15100472595105     -0.04130594581413
  C   0.50690438001757      -0.11832482959645      1.40264769140447
  H   0.52457473191125       0.85687831939832      1.88207056282805
  H   0.07168750710887      -0.99657260245719      1.88410727472531
  F   -1.36727841546315       0.33007813712966     -0.29846454444995
  F   1.50887576634593      -0.56246429852329     -0.68521203869374
6
CI_4
  C   -0.05502985263486       0.08607085008324     -0.01143875182023
  C   -0.10630921801640      -0.09190589559399      1.34379986948128
  H   0.46709148435737       0.54812650849013      1.99923747541405
  H   0.23853309411089      -1.08674677723805      1.70188049993324
  F   -1.05858310606650       0.31804881402709     -1.01339366271936
  F   1.06834681424951       0.01191028623159     -0.72960801528897
6
CI_5
  C   -0.03038733142042      -0.04826989806666      0.01345416420237
  C   0.04763599310920       0.20857248735486      1.38345416053690
  H   -0.02336820591152       1.25371644569496      1.70570147830225
  H   -0.20086728078286      -0.60929091798683      2.07641850564283
  F   -1.18222910669082      -0.14830914899373     -1.10527093123252
  F   1.02127383169643      -0.28595730800261     -0.75760872845183
6
CI_a
  C   0.00100471367411      -0.01587287825003     -0.09501840353764
  C   0.03069259814874      -0.08693103934330      1.34697986049651
  H   1.00614490636721      -0.03156565769486      1.84726641928832
  H   -0.92652464542920      -0.21087690646326      1.87256405197706
  F   -1.10590443919152       0.04702327287974     -0.75250336154911
  F   1.07220819043065      -0.00748215012829     -0.81230051367515
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