Supporting Information for: Assessment of density functional methods for obtaining geometries at conical intersections in organic molecules

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1 Cartesian coordinates and total energies of species obtained using the 6-31G* basis set

Cartesian coordinates and total energies of species reported in Table 1 of the main article. The geometries at conical intersections were optimized by the SI-SA-REKS method. The ground state equilibrium geometries were optimized by the REKS and the total energies at Franck-Condon points were calculates by the SI-SA-REKS method. All calculations reported in this section employ the 6-31G* basis set.

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1.1 Ethylene

Table 1: Cartesian coordinates (Å) of twisted-pyramidalized MECI in C_2H_4.

	HF			CAM-B3LYP		
	X	Y	Z	X	Y	Z
C	-0.025100	-0.474900	0.743800	0.006100	-0.457800	0.732800
C	-0.209100	-0.024600	-0.554800	-0.214700	-0.029800	-0.562200
H	-0.140100	1.012200	-0.891100	-0.155400	1.024500	-0.925400
H	1.007300	0.057200	0.510100	1.031400	0.044100	0.578400
H	-0.330600	0.144600	1.577900	-0.337900	0.138100	1.586800
H	-0.302300	-0.714500	-1.385700	-0.329400	-0.719000	-1.410400

	M06-2X			BH&HLYP		
	X	Y	Z	X	Y	Z
C	0.025000	-0.462500	0.719100	0.003300	-0.463400	0.726300
C	-0.219700	-0.021600	-0.564500	-0.215800	-0.024800	-0.559700
H	-0.163800	1.024800	-0.941600	-0.153300	1.018900	-0.919900
H	1.043900	0.039100	0.618300	1.020000	0.044900	0.572600
H	-0.341600	0.137400	1.572600	-0.331300	0.140200	1.577600
H	-0.343800	-0.717200	-1.403800	-0.322800	-0.715700	-1.396900

Table 2: Cartesian coordinates (Å) of ethylidene MECI in C_2H_4.

	HF			CAM-B3LYP		
	X	Y	Z	X	Y	Z
C	0.016700	0.081800	-0.451000	0.013100	0.076800	-0.424800
C	-0.306400	-0.107000	0.960200	-0.438500	-0.082800	0.950700
H	1.076600	-0.159800	-0.568200	1.082400	-0.176000	-0.509600
H	-0.118500	1.105200	-0.798900	-0.111500	1.106300	-0.797300
H	-0.537000	-0.573900	-1.119900	-0.527200	-0.573500	-1.128000
H	-0.131400	-0.346300	1.977800	-0.018200	-0.350900	1.909000

	M06-2X			BH&HLYP		
	X	Y	Z	X	Y	Z
C	-0.138800	0.077500	-0.428600	0.016600	0.076800	-0.426700
C	-0.442100	-0.052600	0.873200	-0.428200	-0.068300	0.949600
H	0.829100	-0.254900	-0.029500	1.078400	-0.173300	-0.509100
H	-0.089700	1.121300	-0.798000	-0.113800	1.098100	-0.796500
H	-0.433500	-0.567200	-1.296900	-0.526700	-0.572400	-1.117100
H	0.274900	-0.324000	1.679800	-0.026300	-0.360900	1.899700

Table 3: Total energies (a.u.) of the Franck-Condon point and MECIs of C_2H_4.

	S_0	S_1	S_0	S_1
	HF		CAM-B3LYP	
FC	-78.031115	-77.676717	-78.530333	-78.241685
tw-pyr MECI	-77.840251	-77.840186	-78.341711	-78.341708
eth MECI	-77.883906	-77.883902	-78.378555	-78.378549

	M06-2X		BH&HLYP	
FC	-78.535986	-78.248638	-78.528649	-78.222229
tw-pyr MECI	-78.345516	-78.345512	-78.339098	-78.339091
eth MECI	-78.326729	-78.324540	-78.380168	-78.380166

1.2 Methyliminium cation

Table 4: Cartesian coordinates (Å) of twisted-pyramidalized MECI in $CH_2NH_2^+$.

	HF			CAM-B3LYP		
	X	Y	Z	X	Y	Z
N	-0.015700	0.010500	-0.001500	-0.014100	0.045300	0.011700
C	0.009900	0.027800	1.378800	0.007300	0.202900	1.364800
H	0.967400	0.048800	1.872000	0.951500	-0.047700	1.876900
H	-0.040000	0.859700	-0.550400	-0.042700	0.859900	-0.619700
H	-0.003300	-0.859000	-0.517400	-0.003300	-0.876800	-0.453800
H	-0.927900	0.009000	1.905700	-0.908300	-0.086800	1.907300

	M06-2X			BH&HLYP		
	X	Y	Z	X	Y	Z
N	-0.017600	-0.034700	0.015700	-0.015900	0.038000	0.013700
C	0.009200	-0.180800	1.379200	0.007300	0.181300	1.385400
H	0.938500	0.165100	1.856800	0.962100	-0.033100	1.863500
H	-0.033900	0.876000	-0.467300	-0.041400	0.849300	-0.602900
H	0.000700	-0.856000	-0.605200	-0.002900	-0.866200	-0.466700
H	-0.906500	0.127200	1.907900	-0.918800	-0.072600	1.894100

Table 5: Cartesian coordinates (Å) of methylimine MECI in $CH_2NH_2^+$.

	HF			CAM-B3LYP		
	X	Y	Z	X	Y	Z
N	-0.278500	-0.103800	0.905900	-0.393200	-0.092000	0.873100
C	0.048000	0.076800	-0.467400	0.040400	0.059800	-0.409000
H	1.101500	-0.169200	-0.546200	1.109800	-0.187700	-0.477200
H	-0.143600	1.110600	-0.726500	-0.148100	1.099800	-0.725700
H	-0.570000	-0.592600	-1.053400	-0.565500	-0.570200	-1.075900
H	-0.157300	-0.322000	1.887500	-0.043400	-0.309900	1.814700

	M06-2X			BH&HLYP		
	X	Y	Z	X	Y	Z
N	-0.369300	-0.074200	0.864900	-0.389100	-0.087900	0.876200
C	-0.085400	0.093100	-0.389700	0.039200	0.059700	-0.410000
H	1.093000	-0.210500	-0.380900	1.109700	-0.184500	-0.475500
H	-0.119000	1.128900	-0.765900	-0.146000	1.100100	-0.729200
H	-0.534800	-0.600200	-1.114800	-0.568000	-0.572700	-1.075200
H	0.015500	-0.337200	1.786500	-0.045700	-0.314900	1.813700

Table 6: Total energies (a.u.) of the Franck-Condon point and MECIs of $CH_2NH_2^+$.

	S_0	S_1	S_0	S_1
	HF		CAM-B3LYP	
FC	-94.364737	-94.040703	-94.906607	-94.588916
tw-pyr MECI	-94.246178	-94.245730	-94.759025	-94.758209
meth MECI	-94.203907	-94.203907	-94.736077	-94.736072
	M06-2X		BH&HLYP	
FC	-94.908694	-94.579666	-94.895292	-94.574135
tw-pyr MECI	-94.751564	-94.750705	-94.755529	-94.755422
meth MECI	-94.713243	-94.713224	-94.730096	-94.730019

1.3 Styrene

Table 7: Cartesian coordinates (Å) of MECI1 in styrene.

	HF			CAM-B3LYP		
	X	Y	Z	X	Y	Z
C	0.837200	-0.168100	0.392700	0.896900	-0.164900	0.408300
C	1.772200	-0.623600	-0.627900	1.777000	-0.600400	-0.623000
C	1.301500	-1.443000	-1.655500	1.295500	-1.424200	-1.652300
C	2.155800	-1.830800	-2.668600	2.146600	-1.826800	-2.664200
C	3.484800	-1.429800	-2.638200	3.484700	-1.441200	-2.637100
C	3.975000	-0.641600	-1.603800	3.979500	-0.634200	-1.609200
C	3.116600	-0.236500	-0.602200	3.125600	-0.205500	-0.610400
C	-0.455100	-0.614700	0.574300	-0.421400	-0.651800	0.574600
H	-1.136700	0.168000	0.915600	-1.134700	0.138400	0.876300
H	1.352500	0.534100	1.080200	1.389700	0.543300	1.094700
H	0.273800	-1.735800	-1.588000	0.249600	-1.705200	-1.584900
H	1.802400	-2.443700	-3.473000	1.772600	-2.446300	-3.471200
H	4.150100	-1.731900	-3.428100	4.160000	-1.773300	-3.419000
H	5.006800	-0.350600	-1.592800	5.024500	-0.353700	-1.604500
H	3.479600	0.375800	0.205000	3.490900	0.425200	0.191800
H	-0.075300	-0.956500	1.608700	-0.195600	-1.007900	1.628600

	M06-2X			BH&HLYP		
	X	Y	Z	X	Y	Z
C	0.923900	-0.153200	0.384600	0.882048	-0.160780	0.401175
C	1.774000	-0.619500	-0.619600	1.778251	-0.603064	-0.627255
C	1.287600	-1.448900	-1.654100	1.298809	-1.422055	-1.652280
C	2.148600	-1.836000	-2.664800	2.151171	-1.828716	-2.665207
C	3.485300	-1.432200	-2.635500	3.483747	-1.439772	-2.635226
C	3.971500	-0.640400	-1.598300	3.977015	-0.642940	-1.606264
C	3.123300	-0.229000	-0.593200	3.123828	-0.218428	-0.611414
C	-0.410300	-0.631400	0.571700	-0.425567	-0.646490	0.575038
H	-1.137100	0.150600	0.908600	-1.129941	0.139181	0.879659
H	1.343400	0.552200	1.098400	1.394191	0.538988	1.086184
H	0.241600	-1.740200	-1.636500	0.258649	-1.699490	-1.564131
H	1.760800	-2.449400	-3.482700	1.788762	-2.447617	-3.471336
H	4.168800	-1.751200	-3.423900	4.148727	-1.756473	-3.421824
H	5.007500	-0.339400	-1.591900	5.014602	-0.353430	-1.597675
H	3.472100	0.406900	0.218300	3.484372	0.415728	0.184509
H	-0.119500	-0.967600	1.617200	-0.187296	-1.003182	1.624295

Table 8: Cartesian coordinates (Å) of MECI2 in styrene.

	HF			CAM-B3LYP		
	X	Y	Z	X	Y	Z
C	0.856700	-0.202000	0.407100	0.901300	-0.189400	0.418600
C	1.742400	-0.584100	-0.641500	1.763000	-0.594600	-0.612200
C	1.298300	-1.413800	-1.686300	1.296700	-1.407900	-1.663700
C	2.177400	-1.840600	-2.665000	2.162700	-1.838800	-2.651100
C	3.508200	-1.453200	-2.644900	3.495100	-1.448700	-2.642800
C	3.957100	-0.642100	-1.612300	3.964900	-0.639300	-1.618300
C	3.096200	-0.212600	-0.619000	3.117300	-0.227900	-0.610100
C	-0.353800	0.357600	0.581600	-0.366000	0.365100	0.544400
H	-0.755100	1.129100	-0.071200	-0.793800	1.129000	-0.106400
H	1.086300	0.923500	0.763100	1.115000	0.918900	0.777200
H	0.264800	-1.720200	-1.709700	0.265000	-1.707800	-1.673600
H	1.817000	-2.482000	-3.453100	1.791300	-2.469400	-3.437200
H	4.177300	-1.781800	-3.418000	4.162500	-1.768600	-3.425500
H	4.998100	-0.347500	-1.576700	4.998600	-0.333800	-1.607100
H	3.455700	0.401400	0.183200	3.492500	0.382100	0.202100
H	-0.982300	0.157100	1.440400	-1.021400	0.120000	1.383600

	M06-2X			BH&HLYP		
	X	Y	Z	X	Y	Z
C	0.935500	-0.154600	0.421000	0.871200	-0.188700	0.420500
C	1.755500	-0.590200	-0.615700	1.768700	-0.599600	-0.612700
C	1.291100	-1.424000	-1.656500	1.300100	-1.408400	-1.659900
C	2.155300	-1.834400	-2.657800	2.162400	-1.833300	-2.651400
C	3.492800	-1.445900	-2.649800	3.494400	-1.444400	-2.647100
C	3.965700	-0.640800	-1.615100	3.965200	-0.639400	-1.618500
C	3.111900	-0.226700	-0.611000	3.122100	-0.229900	-0.608100
C	-0.382200	0.361200	0.535400	-0.361700	0.362300	0.549300
H	-0.789800	1.119500	-0.125100	-0.791900	1.129800	-0.107900
H	1.156100	0.936700	0.813700	1.117100	0.920300	0.775300
H	0.256100	-1.733400	-1.671500	0.266300	-1.708300	-1.673000
H	1.788400	-2.476700	-3.449300	1.792100	-2.471300	-3.436500
H	4.160400	-1.761000	-3.437300	4.163300	-1.770700	-3.426100
H	5.004400	-0.333900	-1.590400	5.000000	-0.334500	-1.609100
H	3.479400	0.380700	0.209200	3.494400	0.382900	0.200000
H	-1.036100	0.112400	1.378200	-1.019100	0.122000	1.383000

Table 9: Total energies (a.u.) of the Franck-Condon point and MECIs of styrene.

	S_0	S_1	S_0	S_1
	HF		CAM-B3LYP	
FC	-307.582655	-307.343116	-309.454902	-309.263606
MECI1	-307.415630	-307.415629	-309.293249	-309.293246
MECI2	-307.393142	-307.393127	-309.271795	-309.271785

	M06-2X		BH&HLYP	
FC	-309.498779	-309.311239	-309.448569	-309.249950
MECI1	-309.330352	-309.330351	-309.286196	-309.286195
MECI2	-309.314869	-309.314864	-309.263292	-309.263291

1.4 Stilbene

Table 10: Cartesian coordinates (Å) of MECI in stilbene.

	HF			CAM-B3LYP		
	X	Y	Z	X	Y	Z
C	0.766100	-0.143400	0.405600	0.883600	-0.153800	0.391400
C	1.733300	-0.608200	-0.634600	1.736400	-0.658500	-0.613700
C	1.266600	-1.394400	-1.689900	1.271100	-1.438500	-1.683400
C	2.123400	-1.769800	-2.704800	2.137500	-1.789100	-2.696600
C	3.458000	-1.384500	-2.657200	3.460300	-1.337500	-2.660500
C	3.950100	-0.617200	-1.605400	3.922700	-0.592600	-1.605100
C	3.079900	-0.224600	-0.599200	3.069200	-0.248300	-0.587600
C	-0.496600	-0.598500	0.576400	-0.490400	-0.563500	0.559300
C	-1.589200	0.259800	1.026000	-1.598300	0.262700	1.028000
C	-1.855300	1.498900	0.423000	-1.882500	1.490500	0.412800
C	-2.946000	2.264200	0.807500	-2.953700	2.271300	0.803000
C	-3.807600	1.835800	1.803700	-3.803100	1.856000	1.813800
C	-3.549600	0.614000	2.410500	-3.567600	0.627200	2.420500
C	-2.472900	-0.156400	2.032400	-2.495400	-0.159800	2.030800
H	1.343100	0.502500	1.114700	1.354800	0.472000	1.147100
H	0.231000	-1.674800	-1.632700	0.240900	-1.751900	-1.698800
H	1.768400	-2.363700	-3.526200	1.784700	-2.387900	-3.522000
H	4.124400	-1.684900	-3.446200	4.133300	-1.647700	-3.455200
H	4.987300	-0.333500	-1.580300	4.951300	-0.269300	-1.588000
H	3.453500	0.378800	0.211200	3.417400	0.359200	0.232000
H	-0.054500	-1.025600	1.546400	-0.017700	-1.023700	1.509500
H	-1.225800	1.851300	-0.378800	-1.236100	1.833300	-0.382000
H	-3.119400	3.208400	0.316500	-3.124900	3.219100	0.314500
H	-4.657300	2.426200	2.095300	-4.634700	2.469200	2.120700
H	-4.205800	0.250100	3.182300	-4.222300	0.278300	3.203500
H	-2.305300	-1.110300	2.504300	-2.336900	-1.116700	2.506200

	M06-2X			BH&HLYP		
	X	Y	Z	X	Y	Z
C	0.895200	-0.122000	0.364100	0.874800	-0.150700	0.392200
C	1.741400	-0.653400	-0.615700	1.738200	-0.655000	-0.613800
C	1.271300	-1.438300	-1.683200	1.271400	-1.436000	-1.684100
C	2.136300	-1.791600	-2.694900	2.130400	-1.791200	-2.695600
C	3.460000	-1.369000	-2.662500	3.454800	-1.363700	-2.659000
C	3.931000	-0.602200	-1.603600	3.925500	-0.591800	-1.604800
C	3.082600	-0.238700	-0.585900	3.071500	-0.243100	-0.587300
C	-0.509800	-0.563800	0.559900	-0.489900	-0.563900	0.558600
C	-1.599400	0.262000	1.029100	-1.598100	0.262600	1.027500
C	-1.883500	1.490400	0.415100	-1.878400	1.493400	0.412900
C	-2.954800	2.270900	0.805800	-2.952800	2.272600	0.803200
C	-3.804400	1.854600	1.815900	-3.802200	1.854800	1.815300
C	-3.569000	0.625200	2.421500	-3.563700	0.625700	2.419800
C	-2.496700	-0.161500	2.031200	-2.495500	-0.160800	2.029900
H	1.353700	0.471300	1.149200	1.354700	0.473000	1.147500
H	0.240500	-1.749900	-1.699200	0.242300	-1.749800	-1.699900
H	1.784700	-2.384100	-3.522600	1.786800	-2.384200	-3.523100
H	4.133300	-1.644100	-3.454500	4.135100	-1.643200	-3.455300
H	4.950800	-0.267400	-1.585900	4.952000	-0.265500	-1.587300
H	3.416500	0.359200	0.234300	3.417700	0.361500	0.232700
H	-0.018900	-1.024800	1.509700	-0.017400	-1.023400	1.508700
H	-1.236900	1.834100	-0.379200	-1.236300	1.834200	-0.381500
H	-3.125800	3.219000	0.318200	-3.125800	3.218700	0.315300
H	-4.636100	2.467500	2.123400	-4.635800	2.467400	2.120700
H	-4.224000	0.275500	3.204100	-4.222800	0.276200	3.202500
H	-2.338300	-1.118800	2.505900	-2.336700	-1.117800	2.504900

Table 11: Total energies (a.u.) of the Franck-Condon points and MECI of stilbene.

	S_0	S_1	S_0	S_1
	HF		CAM-B3LYP	
trans-FC	-537.137837	-536.927428	-540.380313	-540.222826
cis-FC	-537.131724	-536.909037	-540.373610	-540.206921
MECI	-536.966146	-536.966112	-540.215931	-540.215925
	M06-2X		BH&HLYP	
trans-FC	-540.462963	-540.307726	-540.369326	-540.208889
cis-FC	-540.458135	-540.295896	-540.362270	-540.191193
MECI	-540.293796	-540.293789	-540.205066	-540.205049

1.5 Protonated Schiff base, PSB3

Table 12: Cartesian coordinates (Å) of MECI in PSB3.

	HF			CAM-B3LYP		
	X	Y	Z	X	Y	Z
C	-2.843500	-0.901100	0.810600	-2.849300	-0.907500	0.809900
C	-1.502900	-0.886600	0.826300	-1.500000	-0.856600	0.786800
C	-0.725200	0.000600	0.026500	-0.757200	0.068000	0.039000
C	0.730800	-0.035100	0.002400	0.687300	-0.042000	0.005800
C	1.516800	0.803200	0.847700	1.527600	0.823600	0.870500
N	2.805500	0.796200	0.853400	2.811200	0.784100	0.865400
H	1.270400	-0.697500	-0.654900	1.260200	-0.738600	-0.627000
H	-1.205200	0.648800	-0.688100	-1.185300	0.649300	-0.765900
H	1.025000	1.479900	1.523300	1.028200	1.526200	1.539600
H	-0.983000	-1.572000	1.474900	-0.963800	-1.552600	1.432300
H	3.330500	1.393300	1.461500	3.366900	1.390600	1.472700
H	3.339000	0.194800	0.252500	3.339300	0.150900	0.254700
H	-3.405400	-1.584800	1.418400	-3.340200	-1.638100	1.437500
H	-3.405200	-0.243000	0.167800	-3.477500	-0.261000	0.201100

	M06-2X			BH&HLYP		
	X	Y	Z	X	Y	Z
C	-2.868600	-0.912800	0.817000	-2.854200	-0.909900	0.821700
C	-1.508000	-0.876700	0.792100	-1.506600	-0.870600	0.782600
C	-0.728100	0.037300	0.051100	-0.727400	0.025700	0.066500
C	0.723600	-0.037100	-0.016600	0.707100	-0.038800	-0.007300
C	1.552700	0.842300	0.859100	1.515100	0.817700	0.863200
N	2.795100	0.789300	0.868800	2.796700	0.789400	0.858000
H	1.299600	-0.705500	-0.671300	1.281900	-0.691600	-0.664800
H	-1.150300	0.633400	-0.751700	-1.144500	0.648700	-0.732100
H	0.990600	1.530100	1.516600	1.014100	1.505300	1.527700
H	-0.978200	-1.591400	1.433700	-0.988400	-1.560400	1.437200
H	3.354300	1.384500	1.486700	3.342800	1.379400	1.472900
H	3.320100	0.152600	0.260400	3.319500	0.168000	0.253300
H	-3.379500	-1.610800	1.459200	-3.374800	-1.589700	1.466100
H	-3.475800	-0.238900	0.217300	-3.433800	-0.276800	0.177400

Table 13: Total energies (a.u.) of the Franck-Condon points and MECI of PSB3.

	S_0	S_1	S_0	S_1
	HF		CAM-B3LYP	
trans-FC	-248.189000	-248.012309	-249.667850	-249.516445
cis-FC	-248.183100	-248.010690	-249.662935	-249.514426
MECI	-248.098025	-248.098007	-249.555747	-249.555667
	M06-2X		BH&HLYP	
trans-FC	-249.687607	-249.533192	-249.659245	-249.503585
cis-FC	-249.682897	-249.530867	-249.654007	-249.501458
MECI	-249.564518	-249.564432	-249.548551	-249.548508

1.6 HBI anion

Table 14: Cartesian coordinates (Å) of $MECI_{ph}$ in HBI anion.

	HF			CAM-B3LYP		
	X	Y	Z	X	Y	Z
N	-0.739464	0.266736	3.537723	-0.701300	0.361000	3.540200
N	-0.309361	1.007690	1.499933	-0.208200	0.983500	1.474800
H	-1.023882	0.238377	4.479172	-0.954500	0.381000	4.513100
H	-1.275778	2.268700	2.840841	-1.257400	2.322300	2.789500
H	0.895256	-2.102895	0.677710	0.812500	-2.114000	0.442900
H	2.301623	0.512759	-1.136059	2.306100	0.477600	-1.125400
H	1.654482	1.231159	-3.431305	1.632500	1.315800	-3.382700
H	-2.157323	-0.629246	-2.941418	-2.126200	-0.702000	-2.957300
H	-1.517895	-1.334600	-0.641659	-1.475800	-1.326100	-0.574100
C	-0.781005	1.340385	2.627105	-0.761400	1.378900	2.613000
C	0.230744	-0.286533	1.659993	0.247600	-0.321600	1.657800
C	-0.014105	-0.742661	2.942000	-0.041200	-0.749400	2.961000
C	0.933800	-1.009100	0.570800	0.958800	-1.032100	0.573000
C	0.462839	-0.530033	-0.748756	0.483600	-0.504200	-0.729500
C	1.341539	0.272100	-1.556300	1.344700	0.259200	-1.542300
C	0.997200	0.676800	-2.792000	0.990800	0.703300	-2.775000
C	-0.304000	0.369800	-3.362800	-0.289500	0.350800	-3.339400
C	-1.192400	-0.396000	-2.523500	-1.187100	-0.414900	-2.501500
C	-0.834000	-0.790900	-1.268000	-0.826500	-0.784500	-1.242300
O	0.179100	-1.792000	3.562300	0.152400	-1.819200	3.595800
O	-0.576700	0.669000	-4.513600	-0.616800	0.674800	-4.486200

	M06-2X			BH&HLYP		
	X	Y	Z	X	Y	Z
N	-0.551071	0.458226	3.551593	-0.668547	0.372949	3.522406
N	-0.281721	0.965224	1.445493	-0.242636	0.990664	1.475466
H	-0.862712	0.469339	4.512328	-0.968516	0.390639	4.478737
H	-1.178633	2.338353	2.833049	-1.273624	2.299057	2.797124
H	0.765800	-2.085700	0.414239	0.805541	-2.081806	0.637036
H	2.298339	0.485614	-1.088567	2.298394	0.505248	-1.147056
H	1.632321	1.333000	-3.382433	1.674226	1.281888	-3.427079
H	-2.105253	-0.750653	-2.989647	-2.132369	-0.641370	-2.945212
H	-1.512500	-1.343400	-0.604500	-1.513315	-1.338300	-0.634574
C	-0.787800	1.360571	2.615797	-0.780289	1.358554	2.610560
C	0.199037	-0.298900	1.652000	0.213405	-0.295689	1.639532
C	-0.030200	-0.740400	2.961300	-0.027158	-0.747246	2.948357
C	0.938600	-1.006400	0.588600	0.940800	-1.008354	0.572562
C	0.468600	-0.510700	-0.724500	0.470027	-0.515354	-0.741000
C	1.358700	0.273400	-1.567000	1.343600	0.279000	-1.577023
C	1.002400	0.688300	-2.772500	1.002059	0.715271	-2.795636
C	-0.276000	0.334300	-3.316900	-0.296213	0.381188	-3.340170
C	-1.187400	-0.421200	-2.508300	-1.172006	-0.409507	-2.515373
C	-0.837700	-0.797800	-1.251200	-0.835423	-0.795154	-1.264250
O	0.185500	-1.802900	3.591300	0.186742	-1.810700	3.575100
O	-0.583700	0.678900	-4.503600	-0.583599	0.680707	-4.511389

Table 15: Cartesian coordinates (Å) of MECI$_{Im}$ in HBI anion.

	HF			CAM-B3LYP		
	X	Y	Z	X	Y	Z
N	-1.299238	0.339759	3.240790	-1.287922	0.402073	3.278159
N	0.800305	0.626897	2.525228	0.830948	0.572276	2.493404
H	-2.122071	0.455012	3.781467	-2.110952	0.566254	3.836826
H	0.038099	1.754079	4.105047	0.099410	1.787742	4.093722
H	1.099560	-2.022827	0.687073	1.045972	-2.035327	0.707600
H	0.959670	-2.403094	-1.714407	0.967665	-2.420451	-1.711049
H	0.409491	-1.703268	-3.978660	0.419112	-1.695268	-3.998581
H	-0.603061	2.185834	-2.517401	-0.626991	2.185234	-2.528401
H	-0.050405	1.487575	-0.271779	-0.029165	1.493660	-0.254918
C	-0.124282	0.991103	3.362959	-0.092378	1.003102	3.369336
C	0.246407	-0.334347	1.718648	0.255259	-0.339442	1.711209
C	-1.154938	-0.569372	2.192501	-1.154176	-0.542918	2.203256
C	0.867944	-0.978686	0.560437	0.885655	-0.974423	0.556495
C	0.492588	-0.535990	-0.764801	0.493550	-0.542072	-0.762627
C	0.616064	-1.392546	-1.885217	0.611174	-1.404178	-1.882954
C	0.310590	-1.008605	-3.161018	0.305053	-1.004285	-3.164619
C	-0.152080	0.319585	-3.489360	-0.176530	0.306889	-3.484531
C	-0.266771	1.178200	-2.340575	-0.279624	1.170533	-2.343243
C	0.040777	0.768040	-1.070449	0.043965	0.763826	-1.062609
O	-1.995962	-1.338632	1.847477	-2.000929	-1.330200	1.877880
O	-0.422291	0.682882	-4.647042	-0.482761	0.669331	-4.655949

	M06-2X			BH&HLYP		
	X	Y	Z	X	Y	Z
N	-1.204597	0.489064	3.298271	-1.295805	0.397677	3.246615
N	0.812950	0.558973	2.503115	0.810632	0.575651	2.493733
H	-2.068901	0.726013	3.790986	-2.115205	0.537682	3.804203
H	0.149926	1.793804	4.106972	0.082341	1.772595	4.076561
H	1.054306	-2.042393	0.659729	1.046801	-2.025598	0.701371
H	0.966519	-2.414797	-1.710006	0.961747	-2.403489	-1.710006
H	0.393884	-1.712279	-3.986453	0.406472	-1.706008	-3.979371
H	-0.621482	2.197001	-2.519316	-0.617005	2.177215	-2.523692
H	-0.034184	1.491188	-0.254934	-0.018788	1.492185	-0.267427
C	-0.097892	1.018302	3.398559	-0.102597	1.000722	3.351744
C	0.247536	-0.338187	1.718474	0.243054	-0.341700	1.710850
C	-1.157098	-0.553669	2.193144	-1.155350	-0.548029	2.198789
C	0.885622	-0.972496	0.554024	0.883311	-0.969317	0.557519
C	0.494677	-0.538084	-0.765028	0.492253	-0.538589	-0.763747
C	0.621323	-1.395777	-1.882804	0.609226	-1.394012	-1.882551
C	0.304979	-1.004285	-3.164584	0.302124	-1.007155	-3.161728
C	-0.164026	0.314880	-3.485871	-0.181333	0.305903	-3.486463
C	-0.271497	1.182820	-2.344628	-0.280635	1.166843	-2.343438
C	0.048695	0.768756	-1.068760	0.053315	0.769557	-1.069520
O	-1.986677	-1.332173	1.855749	-1.994467	-1.333938	1.869181
O	-0.467564	0.675800	-4.651297	-0.478928	0.667023	-4.653616

Table 16: Total energies (a.u.) of the Franck-Condon point and MECIs of HBI anion.

	S_0	S_1	S_0	S_1
	HF		CAM-B3LYP	
FC	-641.398504	-641.256916	-644.958011	-644.846930
MECI$_{Ph}$	-641.278669	-641.278664	-644.830087	-644.830083
MECI$_{Im}$	-641.299331	-641.299330	-644.849232	-644.849200

	M06-2X		BH&HLYP	
FC	-645.017015	-644.903551	-644.898242	-644.784381
MECI$_{Ph}$	-644.871432	-644.871412	-644.773107	-644.773094
MECI$_{Im}$	-644.883112	-644.883084	-644.788948	-644.788928

2 Cartesian coordinates and total energies of ethylene and stilbene obtained using the 6-311G** basis set

Cartesian coordinates and total energies of conical intersections in ethylene and stilbene. The geometries at conical intersections were optimized by the SI-SA-REKS/BH&HLYP method. The ground state equilibrium geometries were optimized by the REKS/BH&HLYP and the total energies at Franck-Condon points were calculates by the SI-SA-REKS/BH&HLYP method. All calculations reported in this section employ the 6-311G** basis set.

Table 17: Cartesian coordinates (Å) of MECIs in C_2H_4.

	twisted-pyramidalized MECI			ethylidene MECI		
	X	Y	Z	X	Y	Z
C	0.025336	-0.470871	0.728637	0.005410	-0.048119	-0.000395
C	-0.205102	-0.036602	-0.554744	-0.000151	0.014408	1.452711
H	-0.148920	1.008391	-0.902373	1.025140	-0.020213	1.831361
H	1.044934	0.046157	0.601632	-0.459237	0.929634	1.830993
H	-0.340180	0.112753	1.567130	0.706302	-0.110984	-0.807215
H	-0.306501	-0.724690	-1.395197	-0.545302	-0.819841	1.898384

Table 18: Total energies (a.u.) and relative energies (eV) of the Franck-Condon point and MECIs of C_2H_4.

	S_0	S_1	$\Delta E(S_0)$	$\Delta E(S_1)$
FC	-78.553132	-78.255034	0.000	8.112
tw-pyr MECI	-78.368899	-78.368831	5.013	5.015
eth MECI	-78.405510	-78.405420	4.017	4.019

Table 19: Cartesian coordinates (Å) of MECI in stilbene.

	twisted-pyramidalized MECI		
	X	Y	Z
C	0.900782	-0.167909	0.391671
C	1.753047	-0.637294	-0.632764
C	1.291459	-1.438599	-1.683505
C	2.160524	-1.827600	-2.678019
C	3.492801	-1.437539	-2.647992
C	3.969700	-0.647566	-1.611287
C	3.106082	-0.256579	-0.613336
C	-0.458885	-0.565289	0.553301
C	-1.577290	0.260067	1.007881
C	-1.842897	1.503854	0.415199
C	-2.928140	2.266853	0.798267
C	-3.783450	1.833785	1.798997
C	-3.523111	0.618334	2.410729
C	-2.450219	-0.158944	2.022563
H	1.381515	0.481549	1.133255
H	0.260110	-1.744784	-1.666010
H	1.794907	-2.439384	-3.482975
H	4.159780	-1.766766	-3.426931
H	5.000652	-0.349518	-1.574213
H	3.465072	0.349535	0.202823
H	-0.026988	-1.026869	1.508900
H	-1.207180	1.855094	-0.377008
H	-3.099901	3.211426	0.315500
H	-4.629002	2.424660	2.098154
H	-4.174140	0.270673	3.195967
H	-2.275287	-1.105521	2.505100

Table 20: Total energies (a.u.) and relative energies (eV) of the Franck-Condon points and MECI of stilbene.

	S_0	S_1	$\Delta E(S_0)$	$\Delta E(S_1)$
trans-FC	-540.492552	-540.334363	0.000	4.305
cis-FC	-540.485771	-540.315338	0.185	4.822
tw-pyr MECI	-540.333370	-540.333364	4.332	4.332