Supplementary Information for

Non-Adiabatic Dynamics Simulation Exploration on Wavelength-Dependent Photoinduced Relaxation Mechanism of Trans-N-1-Methyl-2-(Tolylazo) Imidazole in Gas Phase

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CONTENTS

dihedral angle CNNC (ordinate) and bond angle C6NN (abscissa) at hopping points from the S_1 to S_0 state. The blue hexagons show the four twist MECIs and red quadrangle shows MECI5 optimized at SA3-CASSCF(12,10)/6-31G* level. The dynamics simulations were started from the S_1 state performed at SA3-CASSCF(6,5)/6-31G level, shown in Figure 4S……p.S13

j. Time-dependent potential energies of the S_0, S_1 and S_2 states for a typical trajectory, shown in Figure 5S……………p.S14

k. Figure 6S. Time-dependent parameter variables of a typical trajectory started from the S_1 state performed at SA3-CASSCF(6,5)/6-31G level. top: the lengths of twist bonds NC9, NN and C6N; middle: time evolution of the two key bond angles NNC9 and C6NN; bottom: the dihedral angle C6NNC9 related with the twist motion around NN bond over the simulation time of 900 fs. The vertical dashed lines indicate the hopping time…………p.S15

l. The coordinates of endpoints used in LIIC were presented in Table 5S-6S in Z-matrices form…………………p.S16- S17

m. Cartesian coordinates of optimized structures calculated at SA3-CASSCF(12,10)/6-31G* level: Table 7S-11S…………...p. S18-S22

n. The Cartesian coordinates of optimized structures calculated at SA3-CASSCF(12,10)/ 6-311G** level: Table 12S-16S…………...p. S23-S27

12e10o

| 48 | 49 | 50 | 51 | 52 |

| 53(HOMO) | 54(LOMO) | 55 | 56 | 57 |

6e5o

| 51 | 52 | 53(HOMO) | 54(LOMO) | 55 |
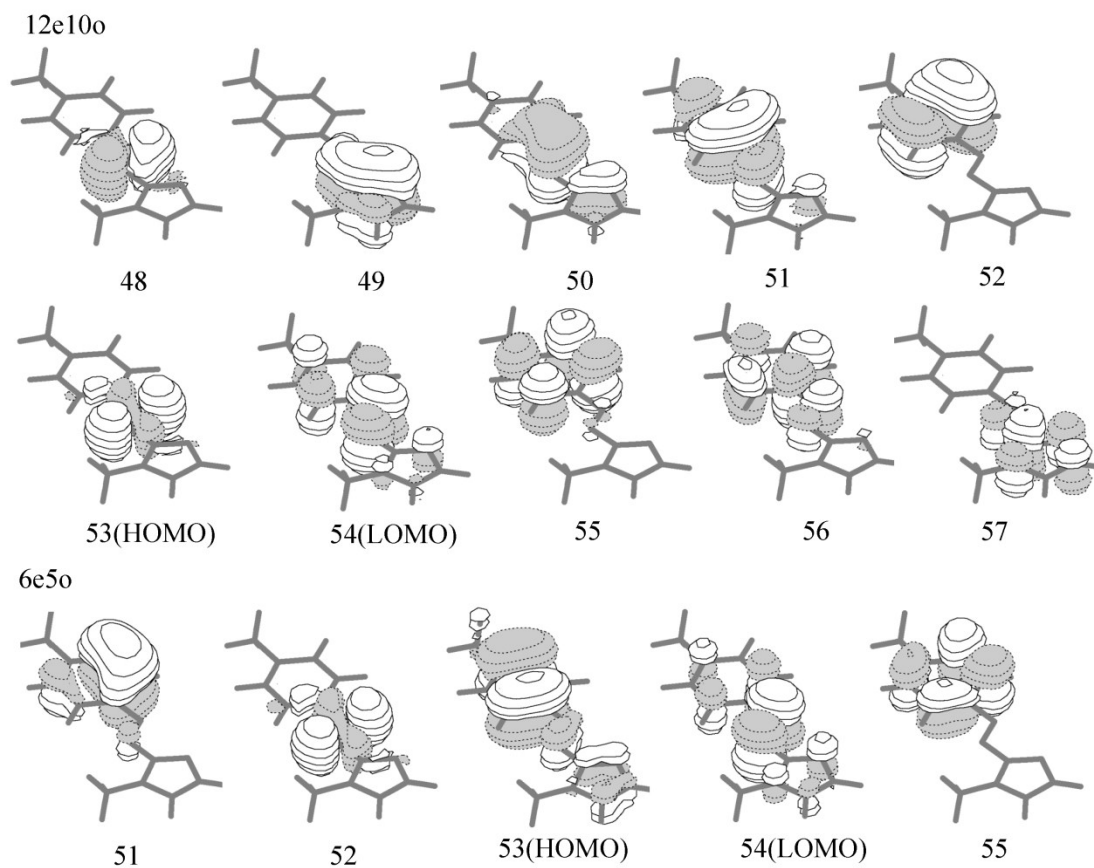
Figure 1S. The active spaces included in CASSCF(12,10) and CASSCF (6,5) calculation levels, Figure 1S shows the active orbitals for the most stable ground-state conformation of trans-MTAI.
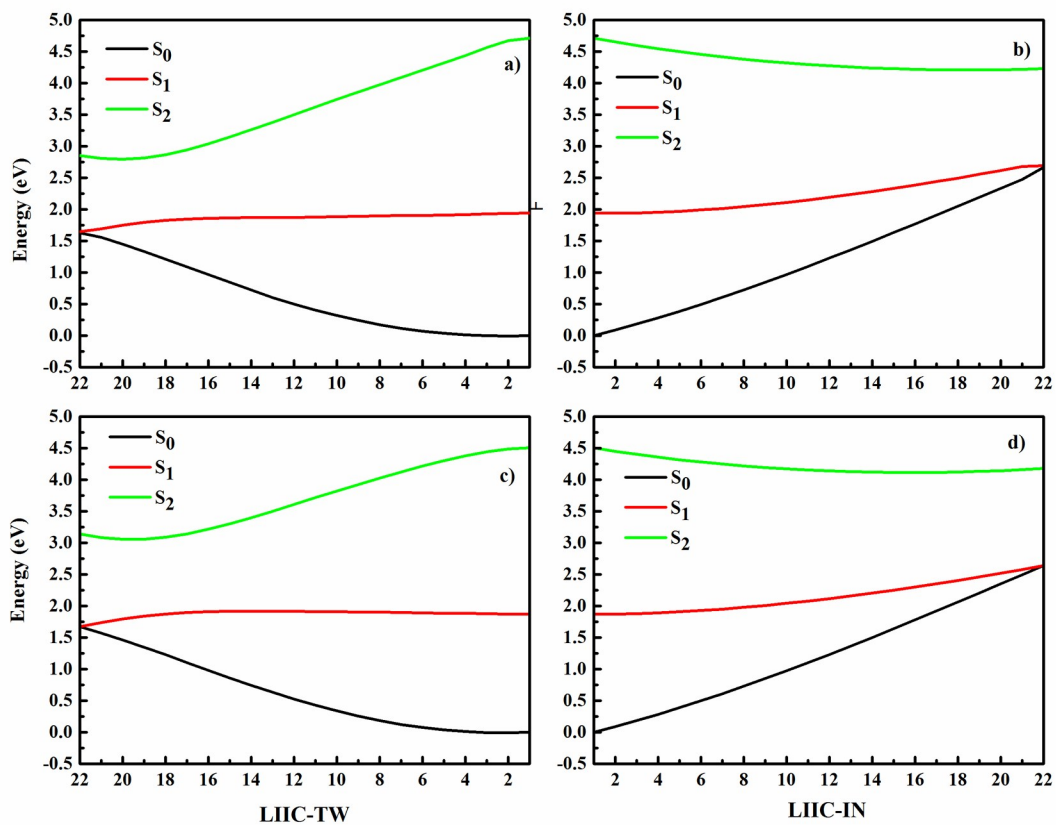
Figure 2S. The energy profiles along constructed linearly interpolated internal coordinate (LIIC) pathway between FC and MECI1 (left) and MECI5 (right) at SA3-CASSCF(12,10) /6-31G* (a and b) CASPT2 (c and d) calculation levels.
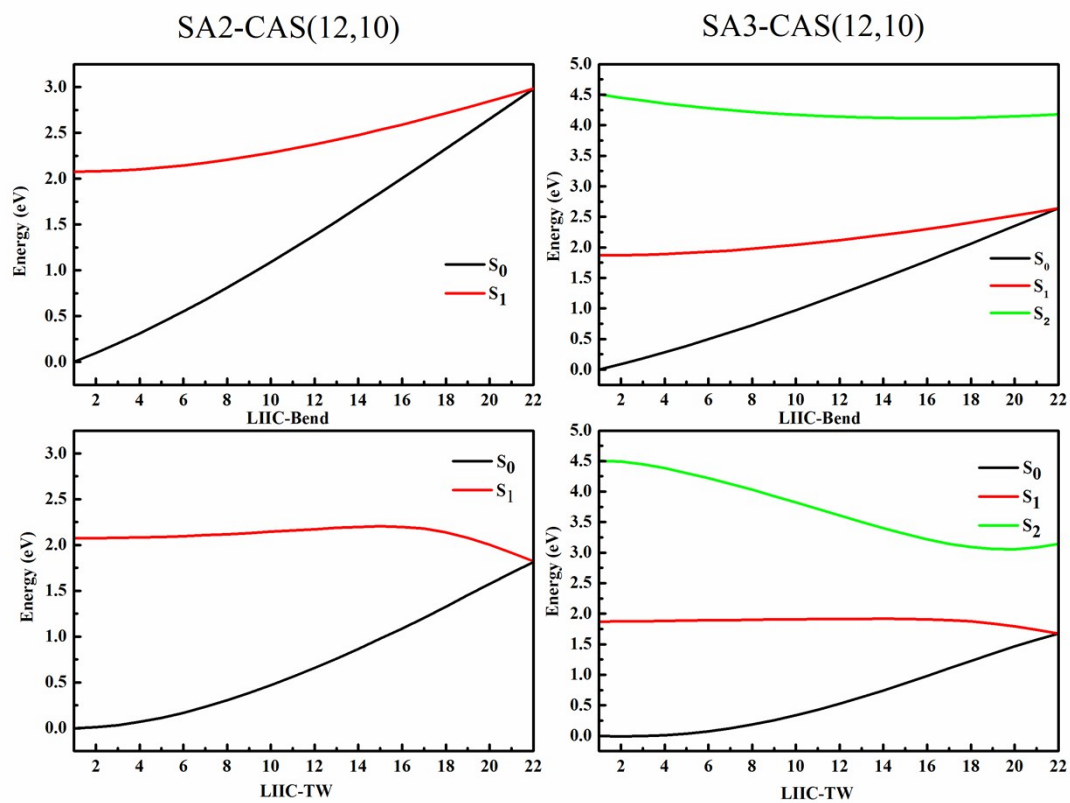
Figure 3S. The energy profiles along constructed linearly interpolated internal coordinate (LIIC) pathway between FC and MECI1 (bottom) and MECI5 (top) at SA2-CASSCF(12,10)/6-31G* (left) and SA3-CASSCF(12,10)/6-31G* (right) calculation levels.

Calculation Details of Different CASSCF parameters (continued)

Firstly, in order to check the accuracy of calculation results we obtained with 6-31G*, larger basis set 6-311G** was employed to examine the effect of the size of basis set on the optimized configurations. The most relevant geometrical parameters calculated at SA3-CASSCF(12,10)/6-311G** and 6-31G* levels are summarized in Table 1S, and the relevant Cartesian coordinates are provided in Table12S-16S . The calculation results indicated that the size of basis set do not have much effect on the optimized geometries.

In order to determine a reasonable calculation level which can provide a balanced description of results accuracy and calculation cost, different CASSCF parameters SA3-CASSCF(10,8)/6-31G*, SA3-CASSCF(6,5)/6-31G, SA2-CASSCF (12,10)/6-31G*, SA2-CASSCF(10,8)/6-31G* and SA2-CASSCF(6,5)/6-31G were employed to compare the results obtained by SA3-CASSCF(12,10)/6-31G* method. The most relevant parameters are summarized in Table 2S, and the relative energies at different geometries are presented in Table 3S. The results computed at all levels we performed present essentially the same qualitative features.

Next, We compared the energy profiles of the S_1 state at SA3- CASSCF(12,10)/6-31G* and SA2-CASSCF(12,10)/6-31G* levels to test the influence of numbers of states included in the averaging procedure, which has been presented in Figure 3S. Obviously, the two levels give essentially the same qualitative features, which should lead to similar dynamics behaviors. For further confirmation, 20 trajectories performed at SA3-CASSCF(6,5)/6-31G level have been performed to compare the results obtained at SA2-CASSCF(6,5)/6-31G level. The results are presented in Figure 4S -6S. All hopping structures are around the four twisting related MECIs, but far away from MECI5. The results are consistent with those obtained at SA2-CASSCF(6,5)/6-31G level.

In sum, the SA3-CASSCF(6,5)/6-31G method used for the S_2 state dynamics simulation and SA2-CASSCF(6,5)/6-31G used for the S_1 state dynamics simulations are reasonable based on the calculations we performed before.

Table 1S Key geometrical parameters of optimal structures in the S_0, S_1 and S_2 states and the six

minimum energy conical intersections calculated at SA3-CASSCF(12,10)/6-31G* and SA3-

CASSCF(12,10)/6-311G** levels, with the bond lengths in angstroms, angles in degree.

Geo.	Method	C6N7	NN	N8C9	C6N7N8	N7N8C9	C6N7N8C9
S_0-min	a	1.418	1.244	1.405	115.2	114.4	-180.0
	b	1.447	1.238	1.409	114.7	114.3	-180.0
S_1-min	a	1.359	1.257	1.359	130.5	124.6	180.0
	b	1.359	130.5	1.376	130.5	124.6	180.0
S_2-min	a	1.308	1.361	1.341	113.4	112.8	179.9
	b	1.307	1.364	1.389	112.8	112.1	179.9
MECI1	a	1.391	1.272	1.358	118.9	135.7	94.1
	b	1.403	1.258	1.352	118.6	139.7	95.7
MECI2	a	1.398	1.265	1.356	118.9	135.7	-93.2
	b	1.406	1.256	1.353	118.5	140.4	-95.3
MECI3	a	1.359	1.254	1.405	143.6	116.5	95.4
	b	1.359	1.251	1.406	143.5	116.6	95.3
MECI4	a	1.357	1.253	1.406	144.1	116.5	-95.7
	b	1.358	1.252	1.395	143.5	116.9	-95.1
MECI5	a	1.286	1.210	1.350	156.5	144.1	179.9
	b	1.281	1.202	1.356	157.8	147.6	179.9
MECI6	a	1.317	1.348	1.334	111.7	113.9	-179.9
	b	1.289	1.443	1.383	105.1	106.4	-179.9

a.SA3-CASSCF(12,10)/6-31G*; b.SA3-CASSCF(12,10)/6-311G**

Table 2S Key geometrical parameters of optimal structures in S_0, S_1 and S_2 states optimized at different CASSCF levels, with the bond lengths in angstroms, angles in degree.

Geometry	Method	C6-N7	N7-N8	N8-C9	C6-N7-N8	N7-N8-C9	C6-N7-N8-C9
S_0-min	SA2-CASSCF(6,5)[a]	1.428	1.246	1.408	115.2	114.1	-180.0
	SA2-CASSCF(10,8)[b]	1.419	1.246	1.413	115.0	114.2	-180.0
	SA2-CASSCF(12,10)[b]	1.419	1.246	1.413	115.1	114.0	-180.0
	SA3-CASSCF(6,5)[a]	1.383	1.239	1.394	118.8	117.6	-180.0
	SA3-CASSCF(10,8)[b]	1.419	1.243	1.409	115.2	114.1	-180.0
	SA3-CASSCF(12,10)[b]	1.418	1.244	1.405	115.2	114.4	-180.0
S_1-min	SA2-CASSCF(6,5)[a]	1.377	1.292	1.379	136.7	117.8	180.0
	SA2-CASSCF(10,8)[b]	1.359	1.257	1.378	130.7	124.2	180.0
	SA2-CASSCF(12,10)[b]	1.359	1.257	1.378	130.5	124.5	180.0
	SA3-CASSCF(6,5)[a]	1.367	1.245	1.367	134.1	127.6	180.0
	SA3-CASSCF(10,8)[b]	1.359	1.257	1.377	130.7	124.3	180.0
	SA3-CASSCF(12,10)[b]	1.359	1.257	1.359	130.5	124.6	180.0
S_2-min	SA3-CASSCF(6,5)[a]	1.291	1.365	1.376	114.5	114.5	-179.9
	SA3-CASSCF(10,8)[b]	1.305	1.343	1.382	113.4	112.9	179.9
	SA3-CASSCF(12,10)[b]	1.308	1.361	1.341	113.4	112.8	179.9

[a] 6-31G basis set; [b] 6-31G* basis set;

Table 3S Key geometrical parameters of six minimum energy conical intersections (MECIs) optimized at different CASSCF levels, with the bond lengths in angstroms, angles in degree.

Geometry	Method[a]	C6-N7	N7-N8	N8-C9	C6-N7-N8	N7-N8-C9	C6-N7-N8-C9
MECI1	SA2-CASSCF(10,8)	1.393	1.271	1.358	118.8	133.6	94.2
	SA2-CASSCF(12,10)	1.390	1.272	1.358	118.9	132.5	93.7
	SA3-CASSCF(10,8)	1.400	1.264	1.357	118.7	136.9	94.8
	SA3-CASSCF(12,10)	1.391	1.272	1.358	118.9	132.5	-92.9
MECI2	SA2-CASSCF(10,8)	1.395	1.270	1.358	118.7	133.8	-93.3
	SA2-CASSCF(12,10)	1.391	1.272	1.358	118.9	132.5	-92.9
	SA3-CASSCF(10,8)	1.400	1.264	1.357	118.7	136.8	-94.7
	SA3-CASSCF(12,10)	1.398	1.265	1.356	118.9	135.7	-93.2
MECI3	SA2-CASSCF(10,8)	1.357	1.263	1.399	138.8	116.4	94.3
	SA2-CASSCF(12,10)	1.356	1.261	1.403	139.5	116.4	94.5
	SA3-CASSCF(10,8)	1.359	1.255	1.402	142.9	116.6	95.2
	SA3-CASSCF(12,10)	1.359	1.254	1.405	143.6	116.5	95.4
MECI4	SA2-CASSCF(10,8)	1.357	1.262	1.389	139.1	116.9	-93.9
	SA2-CASSCF(12,10)	1.355	1.260	1.403	140.1	116.3	-94.5
	SA3-CASSCF(10,8)	1.357	1.255	1.402	143.5	116.6	-95.6
	SA3-CASSCF(12,10)	1.357	1.253	1.406	144.1	116.5	-95.7
MECI5	SA2-CASSCF(10,8)	1.276	1.204	1.355	160.3	146.7	-179.8
	SA2-CASSCF(12,10)	1.277	1.206	1.353	159.3	146.2	-179.4
	SA3-CASSCF(10,8)	1.285	1.208	1.352	157.4	144.3	179.7
	SA3-CASSCF(12,10)	1.286	1.210	1.350	156.5	144.1	179.9
MECI6	SA3-CASSCF(10,8)	1.296	1.357	1.379	111.4	109.2	-177.6
	SA3-CASSCF(12,10)	1.317	1.348	1.334	111.7	113.9	-179.9

[a] 6-31G* basis set;

Table 4S Relative and vertical energies (in eV) of S_0-min, S_1-min, S_2-min and six minimal energy conical intersections calculated at different CASSCF levels.

Geo.	Method	(S1-S0)VE[b]	E[c]	E[d]	(S2-S0)VE[e]	E[f]
S_0-min	SA2-CASSCF(6,5)[a]	3.74	3.74	0.0	----	----
	SA2-CASSCF(10,8)[b]	3.22	3.22	0.0	----	----
	SA2-CASSCF(12,10)[b]	3.18	3.18	0.0	----	----
	SA3-CASSCF(6,5)[a]	3.67	3.67	0.0	5.23	5.23
	SA3-CASSCF(10,8)[b]	3.30	3.30	0.0	5.64	5.64
	SA3-CASSCF(12,10)[b]	3.24	3.24	0.0	5.59	5.59
S_1-min	SA2-CASSCF(6,5)[a]	2.54	3.14	-0.59	----	----
	SA2-CASSCF(10,8)[b]	2.12	2.74	-0.48	----	----
	SA2-CASSCF(12,10)[b]	2.07	2.69	-0.49	----	----
	SA3-CASSCF(6,5)[a]	1.71	2.64	-1.03	3.20	4.12
	SA3-CASSCF(10,8)[b]	1.91	2.68	-0.62	4.59	5.35
	SA3-CASSCF(12,10)[b]	1.87	2.72	----	4.51	5.35
S2-min	SA3-CASSCF(6,5)[a]	3.09	3.96	0.29	3.53	4.41
	SA3-CASSCF(10,8)[b]	2.97	3.86	0.56	4.26	4.93
	SA3-CASSCF(12,10)[b]	1.87	2.72	----	4.51	5.35
MECI1	SA2-CASSCF(6,5)[a]	0.00	2.44	-1.29	----	----
	SA2-CASSCF(10,8)[b]	0.00	2.40	-0.82	----	----
	SA2-CASSCF(12,10)[b]	0.00	2.43	-0.26	----	----
	SA3-CASSCF(6,5)[a]	0.00	1.77	-1.9	1.55	3.32
	SA3-CASSCF(10,8)[b]	0.00	2.47	-0.83	1.46	3.93
	SA3-CASSCF(12,10)[b]	0.00	2.50	-0.22	1.47	3.97
MECI2	SA2-CASSCF(6,5)[a]	0.00	2.35	-0.33	----	----
	SA2-CASSCF(10,8)[b]	0.00	2.51	-0.21	----	----
	SA2-CASSCF(12,10)[b]	0.00	2.35	-0.83	----	----
	SA3-CASSCF(6,5)[a]	0.00	1.77	-1.9	1.55	3.32
	SA3-CASSCF(10,8)[b]	0.00	2.47	-0.83	1.46	3.93
	SA3-CASSCF(12,10)[b]	0.00	2.59	-0.66	1.48	3.98
MECI3	SA2-CASSCF(6,5)[a]	0.01	2.43	-1.31	----	----
	SA2-CASSCF(10,8)[b]	0.00	2.44	-0.78	----	----
	SA2-CASSCF(12,10)[b]	0.00	2.43	-0.26	----	----
	SA3-CASSCF(6,5)[a]	0.25	2.34	-1.33	1.56	3.65
	SA3-CASSCF(10,8)[b]	0.00	2.52	-0.78	1.53	4.05
	SA3-CASSCF(12,10)[b]	0.002	2.60	-0.12	1.50	4.09
MECI4	SA2-CASSCF(6,5)[a]	0.00	2.31	-1.43	----	----
	SA2-CASSCF(10,8)[b]	0.00	2.54	-0.68	----	----
	SA2-CASSCF(12,10)[b]	0.00	2.43	-0.26	----	----
	SA3-CASSCF(6,5)[a]	0.13	2.15	-1.52	1.40	3.42

	SA3-CASSCF(10,8)[b]	0.00	2.52	-0.78	1.57	4.08
	SA3-CASSCF(12,10)[b]	0.00	2.59	-0.13	1.53	4.12
MECI5	SA2-CASSCF(6,5)[a]	0.00	4.38	0.64	----	----
	SA2-CASSCF(10,8)[b]	0.00	3.68	0.46	----	----
	SA2-CASSCF(12,10)[b]	0.002	3.59	0.90	----	----
	SA3-CASSCF(6,5)[a]	0.12	3.84	0.18	1.36	5.08
	SA3-CASSCF(10,8)[b]	0.00	3.48	0.18	1.56	5.03
	SA3-CASSCF(12,10)[b]	0.0002	3.49	0.77	1.53	5.02
MECI6	SA3-CASSCF(6,5)[a]	3.27	4.54	0.87	3.27	4.54
	SA3-CASSCF(10,8)[b]	3.69	4.78	1.58	3.73	4.83
	SA3-CASSCF(12,10)[b]	4.00	4.72	2.00	4.00	4.72

[a] 6-31G* basis set; [b] vertical energies excited to S_1 state; [c] S_1 state energies relative to ground state energy of S_0-min;

[d] S_1 state energies relative to S_1 state energy of S_1-min geometry; [e]vertical energies excited to S_2state

[f] S_2 state energies relative to ground state energy of S_0-min;
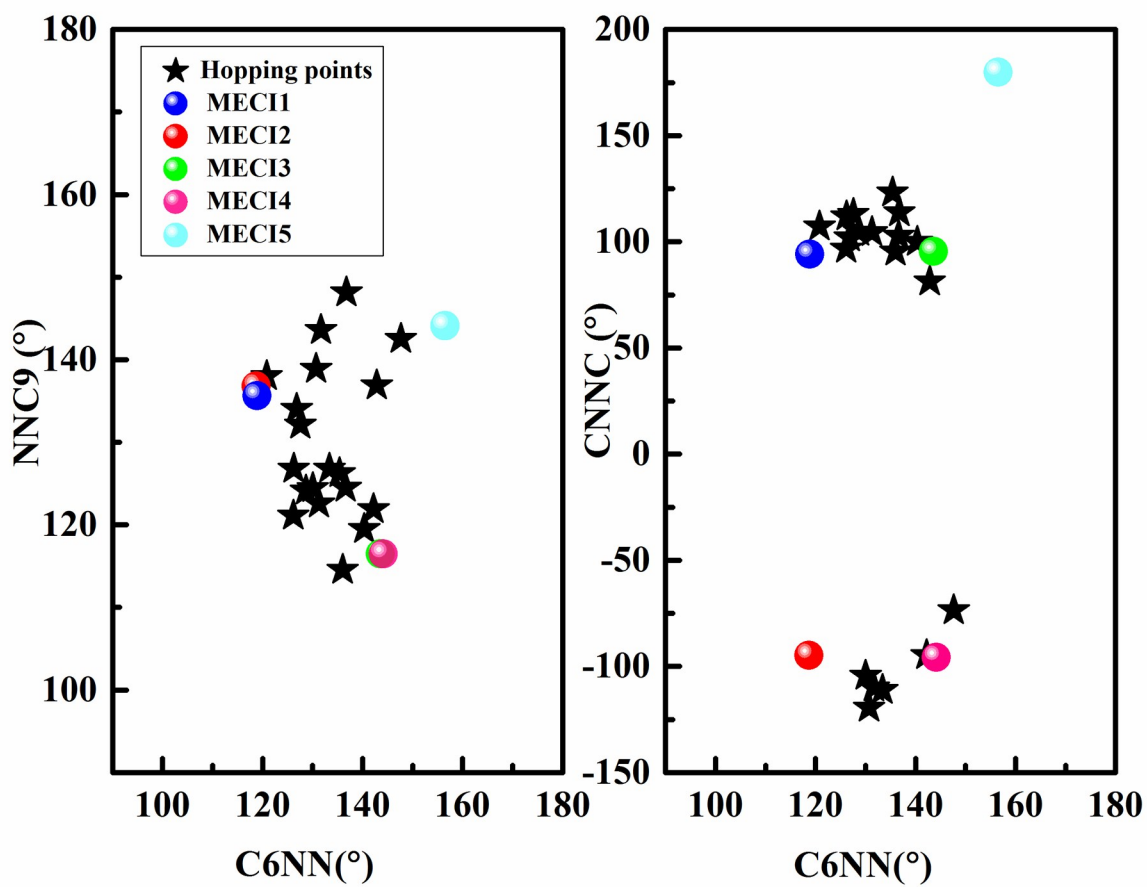
Figure 4S. Diagram (left) for bond angles NNC9 (ordinate) and C6NN (abscissa), and (right) for dihedral angle CNNC (ordinate) and bond angle C6NN (abscissa) at hopping points from the S_1 to S_0 state. The five MECIs were optimized at the SA3-CASSCF(12,10)/6-31G* level.
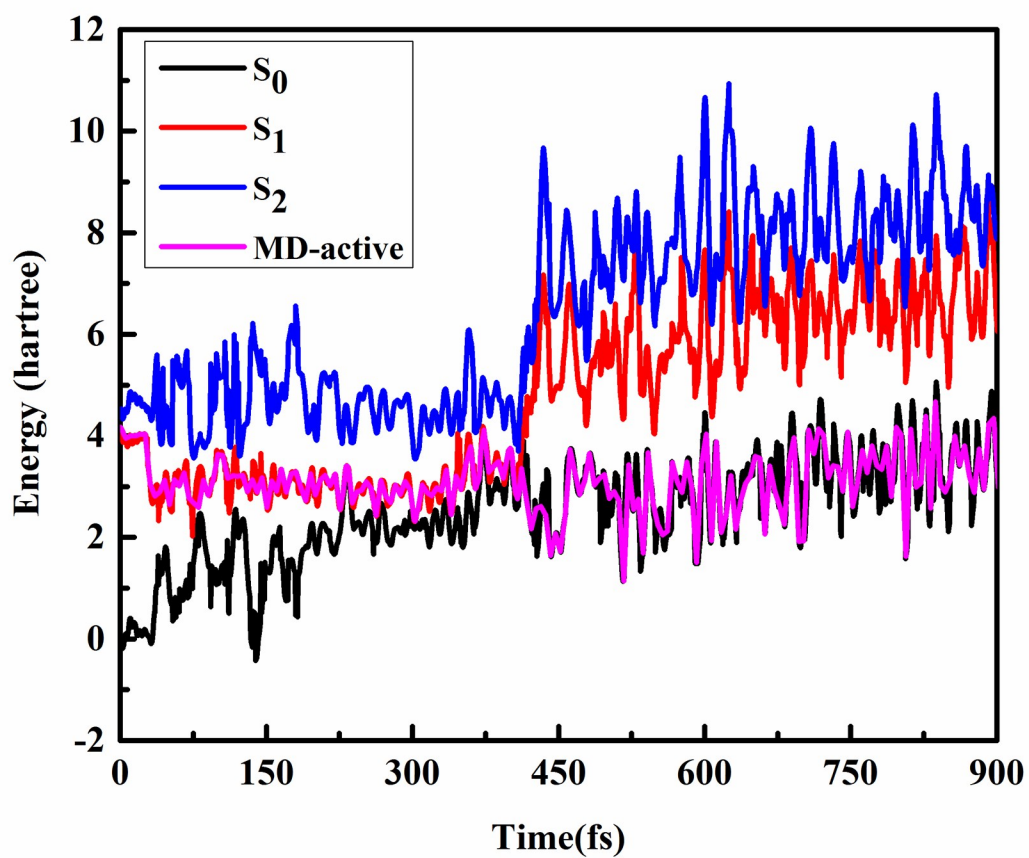
Figure 5S. Time-dependent potential energies of S_0, S_1 and S_2 states for a typical trajectory.
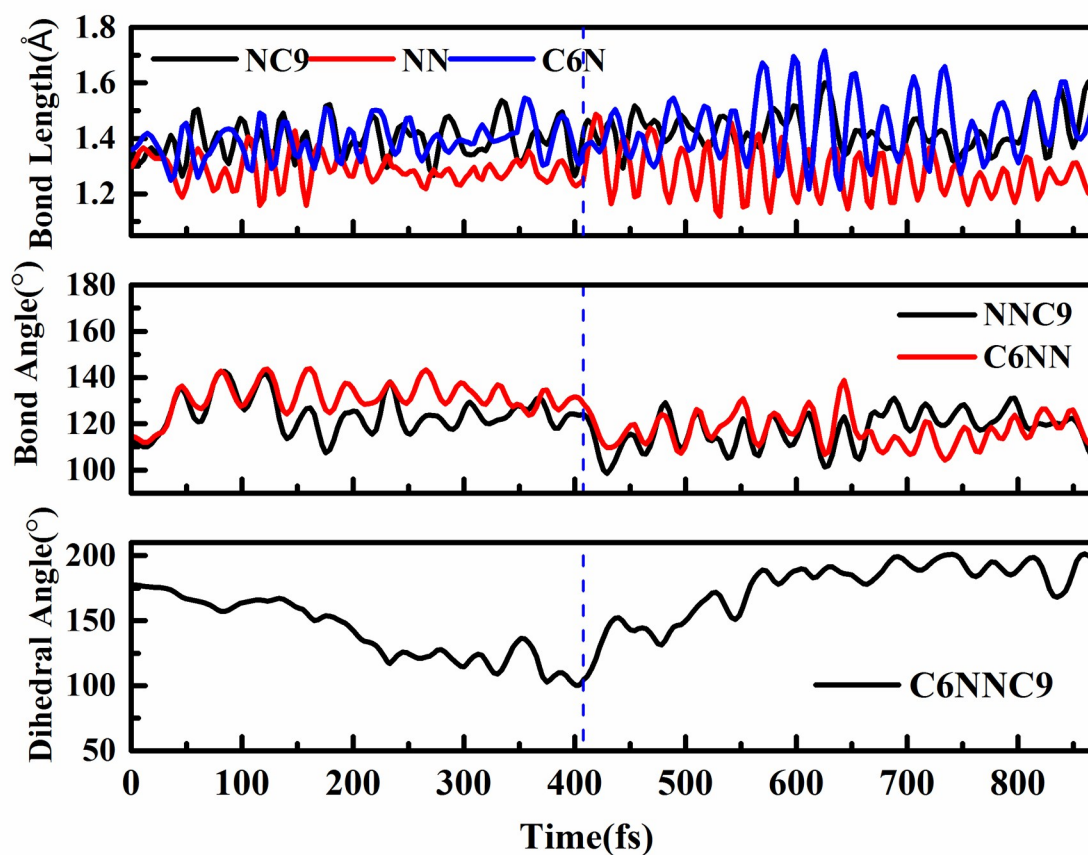
Figure 6S. Time-dependent parameter variables of a typical trajectory started from S_1 state performed with SA3-CASSCF(6,5)/6-31G level. top: the lengths of twist bonds NC9, NN and C6N; middle: time evolution of the two key bond angles NNC9 and C6NN; bottom: the dihedral angle C6NNC9 related with the twist motion around NN bond over the simulation time of 900 fs. The vertical dashed lines indicate the hopping time.

Table 5S. The ground state coordinates of S_1-min (left), MECI1(middle) and MECI5(right) used in LIIC in Z-matrices form at SA3-CASSCF(12,10)/6-31G* level.

C								C								C		

<table>
<tr><td colspan="7">Left</td><td colspan="7">Middle</td><td colspan="5">Right</td></tr>
<tr><td>C</td><td></td><td></td><td></td><td></td><td></td><td></td><td>C</td><td></td><td></td><td></td><td></td><td></td><td></td><td>C</td><td></td><td></td><td></td><td></td></tr>
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<tr><td>N</td><td>9</td><td>1.28615</td><td>8</td><td>126.7276</td><td>7</td><td>-0.0000</td><td>N</td><td>9</td><td>1.28906</td><td>8</td><td>125.8154</td><td>7</td><td>-12.9310</td><td>N</td><td>9</td><td>1.28703</td><td>8</td><td>125.4951 7 -0.0000</td></tr>
<tr><td>C</td><td>10</td><td>1.38071</td><td>9</td><td>104.4730</td><td>8</td><td>-180.0000</td><td>C</td><td>10</td><td>1.38364</td><td>9</td><td>104.3051</td><td>8</td><td>-180.0000</td><td>C</td><td>10</td><td>1.38724</td><td>9</td><td>103.8408 8 -180.0000</td></tr>
<tr><td>C</td><td>11</td><td>1.35688</td><td>10</td><td>110.5165</td><td>9</td><td>0.0000</td><td>C</td><td>11</td><td>1.35570</td><td>10</td><td>110.6805</td><td>9</td><td>0.0000</td><td>C</td><td>11</td><td>1.35344</td><td>10</td><td>110.9612 9 0.0000</td></tr>
<tr><td>H</td><td>1</td><td>1.07332</td><td>2</td><td>120.6459</td><td>6</td><td>-180.0000</td><td>H</td><td>1</td><td>1.07250</td><td>2</td><td>120.3251</td><td>6</td><td>-180.0000</td><td>H</td><td>1</td><td>1.07475</td><td>2</td><td>121.5366 6 -180.0000</td></tr>
<tr><td>H</td><td>2</td><td>1.07629</td><td>1</td><td>118.5221</td><td>3</td><td>180.0000</td><td>H</td><td>2</td><td>1.07553</td><td>1</td><td>119.1610</td><td>3</td><td>180.0000</td><td>H</td><td>2</td><td>1.07678</td><td>1</td><td>118.8399 3 -180.0000</td></tr>
<tr><td>H</td><td>4</td><td>1.07615</td><td>5</td><td>119.0472</td><td>3</td><td>-180.0000</td><td>H</td><td>4</td><td>1.07619</td><td>5</td><td>119.4329</td><td>3</td><td>-180.0000</td><td>H</td><td>4</td><td>1.07607</td><td>5</td><td>118.2237 3 -180.0000</td></tr>
<tr><td>H</td><td>5</td><td>1.07386</td><td>4</td><td>121.1098</td><td>6</td><td>180.0000</td><td>H</td><td>5</td><td>1.07407</td><td>4</td><td>121.1904</td><td>6</td><td>180.0000</td><td>H</td><td>5</td><td>1.07293</td><td>4</td><td>121.4473 6 -180.0000</td></tr>
<tr><td>H</td><td>11</td><td>1.06941</td><td>10</td><td>121.0578</td><td>12</td><td>-180.0000</td><td>H</td><td>11</td><td>1.06947</td><td>10</td><td>120.9611</td><td>12</td><td>-180.0000</td><td>H</td><td>11</td><td>1.06926</td><td>10</td><td>120.7327 12 -180.0000</td></tr>
<tr><td>H</td><td>12</td><td>1.06833</td><td>11</td><td>132.5757</td><td>17</td><td>-0.0000</td><td>H</td><td>12</td><td>1.06813</td><td>11</td><td>132.6729</td><td>17</td><td>0.0000</td><td>H</td><td>12</td><td>1.06773</td><td>11</td><td>132.9684 17 0.0000</td></tr>
<tr><td>N</td><td>9</td><td>1.35262</td><td>8</td><td>119.1039</td><td>7</td><td>180.0000</td><td>N</td><td>9</td><td>1.35257</td><td>8</td><td>119.9456</td><td>7</td><td>167.6279</td><td>N</td><td>9</td><td>1.35060</td><td>8</td><td>119.5559 7 180.0000</td></tr>
<tr><td>C</td><td>19</td><td>1.44399</td><td>9</td><td>128.4652</td><td>8</td><td>0.0000</td><td>C</td><td>19</td><td>1.44235</td><td>9</td><td>127.3064</td><td>8</td><td>1.4119</td><td>C</td><td>19</td><td>1.44175</td><td>9</td><td>126.9774 8 0.0000</td></tr>
<tr><td>H</td><td>20</td><td>1.08354</td><td>19</td><td>110.5166</td><td>12</td><td>-60.4980</td><td>H</td><td>20</td><td>1.08162</td><td>19</td><td>109.0987</td><td>12</td><td>31.3665</td><td>H</td><td>20</td><td>1.08439</td><td>19</td><td>111.1606 12 -118.1860</td></tr>
<tr><td>H</td><td>20</td><td>1.08353</td><td>21</td><td>109.0451</td><td>19</td><td>-121.6583</td><td>H</td><td>20</td><td>1.08093</td><td>21</td><td>108.5658</td><td>19</td><td>-119.3806</td><td>H</td><td>20</td><td>1.08017</td><td>21</td><td>108.5056 19 -119.3510</td></tr>
<tr><td>H</td><td>20</td><td>1.07887</td><td>22</td><td>108.7069</td><td>21</td><td>118.3697</td><td>H</td><td>20</td><td>1.08496</td><td>22</td><td>108.9054</td><td>21</td><td>118.3838</td><td>H</td><td>20</td><td>1.08429</td><td>22</td><td>108.4690 21 118.2371</td></tr>
<tr><td>C</td><td>3</td><td>1.50975</td><td>2</td><td>121.7472</td><td>4</td><td>-180.0000</td><td>C</td><td>3</td><td>1.50976</td><td>2</td><td>121.3130</td><td>4</td><td>-179.1102</td><td>C</td><td>3</td><td>1.50545</td><td>2</td><td>119.9736 4 180.0000</td></tr>
<tr><td>H</td><td>24</td><td>1.08639</td><td>3</td><td>111.2548</td><td>15</td><td>-59.9036</td><td>H</td><td>24</td><td>1.08663</td><td>3</td><td>110.9763</td><td>15</td><td>-72.4012</td><td>H</td><td>24</td><td>1.08773</td><td>3</td><td>111.5446 15 -120.1764</td></tr>
<tr><td>H</td><td>24</td><td>1.08638</td><td>25</td><td>107.3539</td><td>3</td><td>-121.9438</td><td>H</td><td>24</td><td>1.08518</td><td>25</td><td>107.4786</td><td>3</td><td>-121.7127</td><td>H</td><td>24</td><td>1.08426</td><td>25</td><td>107.6088 3 -122.2146</td></tr>
<tr><td>H</td><td>24</td><td>1.08397</td><td>25</td><td>107.7486</td><td>26</td><td>-115.8096</td><td>H</td><td>24</td><td>1.08371</td><td>25</td><td>107.7639</td><td>26</td><td>-116.1072</td><td>H</td><td>24</td><td>1.08773</td><td>25</td><td>107.1207 26 -115.4589</td></tr>
</table>

Table 6S. The ground state coordinates of S0-min (left), MECI1(middle)and MECI5(right) used in LIIC in Z-matrices form at SA2-CASSCF(12,10)/6-31G*level.

S0-min	MECI1	MECI5
C	C	C
C 1 1.38003	C 1 1.38607	C 1 1.33197
C 2 1.38841 1 122.1299	C 2 1.38286 1 122.1557	C 2 1.45424 1 122.7992
C 3 1.40624 2 117.8773 1 0.0000	C 3 1.40527 2 117.7472 1 -0.0000	C 3 1.40481 2 117.3463 1 -0.0000
C 4 1.38311 3 121.4977 2 -0.0000	C 4 1.38311 3 121.6175 2 -0.0000	C 4 1.38289 3 122.7384 2 -0.0000
C 1 1.40802 5 30.4707 2 -180.0000	C 1 1.40333 5 30.5555 2 -180.0000	C 1 1.46716 5 30.6326 2 -180.0000
N 6 1.35886 1 122.4666 5 -180.0000	N 6 1.35615 1 121.4923 5 180.0000	N 6 1.27682 1 120.4142 5 -180.0000
N 7 1.25712 6 130.5222 1 0.0000	N 7 1.26134 6 139.4715 1 -4.6951	N 7 1.20566 6 159.2844 1 -0.0000
C 8 1.37734 7 124.4559 6 180.0000	C 8 1.40253 7 116.3603 6 94.4852	C 8 1.35285 7 146.1875 6 -180.0000
N 9 1.28576 8 126.7519 7 -0.0000	N 9 1.28628 8 127.7831 7 -7.9955	N 9 1.28445 8 125.3120 7 -0.0000
C 10 1.38089 9 104.4787 8 -180.0000	C 10 1.37192 9 104.8450 8 -178.2781	C 10 1.38912 9 103.7913 8 -180.0000
C 11 1.35676 10 110.5062 9 -0.0000	C 11 1.36241 10 110.1848 9 -0.0000	C 11 1.35243 10 110.9329 9 0.0000
H 1 1.07328 2 120.6573 6 -180.0000	H 1 1.07370 2 120.5210 6 -180.0000	H 1 1.07471 2 121.6892 6 180.0000
H 2 1.07628 1 118.5295 3 180.0000	H 2 1.07632 1 118.3585 3 180.0000	H 2 1.07671 1 118.8986 3 -180.0000
H 4 1.07614 5 119.0473 3 -180.0000	H 4 1.07636 5 118.9241 3 180.0000	H 4 1.07610 5 118.2025 3 -180.0000
H 5 1.07382 4 121.1090 6 180.0000	H 5 1.07392 4 120.9678 6 180.0000	H 5 1.07261 4 121.6645 6 180.0000
H 11 1.06941 10 121.0562 12 -180.0000	H 11 1.06939 10 121.4084 12 -180.0000	H 11 1.06922 10 120.6979 12 180.0000
H 12 1.06833 11 132.5828 17 -0.0000	H 12 1.06861 11 132.2059 17 0.0000	H 12 1.06770 11 133.0329 17 -0.0000
N 9 1.35236 8 119.0717 7 180.0000	N 9 1.35259 8 118.4096 7 173.5326	N 9 1.34896 8 119.5733 7 180.0000
C 19 1.44403 9 128.4823 8 0.0000	C 19 1.44782 9 128.3178 8 -0.0000	C 19 1.44196 9 127.0702 8 0.0000
H 20 1.08354 19 110.5111 12 -60.4932	H 20 1.07753 19 109.0782 12 173.6129	H 20 1.08436 19 111.1839 12 -117.7295
H 20 1.08353 21 109.0431 19 -121.6465	H 20 1.08353 21 109.0930 19 -120.8664	H 20 1.08011 21 108.4978 19 -119.3395
H 20 1.07882 22 108.7104 21 118.3746	H 20 1.08274 22 109.0792 21 119.1061	H 20 1.08423 22 108.4494 21 118.2487
C 3 1.50971 2 121.7380 4 -180.0000	C 3 1.51016 2 121.8508 4 180.0000	C 3 1.50438 2 119.8583 4 -180.0000
H 24 1.08638 3 111.2530 15 -59.9130	H 24 1.08646 3 111.3004 15 60.1149	H 24 1.08796 3 111.5630 15 -120.1029
H 24 1.08637 25 107.3543 3 -121.9410	H 24 1.08410 25 107.7100 3 -122.1816	H 24 1.08430 25 107.6027 3 -122.2465
H 24 1.08397 25 107.7493 26 -115.8111	H 24 1.08652 25 107.3520 26 -115.7540	H 24 1.08796 25 107.0714 26 -115.4256

Table 7S. Cartesian coordinates of S_0-min (left) and S_1-min (right) optimized at SA3-CASSCF(12,10)/6-31G* level

	SA3-CASSCF(12,10)/6-31G*				SA3-CASSCF(12,10)/6-31G*		
	X	Y	Z		X	Y	Z
C	0.0544038497	0.0554497516	0.0000253141	C	-0.0325077552	-0.0063230476	0.0001931290
C	-0.6970951794	-1.1152518390	0.0000258311	C	-0.7402011976	-1.1914047195	0.0002805914
C	-0.1009631911	-2.3624324416	0.0000540782	C	-0.1095043478	-2.4277969151	0.0000978391
C	1.2986041821	-2.4319708770	0.0001158851	C	1.2966973219	-2.4485659323	-0.0001708369
C	2.0663516046	-1.2751324583	0.0001219536	C	2.0365874009	-1.2800238291	-0.0002678989
C	1.4459368503	-0.0210708290	0.0000669821	C	1.3747852599	-0.0344259199	-0.0000838673
N	2.3276967284	1.0903156887	0.0000966714	N	2.1274296581	1.0972771474	-0.0001937529
N	1.7750380562	2.2048988004	-0.0001129565	N	1.7835747051	2.3058700444	-0.0000576337
C	2.6635528758	3.2928410304	-0.0001040718	C	2.6602593638	3.3671135444	0.0000329293
N	3.9598145897	3.2909584820	-0.0001519621	N	3.9448410598	3.3035635104	0.0002719183
C	4.3154147433	4.6212781944	-0.0001301275	C	4.3555498477	4.6217785504	0.0002658165
C	3.2122670272	5.3955390137	-0.0000731519	C	3.2837215769	5.4538227350	0.0000599072
H	-0.4318423961	1.0108495504	0.0000175510	H	-0.5448110609	0.9368388695	0.0003528880
H	-1.7707108848	-1.0424775289	0.0000094079	H	-1.8156034237	-1.1477951228	0.0005033688
H	1.7845591658	-3.3919051222	0.0001702852	H	1.8120386586	-3.3933010072	-0.0002953328
H	3.1394128156	-1.3199957577	0.0001860091	H	3.1102041735	-1.3030958715	-0.0004601902
H	5.3413447744	4.9224846331	-0.0001782682	H	5.3943031095	4.8760109178	0.0003823912
H	3.0933915598	6.4585658110	-0.0000498007	H	3.1951795854	6.5184794566	0.0000036324
N	2.1371359687	4.5517618830	-0.0000724629	N	2.1681220927	4.6270244779	-0.0001468392
C	0.7455785500	4.9484324447	0.0001420412	C	0.7881845535	5.0523127453	-0.0001750003
H	0.5205715046	5.5343399016	0.8832933258	H	0.5723975477	5.6416053456	0.8831361352
H	0.5213516055	5.5373898745	-0.8811631644	H	0.5736527342	5.6448461058	-0.8816056162
H	0.1284203329	4.0657534062	-0.0016574596	H	0.1472949635	4.1844293739	-0.0022516600
C	-0.9231188848	-3.6297791541	-0.0001086980	C	-0.8921858176	-3.7188240235	0.0000504297
H	-0.7085407960	-4.2342927627	-0.8763709892	H	-0.6623169305	-4.3187027658	-0.8760424074
H	-0.7061830194	-4.2360854167	0.8743192315	H	-0.6600281823	-4.3201599752	0.8745283302
H	-1.9846275329	-3.4116969783	0.0015290452	H	-1.9598999966	-3.5317863946	0.0015922294

Table 8S. Cartesian coordinates of S$_2$-min (left) and MECI1 (right) optimized at SA3-CASSCF(12,10)/6-31G* level

	SA3-CASSCF(12,10)/6-31G*			SA3-CASSCF(12,10)/6-31G*	
X	Y	Z	X	Y	Z
C	0.0884015398	0.0791032768	0.0001620763	C	-0.6716001318	4.0752321408	-1.0626866360
C	-0.6920454230	-1.1184695370	0.0004391088	C	-1.8976769446	3.3958872309	-1.0786906277
C	-0.1461954585	-2.3495263645	0.0001862871	C	-1.9513765179	2.0273090578	-1.1112270702
C	1.3044435981	-2.4539772278	-0.0003840699	C	-0.7686268119	1.2721176990	-1.1211264979
C	2.1413159542	-1.2974780978	-0.0006922771	C	0.4671174389	1.9280819382	-1.1096249797
C	1.5837439231	0.0167615868	-0.0004340880	C	0.5034963897	3.3189859669	-1.0791711667
N	2.4135215122	1.0274895955	-0.0007367206	H	-2.8135167575	3.9608907737	-1.0647316140
N	1.7792070769	2.2319274695	-0.0006748159	H	-2.8912876688	1.5076145346	-1.1220002458
C	2.6195633015	3.2763859781	-0.0001674408	H	1.3783984248	1.3626616856	-1.1205836945
N	3.9464259516	3.2910354381	0.0003081910	H	1.4560785772	3.8181255426	-1.0646348402
C	4.2951972689	4.6146636539	0.0006489636	C	0.9169934847	-1.4820968857	-0.3424437521
C	3.1883421129	5.3888356773	0.0003939719	C	1.9575507845	-2.1346783020	1.3748038425
H	-0.3882349170	1.0349323031	0.0003548343	C	2.4903429300	-2.8296624043	0.3398938064
H	-1.7626865759	-1.0096419673	0.0008672160	H	2.2136287774	-2.1879158861	2.4117955870
H	1.7624068642	-3.4254841768	-0.0005583268	H	3.2580835206	-3.5701760054	0.2840208375
H	3.2090340121	-1.3961766154	-0.0011089624	N	-0.9331069267	-0.1162133929	-1.1224203133
H	5.3194457703	4.9217744507	0.0010301029	N	0.0918910457	-0.8525617356	-1.2158602052
H	3.0791801657	6.4535470442	0.0005323412	N	0.9662067639	-1.2783056230	0.9294564342
N	2.1099103163	4.5605561284	-0.0001495505	N	1.7948305698	-2.4083085207	-0.7907407577
C	0.7219657796	4.9594205038	-0.0003266660	C	2.0052800921	-2.8248717440	-2.1555011124
H	0.4916401550	5.5440731561	0.8831046477	H	2.3544049303	-3.8485658228	-2.1632278875
H	0.4931284253	5.5477712809	-0.8816708983	H	1.0713975793	-2.7756410329	-2.6975760397
H	0.1081932305	4.0739970747	-0.0026966614	H	2.7368938872	-2.2011030202	-2.6582901711
C	-0.9588976602	-3.6162426928	0.0003652152	C	-0.6332886327	5.5844424372	-1.0485789062
H	-0.7400864181	-4.2226363640	-0.8750801413	H	-0.9296459062	5.9901072041	-2.0120955145
H	-0.7385797444	-4.2233708743	0.8749181324	H	-1.3118899618	5.9862052979	-0.3031263012
H	-2.0205758611	-3.4005034002	0.0013700302	H	0.3617665685	5.9521166605	-0.8269552039

Table 9S. Cartesian coordinates of MECI2 (left) and MECI3 (right) optimized at SA3-CASSCF(12,10)/6-31G* level.

	SA3-CASSCF(12,10)/6-31G*-				SA3-CASSCF(12,10)/6-31G*-		
	X	Y	Z		X	Y	Z
C	-2.4194027783	1.1611388458	2.7893942975	C	0.3262075256	2.4792566142	0.6131421758
C	-3.0774176232	1.4969379789	1.6000608416	C	-0.9181577240	2.8180766500	1.1280940501
C	-2.6351531361	1.0340168350	0.3873238598	C	-2.0958619976	2.3934713543	0.5451870990
C	-1.5002397762	0.2135824699	0.3140277785	C	-2.0035862704	1.5967719147	-0.6076275025
C	-0.8299022707	-0.1413349494	1.4905906615	C	-0.7809268141	1.2470418566	-1.1530680462
C	-1.2938410565	0.3346238176	2.7122583346	C	0.4063605817	1.6881613904	-0.5400534779
H	-3.9481930591	2.1279414264	1.6389965826	N	1.6075882752	1.3494547770	-1.0773442861
H	-3.1420997323	1.2905490017	-0.5241396206	N	2.8423158805	1.5498018481	-0.9941563422
H	0.0330987360	-0.7769170281	1.4495809619	C	3.5763246339	0.6292118700	-0.2269245220
H	-0.7744607728	0.0603420171	3.6133495765	N	3.1217633584	-0.3192958314	0.5116421176
C	1.1898316840	-0.8683326976	-1.2960403566	C	4.2359638187	-0.8953416545	1.0687965479
C	3.1668509840	-0.1645254341	-1.5253445500	C	5.3599320890	-0.2594081965	0.6356065116
C	3.2297172103	-1.5019024137	-1.7359749034	H	1.2254852440	2.8156695724	1.0935208479
H	3.9632985635	0.5489122799	-1.5455381188	H	-0.9543323379	3.4290029996	2.0134779578
H	4.0399748916	-2.1627623626	-1.9543318305	H	-2.9036266399	1.2492023323	-1.0848085261
N	-1.1163404739	-0.1813859949	-0.9711799711	H	-0.7248609726	0.6390903394	-2.0365327115
N	-0.1470464253	-0.9843468969	-1.0992706418	H	4.1583028687	-1.7257854227	1.7380156115
N	1.8691082200	0.2252743817	-1.2415785201	H	6.3972756168	-0.4165445592	0.8383854027
N	1.9278755485	-1.9694993190	-1.5674801876	N	4.9241647613	0.7338480995	-0.2145470835
C	1.4353311057	-3.2990322752	-1.8359039655	C	5.7581372602	1.6883546732	-0.9144772486
H	2.2415124839	-4.0053245363	-1.6931616484	H	5.1453097225	2.2658908725	-1.5866901537
H	0.6389720355	-3.5453245093	-1.1473905247	H	6.2418473100	2.3573009008	-0.2127329329
H	1.0621086024	-3.3904614300	-2.8500301791	H	6.5156106979	1.1662554305	-1.4853702854
C	-2.9016139337	1.7003977718	4.1145691440	C	-3.4456665347	2.7614159024	1.1144286785
H	-2.5461524320	2.7153076888	4.2714167969	H	-4.0106440854	1.8767924216	1.3947683834
H	-3.9851835147	1.7231654259	4.1592031359	H	-3.3431447041	3.3806974765	1.9983110587
H	-2.5448749809	1.0957146069	4.9404232468	H	-4.0426668089	3.3120107745	0.3926726849

Table 10S. Cartesian coordinates of MECI4 (left) and MECI5 (right) optimized at SA3-CASSCF(12,10)/6-31G* level.

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	SA3-CASSCF(12,10)/6-31G*-				SA3-CASSCF(12,10)/6-31G*-		
	X	Y	Z		X	Y	Z
C	-2.4818476687	1.9414360905	2.4322699877	C	-0.4123961345	0.1522073975	-0.0388874000
C	-2.9458291100	2.2067523482	1.1335007756	C	-1.1072892764	-0.9889735067	-0.0347416839
C	-2.4456618398	1.5594059422	0.0378729214	C	-0.4760132562	-2.2883432473	0.0330486819
C	-1.4267250645	0.5989775613	0.1912120341	C	0.9234502143	-2.3215679591	0.0961864426
C	-0.9397107104	0.3175054670	1.4745520132	C	1.6987402477	-1.1723322052	0.0953977449
C	-1.4764860518	0.9878159080	2.5736200909	C	1.0455831216	0.1126441973	0.0269876819
H	-3.7217333978	2.9398844787	0.9923973879	N	1.7249475325	1.2045724134	0.0236226269
H	-2.8169580379	1.7756023087	-0.9465933609	N	1.9011033637	2.4014672761	-0.0050304155
H	-0.1569031766	-0.4059246741	1.6031510359	C	2.8434428461	3.3681420203	0.0072212916
H	-1.0940596083	0.7581496614	3.5528443655	N	4.1138894243	3.1725172036	0.0715412251
C	1.1242928776	-0.6270885745	-1.6205616847	C	4.6480079405	4.4527184414	0.0558089408
C	2.9902926907	0.3105251059	-1.8984952725	C	3.6694149437	5.3847485645	-0.0181343129
C	3.1409915446	-0.9653482032	-2.3508537594	H	-0.9013660195	1.1079314541	-0.0898050485
H	3.7147662063	1.0966646278	-1.8729723901	H	-2.1819656906	-0.9428760662	-0.0838073625
H	3.9737435103	-1.4830868312	-2.7755801785	H	1.4237291179	-3.2728924089	0.1475579929
N	-0.9387265207	-0.0406964803	-0.9020999062	H	2.7695216386	-1.2194309413	0.1443474696
N	-0.1959576285	-0.9743278893	-1.2847291485	H	5.7056018927	4.6041265030	0.0992874431
N	1.7100222853	0.5027762462	-1.4423145201	H	3.6817640362	6.4518934257	-0.0512751530
N	1.9182791891	-1.5744529729	-2.1680362715	N	2.4688703266	4.6644483319	-0.0511211934
C	1.5831082289	-2.9404087641	-2.5122067480	C	1.1228878404	5.1756862063	-0.1259447831
H	2.2035006482	-3.6312693885	-1.9543015417	H	0.5478137046	4.8936202152	0.7490577394
H	0.5488206154	-3.1209640062	-2.2701633741	H	1.1661605557	6.2538812736	-0.1748228459
H	1.7334073142	-3.1059648431	-3.5720038544	H	0.6164027822	4.8116832304	-1.0128811832
C	-3.0586902141	2.6740336690	3.6202873545	C	-1.3195877279	-3.5352384294	0.0339783060
H	-2.8949540722	3.7452755207	3.5421025146	H	-1.9253029773	-3.6083866351	-0.8665254221
H	-4.1303389474	2.5147835863	3.7017865961	H	-0.7030869943	-4.4255482428	0.0878171568
H	-2.6048377481	2.3388105277	4.5460797212	H	-2.0015567140	-3.5555101496	0.8811315162

Table 11S. Cartesian coordinates of MECI6 optimized at SA3-CASSCF(12,10)/6-31G* level.

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SA3-CASSCF(12,10)/6-31G* -		
X	Y	Z
C	0.4572080171	2.8177051227	0.1425276934
C	-0.7373484269	3.5857103704	0.2428595028
C	-2.0097299704	2.9913184832	0.2540581368
C	-2.0911814859	1.6120165057	0.1638416321
C	-0.9508114395	0.8124776687	0.0635502383
C	0.3751003608	1.3858669404	0.0488273857
N	1.3874814448	0.5491168419	-0.0488193586
N	2.5934767315	1.1507094248	-0.0567923891
C	3.5856404462	0.2637843751	-0.1570812272
N	3.5588961277	-1.0931538494	-0.2483057722
C	4.8126832510	-1.4700646798	-0.3248832131
C	5.6856909017	-0.3868206308	-0.2866418825
H	1.4136671381	3.2947651519	0.1361167108
H	-0.6561144376	4.6559332948	0.3120377989
H	-3.0555282555	1.1360834432	0.1705311807
H	-1.0291269521	-0.2553134347	-0.0056989822
H	5.0882492130	-2.5028333100	-0.4063219261
H	6.7508068844	-0.3234007594	-0.3254545967
N	4.8784636940	0.7124111492	-0.1787959033
C	5.2826859846	2.0977134824	-0.1020738598
H	4.9370841378	2.5405367395	0.8220749149
H	6.3619743409	2.1464475863	-0.1396769969
H	4.8707306766	2.6572640224	-0.9308538834
C	-3.2439708861	3.8523131864	0.3630246491
H	-3.3037540179	4.5569819962	-0.4614933583
H	-4.1450631487	3.2508594799	0.3526382604
H	-3.2387059498	4.4292257186	1.2834588548

Table 12S. Cartesian coordinates of S_0-min (left), S_1-min (right) optimized at SA3-CASSCF(12,10)/6-311G** level.

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	SA3-CASSCF(12,10)/6-311G**			SA3-CASSCF(12,10)/6-311G**	
X	Y	Z	X	Y	Z
C	0.0479931882	0.0513914898	-0.0000376269	C	-0.0323900065	-0.0062543593	0.0001908243
C	-0.7024611552	-1.1179668403	-0.0000297206	C	-0.7401405913	-1.1912706983	0.0002793529
C	-0.1029257817	-2.3650960030	0.0000525245	C	-0.1095273575	-2.4277111078	0.0000982619
C	1.2937688248	-2.4340406612	0.0001590409	C	1.2966808634	-2.4485726402	-0.0001723451
C	2.0617649654	-1.2787707287	0.0001582817	C	2.0366170357	-1.2801041548	-0.0002711208
C	1.4398181330	-0.0275027233	0.0000502103	C	1.3748764804	-0.0344422029	-0.0000890647
N	2.3420360300	1.1042630806	0.0000764292	N	2.1275955569	1.0971991203	-0.0002026672
N	1.7858817392	2.2110922511	-0.0001383414	N	1.7837731673	2.3057861256	-0.0000568184
C	2.6720187211	3.3066961456	-0.0001336888	C	2.6603382554	3.3670794248	0.0000153369
N	3.9600704035	3.3079152991	-0.0002157858	N	3.9449337057	3.3036439560	0.0002272331
C	4.3145753544	4.6225131774	-0.0001799550	C	4.3555153478	4.6218905297	0.0002764217
C	3.2108820502	5.4061269868	-0.0000823007	C	3.2836247785	5.4538295033	0.0000507722
H	-0.4369318812	1.0075973981	-0.0000857728	H	-0.5446431255	0.9369324495	0.0003525327
H	-1.7764287693	-1.0481777271	-0.0000813270	H	-1.8155385284	-1.1476257611	0.0005018913
H	1.7785919525	-3.3948234619	0.0002548177	H	1.8119375959	-3.3933472080	-0.0002971301
H	3.1349417906	-1.3229209653	0.0002550224	H	3.1102337934	-1.3031407275	-0.0004636879
H	5.3409566734	4.9246928380	-0.0002495767	H	5.3942482145	4.8761927040	0.0004422275
H	3.0868938719	6.4680353834	-0.0000377603	H	3.1949671835	6.5184723655	-0.0000208276
N	2.1445061442	4.5506432586	-0.0000740612	N	2.1681089064	4.6269489431	-0.0001541150
C	0.7480142000	4.9411484400	0.0002069810	C	0.7881410544	5.0520859827	-0.0001672977
H	0.5257992182	5.5263732450	0.8846695062	H	0.5722764954	5.6413359535	0.8831470524
H	0.5264770615	5.5294688679	-0.8823564336	H	0.5735293804	5.6445995292	-0.8815855584
H	0.1344794492	4.0557806515	-0.0015779817	H	0.1473557095	4.1841384053	-0.0022550234
C	-0.9247712759	-3.6320871288	-0.0001013247	C	-0.8922507781	-3.7186855722	0.0000561003
H	-0.7071207107	-4.2341801668	-0.8773675175	H	-0.6624142516	-4.3185928447	-0.8760232530
H	-0.7049064203	-4.2358763904	0.8754312057	H	-0.6601400332	-4.3200367601	0.8745335251
H	-1.9861588769	-3.4135284158	0.0014356548	H	-1.9599439517	-3.5315836550	0.0015878770

Table 13S. Cartesian coordinates of S$_2$-min (left) and MECI1(right) optimized at SA3-CASSCF(12,10)/6-311G** level.

SA3-CASSCF(12,10)/6-31G**			SA3-CASSCF(12,10)/6-31G**		
X	Y	Z	X	Y	Z
C	0.0943025738	0.0675530102	0.0005215500	C	-0.6716001318	4.0752321408	-1.0626866360
C	-0.6840355895	-1.1340128463	0.0011869340	C	-1.8976769446	3.3958872309	-1.0786906277
C	-0.1396570555	-2.3696853213	0.0003855624	C	-1.9513765179	2.0273090578	-1.1112270702
C	1.2935754070	-2.4755384474	-0.0012156351	C	-0.7686268119	1.2721176990	-1.1211264979
C	2.1428526271	-1.2982533707	-0.0019683854	C	0.4671174389	1.9280819382	-1.1096249797
C	1.5707041075	0.0243851790	-0.0010301627	C	0.5034963897	3.3189859669	-1.0791711667
N	2.3931394271	1.0401526130	-0.0016187754	H	-2.8135167575	3.9608907737	-1.0647316140
N	1.7486585296	2.2417134848	-0.0014014158	H	-2.8912876688	1.5076145346	-1.1220002458
C	2.6364538080	3.3104185003	-0.0001208762	H	1.3783984248	1.3626616856	-1.1205836945
N	3.9295792903	3.3073444591	0.0012713309	H	1.4560785772	3.8181255426	-1.0646348402
C	4.2925850260	4.6200400297	0.0020734491	C	0.9169934847	-1.4820968857	-0.3424437521
C	3.1972214018	5.4132992985	0.0011471455	C	1.9575507845	-2.1346783020	1.3748038425
H	-0.3924290939	1.0186207044	0.0010674120	C	2.4903429300	-2.8296624043	0.3398938064
H	-1.7545681912	-1.0249864958	0.0024000876	H	2.2136287774	-2.1879158861	2.4117955870
H	1.7590170261	-3.4434497659	-0.0018476405	H	3.2580835206	-3.5701760054	0.2840208375
H	3.2102654821	-1.3952476687	-0.0031940374	N	-0.9331069267	-0.1162133929	-1.1224203133
H	5.3215417286	4.9145886177	0.0032410241	N	0.0918910457	-0.8525617356	-1.2158602052
H	3.0825453078	6.4764014826	0.0013558375	N	0.9662067639	-1.2783056230	0.9294564342
N	2.1229315549	4.5658846466	-0.0003085647	N	1.7948305698	-2.4083085207	-0.7907407577
C	0.7318127136	4.9652775891	-0.0014094567	C	2.0052800921	-2.8248717440	-2.1555011124
H	0.5087565553	5.5515979202	0.8829064805	H	2.3544049303	-3.8485658228	-2.1632278875
H	0.5115411716	5.5557340492	-0.8836512900	H	1.0713975793	-2.7756410329	-2.6975760397
H	0.1131679055	4.0831693624	-0.0044541529	H	2.7368938872	-2.2011030202	-2.6582901711
C	-0.9635374485	-3.6303418333	0.0010449359	C	-0.6332886327	5.5844424372	-1.0485789062
H	-0.7491444183	-4.2358623980	-0.8758432219	H	-0.9296459062	5.9901072041	-2.0120955145
H	-0.7467458676	-4.2365251241	0.8768819875	H	-1.3118899618	5.9862052979	-0.3031263012
H	-2.0227690791	-3.4035103753	0.0025803774	H	0.3617665685	5.9521166605	-0.8269552039

Table 14S. Cartesian coordinates of MECI2 (left) and MECI3 (right) optimized at SA3-CASSCF(12,10)/6-311G** level.

	SA3-CASSCF(12,10)/6-31G**				SA3-CASSCF(12,10)/6-31G*-*		
	X	Y	Z		X	Y	Z
C	-2.4545528076	1.1760303216	2.8018439738	C	0.3267652454	2.4742520060	0.6144826033
C	-3.1396343272	1.4311154632	1.6145876560	C	-0.9169967363	2.8142586707	1.1292154890
C	-2.6754838356	0.9610431603	0.4088697365	C	-2.0938784161	2.3934396556	0.5452751810
C	-1.4955203482	0.2148215800	0.3510862111	C	-2.0019346099	1.5996700476	-0.6089006735
C	-0.7930005768	-0.0572117991	1.5291213141	C	-0.7811413663	1.2498677156	-1.1541756031
C	-1.2761262785	0.4241835251	2.7378490955	C	0.4061019779	1.6871946134	-0.5399276585
H	-4.0499096763	2.0047698650	1.6414337111	N	1.6065471656	1.3463340695	-1.0786993931
H	-3.2050483439	1.1565766303	-0.5053358763	N	2.8390899149	1.5459104501	-0.9975147703
H	0.1127438583	-0.6313467509	1.4971871528	C	3.5756281437	0.6280737042	-0.2271886768
H	-0.7315330517	0.2146682553	3.6419923001	N	3.1211059690	-0.3168178955	0.5117738822
C	1.2474896254	-0.8654255684	-1.2589260526	C	4.2354062575	-0.8919834992	1.0723957652
C	3.2537012073	-0.2325521674	-1.5160397403	C	5.3580487826	-0.2568082985	0.6386018663
C	3.2503186657	-1.5485586502	-1.7658207300	H	1.2260438668	2.8069923701	1.0976293829
H	4.0789059418	0.4472227898	-1.5357491788	H	-0.9525244992	3.4230242710	2.0164358322
H	4.0354711410	-2.2221825813	-2.0358117612	H	-2.9025107752	1.2543896780	-1.0873373121
N	-1.0906618797	-0.1928748183	-0.9321646564	H	-0.7252250447	0.6438835140	-2.0392052729
N	-0.0848360408	-0.9382454840	-1.0342343883	H	4.1575499459	-1.7209413954	1.7436277084
N	1.9763363732	0.2037058733	-1.1812011511	H	6.3951707374	-0.4141834917	0.8432419111
N	1.9497722768	-1.9836958347	-1.5908803717	N	4.9220467106	0.7343110900	-0.2147566052
C	1.4046159387	-3.2817879696	-1.9084773262	C	5.7562649916	1.6888481346	-0.9168671010
H	2.2114375173	-4.0024993422	-1.9275806295	H	5.1419625083	2.2646501505	-1.5901394896
H	0.6931296355	-3.5858959915	-1.1508287446	H	6.2388636667	2.3604769535	-0.2156755844
H	0.9092080185	-3.2814493546	-2.8745676399	H	6.5140200149	1.1657795509	-1.4878898310
C	-2.9530004352	1.7224358861	4.1175455058	C	-3.4433348397	2.7615075172	1.1143368913
H	-2.5565633341	2.7190549730	4.2946572297	H	-4.0076576174	1.8751161016	1.3913474790
H	-4.0352183296	1.7911768736	4.1293003721	H	-3.3391057161	3.3782402445	1.9998414277
H	-2.6462828345	1.0936758164	4.9459741881	H	-4.0371915230	3.3149184779	0.3917885606

Table 15S. Cartesian coordinates of MECI4 (left) and MECI5 (right) optimized at SA3-CASSCF(12,10)/6-311G** level.

	SA3-CASSCF(12,10)/6-311G**				SA3-CASSCF(12,10)/6-311G**		
	X	Y	Z		X	Y	Z
C	-2.4761176821	1.9340920052	2.4309977368	C	-0.4123961345	0.1522073975	-0.0388874000
C	-2.9474869720	2.2227240390	1.1405581712	C	-1.1072892764	-0.9889735067	-0.0347416839
C	-2.4513358437	1.5763026095	0.0244948665	C	-0.4760132562	-2.2883432473	0.0330486819
C	-1.4410843013	0.6083955048	0.1720820084	C	0.9234502143	-2.3215679591	0.0961864426
C	-0.9595266053	0.3166758104	1.4534304785	C	1.6987402477	-1.1723322052	0.0953977449
C	-1.4880437248	0.9792056842	2.5530874943	C	1.0455831216	0.1126441973	0.0269876819
H	-3.7179462926	2.9637122773	1.0117115976	N	1.7249475325	1.2045724134	0.0236226269
H	-2.8234985373	1.8051869471	-0.9567418781	N	1.9011033637	2.4014672761	-0.0050304155
H	-0.1825851618	-0.4137283317	1.5794354901	C	2.8434428461	3.3681420203	0.0072212916
H	-1.1032169787	0.7352088306	3.5285087651	N	4.1138894243	3.1725172036	0.0715412251
C	1.1080574619	-0.6199041178	-1.6252721498	C	4.6480079405	4.4527184414	0.0558089408
C	2.9879591833	0.3141183898	-1.9166146105	C	3.6694149437	5.3847485645	-0.0181343129
C	3.1273501293	-0.9580770822	-2.3404083953	H	-0.9013660195	1.1079314541	-0.0898050485
H	3.7164760265	1.0964963924	-1.9047017367	H	-2.1819656906	-0.9428760662	-0.0838073625
H	3.9689939790	-1.4749432669	-2.7518141824	H	1.4237291179	-3.2728924089	0.1475579929
N	-0.9554995163	-0.0289775849	-0.9242477301	H	2.7695216386	-1.2194309413	0.1443474696
N	-0.2053586562	-0.9590932650	-1.2978875857	H	5.7056018927	4.6041265030	0.0992874431
N	1.7028375914	0.5214874719	-1.4660345737	H	3.6817640362	6.4518934257	-0.0512751530
N	1.9213704803	-1.5737646447	-2.1607437225	N	2.4688703266	4.6644483319	-0.0511211934
C	1.5989868776	-2.9491701657	-2.4830238884	C	1.1228878404	5.1756862063	-0.1259447831
H	2.2082928014	-3.6282848144	-1.8974653013	H	0.5478137046	4.8936202152	0.7490577394
H	0.5598052286	-3.1258131655	-2.2567686313	H	1.1661605557	6.2538812736	-0.1748228459
H	1.7678959125	-3.1368082345	-3.5370798865	H	0.6164027822	4.8116832304	-1.0128811832
C	-3.0405160375	2.6568304847	3.6307399860	C	-1.3195877279	-3.5352384294	0.0339783060
H	-2.8668207874	3.7274280556	3.5620367638	H	-1.9253029773	-3.6083866351	-0.8665254221
H	-4.1132799455	2.5041438148	3.7133717978	H	-0.7030869943	-4.4255482428	0.0878171568
H	-2.5839033163	2.3054227777	4.5491139042	H	-2.0015567140	-3.5555101496	0.8811315162

Table 16S. Cartesian coordinates of MECI6 optimized at SA3-CASSCF(12,10)/6-311G** level.

SA3-CASSCF(12,10)/6-311G**		
X	Y	Z
C 0.5097743860	2.7393197526	0.1321490836
C -0.7481617897	3.5674256800	0.2415913908
C -2.0720904039	2.9823657947	0.2566276089
C -2.1678332664	1.6497182384	0.1685334361
C -1.0117725601	0.7836480675	0.0598707829
C 0.4296537094	1.3084019198	0.0392444247
N 1.3546287287	0.4161013344	-0.0567857456
N 2.5922107941	1.1580652348	-0.0566977331
C 3.6076345030	0.2245389711	-0.1603153575
N 3.5948858988	-1.0714266192	-0.2470340730
C 4.8885355941	-1.4496142121	-0.3244897176
C 5.7019994001	-0.3580734397	-0.2837473756
H 1.4493834654	3.2408707169	0.1265971606
H -0.6309528600	4.6320813981	0.3102939720
H -3.1339054815	1.1761600175	0.1762073892
H -1.1267724557	-0.2789791295	-0.0118307337
H 5.1714837708	-2.4787373351	-0.4050796640
H 6.7665735760	-0.2627839445	-0.3201442200
N 4.8807218473	0.7133494198	-0.1785516366
C 5.2867984232	2.1028773158	-0.1018535582
H 4.9476020857	2.5493328206	0.8227823350
H 6.3669325618	2.1437536719	-0.1400871265
H 4.8811287015	2.6657226395	-0.9313481445
C -3.2610297821	3.8984887788	0.3696782793
H -3.2934158330	4.6001669970	-0.4602012638
H -4.1858701308	3.3345454238	0.3700556178
H -3.2196385027	4.4803348082	1.2871884793