Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Analyzing Torquoselectivity in Electrocyclic Ring Opening Reactions of *trans*-3,4-Dimethylcyclobutene and 3-Formylcyclobutene through Electronic Structure Principles

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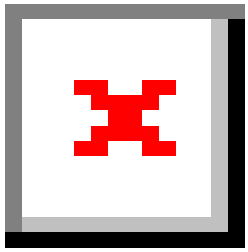
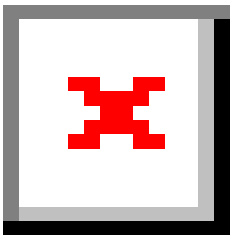
Supporting information



TSIC



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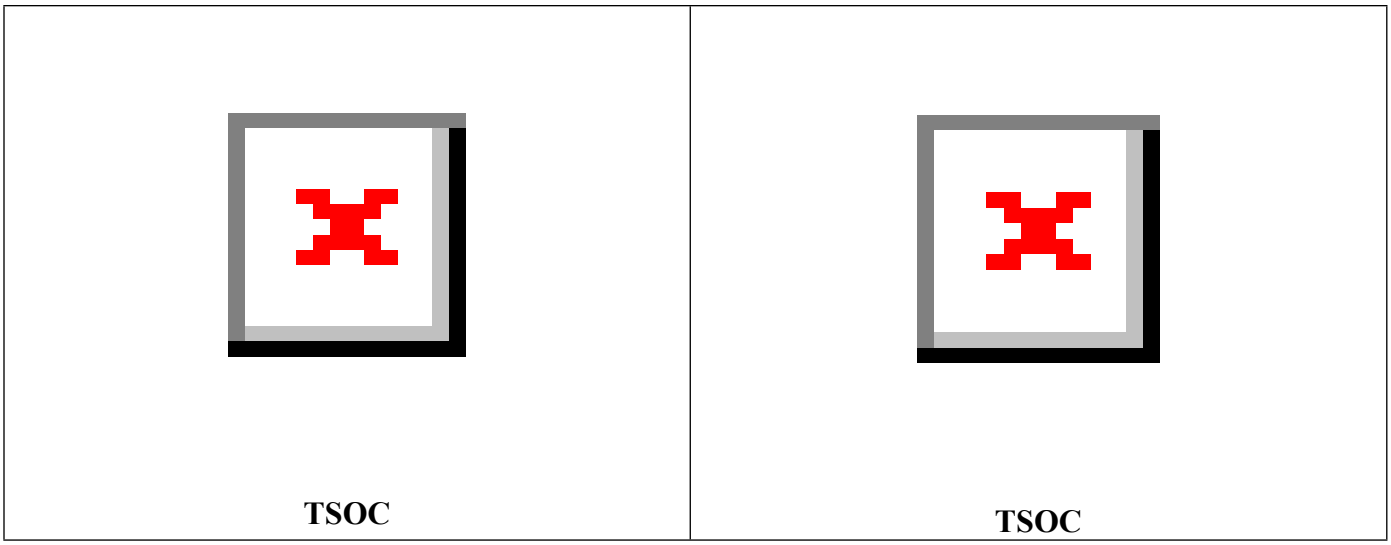

Figure S1. ω^{+} and ω^{-} profiles at C1 and C2 centers of *trans*-3,4-dimethylcyclobutene along IRC (ξ, amu$^{1/2}$bohr) at the B3LYP/6-31G(d,p) level.

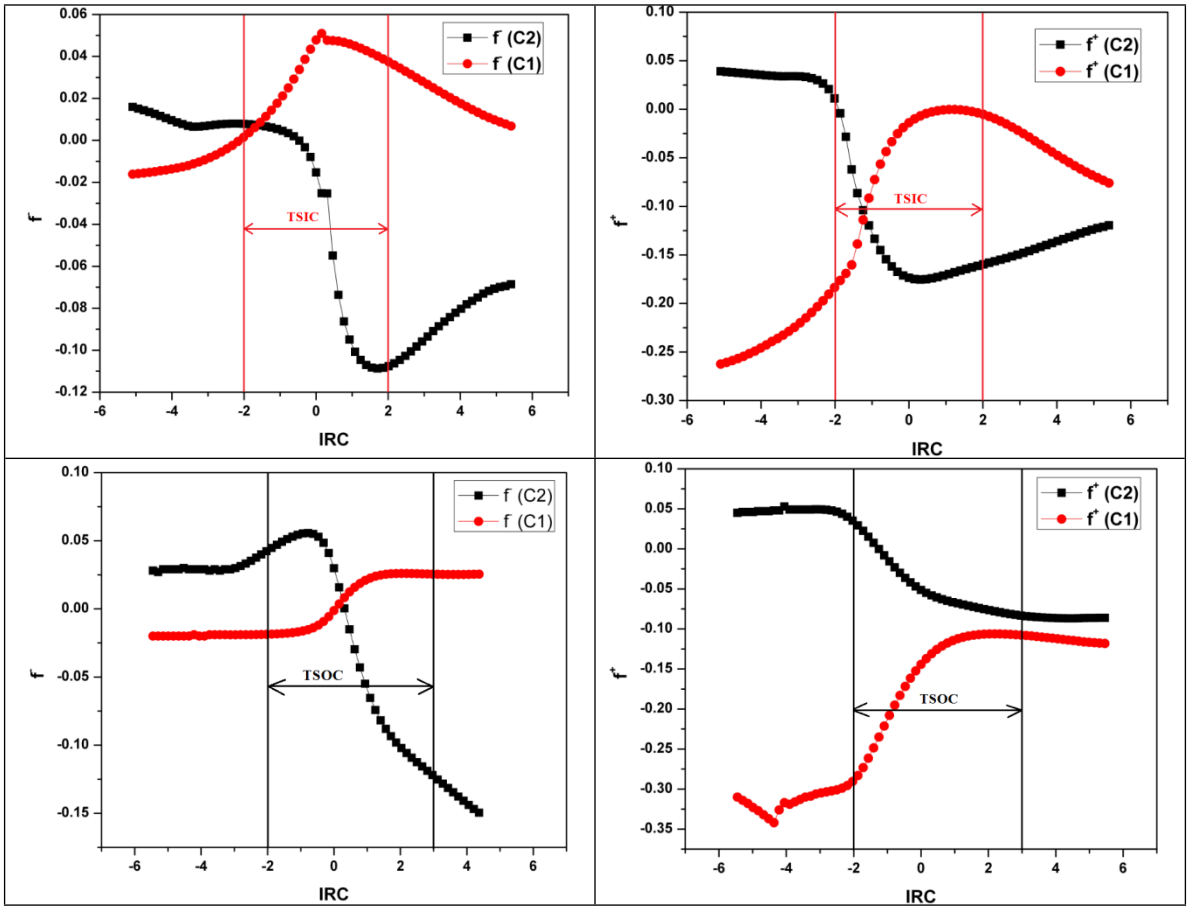

Figure S2. f^+ and f^- (au) profiles at C1 and C2 centers of 3-formylcyclobutene along IRC (ξ, $amu^{1/2}bohr$) at the B3LYP/6-31G(d,p) level.

Ring opening reaction of trans-3,4- dimethylcyclobutene.

I. Trans-3,4- dimethylcyclobutene.

E = -234.5543905 au

C	0.676255000	1.383078000	-0.216260000
C	0.803129000	0.032533000	0.498796000
C	-0.802960000	0.034038000	0.498580000
C	-0.673244000	1.384284000	-0.216789000
H	1.424540000	2.084785000	-0.570887000
H	1.201735000	0.121446000	1.520188000
H	-1.201627000	0.124333000	1.519917000
H	-1.420015000	2.087552000	-0.571489000
C	1.535548000	-1.095600000	-0.231935000
H	2.613060000	-0.889170000	-0.271595000
H	1.399431000	-2.055447000	0.282681000
H	1.181032000	-1.205839000	-1.262813000
C	-1.537888000	-1.092725000	-0.231600000
H	-1.404338000	-2.052883000	0.283226000
H	-2.614954000	-0.883838000	-0.271458000
H	-1.183902000	-1.204584000	-1.262526000

II. TSIC

E = -234.4901987 au, Imaginary Frequency: 637.22 *i*

C	-1.039407000	0.223468000	-0.989662000
C	-0.675556000	0.046317000	0.490331000
C	0.827685000	-0.106414000	-0.031944000
C	0.229287000	0.093567000	-1.430860000
H	-1.989669000	0.401731000	-1.482968000
H	1.454563000	0.734092000	0.300370000
H	0.685697000	0.108854000	-2.416038000
C	1.533513000	-1.434914000	0.250957000

H	2.478905000	-1.504803000	-0.303670000
H	1.763701000	-1.541281000	1.318997000
H	0.904478000	-2.283014000	-0.050005000
C	-0.969042000	1.214694000	1.434168000
H	-2.049075000	1.341769000	1.581644000
H	-0.513846000	1.051717000	2.419827000
H	-0.573707000	2.153045000	1.025427000
H	-1.048745000	-0.892708000	0.923021000

III. Z,Z-butadiene

E = -234.579384 au

C	-0.072354000	0.158095000	-0.023400000
C	-0.225897000	0.187373000	1.318647000
C	2.374711000	-0.081751000	-0.662124000
C	1.143054000	0.455151000	-0.804533000
H	-0.958627000	-0.061227000	-0.622279000
H	3.153242000	0.261016000	-1.344818000
H	0.998002000	1.160067000	-1.625685000
C	2.789388000	-1.155214000	0.307523000
H	3.372068000	-1.931175000	-0.206186000
H	3.431547000	-0.755594000	1.106277000
H	1.924559000	-1.630034000	0.780042000
C	0.806215000	0.579624000	2.341085000
H	0.377957000	1.282877000	3.067418000
H	1.160868000	-0.289338000	2.914842000
H	1.677042000	1.051621000	1.876824000
H	-1.211553000	-0.057870000	1.716150000

IV. TSOC

E = -234.5108830 au, Imaginary Frequency: 523.90 *i*

C	-1.306166000	0.263822000	-0.506454000
H	-2.101368000	0.690637000	-1.113417000
C	-1.219408000	-1.144661000	-0.084873000
H	-2.101723000	-1.749514000	0.119219000
C	0.868639000	-0.213141000	0.245363000
H	0.501859000	0.374789000	1.098245000
C	2.200514000	0.349407000	-0.250007000

H	3.022593000	0.013219000	0.404182000
H	2.426670000	-0.021926000	-1.257546000
H	2.252920000	1.459136000	-0.295027000
C	-0.965646000	1.505834000	0.282108000
H	-1.191416000	2.444441000	-0.234838000
H	-1.457250000	1.543431000	1.268738000
H	0.113708000	1.472727000	0.468961000
C	0.110771000	-1.465104000	0.077760000
H	0.401783000	-2.003880000	0.958098000

V. E,E-butadiene

E = -234.5841007 au

C	0.147141000	0.055466000	0.221730000
C	-0.007064000	0.167323000	1.557319000
C	2.642373000	-0.106294000	-0.074268000
C	1.377404000	-0.330902000	-0.485960000
H	-0.719489000	0.247428000	-0.414051000
H	2.808257000	0.443989000	0.853303000
H	1.229742000	-0.830113000	-1.445699000
C	3.877206000	-0.546288000	-0.812299000
H	3.624812000	-1.066804000	-1.743284000
H	4.519719000	0.309267000	-1.064004000
H	4.486114000	-1.227479000	-0.200560000
C	-1.275210000	0.597236000	2.242943000
H	-2.074125000	0.799198000	1.520227000
H	-1.634044000	-0.172352000	2.940885000
H	-1.118705000	1.510355000	2.835172000
H	0.831856000	-0.078594000	2.210353000

Ring opening reaction of Formyl-cyclobutene.

I. 3-formylcyclobutene

E = -269.299032 au

C	1.111979000	-0.979380000	-0.220193000
C	-0.024326000	-0.229907000	0.472376000
C	0.963926000	1.005370000	0.443290000

C	1.930798000	0.079920000	-0.265056000
H	1.185943000	-2.008534000	-0.556834000
H	0.613181000	1.875677000	-0.124793000
H	2.931784000	0.236293000	-0.655192000
H	-0.317291000	-0.580872000	1.466683000
H	1.260729000	1.340162000	1.442759000
C	-1.255373000	-0.037897000	-0.379060000
H	-1.042806000	0.370822000	-1.395093000
O	-2.386243000	-0.298223000	-0.032268000

II. TSIC

E = -269.257045 au, Imaginary Frequency: 651.85 *i*

C	-0.017477000	-0.017582000	-0.005669000
C	0.014568000	-0.058041000	1.431061000
C	2.055347000	0.119161000	0.774091000
C	1.237035000	0.388235000	-0.371552000
H	-0.868445000	-0.283641000	-0.627162000
H	2.883838000	0.764171000	1.075706000
H	1.566563000	0.877035000	-1.285240000
H	-0.481165000	-0.846342000	2.005419000
H	2.144950000	-0.901415000	1.126797000
C	0.226806000	1.173464000	2.225698000
H	0.517327000	2.056840000	1.616871000
O	0.061163000	1.241514000	3.429475000

III. TSOC

E = -269.2504837 au, Imaginary Frequency: 651.85 *i*

C	0.651001000	1.223325000	0.109334000
C	0.974717000	-0.148212000	0.365868000
C	-1.022033000	-0.147391000	-0.382291000
C	-0.703358000	1.227630000	-0.084977000
H	1.367658000	2.033771000	-0.002917000
H	-0.592208000	-0.612480000	-1.264536000
H	-1.412589000	2.047936000	-0.001953000
H	0.563162000	-0.632161000	1.242640000
C	-2.236506000	-0.812304000	0.125181000
O	-2.529120000	-1.975257000	-0.093363000

H	-2.884149000	-0.170452000	0.767312000
H	1.882595000	-0.623586000	-0.015073000

IV. Z-2,4-pentadienal

E = -269.3139908 au

C	0.998715000	-0.893274000	0.076360000
C	-0.315782000	-1.051105000	0.367543000
C	1.493666000	1.545516000	-0.499594000
C	1.820097000	0.257102000	-0.311454000
H	1.583179000	-1.810446000	0.139797000
H	2.255961000	2.261417000	-0.790546000
H	2.865449000	-0.005189000	-0.466589000
H	-0.662340000	-2.048010000	0.630996000
H	0.491629000	1.939374000	-0.378848000
C	-1.390830000	-0.051722000	0.384950000
H	-1.129356000	0.992243000	0.128708000
O	-2.541651000	-0.341199000	0.669602000

V. E-2,4-pentadienal

E = -269.322729 au

C	2.008803000	0.020728000	-0.129302000
C	2.273867000	1.308139000	0.138270000
C	-0.514845000	-0.004744000	-0.025395000
C	0.685204000	-0.595169000	-0.205412000
H	2.845371000	-0.650858000	-0.311154000
H	-0.624011000	1.051163000	0.208218000
H	0.680036000	-1.661101000	-0.436240000
H	1.491542000	2.036550000	0.330089000
C	-1.754467000	-0.778443000	-0.139348000
O	-2.871251000	-0.315252000	0.009435000
H	-1.607366000	-1.856716000	-0.379460000
H	3.294886000	1.673055000	0.173097000

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