

## Unveiling the Reaction Mechanism and the Regioselectivity of Diels-Alder Cycloadditions between 2-methoxy-3-thiophenylbutadiene and methyl vinyl ketone Using Topological Tools

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Table S1 Energies (E, in a.u.), enthalpies (H<sup>0</sup>, in a.u.), Gibbs free energy (G<sup>0</sup>, in a.u.), and Maxwell-Boltzmann weights (P, in %) of the *s-cis* and *s-trans* conformers of methyl vinyl ketone **2** calculated at the IEFPCM(Diethylether)/M06-2X-D3/6-311+G(d,p) level. [ $\Delta X = X(2 \text{ s-cis}) - X(2 \text{ s-trans})$  in kcal mol<sup>-1</sup>, with X = E, H<sup>0</sup>, and G<sup>0</sup>]

	E	$\Delta E$	H <sup>0</sup>	$\Delta H^0$	G <sup>0</sup>	$\Delta G^0$	P
<b>2 s-cis</b>	-231.193539	0.07	-231.096775	0.01	-231.132371	-0.17	57
<b>2 s-trans</b>	-231.193655		-231.096797		-231.132105		43

Table S2 Energies, enthalpies, entropies, and Gibbs enthalpies of reactants, transition states, and products calculated at the DFT level using the M06-2X-D3/6-311+G(d,p) (T = 298.15K and P = 1 atm). Solvent (Diethylether) effects were described using IEFPCM

	E (u.a.)	H (u.a.)	G (u.a.)	S (cal mol <sup>-1</sup> K <sup>-1</sup> )
<b>In vacuo</b>				
<b>1</b>	-899.651864	-899.435937	-899.490616	115.082
<b>2</b>	-231.189354	-231.092389	-231.127594	74.095
<b>TS-on</b>	-1130.827118	-1130.512558	-1130.578215	138.185
<b>TS-ox</b>	-1130.821348	-1130.507001	-1130.574670	142.422
<b>TS-mn</b>	-1130.825675	-1130.511104	-1130.576325	137.269
<b>TS-mx</b>	-1130.820219	-1130.505877	-1130.573499	142.322
<b>CA-on</b>	-1130.912259	-1130.592851	-1130.659746	140.793
<b>CA-ox</b>	-1130.908606	-1130.589312	-1130.656809	142.059
<b>CA-mn</b>	-1130.919119	-1130.600087	-1130.667829	142.575
<b>CA-mx</b>	-1130.908737	-1130.589426	-1130.657267	142.784
<b>Diethylether (<math>\epsilon = 4.33</math>)</b>				

<b>1</b>	-899.656647	-899.440852	-899.495360	114.720
<b>2</b>	-231.193655	-231.096797	-231.132105	74.313
<b>TS-on</b>	-1130.835679	-1130.521275	-1130.586926	138.174
<b>TS-ox</b>	-1130.830436	-1130.516261	-1130.583872	142.299
<b>TS-mn</b>	-1130.834556	-1130.520129	-1130.585748	138.108
<b>TS-mx</b>	-1130.829940	-1130.515796	-1130.583394	142.273
<b>CA-on</b>	-1130.920256	-1130.600958	-1130.667673	140.414
<b>CA-ox</b>	-1130.916766	-1130.597416	-1130.664940	142.115
<b>CA-mn</b>	-1130.918526	-1130.599290	-1130.667741	144.067
<b>CA-mx</b>	-1130.916997	-1130.597658	-1130.666161	144.177

Table S3 M06-2X-D3/6-311+G(d,p) local reactivity descriptors namely the nucleophilic and electrophilic indices ( $N_k$ ,  $\omega_k$ ), and Local reactivity difference index ( $R_k$ ), in eV. k corresponds to each of the two reactive centers of **1** and **2**, in *vacuo*

Reactants	k	$P_k^-$	$N_k$	$P_k^+$	$\omega_k$	$R_k$
<b>1</b>	C1	0.008	0.02	0.17	0.15	0.13
	C2	0.006	0.01	0.02	0.02	0.01
	C3	-0.03	-0.06	0.20	0.18	0.24
	C4	0.08	0.17	0.60	0.54	0.37
<b>2</b>	C5	-0.04	-0.02	0.50	0.70	0.72
	C6	0.14	0.04	0.05	0.07	0.03

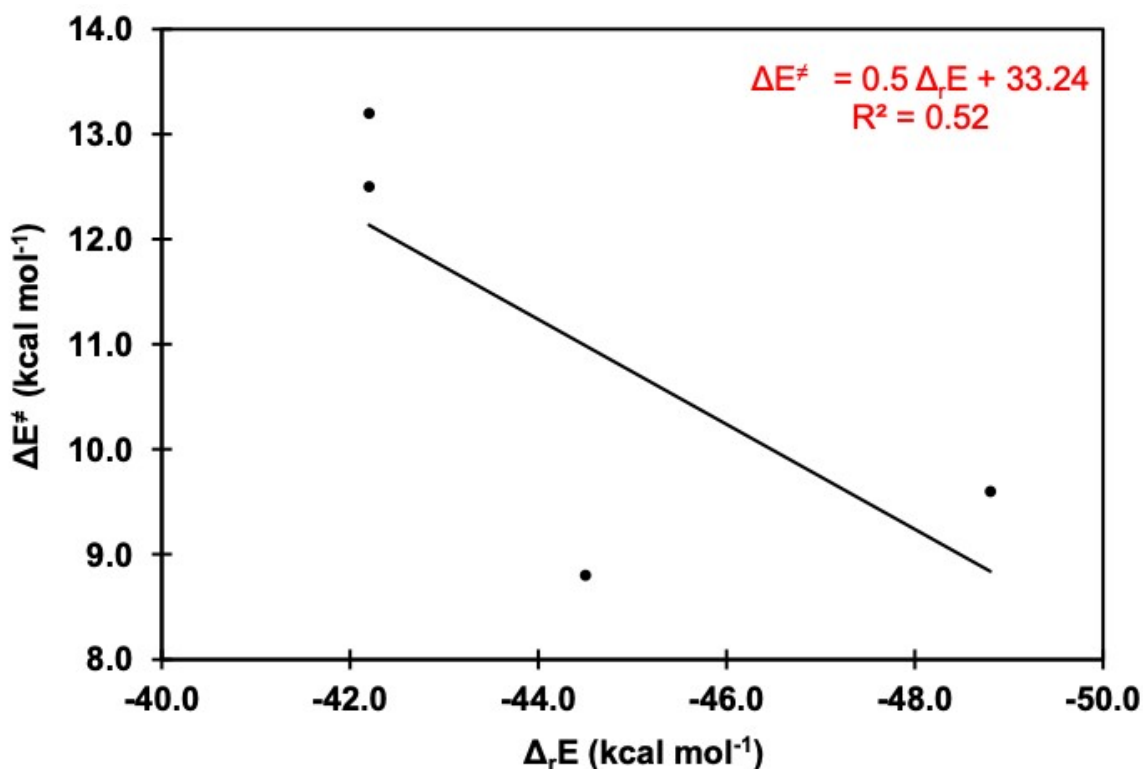


Fig. S1 Activation energy ( $\Delta E^\ddagger$ , in kcal mol<sup>-1</sup>) versus the energy reaction ( $\Delta_r E$ , in kcal mol<sup>-1</sup>) as evaluated at the M06-2X-D3/6-311+G(d,p) level, in *vacuo*.

**Cartesian Coordinates of all the Stationary Points as Computed at the M06-2X-D3/6-311+G(d,p) level in *vacuo***

**1**

0 1

C	-3.6331640000	-0.5526550000	0.4531470000
H	-3.7750750000	-1.5718660000	0.7802660000
H	-4.5078210000	0.0710840000	0.3372430000
C	-2.3937140000	-0.1252090000	0.1943610000
C	-1.1983170000	-0.9829300000	0.3885460000
C	-0.9699730000	-1.6321770000	1.5262060000
H	-1.6293020000	-1.4967300000	2.3764080000
H	-0.1122240000	-2.2845710000	1.6355730000
S	-0.0761450000	-1.1212990000	-1.0054410000
C	1.3719910000	-0.2916240000	-0.3696580000
C	2.6202740000	-0.8596280000	-0.6122890000
C	1.2764070000	0.9271550000	0.3030520000
C	3.7729830000	-0.2066890000	-0.1856210000
H	2.6863010000	-1.8118220000	-1.1251990000
C	2.4305810000	1.5588100000	0.7450430000
H	0.3005560000	1.3677240000	0.4700600000
C	3.6817850000	0.9985160000	0.4988300000
H	4.7418340000	-0.6521710000	-0.3777980000
H	2.3532720000	2.5016380000	1.2736690000
H	4.5792390000	1.5002330000	0.8396310000
O	-2.0518650000	1.1004340000	-0.2687590000
C	-3.1086380000	1.9790800000	-0.5951340000
H	-3.6920300000	2.2369710000	0.2942480000
H	-2.6459300000	2.8743000000	-1.0030210000
H	-3.7668810000	1.5266290000	-1.3428580000

**2**

0 1

C	1.9240280000	0.1691430000	0.0000000000
H	1.8143740000	1.2482210000	0.0000000000
H	2.9358680000	-0.2180130000	0.0000000000
C	0.8732060000	-0.6444520000	0.0000000000
H	0.9894350000	-1.7233780000	0.0000000000
C	-0.5478480000	-0.1899930000	0.0000000000
O	-1.4352860000	-1.0086750000	0.0000000000
C	-0.8381160000	1.2957960000	0.0000000000
H	-0.4043310000	1.7713560000	0.8824870000
H	-0.4042770000	1.7713910000	-0.8824500000
H	-1.9163990000	1.4368640000	0.0000000000

**CA-ox**

0 1

C	-2.2740200000	0.3879700000	0.7603370000
H	-2.0656260000	-0.3548680000	1.5409630000

H	-3.0550440000	1.0419060000	1.1511900000
C	-1.0109560000	1.1663630000	0.4960570000
C	-0.0209940000	0.5657960000	-0.1721590000
C	-0.2555050000	-0.8583580000	-0.6157450000
H	-0.2372760000	-1.5269130000	0.2537170000
H	0.5447000000	-1.1870980000	-1.2798530000
S	1.4422890000	1.4387460000	-0.6499510000
C	2.6799640000	0.2506610000	-0.1620990000
C	3.7592410000	0.0117690000	-1.0105170000
C	2.6019170000	-0.4076460000	1.0655370000
C	4.7583590000	-0.8773170000	-0.6279750000
H	3.8091960000	0.5164400000	-1.9681690000
C	3.5908830000	-1.3117910000	1.4298350000
H	1.7690320000	-0.2011070000	1.7285020000
C	4.6741380000	-1.5463570000	0.5874160000
H	5.5968840000	-1.0563890000	-1.2903820000
H	3.5227040000	-1.8243350000	2.3821230000
H	5.4476240000	-2.2465450000	0.8781290000
O	-0.9227430000	2.4353850000	0.9856850000
C	-1.6873440000	3.3835840000	0.2555000000
H	-2.7458030000	3.1034680000	0.2203130000
H	-1.5852180000	4.3348890000	0.7732890000
H	-1.3037570000	3.4761770000	-0.7653890000
C	-1.6153160000	-0.9567750000	-1.3301320000
H	-1.8258110000	-2.0010900000	-1.5745100000
H	-1.5305180000	-0.4257320000	-2.2798570000
C	-2.7771170000	-0.3324170000	-0.5186450000
H	-3.2999100000	0.4072940000	-1.1271770000
C	-3.8418300000	-1.3275070000	-0.0801630000
O	-5.0108370000	-1.0406900000	-0.1156500000
C	-3.3817340000	-2.6763270000	0.4442100000
H	-3.3936570000	-3.3942240000	-0.3805460000
H	-2.3683140000	-2.6483900000	0.8476400000
H	-4.0853110000	-3.0208650000	1.2002040000

**CA-on**

0 1

C	2.2349670000	0.4072440000	-1.2425760000
H	1.8363570000	0.3855910000	-2.2621470000
H	3.1025510000	1.0720900000	-1.2522600000
C	1.1921190000	0.9348170000	-0.2923490000
C	0.1468280000	0.1596630000	0.0081700000
C	0.1110000000	-1.2176570000	-0.6078310000
H	-0.1065450000	-1.1442730000	-1.6796420000
H	-0.6857240000	-1.8163920000	-0.1648100000
S	-1.0226100000	0.6567540000	1.2416130000
C	-2.5342680000	0.0994170000	0.4778850000
C	-3.4992800000	-0.5199190000	1.2697630000
C	-2.7843310000	0.3156440000	-0.8777960000
C	-4.7093710000	-0.9140880000	0.7084060000

H	-3.2961550000	-0.6975270000	2.3192420000
C	-3.9848060000	-0.1023280000	-1.4365660000
H	-2.0357470000	0.8116440000	-1.4859320000
C	-4.9531920000	-0.7136130000	-0.6451440000
H	-5.4564620000	-1.3923770000	1.3304900000
H	-4.1700400000	0.0618050000	-2.4915180000
H	-5.8914600000	-1.0320400000	-1.0824750000
O	1.4074250000	2.1408610000	0.3156680000
C	1.2713180000	3.2500440000	-0.5622720000
H	0.2435140000	3.3152180000	-0.9317650000
H	1.5102480000	4.1398100000	0.0161040000
H	1.9604210000	3.1728610000	-1.4098790000
C	1.4719450000	-1.9061940000	-0.4002400000
H	1.4895550000	-2.8635340000	-0.9233290000
H	1.5673550000	-2.1322190000	0.6653830000
C	2.6680400000	-1.0361540000	-0.8704210000
H	3.1339640000	-1.4932670000	-1.7443150000
C	3.7569610000	-1.0230110000	0.1996780000
O	4.7762270000	-1.6464200000	0.0423770000
C	3.5071590000	-0.2092290000	1.4532550000
H	4.3259140000	-0.3766610000	2.1496230000
H	3.4394030000	0.8543960000	1.2084440000
H	2.5548550000	-0.4765290000	1.9168480000

#### CA-mn

0 1

C	-3.0290450000	0.0395590000	0.0258800000
H	-3.0988140000	-0.2985550000	1.0616090000
H	-3.9454000000	0.5958340000	-0.1990810000
C	-1.8668650000	0.9899850000	-0.0825990000
C	-0.7642220000	0.7272040000	-0.7968330000
C	-0.6051560000	-0.5347120000	-1.6081770000
H	0.4487310000	-0.8229810000	-1.6181000000
H	-0.8782440000	-0.3390410000	-2.6507040000
S	0.5563310000	1.9124080000	-0.8898950000
C	1.8788660000	0.9191600000	-0.2163520000
C	3.1538530000	1.0292900000	-0.7707310000
C	1.6698470000	0.0700250000	0.8720320000
C	4.2113730000	0.3022580000	-0.2351340000
H	3.3106810000	1.6785510000	-1.6242530000
C	2.7281580000	-0.6681740000	1.3888200000
H	0.6805280000	-0.0102990000	1.3100620000
C	4.0023140000	-0.5534690000	0.8410170000
H	5.1990410000	0.3961210000	-0.6709790000
H	2.5548390000	-1.3267640000	2.2322900000
H	4.8257040000	-1.1258110000	1.2504090000
O	-1.9913120000	2.1883690000	0.5493220000
C	-2.5576470000	2.1663040000	1.8503360000
H	-2.0324090000	1.4535000000	2.4935490000
H	-2.4316660000	3.1712360000	2.2466650000

H	-3.6228070000	1.9205670000	1.8266420000
C	-2.9176050000	-1.1786130000	-0.8978760000
H	-3.2896240000	-0.9136440000	-1.8918150000
H	-3.5539090000	-1.9792700000	-0.5153350000
C	-1.4811790000	-1.6771290000	-1.0640970000
H	-1.4587340000	-2.4922450000	-1.7962110000
C	-0.8829030000	-2.2240730000	0.2278350000
O	-1.3678700000	-1.9934900000	1.3095370000
C	0.3486620000	-3.0935330000	0.0913770000
H	0.0718430000	-4.0254170000	-0.4102680000
H	1.1185210000	-2.6074960000	-0.5107630000
H	0.7431580000	-3.3163330000	1.0807360000

**CA-mx**

0 1

C	-2.2960000000	1.5008890000	0.8983820000
H	-2.1962610000	1.3890650000	1.9844820000
H	-2.8901570000	2.4068220000	0.7406450000
C	-0.9198170000	1.7246430000	0.3315330000
C	-0.2815340000	0.8237330000	-0.4233920000
C	-0.8560160000	-0.5340560000	-0.7359210000
H	-0.0679350000	-1.2875640000	-0.6494590000
H	-1.1888800000	-0.5701070000	-1.7778260000
S	1.2996360000	1.2141020000	-1.1444890000
C	2.3114190000	0.0088850000	-0.2974990000
C	3.2021910000	-0.7721900000	-1.0294490000
C	2.2375300000	-0.1286690000	1.0885660000
C	4.0221270000	-1.6851200000	-0.3733500000
H	3.2422600000	-0.6700710000	-2.1073420000
C	3.0433840000	-1.0575660000	1.7336270000
H	1.5533780000	0.4994070000	1.6482530000
C	3.9404230000	-1.8349840000	1.0058330000
H	4.7143630000	-2.2905710000	-0.9462020000
H	2.9806590000	-1.1653320000	2.8100690000
H	4.5720190000	-2.5542240000	1.5128450000
O	-0.3490920000	2.9088280000	0.7172930000
C	-0.5612920000	3.9839480000	-0.1850480000
H	-1.6297630000	4.1360940000	-0.3739210000
H	-0.1487210000	4.8742350000	0.2856910000
H	-0.0460490000	3.7993190000	-1.1318550000
C	-2.9951740000	0.2869630000	0.2909910000
H	-3.3485670000	0.5294910000	-0.7171540000
H	-3.8697600000	0.0273300000	0.8915180000
C	-2.0144920000	-0.8914450000	0.1895000000
H	-1.6252250000	-1.0863350000	1.1993920000
C	-2.7150300000	-2.1652910000	-0.2631120000
O	-2.3826370000	-2.7541810000	-1.2597520000
C	-3.8675690000	-2.6571140000	0.5902470000
H	-3.7093850000	-2.4473350000	1.6495720000
H	-4.7824040000	-2.1439430000	0.2804660000

H	-4.0008170000	-3.7248360000	0.4268820000
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**TS-ox**

0 1

C	-2.4066090000	0.7025350000	0.8727990000
H	-2.3573450000	-0.1294560000	1.5562470000
H	-3.3789390000	1.1639560000	0.7704740000
C	-1.2538310000	1.3430690000	0.5008950000
C	-0.0174680000	0.6450740000	0.4492560000
C	0.0212560000	-0.7076220000	0.7391340000
H	-0.6244270000	-1.0862010000	1.5209270000
H	0.9546590000	-1.2467460000	0.6325190000
S	1.2629220000	1.4796450000	-0.4630740000
C	2.6369100000	0.3720590000	-0.2005720000
C	3.0716610000	-0.4507920000	-1.2367860000
C	3.2972420000	0.3541880000	1.0284270000
C	4.1628080000	-1.2935620000	-1.0424870000
H	2.5540510000	-0.4272270000	-2.1884180000
C	4.3774820000	-0.4968170000	1.2210140000
H	2.9539510000	1.0049860000	1.8238560000
C	4.8125300000	-1.3203170000	0.1854610000
H	4.5006540000	-1.9303840000	-1.8511590000
H	4.8868660000	-0.5113610000	2.1770910000
H	5.6593820000	-1.9787470000	0.3365730000
O	-1.2232250000	2.5634010000	-0.0994030000
C	-2.4274850000	3.2995060000	-0.1542540000
H	-2.8447340000	3.4402410000	0.8476220000
H	-2.1707500000	4.2642560000	-0.5847330000
H	-3.1664120000	2.8018030000	-0.7894290000
C	-1.1353270000	-1.5645810000	-0.7643080000
H	-1.0236360000	-2.5595240000	-0.3465950000
H	-0.4292720000	-1.3220900000	-1.5500500000
C	-2.3996690000	-0.9899920000	-0.8126160000
H	-2.6229930000	-0.2273540000	-1.5485860000
C	-3.5980710000	-1.5988000000	-0.2041370000
O	-4.7118140000	-1.1915820000	-0.4573760000
C	-3.4002810000	-2.7543900000	0.7638500000
H	-4.3370520000	-2.9300550000	1.2882650000
H	-3.1261960000	-3.6570690000	0.2118480000
H	-2.6011370000	-2.5552270000	1.4828970000

**TS-on**

0 1

C	-2.3663770000	0.4885320000	1.5405190000
H	-2.0379200000	0.0342000000	2.4598930000
H	-3.4207450000	0.7191510000	1.4798780000
C	-1.4481710000	1.0758310000	0.7075460000
C	-0.1078240000	0.6092550000	0.6642910000
C	0.2656260000	-0.4775430000	1.4367380000
H	-0.1669260000	-0.5828170000	2.4223620000

H	1.2698620000	-0.8731880000	1.3466770000
S	0.8364320000	1.1893790000	-0.7332950000
C	2.4201060000	0.4371840000	-0.4026530000
C	2.8122120000	-0.6936790000	-1.1153260000
C	3.2761950000	0.9952500000	0.5469300000
C	4.0566610000	-1.2689220000	-0.8741090000
H	2.1412360000	-1.1167100000	-1.8536440000
C	4.5127850000	0.4117270000	0.7911090000
H	2.9623690000	1.8791000000	1.0894710000
C	4.9045200000	-0.7198760000	0.0804680000
H	4.3600690000	-2.1470920000	-1.4312090000
H	5.1752070000	0.8448760000	1.5308790000
H	5.8716940000	-1.1698540000	0.2692050000
O	-1.7740640000	1.9179620000	-0.3115250000
C	-3.1365700000	2.2709900000	-0.4601020000
H	-3.5077240000	2.7772180000	0.4363580000
H	-3.1780950000	2.9504740000	-1.3076900000
H	-3.7519780000	1.3882160000	-0.6631000000
C	-0.8870510000	-2.0524740000	0.6983190000
H	-0.4681000000	-2.7457040000	1.4186720000
H	-0.4038270000	-2.0631750000	-0.2724300000
C	-2.2422640000	-1.7568220000	0.7836080000
H	-2.8170020000	-2.0869290000	1.6420910000
C	-3.0755740000	-1.3744610000	-0.3766640000
O	-4.2867870000	-1.3308030000	-0.2965650000
C	-2.3712800000	-1.0452390000	-1.6792080000
H	-3.0979490000	-0.6203640000	-2.3693630000
H	-1.5404470000	-0.3514450000	-1.5343170000
H	-1.9637860000	-1.9618160000	-2.1151080000

**TS-mn**

0 1

C	-2.3663770000	0.4885320000	1.5405190000
H	-2.0379200000	0.0342000000	2.4598930000
H	-3.4207450000	0.7191510000	1.4798780000
C	-1.4481710000	1.0758310000	0.7075460000
C	-0.1078240000	0.6092550000	0.6642910000
C	0.2656260000	-0.4775430000	1.4367380000
H	-0.1669260000	-0.5828170000	2.4223620000
H	1.2698620000	-0.8731880000	1.3466770000
S	0.8364320000	1.1893790000	-0.7332950000
C	2.4201060000	0.4371840000	-0.4026530000
C	2.8122120000	-0.6936790000	-1.1153260000
C	3.2761950000	0.9952500000	0.5469300000
C	4.0566610000	-1.2689220000	-0.8741090000
H	2.1412360000	-1.1167100000	-1.8536440000
C	4.5127850000	0.4117270000	0.7911090000
H	2.9623690000	1.8791000000	1.0894710000
C	4.9045200000	-0.7198760000	0.0804680000
H	4.3600690000	-2.1470920000	-1.4312090000

H	5.1752070000	0.8448760000	1.5308790000
H	5.8716940000	-1.1698540000	0.2692050000
O	-1.7740640000	1.9179620000	-0.3115250000
C	-3.1365700000	2.2709900000	-0.4601020000
H	-3.5077240000	2.7772180000	0.4363580000
H	-3.1780950000	2.9504740000	-1.3076900000
H	-3.7519780000	1.3882160000	-0.6631000000
C	-0.8870510000	-2.0524740000	0.6983190000
H	-0.4681000000	-2.7457040000	1.4186720000
H	-0.4038270000	-2.0631750000	-0.2724300000
C	-2.2422640000	-1.7568220000	0.7836080000
H	-2.8170020000	-2.0869290000	1.6420910000
C	-3.0755740000	-1.3744610000	-0.3766640000
O	-4.2867870000	-1.3308030000	-0.2965650000
C	-2.3712800000	-1.0452390000	-1.6792080000
H	-3.0979490000	-0.6203640000	-2.3693630000
H	-1.5404470000	-0.3514450000	-1.5343170000
H	-1.9637860000	-1.9618160000	-2.1151080000

**TS-mx**

0 1

C	2.9416390000	-0.3395440000	0.7482310000
H	2.7623930000	0.4169100000	1.4961680000
H	3.9764400000	-0.6424980000	0.6575140000
C	1.9272690000	-1.2364340000	0.4617640000
C	0.5706480000	-0.8236830000	0.4834480000
C	0.2561050000	0.4548180000	0.8658180000
H	0.8669640000	0.9556620000	1.6046340000
H	-0.7455460000	0.8486210000	0.7503100000
S	-0.5462940000	-1.8836820000	-0.4272620000
C	-2.0797850000	-1.0006310000	-0.1984560000
C	-2.4915730000	-0.0654750000	-1.1461410000
C	-2.8657580000	-1.2476960000	0.9262110000
C	-3.6828050000	0.6285450000	-0.9630240000
H	-1.8716570000	0.1227710000	-2.0144490000
C	-4.0563440000	-0.5531010000	1.1038600000
H	-2.5342320000	-1.9777370000	1.6547080000
C	-4.4642530000	0.3857660000	0.1610050000
H	-3.9933550000	1.3640210000	-1.6948110000
H	-4.6655730000	-0.7447840000	1.9790040000
H	-5.3904870000	0.9291560000	0.3037930000
O	2.1325840000	-2.4291450000	-0.1524660000
C	3.4557970000	-2.9086220000	-0.2620130000
H	3.9343080000	-2.9653680000	0.7204510000
H	3.3794340000	-3.9045980000	-0.6910910000
H	4.0541260000	-2.2748700000	-0.9237250000
C	1.3681710000	1.6212800000	-0.7629450000
H	3.4722010000	1.7673680000	-0.3702160000
H	0.6578830000	1.2535220000	-1.4942770000
C	2.6774600000	1.1547210000	-0.7807680000

H	2.9825110000	0.4953170000	-1.5833410000
C	0.9773810000	2.9080190000	-0.1516960000
O	-0.0946220000	3.4198460000	-0.3910490000
C	1.9571330000	3.5756350000	0.8000750000
H	1.4298210000	4.3521980000	1.3499670000
H	2.4052410000	2.8625640000	1.4969590000
H	2.7700110000	4.0334650000	0.2305090000

**Cartesian Coordinates of all the Stationary Points as Computed at the IEFPCM(diethylether)/M06-2X-D3/6-311+G(d,p) level**

**1**

0 1

C	-3.6413880000	-0.4882600000	0.4391270000
H	-3.8169210000	-1.4966870000	0.7838800000
H	-4.4943750000	0.1631200000	0.3129790000
C	-2.3882950000	-0.1038220000	0.1762130000
C	-1.2212340000	-0.9966650000	0.3883030000
C	-1.0340620000	-1.6685930000	1.5207390000
H	-1.7074080000	-1.5295000000	2.3593530000
H	-0.1993710000	-2.3488980000	1.6383980000
S	-0.0703990000	-1.1612560000	-0.9812290000
C	1.3677120000	-0.3076870000	-0.3519820000
C	2.6232710000	-0.8382390000	-0.6424240000
C	1.2602960000	0.8867770000	0.3615750000
C	3.7706750000	-0.1712620000	-0.2225400000
H	2.7016740000	-1.7721130000	-1.1866300000
C	2.4109990000	1.5327880000	0.7951950000
H	0.2807470000	1.3017160000	0.5668460000
C	3.6687690000	1.0106090000	0.5019340000
H	4.7442200000	-0.5882470000	-0.4513330000
H	2.3240260000	2.4565570000	1.3550100000
H	4.5624190000	1.5226450000	0.8372230000
O	-2.0079090000	1.1032570000	-0.3047820000
C	-3.0391300000	2.0207810000	-0.6239730000
H	-3.6035900000	2.2982840000	0.2707030000
H	-2.5487960000	2.8984140000	-1.0368240000
H	-3.7186520000	1.5901850000	-1.3646890000

**2**

0 1

C	1.9227380000	0.1672070000	0.0000000000
H	1.8147900000	1.2463420000	0.0000000000
H	2.9335540000	-0.2226420000	0.0001260000
C	0.8708970000	-0.6462280000	0.0000000000
H	0.9888940000	-1.7250650000	0.0000000000
C	-0.5462830000	-0.1873950000	-0.0001070000
O	-1.4381650000	-1.0073910000	0.0000000000
C	-0.8347030000	1.2959820000	0.0000000000

H	-0.3978360000	1.7695260000	0.8818040000
H	-0.3978570000	1.7696400000	-0.8817600000
H	-1.9121200000	1.4439300000	0.0000000000

**CA-on**

0 1

C	-2.2232510000	0.4191040000	1.2337650000
H	-1.8193810000	0.3958530000	2.2506490000
H	-3.0834420000	1.0926790000	1.2479780000
C	-1.1767190000	0.9314470000	0.2786690000
C	-0.1458760000	0.1374050000	-0.0247070000
C	-0.1266170000	-1.2388810000	0.5939200000
H	0.0936460000	-1.1653680000	1.6648530000
H	0.6594090000	-1.8501790000	0.1489370000
S	1.0308680000	0.6091110000	-1.2617170000
C	2.5460560000	0.0845150000	-0.4795980000
C	3.5356760000	-0.5053990000	-1.2644690000
C	2.7719780000	0.2978340000	0.8808970000
C	4.7485090000	-0.8730520000	-0.6900820000
H	3.3524310000	-0.6810280000	-2.3180520000
C	3.9767960000	-0.0932880000	1.4517590000
H	2.0041130000	0.7688050000	1.4848250000
C	4.9704290000	-0.6748930000	0.6684360000
H	5.5148020000	-1.3284720000	-1.3059280000
H	4.1439450000	0.0679400000	2.5101480000
H	5.9108990000	-0.9725650000	1.1155990000
O	-1.3702660000	2.1412170000	-0.3270050000
C	-1.3131080000	3.2468600000	0.5704770000
H	-0.3159880000	3.3202200000	1.0136850000
H	-1.5209330000	4.1378380000	-0.0173460000
H	-2.0602050000	3.1539160000	1.3639130000
C	-1.4962730000	-1.9105220000	0.3927840000
H	-1.5240880000	-2.8657850000	0.9186070000
H	-1.6005210000	-2.1362870000	-0.6720860000
C	-2.6755580000	-1.0211780000	0.8714290000
H	-3.1345540000	-1.4675340000	1.7543570000
C	-3.7692800000	-1.0042250000	-0.1893630000
O	-4.7892540000	-1.6329190000	-0.0304350000
C	-3.5302160000	-0.1876000000	-1.4405760000
H	-4.3524700000	-0.3475630000	-2.1346190000
H	-3.4590060000	0.8739250000	-1.1884060000
H	-2.5816750000	-0.4573120000	-1.9101710000

**CA-ox**

0 1

C	-2.2544230000	0.4328490000	0.6450090000
H	-2.0202180000	-0.2519180000	1.4694120000
H	-3.0550580000	1.0829020000	0.9942530000

C	-1.0006550000	1.2007510000	0.3064600000
C	-0.0130730000	0.5331080000	-0.3062090000
C	-0.2509500000	-0.9213800000	-0.6315110000
H	-0.2347540000	-1.5235690000	0.2855570000
H	0.5484020000	-1.3015370000	-1.2687820000
S	1.4621620000	1.3501240000	-0.8433990000
C	2.7053060000	0.2425370000	-0.2039710000
C	3.8607860000	0.0333820000	-0.9565680000
C	2.5643490000	-0.3782610000	1.0378270000
C	4.8717180000	-0.7853070000	-0.4638430000
H	3.9630960000	0.5060220000	-1.9265760000
C	3.5691790000	-1.2124420000	1.5129390000
H	1.6711760000	-0.2016800000	1.6266640000
C	4.7275120000	-1.4158440000	0.7675240000
H	5.7677570000	-0.9402850000	-1.0530270000
H	3.4507940000	-1.6959870000	2.4754820000
H	5.5109750000	-2.0619570000	1.1440490000
O	-0.8543860000	2.4990440000	0.6723690000
C	-2.0121080000	3.3250500000	0.6794490000
H	-2.6343340000	3.1383790000	1.5577030000
H	-1.6466810000	4.3486790000	0.7165650000
H	-2.6028030000	3.1854320000	-0.2298440000
C	-1.6083830000	-1.0759130000	-1.3376750000
H	-1.8230660000	-2.1353610000	-1.4958700000
H	-1.5253760000	-0.6219630000	-2.3263980000
C	-2.7623960000	-0.3827820000	-0.5749240000
H	-3.2838140000	0.3106810000	-1.2364390000
C	-3.8273610000	-1.3310820000	-0.0458640000
O	-4.9956810000	-1.0256260000	-0.0764870000
C	-3.3772510000	-2.6446940000	0.5587060000
H	-3.3932370000	-3.4103060000	-0.2221190000
H	-2.3620770000	-2.5968210000	0.9550980000
H	-4.0783300000	-2.9398760000	1.3375040000

### CA-mn

0 1

C	-2.2147730000	1.3009680000	1.2529070000
H	-1.7493670000	1.2558470000	2.2442520000
H	-2.9217300000	2.1294740000	1.2706710000
C	-1.1422340000	1.5042740000	0.2108250000
C	-0.3438450000	0.4638650000	-0.0663670000
C	-0.5121700000	-0.7975470000	0.7443950000
H	-0.0998280000	-0.6412950000	1.7474700000
H	0.0551530000	-1.6074520000	0.2859730000
S	0.8759780000	0.5435690000	-1.3467460000
C	2.3362240000	0.0687800000	-0.4387270000
C	3.2885880000	-0.7271160000	-1.0750040000
C	2.5617050000	0.5089390000	0.8663880000
C	4.4622550000	-1.0708610000	-0.4118540000

H	3.1050540000	-1.0809680000	-2.0828420000
C	3.7264050000	0.1430390000	1.5301640000
H	1.8251670000	1.1388150000	1.3530420000
C	4.6829160000	-0.6434300000	0.8932570000
H	5.1982620000	-1.6873410000	-0.9142570000
H	3.8921490000	0.4843060000	2.5453080000
H	5.5922910000	-0.9218500000	1.4116120000
O	-0.9657370000	2.7104700000	-0.3873040000
C	-2.1254820000	3.4748930000	-0.6902860000
H	-2.5217310000	3.9759900000	0.1960220000
H	-1.8082840000	4.2276280000	-1.4085260000
H	-2.9019690000	2.8514010000	-1.1418580000
C	-2.9592300000	-0.0104040000	0.9673010000
H	-3.4825590000	0.1112470000	0.0137380000
H	-3.7202890000	-0.1847390000	1.7295760000
C	-1.9868100000	-1.2206910000	0.8864660000
H	-2.0945100000	-1.8093220000	1.8033540000
C	-2.4241790000	-2.1121480000	-0.2692270000
O	-1.7563040000	-2.2498020000	-1.2647800000
C	-3.7494930000	-2.8191420000	-0.0962250000
H	-3.6339490000	-3.5911940000	0.6698980000
H	-4.5230530000	-2.1314840000	0.2512010000
H	-4.0493930000	-3.2820220000	-1.0340920000

### CA-mx

0 1

C	-2.5259460000	1.0803200000	0.6420360000
H	-2.3373790000	0.6564590000	1.6346160000
H	-3.2579080000	1.8770300000	0.7686260000
C	-1.2375350000	1.6057490000	0.0594480000
C	-0.3291860000	0.7086060000	-0.3489670000
C	-0.6524610000	-0.7528990000	-0.1658690000
H	-0.5915690000	-1.0118900000	0.8989340000
H	0.0773930000	-1.3777470000	-0.6821600000
S	1.1371170000	1.2066010000	-1.2050070000
C	2.3672150000	0.2540130000	-0.3312810000
C	3.4378330000	-0.2725480000	-1.0532380000
C	2.3018710000	0.0656060000	1.0497890000
C	4.4404050000	-0.9765310000	-0.3940730000
H	3.4795810000	-0.1368920000	-2.1277490000
C	3.2956580000	-0.6580600000	1.6977520000
H	1.4745860000	0.4880360000	1.6092790000
C	4.3700840000	-1.1774800000	0.9804490000
H	5.2701360000	-1.3809620000	-0.9615090000
H	3.2354320000	-0.8067790000	2.7694590000
H	5.1453140000	-1.7365810000	1.4898420000
O	-1.0523320000	2.9332030000	-0.1546230000
C	-1.6345600000	3.8379550000	0.7762090000
H	-1.4837850000	3.4990770000	1.8042430000

H	-1.1221350000	4.7863460000	0.6319230000
H	-2.7007800000	3.9783300000	0.5854170000
C	-3.1074720000	-0.0038050000	-0.2881810000
H	-3.4681750000	0.4887090000	-1.1922290000
H	-3.9803810000	-0.4528520000	0.1909050000
C	-2.0754660000	-1.0813800000	-0.6945100000
H	-2.0122750000	-1.1449160000	-1.7815060000
C	-2.4192090000	-2.4793130000	-0.2089590000
O	-2.2600620000	-3.4425280000	-0.9201950000
C	-2.9298160000	-2.6343280000	1.2100180000
H	-2.6223460000	-1.8137900000	1.8596870000
H	-4.0230270000	-2.6519130000	1.1854780000
H	-2.5858810000	-3.5861050000	1.6116630000

**TS-on**

0 1

C	-2.3772600000	0.5121830000	1.5278990000
H	-2.0580140000	0.0334040000	2.4379850000
H	-3.4276990000	0.7609050000	1.4696980000
C	-1.4515300000	1.0941840000	0.7017810000
C	-0.1134720000	0.6176970000	0.6614810000
C	0.2548240000	-0.4720570000	1.4334620000
H	-0.1816000000	-0.5786410000	2.4173920000
H	1.2607170000	-0.8644330000	1.3487920000
S	0.8428320000	1.1985400000	-0.7270960000
C	2.4228340000	0.4355590000	-0.4011930000
C	2.7986000000	-0.7047320000	-1.1083220000
C	3.2877580000	0.9939540000	0.5403540000
C	4.0391760000	-1.2896640000	-0.8686850000
H	2.1203800000	-1.1293960000	-1.8390470000
C	4.5209020000	0.4006710000	0.7817730000
H	2.9867730000	1.8838880000	1.0802900000
C	4.8976880000	-0.7403410000	0.0772330000
H	4.3308780000	-2.1753710000	-1.4199190000
H	5.1909130000	0.8328260000	1.5151340000
H	5.8614890000	-1.1980750000	0.2644380000
O	-1.7639360000	1.9546880000	-0.3077830000
C	-3.1260620000	2.3151450000	-0.4622500000
H	-3.5024900000	2.8120180000	0.4363700000
H	-3.1617000000	3.0017440000	-1.3039880000
H	-3.7400420000	1.4348230000	-0.6782320000
C	-0.8612980000	-2.0338610000	0.6776550000
H	-0.4235620000	-2.7274420000	1.3865400000
H	-0.3898850000	-2.0299220000	-0.2992300000
C	-2.2239650000	-1.7745410000	0.7791320000
H	-2.7738520000	-2.1114770000	1.6511620000
C	-3.0758280000	-1.4086590000	-0.3643060000
O	-4.2925590000	-1.4357460000	-0.2843710000
C	-2.3975520000	-1.0208520000	-1.6633020000

H	-3.1376530000	-0.5828450000	-2.3309140000
H	-1.5737860000	-0.3221880000	-1.5061950000
H	-1.9831200000	-1.9161060000	-2.1357910000

**TS-ox**

0 1

C	-2.4149460000	0.7243870000	0.8811120000
H	-2.3653540000	-0.1075910000	1.5645160000
H	-3.3840950000	1.1928580000	0.7806330000
C	-1.2631040000	1.3580460000	0.4977170000
C	-0.0266620000	0.6578310000	0.4545980000
C	0.0156870000	-0.6911150000	0.7633150000
H	-0.6284570000	-1.0596340000	1.5511840000
H	0.9521410000	-1.2269610000	0.6684610000
S	1.2555140000	1.4807710000	-0.4657200000
C	2.6307020000	0.3728730000	-0.2073020000
C	3.0307080000	-0.4849620000	-1.2295350000
C	3.3206940000	0.3884380000	1.0053460000
C	4.1199880000	-1.3308050000	-1.0362520000
H	2.4891610000	-0.4890330000	-2.1680460000
C	4.4001810000	-0.4650730000	1.1962360000
H	3.0040040000	1.0644580000	1.7907470000
C	4.8015040000	-1.3239930000	0.1755030000
H	4.4311230000	-1.9960380000	-1.8325580000
H	4.9334130000	-0.4546110000	2.1391730000
H	5.6467700000	-1.9846990000	0.3254480000
O	-1.2300400000	2.5754440000	-0.1094920000
C	-2.4386790000	3.3112270000	-0.1749940000
H	-2.8587820000	3.4583310000	0.8240190000
H	-2.1824040000	4.2728460000	-0.6119490000
H	-3.1718520000	2.8055950000	-0.8093960000
C	-1.1078880000	-1.5691700000	-0.7270440000
H	-0.9937750000	-2.5574280000	-0.2940760000
H	-0.3974220000	-1.3356940000	-1.5118170000
C	-2.3790630000	-1.0097450000	-0.8052720000
H	-2.5960410000	-0.2550610000	-1.5516940000
C	-3.5732950000	-1.6220400000	-0.2049240000
O	-4.6944610000	-1.2523680000	-0.5047120000
C	-3.3780150000	-2.7379630000	0.8051580000
H	-4.3161390000	-2.9023060000	1.3311170000
H	-3.0967100000	-3.6577780000	0.2858350000
H	-2.5846720000	-2.5118310000	1.5215780000

**TS-mn**

0 1

C	2.9060850000	-0.4266630000	1.3586950000
H	2.5780130000	-0.2018000000	2.3617430000
H	3.9618880000	-0.6469650000	1.2731060000

C	2.0040020000	-1.0403420000	0.5034970000
C	0.6218470000	-0.7193860000	0.5522240000
C	0.1768840000	0.2248010000	1.4403540000
H	0.6859070000	0.3655940000	2.3816930000
H	-0.8377810000	0.6001460000	1.3945810000
S	-0.3558090000	-1.3293240000	-0.8216600000
C	-1.9873600000	-0.7864720000	-0.3412240000
C	-2.4611550000	0.4539660000	-0.7660390000
C	-2.7892700000	-1.6126820000	0.4459020000
C	-3.7376480000	0.8672650000	-0.3962860000
H	-1.8249820000	1.1043910000	-1.3540870000
C	-4.0646720000	-1.1950820000	0.8093760000
H	-2.4088190000	-2.5739370000	0.7699150000
C	-4.5391190000	0.0443000000	0.3882860000
H	-4.1007610000	1.8352920000	-0.7194980000
H	-4.6874380000	-1.8374570000	1.4202800000
H	-5.5326970000	0.3685920000	0.6736540000
O	2.3681440000	-1.7413360000	-0.6007130000
C	3.7310850000	-2.1041580000	-0.7468550000
H	4.0795420000	-2.6633530000	0.1254200000
H	3.7800240000	-2.7329250000	-1.6318750000
H	4.3583540000	-1.2208510000	-0.8933360000
C	2.8076340000	1.6251480000	0.8654530000
H	3.3280780000	1.5041830000	-0.0765440000
H	3.4455200000	1.8918420000	1.6997360000
C	1.4927910000	2.0802800000	0.8686400000
H	1.0986580000	2.5967460000	1.7364680000
C	0.7252320000	2.2940460000	-0.3697480000
O	-0.3170370000	2.9268920000	-0.3746560000
C	1.2897760000	1.7264450000	-1.6572710000
H	1.7145130000	0.7305740000	-1.5198930000
H	0.5026390000	1.6896460000	-2.4082830000
H	2.0867530000	2.3862160000	-2.0135950000

### TS-mx

0 1

C	-2.9266710000	-0.3912900000	-0.7473570000
H	-2.7638240000	0.3649790000	-1.4996130000
H	-3.9540570000	-0.7177990000	-0.6556310000
C	-1.8937420000	-1.2668440000	-0.4597290000
C	-0.5439300000	-0.8259630000	-0.4897790000
C	-0.2501850000	0.4526630000	-0.8788340000
H	-0.8787170000	0.9502560000	-1.6044720000
H	0.7445110000	0.8636130000	-0.7630770000
S	0.5985830000	-1.8675870000	0.4153420000
C	2.1185630000	-0.9603740000	0.1904320000
C	2.5320320000	-0.0500050000	1.1616110000
C	2.8925310000	-1.1666590000	-0.9511870000
C	3.7168800000	0.6583450000	0.9863940000

H	1.9217940000	0.1065510000	2.0431160000
C	4.0746290000	-0.4552240000	-1.1221090000
H	2.5611970000	-1.8772550000	-1.6989180000
C	4.4867010000	0.4572460000	-0.1544850000
H	4.0330520000	1.3701380000	1.7390480000
H	4.6744480000	-0.6144750000	-2.0100650000
H	5.4075340000	1.0114060000	-0.2905350000
O	-2.0721600000	-2.4607650000	0.1560700000
C	-3.3914380000	-2.9660860000	0.2738710000
H	-3.8683360000	-3.0370690000	-0.7072880000
H	-3.2944520000	-3.9571520000	0.7089960000
H	-3.9957680000	-2.3370500000	0.9326710000
C	-1.4291130000	1.6034690000	0.7772100000
H	-3.5345680000	1.6588260000	0.3715930000
H	-0.7032050000	1.2564030000	1.5035850000
C	-2.7163190000	1.0760200000	0.7796170000
H	-2.9968600000	0.4018020000	1.5790860000
C	-1.0898210000	2.8941650000	0.1592850000
O	-0.0401880000	3.4593240000	0.4073250000
C	-2.0844190000	3.5119980000	-0.8068100000
H	-1.5871910000	4.3043240000	-1.3624260000
H	-2.4982110000	2.7752670000	-1.4994030000
H	-2.9200750000	3.9413890000	-0.2480890000