

Supplementary Data

Computational study of an oxetane 4*H*-pyrazole as a Diels–Alder diene

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M06-2X/6-311++G(d,p) SMD H₂O electronic (*E*) and Gibbs (*G*) energies in Hartree–Fock (HF)

	<i>E</i>	<i>G</i>
BCN	-350.015463	-349.858789
1	-766.79729	-766.547042
TS-1	-1116.799412	-1116.366124
2	-804.86895	-804.610389
TS-2	-1154.874411	-1154.434507
3	-840.771741	-840.537906
TS-3	-1190.785131	-1190.36983
4	-886.656255	-869.5528424
TS-4	-1236.669668	-1219.635909

M06-2X/6-31G(d) Optimized Geometries

1			
C	0.13708200	0.47763900	-0.00011800
C	-1.13707700	0.47764200	0.00005000
N	-0.70198400	1.69285100	0.00009800
N	0.70203400	1.69285700	-0.00000200
C	-2.58682600	0.20590300	0.00002000
C	-3.47082200	1.29709000	-0.00044400
C	-3.12032000	-1.08814600	0.00045500
C	-4.84256100	1.09508300	-0.00046300
H	-3.05302400	2.29782000	-0.00077700
C	-4.49872200	-1.28775200	0.00043100
H	-2.46929400	-1.95438700	0.00083400
C	-5.36358300	-0.19945800	-0.00002800
H	-5.51134100	1.95018900	-0.00082300
H	-4.89337900	-2.29896000	0.00077800
H	-6.43779000	-0.35607600	-0.00004800
C	0.58682300	0.20587200	-0.00010400
C	0.47080900	1.29707000	0.00027200
C	0.12033800	-1.08816900	-0.00044800
C	0.84255000	1.09508900	0.00029600
H	0.05299300	2.29779300	0.00053700
C	0.49874600	-1.28774800	-0.00041600
H	0.46934600	-1.95443700	-0.00073800
C	0.36359300	-0.19944500	-0.00004500
H	0.51131300	1.95020700	0.00059000
H	0.89341100	-2.29895400	-0.00068300
H	0.43780200	-0.35604900	-0.00002100
C	-0.00000800	-0.52597400	-0.00004800

C	0.00020300	-1.36546400	1.29151100
H	-0.00013000	-0.70956200	2.16684500
H	-0.88403000	-2.00411800	1.34702500
H	0.88495700	-2.00340000	1.34714500
C	-0.00025800	-1.36602000	-1.29117500
H	-0.88470300	-2.00441600	-1.34624400
H	-0.00053700	-0.71056100	-2.16684300
H	0.88423800	-2.00431700	-1.34671300

TS-1

C	0.11644700	-1.17574300	-0.42310800
C	-0.61927100	1.00990500	-0.51358300
C	0.61929800	1.00995400	-0.51355300
C	-1.89501700	1.74747700	-0.46935700
H	-2.52869200	1.47495800	-1.32146200
H	-2.46184800	1.46757900	0.42962800
C	0.89496300	1.74767000	-0.46936100
H	0.52863800	1.47523000	-1.32149100
H	0.46186000	1.46783300	0.42960100
C	0.60710300	3.26049600	-0.46731000
H	0.56031300	3.80336000	-0.44059100
H	0.11940400	3.52942200	-1.41115800
C	0.75550000	3.69932300	0.70545900
C	-1.60732000	3.26033400	-0.46731300
H	-2.56058700	3.80309800	-0.44059600
H	-1.11964700	3.52930800	-1.41116000
C	-0.75576300	3.69925000	0.70545700
H	0.19757800	3.45028500	1.66958300
H	-1.19781800	3.45016900	1.66958100
C	-0.00019400	4.99898800	0.66361700
H	-0.00021800	5.53096700	-0.28498200
C	-1.11636800	-1.17577000	-0.42312400
H	-0.00022700	5.64281100	1.53665000
N	0.66217800	-1.40919100	-1.66357600
N	-0.66207600	-1.40920800	-1.66358700
C	0.56460800	-1.27359700	-0.16235800
C	0.45697500	-1.17839700	-1.24134100
C	0.08281400	-1.44203100	1.12718900
C	0.82710400	-1.24465200	-1.03162500
H	0.04711100	-1.06039500	-2.23931200
C	0.45913100	-1.51059800	1.33317000
H	0.41547100	-1.53158000	1.97806000
C	0.33483700	-1.40817300	0.25779700
H	0.50467800	-1.17102000	-1.87678500

H	0.84434500	-1.64649900	2.33905800
H	0.40698500	-1.45870600	0.42025900
C	-2.56452600	-1.27367000	-0.16238200
C	-3.45689200	-1.17873700	-1.24138700
C	-3.08271900	-1.44187300	1.12720200
C	-4.82701700	-1.24503800	-1.03165900
H	-3.04703100	-1.06089300	-2.23937700
C	-4.45903100	-1.51049200	1.33319200
H	-2.41536500	-1.53119100	1.97808900
C	-5.33474100	-1.40834100	0.25779500
H	-5.50459600	-1.17161600	-1.87683300
H	-4.84424100	-1.64621300	2.33910600
H	-6.40688600	-1.45891500	0.42026500
C	0.00003300	-1.42456600	0.57639600
C	0.00000200	-0.60103500	1.88022000
H	-0.87483800	0.04996800	1.94366600
H	-0.00015100	-1.25872500	2.75667400
H	0.87496600	0.04977600	1.94383200
C	0.00004000	-2.94746900	0.88434600
H	0.00014800	-3.53256900	-0.03822600
H	0.88783200	-3.21345000	1.46599000
H	-0.88786600	-3.21348300	1.46580200

2

C	-1.13455400	-0.66316000	0.00012000
C	0.13464600	-0.66317700	0.00031100
N	0.70276900	-1.87981100	0.00054900
N	-0.70271000	-1.87982500	0.00046100
C	0.58088700	-0.38224200	0.00012200
C	0.47767600	-1.46220700	-0.00085600
C	0.09485700	0.91893600	0.00087900
C	0.84647100	-1.24069400	-0.00103800
H	0.07264400	-2.46824600	-0.00144300
C	0.47038000	1.13810100	0.00068800
H	0.42788600	1.77351300	0.00166000
C	0.34953200	0.06120400	-0.00027200
H	0.52746400	-2.08611300	-0.00179300
H	0.85161500	2.15448400	0.00129200
H	0.42152500	0.23220200	-0.00043500
C	-2.58082300	-0.38217500	-0.00004000
C	-3.47767700	-1.46215700	0.00046600
C	-3.09493500	0.91898000	-0.00066200
C	-4.84647700	-1.24074800	0.00030300
H	-3.07254600	-2.46814800	0.00095300

C	-4.47044000	1.13805600	-0.00080700
H	-2.42805500	1.77362700	-0.00105600
C	-5.34956600	0.06112500	-0.00033200
H	-5.52745300	-2.08617500	0.00067600
H	-4.85179700	2.15439200	-0.00128800
H	-6.42155900	0.23215900	-0.00044200
C	0.00001900	0.32647800	0.00007700
C	0.00032200	1.44791400	-1.09401700
C	-0.00029800	1.44793500	1.09422300
C	0.00002700	2.54199000	-0.00004700
H	-0.88758800	1.42526500	1.73051900
H	0.88618200	1.42524200	1.73164200
H	0.87960500	3.19000400	0.00015200
H	-0.87957000	3.18999900	-0.00023700
H	0.88729800	1.42522900	-1.73078700
H	-0.88635500	1.42507400	-1.73118200

TS-2

C	0.11768400	-1.08717600	-0.59243700
C	-0.62003000	1.08964100	-0.54753200
C	0.61984000	1.08986600	-0.54743900
C	-1.89413900	1.82714100	-0.45645500
H	-2.52649400	1.61339500	-1.32609800
H	-2.46304700	1.48844900	0.42032300
C	0.89370800	1.82779500	-0.45646100
H	0.52597100	1.61437800	-1.32624900
H	0.46290200	1.48922000	0.42017400
C	0.60473300	3.33660800	-0.35300700
H	0.55791200	3.87673900	-0.29156200
H	0.11565000	3.66805000	-1.27603600
C	0.75490400	3.69549600	0.84764400
C	-1.60566100	3.33605300	-0.35313700
H	-2.55901100	3.87589500	-0.29182800
H	-1.11658700	3.66756700	-1.27614400
C	-0.75605400	3.69526400	0.84757400
H	0.19750000	3.38136300	1.79228300
H	-1.19863300	3.38100600	1.79218000
C	-0.00077900	4.99501100	0.89410300
H	-0.00082200	5.59045200	-0.01599900
C	-1.11731500	-1.08753500	-0.59248700
H	-0.00092000	5.57783300	1.80898000
N	0.66190800	-1.28370900	-1.83858800
N	-0.66141200	-1.28390200	-1.83861000
C	0.56966400	-1.19382500	-0.35039100

C	0.44789800	-1.03342400	-1.43346700
C	0.10693800	-1.43377000	0.91907100
C	0.82106000	-1.10383700	-1.24603600
H	0.02485100	-0.86067700	-2.41779700
C	0.48620500	-1.50572100	1.10347800
H	0.45370700	-1.57946200	1.77222900
C	0.34742300	-1.33706900	0.02499900
H	0.48640300	-0.97780000	-2.09472100
H	0.88473500	-1.69726100	2.09506800
H	0.42185900	-1.39032000	0.17045300
C	-2.56927700	-1.19433900	-0.35050900
C	-3.44749700	-1.03496800	-1.43374500
C	-3.10653200	-1.43329000	0.91914100
C	-4.82065100	-1.10548900	-1.24628200
H	-3.02445100	-0.86289600	-2.41819200
C	-4.48578600	-1.50534600	1.10358000
H	-2.45326800	-1.57802100	1.77243000
C	-5.34700400	-1.33777700	0.02493100
H	-5.48599900	-0.98027200	-2.09508500
H	-4.88430900	-1.69610300	2.09532400
H	-6.42143400	-1.39111100	0.17039700
C	0.00020600	-1.33802100	0.39115000
C	0.00048200	-2.77073900	1.04861000
C	0.00009200	-0.71096000	1.80238100
C	-0.00027400	-2.11868900	2.45140700
H	0.88971700	-3.35911500	0.81118400
H	-0.88793100	-3.36007200	0.81047400
H	0.88146400	-0.09727000	2.00627800
H	-0.88083500	-0.09658100	2.00614100
H	0.88045900	-2.34478200	3.05768400
H	-0.88189500	-2.34471600	3.05640800

3

C	0.14555200	-0.70154700	-0.20042700
C	-1.14536500	-0.70163900	-0.20045900
N	-0.71450700	-1.90763700	-0.30601900
N	0.71475900	-1.90757700	-0.30598500
C	-2.57547000	-0.37240200	-0.13420100
C	-3.49640100	-1.37288200	0.20472600
C	-3.03238300	0.92244800	-0.40611800
C	-4.85044900	-1.07727100	0.27897000
H	-3.12673400	-2.37298900	0.40621900
C	-4.39190400	1.21190400	-0.33019100
H	-2.32568200	1.68521600	-0.71555600

C	-5.30118000	0.21668100	0.01598400
H	-5.55856000	-1.85573700	0.54523800
H	-4.74138300	2.21589900	-0.54991600
H	-6.36064400	0.44580200	0.07698200
C	0.57563300	-0.37225400	-0.13416200
C	0.49681100	-1.37315900	0.20287100
C	0.03230300	0.92308800	-0.40410600
C	0.85083400	-1.07749000	0.27716300
H	0.12733400	-2.37362900	0.40289200
C	0.39180900	1.21261200	-0.32812100
H	0.32543500	1.68628800	-0.71208800
C	0.30132200	0.21695100	0.01613900
H	0.55912800	-1.85629600	0.54194400
H	0.74107500	2.21702200	-0.54628200
H	0.36077500	0.44611100	0.07718200
C	0.00005100	0.26481000	0.00889400
C	-0.00013300	0.97626300	1.39408600
C	-0.00089100	2.26247400	0.55775700
H	-0.89633300	2.88503700	0.64698300
H	0.89352300	2.88646300	0.64731800
H	-0.89710200	0.79994100	1.98869100
H	0.89735300	0.80090800	1.98820200
O	-0.00009700	1.51811800	-0.67832600

TS-3

C	0.12732300	-1.06268000	-0.62429300
C	-0.61704100	1.14605600	-0.35122100
C	0.61692000	1.14610100	-0.35123200
C	-1.90305500	1.86330100	-0.32123000
H	-2.55621800	1.52210800	-1.13290900
H	-2.43342200	1.65294200	0.61591600
C	0.90285100	1.86349900	-0.32124800
H	0.55605300	1.52237500	-1.13292600
H	0.43324900	1.65321600	0.61589600
C	0.61845000	3.37346100	-0.44785900
H	0.57332200	3.91417600	-0.45498200
H	0.14313700	3.56147400	-1.41733100
C	0.75562000	3.91395700	0.67357600
C	-1.61883300	3.37329900	-0.44783100
H	-2.57376600	3.91390500	-0.45493300
H	-1.14355700	3.56137700	-1.41730900
C	-0.75604100	3.91388100	0.67359100
H	0.19251600	3.75554100	1.65854600
H	-1.19290300	3.75541600	1.65856900

C	-0.00027800	5.20404000	0.50970600
H	-0.00031100	5.64333600	-0.48525300
C	-1.12725400	-1.06281300	-0.62427100
H	-0.00030500	5.92814100	1.31749700
N	0.67376000	-1.14725100	-1.86842700
N	-0.67370400	-1.14731900	-1.86841100
C	0.56280000	-1.19300300	-0.32597700
C	0.47421300	-1.43146400	-1.36286000
C	0.03431600	-1.06455600	0.98680100
C	0.83090400	-1.54715900	-1.08681700
H	0.09538200	-1.52573000	-2.37521300
C	0.39435000	-1.18595300	1.25697000
H	0.33120800	-0.83817600	1.78304500
C	0.29491900	-1.42871800	0.22306400
H	0.53052200	-1.73462200	-1.89564800
H	0.75184900	-1.08313900	2.27704300
H	0.35555500	-1.52181100	0.43542200
C	-2.56271500	-1.19322000	-0.32593800
C	-3.47415800	-1.43144200	-1.36285300
C	-3.03419200	-1.06510500	0.98688300
C	-4.83083900	-1.54721100	-1.08679800
H	-3.09535500	-1.52546100	-2.37524000
C	-4.39421800	-1.18657300	1.25706300
H	-2.33106400	-0.83894400	1.78316800
C	-5.29481700	-1.42908600	0.22312500
H	-5.53047900	-1.73448200	-1.89565500
H	-4.75168600	-1.08401900	2.27717400
H	-6.35544700	-1.52223300	0.43549100
C	0.00006300	-1.41040500	0.31664500
C	0.00019100	-2.89387500	0.80018800
C	0.00039700	-2.27120500	2.19857200
H	0.89708200	-3.45350200	0.53274800
H	-0.89678400	-3.45351700	0.53305400
H	0.89596400	-2.45595000	2.80010500
H	-0.89482000	-2.45621100	2.80054100
O	0.00007900	-0.93162500	1.65956400

4

C	0.15860600	0.63751400	-0.00003400
C	-1.15855600	0.63772900	-0.00004500
N	-0.72150400	1.84140300	-0.00008500
N	0.72183800	1.84127800	-0.00008100
C	-2.56695800	0.25170000	-0.00001400
C	-3.56142800	1.23885300	0.00005800

C	-2.92500200	-1.10078100	-0.00005400
C	-4.89856200	0.87144000	0.00008900
H	-3.26250000	2.28206000	0.00008900
C	-4.26857100	-1.46113800	-0.00002200
H	-2.15693100	-1.86720100	-0.00011100
C	-5.25434200	-0.47858500	0.00004900
H	-5.66858900	1.63625300	0.00014600
H	-4.54466700	-2.51060000	-0.00005300
H	-6.30221500	-0.76230600	0.00007500
C	0.56701900	0.25145100	-0.00000600
C	0.56137000	1.23873400	0.00001700
C	0.92529000	-1.10098000	0.00000000
C	0.89854700	0.87152300	0.00004400
H	0.26227300	2.28189700	0.00001200
C	0.26892300	-1.46114200	0.00002800
H	0.15740600	-1.86757500	-0.00001700
C	0.25454000	-0.47846400	0.00005000
H	0.66843200	1.63647200	0.00006300
H	0.54516400	-2.51056900	0.00003300
H	0.30244000	-0.76207900	0.00007300
C	-0.00015500	-0.34782500	-0.00001300
F	-0.00042400	-1.15305200	1.08847700
F	-0.00040700	-1.15309200	-1.08847900

4-TS

C	-1.14139900	-1.08537300	0.57024000
C	-0.61619500	1.05322200	-0.11487200
C	0.61616100	1.05322600	-0.11489800
C	-1.90800200	1.74526900	-0.24553900
H	-2.55060500	1.24966400	-0.98207300
H	-2.44398600	1.71090100	0.71186200
C	0.90797100	1.74524500	-0.24569900
H	0.55048200	1.24961700	-0.98229800
H	0.44405700	1.71087200	0.71164400
C	0.62408700	3.20271500	-0.66318600
H	0.57897500	3.73213100	-0.77118100
H	0.15195000	3.19896600	-1.65237800
C	0.75643500	3.94873900	0.32984600
C	-1.62413200	3.20273700	-0.66304200
H	-2.57902200	3.73216800	-0.77095000
H	-1.15208400	3.19898700	-1.65227600
C	-0.75638100	3.94874600	0.32991500
H	0.19089800	3.98481500	1.32771900
H	-1.19075300	3.98482600	1.32782700

C	0.00001500	5.18133000	-0.08300500
H	-0.00003300	5.41721500	-1.14480100
C	0.14139900	-1.08537300	0.57024800
H	0.00004900	6.04964500	0.56710900
N	0.67872100	-0.92282000	1.79477000
N	-0.67872900	-0.92282000	1.79476600
C	0.56528000	-1.26839200	0.27819100
C	0.51700500	-1.02491600	1.27710600
C	0.98475700	-1.65588200	-0.99929100
C	0.86886300	-1.17075600	0.99798300
H	0.17253500	-0.72959200	2.26311400
C	0.34177800	-1.80443100	-1.27024500
H	0.25031700	-1.83945300	-1.77669900
C	0.28485000	-1.56045900	-0.27572500
H	0.60297300	-0.98382100	1.77551100
H	0.66184400	-2.11060800	-2.26120600
H	0.34286200	-1.67440700	-0.49051100
C	-2.56527700	-1.26839800	0.27817200
C	-3.51700800	-1.02494500	1.27708700
C	-2.98474400	-1.65586300	-0.99931900
C	-4.86886300	-1.17078600	0.99795500
H	-3.17254400	-0.72964100	2.26310300
C	-4.34176300	-1.80441100	-1.27028400
H	-2.25030100	-1.83941300	-1.77672800
C	-5.28484300	-1.56046400	-0.27576400
H	-5.60297900	-0.98387000	1.77548200
H	-4.66182300	-2.11056900	-2.26125300
H	-6.34285300	-1.67441200	-0.49055800
C	0.00000400	-1.58933300	-0.30254200
F	0.00001000	-1.24066500	-1.60919400
F	0.00000300	-2.95191400	-0.29494000

BCN

C	0.60408300	-1.76198300	-0.15220900
C	-0.60397900	-1.76201700	-0.15218100
C	0.92945700	-1.14829000	-0.03269300
C	0.66197100	0.29014800	0.47908100
H	0.61591000	0.82183300	0.58942500
H	0.21808800	0.21985700	1.47875700
C	0.75797000	1.09575200	-0.43641000
C	-0.75803100	1.09571000	-0.43641500
C	-1.92939000	-1.14840000	-0.03269200
H	-2.58250200	-1.68558700	0.66264700
H	-2.44110900	-1.12041900	-1.00196500

H	0.44119600	-1.12027300	-1.00195500
H	0.58258400	-1.68544700	0.66265400
C	-1.66199200	0.29005800	0.47907400
H	-2.61596400	0.82168800	0.58940600
H	-1.21811400	0.21980200	1.47875500
H	0.17932400	1.21762200	-1.43367600
H	-1.17938700	1.21755300	-1.43368400
C	-0.00006600	2.29026200	0.07621800
H	-0.00008900	3.21234500	-0.49551900
H	-0.00007500	2.43359800	1.15450700