# Can the ene reaction of nitroso compounds go concertedly? 

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S1 Cartesian coordinates, electronic energies and number of imaginary frequencies for each structure

MeNO
$E($ RB + HF-LYP $)=-169.7905493$ Hartree; NIMAG $=0$
$\mathrm{N}, 0,0.0197617768,-0.5742886423,-0.0003852223$
O,0,1.168225373,-0.1910700162,0.0004682682
C,0,-0.96776809,0.5382320718,-0.0001028971
H,0,-1.6015769964,0.4035926817,-0.884661041
H,0,-0.4725966524,1.5138674043,0.0013513391
Н,0,-1.6033532327,0.4017281085,0.8828774946

OIT
$E($ RB + HF-LYP $)=-271.5049298$ Hartree; NIMAG $=0$

C, $0,-0.0065938845,-0.1427396007,-2.371130234$
C, $0,0.0056341352,0.0116982134,-1.0340155731$
C, $0,1.2621266111,0.0538616485,-0.2896142677$
C, $0,1.295642329,0.0125253443,1.0606530235$
C,0,0.0681863993,-0.0804437724,1.8477500083
C, $0,-1.1355036626,-0.0343862244,1.2548051028$
$\mathrm{H}, 0,0.9169782357,-0.2056408187,-2.9407121633$
Н,0,-0.933332693,-0.2071191596,-2.9355820651
H,0,2.1852614231,0.0759659446,-0.864709946
H,0,2.248917304,0.0175254012,1.5830671085
Н,0,0.1500750129,-0.1918878393,2.9261183095
H,0,-2.0487846993,-0.0975571095,1.8423141951
C,0,-1.2854889758,0.1674635302,-0.2328492213
H,0,-1.6839625048,1.1841676132,-0.3943465209
H,0,-2.0591697885,-0.5033288654,-0.6297419481

TS1
E (RB+HF-LYP $)=-441.2929546$ hartree; NIMAG=1
$\mathrm{C}, 0,1.0806052078,1.0471863881,-1.1241700069$
$\mathrm{C}, 0,-0.1444726729,0.5410627889,-0.723916872$
$\mathrm{C}, 0,-1.0466276199,1.2914313926,0.1016751514$
$\mathrm{C}, 0,-2.2124914923,0.7498202054,0.5616022219$
$\mathrm{C}, 0,-2.5947101426,-0.6024833041,0.2239308984$
$\mathrm{C}, 0,-1.7759697544,-1.3827414307,-0.5159753155$
$\mathrm{C}, 0,-0.4289763239,-0.9140218379,-0.9445167901$
$\mathrm{H}, 0,1.3318780981,2.0867638179,-0.9317885714$
$\mathrm{H}, 0,1.6446339292,0.5647904441,-1.9144544479$
$\mathrm{H}, 0,-0.7976738959,2.3258002431,0.3293953606$
$\mathrm{H}, 0,-2.8898974135,1.3524410113,1.1609806969$
$\mathrm{H}, 0,-3.5590785128,-0.9741920477,0.560266973$
$\mathrm{H}, 0,-2.0655553686,-2.3966886333,-0.7808890319$
$\mathrm{H}, 0,0.3677644594,-1.452771019,-0.3331293894$
$\mathrm{H}, 0,-0.1861620954,-1.2371010147,-1.9655051415$
$\mathrm{~N}, 0,2.2443512937,0.059794476,0.2716225724$
$\mathrm{O}, 0,2.1535588683,-1.1698950648,0.0847704209$
$\mathrm{C}, 0,1.7982849616,0.4476710833,1.644544979$
$\mathrm{H}, 0,0.8659123815,-0.0486972148,1.9350524036$
$\mathrm{H}, 0,2.5974156167,0.1188563055,2.3180368447$
$\mathrm{H}, 0,1.6979798186,1.5338455803,1.7034673315$

Pro 1
$E($ RB + HF-LYP $)=-441.3723011$ Hartree; NIMAG $=0$

C,0,0.0475373894,0.5837922455,-1.5579400577
C, $, 0.0 .0537827094,0.6573650084,-0.0404667844$
C,0,1.2552892195,0.6756904732,0.6829389377
C,0,1.2524624688,0.6963884795,2.0783546817
C, $0,0.0423615869,0.6942660113,2.7762182845$
C,0,-1.1620554915,0.6775850554,2.070705689
C,0,-1.1553404795,0.661246028,0.6739503496
H, $0,-0.7886299612,1.1641813045,-1.9605352424$
H,0,0.9740380467,1.005908698,-1.9643363193
H,0,-2.0950992107,0.670124668,0.1268955794
$\mathrm{H}, 0,2.2017633156,0.6844924409,0.1464590435$
H,0,-2.1077427511,0.6860137804,2.6063837797
$\mathrm{H}, 0,2.1940010245,0.7187594605,2.6209125279$
H,0,0.0388530953,0.7132024971,3.8627256455
$\mathrm{N}, 0,-0.0804130425,-0.7672037342,-2.1370745887$
C, $, 1.1 .0027449181,-1.6855118689,-1.8130853127$

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H,0,0.8137913568,-2.6294587169,-2.3302891634
H,0,1.9453018026,-1.2642606642,-2.1799069536
H,0,1.1065556101,-1.8872598551,-0.7316934023
O,0,-1.3114351483,-1.3499014712,-1.7151044812
H,0,-1.2491537711,-1.456994299,-0.7403122507
TS2
E(RB+HF-LYP)= -441.2826089 Hartree; NIMAG=1
C,0,-0.50376728,-0.8683843108,-0.6487499551
C,0,-1.868641852,-1.3672528361,-0.3720823071
C,0,-2.8047619821,-0.5689632295,0.201720639
C,0,-2.5110103303,0.8067897765,0.490696282
C,0,-1.3011828629,1.3582797258,0.1501052694
C,0,-0.3019251166,0.5970840637,-0.5163460328
C,0,0.9777320775,1.1065786542,-0.7707507018
N,0,2.1079397534,0.2262352095,0.5673303597
O,0,1.4951887244,-0.7104256671,1.1583981459
C,0,3.2943040437,-0.2953866558,-0.1724464912
H,0,-3.7924895741,-0.9573942364,0.4361239107
H,0,-2.0917131241,-2.4063443277,-0.6005397888
H,0,-3.2720946373,1.4216063022,0.9635994491
H,0,-1.1037181656,2.408432005,0.3525533769
H,0,1.5390011058,0.6907414077,-1.6029917496
H,0,1.1725362552,2.1572049846,-0.5760191618
H,0,-0.0728778971,-1.2919578943,-1.5653812342
H,0,0.2287555245,-1.2654231102,0.1655091791
H,0,3.7323687849,0.5058787122,-0.7745706728
H,0,4.0155278199,-0.6133951497,0.5874806533
H,0,3.0431356555,-1.162060951,-0.797141861
Pro2
\(\mathrm{E}(\mathrm{RB}+\) HF-LYP \()=-441.3709052\) Hartree; NIMAG=0
C,0,0.1302204937,-0.7593643598,-1.667328646
C, \(0,0.0755864743,-0.4479475617,-0.3048509177\)
C, \(0,1.2721790094,-0.2296133014,0.3890278637\)
C,0,2.49745454,-0.3243874198,-0.2700809748
С, \(0,2.5449427465,-0.644088976,-1.6297413404\)
C,0,1.3567081536,-0.8618334932,-2.3278664907
C,0,-1.2593395933,-0.4057140858,0.4118882231
\(\mathrm{N}, 0,-1.3233602905,0.6114432787,1.4564267667\)
C,0,-2.5654651886,0.5673138094,2.2132693186
O,0,-1.2072753111,1.9004280631,0.8609997418
\(\mathrm{H}, 0,1.2291228767,0.032236596,1.4415177717\)
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H, $0,1.3812457276,-1.1038963698,-3.3872770538$
H,0,3.5010619161,-0.7170800784,-2.1413878189
Н,0,3.4188098139,-0.145744114,0.2784651805
Н,0,-1.9509113995,1.9799575086,0.2216841441
H,0,-0.7940693915,-0.9225864868,-2.2184169709
H,0,-2.0774708023,-0.2696997925,-0.3264218012
Н,0,-1.4485666244,-1.368215259,0.9075562237
H,0,-2.5552617774,1.375484965,2.9478279002
H,0,-2.6350219498,-0.3915045486,2.7374048091
Н, $0,-3.4609336821,0.6813324534,1.5701600989$

