

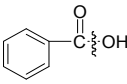
Supporting Information

Computational study on alkenyl/aryl C(sp²)-O homolytic cleavage of carboxylates and carbamates

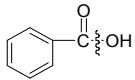
Wenrui Zheng*, Lanlan Ding, Jiaoyang Wang and Yingxing Wang


College of Chemistry and Chemical Engineering, Shanghai University of Engineering Science, Shanghai 201620, China

Table 1. The 19 C-O calculated BDEs using 14 DFTs (kJ/mol)

entry	compounds	B3LYP	X3LYP	M06	M06-2X	M06-L	t-HTCH
1	$\text{H}_3\text{C}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	345.7	350.7	382.9	407.9	344.2	335.3
2	$\text{HC}(\text{O})-\text{OH}$	436.8	439.1	469.3	464.2	451.9	457.7
3	$\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	432.3	435.1	469.3	464.6	449.7	449.2
4	$\text{C}_2\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	417.5	421.0	441.4	452.1	419.5	423.5
5	$\text{C}_2\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	433.5	436.5	473.5	467.5	453.8	449.7
6	$\text{HO}-\text{CH}(\text{O})\text{OH}$	332.2	334.7	361.5	364.6	341.9	344.1
7	$\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_3$	328.0	333.0	367.5	392.5	328.2	317.1
8	$\text{HC}(\text{O})-\text{OCH}_3$	384.6	387.7	420.6	423.8	400.7	395.3
9	$\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}-\text{OCH}_3$	377.8	381.4	418.5	422.2	396.3	384.4
10	$\text{C}_2\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{OCH}_3$	361.4	365.7	388.7	413.4	364.5	356.7
11	$\text{C}_2\text{H}_5-\text{OC}(\text{O})\text{CH}_3$	328.6	384.8	369.0	382.8	326.9	311.6
12	$i\text{C}_3\text{H}_7-\text{OC}(\text{O})\text{CH}_3$	324.8	293.6	368.9	399.3	324.0	323.1
13		430.6	433.8	470.3	446.1	450.1	445.7
14	$\text{H}_3\text{C}-\text{OC}(\text{O})\text{C}_6\text{H}_5$	327.8	333.0	367.3	393.2	328.8	317.0
15	$\text{HC}(\text{O})-\text{OC}_6\text{H}_5$	280.6	284.5	312.5	329.4	298.0	287.0
16	$\text{C}_4\text{H}_9-\text{OC}(\text{O})\text{CH}_3$	329.3	335.4	372.2	398.6	321.7	312.2
17	$\text{H}_3\text{C}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OC}_6\text{H}_5$	279.6	284.2	317.0	335.6	300.5	280.4
18	$\text{C}_6\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{OCH}_3$	375.8	379.9	419.4	423.8	396.7	380.6
19	$\text{C}_6\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{OC}_6\text{H}_5$	280.5	285.4	320.0	339.6	303.5	279.6

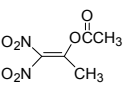
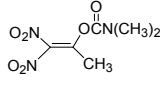
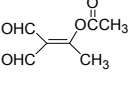
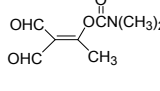
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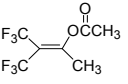
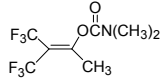
entry	compounds	wB97	wB97X	wB97X-D	MPWKCIS1K
1	$\text{H}_3\text{C}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	392.0	385.8	376.1	373.7
2	$\text{HC}(\text{O})-\text{OH}$	457.9	457.6	455.9	446.0
3	$\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	457.7	456.5	454.4	443.4
4	$\text{C}_2\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	445.8	444.3	440.0	422.9
5	$\text{C}_2\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	460.8	459.1	456.9	445.2
6	$\text{HO}-\text{CH}_2-\text{CH}(\text{O})\text{OH}$	357.4	354.7	353.1	336.4
7	$\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{CH}_3$	376.4	369.6	359.9	355.9
8	$\text{HC}(\text{O})-\text{O}-\text{CH}_3$	412.5	410.3	407.3	396.9
9	$\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{CH}_3$	410.3	407.0	404.0	392.1
10	$\text{C}_2\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{CH}_3$	396.7	393.2	388.1	370.3
11	$\text{C}_2\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{C}(\text{O})\text{CH}_3$	379.8	372.0	360.0	357.8
12	$i\text{C}_3\text{H}_7-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{C}(\text{O})\text{CH}_3$	381.0	372.0	363.8	370.3
13		459.2	457.3	454.7	442.6
14	$\text{H}_3\text{C}-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{C}_6\text{H}_5$	377.7	370.8	375.0	356.4
15	$\text{HC}(\text{O})-\text{O}-\text{C}_6\text{H}_5$	305.9	306.7	307.0	302.0
16	$\text{C}_4\text{H}_9-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{C}(\text{O})\text{CH}_3$	382.4	374.4	423.2	359.9
17	$\text{H}_3\text{C}-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{C}_6\text{H}_5$	310.9	310.6	310.5	302.7
18	$\text{C}_6\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{CH}_3$	412.0	408.1	392.6	391.3
19	$\text{C}_6\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{C}_6\text{H}_5$	314.7	313.7	314.1	304.5

entry	compounds	MPWB1K	MPW1KCIS	MPW1K	B98	(wB97)
1	$\text{H}_3\text{C}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	392.1	349.1	440.6	360.6	384.3
2	$\text{HC}(\text{O})-\text{OH}$	456.3	455.3	441.6	450.5	458.0
3	$\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	454.4	450.0	439.4	445.8	457.6
4	$\text{C}_2\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	439.2	427.3	420.7	431.4	445.4
5	$\text{C}_2\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	457.0	451.1	441.5	447.2	460.5
6	$\text{HO}-\text{CH}_2-\text{CH}(\text{O})\text{OH}$	353.0	315.3	330.4	347.1	356.6
7	$\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{CH}_3$	375.3	331.0	357.4	343.3	372.0
8	$\text{HC}(\text{O})-\text{O}-\text{CH}_3$	409.1	423.8	395.8	397.2	413.9
9	$\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{CH}_3$	405.4	389.5	391.6	390.4	411.5
10	$\text{C}_2\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{CH}_3$	389.2	365.2	371.3	374.4	397.7
11	$\text{C}_2\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{C}(\text{O})\text{CH}_3$	377.4	330.0	360.3	342.9	373.0
12	$i\text{C}_3\text{H}_7-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{C}(\text{O})\text{CH}_3$	376.0	324.7	358.3	338.8	373.0
13		456.0	448.0	439.2	444.6	454.6
14	$\text{H}_3\text{C}-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{C}_6\text{H}_5$	376.7	331.5	357.9	343.4	373.8
15	$\text{HC}(\text{O})-\text{O}-\text{C}_6\text{H}_5$	314.5	294.9	301.1	293.0	304.9
16	$\text{C}_4\text{H}_9-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{C}(\text{O})\text{CH}_3$	379.5	331.4	362.4	344.0	346.6
17	$\text{H}_3\text{C}-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{C}_6\text{H}_5$	317.4	290.2	362.8	291.7	309.7
18	$\text{C}_6\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{CH}_3$	407.1	384.7	391.4	389.1	435.2
19	$\text{C}_6\text{H}_5-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{C}_6\text{H}_5$	321.9	292.7	305.2	293.0	333.0

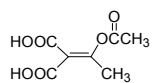
Note: The values of (wB97) are calculated at wB97/6-311++G(2df,2p)//wB97/6-31+G(d) level.

Table 2. The Cartesian coordinates of optimized geometries

 <p>SCF energy=-754.9123076</p>	 <p>SCF energy=-849.6078855</p>
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C -0.84924000 0.03403700 -0.11678000	C 1.50176400 0.00920600 -0.03679200
O 1.35448600 0.05434000 -0.77252900	O -0.74031000 0.05322300 -0.35984900
C 2.54461500 -0.04067300 -0.00632200	C -1.91231700 0.56582700 0.23406700
O 3.53106600 -0.39190900 -0.58068200	O -1.88458800 1.52853800 0.97338100
C 2.39833000 0.24027700 1.46462100	C 0.39465700 2.23267500 -0.63482200
H 3.36853700 0.09960300 1.94235900	N 1.33297400 -1.43898300 0.22694600
H 2.05195700 1.26377200 1.64502400	O 1.18693800 -1.77326300 1.39643900
H 1.66512500 -0.44817400 1.89869100	O 1.33136000 -2.18084700 -0.74922100
C 0.36984600 2.25877600 -0.42694700	N 2.87440400 0.43744000 -0.00017900
H -0.11271300 2.73581200 0.42877000	O 3.10834300 1.64208300 -0.13622500
H 1.42445100 2.54082900 -0.47897900	O 3.72254800 -0.43770700 0.17548300
H -0.13186300 2.63951200 -1.32434500	N -2.98501800 -0.17100800 -0.12655100
N -0.80050400 -1.44317800 -0.13999000	C -2.94282600 -1.36090000 -0.97650100
O -1.39353600 -1.99350200 -1.05618600	H -3.11016600 -2.26356600 -0.37516100
O -0.15999800 -1.99302300 0.75261800	H -3.73610300 -1.28886900 -1.72892100
N -2.15554100 0.56457800 0.20646700	H -1.98219300 -1.44352900 -1.47939500
O -2.34322800 1.76922500 0.01493300	C -4.27300700 0.13261500 0.49397300
O -2.97597800 -0.22279100 0.67143000	H -5.02788300 0.29338600 -0.28420000
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C -1.00166600 0.12308600 -0.17473000	H -0.55016000 2.48454400 -1.11914700
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C 2.16738000 -0.25215800 0.02530000	H 0.48435900 2.83476200 0.27511100
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	C 1.67092500 -0.17119100 -0.09593600

H	2.72401200	-0.87548300	1.96994300	O	-0.37961900	1.05128200	-0.29496400
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H	0.39728000	2.95051900	-0.95871600	H	3.58273000	0.80231900	0.43318100
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O	-3.36382300	-0.05796700	0.16242900	O	-0.09782600	-1.71255400	-0.64695000
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O	-1.40516600	-2.23775200	-0.06784900	C	-2.65170400	0.19940600	-1.45577100
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H	2.02569100	-0.07834100	1.98331300		SCF energy=-1114.7813743		
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C	-1.93788200	0.68390400	0.09175000	C	-0.08602800	0.86442300	-0.38020600
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H	1.72145300	2.57673400	-0.65820600	O	2.09132900	1.50438800	1.08962100
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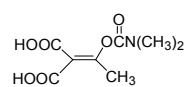
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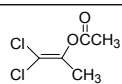
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 H -0.26207400 2.97682400 0.49450800
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 O 2.55658200 -1.65770600 -0.05648100
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C 3.39852900 -1.10585800 -1.08303400
 H 4.22432600 -0.92245200 -1.78051800
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 H 2.46847000 -1.17862600 -1.64195300
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 H 4.82592500 -0.62834000 1.24438500
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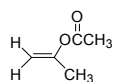
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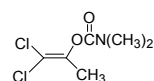
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 O 3.26938900 -0.32299200 -0.44231200
 C 1.92227400 0.01299500 1.52884800
 H 2.85936100 -0.15011600 2.06257500
 H 1.48061800 0.96417700 1.84256000
 H 1.21655300 -0.78332300 1.78880800
 C -0.18951900 2.26862100 -0.35152800
 H -1.18782400 2.58948000 -0.05297100
 H 0.54293800 2.71398400 0.33383700
 H 0.02587300 2.66042300 -1.35344900
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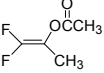
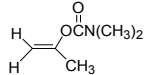
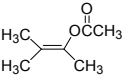
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 C -1.27913000 -0.11220300 -0.08184200
 O -2.29450000 -0.59163400 -0.52291100
 C -1.23861200 0.89231600 1.05038200
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 H -0.50415100 0.61990900 1.81470300
 H -0.96318700 1.88303400 0.67442700
 C 1.88000500 -0.97286900 0.67833700
 H 2.87369300 -0.59853500 0.93996300

O -0.75344500 1.89402800 1.30747500
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 C -2.89799300 -0.36033800 0.09070600
 O -3.76561600 0.43105300 0.41302700
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 H 2.12622600 1.26403600 -1.66275200
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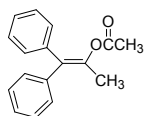
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C 1.54511300	-0.44222000	1.39358300	H 0.27756600	-2.70462300	0.01049600
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O 0.75375500	0.20864700	-0.81869300	H -2.72894400	1.51098400	1.23088200
C 1.82330100	-0.11256200	-0.02640000	H -1.06398900	1.98985300	0.82734700
O 2.87735100	-0.36702700	-0.55946700	C -2.80682400	-0.72974800	-0.22613900
C 1.60549900	-0.15864300	1.47241300	H -3.50492800	-0.74978400	0.61954400
H 2.57447600	-0.30373900	1.95192200	H -3.33745800	-0.34136500	-1.10732900
			H -2.46009500	-1.74103300	-0.43564400

H 1.13991600	0.75760700	1.84804100	H 1.88589500	-1.71023800	0.91277300
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C -1.18140800	-1.82223000	-0.35408200	H 2.13250900	-0.36076500	2.03751700
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H -3.57626700	-0.32428700	-0.36288300	N -2.24466600	-0.10548600	0.09578400
C -0.60975200	2.07790000	-0.17307500	C -2.47970200	-1.10074200	1.13624600
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C -1.38931800	-0.42211800	-0.09196100	H -4.21135400	0.58922700	-0.13938100
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C 1.78620700	-0.08374800	-0.00989800	C 1.57691900	1.74376400	0.88445400
O 2.83962700	-0.37642200	-0.52551100	H 0.98973400	2.48744500	0.33457300
C 1.53842000	-0.09562900	1.48286300	H 1.33479200	1.83182800	1.95131700
H 2.48575500	-0.30394000	1.98230500	H 2.63786300	1.96961300	0.75007500
H 1.13833400	0.86068300	1.83451100	F 1.84047000	-1.70479700	-0.57542100
H 0.81043700	-0.87411300	1.73514500	F 3.42392200	-0.21027500	-0.31798200
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H -0.23833300	2.55075500	0.62035400	C -1.24649700	-0.41607800	0.37089900
H -0.46071200	2.56651700	-1.13231400	O 0.06282300	0.08696100	0.57187900
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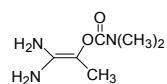
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N	-1.02313200	-1.74929500	-0.34033100
H	-1.75852500	-2.43258900	-0.21577100
H	-0.45803500	-1.90043400	-1.16758900



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C	-0.33366700	-1.49054400	-0.60519400
C	0.21447400	-0.28849900	-0.31540700
O	-1.72117700	-1.62423800	-0.76949600
C	-2.59940200	-1.76551800	0.27869900
O	-3.77454300	-1.86523200	0.02345600
C	-2.02823700	-1.78372500	1.67905300
H	-1.18009400	-2.47049000	1.76487200
H	-1.67643900	-0.78407100	1.95536100
H	-2.82127000	-2.08669700	2.36421400
C	0.36820600	-2.77156200	-0.94892900
H	0.16916700	-3.55232000	-0.20142800
H	-0.02177800	-3.14440200	-1.90468300
H	1.44778600	-2.64105100	-1.03434300
C	1.69513400	-0.15814500	-0.13748200
C	2.41909300	0.76099000	-0.91753700
C	2.39229900	-0.91210600	0.82046200
C	3.79853600	0.90219700	-0.76151500
H	1.89341500	1.36414400	-1.65329700
C	3.77325800	-0.76772100	0.98297400
H	1.84648000	-1.61017900	1.45049100
C	4.48197000	0.13783700	0.19009500
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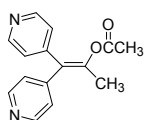
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C	2.51627600	0.97463800	1.24005000
H	3.36910700	0.58688600	1.81138600
H	2.75506300	1.99982000	0.92072500
H	1.64005600	0.99963200	1.88459800
C	3.41402700	-0.13615500	-0.78070600
H	3.78392800	0.80268600	-1.21734900
H	4.22857000	-0.59579000	-0.20660500
H	3.11082900	-0.80856600	-1.58243500
C	-1.37458400	-1.84652000	0.80401400
H	-0.74563000	-2.48956500	0.17750700
H	-1.03814600	-1.95855000	1.84352300
H	-2.40158000	-2.20985500	0.73909500
C	-3.63767100	0.04826700	-0.23227900
H	-3.85677800	-0.98154500	0.05638800
H	-4.27751600	0.70904700	0.36985000
H	-3.95187700	0.17550100	-1.27772800
C	-1.87601400	1.85608200	-0.46737200
H	-2.49065000	2.55926600	0.11261600
H	-0.82666900	2.11509200	-0.31693800
H	-2.12272500	2.02124300	-1.52565900



SCF energy=-551.2594314

C	1.18537000	0.45792000	0.43217900
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O	0.02478800	0.32500200	1.23409100
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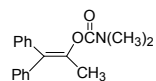
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C	-0.25246600	1.87273900	0.87098200
C	-2.36455000	2.47874200	-0.84131300
H	-1.92444200	0.61091700	-1.80987100
C	-0.97125300	3.05689700	1.04311000
H	0.57950900	1.65030400	1.53379700
C	-2.03150500	3.36557100	0.18661800
H	-3.18250400	2.71104100	-1.51855500
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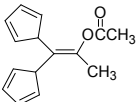
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C	-2.63740400	-1.72424000	0.26643100
O	-3.80653700	-1.79616100	-0.01371600
C	-2.08769100	-1.76247600	1.67397800
H	-1.25730400	-2.46941600	1.76881600
H	-1.71875900	-0.77260600	1.96305700
H	-2.89721300	-2.05094500	2.34579400
C	0.33302800	-2.78297900	-0.91530300
H	0.10061200	-3.55478000	-0.16887900
H	-0.04660200	-3.15108900	-1.87672400
H	1.41645100	-2.67699600	-0.98059100
C	-0.56630500	0.96902700	-0.14646200
C	-1.64657300	1.31336500	-0.97615300
C	-0.21155600	1.89965100	0.84572700

C	1.89731100	1.75187200	0.67767900
N	2.71937400	-0.54991200	-1.17889900
H	3.05186300	0.39099400	-1.35421000
H	3.50012300	-1.14821600	-0.91233000
N	1.01288000	-1.85244500	-0.24735000
H	1.41221100	-2.56823700	-0.83696000
H	0.59376700	-2.17127700	0.61771100
N	-1.70938800	0.35384800	-0.32735300
C	-1.29872200	1.63825100	-0.87433700
H	-0.66114100	1.51967700	-1.76081200
H	-2.19644100	2.19832700	-1.16217800
H	-0.76398200	2.21806500	-0.12305600
C	-2.84499900	-0.29065500	-0.97535500
H	-3.76647700	0.28387000	-0.80835700
H	-2.66468900	-0.35881700	-2.05573400
H	-2.97168200	-1.29070000	-0.56279700
H	2.94772300	1.69972300	0.37140100
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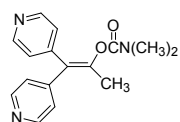
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O	-1.54129800	-0.81522100	-0.73752000
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O	-1.93511400	-1.81180000	1.28027700
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C	-4.11534300	-0.13724700	-1.08887100
H	-5.07466300	-0.53238500	-1.44285900
H	-4.25696300	0.91514900	-0.80306300

C	-2.30210200	2.52877600	-0.77224800	H	-3.39195000	-0.18846800	-1.90050900
H	-1.97437000	0.65137300	-1.76965900	C	-4.64175700	-1.18002200	1.09606500
C	-0.93888000	3.08406600	0.96918800	H	-4.96371700	-0.23519200	1.55727000
H	0.62252000	1.70843800	1.51473500	H	-5.52208600	-1.67998000	0.67459200
N	-1.97122900	3.41119200	0.18085000	H	-4.19430700	-1.81465600	1.86019700
H	-3.13762000	2.80731000	-1.41154300	C	0.10362000	-2.57016500	-1.01591500
H	-0.67614000	3.80786200	1.73865500	H	-0.27746200	-3.26169100	-0.25489300
C	1.69464900	-0.17967100	-0.13023000	H	-0.41234900	-2.79890800	-1.95794400
C	2.43960000	0.72373400	-0.90419600	H	1.17129800	-2.75065100	-1.15185600
C	2.40056100	-0.93086300	0.82004600	C	0.27384600	1.23772400	-0.06643100
C	3.81850100	0.81344400	-0.71187200	C	-0.48100100	1.95282400	-1.01178800
H	1.95294500	1.34544800	-1.65043000	C	0.66979000	1.89998900	1.10853400
C	3.78261900	-0.76203900	0.93859500	C	-0.83795700	3.28394100	-0.78449200
H	1.88298800	-1.63134200	1.46976500	H	-0.78084600	1.46184000	-1.93290500
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H	4.41043000	1.50156900	-1.31237300	H	1.26354500	1.36587900	1.84560900
H	4.34206200	-1.33707100	1.67450300	C	-0.45082400	3.92555900	0.39559200
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SCF energy= -731.6858103				H	0.61224900	3.71561500	2.26333200
C	-0.45776800	-1.23208400	-0.50155700	H	-0.72905900	4.96151400	0.57262900
C	0.56318900	-0.40445200	-0.22754900	C	2.15462900	-0.46958500	-0.14007600
O	-1.73432900	-0.65159500	-0.66023100	C	3.11526600	0.29291400	-0.82800200
C	-2.67831900	-0.86663100	0.30190800	C	2.60186900	-1.47438500	0.73437700
C	-0.46606400	-2.70763700	-0.77466800	C	4.47829000	0.03803800	-0.67062700
H	0.53364600	-3.14555700	-0.76855600	H	2.78732500	1.08874700	-1.49199600
H	-1.07163200	-3.22863900	-0.02437400	C	3.96689700	-1.72685400	0.89723100
H	-0.91418500	-2.89973400	-1.75844200	H	1.87238100	-2.04840700	1.29963700
C	0.36560300	1.09468900	-0.00591700	C	4.90997300	-0.97491800	0.19213700
H	1.36495000	1.50254700	0.22920700	H	5.20441200	0.63259300	-1.21972800
C	-0.14649300	1.92318700	-1.16746700	H	4.29150400	-2.50659800	1.58202700

C	-0.52954600	1.54205200	1.13214500
H	0.25277000	1.84707200	-2.17278700
C	-1.09471200	2.77813800	-0.72606900
H	-0.46557500	1.13384100	2.13445500
C	-1.33244600	2.54132300	0.70393400
H	-1.60599800	3.52968800	-1.32003700
H	-2.04039700	3.09704200	1.31166400
C	1.99802400	-0.89850500	-0.10971300
H	2.03316800	-1.98012100	-0.30158100
C	2.98128100	-0.23019600	-1.05207700
C	2.63369400	-0.65365500	1.24607900
H	2.84595500	-0.19746000	-2.12779800
C	4.01969500	0.26676700	-0.34464000
H	2.19080900	-0.99052700	2.17700600
C	3.80302700	0.00388800	1.08563000
H	4.88806700	0.77620800	-0.75098300
H	4.48993300	0.29415500	1.87461900
O	-2.47790000	-1.50929100	1.30892100
C	-3.97892000	-0.20862800	-0.08217900
H	-4.69678500	-0.31804000	0.73204600
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H	-4.37824300	-0.67346200	-0.99088600

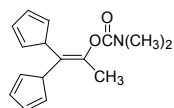
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O	-1.54415800	-0.78759500	-0.72525800
C	-2.37397000	-1.20093200	0.29969900
O	-1.95689900	-1.77009200	1.29547900
N	-3.67620300	-0.90153100	0.03892700
C	-4.12093200	-0.12776300	-1.11454500
H	-5.07127500	-0.53964700	-1.47279200
H	-4.27777900	0.92721700	-0.84851200
H	-3.38762100	-0.18632500	-1.91670800
C	-4.66715200	-1.14002000	1.08175400
H	-5.01275800	-0.19039200	1.51363900
H	-5.53052500	-1.66606400	0.65753600
H	-4.22105400	-1.74837700	1.86759200
C	0.06999500	-2.57508800	-0.97311600
H	-0.32351300	-3.24680400	-0.20122400
H	-0.45005800	-2.80879300	-1.91115300
H	1.13408200	-2.77593800	-1.10690800
C	0.29515500	1.23698300	-0.06440300
C	-0.47208300	1.96383700	-0.98720400
C	0.71316400	1.91994900	1.08784300
C	-0.78436300	3.29689700	-0.71659300
H	-0.81381900	1.50037900	-1.90710200
C	0.33775400	3.25183600	1.26882500
H	1.31688000	1.41964800	1.83963700
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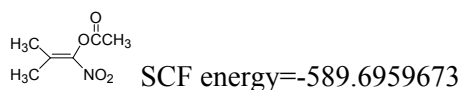
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C	2.61147700	-1.49610100	0.72181000
C	4.47521700	-0.04331500	-0.62833800
H	2.83996000	1.06926900	-1.48306300
C	3.98544100	-1.71772900	0.84264100
H	1.90971900	-2.08834300	1.30203300
N	4.91610500	-1.01566700	0.18311900
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H	4.35612600	-2.49557400	1.50806600



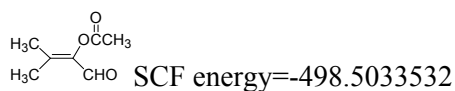
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C	2.57694800	-0.34453900	-0.37682300
O	2.36566300	-0.44836600	-1.57561000
N	3.73940400	0.09728200	0.18494700
C	3.93662800	0.29107900	1.61619700
H	4.92928400	-0.08164800	1.89646700
H	3.88110100	1.35690100	1.88148500
H	3.18204300	-0.25375500	2.17992200
C	4.78991600	0.60465400	-0.68757600
H	4.89008200	1.69438600	-0.58333600
H	5.74819500	0.14072600	-0.42340200
H	4.54334100	0.36534300	-1.72135800
C	0.65628300	-2.74804300	-0.13555300
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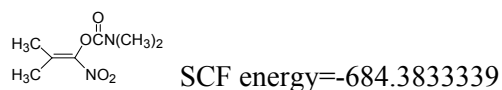
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C	-2.94154600	-1.50858700	0.87753700
C	-2.91587200	-0.39520300	-1.20717000
H	-2.62178900	-2.05277900	1.75974800
C	-4.18964300	-1.08429100	0.58172500
H	-2.57841800	0.03323900	-2.14336700
C	-4.17362000	-0.39518200	-0.71447100
H	-5.07621900	-1.22505600	1.19277300
H	-5.04695000	0.04013700	-1.19009500
C	-0.60571400	0.94602700	0.40985800
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C	-0.48555800	1.86661500	-0.79182900
C	-1.73340700	1.57824900	1.19527300
H	0.22235500	1.69386600	-1.59490400
C	-1.34012300	2.90318600	-0.64593600
H	-2.11575900	1.17441100	2.12535200
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H	-1.45052400	3.74316800	-1.32524000
H	-2.86398900	3.42078900	0.95078800



C	-0.37986500	0.01033000	-0.28727900
C	-1.32761500	-0.92097000	-0.04209800
O	0.85387300	-0.29516900	-0.78769400
C	2.01306700	-0.31155200	-0.00182300
O	3.04744800	-0.53537400	-0.56636000
C	1.85209900	-0.08323400	1.48025800
H	2.80860300	-0.29233200	1.96094400
H	1.57359600	0.95821800	1.67047800
H	1.07669100	-0.72809900	1.90613000
C	-2.73632900	-0.64439400	0.41793300
H	-3.34060500	-0.24257600	-0.40429300
H	-3.19845700	-1.57517700	0.76162800
H	-2.78065100	0.09739700	1.21896000
C	-0.98664000	-2.37542200	-0.24020000
H	-0.00191300	-2.53189100	-0.68164600
H	-1.03886200	-2.90693800	0.72024000
H	-1.74086600	-2.83736500	-0.89090000
N	-0.60390800	1.46150300	-0.17817700
O	0.39261400	2.18458600	-0.22250600
O	-1.76124500	1.86842000	-0.04532000



C	-0.49503300	0.27979800	-0.24105900
C	-1.66900400	-0.36115900	-0.00720400
O	0.59247200	-0.45752400	-0.69128600
C	1.78253000	-0.57453800	0.00299900
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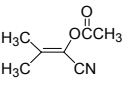
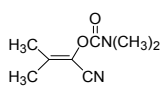
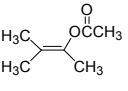


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O	0.13265000	-0.63008300	-1.00113300
C	1.50001100	-0.41740800	-0.72865600
O	2.26131000	-0.35985500	-1.66382800
C	-3.27121400	0.10317900	0.48713600
H	-3.36896800	1.14080100	0.16330000
H	-4.16183600	-0.45597200	0.17987900
H	-3.24902600	0.11705300	1.58464600
C	-2.19920600	-2.05042300	-0.34887800
H	-1.26021100	-2.53676000	-0.61658800
H	-2.63668800	-2.55658300	0.52209700
H	-2.90374000	-2.19182500	-1.18024100
N	1.83642500	-0.30512600	0.59097400
C	1.15762800	-1.00387800	1.68275600
H	1.83520100	-1.75542100	2.11034100
H	0.87073000	-0.30155800	2.47417600
H	0.26704600	-1.51723600	1.32568100
C	3.21321800	0.09976500	0.87482700
H	3.23695800	0.58249100	1.85687200
H	3.89250700	-0.76404000	0.88152500
H	3.54977900	0.80561000	0.11562000
N	-0.63227800	1.45916000	-0.13072300
O	0.21116500	2.00070700	-0.84359500
O	-1.28709300	2.03036400	0.74757500

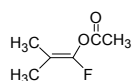
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H 0.90336600	-0.19382400	1.95882100	C -1.03995700	-0.20782600	0.43085400
C -2.95539600	0.33059900	0.36768700	O -0.76913900	-0.10567200	1.61484700
H -2.87324200	1.40864400	0.50798800	C 3.64652300	-0.03037300	0.20010900
H -3.71459600	0.14577300	-0.40435800	H 3.73965800	1.04937200	0.32005500
H -3.34776300	-0.10031100	1.29843600	H 4.02442400	-0.50560600	1.11509400
C -1.77612300	-1.85809300	-0.12190500	H 4.31728500	-0.33856900	-0.61337600
H -0.86022200	-2.31662900	-0.49585100	C 2.11994600	-2.00627200	-0.23206600
H -2.01880000	-2.29588800	0.85692900	H 1.10080200	-2.31789100	-0.46274500
H -2.60318200	-2.12415900	-0.79384600	H 2.78800200	-2.36584600	-1.02684400
C -0.30291200	1.74209700	-0.22010900	H 2.43726500	-2.50318800	0.69511900
O 0.76957900	2.28239400	-0.43646000	N -2.28229400	-0.38839900	-0.09429000
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	SCF energy= -573.7764375		H -3.32452100	-1.01496500	-1.79709000
C -0.38268400	-0.01880200	-0.26287700	H -3.01164700	0.73908300	-1.72883400
C -1.24312000	-1.03756100	-0.02787000	H -1.68924200	-0.38790000	-2.11083800
O 0.88390400	-0.30909000	-0.76685400	C -3.42104600	-0.35338300	0.81518600
C 2.03590100	-0.23699900	-0.00700000	H -3.90676200	0.63281900	0.79865600
O 3.08145400	-0.46440900	-0.56054500	H -4.15228800	-1.11033800	0.50965200
C 1.89636900	0.09134500	1.46089400	H -3.08048500	-0.56132300	1.82902700
H 2.85204400	-0.11030700	1.94673800	C 1.17135600	1.76715900	-0.05231700
H 1.64962000	1.15136300	1.57846500	O 0.17977900	2.45500600	-0.23269000
H 1.10579300	-0.49707300	1.93719800	H 2.13020700	2.23724600	0.22721400
C -2.66745300	-0.88962500	0.44466500		SCF energy=-668.4533237	
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H -2.91618900	-1.72471000	1.11036500	C -2.03168000	-0.64746200	-0.04937500
H -2.86561900	0.04882800	0.95921400	O 0.13826900	-0.70867100	-0.94518400
C -0.80433400	-2.46469400	-0.24037500	C 1.48699500	-0.45422500	-0.71297500

H	0.13028100	-2.54322500	-0.79694700	O	2.24961200	-0.44285100	-1.65271600
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C	-0.62665100	1.44723600	-0.19375400	H	-4.15716000	-0.43918300	-0.10578000
O	0.26082500	2.27680600	-0.25172400	H	-3.46581200	-0.26514300	1.50485300
O	-1.93150100	1.80695600	-0.07878800	C	-2.13175500	-2.13453400	-0.28424800
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C	-1.51056400	-0.58156400	0.01435500	N	1.84750900	-0.25899800	0.59904700
O	0.74552200	-0.37738200	-0.75129400	C	1.22754400	-0.96615600	1.71807700
C	1.92546600	-0.31380000	-0.01998700	H	1.86025600	-1.81034700	2.03099900
O	2.90063400	-0.82338600	-0.50566300	H	1.10828400	-0.28817600	2.57133700
C	1.88375500	0.38105500	1.31965600	H	0.24868000	-1.35262400	1.44296700
H	2.83660600	0.20879800	1.82158300	C	3.23358100	0.14465200	0.82460100
H	1.73719000	1.45905900	1.18894200	H	3.29731500	0.63773400	1.80015700
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C	-2.83996400	0.01758800	0.38334800	H	3.54198000	0.84071900	0.04442400
H	-2.82563900	1.10988500	0.40764400	C	-0.61391700	1.47160000	-0.23446500
H	-3.60788900	-0.30027900	-0.33464900	O	0.23768700	2.04838400	-0.87915700
H	-3.15888500	-0.34716500	1.36874300	O	-1.39580300	2.12713000	0.66611700
C	-1.42801100	-2.08235500	-0.00515000	H	-1.13746500	3.06677300	0.60872800
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H	-1.63705000	-2.48683300	0.99486200	C	1.15983300	0.27986100	-0.24707500
H	-2.19760400	-2.48997300	-0.67414700	C	2.05361100	-0.72017500	-0.12661900
C	-0.49334800	1.62176400	-0.34380100	O	-0.16388700	0.05816800	-0.63339800
N	-0.49556200	2.78604500	-0.37235200	C	-1.09401400	-0.04918900	0.39714100
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				C	3.49379400	-0.45426300	0.21582100

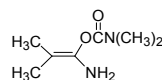
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H	-3.64538500	-0.34867500	-0.19088200
H	-3.02561500	0.04186700	1.41286500
C	-1.36024100	-1.81377500	-0.17780000
H	-0.37237800	-2.12539800	-0.52424300
H	-1.55057300	-2.28988400	0.79625600
H	-2.10344000	-2.22528400	-0.87538100
N	-0.40198700	1.90818000	-0.18040300
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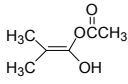
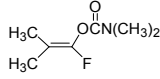
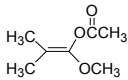
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O	-0.71141000	0.35116700	-0.73154500
C	-1.89310700	0.19474500	-0.00297800
O	-2.87441500	0.74709700	-0.42068200
C	-1.82411300	-0.64619300	1.24749800
H	-2.75990000	-0.52449700	1.79420900
H	-1.69006300	-1.70106800	0.98574600
H	-0.97892000	-0.35248800	1.87875100
C	2.82047800	-0.54255800	0.24588400
H	2.67058900	-1.60806700	0.05839700
H	3.62808900	-0.18919300	-0.40978500
H	3.17435000	-0.42055400	1.27877000
C	1.65834300	1.75497200	0.24470600
H	0.72030100	2.26852600	0.02178400

H	0.63916200	-2.27066900	-0.67831900
H	2.34481300	-2.65518700	-1.00760000
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N	-2.36347300	-0.06400500	-0.08601000
C	-2.72522800	0.10101300	-1.48939000
H	-3.23287900	-0.80031200	-1.85823400
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H	-1.83842200	0.28253700	-2.09226500
C	-3.46858100	-0.22318200	0.85142800
H	-4.10975800	0.66782200	0.83735900
H	-4.07514300	-1.09439200	0.57244600
H	-3.07092300	-0.36364100	1.85580700
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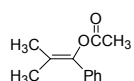


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C	-1.11205100	-0.44248900	-0.16083300
O	-1.00562300	-1.50130300	-0.76959100
C	3.65700600	-0.15250500	-0.20723700
H	3.70813700	-1.24695700	-0.23148000
H	4.14993000	0.20826700	-1.11980800
H	4.27204600	0.19061800	0.63908400
C	2.08317800	1.83013300	-0.52531700
H	1.05635500	2.18134800	-0.40562500
H	2.73606900	2.47632900	0.08108300
H	2.37693600	1.98534900	-1.57382800
N	1.26702800	-1.64819300	0.88154100

H 1.93568900	1.97162400	1.28568100	H 0.61324500	-2.28620800	0.43055500
H 2.44305500	2.18966700	-0.38925000	H 2.19972100	-2.04263000	0.89969500
F 0.32794800	-1.64222000	-0.60954100	N -2.28337400	0.21860600	0.05634400
	SCF energy=-460.4068298		C -2.39097400	1.49729700	0.74730200
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C 1.51462300	0.29440600	-0.06887000	H -3.20648900	1.44610600	1.47936500
O -0.74340500	0.02467000	-0.84213600	H -1.46344900	1.72579900	1.26790900
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C -1.64453300	-0.05880500	1.46073900	H -3.90282900	0.39511500	-1.28284200
H -2.60651800	0.05159000	1.96266200	H -3.29720700	-1.26060400	-1.00955700
H -1.22758000	-1.05007000	1.66409800		SCF energy=-579.11451079	
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C 2.83285000	-0.31260800	0.33832700	C -2.17057300	0.07081700	0.06353000
H 2.81707500	-1.40342700	0.28733200	O 0.00426400	-0.51692400	0.87642800
H 3.64043900	0.05597900	-0.30942300	C 1.36741700	-0.59303800	0.51198200
H 3.09589700	-0.02233800	1.36575300	O 1.99462300	-1.58979800	0.79212200
C 1.44552700	1.79868600	-0.12845000	C -3.21255900	-0.02874600	-1.02135100
H 0.47518300	2.16259400	-0.47465600	H -2.84370800	-0.54725500	-1.90943300
H 1.65087700	2.24012000	0.85777800	H -4.09879700	-0.56678700	-0.65634700
H 2.21361000	2.18839300	-0.81061200	H -3.55217400	0.97136900	-1.32545900
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C -0.44618200	0.22323900	-0.10571200	H -3.41020000	0.23640000	1.81848000
C -1.50222400	-0.60151100	-0.08052500	N 1.85918200	0.52740700	-0.07820600
O 0.74513200	-0.11657100	-0.74693000	C 1.13650400	1.78475600	-0.23556000
C 1.88751800	-0.40477400	-0.02151600	H 1.80732200	2.61066900	0.02820700
			H 0.80176200	1.92549700	-1.27191900

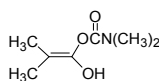
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H	2.70426800	-0.85121600	1.88736500
H	1.36936900	0.33966300	1.93568200
H	1.00400400	-1.36955000	1.69205800
C	-2.81912500	-0.17062300	0.51291500
H	-2.79191300	0.86006800	0.87277500
H	-3.62468400	-0.26211700	-0.22918800
H	-3.09461700	-0.82022900	1.35603500
C	-1.43418800	-2.00593800	-0.62363100
H	-0.46954900	-2.23244700	-1.08313900
H	-1.62300400	-2.74146500	0.17194200
H	-2.21480200	-2.15929600	-1.38149100
O	-0.43555500	1.46818500	0.45434500
C	-0.19978000	2.55521100	-0.46052800
H	-0.21447800	3.46254800	0.14563100
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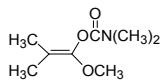
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C	-1.63421700	-1.74698500	0.18552400
O	-2.13870900	-2.74649900	-0.26729400
C	-1.29263200	-1.55309500	1.64598100
H	-1.72458400	-2.37974700	2.21175300
H	-0.20631000	-1.54913500	1.78670600
H	-1.67562300	-0.59877400	2.02157400
C	-0.62289600	2.93972100	-0.01653300

H	0.27279700	1.81889900	0.42605600
C	3.23474200	0.51027000	-0.56817400
H	3.25847700	0.85401700	-1.60942100
H	3.86661900	1.17349300	0.03701000
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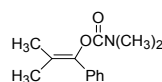


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C	-1.12787800	-0.44153600	0.11126900
O	-1.05108200	-1.57895200	0.58028600
C	3.66283300	-0.26000600	0.13183700
H	3.63544200	-1.32644400	-0.10156600
H	4.32630300	0.23258700	-0.59424500
H	4.12598700	-0.13133900	1.12056500
C	2.19663000	1.81767600	0.47195500
H	1.17236800	2.19599300	0.44187400
H	2.59267800	1.98694600	1.48350000
H	2.80621100	2.42907800	-0.20962300
N	-2.28072200	0.26193400	-0.02375100
C	-2.36290500	1.61376000	-0.56425900
H	-3.08062500	1.63558300	-1.39407700
H	-2.70748400	2.31256400	0.20978700
H	-1.39036000	1.93560400	-0.92968500
C	-3.53350400	-0.33430800	0.42306200
H	-3.98359700	0.28064900	1.21318900
H	-4.23933600	-0.39816400	-0.41495200
H	-3.33862800	-1.33337600	0.81043200

H 0.45488100	2.89522900	-0.18584900	O 1.27229600	-1.64851000	-0.70096400
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H -3.25068600	2.20653800	0.51599000	O -0.07832000	-0.03436200	0.98274400
H -3.07215600	2.29162800	-1.23350300	C -1.38933800	0.28415700	0.61218200
C 0.81194900	0.19509600	-0.17346600	O -1.92152100	1.28554100	1.05381800
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C 2.81439900	-0.91196600	-1.00978000	H 4.12351000	-0.00834900	-0.28411100
H 0.85315800	-1.13211600	-1.87450700	H 3.43761000	-1.07607600	-1.50703500
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H 3.28507400	-1.57195700	-1.73400600	H 3.10737900	-1.59078300	1.62058500
H 3.54362200	0.97830500	1.72470800	N -1.99205600	-0.64325800	-0.17870100
H 4.64731900	-0.51195300	0.06240900	C -1.35925700	-1.86110600	-0.66941800
			H -2.07176200	-2.69012000	-0.58325800
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			H -0.47658300	-2.09753500	-0.07949700
			C -3.34204400	-0.38319700	-0.66665800
			H -3.34099600	-0.31214200	-1.76252500
			H -4.01277400	-1.19916000	-0.36934700
			H -3.70192000	0.55318800	-0.24267800
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			C 0.80768900	2.56300400	-0.19738400
			H 0.59877600	3.26243900	-1.00896600
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H 1.82289400 2.72436900 0.18465200



SCF energy=-710.9147988

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C -1.44852000 -1.07440000 -0.72666300

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H 1.58305200 2.86212000 0.31446400

H 0.58165500 4.17518800 -0.32692600

H 0.37927800 3.66079400 1.34445400

C -1.83974900 2.95124400 -0.37513300

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H -2.16517900 3.52927000 0.50197700

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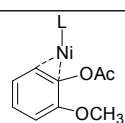
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C 1.70706700 0.32888500 1.07182800

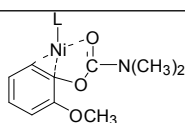
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H 1.04940900 -0.52890800 -2.15526600

	C	2.91527200	-0.35050100	1.24202700
	H	1.28089100	0.88953400	1.89955700
	C	3.45715100	-1.09198500	0.18839600
	H	3.19204800	-1.73045000	-1.85700900
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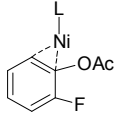
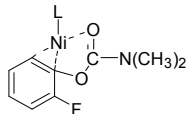


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C	1.34864500	-0.13248100	-0.53678300
C	0.15706800	1.19126200	-2.21656500
C	1.20612000	0.91228800	0.41572700
C	-0.00130400	2.22778700	-1.27367800
C	0.50893500	2.08821400	0.04225700
Ni	-0.85581800	0.38569600	-0.40141700
P	-2.65337700	-0.55850300	0.21635100
H	0.93658700	-0.82505500	-2.53172100
H	-0.24006800	1.29488100	-3.22084900
O	1.95825400	-1.32816600	-0.17748400
C	3.32773300	-1.45198700	-0.07712500
O	3.77077100	-2.50739400	0.30302100
C	4.17061700	-0.25998300	-0.47165000
H	3.88320000	0.12882600	-1.45392600
H	4.04338700	0.54664300	0.25791100
H	5.21601400	-0.57178200	-0.48659200
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H	-1.97763500	-1.80897500	2.21844200

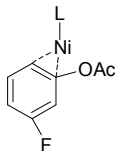


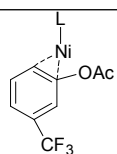
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C	-0.48070000	-1.70293600	0.52142700
C	1.47791700	-2.65728100	-0.61952400
C	0.72199800	-2.44844400	0.56535700
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P	2.35926000	1.30486600	0.11575800
H	-0.45264100	-0.82911400	-2.79130400
H	1.63021300	-2.24377600	-2.74986200
O	-2.10144100	-0.46945700	-0.80646600
C	-2.29166500	0.75046500	-0.18637900
O	-1.38991900	1.42208400	0.28230100
C	1.96024700	2.09561600	1.75295100
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H	2.28059100	1.43624600	2.56744100
H	2.45188400	3.07064700	1.87137300
C	4.21999300	1.38886700	0.15331200
H	4.60350700	0.68777500	0.90273800

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P	2.44647200	-0.99532800	-0.13643700	P	1.59970500	-2.01611900	0.02263200
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C	-3.55560500	-1.47725200	-0.39103500	C	-2.72313100	0.03299300	-0.41197700
O	-4.04145100	-2.48936500	-0.83244300	O	-2.05736500	-0.53874700	-1.25813100
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H	2.57589400	-0.83561800	-2.58365800	H	3.80386100	-2.41880300	1.03606100
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C	4.07813400	-0.11363100	0.03998200	C	0.85105300	-3.37086600	1.06033800
H	4.09341900	0.76440800	-0.61485000	H	1.14215300	-4.36986500	0.70855000
H	4.19736700	0.23413700	1.07189400	H	1.16792700	-3.25347600	2.10241200
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C	2.80703400	-2.53739400	0.84215000	H	2.85168000	2.38019000	0.95501000
H	3.74156100	-3.01811100	0.52378500	H	-0.61812500	1.64356900	-1.53856500
H	2.87997300	-2.28799200	1.90627000	O	1.76372500	2.54325100	-1.57210500
H	1.98211700	-3.24714600	0.71896300	C	3.15841900	2.81980300	-1.56141600
H	0.36845000	2.85948400	1.51987500	H	3.41495300	3.08756600	-2.58808100
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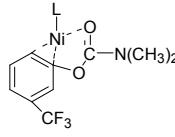
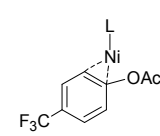
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H	5.84876100	-0.80794200	-0.90522200	H	-0.80911000	1.11608900	-2.00802900
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C	0.98401600	0.77187900	-1.47838400	C	3.53340300	3.56286200	-0.35076000
C	1.43486300	0.11774000	-0.30831500	H	3.17213200	4.14232400	0.51016900
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C	1.16535900	0.70082600	0.94895000	H	3.05973200	3.94391300	-1.26579600
C	0.07784600	2.59641800	-0.11444600	N	-4.23738100	0.20911400	0.05466400
C	0.49892400	1.93513000	1.06443200	C	-4.74321800	0.99306600	1.17398000
Ni	-0.75220400	0.51394800	-0.10624500	H	-5.49826400	1.71094700	0.82436200
P	-2.56665300	-0.59970200	0.01422700	H	-5.21598700	0.32968700	1.91065100
H	1.17263600	0.30755100	-2.44089500	H	-3.93392600	1.53761300	1.65452400
H	-0.01358100	2.52029400	-2.28203000	C	-5.21717400	-0.60442700	-0.65161800
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O	3.89188000	-2.36314200	-0.33040600	H	-4.72275300	-1.14053200	-1.46081500
C	4.24287500	0.00106900	-0.01154700				
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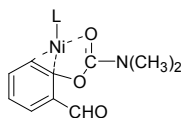
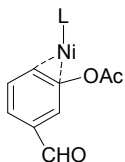




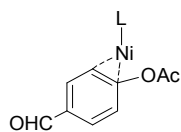
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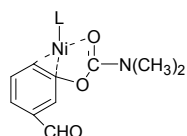


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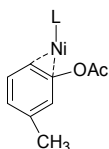
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C	-1.18118000	0.82056800	-0.73867300
C	-0.15883900	2.01823400	1.15267100
C	-0.47259800	1.94787600	-0.23282000
Ni	0.64869500	0.09213400	0.29573500
P	2.46796400	-0.96100300	-0.12617300
H	0.38124000	2.88403000	1.52051800
H	-1.45538300	-1.00663800	2.14516800
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O	-2.23676000	-1.32301100	-0.36186900
C	-3.61680000	-1.39309900	-0.38980000
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C	2.80957400	-1.40715800	-1.89804400
H	1.99253400	-2.02617600	-2.28361100
H	2.85766900	-0.49621200	-2.50416600
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C	4.07242100	-0.14468200	0.33526300
H	4.16251100	0.81157500	-0.19082400
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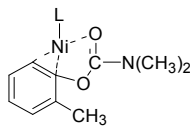
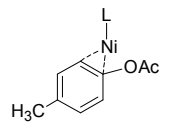
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H	1.76793400	2.90384200	1.33045500
C	0.24811400	0.80042600	2.02594700
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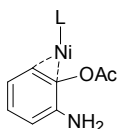
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H	-3.72565000	-0.14322400	1.68863600	C	0.75117900	-3.92347100	0.53655300
H	-4.19109300	0.32210800	0.04659100	H	0.37245200	-3.86654000	1.56280500
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H	0.04590600	2.23039300	1.96216400	C	2.89636700	-2.10522300	1.09602500
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C	1.44029600	0.11416900	-0.16155500				
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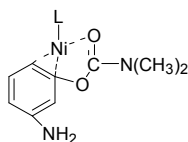
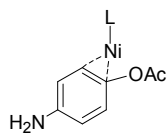


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C	3.44831200	-1.23550100	-0.29126900	C	-0.78404700	1.15839300	-0.30234600	
O	3.93382700	-2.34014500	-0.27719200	C	0.14781700	3.15846400	0.70493600	
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H	-2.17010100	-2.25636400	1.71507900	H	0.17693700	3.87839300	1.52084600	
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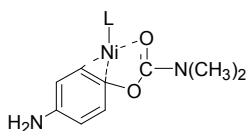


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C	-4.02022700	-0.09602900	-0.60003600	C	1.69613800	-2.87776300	1.30424900
H	-4.26248700	0.77396900	0.02021800	H	2.19845300	-3.82716600	1.07404600
H	-3.89062300	0.25131400	-1.63083100	H	1.99946800	-2.54829100	2.30396600
H	-4.86111700	-0.80155900	-0.56636500	H	0.61346200	-3.04331000	1.31896300
C	-2.42022400	-2.41591000	-1.03692100	H	2.54382900	3.07855500	0.35572700
H	-3.36847600	-2.96589200	-0.97131000	H	-0.86900000	1.42847300	-1.74881500
H	-2.23351900	-2.15309600	-2.08380700	N	1.38854500	2.83809300	-2.05855400
H	-1.60563600	-3.06897400	-0.70619600	H	2.39475900	2.96369000	-2.07723900
H	1.43239600	0.05278800	2.16020400	H	1.08016400	2.32829000	-2.87945300

H	0.23487400	2.24988600	2.16399100	N	-3.88263900	-0.68912100	0.00867500
N	-0.37638600	3.71640200	-0.00332800	C	-4.63208500	-0.14552800	1.13472700
H	-0.91159700	3.93588500	-0.83637400	H	-5.41794100	0.54175100	0.78862200
H	-0.91036500	3.93961600	0.82949600	H	-5.11033100	-0.96843300	1.67978500
				H	-3.96879700	0.38922400	1.81094400
				C	-4.61057800	-1.59183200	-0.87266600
				H	-5.00899800	-2.43404200	-0.29361800
				H	-5.45150200	-1.07269200	-1.35492100
				H	-3.93491700	-1.96685300	-1.64055400



C	-0.47269300	1.06135500	1.21883700
C	-1.00593600	0.61101800	-0.00135600
C	0.56743700	2.02122500	1.21759100
C	-0.47124800	1.06114400	-1.22122500
C	1.06983500	2.54281700	-0.00039900
C	0.56910400	2.02056100	-1.21901800
Ni	1.20057600	0.23674900	-0.00033300
P	2.60390000	-1.33983800	0.00047200
H	-0.87809600	0.69041400	2.15402900
H	0.95406400	2.39130800	2.16301700
O	-2.01781200	-0.35456700	-0.00195700
C	-3.31720000	0.11026300	-0.00002000
O	-3.60356300	1.29554700	0.00372300
C	2.73185800	-2.39953600	-1.52871200
H	1.75840000	-2.85545500	-1.73945500
H	3.00017600	-1.77294900	-2.38636700
H	3.48141000	-3.19520500	-1.42064600
C	4.40890000	-0.93810400	0.24592600

H	4.74299800	-0.25791100	-0.54531300
H	4.54255100	-0.42783100	1.20610900
H	5.03926700	-1.83745800	0.23061100
C	2.40903000	-2.67536200	1.28712500
H	3.17746600	-3.45503300	1.19657700
H	2.47021400	-2.23124800	2.28667800
H	1.42072400	-3.13698600	1.18642700
H	-0.87537900	0.68986700	-2.15683800
H	0.95738100	2.38973700	-2.16410600
N	2.00708500	3.58637500	0.00019100
H	2.58517600	3.62482000	0.83253000
H	2.58385600	3.62722600	-0.83294300
N	-4.21004600	-0.92193800	-0.00360300
C	-3.84801100	-2.33316000	-0.00261900
H	-4.25014500	-2.82624300	0.89326700
H	-4.27019200	-2.83096000	-0.88639600
H	-2.76616800	-2.44631100	-0.01449700
C	-5.63405000	-0.61903000	0.00307000
H	-6.11909500	-1.04946000	-0.88346400
H	-6.11016600	-1.04181500	0.89826100
H	-5.76950600	0.46204000	-0.00067900

Figures . Correlations between the experimental and theoretical C-O BDEs calculated by other DFT methods.

