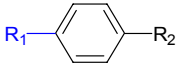
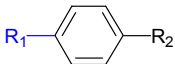


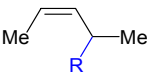
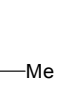








Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	R ₁ = SC ₇ H ₇ , R ₂ = NO ₂	C-R ₁ heterol.	12.95
		homolysis	26.95
		radical cation	-14.3
	R ₁ = SC ₇ H ₇ , R ₂ = Br	heterolysis	17.85
		homolysis	25.74
		radical cation	-18.1
	R ₁ = SC ₇ H ₇ , R ₂ = Cl	heterolysis	18.38
		homolysis	23.96
		radical cation	-24.3
	R ₁ = SC ₇ H ₇ , R ₂ = H	heterolysis	20.17
		homolysis	24.57
		radical cation	-21.9
	R ₁ = SC ₇ H ₇ , R ₂ = Me	heterolysis	20.75
		homolysis	23.68
		radical cation	-24.8
	R ₁ = SC ₇ H ₇ , R ₂ = OMe	heterolysis	21.61
		homolysis	23.50
		radical cation	-24.8
	R ₁ = S-TPCP, R ₂ = NO ₂	heterolysis	14.44
		homolysis	44.16
	radical cation	-14.3	
R ₁ = S-TPCP, R ₂ = Br	heterolysis	17.80	
	homolysis	41.41	
	radical cation	-17.3	
R ₁ = S-TPCP, R ₂ = Cl	heterolysis	18.09	
	homolysis	39.40	
	radical cation	-19.5	
R ₁ = S-TPCP, R ₂ = H	heterolysis	20.14	
	homolysis	40.27	
	radical cation	-18.6	
R ₁ = S-TPCP, R ₂ = Me	heterolysis	20.75	
	homolysis	39.38	
	radical cation	-19.6	
R ₁ = S-TPCP, R ₂ = OMe	heterolysis	21.90	
	homolysis	39.52	
	radical cation	-19.6	

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Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	R ₁ = S-9-PhXan, R ₂ = NO ₂	C-R ₁ heterol.	18.33
		homolysis	26.1
		radical cation	-10.4
	R ₁ = S-9-PhXan, R ₂ = Br	heterolysis	23.05
		homolysis	24.71
		radical cation	-13.1
	R ₁ = S-9-PhXan, R ₂ = Cl	heterolysis	24.36
		homolysis	23.71
		radical cation	-14.6
	R ₁ = S-9-PhXan, R ₂ = H	heterolysis	26.11
		homolysis	24.29
		radical cation	-13.6
	R ₁ = S-9-PhXan, R ₂ = Me	heterolysis	26.94
		homolysis	23.64
		radical cation	-14.8
	R ₁ = S-9-PhXan, R ₂ = OMe	heterolysis	27.85
		homolysis	23.51
		radical cation	-15.0
	R ₁ = S-Xan, R ₂ = NO ₂	heterolysis	21.66
		homolysis	29.32
		radical cation	-6.27
	R ₁ = S-Xan, R ₂ = Br	heterolysis	24.70
		homolysis	26.25
		radical cation	-9.45
	R ₁ = S-Xan, R ₂ = Cl	heterolysis	25.87
		homolysis	25.11
		radical cation	-10.4
	R ₁ = S-Xan, R ₂ = H	heterolysis	26.43
	homolysis	24.49	
	radical cation	-11.1	
R ₁ = S-Xan, R ₂ = Me	heterolysis	27.16	
	homolysis	23.75	
	radical cation	-11.8	
R ₁ = S-Xan, R ₂ = OMe	heterolysis	27.67	
	homolysis	23.22	
	radical cation	-12.3	
R ₁ = S-CPH ₃ , R ₂ = NO ₂	radical cation	-11.0	
R ₁ = S-CPH ₃ , R ₂ = Br	radical cation	-14.7	
R ₁ = S-CPH ₃ , R ₂ = Cl	radical cation	-15.0	
R ₁ = S-CPH ₃ , R ₂ = H	radical cation	-14.5	
R ₁ = S-CPH ₃ , R ₂ = H	radical cation	-15.3	
R ₁ = S-CPH ₃ , R ₂ = Me	radical cation	-15.3	
R ₁ = S-CPH ₃ , R ₂ = OMe	radical cation	-16.0	

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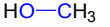
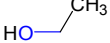


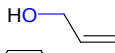
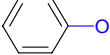
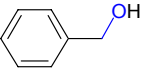

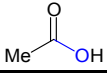
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level

	R = OO·	dissociated radical as trans or cis	C-OO·	<i>trans, cis</i> 19.6, 23.1	B3P86-HLM
				20.5, 21.3	B3P86-HLM
				7.9, 7.4	B3P86-HLM
				8.4,	B3P86-HLM
				14.2, 77.4	B3P86-HLM
				14.6, 77.7	B3P86-HLM
				4.2	B3P86-HLM
				6.0	B3P86-HLM
				9.8, 11.2	B3P86-HLM
				11.7, 12.9	B3P86-HLM


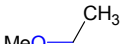


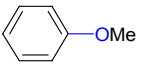
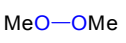

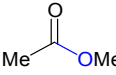
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HO-CH ₃	C-O	92.1
MeO-CH ₃		83.2
H ₂ N-CH ₃	C-N	85.2
O ₂ N-CH ₃		61.0


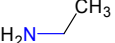


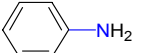
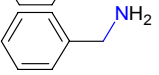
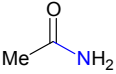
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Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-O	92.1	
		94.0	
		95.5	
		95.8	
		80.1	
		112.4	
		82.6	
		109.5	
		109.9	

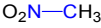
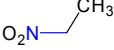
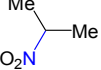
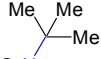
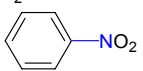
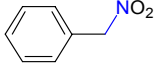
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	C-OMe	83.2	
		85	
		85.8	
		84	
		101	
		38	
		99.6	
		100	




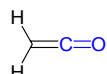
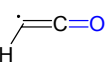

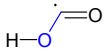
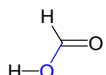

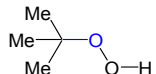
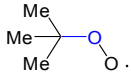
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	C-NH ₂	85.2	
		84.8	
		86.0	
		85.7	
		104.2	
		71.7	
		99.1	

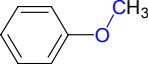
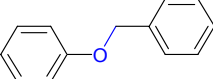
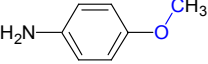
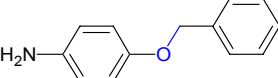
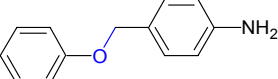
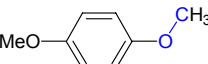
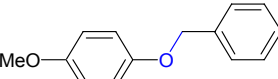
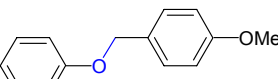
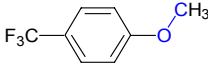
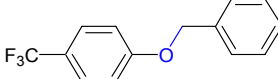
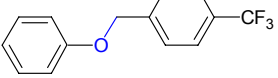
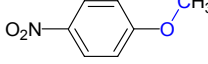
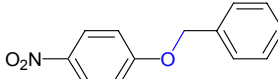
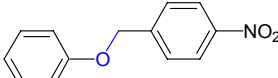
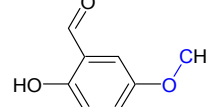
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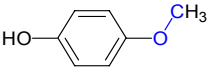
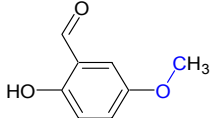
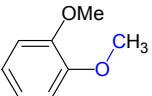
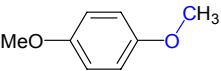
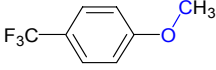
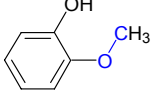
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-NO ₂	61.0	
		61.6	
		62.9	
		62.8	
		72.5	
		50.5	

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	C-O	106.3	
		92.1	
		90.5	
		174	
		154	
		178.8	
		28	
		109.3	
		100	
		74	
		38	

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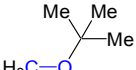
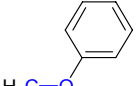
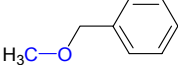
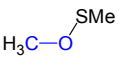
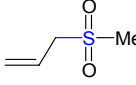
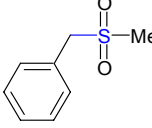
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-O	59.3	DFT I
		65.2	DFT II
		63.5	DFT III
		65.3	Experimental
		52.8; 52.5	DFT II
		-9.2	DFT I
		-9.5	DFT II
		-8.9	DFT III
		-9.3	DFT II
		-1.4	DFT II
		-6.0	DFT I
		-6.1	DFT II
		-5.5	DFT III
		-6.1	DFT II
		-0.5	DFT II
		3.7	DFT I
		3.0	DFT II
		2.8	DFT III
		3.0	DFT II
		-0.1	DFT II
		5.2	DFT I
		4.6	DFT II
		4.5	DFT III
		4.7	DFT II
		-0.9	DFT II
		-4.5	DFT II
		-4.7	DFT III

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-O	62.6	Experimental
		62.3	Experimental
		61.2	Experimental
		62.2	Experimental
		67.5	Experimental
		58.1	Experimental

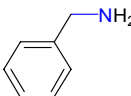
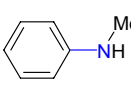
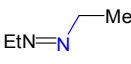
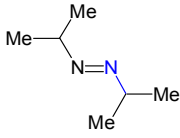
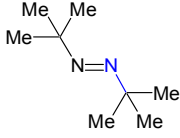
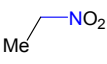
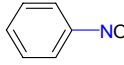
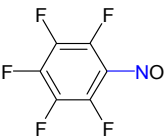
Pratt, D. A.; de Heer, M. I.; Mulder, P.; Ingold, K. UJ. *Am. Chem. Soc.* **2001**, *123*, 5518-5526

(kJ/mol)		
H ₃ C-N	C-N	356
H ₃ C-O	C-O	385.7
H ₃ C-S	C-S	307.8

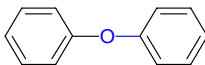
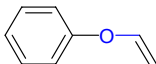
Cherkasov, A.; Jonsson, M.J. *Chem. Inf. Comput. Sci.* **2000**, *40*, 1222-1226

	C-O	80.9	DFT-AM1
		66.3	Experimental
		68.8	Corrected
		65.1	DFT-AM1
		57.0	Experimental
		55.3	Corrected
		83.2	DFT-AM1
		67.0	Experimental
		70.7	Corrected
		72.6	DFT-AM1
		66.8	Experimental
		61.7	Corrected
	C-S	56.3	DFT-AM1
		49.6	Experimental
		47.4	Corrected
		63.7	DFT-AM1
		52.9	Experimental
		54.1	Corrected



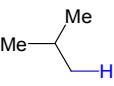
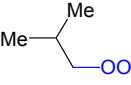
Jursic, B. S. *J. Chem. Soc. Perkin Trans.* **1999**, *2*, 369-372



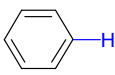
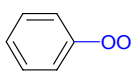

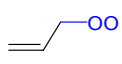
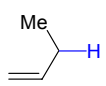
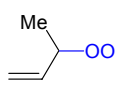
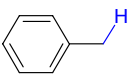
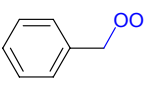
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
$\text{H}_3\text{C}-\text{NH}_2$	C-N	89.4	DFT-AM1
		84.9	Experimental
		84.9	Corrected
	C-N	74.0	DFT-AM1
		71.9	Experimental
		70.3	Corrected
	C-N	73.3	DFT-AM1
		67.7	Experimental
		69.6	Corrected
$\text{MeN}=\text{N}-\text{CH}_3$	C-N	56.4	DFT-AM1
		52.5	Experimental
		53.6	Corrected
	C-N	52.5	DFT-AM1
		50.0	Experimental
		49.9	Corrected
	C-N	48.4	DFT-AM1
		47.5	Experimental
		46.0	Corrected
	C-N	46.9	DFT-AM1
		43.5	Experimental
		44.6	Corrected
	C-N	63.4	DFT-AM1
		62.0	Experimental
		60.2	Corrected
	C-N	54.8	DFT-AM1
		51.5	Experimental
		52.1	Corrected
	C-N	51.7	DFT-AM1
		50.5	Experimental
		49.1	Corrected

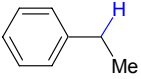
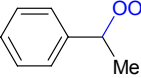
Jursic, B. S. *J. Chem. Soc. Perkin Trans.* **1999**, 2, 369-372

	C-O	78.8	Experimental
		74.3	B3LYP/6-31G(d), 298K
	C-O	76.0	Experimental
		73.4	B3LYP/6-31G(d), 298K


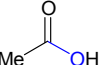
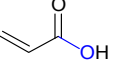
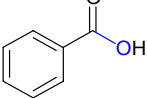
van Scheppingen, W.; Dorrestijn, E.; Arends, I.; Mulder, P.J. *Phys. Chem. A* **1997**, 101, 5404-5411

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
c-C ₆ H ₁₁	C-H	97	Photoacoustic Calorimetry (PAC)
	C-OO	24	
c-C ₆ H ₇	C-H	77	Photoacoustic Calorimetry (PAC)
	C-OO	12, 13	
c-C ₄ H ₈ N	C-H	88.2, (87)	DFT, (Expt)
	C-OO	27.8, (10)	DFT, (Expt)
N(Et) ₂ CHCH ₃	C-H	89.9, 89	DFT, (Expt)
	C-OO	30.2 (25,24)	DFT, (Expt)
C ₄ H ₇ O	C-H	90.7, 91.6, (92)	DFT, (Expt)
	C-OO	32.4, (32)	DFT, (Expt)
C ₄ H ₇ O ₂	C-H	94.6, (96)	DFT, (Expt)
	C-OO	31.6, (34)	DFT, (Expt)
H ₃ C—H	C-H	105.0, 105.7	DFT
		105	Experimental
H ₃ C—OO	C-OO	31.4, 31.1	DFT
		33	Experimental
C ₂ H ₅ —H	C-H	100.3, 101.0	DFT
		101	Experimental
C ₂ H ₅ —OO	C-OO	32.4	DFT
		35	Experimental
C ₃ H ₇ —H	C-H	100.9, 101.6	DFT
		101	Experimental
C ₃ H ₇ —OO	C-OO	33.0	DFT
	C-H	96.4, 97.1	DFT
		98	Experimental
	C-OO	32.3	DFT
		37	Experimental
	C-H	93.2, 94.0	DFT
		96	Experimental
	C-OO	31.4	DFT
		37	Experimental
c-C ₃ H ₅ —H	C-H	106.4, 107.2	DFT
c-C ₃ H ₅ —OO	C-OO	39.5	DFT

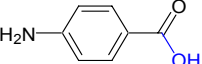
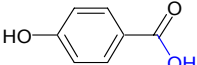
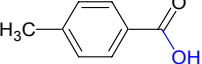
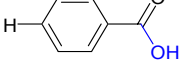
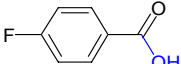
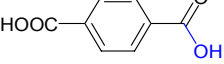
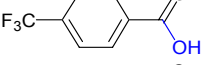
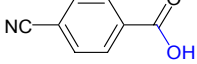
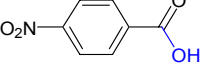
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
<chem>c-C4H7-H</chem>	C-H	97.3, 98.0	DFT
<chem>c-C4H7-OO</chem>	C-OO	34.2	DFT
<chem>c-C6H11-H</chem>	C-H	96.9, 97.6 97	DFT Experimental
<chem>c-C6H11-OO</chem>	C-OO	32.7 24	DFT Experimental
<chem>C2H3-H</chem>	C-H	109.3 111	DFT Experimental
<chem>C2H3-OO</chem>	C-OO	45.2	DFT
	C-H	105.7	DFT
	C-OO	44.1	DFT
	C-H	110.8 113	DFT Experimental
	C-OO	46.2	DFT
	C-H	85.0, 85.9 88	DFT Experimental
	C-OO	14.8 18	DFT Experimental
	C-H	80.2, 81.5 84	DFT Experimental
	C-OO	14.9	DFT
<chem>c-C6H7-H</chem>	C-H	71.4, 72.3 77	DFT Experimental
<chem>c-C6H7-OO</chem>	C-OO	5.9 12	DFT Experimental
	C-H	87.8, 88.6 90	DFT Experimental
	C-OO	18.2 22	DFT Experimental

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	84.8, 85.7 87	DFT Experimental
	C-OO	18.9	DFT
$\text{Cl}_3\text{C}-\text{H}$	C-H	92.1 96	DFT Experimental
$\text{Cl}_3\text{C}-\text{OO}$	C-OO	17.2 20	DFT Experimental

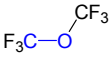
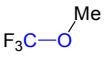
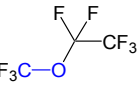
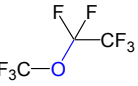
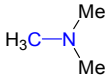
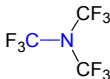
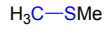
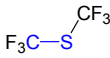
Kranenburg, M.; Ciriano, M. V.; Cherkasov, A.; Mulder, P.J. *Phys. Chem. A* **2000**, *104*, 915-921

	C-OH	108.7	G3
		109.2	G3
		108.9	G3
		109.9	CBS-4M

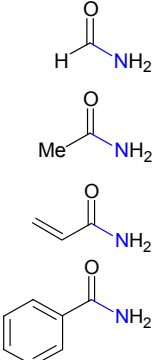
Feng, Y.; Huang, H.; Liu, L.; Guo, Q.-X. *Phys. Chem. Chem. Phys.* **2003**, *5*, 685-690

	C-OH	109.2	
		109.7	
		109.8	
		109.9	
		110.1	
		110.4	
		110.6	
		110.7	
		110.9	

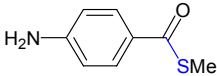
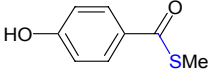
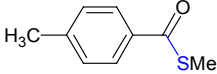
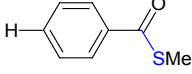
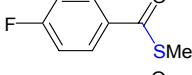
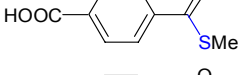
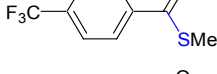
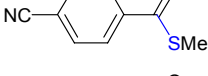
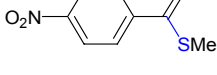
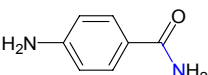
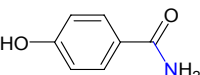
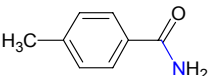
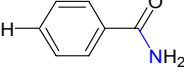
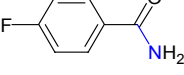
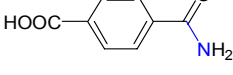
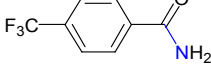
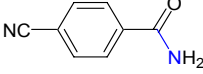
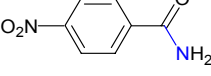
Feng, Y.; Huang, H.; Liu, L.; Guo, Q.-X. *Phys. Chem. Chem. Phys.* **2003**, *5*, 685-690

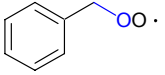
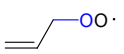
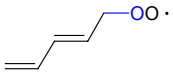
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-O	110.2	G2
		110.5	G2MP2
		110.3	G2MS
	C-O	108.8	G2
		109.3	G2MP2
		109.1	G2MS
	C-O	109.9	G2MP2
		109.8	G2MS
	C-O	108.1	G2MP2
		108.1	G2MS
	C-N	80.8	G2
		81.4	G2MP2
		83.2	G2MS
		75.3	Experimental
	C-N	99.8	Experimental
	C-S	73.2	G2
		74.1	G2MP2
		74.7	G2MS
		73.6	Experimental
	C-S	78.4	Experimental

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	C-N	99.1	G3
		98.5	G3
		98.9	G3
		99.8	CBS-4M

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Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-SMe		
		77.5	ALL <i>ab-initio</i>
		77.9	
		78.1	
		78.3	
		78.4	
		78.9	
		79.1	
		79.3	
		79.5	
	C-NH₂		
		98.2	
		99.1	
		99.4	
		99.8	
		99.7	
		100.7	
		100.8	
		101.0	
		101.3	

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-O	22.2	B3P86-MLM
		21.8	Experimental
		20.6	B3P86-LLM
		21.2	B3P86-MLM
		19.8	B3P86-MLM
		19.7	G3MP2
		19.0	G3
		18.4	Experimental
		15.3	B3P86-LLM
		15.0	B3P86-MLM
		14.0	B3P86-MLM
		15.1	G3MP2
		13.9	G3
		13.4	Experimental

Pratt, D. A.; Mills, J. H.; Porter, N. A. *J. Am. Chem. Soc.* **2003**, *125*, 5801-5810 Reference includes radical stabilization energies