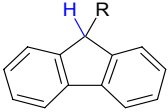
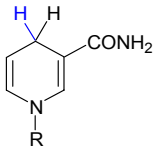
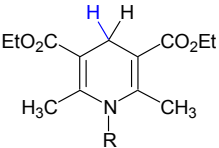
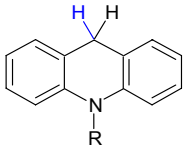


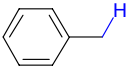

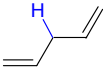
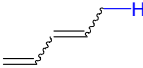
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level

	R = H	C-H	79.5
	R = Me ₃ C		79.4
	R = Ph ₃ C		77.2
	R = Me ₃ Si		82.5
	R = Et ₃ Si		81.2
	R = Ph ₃ Si		80.6
	R = PhSO ₂ CH ₄		99
	R = PhSO ₂ CH ₂ SiMe ₃		99.4
	R = PhSO ₂ CH ₂ SiPh ₃		97.4
	R = PhSO ₂ CH(SiMe ₃) ₂		96.5
	R = PhS(O)(=NSO ₂ Tol)CH ₃		103.1
R = PhS(O)(=NSO ₂ Tol)CH(SiMe ₃) ₂		99.8	
R = PhSO ₂ CH ₂ Ph		90.2	
R = PhSO ₂ CH(CH=CH ₂)(SiMe ₃)		91.1	

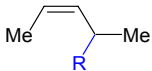
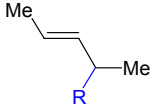
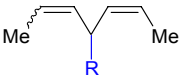
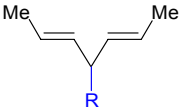


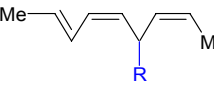
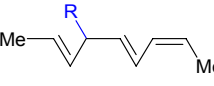
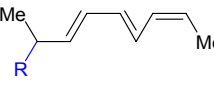

Zhang, S.; Zhang, X-M.; Bordwell, F. G. *J. Am. Chem. Soc.* **1995**, *117*, 602-606.

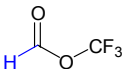
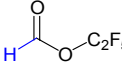
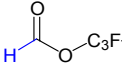
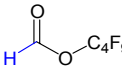
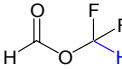
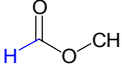
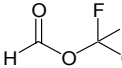
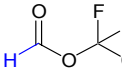
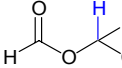
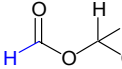
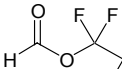
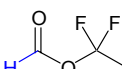
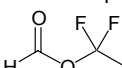
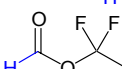
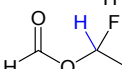
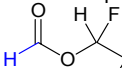
	R = PhCH ₂	C-H heterol. homolysis	64.2 67.9	
	R = 4-CH ₃ OPh	heterolysis homolysis	66.9 69.4	
	R = 4-CH ₃ Ph	heterolysis homolysis	67.5 69.2	
	R = Ph	heterolysis homolysis	68.8 69.2	
	R = 4-ClPh	heterolysis homolysis	70.2 69.1	
	R = 4-BrPh	heterolysis homolysis	70.4 69.2	
	R = 4-CF ₃ Ph	heterolysis homolysis	72.6 69.5	
		R = H	C-H heterol. homolysis	69.3 69.4
		R = CH ₃	heterolysis homolysis	69.9 68.8
			R = CH ₃	C-H heterol. homolysis

Chem. Eur. J. **2003**, *9*(4), 871-880

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
H ₃ C-H	C-H	105.5	B3LYP-LLM
		105.5	B3LYP-MLM1
		105.5	B3LYP-MLM2
		105.8	B3LYP-HLM
		104.9	G3
		105.3	G3MP2
		104.9	Experimental
	C-H	89.3	B3LYP-LLM
		89.4	B3LYP-MLM1
		90.1	B3LYP-MLM2
		90.6	B3LYP-HLM
		91.1	G3
		93.1	G3MP2
		88.5	Experimental
	C-H	86.9	B3LYP-LLM
		87.1	B3LYP-MLM1
		87.9	B3LYP-MLM2
		88.1	B3LYP-HLM
		87.5	G3
		88.6	G3MP2
		88.2	Experimental
	C-H	71.9	B3LYP-LLM
		72.6	B3LYP-MLM1
		74.1	B3LYP-MLM2
		74.2	B3LYP-HLM
		75.6	G3
		77.3	G3MP2
		76.4	Experimental
	C-H	80.7	B3LYP-LLM
		80.8	B3LYP-MLM1
		82.0	B3LYP-MLM2
		82.3	B3LYP-HLM
		82.1	G3
		83.7	G3MP2
		83.5	Experimental
H ₃ C-OO·	C-O	32.7	B3P86-LLM
		35.9	B3P86-MLM
		34.1	B3P86-MLM
		32.4	G3MP2
		32.2	G3
		32.7	Experimental

Pratt, D. A.; Mills, J. H.; Porter, N. A. *J. Am. Chem. Soc.* **2003**, *125*, 5801-581 Reference includes radical stabilization energies

Compound	Bond Dissociation Enthalpy (kcal/mol)			
	Bond (C-Y)	Energy	Theory Level	
	R = OO· R = H	dissociated radical as trans or cis	C-R <i>trans, cis</i> 19.6, 23.1 83.4, 87.0	B3P86-HLM B3LYP-HLM
	R = OO· R = H		20.5, 21.3 84.0, 84.9	B3P86-HLM B3LYP-HLM
	R = OO· R = H		7.9, 7.4 73.1, 72.7	B3P86-HLM B3LYP-HLM
	R = OO· R = H		8.4, 73.5,	B3P86-HLM B3LYP-HLM
	R = OO· R = H		14.2, 77.4 15.3, 78.5	B3P86-HLM B3LYP-HLM
	R = OO· R = H		14.6, 77.7 15.7, 78.8	B3P86-HLM B3LYP-HLM
	R = OO· R = H		4.2 69.8	B3P86-HLM B3LYP-HLM
	R = OO· R = H		6.0 71.5	B3P86-HLM B3LYP-HLM
	R = OO· R = H		9.8, 11.2 72.9, 74.3	B3P86-HLM B3LYP-HLM
	R = OO· R = H		11.7, 12.9 75.1, 76.3	B3P86-HLM B3LYP-HLM

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H Syn Anti	100.4 96.5	All Calculated with DFT (RO)B3LYP/6-311G
	Syn Anti	100.2 96.7	
	Syn Anti	100.2 96.7	
	Syn Anti	100.1 96.8	
	Syn Anti	104.3 105.0	
	Syn Anti	100.2 96.0	
	Syn Anti	102.2 101.9	
	Syn Anti	99.8 96.6	
	Syn Anti	102.2 99.7	
	Syn Anti	100.8 95.3	
	Syn Anti	101.6 101.0	
	Syn Anti	100.1 96.6	
	Syn Anti	100.8 100.9	
	Syn Anti	99.6 96.6	
	Syn Anti	101.8 99.3	
	Syn Anti	100.8 95.4	

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
CH ₃ OCH ₃	C-H	95.7	
CF ₃ OCH ₃		100.7	
CF ₃ OCHF ₂		103.5	
CHF ₂ OCHF ₂		103.4	
CF ₃ CF ₂ OCH ₃		100.9	
CF ₃ CF ₂ CF ₂ OCH ₃		101.1	
(CF ₃) ₂ CFOCH ₃		99.8	
CF ₃ CH ₃		106.0	
CF ₃ CH ₂ F		101.1	
CF ₃ CHF ₂		102.0	
CF ₃ CH ₂ Cl		99.5	
CF ₃ CHCl ₂		95.3	
CF ₃ CHFCI		98.9	
CF ₂ CICH ₃		104.0	
CF ₂ CICH ₂ F		99.6	
CF ₂ CICHF ₂		100.7	
CF ₂ CICH ₂ Cl		98.6	
CF ₂ CICHCl ₂		93.7	
CF ₂ CICHFCI		97.5	
CFCl ₂ CH ₃		102.9	
CFCl ₂ CH ₂ F		98.9	
CFCl ₂ CHF ₂		100.9	
CFCl ₂ CH ₂ Cl		97.5	
CFCl ₂ CHCl ₂		93.7	
CFCl ₂ CHFCI		97.3	
CCl ₃ CH ₃		102.6	
CCl ₃ CH ₂ F		98.6	
CCl ₃ CHF ₂		101.0	
CCl ₃ CH ₂ Cl		97.2	
CCl ₃ CHCl ₂		94.1	
CCl ₃ CHFCI		97.5	
CHF ₂ CHF ₂		102.8	
CF ₃ CHFCF ₃		101.0	
CF ₃ CH ₂ CHF ₂		101.3	
CF ₃ CH ₂ CHF ₂		104.8	
CF ₃ CH ₂ CH ₂ CF ₃		102.3	
CF ₃ CH ₂ CF ₂ CH ₃		102.6	
CF ₃ CH ₂ CF ₂ CH ₃		104.5	
CHF ₂ CF ₂ CF ₂ CHF ₂		102.0	
CF ₃ CF ₂ CH ₂ CH ₂ CF ₂ CF ₃		103.2	
CH ₃ OCH ₂ F		97.4	
CH ₃ OCH ₂ F		97.9	
CH ₃ OCHF ₂		102.8	
CH ₃ OCHF ₂		100.0	
CF ₃ OCH ₃		100.7	
CF ₃ OCHF ₂		103.5	
CH ₂ FOCH ₂ F		99.7	
CHF ₂ OCHF ₂		103.4	
CF ₃ CF ₂ OCH ₃		100.9	

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
CF ₃ CF ₂ CF ₂ OCH ₃	C-H	101.1	
(CF ₃) ₂ CFOCH ₃		99.8	
CH ₃ OCF ₂ CHF ₂		101.8	
CH ₃ OCF ₂ CHF ₂		100.5	
CH ₂ FCF ₂ OCHF ₂		103.9	
CH ₂ FCF ₂ OCHF ₂		101.5	
CHF ₂ CF ₂ OCH ₂ CF ₃		99.5	
CHF ₂ CF ₂ OCH ₂ CF ₃		102.3	
CF ₃ CHF ₂ CF ₂ OCH ₃		100.7	
CF ₃ CHF ₂ CF ₂ OCH ₃		100.6	
CF ₃ CH ₂ OCH ₂ CF ₃		96.9	
CF ₃ CF ₂ CH ₂ OCHF ₂		103.9	
CF ₃ CF ₂ CH ₂ OCHF ₂		98.4	
CHFClCF ₂ OCH ₃		98.8	
CHFClCF ₂ OCH ₃		100.6	
CHF ₂ OCF ₂ CH ₂ Cl		99.1	
CHF ₂ OCF ₂ CH ₂ Cl		103.8	
CHF ₂ OCHClCF ₃		98.3	
CHF ₂ OCHClCF ₃		103.7	

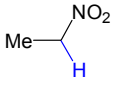
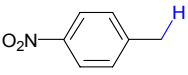
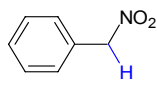
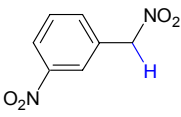
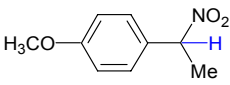
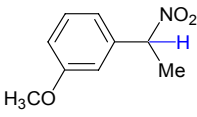
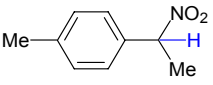
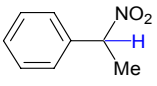
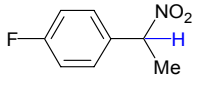
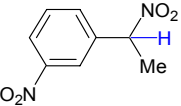
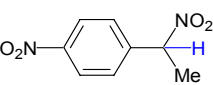
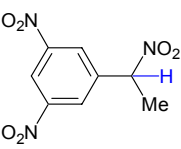
Chandra, A. K.; Uchimaru, T.; Urata, S.; Sugie, M.; Sekiya, A. *J. Chem. Kinetics* **2003**, *35*(3), 130-138


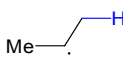
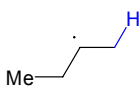
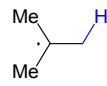
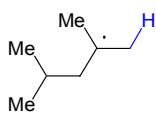
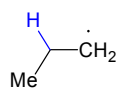
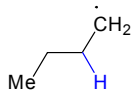
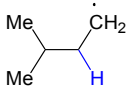
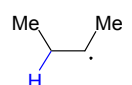
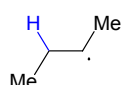


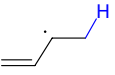
α -Naphthalene	C-H	111.2	
		110.7	B3LYP/6-31+G(d)
β -Naphthalene		111.9	
		110.6	B3LYP/6-31+G(d)

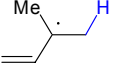
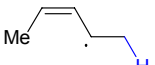
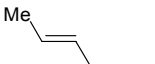
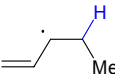

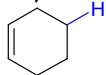
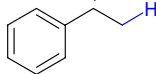
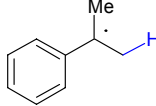
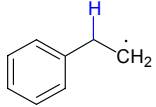




Reed, D. R.; Kass, S. R. *J. Mass Spectrom.* **2000**, *35*, 534-539









CF ₃ -CH ₃	C-H	106.0	
F ₃ C-CH ₂ F		101.1	
F ₃ C-CHF ₂		102.0	
F ₃ C-CH ₂ Cl		99.5	
F ₃ C-CHCl ₂		95.3	
F ₃ C-CH ₂ Cl		98.9	
CF ₂ Cl-CHCl ₂		93.7	
CF ₂ Cl-CH ₂ Cl		97.5	
CFCl ₂ -CH ₂ Cl		97.3	
CCl ₃ -CH ₃		102.6	
CH ₃ OCH ₃		95.7	
CF ₃ OCH ₃		100.7	

Chandra, A. K.; Uchimaru, T.; Urata, S.; Sugie, M.; Sekiya, A. *J. Chem. Kinetics* **2003**, *35*(3), 130-138

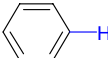

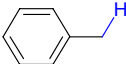
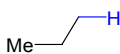
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H homolytic	87	
		86.5	
		85	
		87	
		85	
		87	
		85.5	
		86	
		86	
		87	
		87	
		89	

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H (0°K)	35.6	CBS-4
	298°K	36.3	CBS-4
	Experimental	35.2	
	0°K	35.6	CBS-4
	298°K	36.4	CBS-4
	Experimental	35.0	
	0°K	35.6	CBS-4
	298°K	36.3	CBS-4
	Experimental	34.9	
	0°K	35.4	CBS-4
	298°K	36.2	CBS-4
	Experimental	34.9	
	0°K	35.4	CBS-4
	298°K	36.2	CBS-4
	Experimental	33.3	
	0°K	32.3	CBS-4
	298°K	33.2	CBS-4
	Experimental	31.9	
	0°K	32.6	CBS-4
	298°K	33.4	CBS-4
	Experimental	32.0	
	0°K	29.8	CBS-4
	298°K	30.8	CBS-4
	Experimental	29.7	
 	0°K <i>cis</i>	34.1	CBS-4
	<i>trans</i>	32.5	CBS-4
	298°K <i>cis</i>	35.0	CBS-4
	<i>trans</i>	33.5	CBS-4
	Experimental <i>cis</i>	33.2	
	<i>trans</i>	32.2	
	0°K	33.9	CBS-4
	298°K	35.0	CBS-4
	Experimental	34.0	
	0°K	33.1	CBS-4
	298°K	34.2	CBS-4
	Experimental	32.5	
	0°K	48.1	CBS-4
	298°K	49.2	CBS-4
	Experimental	47.6	

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H (0°K)	47.7	CBS-4
	298°K	48.5	CBS-4
	Experimental	47.5	
	0°K	45.2	CBS-4
	298°K	46.4	CBS-4
	Experimental	44.2	
	0°K	47.5	CBS-4
	298°K	48.5	CBS-4
	Experimental	44.6	
	0°K <i>cis</i>	45.7	CBS-4
	<i>trans</i>	44.8	CBS-4
	298°K <i>cis</i>	46.9	CBS-4
	<i>trans</i>	46.0	CBS-4
	Experimental <i>cis</i>	45.5	
	<i>trans</i>	44.3	
	0°K	44.6	CBS-4
	298°K	45.6	CBS-4
	Experimental	45.8	
	0°K	49.4	CBS-4
	298°K	50.6	CBS-4
	Experimental	49.3	
	0°K	44.6	CBS-4
	298°K	45.5	CBS-4
	Experimental	47.5	
	0°K	44.3	CBS-4
	298°K	45.2	CBS-4
	0°K	29.7	CBS-4
	298°K	30.5	CBS-4
	Experimental	32.5	
	0°K	109.0	CBS-4
	298°K	110.6	CBS-4
	Experimental	110	
	0°K	37.9	CBS-4
	298°K	39.1	CBS-4
	Experimental	35.6	
	0°K	105.8	CBS-4
	298°K	107.4	CBS-4
	0°K	35.0	CBS-4
	298°K	36.1	CBS-4
	Experimental	36.2	

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H (0°K)	110.0	CBS-4
	298°K	111.5	CBS-4
	0°K	30.7	CBS-4
	298°K	31.9	CBS-4
	0°K	109.6	CBS-4
	298°K	111.1	CBS-4
	0°K	31.1	CBS-4
	298°K	32.3	CBS-4
	0°K	57.2	CBS-4
	298°K	58.6	CBS-4
	0°K	54.0	CBS-4
	298°K	55.0	CBS-4
	Experimental	60.0	
	0°K	53.5	CBS-4
	298°K	54.7	CBS-4

Zhang, X.-M.J. *Org. Chem.* **1998**, *63*, 1872-1877

	C-H	111.4	Experimental
		110.9	B3LYP/6-31G(d), 298K
		110.6	B3LYP/6-311++G(d,p), 298K
		108.9	Experimental
		109.3	B3LYP/6-31G(d), 298K
		108.3	B3LYP/6-311++G(d,p), 298K
		88.5	Experimental
		87.9	B3LYP/6-31G(d), 298K
		88.1	Experimental
		85.1	B3LYP/6-31G(d), 298K
		84.1	B3LYP/6-311++G(d,p), 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
CH ₄	C-H	106.0	(RO) B3LYP
		118.9	(RO) B3PW86
		106.2	(RO) B3PW91
		102.3	(RO) PW91LYP
		105.1	B3LYP 6-311G(d,p)
		105.5	(RO)B3LYP 6-311++G(3df,2p)
		102.8	MP2/cc-pVtz
		104.9	Experimental
CH ₃ F		100.6	(RO) B3LYP
		113.3	(RO) B3PW86
		100.7	(RO) B3PW91
		95.3	(RO) PW91LYP
		99.7	B3LYP 6-311G(d,p)
		101.1	(RO)B3LYP 6-311++G(3df,2p)
		99.7	MP2/cc-pVtz
101.3	Experimental		
CH ₂ F ₂		100.3	(RO) B3LYP
		113.1	(RO) B3PW86
		100.4	(RO) B3PW91
		94.4	(RO) PW91LYP
		99.7	B3LYP 6-311G(d,p)
		100.7	(RO)B3LYP 6-311++G(3df,2p)
		100.0	MP2/cc-pVtz
103.2	Experimental		
CHF ₃		104.9	B3LYP 6-311G(d,p)
		105.4	(RO)B3LYP 6-311G(d,p)
		105.3	(RO)B3LYP 6-311++G(3df,2p)
		105.1	MP2/cc-pVtz
		106.7	Experimental
CH ₃ Cl		100.6	(RO) B3LYP
		113.1	(RO) B3PW86
		100.6	(RO) B3PW91
		95.7	(RO) PW91LYP
		99.6	B3LYP 6-311G(d,p)
		99.5	(RO)B3LYP 6-311++G(3df,2p)
		97.7	MP2/cc-pVtz
100.1	Experimental		
CHCl ₃		93.1	B3LYP 6-311G(d,p)
		93.9	(RO)B3LYP 6-311G(d,p)
		92.1	(RO)B3LYP 6-311++G(3df,2p)
		93.2	MP2/cc-pVtz
		93.8	Experimental

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
CH ₂ Cl ₂	C-H	96.9	(RO) B3LYP
		109.3	(RO) B3PW86
		96.8	(RO) B3PW91
		91.6	(RO) PW91LYP
		96.0	B3LYP 6-311G(d,p)
		95.4	(RO)B3LYP 6-311++G(3df,2p)
		93.8	MP2/cc-pVtz
		96.2	Experimental
CH ₂ FCI		98.2	B3LYP 6-311G(d,p)
		99.0	(RO)B3LYP 6-311G(d,p)
		98.4	(RO)B3LYP 6-311++G(3df,2p)
		100.8	Experimental
CHF ₂ Cl		100.5	B3LYP 6-311G(d,p)
		101.1	(RO)B3LYP 6-311G(d,p)
		100.4	(RO)B3LYP 6-311++G(3df,2p)
		100.7	Experimental
CHFCl ₂		96.8	B3LYP 6-311G(d,p)
		97.5	(RO)B3LYP 6-311G(d,p)
		96.2	(RO)B3LYP 6-311++G(3df,2p)
		98.9	Experimental
CH ₃ Br		100.2	B3LYP 6-311G(d,p)
		101.2	(RO)B3LYP 6-311G(d,p)
		100.9	(RO)B3LYP 6-311++G(3df,2p)
		98.9	MP2/cc-pVtz
		101.6	Experimental
CH ₂ Br ₂		96.1	B3LYP 6-311G(d,p)
		97.0	(RO)B3LYP 6-311G(d,p)
		96.8	(RO)B3LYP 6-311++G(3df,2p)
		96.3	MP2/cc-pVtz
		99.7	Experimental
CHBr ₃		91.7	B3LYP 6-311G(d,p)
		92.6	(RO)B3LYP 6-311G(d,p)
		92.4	(RO)B3LYP 6-311++G(3df,2p)
		93.2	MP2/cc-pVtz
		96.0	Experimental
CH ₂ FBr		98.1	B3LYP 6-311G(d,p)
		98.8	(RO)B3LYP 6-311G(d,p)
		98.5	(RO)B3LYP 6-311++G(3df,2p)

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
CHF ₂ Br	C-H	98.9	B3LYP 6-311G(d,p)
		99.5	(RO)B3LYP 6-311G(d,p)
		99.1	(RO)B3LYP 6-311++G(3df,2p)
CHFBr ₂		94.9	B3LYP 6-311G(d,p)
		95.6	(RO)B3LYP 6-311G(d,p)
		94.6	(RO)B3LYP 6-311++G(3df,2p)
CH ₂ ClBr		96.1	B3LYP 6-311G(d,p)
		97.0	(RO)B3LYP 6-311G(d,p)
		96.2	(RO)B3LYP 6-311++G(3df,2p)
CHCl ₂ Br		92.6	B3LYP 6-311G(d,p)
		93.4	(RO)B3LYP 6-311G(d,p)
		92.2	(RO)B3LYP 6-311++G(3df,2p)
CHBr ₂ Cl		92.2	B3LYP 6-311G(d,p)
		93.0	(RO)B3LYP 6-311G(d,p)
		92.2	(RO)B3LYP 6-311++G(3df,2p)
CHFClBr		95.8	B3LYP 6-311G(d,p)
		96.6	(RO)B3LYP 6-311G(d,p)
		95.9	(RO)B3LYP 6-311++G(3df,2p)
HOH		114.2	B3LYP 6-311G(d,p)
		115.1	(RO)B3LYP 6-311G(d,p)
		118.4	(RO)B3LYP 6-311++G(3df,2p)
		119.0	Experimental

Chandra, A. K.; Uchimaru, T. *J. Phys. Chem. A* **2000**, *104*, 9244-9249





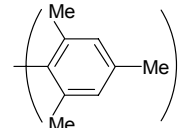
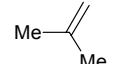
F ₃ C—CH ₃	C-H	106.0	(RO)B3LYP 6-311G(d,p)
		105.8	(RO)B3LYP 6-311++G(3df,2p)
		106.7	Experimental
F ₃ C—CH ₂ F		101.1	(RO)B3LYP 6-311G(d,p)
		101.1	(RO)B3LYP 6-311++G(3df,2p)
F ₃ C—CHF ₂		102.0	(RO)B3LYP 6-311G(d,p)
		101.7	(RO)B3LYP 6-311++G(3df,2p)
		102.7	Experimental
F ₃ C—CH ₂ Cl		99.5	(RO)B3LYP 6-311G(d,p)
		98.3	(RO)B3LYP 6-311++G(3df,2p)
		101.8	Experimental
F ₃ C—CHCl ₂		95.3	(RO)B3LYP 6-311G(d,p)
		93.6	(RO)B3LYP 6-311++G(3df,2p)
		95.3	Experimental
F ₃ C—CHFCI		98.9	(RO)B3LYP 6-311G(d,p)
		97.8	(RO)B3LYP 6-311++G(3df,2p)
		99.2	Experimental

Chandra, A. K.; Uchimaru, T. *J. Phys. Chem. A* **2000**, *104*, 9244-9249

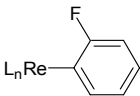
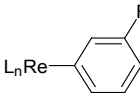
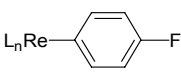
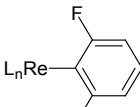
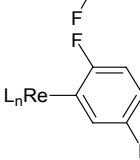
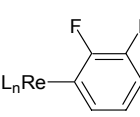
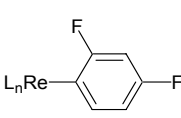
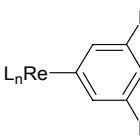
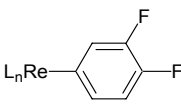
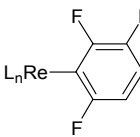
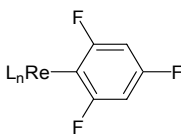
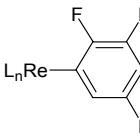
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
CF ₂ Cl—CH ₃	C-H	104.0	(RO)B3LYP 6-311G(d,p)
		103.8	(RO)B3LYP 6-311++G(3df,2p)
CF ₂ Cl—CH ₂ F		99.6	(RO)B3LYP 6-311G(d,p)
		100.0	(RO)B3LYP 6-311++G(3df,2p)
CF ₂ Cl—CHF ₂		100.7	(RO)B3LYP 6-311G(d,p)
		100.4	(RO)B3LYP 6-311++G(3df,2p)
CF ₂ Cl—CH ₂ Cl		98.6	(RO)B3LYP 6-311G(d,p)
		97.6	(RO)B3LYP 6-311++G(3df,2p)
CF ₂ Cl—CHCl ₂		93.7	(RO)B3LYP 6-311G(d,p)
		92.1	(RO)B3LYP 6-311++G(3df,2p)
CF ₂ Cl—CHFCI		97.5	(RO)B3LYP 6-311G(d,p)
		96.4	(RO)B3LYP 6-311++G(3df,2p)
CFCl ₂ —CH ₃		102.9	(RO)B3LYP 6-311G(d,p)
		102.9	(RO)B3LYP 6-311++G(3df,2p)
CFCl ₂ —CH ₂ F		98.9	(RO)B3LYP 6-311G(d,p)
		98.9	(RO)B3LYP 6-311++G(3df,2p)
CFCl ₂ —CHF ₂		100.9	(RO)B3LYP 6-311G(d,p)
		100.6	(RO)B3LYP 6-311++G(3df,2p)
CFCl ₂ —CH ₂ Cl		97.5	(RO)B3LYP 6-311G(d,p)
		96.7	(RO)B3LYP 6-311++G(3df,2p)
CFCl ₂ —CHCl ₂		93.7	(RO)B3LYP 6-311G(d,p)
		92.2	(RO)B3LYP 6-311++G(3df,2p)
CFCl ₂ —CHFCI		97.3	(RO)B3LYP 6-311G(d,p)
		96.2	(RO)B3LYP 6-311++G(3df,2p)
CCl ₃ —CH ₃		102.6	(RO)B3LYP 6-311G(d,p)
		102.5	(RO)B3LYP 6-311++G(3df,2p)
CCl ₃ —CH ₂ F		98.6	(RO)B3LYP 6-311G(d,p)
		98.7	(RO)B3LYP 6-311++G(3df,2p)
CCl ₃ —CHF ₂		101.0	(RO)B3LYP 6-311G(d,p)
		100.7	(RO)B3LYP 6-311++G(3df,2p)
CCl ₃ —CH ₂ Cl		97.2	(RO)B3LYP 6-311G(d,p)
		96.2	(RO)B3LYP 6-311++G(3df,2p)
CCl ₃ —CHCl ₂		94.1	(RO)B3LYP 6-311G(d,p)
		92.5	(RO)B3LYP 6-311++G(3df,2p)
		94.9	Experimental
CCl ₃ —CHFCI		97.5	(RO)B3LYP 6-311G(d,p)
		96.4	(RO)B3LYP 6-311++G(3df,2p)

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
CH ₃ —H	C-H	102.8	corrected MP2/cc-pVtz
		103.8	CCSD(T)/6-311++G(3df,3pd)
		105.1	Experimental
CH ₂ F—H		99.7	corrected MP2/cc-pVtz
		98.5	CCSD(T)/6-311++G(3df,3pd)
		101.3	Experimental
CH ₂ Cl—H		97.7	corrected MP2/cc-pVtz
		96.6	CCSD(T)/6-311++G(3df,3pd)
		99.5	Experimental
CH ₂ Br—H		98.9	corrected MP2/cc-pVtz
		97.6	CCSD(T)/6-311++G(3df,3pd)
		101.6	Experimental
CHF ₂ —H		100.0	corrected MP2/cc-pVtz
		101.3	Experimental
CHCl ₂ —H		93.8	corrected MP2/cc-pVtz
		95.6	Experimental
CHBr ₂ —H		96.3	corrected MP2/cc-pVtz
		99.7	Experimental
CF ₃ —H		105.1	corrected MP2/cc-pVtz
		106.7	Experimental
CCl ₃ —H		93.2	corrected MP2/cc-pVtz
		95.8	Experimental
CBr ₃ —H		93.2	corrected MP2/cc-pVtz
		96	Experimental

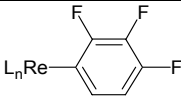
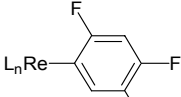
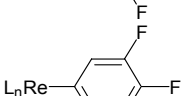
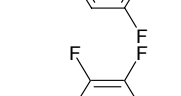
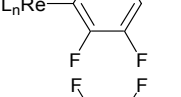
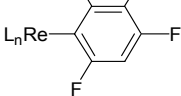
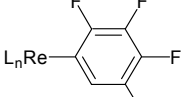
McGovern, W. S.; D.-K., A.; North, S. W.; Francisco, J. S. *J. Phys. Chem. A* **2000**, *104*, 436-442

Tp ⁺ Rh(CNneo)(R)H	R = Ph	C-H	113.5
	R = 		109.7
	R = Me		104.9
	R = <i>n</i> -pentyl 		98
	R = cyclopentyl 		96.4
	R = cyclohexyl 		96
	R = Mesityl 		88.5
	R = Methallyl 		85.6

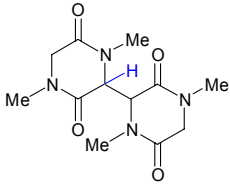
Wick, D. D.; Jones, W. D. *Organometallics* **1999**, *18*, 495-505

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
$\text{Re}(\text{Cp})(\text{CO})_2(\text{H})(\text{R})$ R = Ph	C-Re	252.0	All calculated with B3PW91 (Hybrid DFT)
	C-H	489.8	
R = 	C-Re	276.9	
	C-H	500.5	
R = 	C-Re	253.5	
	C-H	490.6	
R = 	C-Re	255.3	
	C-H	494.3	
R = 	C-Re	300.0	
	C-H	512.0	
R = 	C-Re	278.7	
	C-H	501.2	
R = 	C-Re	278.1	
	C-H	500.3	
R = 	C-Re	279.9	
	C-H	504.6	
R = 	C-Re	255.4	
	C-H	492.0	
R = 	C-Re	256.1	
	C-H	494.5	
R = 	C-Re	301.2	
	C-H	511.8	
R = 	C-Re	302.7	
	C-H	515.5	
R = 	C-Re	280.4	
	C-H	501.7	

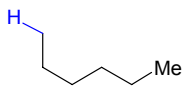
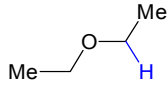
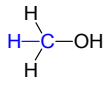
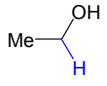
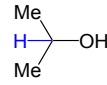
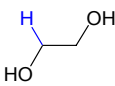

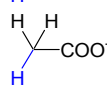
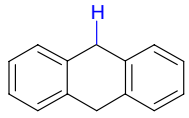
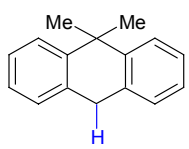
Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level

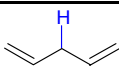
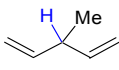
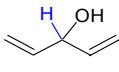
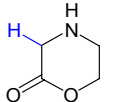
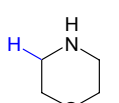
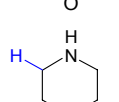
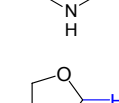
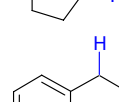
$\text{Re}(\text{Cp})(\text{CO})_2(\text{H})(\text{R})$	 $\text{R} = \text{L}_n\text{Re}-\text{C}_6\text{H}_2\text{F}_5$	C-Re C-H	280.8 503.6	All calculated with B3PW91 (Hybrid DFT)
	 $\text{R} = \text{L}_n\text{Re}-\text{C}_6\text{H}_2\text{F}_5$	C-Re C-H	281.0 504.8	
	 $\text{R} = \text{L}_n\text{Re}-\text{C}_6\text{H}_2\text{F}_5$	C-Re C-H	257.4 495.0	
	 $\text{R} = \text{L}_n\text{Re}-\text{C}_6\text{H}_2\text{F}_5$	C-Re C-H	304.7 512.4	
	 $\text{R} = \text{L}_n\text{Re}-\text{C}_6\text{H}_2\text{F}_5$	C-Re C-H	304.0 514.7	
	 $\text{R} = \text{L}_n\text{Re}-\text{C}_6\text{H}_2\text{F}_5$	C-Re C-H	283.0 504.4	
	 $\text{R} = \text{L}_n\text{Re}-\text{C}_6\text{H}_2\text{F}_5$	C-Re C-H	306.7 514.7	

Clot, E.; Besora, M.; Maseras, F.; Megret, C.; Eisenstein, O.; Oelckers, B.; Perutz, R. N. *Chem. Commun.* **2003**, 490-491
(kcal/mol)

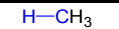

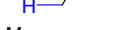



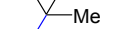

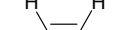

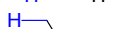
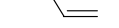
	RSE	6.3	C-H	92.4
---	-----	-----	-----	------

Brocks, J. J.; Welle, F. M.; Beckhaus, H.-D.; Rüchardt, C. *Tet. Lett.* **1997**, 38(44), 7721-7724










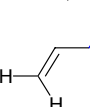

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Solvent
	C-H	77	isooctane
		93	isooctane
		92	water
		92	water
		89	water
		90	water
$(\text{CH}_2(-\text{H}))_3\text{OH}$		99	water
		96	water
		92	water
		78	benzene
		77	benzene












Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Solvent
	C-H	77	benzene
		77	benzene
		69	benzene
		78	benzene
		94	benzene
		93	benzene
		92	THF
		83	tetralin

Laarhoven, L. J. J.; Mulder, P.; Wayner, D. D. *M.Acc. Chem. Res.* **1999**, 32, 342-349






	C-H	104.9	
		101.1	
		98.6	
		96.5	
		96.5	
		110.7	
		88.8	
		112.9	
		89.7	
		104.6	
		88.1	
		89.4	

Blanksby, S. J.; Ellison, G. B. *Acc. Chem. Res.* **2003**, 36, 255

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
$\text{H}-\text{CH}_3$	C-H	104.99	
$\text{H}-\text{CH}_2$		110.4	
$\text{H}-\text{CH}$		101.3	
$\text{H}-\text{CN}$		126.3	
$\text{H}-\text{C}$		80.9	
		101.1	
		98.6	
		98.2	
		96.5	
		110.7	
$\text{H}-\text{C}\equiv\text{C}-\text{H}$		133.32	
		112.9	
		78	
		94	
		109	
	88.8		
	89.8		

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	101.1	
		110.7	
		35.7	
		83	
		35.4	
		133.32	
		86	
		112.9	
		78	
		94	
		109	

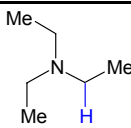
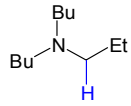
Blanksby, S. J.; Ellison, G. B. *Acc. Chem. Res.* **2003**, *36*, 255

	C-H	96.1	
		22.0	
		105	
		88.0	
		-12	

Blanksby, S. J.; Ellison, G. B. *Acc. Chem. Res.* **2003**, *36*, 255




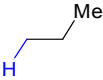
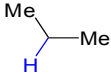




Compound	Resultant Radical	Bond Dissociation Enthalpy (kJ/mol)		
		Bond (C-Y)	Energy	Bond Enthalpy Terms (<i>E</i>)
CH		C-H	341	
HCH			426	
HCH ₂			458	
HCH ₃			439.4	
C ₂ H			485	
C ₂ H ₂			555	
C ₂ H ₄			461	
C ₂ H ₆			421	410.8
C ₃ H ₆			363	410.8
C ₃ H ₈	Pr		418	410.8
	<i>i</i> -Pr		406	407.0
C ₄ H ₁₀	Bu		418	410.8
	<i>s</i> -Bu		406	407.0
Me ₃ CH	<i>i</i> -Bu		420	410.8
	<i>t</i> -Bu		396	403.9
CpH			347	
<i>c</i> -C ₅ H ₁₀			395	
C ₅ H ₁₂			418	410.8
Me ₃ CCH ₃			418	410.8
C ₆ H ₆			465	420.6
<i>c</i> -C ₆ H ₁₂			400	407.0
2,3-Me ₂ C ₄ H ₈	2,3-Me ₂ Bu		418	410.8
PhCH ₃	Bz		368	410.8
	MeC ₆ H ₄		465	420.6
PhCCH			553	435
PhCH ₂ Me			357	407.0
<i>c</i> -C ₅ Me ₅			368	

Simões, J.A.M.; Beauchamp, J.L. *Chem. Rev.* **1990**, *90*, 629-688

	C-H	381	Experimental
		379.5	Estimated
		381	Experimental
		370.2	Estimated
H ₃ C-H		438.56	

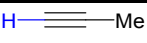


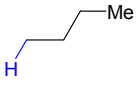
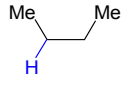
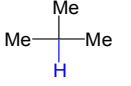
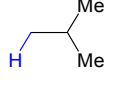
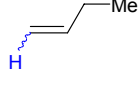
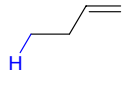
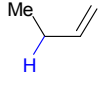
Cherkasov, A.; Jonsson, M.J. *Chem. Inf. Comput. Sci.* **2000**, *40*, 1222-1226

Compound	Resultant Radical	Bond Dissociation Enthalpy (kJ/mol)		
		Bond (C-Y)	Energy	Bond Enthalpy Terms (<i>E</i>)
BuCH ₂ OH		C-H	389	401.7
PhOH			362	451.2
PhC(O)H			371	426.6
CF ₂ H			274	
CF ₃ H			447	420
CH ₂ F			359	
CH ₃ F			424	
CH ₂ F ₂			430	
CF ₃ C(O)H			381	426.6
CF ₃ CH ₂ OH			436	451.2
C ₆ F ₅ OH			362	451.2
HCl			432.0	
HBr			366.3	
HI			298.4	
SiH ₃			304	
SiMe ₄			415	
HCO	H		63	
MeCO	Me		61	
EtCO	Et		49	
PrCO	Pr		46	
PhCO	Ph		104	
Me ₂ CO	MeCO		340	
MeC(O)Cl	MeCO		340	
PhC(O)Cl	PhCO		343	
Mel			238	
C ₂ H ₃ I	C ₂ H ₃		272	
Etl			235	
C ₃ H ₅ I	C ₃ H ₅		180	
Prl			235	
<i>i</i> -Prl			232	
Bul			237	
Phl			273	
Bzl			207	
PhCH ₂ CH ₂ I			237	
Me(CEt) ₂ ⁻			237	
PhCCI			319	
Me ₃ SiCH ₂ I			232	
I ₂			151.3	
PhC(O)I			212	
MeC(O)I	MeCO		209	

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
CH ₄	C-H	421.1	B3LYP
		427.4	KMLYP
		439.5	CBS-Q
		438.9	Experimental
	C-H	411.6	B3LYP
		419.3	KMLYP
		425.5	CBS-Q
		420.7	Experimental
	C-H	465.0	B3LYP
		476.6	KMLYP
		462.0	CBS-Q
		464.7	Experimental
	C-H	563.3	B3LYP
		572.9	KMLYP
		557.6	CBS-Q
		556.1	Experimental
	C-H	413.0	B3LYP
		424.0	KMLYP
		426.9	CBS-Q
		422.7	Experimental
	C-H	394.4	B3LYP
		405.4	KMLYP
		414.9	CBS-Q
		416.8	Experimental
	C-H	350.9	B3LYP
		359.5	KMLYP
		361.3	CBS-Q
		361.9	Experimental
	C-H	458.2	B3LYP
		468.9	KMLYP
		471.7	CBS-Q
	C-H	436.3	B3LYP
		447.7	KMLYP
		452.1	CBS-Q
	C-H	364.1	B3LYP
		377.2	KMLYP
		380.1	CBS-Q
		339.0	Experimental

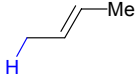
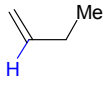

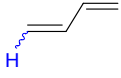

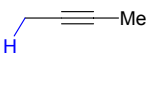
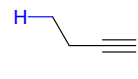
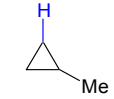
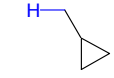
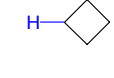
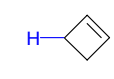
Senosiain, J. P.; Han, J. H.; Musgrave, C. B.; Golden, D. M *Faraday Discuss.* **2001**, *119*, 173-189

Reference includes radical stabilization energies

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	562.2	B3LYP
		570.2	KMLYP
		566.1	CBS-Q
		441.3	B3LYP
		452.6	KMLYP
		458.5	CBS-Q
		444.8	Experimental
		406.5	B3LYP
		413.8	KMLYP
		421.3	CBS-Q
		379.1	Experimental
		409.8	B3LYP
		418.0	KMLYP
		427.6	CBS-Q
		425.4	Experimental
		393.9	B3LYP
		404.0	KMLYP
		413.0	CBS-Q
		411.2	Experimental
		383.9	B3LYP
		396.4	KMLYP
		409.1	CBS-Q
		404.3	Experimental
		413.9	B3LYP
		423.0	KMLYP
		427.6	CBS-Q
		425.2	Experimental
		413.8	B3LYP
		422.2	KMLYP
		471.2	CBS-Q
		415.4	B3LYP
		424.6	KMLYP
		427.9	CBS-Q
		333.9	B3LYP
		343.3	KMLYP
		347.9	CBS-Q



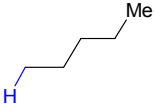
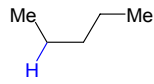
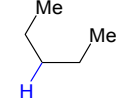
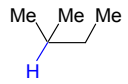
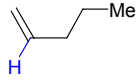
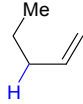
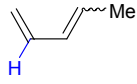
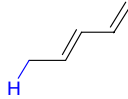
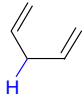
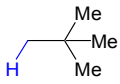
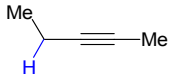
Senosiain, J. P.; Han, J. H.; Musgrave, C. B.; Golden, D. M *Faraday Discuss.* **2001**, *119*, 173-189

Reference includes radical stabilization energies

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	348.1	B3LYP
		357.3	KMLYP
		360.5	CBS-Q
		358.2	Experimental
		447.3	B3LYP
		459.4	KMLYP
		402.1	B3LYP
		414.2	KMLYP
		408.8	CBS-Q
		462.5	B3LYP
		471.7	KMLYP
		468.3	CBS-Q
		357.8	B3LYP
		367.2	KMLYP
		364.5	CBS-Q
		358.2	Experimental
		359.9	B3LYP
		373.7	KMLYP
		355.1	CBS-Q
		364.8	Experimental
		421.1	B3LYP
		429.7	KMLYP
		427.5	CBS-Q
		425.2	B3LYP
		439.0	KMLYP
		399.1	B3LYP
		411.3	KMLYP
		413.8	CBS-Q
		407.5	Experimental
		401.3	B3LYP
		411.3	KMLYP
		419.0	CBS-Q
		403.8	Experimental
		366.2	B3LYP
		373.8	KMLYP
		376.2	CBS-Q

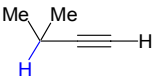





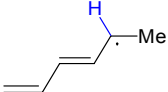





Senosiain, J. P.; Han, J. H.; Musgrave, C. B.; Golden, D. M *Faraday Discuss.* **2001**, *119*, 173-189

Reference includes radical stabilization energies

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	459.0	B3LYP
		472.7	KMLYP
		467.5	CBS-Q
		460.5	B3LYP
		472.8	KMLYP
		474.0	CBS-Q
		413.9	B3LYP
		415.9	KMLYP
		428.3	CBS-Q
		396.6	B3LYP
		398.9	KMLYP
		394.6	B3LYP
		404.9	KMLYP
		386.6	B3LYP
		400.1	KMLYP
		404.0	Experimental
		439.0	B3LYP
		450.8	KMLYP
		338.2	B3LYP
		348.6	KMLYP
		383.0	B3LYP
		402.7	KMLYP
		325.6	B3LYP
		334.5	KMLYP
		333.5	CBS-Q
		347.0	Experimental
		289.9	B3LYP
		296.2	KMLYP
		318.0	Experimental
		415.8	B3LYP
		425.9	KMLYP
		418.0	Experimental
		344.0	B3LYP
		358.2	KMLYP
		365.3	Experimental

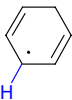
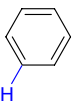
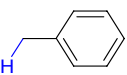
Senosiain, J. P.; Han, J. H.; Musgrave, C. B.; Golden, D. M *Faraday Discuss.* **2001**, *119*, 173-189

Reference includes radical stabilization energies

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	335.4	B3LYP
		350.2	KMLYP
		338.9	Experimental
		324.9	B3LYP
		334.2	KMLYP
		323.0	Experimental
		386.9	B3LYP
		395.1	KMLYP
		406.5	CBS-Q
		403.5	Experimental
		334.1	B3LYP
		336.0	KMLYP
		347.1	CBS-Q
		344.3	Experimental
		389.2	B3LYP
		389.6	KMLYP
		406.4	CBS-Q
		329.9	B3LYP
		344.4	KMLYP
		346.7	Experimental
		308.9	B3LYP
		318.0	KMLYP
		397.9	B3LYP
		409.0	KMLYP
		399.6	Experimental
		446.3	B3LYP
		459.3	KMLYP
		333.1	B3LYP
		342.8	KMLYP
		396.7	B3LYP
		407.5	KMLYP
		296.7	B3LYP
		305.5	KMLYP
		305.0	Experimental

Senosiain, J. P.; Han, J. H.; Musgrave, C. B.; Golden, D. *MFaraday Discuss.* **2001**, *119*, 173-189



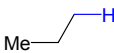

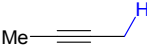
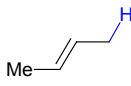

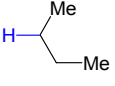


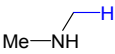
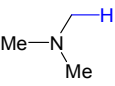
Reference includes radical stabilization energies

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
		296.6	B3LYP
		308.8	KMLYP
		305.4	Experimental
		462.3	B3LYP
		474.0	KMLYP
		473.1	Experimental
		361.7	B3LYP
		371.8	KMLYP
		375.7	Experimental


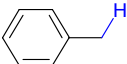
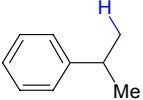
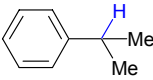



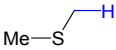


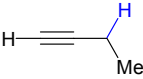


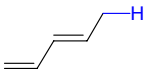

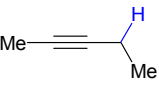
Senosiain, J. P.; Han, J. H.; Musgrave, C. B.; Golden, D. *MFaraday Discuss.* **2001**, *119*, 173-189

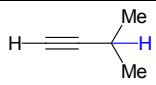
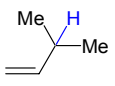
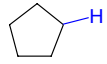
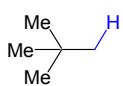
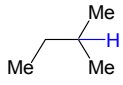
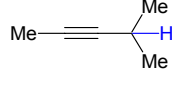
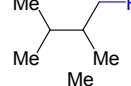
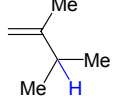
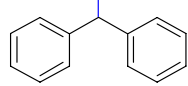
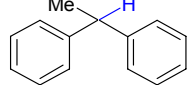
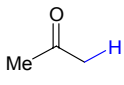
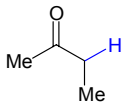
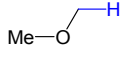
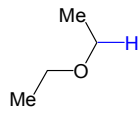


Reference includes radical stabilization energies

















(kJ/mol)


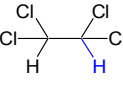
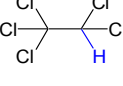
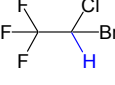
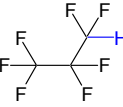
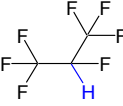
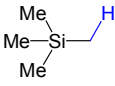
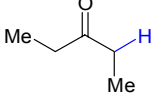
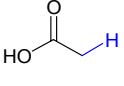

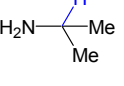
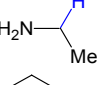
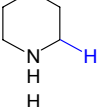
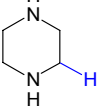
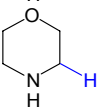
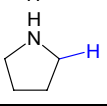
Compound	C-H	Energy	Theory Level
$\text{H}-\text{CH}_3$		438.9	Experimental
		429.7	Estimated
		423	Experimental
		420.7	Estimated
		374	Experimental
		365.6	Estimated
		420	Experimental
		416.7	Estimated
		412.5	Experimental
		411.6	Estimated
		364.8	Experimental
		364.1	Estimated
		358.2	Experimental
		349.0	Estimated
		358.2	Experimental
		347.1	Estimated
		410.9	Experimental
		414.8	Estimated
		403.8	Experimental
		402.6	Estimated
		392.9	Experimental
		386.0	Estimated
		386	Experimental
		396.5	Estimated
		387	Experimental
		392.2	Estimated



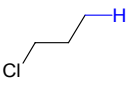
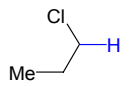


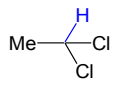



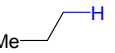

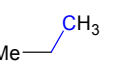
Cherkasov, A.; Jonsson, M.J. *Chem. Inf. Comput. Sci.* **2000**, *40*, 1222-1226

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	394.6	Experimental
		404.6	Estimated
	C-H	370.3	Experimental
		381.9	Estimated
	C-H	357.3	Experimental
		372.8	Estimated
	C-H	353.1	Experimental
		363.8	Estimated
	C-H	376.1	Experimental
		377.0	Estimated
	C-H	361.9	Experimental
		367.9	Estimated
	C-H	392.9	Experimental
		390.4	Estimated
	C-H	384.9	Experimental
		387.4	Estimated
	C-H	446.4	Experimental
		441.9	Estimated
	C-H	361.9	Experimental
		350.7	Estimated
	C-H	347.7	Experimental
		356.6	Estimated
	C-H	403.8	Experimental
		407.5	Estimated
	C-H	345.2	Experimental
		341.7	Estimated
	C-H	347	Experimental
		335.8	Estimated
	C-H	319.7	Experimental
		330.0	Estimated
	C-H	365.3	Experimental
		355.1	Estimated

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	338.9	Experimental
		347.6	Estimated
		323	Experimental
		332.6	Estimated
		403.5	Experimental
		404.1	Estimated
		418	Experimental
		408.8	Estimated
		404	Experimental
		398.6	Estimated
		344.3	Experimental
		346.0	Estimated
		326.4	Experimental
		342.1	Estimated
		319.2	Experimental
		329.0	Estimated
		340.6	Experimental
		334.1	Estimated
		339	Experimental
		325.0	Estimated
		411.3	Experimental
		401.0	Estimated
		386.2	Experimental
		392.0	Estimated
		389	Experimental
		396.1	Estimated
		383.7	Experimental
		382.8	Estimated
		401.9	Experimental
		400.6	Estimated
		389	Experimental
		391.6	Estimated

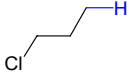
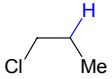
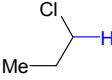
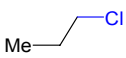
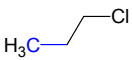
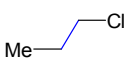
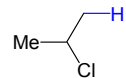
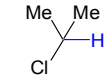
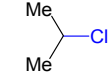
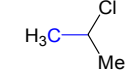
Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	381	Experimental
		382.6	Estimated
		423.8	Experimental
		433.8	Estimated
		431.8	Experimental
		437.9	Estimated
		421.7	Experimental
		424.4	Estimated
		421.3	Experimental
		428.4	Estimated
		413.8	Experimental
		415.0	Estimated
		421.7	Experimental
		420.3	Estimated
		411.7	Experimental
		410.9	Estimated
		392.5	Experimental
		401.5	Estimated
		425.1	Experimental
		421.4	Estimated
		417.2	Experimental
		413.1	Estimated
		401.7	Experimental
		404.9	Estimated
		431	Experimental
		430.5	Estimated
		431	Experimental
		431.3	Estimated
		416.3	Experimental
		428.8	Estimated
		429.7	Experimental
		432.3	Estimated

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	425.9	Experimental
		414.8	Estimated
		393	Experimental
		393.1	Estimated
		397	Experimental
		388.7	Estimated
		404.2	Experimental
		406.2	Estimated
		435	Experimental
		429.2	Estimated
		433.5	Experimental
		422.7	Estimated
		415.1	Experimental
		415.1	Estimated
		383.7	Experimental
		390.3	Estimated
		407	Experimental
		394.9	Estimated
		388	Experimental
		400.8	Estimated
		388	Experimental
		386.4	Estimated
		384	Experimental
		395.4	Estimated
		385	Experimental
		381.2	Estimated
		385	Experimental
		374.3	Estimated
		389	Experimental
		374.5	Estimated
		377	Experimental
		383.8	Estimated

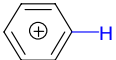
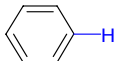
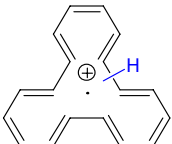
Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	416.6	<i>ab-initio</i>
		422.6	Experimental
		370.7	<i>ab-initio</i>
		375.9	Experimental
		419.4	<i>ab-initio</i>
		423.1	Experimental
		405.2	<i>ab-initio</i>
		406.6	Experimental
		375.4	<i>ab-initio</i>
		375.4	Experimental
		426	<i>ab-initio</i>
		397.8	<i>ab-initio</i>
		390.6	Experimental
		378.0	<i>ab-initio</i>
		365.1	Experimental
		407.3	<i>ab-initio</i>
		375.8	<i>ab-initio</i>
		365.4	Experimental
		419.4	<i>ab-initio</i>
		423.3	Experimental
		407.8	<i>ab-initio</i>
		409.1	Experimental
		371.5	<i>ab-initio</i>
		371.2	Experimental

Seetula, J. A. J. *Chem. Soc Faraday Trans.* **1998**, *94*, 891-898






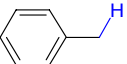




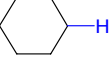
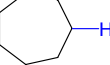

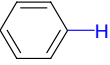
Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level

	C-H	418.7	<i>ab-initio</i>
		406.5	<i>ab-initio</i>
		409.3	Experimental
		407.0	<i>ab-initio</i>
		407.0	Experimental
		345.3	<i>ab-initio</i>
		354.5	Experimental
		376.5	<i>ab-initio</i>
		371.4	Experimental
		378.2	<i>ab-initio</i>
		370.4	Experimental
		420.0	<i>ab-initio</i>
		401.5	<i>ab-initio</i>
		347.8	<i>ab-initio</i>
		352.9	Experimental
		376.3	<i>ab-initio</i>
		367.5	Experimental

Seetula, J. A. *J. Chem. Soc Faraday Trans.* **1998**, *94*, 891-898

	C-H	357	
		453.5	
		359.9 ± 20	

Ling, Y.; Lifshitz, C. *J. Mass Spec.* **1997**, *32*, 1219-1225

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
$\text{H}_3\text{C}-\text{H}$	C-H	112.3 102.0, 102.2	DFT-AM1 Experimental
		108.0 98.0, 98.3	DFT-AM1 Experimental
		105.2 95.0, 95.7	DFT-AM1 Experimental
		102.3 92.0, 93.1	DFT-AM1 Experimental
$\text{H}-\text{C}\equiv\text{C}-\text{H}$		139.0 125.0, 126.4	DFT-AM1 Experimental
		120.0 108.0, 109.2	DFT-AM1 Experimental
		91.3 86.6, 83.1	DFT-AM1 Experimental
		94.1 87.9, 85.6	DFT-AM1 Experimental
		99.6 89.0, 90.6	DFT-AM1 Experimental
		115.7 106.3, 105.2	DFT-AM1 Experimental
		104.1 96.5, 94.7	DFT-AM1 Experimental
		100.6 94.5, 91.5	DFT-AM1 Experimental
		105.2 95.5, 95.7	DFT-AM1 Experimental
		103.5 92.5, 94.2	DFT-AM1 Experimental
		86.4 81.2, 78.6	DFT-AM1 Experimental
		117.7 110.2, 107.1	DFT-AM1 Experimental

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
<chem>NC-H</chem>	C-H	133.0	DFT-AM1
		120.0, 121.0	Experimental
<chem>O=C-H</chem>	C-H	99.0	DFT-AM1
		87.0, 90.1	Experimental
<chem>CC(=O)-H</chem>	C-H	98.8	DFT-AM1
		86.0, 89.9	Experimental
<chem>CO-CH2-H</chem>	C-H	102.4	DFT-AM1
		93.0, 93.2	Experimental






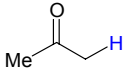
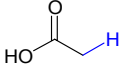
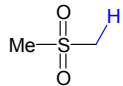
Jursic, B. S. *J. Chem. Soc. Perkin Trans. 1999*, 2, 369-372

<chem>c1ccccc1C=C-H</chem>	C-H	83.3	Calculated
		85.6	Experimental
<chem>c1ccccc1C=CC-H</chem>	C-H	79.9	Calculated
		78.9	Experimental
<chem>C1=CC=CC=C1C=C-H</chem>	C-H	88.3	Calculated
<chem>C=CC-H</chem>	C-H	84.6	Calculated
		86.6	Experimental

Glasovac, Z.; Eckert-Maksic, M.; Dacres, J. E.; Kass, S. R. *J. Chem. Soc. Perkin Trans. 2 2002*, 2, 410-415

<chem>H3C-H</chem>	C-H	79.4	HF
		100.3	MP2
		105.8	B3LYP
		104.7, 104.9	Experimental
<chem>CC-H</chem>	C-H	76.8	HF
		98.9	MP2
		101.1	B3LYP
		100.2, 101.1	Experimental
<chem>CC(C)C-H</chem>	C-H	74.5	HF
		95.3	MP2
		97.1	B3LYP
		99.4, 98.6	Experimental
<chem>CC(C)(C)C-H</chem>	C-H	72.7	HF
		93.7	MP2
		94.0	B3LYP
		95.2, 96.5	Experimental
<chem>FH2C-H</chem>	C-H	77.8	HF
		96.0	MP2
		99.1	B3LYP
		101.7	Experimental Avg

Korth, H.-G.; Sicking, W. *J. Chem. Soc. Perkin Trans. 2 1997*, 715-719

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
ClH ₂ C—H	C-H	76.6	HF
		95.0	MP2
		99.7	B3LYP
		101.5	Experimental Avg
	C-H	74.1	HF
		92.3	MP2
		95.2	B3LYP
		94.1, 96.1	Experimental
	C-H	67.5	HF
		85.0	MP2
		87.7	B3LYP
		92.2	Experimental Avg
	C-H	74.9	HF
		93.1	MP2
		96.3	B3LYP
		94.1	Experimental Avg
	C-H	69.8	HF
		96.2	MP2
		93.8	B3LYP
		92.6, 94.8, (93.4)	Experimental (Avg)
	C-H	67.3	HF
		93.5	MP2
		93.4	B3LYP
		94.2	Experimental Avg
	C-H	69.4	HF
		94.4	MP2
		94.0	B3LYP
		95.1	Experimental Avg
	C-H	73.7	HF
		95.2	MP2
		97.2	B3LYP
		96.0	Experimental Avg
	C-H	80.8	HF
		101.2	MP2
		103.4	B3LYP
		99.0	Experimental Avg
Cl ₃ C—H	C-H	71.8	HF
		89.4	MP2
		92.0	B3LYP
		95.6	Experimental Avg

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
F_3C-H	C-H	106.6	MP2/cc-pVtz (298K)
		106.7	Experimental
Cl_3C-H		94.7	MP2/cc-pVtz (298K)
		95.8	Experimental
Br_3C-H		93.2	MP2/cc-pVtz (298K)
		96	Experimental
H_3C-H		104.4	MP2/cc-pVtz (298K)
		105.1	Experimental
FH_2C-H		101.2	MP2/cc-pVtz (298K)
		101.3	Experimental
ClH_2C-H		99.4	MP2/cc-pVtz (298K)
		99.5	Experimental
BrH_2C-H		98.9	MP2/cc-pVtz (298K)
		101.6	Experimental
F_2HC-H		101.5	MP2/cc-pVtz (298K)
		102.3	Experimental
Cl_2HC-H		95.3	MP2/cc-pVtz (298K)
		95.6	Experimental
Br_2HC-H		97.8	MP2/cc-pVtz (298K)
		99.7	Experimental

McGivern, S. W.; Derecskei-Kovacs, A.; North, S. W.; Francisco, J. S. *J. Phys. Chem. A*, **2000**, *104*, 436

(kJ/mol)

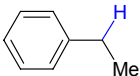
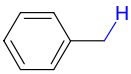
Polycyclic Aromatic Hydrocarbon Borders

C-H


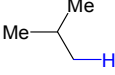

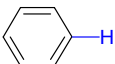

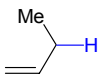
Zigzag border	~480
Armchair border	~477
Second Armchair dissociation	~361

May, K.; Dapprich, S.; Furche, F.; Unterreiner, B. V.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2000**, *2*, 5084-5088

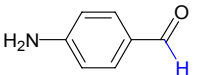
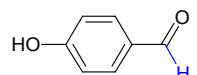
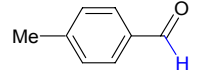
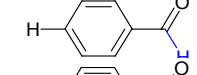
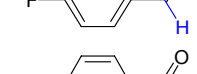
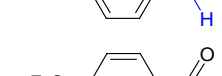
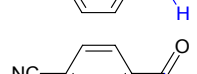
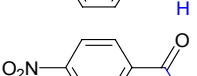
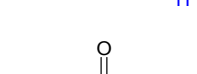

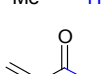
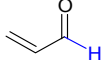
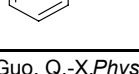
(kcal/mol)

	C-H	84.8, 85.7	DFT
		87	Experimental
Cl_3C-H		92.1	DFT
		96	Experimental
$c-C_6H_7-H$		71.4, 72.3	DFT
		77	Experimental
		87.8, 88.6	DFT
		90	Experimental

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

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
c-C ₆ H ₁₁	C-H	97	Photoacoustic Calorimetry
c-C ₆ H ₇		77	Photoacoustic Calorimetry
c-C ₄ H ₈ N		88.2, (87)	DFT, (Expt)
N(Et) ₂ CHCH ₃		89.9, 89	DFT, (Expt)
C ₄ H ₇ O		90.7, 91.6, (92)	DFT, (Expt)
C ₄ H ₇ O ₂		94.6, (96)	DFT, (Expt)
H ₃ C—H		105.0, 105.7 105	DFT Experimental
C ₂ H ₅ —H		100.3, 101.0 101	DFT Experimental
C ₃ H ₇ —H		100.9, 101.6 101	DFT Experimental
		96.4, 97.1 98	DFT Experimental
		93.2, 94.0 96	DFT Experimental
c-C ₃ H ₅ —H		106.4, 107.2	DFT
c-C ₄ H ₇ —H		97.3, 98.0	DFT
c-C ₆ H ₁₁ —H		96.9, 97.6 97	DFT Experimental
C ₂ H ₃ —H		109.3 111	DFT Experimental
		105.7	DFT
		110.8 113	DFT Experimental
		85.0, 85.9 88	DFT Experimental
		80.2, 81.5 84	DFT Experimental

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

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	91.3	ALL <i>ab-initio</i>
		91.5	
		91.5	
		91.6	
		91.8	
		92.0	
		92.0	
		92.2	
		92.2	
		88.4	G3
		89.4 89.3	G3 Experimental
		91.2	G3
		91.6 88.9	CBS-4M Experimental

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