

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
H <sub>3</sub> C—F	C-X	107.1	CCSD(T)/6-322++G(3df,3pd)
		108.0	corrected MP2/cc-pVtz
		108.1	IB method
		109.2	Experimental
H <sub>3</sub> C—Cl	C-X	79.6	CCSD(T)/6-322++G(3df,3pd)
		81.4	corrected MP2/cc-pVtz
		80.0	IB method
		83.2	Experimental
H <sub>3</sub> C—Br	C-X	65.8	CCSD(T)/6-322++G(3df,3pd)
		70.6	corrected MP2/cc-pVdz
		69.7	corrected MP2/cc-pVtz
		69.5	corrected MP2/cc-pVqz
		69.1	IB method
		70.9	Experimental

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

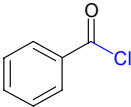
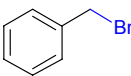
CH <sub>2</sub> F—F	C-X	119.3	corrected MP2/cc-pVtz
		118.8	Experimental
CHF <sub>2</sub> —H	C-H	100.0	corrected MP2/cc-pVtz
		101.3	Experimental
CH <sub>2</sub> Cl—Cl	C-X	78.5	corrected MP2/cc-pVtz
		80.9	Experimental
CHCl <sub>2</sub> —H	C-H	93.8	corrected MP2/cc-pVtz
		95.6	Experimental
CH <sub>2</sub> Br—Br	C-X	67.0	corrected MP2/cc-pVtz
		69.8	Experimental
CHBr <sub>2</sub> —H	C-H	96.3	corrected MP2/cc-pVtz
		99.7	Experimental
CHF <sub>2</sub> —F	C-X	127.8	corrected MP2/cc-pVtz
		127.0	Experimental
CF <sub>3</sub> —H	C-H	105.1	corrected MP2/cc-pVtz
		106.7	Experimental
CHCl <sub>2</sub> —Cl	C-X	75.6	corrected MP2/cc-pVtz
		77.8	Experimental
CCl <sub>3</sub> —H	C-H	93.2	corrected MP2/cc-pVtz
		95.8	Experimental
CHBr <sub>2</sub> —Br	C-X	63.8	corrected MP2/cc-pVtz
		66	Experimental
CBr <sub>3</sub> —H	C-H	93.2	corrected MP2/cc-pVtz
		96	Experimental

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

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

$C_5H_{11}-Cl$	C-Cl	352.5	
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Leal, J. P.; Marques, N.; Takats, J.J. *Organomet. Chem.* **2001**, 632, 209-214

		(kcal/mol)	(solvent)
	C-X	87	benzene
		61	various

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

$H_3C-F$	C-X	115	
$H_3C-Cl$		83.7	
$H_3C-Br$		72.1	
$H_3C-I$		57.6	

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

		(kJ/mol)
$H_3C-F$	C-X	459.69
$H_3C-Cl$		350.7
$H_3C-Br$		291.8

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

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
$\text{H}_3\text{C}-\text{F}$	C-F	115	
		110.6	
		123.3	
		127.2	
		98.7	
		122.2	

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

$\text{H}_3\text{C}-\text{Cl}$	C-Cl	83.7	
		84.8	
		85.2	
		84.9	
		91.2	
		97.1	
		74	
		84.7	

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

$\text{H}_3\text{C}-\text{Br}$	C-Br	72.1	
		72.4	
		73.9	
		72.6	
		80.8	
		59	
		84	
		63	
		71.7	

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

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-I	57.6	
		56.9	
		57	
		55.6	
		45.6	
		67	
		51	
		53.8	





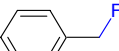
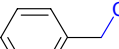
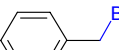
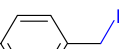
Blanksby, S. J.; Ellison, G. B. *Acc. Chem. Res.* **2003**, *36*, 255

$\text{H}_3\text{C}-\text{F}$	C-X	109.7	MP2/cc-pVtz (298K)
		109.8	Experimental
$\text{H}_3\text{C}-\text{Cl}$		83.0	MP2/cc-pVtz (298K)
		83.8	Experimental
$\text{H}_3\text{C}-\text{Br}$		71.2	MP2/cc-pVtz (298K)
		70.9	Experimental
$\text{FH}_2-\text{C}-\text{F}$		120.7	MP2/cc-pVtz (298K)
		119.4	Experimental
$\text{ClH}_2-\text{C}-\text{Cl}$		80.0	MP2/cc-pVtz (298K)
		80.9	Experimental
$\text{BrH}_2-\text{C}-\text{Br}$		68.2	MP2/cc-pVtz (298K)
		69.8	Experimental
$\text{F}_2\text{HC}-\text{F}$ Fluoroform		129.1	MP2/cc-pVtz (298K)
		127.6	Experimental
$\text{Cl}_2\text{HC}-\text{Cl}$ Chloroform		76.6	MP2/cc-pVtz (298K)
		78.4	Experimental
$\text{Br}_2\text{HC}-\text{Br}$ Bromoform		64.6	MP2/cc-pVtz (298K)
		66	Experimental





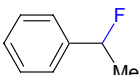
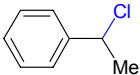
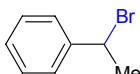
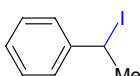




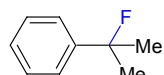
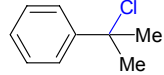
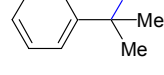
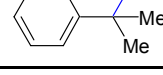
McGivern, S. W.; Derecskei-Kovacs, A.; North, S. W.; Francisco, J. S. *J. Phys Chem. A*, **2000**, *104*, 436

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
H <sub>3</sub> C—Br	C-X	73.6	G2
		74.0	G2MP2
		73.8	G2MS
		70.0	Experimental
F <sub>3</sub> C—Br		74.8	G2
		75.1	G2MP2
		74.8	G2MS
		70.6	Experimental

Fukaya, H.; Ono, T.; Abe, T. *J. Phys. Chem. A* **2001**, *105*, 7401-7404

CH <sub>3</sub> —F	C-X	426.1, 461.9	LLM Method
CH <sub>3</sub> —Cl		354.9, 354.8	LLM Method
CH <sub>3</sub> —Br		312.9, 313.4	LLM Method
		451.5	Experimental
		473.7	LLM Method
		350.2	Experimental
		356.8	LLM Method
		290.8	Experimental
		311.3	LLM Method
		231.4	Experimental
		412.8	Experimental
		416.6, 417.1	LLM Method
		299.9	Experimental
		299.6, 296.2	LLM Method
		239.3	Experimental
		256.5, 257.7	LLM Method
		187.8	Experimental

Verevkin, S. P.; Krashnykh, E. L.; Wright, J. S. *Phys. Chem. Chem. Phys.* **2003**, *5*, 2605-2611

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-X	453.1	Experimental
		482.5	LLM Method
		346.4	Experimental
		358.9	LLM Method
		291.6	Experimental
		310.3	LLM Method
		227.2	Experimental
		425.1	LLM Method
		292.4	Experimental
		297.8	LLM Method
		240.1	Experimental
		250.8	LLM Method
		176.1	Experimental
		483.7	LLM Method
		351.6	Experimental
		359.0	LLM Method
		292.4	Experimental
		304.2	LLM Method
		226.9	Experimental
		434.0	LLM Method
		292.8	Experimental
		294.8	LLM Method
		236.7	Experimental
		243.6	LLM Method
		176.0	Experimental

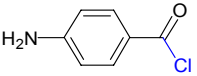
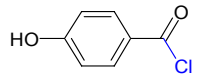
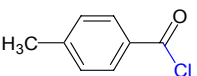
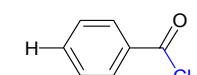
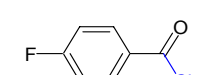
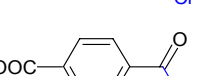
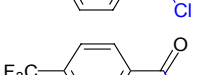
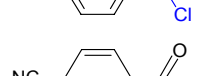
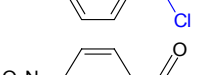
Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-F	120.6	G3
		122.2	G3
		121.7	G3
		121.5	CBS-4M
	C-Cl	83.0	G3
		84.6	G3
		84.6	Experimental
		84.5	G3
		87.8	CBS-4M

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




Compound	Bond (C-F)	Energy	Theory Level
	C-F	121.7	
		121.6	
		121.6	
		121.5	
		121.4	
		121.4	
		121.4	
		121.3	
		121.2	

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

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

Compound	Bond (C-Y)	Energy	Theory Level
	C-Cl	88.3	ALL <i>ab-initio</i>
		88.0	
		88.0	
		87.8	
		87.7	
		87.6	
		87.6	
		87.5	
		87.4	

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

Compound	Bond (C-Y)	Energy	Theory Level
	C-Cl	340.3	<i>ab-initio</i>
		354.1	Experimental
		324.5	<i>ab-initio</i>
		327.9	Experimental
		338.9	<i>ab-initio</i>
		345.1	Experimental

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