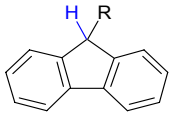
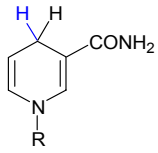
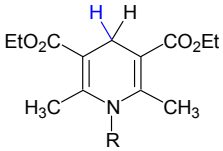
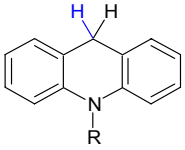
Compound		Bond Dissociation Enthalpy (kcal/mol)		
		Bond (C-Y)	Energy	Theory Level
	R = H	C-H	79.5	
	R = Me_3C		79.4	
	R = Ph_3C		77.2	
	R = Me_3Si		82.5	
	R = Et_3Si		81.2	
	R = Ph_3Si		80.6	
	R = $PhSO2CH_4$		99	
	R = $PhSO_2CH_2SiMe_3$		99.4	
	R = $PhSO_2CH_2SiPh_3$		97.4	
	R = $PhSO_2CH(SiMe_3)_2$		96.5	
	R = $PhS(O)(=NSO_2Tol)CH_3$		103.1	
	R = $PhS(O)(=NSO2Tol)CH(SiMe_3)_2$		99.8	
	R = $PhSO_2CH_2Ph$		90.2	
	R = $PhSO_2CH(CH=CH_2)(SiMe_3)$		91.1	

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

	R = $PhCH_2$	C-H heterol.	64.2	
		homolysis	67.9	
	R = 4-CH_3OPh	heterolysis	66.9	
		homolysis	69.4	
	R = 4-CH_3Ph	heterolysis	67.5	
		homolysis	69.2	
	R = Ph	heterolysis	68.8	
		homolysis	69.2	
	R = 4-ClPh	heterolysis	70.2	
		homolysis	69.1	
	R = 4-BrPh	heterolysis	70.4	
		homolysis	69.2	
	R = 4-CF_3Ph	heterolysis	72.6	
		homolysis	69.5	
	R = H	C-H heterol.	69.3	
		homolysis	69.4	
	R = CH_3	heterolysis	69.9	
		homolysis	68.8	
	R = CH_3	C-H heterol.	81.1	
		homolysis	73.7	

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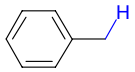
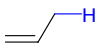
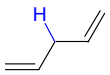
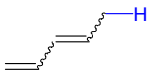
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
$H_3C—H$	C-H	105.5	B3LYP-LLM
		105.5	B3LYP-MLM1
		105.5	B3LYP-MLM2
		105.8	B3LYP-HLM
		104.9	G3
		105.3	G3MP2
		104.9	Experimental
		89.3	B3LYP-LLM
		89.4	B3LYP-MLM1
		90.1	B3LYP-MLM2
		90.6	B3LYP-HLM
		91.1	G3
		93.1	G3MP2
		88.5	Experimental
		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
		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
		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
$H_3C—OO\cdot$	C-O	32.7	B3P86-LLM
		35.9	B3P86-MLM
		34.1	B3P86-MLM
		32.4	G3MP2
		32.2	G3
		32.7	Experimental

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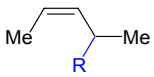
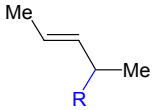
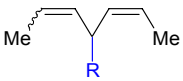
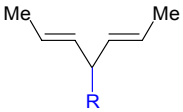
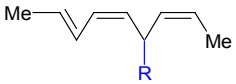
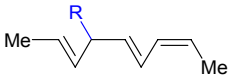
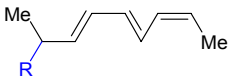
Compound			Bond Dissociation Enthalpy (kcal/mol)		
			Bond (C-Y)	Energy	Theory Level
			C-R	***trans, cis***	
	R = OO·	dissociated radical		19.6, 23.1	B3P86-HLM
	R = H	as trans or cis		83.4, 87.0	B3LYP-HLM
	R = OO·			20.5, 21.3	B3P86-HLM
	R = H			84.0, 84.9	B3LYP-HLM
	R = OO·			7.9, 7.4	B3P86-HLM
	R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

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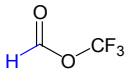
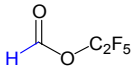
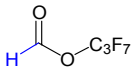
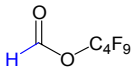
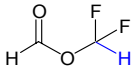
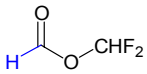
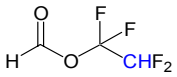
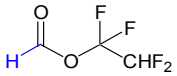
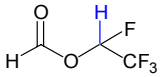
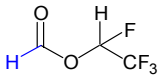
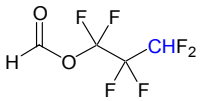
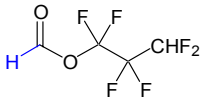
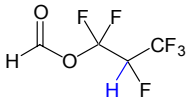
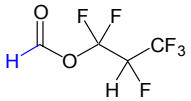
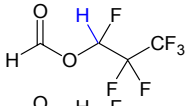
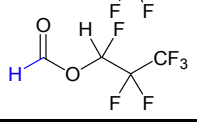
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H Syn	100.4	All Calculated with DFT
	Anti	96.5	(RO)B3LYP/6-311G
	Syn	100.2	
	Anti	96.7	
	Syn	100.2	
	Anti	96.7	
	Syn	100.1	
	Anti	96.8	
	Syn	104.3	
	Anti	105.0	
	Syn	100.2	
	Anti	96.0	
	Syn	102.2	
	Anti	101.9	
	Syn	99.8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

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Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
CH_3OCH_3	C-H	95.7	
CF_3OCH_3		100.7	
CF_3OCHF_2		103.5	
CHF_2OCHF_2		103.4	
$CF_3CF_2OCH_3$		100.9	
$CF_3CF_2CF_2OCH_3$		101.1	
$(CF_3)_2CFOCH_3$		99.8	
CF_3CH_3		106.0	
CF_3CH_2F		101.1	
CF_3CHF_2		102.0	
CF_3CH_2Cl		99.5	
CF_3CHCl_2		95.3	
CF_3CHFCl		98.9	
CF_2ClCH_3		104.0	
CF_2ClCH_2F		99.6	
CF_2ClCHF_2		100.7	
CF_2ClCH_2Cl		98.6	
$CF_2ClCHCl_2$		93.7	
$CF_2ClCHFCl$		97.5	
$CFCl_2CH_3$		102.9	
$CFCl_2CH_2F$		98.9	
$CFCl_2CHF_2$		100.9	
$CFCl_2CH_2Cl$		97.5	
$CFCl_2CHCl_2$		93.7	
$CFCl_2CHFCl$		97.3	
CCl_3CH_3		102.6	
CCl_3CH_2F		98.6	
CCl_3CHF_2		101.0	
CCl_3CH_2Cl		97.2	
CCl_3CHCl_2		94.1	
CCl_3CHFCl		97.5	
CHF_2CHF_2		102.8	
CF_3CHFCF_3		101.0	
$CF_3CH_2CHF_2$		101.3	
$CF_3CH_2CHF_2$		104.8	
$CF_3CH_2CH_2CF_3$		102.3	
$CF_3CH_2CF_2CH_3$		102.6	
$CF_3CH_2CF_2CH_3$		104.5	
$CHF_2CF_2CF_2CHF_2$		102.0	
$CF_3CF_2CH_2CH_2CF_2CF_3$		103.2	
CH_3OCH_2F		97.4	
CH_3OCH_2F		97.9	
CH_3OCHF_2		102.8	
CH_3OCHF_2		100.0	
CF_3OCH_3		100.7	
CF_3OCHF_2		103.5	
CH_2FOCH_2F		99.7	
CHF_2OCHF_2		103.4	
$CF_3CF_2OCH_3$		100.9	

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Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
$CF_3CF_2CF_2OCH_3$	C-H	101.1	
$(CF_3)_2CFOCH_3$		99.8	
$CH_3OCF_2CHF_2$		101.8	
$CH_3OCF_2CHF_2$		100.5	
$CH_2FCF_2OCHF_2$		103.9	
$CH_2FCF_2OCHF_2$		101.5	
$CHF_2CF_2OCH_2CF_3$		99.5	
$CHF_2CF_2OCH_2CF_3$		102.3	
$CF_3CHFCF_2OCH_3$		100.7	
$CF_3CHFCF_2OCH_3$		100.6	
$CF_3CH_2OCH_2CF_3$		96.9	
$CF_3CF_2CH_2OCHF_2$		103.9	
$CF_3CF_2CH_2OCHF_2$		98.4	
$CHFClCF_2OCH_3$		98.8	
$CHFClCF_2OCH_3$		100.6	
CHF_2OCF_2CHFCl		99.1	
CHF_2OCF_2CHFCl		103.8	
$CHF_2OCHClCF_3$		98.3	
$CHF_2OCHClCF_3$		103.7	

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

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CF_3—CH_3	C-H	106.0	
F_3C—CH_2F		101.1	
F_3C—CHF_2		102.0	
F_3C—CH_2Cl		99.5	
F_3C—$CHCl_2$		95.3	
F_3C—CHFCl		98.9	
CF_2Cl—$CHCl_2$		93.7	
CF_2Cl—CHFCl		97.5	
$CFCl_2$—CHFCl		97.3	
CCl_3—CH_3		102.6	
CH_3OCH_3		95.7	
CF_3OCH_3		100.7	

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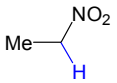
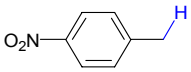
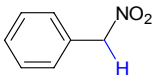
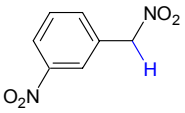
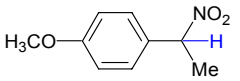
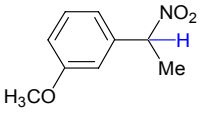
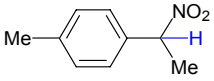
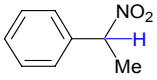
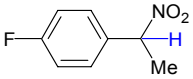
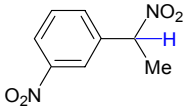
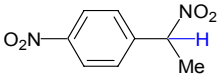
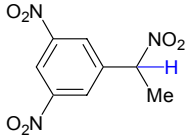
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H homolytic	87	
		86.5	
		85	
		87	
		85	
		87	
		85.5	
		86	
		86	
		87	
		87	
		89	

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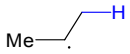
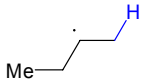
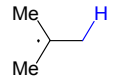
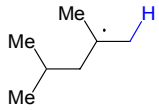
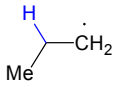
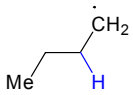
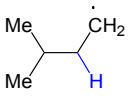
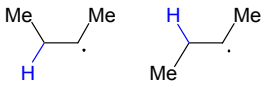
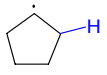
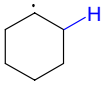
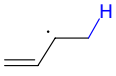
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H (O^oK)	35.6	CBS-4
	298°K	36.3	CBS-4
	Experimental	35.2	
	O^oK	35.6	CBS-4
	298°K	36.4	CBS-4
	Experimental	35.0	
	O^oK	35.6	CBS-4
	298°K	36.3	CBS-4
	Experimental	34.9	
	O^oK	35.4	CBS-4
	298°K	36.2	CBS-4
	Experimental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

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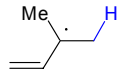
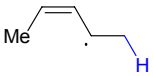
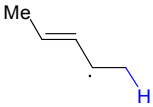
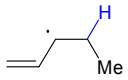
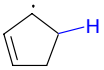
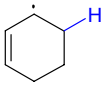
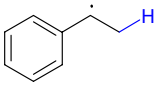
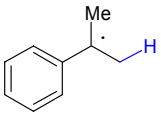
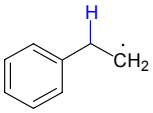
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H (O°K)	47.7	CBS-4
	298°K	48.5	CBS-4
	Experimental	47.5	
	O°K	45.2	CBS-4
	298°K	46.4	CBS-4
	Experimental	44.2	
	O°K	47.5	CBS-4
	298°K	48.5	CBS-4
	Experimental	44.6	
	O°K *cis*	45.7	CBS-4
	trans	44.8	CBS-4
	298°K *cis*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

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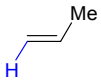
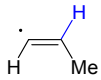
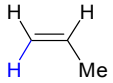
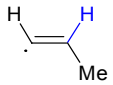
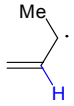
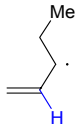
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H (O^oK)	110.0	CBS-4
	298^oK	111.5	CBS-4
	O^oK	30.7	CBS-4
	298^oK	31.9	CBS-4
	Experimental	32.1	
	O^oK	109.6	CBS-4
	298^oK	111.1	CBS-4
	O^oK	31.1	CBS-4
	298^oK	32.3	CBS-4
	Experimental	32.5	
	O^oK	57.2	CBS-4
	298^oK	58.6	CBS-4
	Experimental	58.9	
	O^oK	54.0	CBS-4
	298^oK	55.0	CBS-4
	Experimental	60.0	
	O^oK	53.5	CBS-4
	298^oK	54.7	CBS-4

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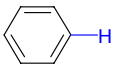
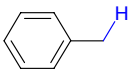
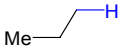
	C-H	111.4	Experimental
		110.9	B3LYP/6-31G(d), 298K
		110.6	B3LYP/6-311++G(d,p), 298K
		108.9	Experimental
		109.3	B3LYP/6-31G(d), 298K
		108.3	B3LYP/6-311++G(d,p), 298K
		88.5	Experimental
		87.9	B3LYP/6-31G(d), 298K
		88.1	Experimental
		85.1	B3LYP/6-31G(d), 298K
		84.1	B3LYP/6-311++G(d,p), 298K

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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_3F		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_2F_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_3Cl		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

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Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
CH_2Cl_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_2FCl		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_2Cl		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_3Br		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_2Br_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_2FBr		98.1	B3LYP 6-311G(d,p)
		98.8	(RO)B3LYP 6-311G(d,p)
		98.5	(RO)B3LYP 6-311++G(3df,2p)

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Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
CHF_2Br	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_2ClBr		96.1	B3LYP 6-311G(d,p)
		97.0	(RO)B3LYP 6-311G(d,p)
		96.2	(RO)B3LYP 6-311++G(3df,2p)
$CHCl_2Br$		92.6	B3LYP 6-311G(d,p)
		93.4	(RO)B3LYP 6-311G(d,p)
		92.2	(RO)B3LYP 6-311++G(3df,2p)
$CHBr_2Cl$		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

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$F_3C—CH_3$	C-H	106.0	(RO)B3LYP 6-311G(d,p)
		105.8	(RO)B3LYP 6-311++G(3df,2p)
		106.7	Experimental
$F_3C—CH_2F$		101.1	(RO)B3LYP 6-311G(d,p)
		101.1	(RO)B3LYP 6-311++G(3df,2p)
$F_3C—CHF_2$		102.0	(RO)B3LYP 6-311G(d,p)
		101.7	(RO)B3LYP 6-311++G(3df,2p)
		102.7	Experimental
$F_3C—CH_2Cl$		99.5	(RO)B3LYP 6-311G(d,p)
		98.3	(RO)B3LYP 6-311++G(3df,2p)
		101.8	Experimental
$F_3C—CHCl_2$		95.3	(RO)B3LYP 6-311G(d,p)
		93.6	(RO)B3LYP 6-311++G(3df,2p)
		95.3	Experimental
$F_3C—CHFCl$		98.9	(RO)B3LYP 6-311G(d,p)
		97.8	(RO)B3LYP 6-311++G(3df,2p)
		99.2	Experimental

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Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
$CF_2Cl—CH_3$	C-H	104.0	(RO)B3LYP 6-311G(d,p)
		103.8	(RO)B3LYP 6-311++G(3df,2p)
$CF_2Cl—CH_2F$		99.6	(RO)B3LYP 6-311G(d,p)
		100.0	(RO)B3LYP 6-311++G(3df,2p)
$CF_2Cl—CHF_2$		100.7	(RO)B3LYP 6-311G(d,p)
		100.4	(RO)B3LYP 6-311++G(3df,2p)
$CF_2Cl—CH_2Cl$		98.6	(RO)B3LYP 6-311G(d,p)
		97.6	(RO)B3LYP 6-311++G(3df,2p)
$CF_2Cl—CHCl_2$		93.7	(RO)B3LYP 6-311G(d,p)
		92.1	(RO)B3LYP 6-311++G(3df,2p)
$CF_2Cl—CHFCl$		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)
$CFCl_2—CH_2F$		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)
$CFCl_2—CH_2Cl$		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)
$CFCl_2—CHFCl$		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)
$CCl_3—CH_2F$		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)
$CCl_3—CH_2Cl$		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
$CCl_3—CHFCl$		97.5	(RO)B3LYP 6-311G(d,p)
		96.4	(RO)B3LYP 6-311++G(3df,2p)

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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_2F—H		99.7	corrected MP2/cc-pVtz
		98.5	CCSD(T)/6-311++G(3df,3pd)
		101.3	Experimental
CH_2Cl—H		97.7	corrected MP2/cc-pVtz
		96.6	CCSD(T)/6-311++G(3df,3pd)
		99.5	Experimental
CH_2Br—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

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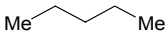
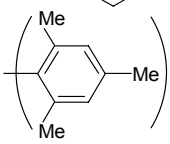
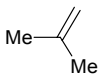
Tp'Rh(CNneo)(R)H	R = Ph	C-H	113.5	
	R = 		109.7	
	R = Me		104.9	
	R = *n*-pentyl 		98	
	R = cyclopentyl 		96.4	
	R = cyclohexyl 		96	
	R = Mesityl 		88.5	
	R = Methallyl 		85.6	

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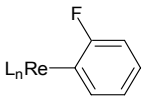
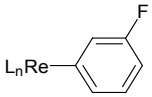
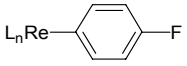
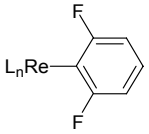
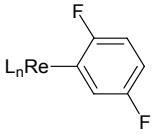
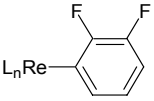
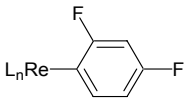
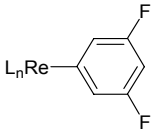
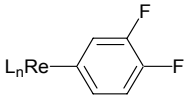
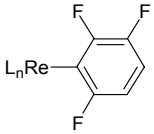
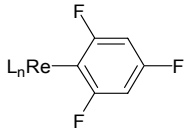
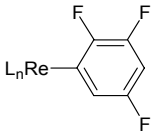
Compound		Bond Dissociation Enthalpy (kcal/mol)		
		Bond (C-Y)	Energy	Theory Level
$Re(Cp)(CO)_2(H)(R)$	R = Ph	C-Re	252.0	All calculated with
		C-H	489.8	B3PW91 (Hybrid DFT)
	R = 	C-Re	276.9	
		C-H	500.5	
	R = 	C-Re	253.5	
		C-H	490.6	
	R = 	C-Re	255.3	
		C-H	494.3	
	R = 	C-Re	300.0	
		C-H	512.0	
	R = 	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	

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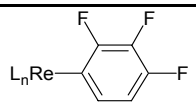
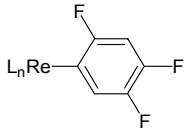
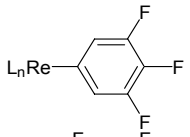
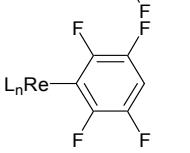
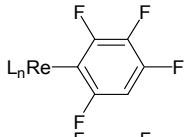
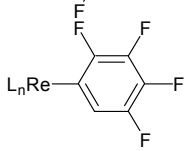
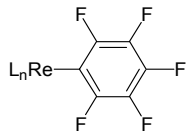
Compound		Bond Dissociation Enthalpy (kJ/mol)		
		Bond (C-Y)	Energy	Theory Level
$Re(Cp)(CO)_2(H)(R)$	R = 	C-Re C-H	280.8 503.6	All calculated with B3PW91 (Hybrid DFT)
	R = 	C-Re C-H	281.0 504.8	
	R = 	C-Re C-H	257.4 495.0	
	R = 	C-Re C-H	304.7 512.4	
	R = 	C-Re C-H	304.0 514.7	
	R = 	C-Re C-H	283.0 504.4	
	R = 	C-Re C-H	306.7 514.7	

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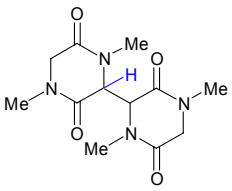
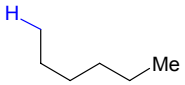
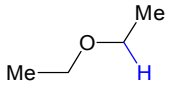
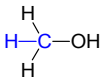
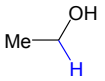
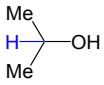
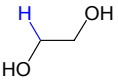
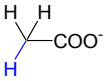
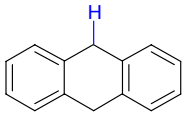
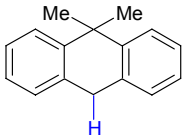
(kcal/mol)

	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
$(CH_2(\text{-}H))_3OH$		99	water
		96	water
		92	water
		78	benzene
		77	benzene

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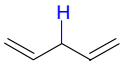
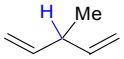
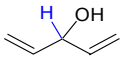
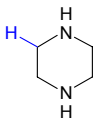
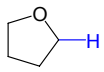
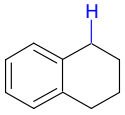
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Solvent
	C-H	77	benzene
		77	benzene
		69	benzene
		78	benzene
		94	benzene
		93	benzene
		92	THF
		83	tetralin

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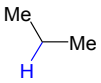
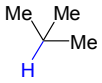
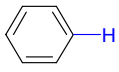
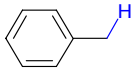
	C-H	104.9	
		101.1	
		98.6	
		96.5	
		110.7	
		88.8	
		112.9	
		89.7	
		104.6	
		88.1	
		89.4	

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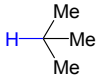
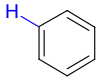
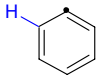
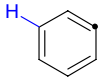
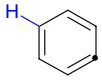
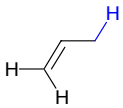
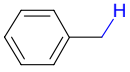
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	104.99	
		110.4	
		101.3	
		126.3	
		80.9	
		101.1	
		98.6	
		98.2	
		96.5	
		110.7	
		133.32	
		112.9	
		78	
		94	
		109	
		88.8	
		89.8	

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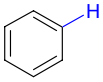
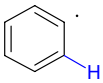
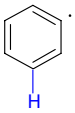
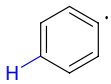
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	101.1	
		110.7	
		35.7	
		83	
		35.4	
		133.32	
		86	
		112.9	
		78	
		94	
		109	

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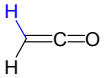
	C-H	96.1	
		22.0	
		105	
		88.0	
		-12	

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Compound	Resultant Radical	Bond Dissociation Enthalpy (kJ/mol)		
		Bond (C-Y)	Energy	Bond Enthalpy Terms (*E*)
CH		C-H	341	
HCH			426	
HCH_2			458	
HCH_3			439.4	
C_2H			485	
C_2H_2			555	
C_2H_4			461	
C_2H_6			421	410.8
C_3H_6			363	410.8
C_3H_8	Pr		418	410.8
	i-Pr		406	407.0
C_4H_{10}	Bu		418	410.8
	s-Bu		406	407.0
Me_3CH	*i*-Bu		420	410.8
	t-Bu		396	403.9
CpH			347	
c-C_5H_{10}			395	
C_5H_{12}			418	410.8
Me_3CCH_3			418	410.8
C_6H_6			465	420.6
c-C_6H_{12}			400	407.0
2,3-$Me_2C_4H_8$	2,3-Me_2Bu		418	410.8
$PhCH_3$	Bz		368	410.8
	MeC_6H_4		465	420.6
PhCCH			553	435
$PhCH_2Me$			357	407.0
c-C_5Me_5			368	

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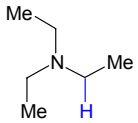
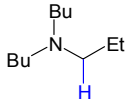
	C-H	381	Experimental
		379.5	Estimated
		381	Experimental
		370.2	Estimated
		438.56	

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Compound	Resultant Radical	Bond Dissociation Enthalpy (kJ/mol)		
		Bond (C-Y)	Energy	Bond Enthalpy Terms (*E*)
$BuCH_2OH$		C-H	389	401.7
PhOH			362	451.2
PhC(O)H			371	426.6
CF_2H			274	
CF_3H			447	420
CH_2F			359	
CH_3F			424	
CH_2F_2			430	
$CF_3C(O)H$			381	426.6
CF_3CH_2OH			436	451.2
C_6F_5OH			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_2CO	MeCO		340	
MeC(O)Cl	MeCO		340	
PhC(O)Cl	PhCO		343	
MeI			238	
C_2H_3I	C_2H_3		272	
EtI			235	
C_3H_5I	C_3H_5		180	
PrI			235	
i-PrI			232	
BuI			237	
PhI			273	
BzI			207	
$PhCH_2CH_2I$			237	
$Me(CHEt)_2^-$			237	
PhCCl			319	
Me_3SiCH_2I			232	
I_2			151.3	
PhC(O)I			212	
MeC(O)I	MeCO		209	

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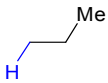
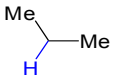
Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
CH_4	C-H	421.1	B3LYP
		427.4	KMLYP
		439.5	CBS-Q
		438.9	Experimental
		411.6	B3LYP
		419.3	KMLYP
		425.5	CBS-Q
		420.7	Experimental
		465.0	B3LYP
		476.6	KMLYP
		462.0	CBS-Q
		464.7	Experimental
		563.3	B3LYP
		572.9	KMLYP
		557.6	CBS-Q
		556.1	Experimental
		413.0	B3LYP
		424.0	KMLYP
		426.9	CBS-Q
		422.7	Experimental
		394.4	B3LYP
		405.4	KMLYP
		414.9	CBS-Q
		416.8	Experimental
		350.9	B3LYP
		359.5	KMLYP
		361.3	CBS-Q
		361.9	Experimental
		458.2	B3LYP
		468.9	KMLYP
		471.7	CBS-Q
		436.3	B3LYP
		447.7	KMLYP
		452.1	CBS-Q
		364.1	B3LYP
		377.2	KMLYP
		380.1	CBS-Q
		339.0	Experimental

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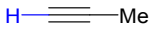
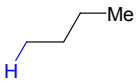
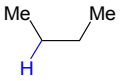
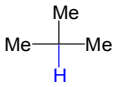
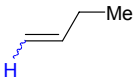
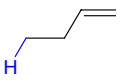
Reference includes radical stabilization energies

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

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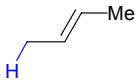
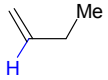
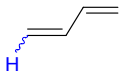
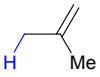
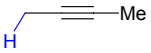
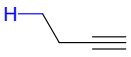
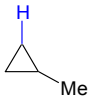
Reference includes radical stabilization energies

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

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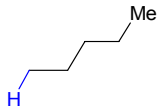
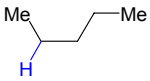
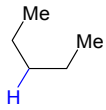
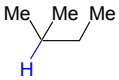
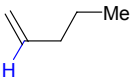
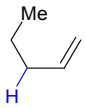
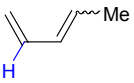
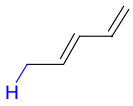
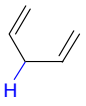
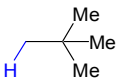
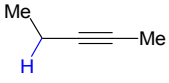
Reference includes radical stabilization energies

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

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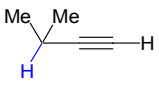
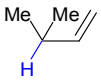
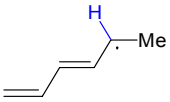
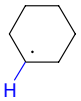
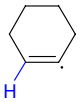
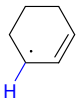
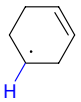
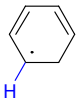
Reference includes radical stabilization energies

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

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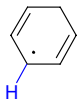
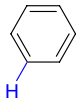
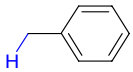
Reference includes radical stabilization energies

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

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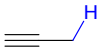
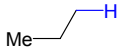
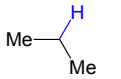
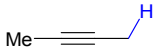
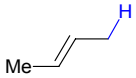
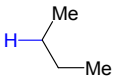
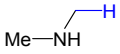
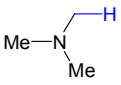
Reference includes radical stabilization energies

		(kJ/mol)	
	C-H	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

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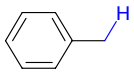
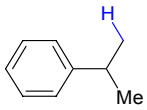
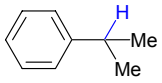
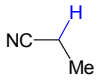
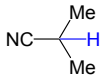
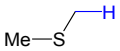
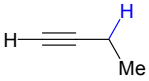
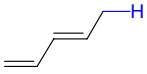
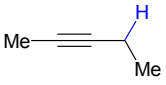
Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	394.6 404.6	Experimental Estimated
		370.3 381.9	Experimental Estimated
		357.3 372.8	Experimental Estimated
		353.1 363.8	Experimental Estimated
		376.1 377.0	Experimental Estimated
		361.9 367.9	Experimental Estimated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

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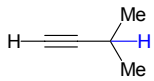
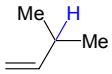
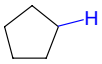
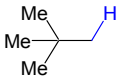
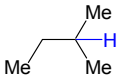
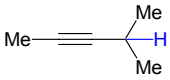
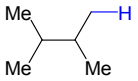
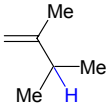
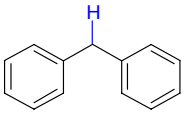
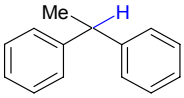
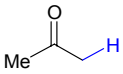
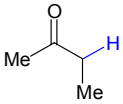
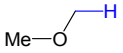
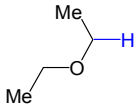
Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	338.9	Experimental
		347.6	Estimated
		323	Experimental
		332.6	Estimated
		403.5	Experimental
		404.1	Estimated
		418	Experimental
		408.8	Estimated
		404	Experimental
		398.6	Estimated
		344.3	Experimental
		346.0	Estimated
		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

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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

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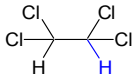
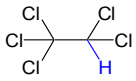
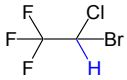
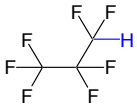
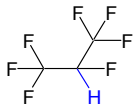
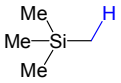
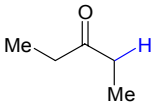
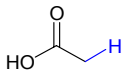
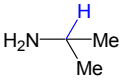
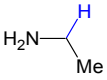
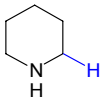
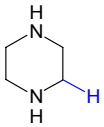
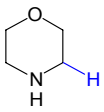
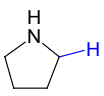
Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	425.9	Experimental
		414.8	Estimated
		393	Experimental
		393.1	Estimated
		397	Experimental
		388.7	Estimated
		404.2	Experimental
		406.2	Estimated
		435	Experimental
		429.2	Estimated
		433.5	Experimental
		422.7	Estimated
		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

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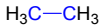
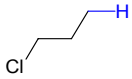
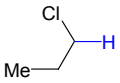
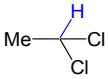
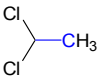
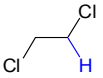
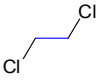
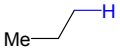
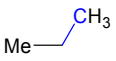
Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	416.6	*ab-initio*
		422.6	Experimental
		370.7	*ab-initio*
		375.9	Experimental
		419.4	*ab-initio*
		423.1	Experimental
		405.2	*ab-initio*
		406.6	Experimental
		375.4	*ab-initio*
		375.4	Experimental
		426	*ab-initio*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

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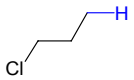
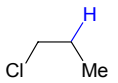
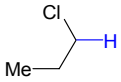
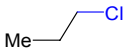
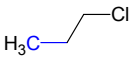
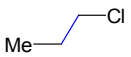
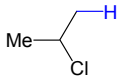
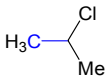
Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	418.7	*ab-initio*
		406.5	*ab-initio*
		409.3	Experimental
		407.0	*ab-initio*
		407.0	Experimental
		345.3	*ab-initio*
		354.5	Experimental
		376.5	*ab-initio*
		371.4	Experimental
		378.2	*ab-initio*
		370.4	Experimental
		420.0	*ab-initio*
		401.5	*ab-initio*
		347.8	*ab-initio*
		352.9	Experimental
		376.3	*ab-initio*
		367.5	Experimental

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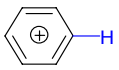
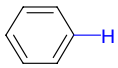
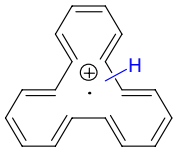
	C-H	357	
		453.5	
		359.9 ± 20	

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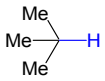
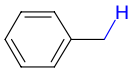
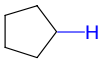
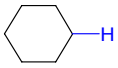
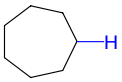
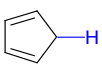
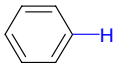
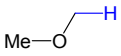
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	112.3 102.0, 102.2	DFT-AM1 Experimental
		108.0 98.0, 98.3	DFT-AM1 Experimental
		105.2 95.0, 95.7	DFT-AM1 Experimental
		102.3 92.0, 93.1	DFT-AM1 Experimental
		139.0 125.0, 126.4	DFT-AM1 Experimental
		120.0 108.0, 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

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

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	133.0	DFT-AM1
		120.0, 121.0	Experimental
		99.0	DFT-AM1
		87.0, 90.1	Experimental
		98.8	DFT-AM1
		86.0, 89.9	Experimental
		102.4	DFT-AM1
		93.0, 93.2	Experimental

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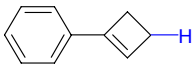
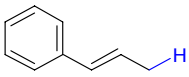
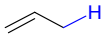
	C-H	83.3	Calculated
		85.6	Experimental
		79.9	Calculated
		78.9	Experimental
		88.3	Calculated
		84.6	Calculated
		86.6	Experimental

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

$H_3C—H$	C-H	79.4	HF
		100.3	MP2
		105.8	B3LYP
		104.7, 104.9	Experimental
		76.8	HF
		98.9	MP2
		101.1	B3LYP
		100.2, 101.1	Experimental
		74.5	HF
		95.3	MP2
		97.1	B3LYP
		99.4, 98.6	Experimental
		72.7	HF
		93.7	MP2
		94.0	B3LYP
		95.2, 96.5	Experimental
$FH_2C—H$		77.8	HF
		96.0	MP2
		99.1	B3LYP
		101.7	Experimental Avg

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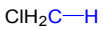
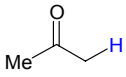
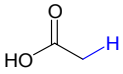
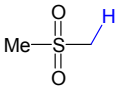
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	76.6	HF
		95.0	MP2
		99.7	B3LYP
		101.5	Experimental Avg
		74.1	HF
		92.3	MP2
		95.2	B3LYP
		94.1, 96.1	Experimental
		67.5	HF
		85.0	MP2
		87.7	B3LYP
		92.2	Experimental Avg
		74.9	HF
		93.1	MP2
		96.3	B3LYP
		94.1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

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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

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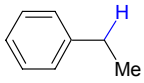
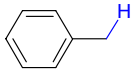
(kJ/mol)

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

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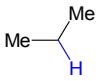
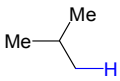
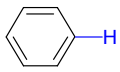
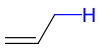
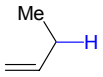
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
c-C_6H_{11}	C-H	97	Photoacoustic Calorimetry
c-C_6H_7		77	Photoacoustic Calorimetry
c-C_4H_8N		88.2, (87)	DFT, (Expt)
$N(Et)_2CHCH_3$		89.9, 89	DFT, (Expt)
C_4H_7O		90.7, 91.6, (92)	DFT, (Expt)
$C_4H_7O_2$		94.6, (96)	DFT, (Expt)
H_3C—H		105.0, 105.7 105	DFT Experimental
C_2H_5—H		100.3, 101.0 101	DFT Experimental
C_3H_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_3H_5—H		106.4, 107.2	DFT
c-C_4H_7—H		97.3, 98.0	DFT
c-C_6H_{11}—H		96.9, 97.6 97	DFT Experimental
C_2H_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

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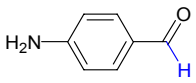
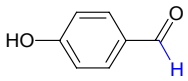
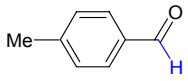
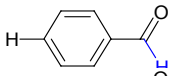
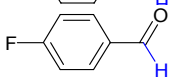
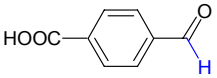
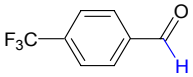
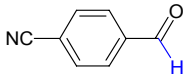
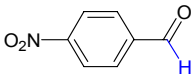
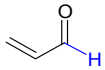
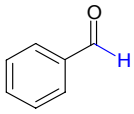
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-H	91.3	ALL *ab-initio*
		91.5	
		91.5	
		91.6	
		91.8	
		92.0	
		92.0	
		92.2	
		92.2	
		88.4	G3
		89.4 89.3	G3 Experimental
		91.2	G3
		91.6 88.9	CBS-4M Experimental

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