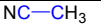
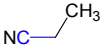
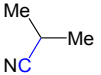
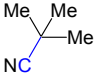
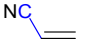
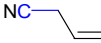
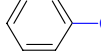
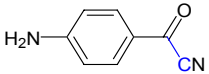
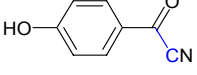
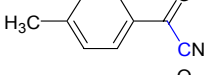
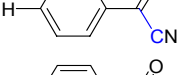
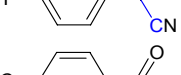
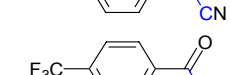
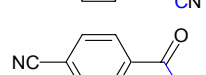
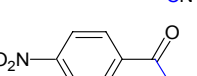
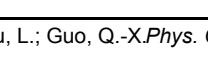
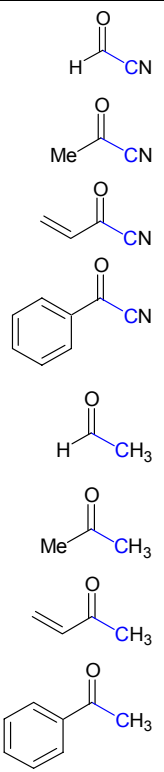


Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-CN	122.4	
		121.6	
		120.9	
		117.8	
		133	
		108.7	
		134	

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

	C-CN	
		111.4
		110.6
		110.5
		110.1
		110.0
		109.7
		109.6
		109.4
		109.1

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

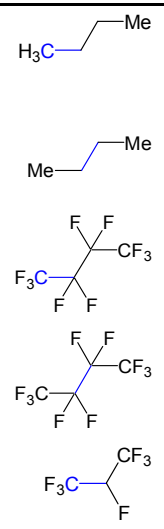
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-CN	104.7	G3
		107.3	G3
		108.9	G3
		110.1	CBS-4M
		83.5	G3
		83.4	G3
		84.4	Experimental
		84.1	G3
	86.4	CBS-4M	

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

Polycyclic Aromatic Hydrocarbon Borders

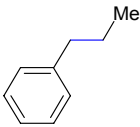
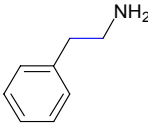
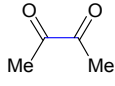
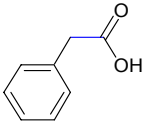
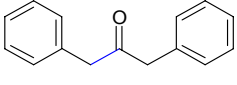
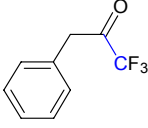
Zigzag border	C-CH ₃	~428
Armchair border		~394
Second Armchair dissociation		~287

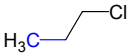
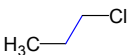
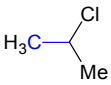
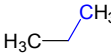



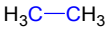
May, K.; Dapprich, S.; Furche, F.; Unterreiner, B. V.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2000**, *2*, 5084-5088

	C-C	91.3	G2
		91.5	G2MP2
		92.3	G2MS
		90.3	G2
		90.6	G2MP2
		91.2	G2MS
		97.0	G2MP2
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		94.4	G2MP2
		94.7	G2MS
		97.8	G2MP2
		98.0	G2MS

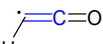
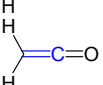






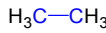
Fukaya, H.; Ono, T.; Abe, T. *J. Phys. Chem. A* **2001**, *105*, 7401-7404

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
CCl ₃ —CH ₃	C-C	89.36	<i>ab-initio</i>
		87.0	Experimental
		87.88	0 K
		89.41	Equilibrium Distance D_e
CFCl ₂ —CH ₃		93.85	<i>ab-initio</i>
		92.36	0 K
		93.68	Equilibrium Distance D_e
CF ₂ Cl—CH ₃		97.30	<i>ab-initio</i>
		95.82	0 K
		97.09	Equilibrium Distance D_e
CF ₃ —CH ₃		100.91	<i>ab-initio</i>
		101	Experimental
		99.42	0 K
		100.58	Equilibrium Distance D_e
CF ₃ —CClH ₂		96.34	<i>ab-initio</i>
		94.86	0 K
		90.07	Equilibrium Distance D_e
CF ₃ —CCl ₂ H		91.85	<i>ab-initio</i>
		90.37	0 K
		91.60	Equilibrium Distance D_e
CF ₃ —CCl ₃		86.87	<i>ab-initio</i>
		85.39	0 K
		86.67	Equilibrium Distance D_e
CF ₃ —CCl ₂ F		90.57	<i>ab-initio</i>
		89.28	0 K
		90.61	Equilibrium Distance D_e
CF ₃ —CClF ₂		93.55	<i>ab-initio</i>
		92.15	0 K
		93.53	Equilibrium Distance D_e
CF ₃ —CF ₃		96.20	<i>ab-initio</i>
		98.7, 97.27	Experimental
		94.27	0 K
		96.73	Equilibrium Distance D_e

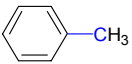
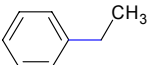
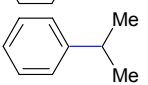
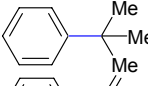
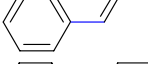
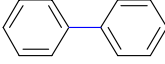
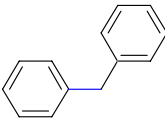
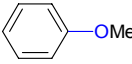
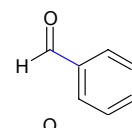
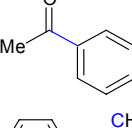
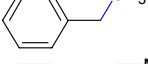
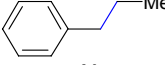
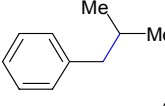
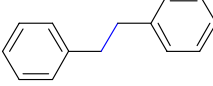
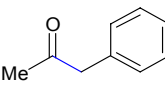
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
$\text{CH}_3\text{—CH}_3$	C-C	95.2	DFT-AM1
		88.0	Experimental
		86.6	Corrected
$\text{CH}_3\text{—CF}_3$		102.3	DFT-AM1
		101.2	Experimental
		93.1	Corrected
$\text{CF}_3\text{—CF}_3$		93.3	DFT-AM1
		96.9	Experimental
		84.9	Corrected
$\text{CF}_3\text{—CN}$		128.5	DFT-AM1
		123.9	Experimental
		116.9	Corrected
CN—CN		146.7	DFT-AM1
		128.0	Experimental
		133.5	Corrected
		73.8	DFT-AM1
		69.0	Experimental
		67.2	Corrected
$\text{H}_3\text{C—CH}_2\text{—CN}$		83.6	DFT-AM1
		72.7	Experimental
		76.0	Corrected
		68.8	DFT-AM1
		65.7	Experimental
		62.6	Corrected
		79.1	DFT-AM1
		67.4	Experimental
		72.0	Corrected
		76.5	DFT-AM1
		68.1	Experimental
		69.6	Corrected
		72.2	DFT-AM1
		65.4	Experimental
		65.7	Corrected
		86.5	DFT-AM1
		73.8	Experimental
		78.7	Corrected

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-C	376.5	<i>ab-initio</i>
		371.4	Experimental
	C-C	378.2	<i>ab-initio</i>
		370.4	Experimental
	C-C	376.3	<i>ab-initio</i>
		367.5	Experimental
	C-C	371.5	<i>ab-initio</i>
		371.2	Experimental
	C-C	375.8	<i>ab-initio</i>
		365.4	Experimental
	C-C	378.0	<i>ab-initio</i>
		365.1	Experimental
	C-C	375.4	<i>ab-initio</i>
		375.4	Experimental
	C-C	370.7	<i>ab-initio</i>
		375.9	Experimental

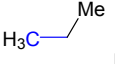
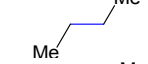
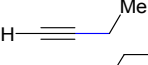
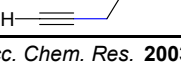
Seetula, J. A. J. *Chem. Soc Faraday Trans.* **1998**, *94*, 891-898

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-C	91	
		78.7	
	C-C	142.4	
		178.2	
		230.7	
	C-C	165	
		99.4	
	C-C	174.1	
		90.1	


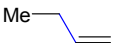
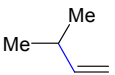
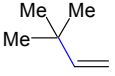


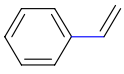
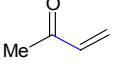
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Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-Ph	103.5	
		102.2	
		101.0	
		98.3	
		116	
		118	
		97	
		101	
		99.3	
		98.8	
		77.6	
		76.7	
		76.4	
		65.2	
		71.4	


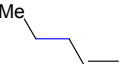
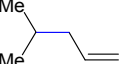
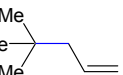
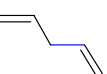
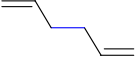
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	C-C	89.0	
		87.9	
		125.1	
		77	

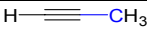
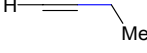
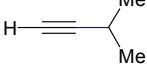
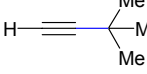
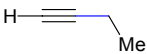
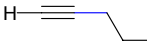
Blanksby, S. J.; Ellison, G. B. *Acc. Chem. Res.* **2003**, *36*, 255

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-CHCH ₂	101.4	
		100.0	
		99.2	
		97.8	
		116	
		87.3	
		116	
		41	

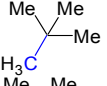
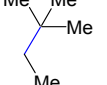
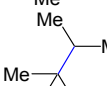
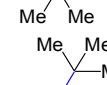

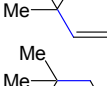
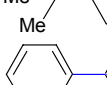
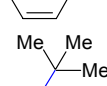
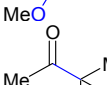
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	C-CH ₂ CHCH ₂	76.5
		75.4
		75.2
		73.2
		87.3
		62.7

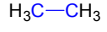


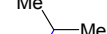

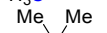



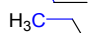
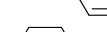

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	C-CCH	126.5
		125.1
		124.5
		122.3
		78
		77

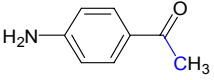
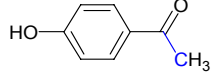
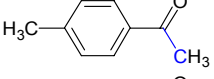
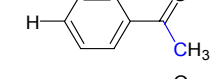
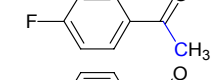
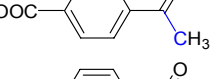
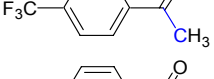
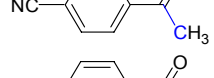
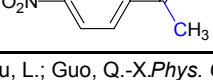
Blanksby, S. J.; Ellison, G. B. *Acc. Chem. Res.* **2003**, *36*, 255

Compound	Bond Dissociation Enthalpy (kcal/mol)	
	Bond (C-Y)	Theory Level
	C-C(CH ₃) ₃	87.5
		85.6
		82.7
		78.6
		97.8
		73.2
		98.3
		84
		79.4

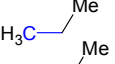
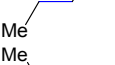
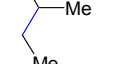
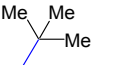
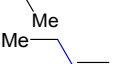
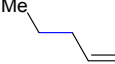
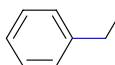
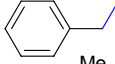
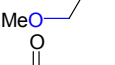
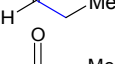
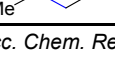
Blanksby, S. J.; Ellison, G. B. *Acc. Chem. Res.* **2003**, *36*, 255

	C-CH ₃	90.1
		89.0
		88.6
		87.5
		87.5
		101.4
		76.5
		103.5
		77.6
		83.2
		84.8
		84.5

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

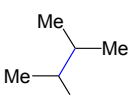
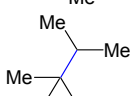
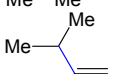
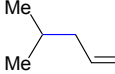
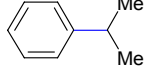
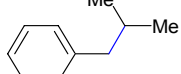
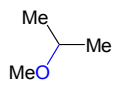
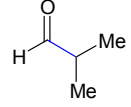
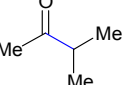
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-CH ₃	85.5	
		86.1	
		86.2	
		86.4	
		86.5	
		87.1	
		87.2	
		87.4	
		87.6	

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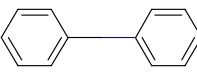
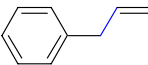
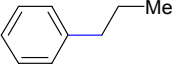
	C-CH ₂ CH ₃	89.0
		87.9
		87.1
		85.6
		100.0
		75.4
		102.2
		76.7
		85
		83.3
		83.5

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
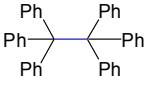
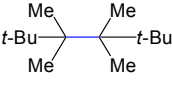
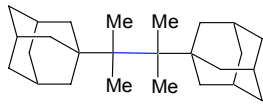
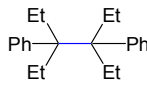
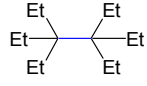
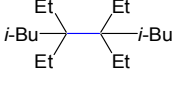
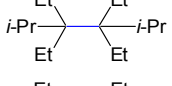
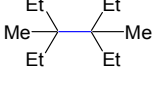
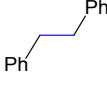
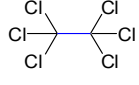
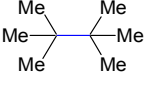

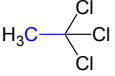
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level

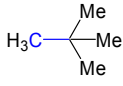
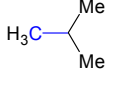
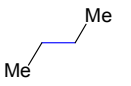
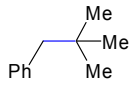
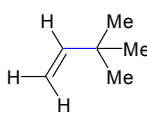
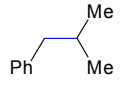
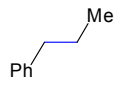
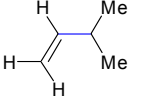
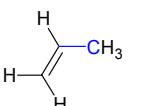
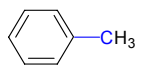
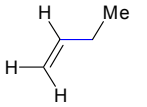
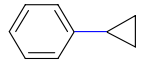
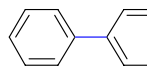
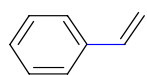
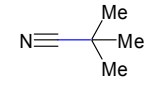
	C-CH(CH ₃) ₂	88.6	
		87.1	
		85.6	
		82.7	
		99.2	
		75.2	
		101.0	
		76.4	
		85.8	
		83.1	
		81.9	

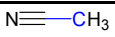
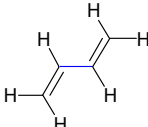
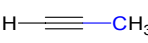
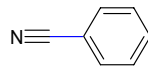
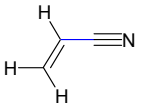
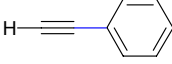
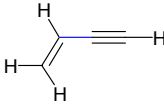


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	C-C	87.8	Experimental
		85.1	Experimental
		82.8	B3LYP/6-31G(d), 298K
		87.3	Experimental
		80.6	B3LYP/6-31G(d), 298K

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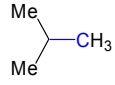
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
$\text{H}_3\text{C}-\text{CH}_3$	C-C	89.68	
		172.2	
$\text{H}-\text{C}\equiv\text{C}-\text{H}$		229.9	
		16.6	
		44.0	
		43.7	
		44.7	
		51.0	
		57.8	
		62.2	
		60.2	
		66.6	
		70.1	
		76.0	
		86.6	
		88.3	

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-C	86.0	
		88.9	
		87.2	
		97.4	
		97.5	
		102.1	
		102.3	
		99.7	
		100.9	
		103.9	
		99.6	
		111.9	
		118.0	
		116.9	
		115.8	

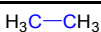
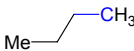
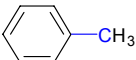
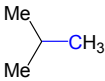
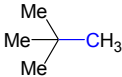
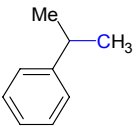
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-C	121.1	
		116.0	
		123.5	
		132.7	
		132.1	
		140.7	
		133.6	
		155.0	
		152.4	

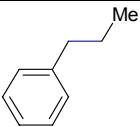
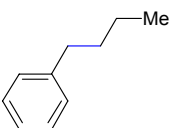
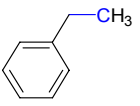
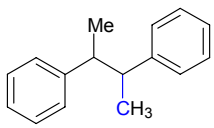
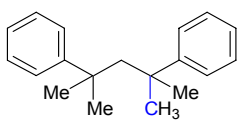
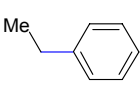
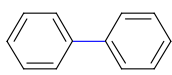
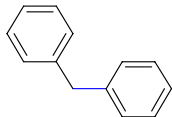
Zavitsas, A. A. *J. Phys. Chem. A* **2003**, *107*, 897-898

Reference includes bond distances in Angstroms

	C-C	66.10	HF and NR
		66.06	HF and RESC
		86.06	B3LYP and NR
		86.04	B3LYP and RESC
		81.77	BOP and NR
		81.76	BOP and RESC

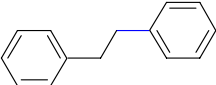
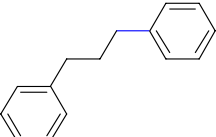
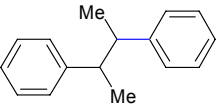
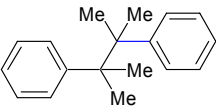
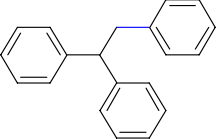
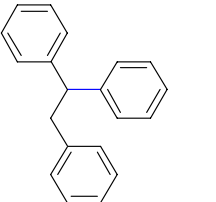
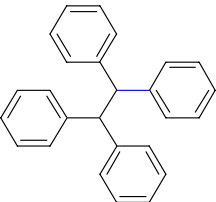
Lie, W.; Fedorov, D. G.; Hirao, K. *J. Phys. Chem. A* **2002**, *106*, 7057-7061

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-C	84.3	B3LYP
		85.9	B3PW91
		86.4	MPW1PW91
		88.6	B3P86
		88.1	CCSD(T)
		87.4	G2MSr
		90.4	Experimental
		81.4	B3LYP
		83.0	B3PW91
		83.8	MPW1PW91
		85.7	B3P86
		87.4	CCSD(T)
		87.0	G2MSr
		85.8	Experimental
		96.5	B3LYP
		97.9	B3PW91
		98.8	MPW1PW91
		100.8	B3P86
		101.8	Experimental
		78.7	B3LYP
		80.3	B3PW91
		81.3	MPW1PW91
		83.2	B3P86
		86.5	CCSD(T)
		86.6	G2MSr
		85.7	Experimental
		76.0	B3LYP
		77.6	B3PW91
		78.8	MPW1PW91
		80.7	B3P86
		85.4	CCSD(T)
		86.0	G2MSr
		84.1	Experimental
		66.4	B3LYP
		68.5	B3PW91
		69.7	MPW1PW91
		71.2	B3P86
		78.1	G2MSr
		74.6	Experimental

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-C	66.3	B3LYP
		68.6	B3PW91
		69.8	MPW1PW91
		71.2	B3P86
		71.8	Experimental
	C-C	66.9	B3LYP
		69.2	B3PW91
		70.5	MPW1PW91
		71.9	B3P86
		72.1	Experimental
	C-C	69.1	B3LYP
		71.4	B3PW91
		72.3	MPW1PW91
		73.9	B3P86
		75.8	Experimental
	C-C	60.2	B3LYP
		62.9	B3PW91
		64.3	MPW1PW91
		65.4	B3P86
		67.6	Experimental
	C-C	66.3, 63.0	B3LYP
		68.9, 65.5	B3PW91
		70.3, 67.2	MPW1PW91
		71.8, 68.9	B3P86
	C-C	92.4	B3LYP
		93.9	B3PW91
		95.1	MPW1PW91
		96.9	B3P86
	C-C	108.0	B3LYP
		109.5	B3PW91
		110.8	MPW1PW91
		112.9	B3P86
		113.7	Experimental
	C-C	79.6	B3LYP
		82.0	B3PW91
		83.4	MPW1PW91
		84.8	B3P86
		89.6	Experimental

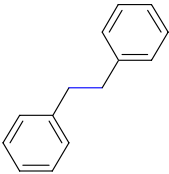
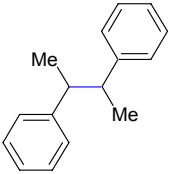
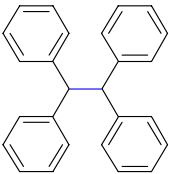
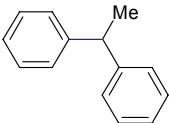
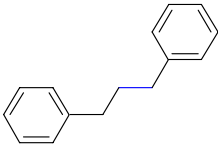
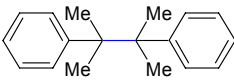
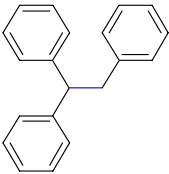
Yao, X.-Q.; Hou, X.-J.; Wu, G.-S.; Xu, Y.-Y.; Xiang, H.-W.; Jiao, H.; Li, Y.-W. *J. Phys. Chem. A* **2002**, *106*, 7184-7189

Reference includes bond distances in Angstroms

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-C	93.1	B3LYP
		94.6	B3PW91
		95.8	MPW1PW91
		97.6	B3P86
		92.6	B3LYP
		94.2	B3PW91
		95.4	MPW1PW91
		97.2	B3P86
		87.4	B3LYP
		89.4	B3PW91
		91.1	MPW1PW91
		92.9	B3P86
		76.2	B3LYP
		78.6	B3PW91
		80.9	MPW1PW91
		82.9	B3P86
		91.0	B3LYP
		92.7	B3PW91
		94.1	MPW1PW91
		95.9	B3P86
		74.8	B3LYP
		77.1	B3PW91
		79.0	MPW1PW91
		80.3	B3P86
		73.3	B3LYP
		76.0	B3PW91
		78.2	MPW1PW91
		79.5	B3P86

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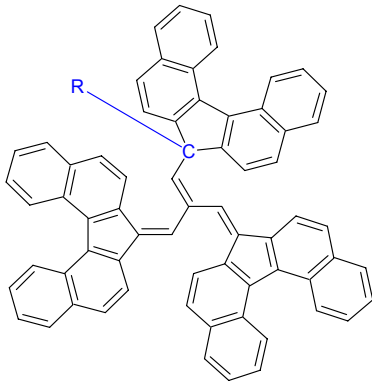
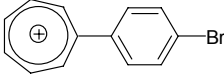
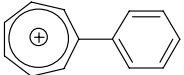

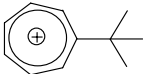
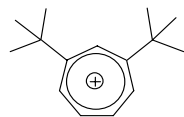
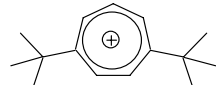
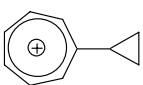
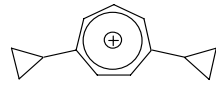
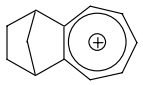
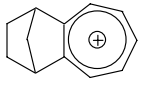
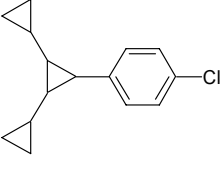
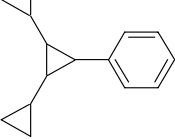
Reference includes bond distances in Angstroms

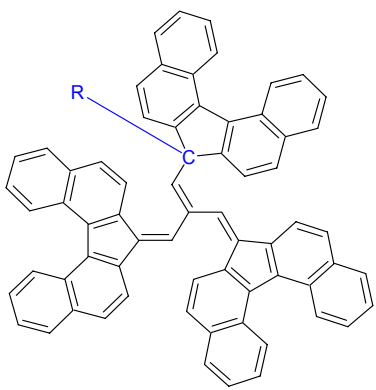
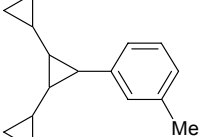
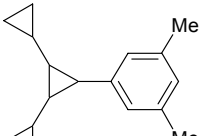
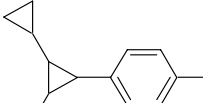
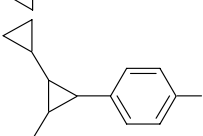
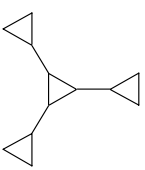
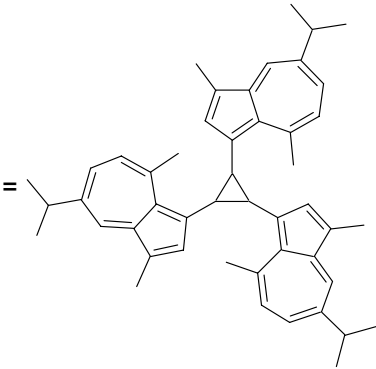




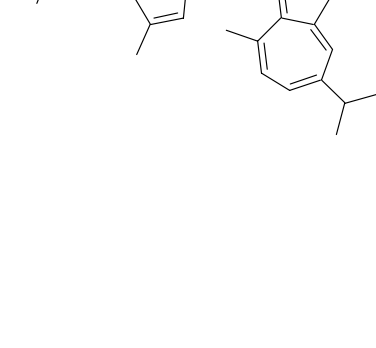
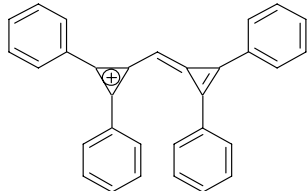
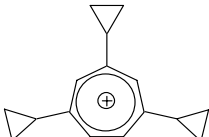
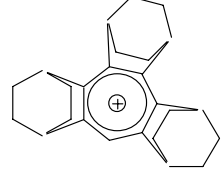
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	C-C	54.1	B3LYP
		57.1	B3PW91
		58.5	MPW1PW91
		59.5	B3P86
		61.4	Experimental
		46.9	B3LYP
		49.9	B3PW91
		52.1	MPW1PW91
		52.9	B3P86
		32.7	B3LYP
		36.9	B3PW91
		39.7	MPW1PW91
		39.8	B3P86
		47.5	Experimental
		75.7	B3LYP
		78.0	B3PW91
		79.7	MPW1PW91
		79.7	B3P86
		66.8	B3LYP
		69.0	B3PW91
		70.3	MPW1PW91
		71.6	B3P86
		73.9	Experimental
		31.8	B3LYP
		35.4	B3PW91
		38.5	MPW1PW91
		39.5	B3P86
		43.4	B3LYP
		46.7	B3PW91
		48.8	MPW1PW91
		49.3	B3P86
		57.8	Experimental

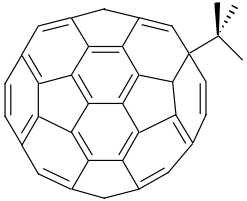

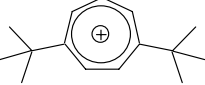
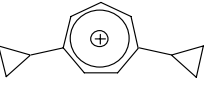
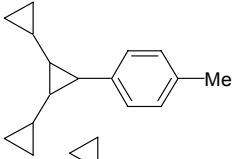
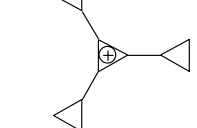
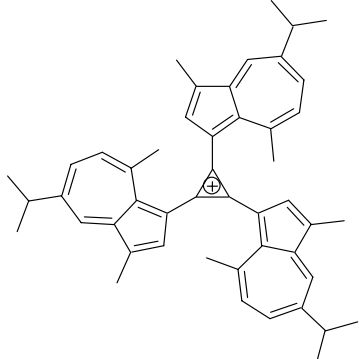
Yao, X.-Q.; Hou, X.-J.; Wu, G.-S.; Xu, Y.-Y.; Xiang, H.-W.; Jiao, H.; Li, Y.-W.J. *Phys. Chem. A* **2002**, *106*, 7184-7189

Reference includes bond distances in Angstroms

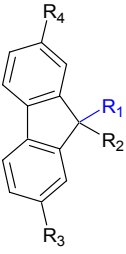
Compound	ΔG° (kcal/mol)		
	Heterolysis	Bond (C-Y)	Energy

Compound	ΔG° (kcal/mol)		
	Heterolysis	Bond (C-Y)	Energy
		C-C	
	R =		8.7 (DMSO)
	R ⁺ =		8.2 (DMSO)
	R ⁺ =		8.3 (DMSO)
		$\Delta H_{\text{het}}^\circ$	19.6
	R ⁺ =		8.2 (DMSO) 9.3 (Sulfolane)
	R ⁺ =		8.2 (DMSO) 9.2 (Sulfolane)
	R ⁺ =		7.7 (DMSO) 8.0 (Sulfolane)
	R ⁺ =		7.1 (DMSO) 8.0 (Sulfolane)
	R ⁺ =		4.9 (DMSO) 6.8 (Sulfolane)
	R ⁺ =		5.2 (DMSO) 6.5 (Sulfolane)
	R ⁺ =		5.4 (DMSO) 6.5 (Sulfolane)
	R =		5.9 (DMSO)
	R =		5.5 (DMSO)
		$\Delta H_{\text{het}}^\circ$	11.9

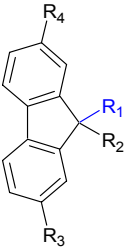
Compound	ΔG° (kcal/mol)		
	Heterolysis	Bond (C-Y)	Energy (Solvent)
	R =		4.6 (DMSO)
	R =		4.8 (DMSO)
	R =		4.6 (DMSO)
	R =		4.6 (DMSO)
	R =		<4 (DMSO)
	R =		4.8 (CH ₃ CN)
	R =		5.7 (ClCH ₂ CH ₂ Cl)
	R =		6.7 (CH ₂ Cl ₂)
	R =		6.6 (THF)
	R =	<4 (DMSO)	<4 (DMSO)
	R ⁺ =		<4 (DMSO)
	R ⁺ =		<4 (DMSO)
	R ⁺ =		<4 (DMSO)

Compound	ΔG° (kcal/mol)		
	Heterolysis	Bond (C-Y)	Energy (Solvent)
	$R^+ =$ 	C-C	ΔG_0 9.3 (DMSO, CS ₂)
	$R^+ =$ 		8.2 (DMSO, CS ₂)
	$R^+ =$ 		7.7 (DMSO, CS ₂)
	$R =$ 		6.2 (DMSO, CS ₂)
	$R^+ =$ 		<4 (DMSO, CS ₂)
	$R^+ =$ 		<4 (DMSO, CS ₂)

Kitagawa, T.; Takeuchi, K.J. *Phys. Org. Chem.* **1998**, *11*, 157-170

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	R ₁ = CPh ₃ , R ₂ = COOMe R ₃ , R ₄ = H	C-R ₁ heterol. homolysis	25.81 16.08
	R ₁ = CPh ₃ , R ₂ = SO ₂ Ph R ₃ , R ₄ = H	heterolysis homolysis	28.35 22.38
	R ₁ = CPh ₃ , R ₂ = SPh R ₃ = H, R ₄ = Br	heterolysis homolysis	29.41 15.60
	R ₁ = CPh ₃ , R ₂ = SPh R ₃ , R ₄ = H	heterolysis homolysis	33.61 12.96
	R ₁ = CPh ₃ , R ₂ = Ph R ₃ , R ₄ = H	heterolysis homolysis	35.51 13.18
	R ₁ = Xan, R ₂ = COOMe R ₃ , R ₄ = Br	heterolysis homolysis	24.62 26.03
	R ₁ = Xan, R ₂ = COOMe R ₃ , R ₄ = H	heterolysis homolysis	27.33 22.53
	R ₁ = Xan, R ₂ = SPh R ₃ = H, R ₄ = Br	heterolysis homolysis	30.13 21.25
	R ₁ = Xan, R ₂ = SPh R ₃ , R ₄ = H	heterolysis homolysis	33.03 20.69
	R ₁ = TPCP, R ₂ = COOMe R ₃ , R ₄ = Br	heterolysis homolysis	16.22 39.70
	R ₁ = TPCP, R ₂ = CN R ₃ , R ₄ = H	heterolysis homolysis	19.56 38.54
	R ₁ = TPCP, R ₂ = COOMe R ₃ , R ₄ = H	heterolysis homolysis	20.62 37.89
	R ₁ = TPCP, R ₂ = SO ₂ Ph R ₃ , R ₄ = H	heterolysis homolysis	22.23 43.26
	R ₁ = TPCP, R ₂ = SPh R ₃ = H, R ₄ = Br	heterolysis homolysis	25.40 38.59
	R ₁ = TPCP, R ₂ = SPh R ₃ , R ₄ = H	heterolysis homolysis	27.49 37.22
	R ₁ = TPCP, R ₂ = Ph R ₃ , R ₄ = H	heterolysis homolysis	29.34 34.02

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

	R ₁ = C ₇ H ₇ , R ₂ = CO ₂ Me R ₃ , R ₄ = Br	C-R ₁ heterol. homolysis	19.45 27.20
	R ₁ = C ₇ H ₇ , R ₂ = CO ₂ Me R ₃ , R ₄ = H	heterolysis homolysis	24.89 26.44
	R ₁ = C ₇ H ₇ , R ₂ = SO ₂ Ph R ₃ , R ₄ = H	heterolysis homolysis	27.17 32.47
	R ₁ = C ₇ H ₇ , R ₂ = SPh R ₃ = H, R ₄ = Br	heterolysis homolysis	28.59 26.05
	R ₁ = C ₇ H ₇ , R ₂ = SPh R ₃ , R ₄ = H	heterolysis homolysis	30.52 24.52
	R ₁ = C ₇ H ₇ , R ₂ = Ph R ₃ , R ₄ = H	heterolysis homolysis	33.84 22.79
	R ₁ = CPh ₃ , R ₂ = COOMe R ₃ , R ₄ = Br	heterolysis homolysis	19.76 16.23

Arnett, E.M.; Venimadhavan, S.J. *Am. Chem. Soc.* **1991**, *113*, 6967-6975

(kJ/mol)

C ₅ H ₁₁ -C ₅ H ₁₁	C-C	361.7
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