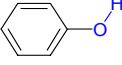
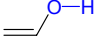


Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
$t\text{Bu}-\text{O}-t\text{Bu}$	O-O	172.5	
		172.3	
I-I	I-I	151.3	
Cl-Cl	Cl-Cl	243.36	

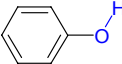
Leal, J. P.; Marques, N.; Takats, J.J. *Organomet. Chem.* **2001**, 632, 209-214

	O-H	87.2	Experimental
		79.3	B3LYP/6-31G(d), 298K
		83.1	B3LYP/6-311++G(d,p), 298K
	O-H	84.3	Experimental
		74.8	B3LYP/6-31G(d), 298K
		79.8	B3LYP/6-311++G(d,p), 298K

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

HOH		114.2	B3LYP 6-311G(d,p)
		115.1	(RO)B3LYP 6-311G(d,p)
		118.4	(RO)B3LYP 6-311++G(3df,2p)
		119.0	Experimental

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

		(Solvent)	
	O-H	86.2	isooctane
		88.0	CCl ₄
		86.3	benzene
		88.3	acetonitrile
		88.3	ethyl acetate
		94	DMSO
		96	NEt ₃
		87.4	solution average
		87	gas phase
		84	benzene
		87	benzene
	87	various	

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

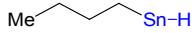
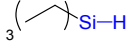
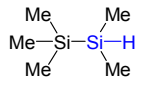
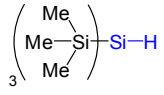
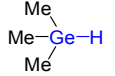





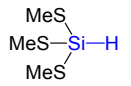
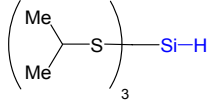
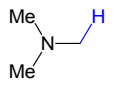
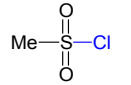
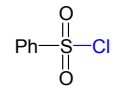
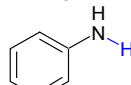
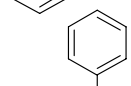
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level (DFT)
Ru—Ru	M-M	40.6	GGA-BP86
		37.1	GGA-BPD91
		46.6	GGA-PD91
		46.1	Experimental
Rh—Rh		33.0	GGA-BP86
		29.7	GGA-BPD91
		32.4	GGA-PD91
		56.8, 32.3, 18.08, 26.7	Experimental
Pd—Pd		33.9	GGA-BP86
		25.5	GGA-BPD91
		31.8	GGA-PD91
		25.0	Experimental
Sn—Sn		60.5	GGA-BP86
		58.9	GGA-BPD91
		61.7	GGA-PD91
		46.9, 44.9	Experimental
Ru—Sn		61.1	GGA-BP86
		58.2	GGA-BPD91
		64.0	GGA-PD91
Rh—Sn		57.6	GGA-BP86
		54.6	GGA-BPD91
		61.0	GGA-PD91
Pd—Sn		66.4	GGA-BP86
		63.2	GGA-BPD91
		65.5	GGA-PD91


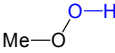
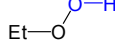
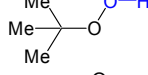


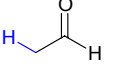
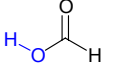
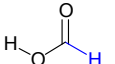
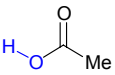
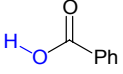



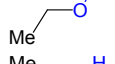
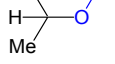
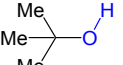

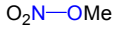
Xavier, E. S.; Duarte, H. A.J. *Quant. Chem.* **2003**, 95(2), 164-176

Compound		Bond Dissociation Enthalpy (kcal/mol)		
		Bond (C-Y)	Energy	Theory (DFT)
M(BMe) ₄	M = Ni	M-BMe	87.2	BP86/II
			87.9	BP86/TZP
	M = Pd		72.5	BP86/II
			70.2	BP86/TZP
			85.5	BP86/II
M = Pt	83.4	BP86/TZP		
M(AlMe) ₄	M = Ni	M-AlMe	59.4	BP86/II
			62.9	BP86/TZP
	M = Pd		50.4	BP86/II
			51.4	BP86/TZP
			60.4	BP86/II
M = Pt	60.6	BP86/TZP		
M(GaMe) ₄	M = Ni	M-GaMe	47.5	BP86/II
			51.5	BP86/TZP
	M = Pd		Experimental	
			38.0	BP86/II
			39.9	BP86/TZP
M = Pt	46.4	BP86/II		
	48.0	BP86/TZP		
		Experimental		
M(InMe) ₄	M = Ni	M-InMe	48.2	BP86/II
			44.9	BP86/TZP
	M = Pd		Experimental	
			40.7	BP86/II
			35.0	BP86/TZP
M = Pt	48.6	BP86/II		
	41.5	BP86/TZP		
M(TlMe) ₄	M = Ni	M-TlMe	35.6	BP86/II
			34.0	BP86/TZP
	M = Pd		25.2	BP86/II
			24.2	BP86/TZP
			29.4	BP86/II
M = Pt	27.8	BP86/TZP		



Doerr, M.; Frenking, G.Z. *Anorg. Allg. Chem.* **2002**, 628, 843-850

Reference includes bond distances





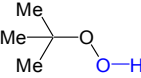
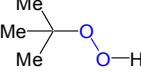
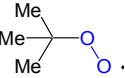
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Solvent
	Sn-H	78	isooctane
	Si-H	96	isooctane
		91	isooctane
		84	isooctane
	Ge-H	87	benzene
		86	benzene
		88	benzene
		86	benzene
		85	benzene
		85	benzene
		87	benzene
	Si-H	90	benzene
	N-H	91	benzene
	S-Cl	70	benzene
		71	benzene
	N-H	90	benzene
		87	benzene

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	O-H	87.8	
		88	
		85	
		84	
		88.144	
		89.4	
		94	
		112	
		≥ 96	
		112	
		111	
		104.6	
	S-H	87.4	
	C-H	94	
	O-H	104.7	
		105.7	
		106.3	
		90	
	N-O	42	

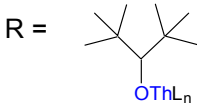
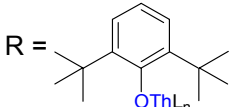
Blanksby, S. J.; Ellison, G. B. *Acc. Chem. Res.* **2003**, *36*, 255

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
H-H	H-Y	104.206	
H-NH ₂		107.6	
H-OH		118.82	
H-O		101.76	
H-O [⊖]		110.21	
H-O [⊕]		115.2	
H-SH		91.2	
H-S		84.1	
H-NO		49.5	
		79.1	
		101.7	
H-SiH ₃		91.7	
H-GeH ₃		83	

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

	O-H	30.2	
		104.6	
		5	
		112	
		85	
	O-O	47	
		65	

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

Compound	Bond Dissociation Enthalpy (kJ/mol)			
	Bond (C-Y)	Energy	Theory Level	
Th(Cp*) ₂ (OR)H	 R = 	Th-O	518.8	
		Th-OR	389	389
			384	384
[Th(Cp*) ₂ H ₂] ₂		Th-H	390	
Ti-Cl ₄		Ti-Cl		430.5
Zr(Cp*) ₂ R ₂	R = H	Zr-Cl		491.4
		Zr-H	339	339
		Hf-Cl		497.6
		Mn-Mn		159
Mn(CO) ₅ R	R = H	Mn-H	245	245
		Re-Re		187
Fe(CO) ₄ H ₂		Fe-H	272	244

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

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Bond Enthalpy Terms (E)
Sc-H	M-H	202	
Ti-H		197	
V-H		172	
Cr-H		172	
Mn-H		126	
Fe-H		191	
Co-H		190	
Ni-H		243	
Cu-H		255	
Zn-H		86	
Mo-H		208	
Ru-H		234	
Rh-H		247	
Pd-H		234	
Ag-H		215	
Cd-H		69.0	
Au-H		292	
Pt-H		352	
Yb-H		159	

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

Sc-H	M ⁺ -H	239	
Ti-H		227	
V-H		202	
Cr-H		136	
Mn-H		203	
Fe-H		208	
Co-H		195	
Ni-H		166	
Cu-H		92	
Zn-H		231	
Y-H		261	
Zr-H		230	
Nb-H		226	
Mo-H		176	
Ru-H		172	
Rh-H		151	
Pd-H		197	
Ag-H		67	
La-H		243	
Lu-H		204	
U-H		208	

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

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Bond Enthalpy Terms (E)
Sc-H	M-H ⁺	918	
Ti-H		881	
V-H		864	
Cr-H		795	
Mn-H		797	
Fe-H		761	
Co-H		749	
Ni-H		741	
Cu-H		658	
Zn-H		637	
Y-H		973	
Zr-H		906	
Nb-H		902	
Mo-H		803	
Ru-H		783	
Rh-H		736	
Pd-H		704	
Ag-H		648	
La-H		1017	
Lu-H		992	
U-H		995	

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

Cr-H	M ⁻ -H	162	
Mn-H		>210	
Fe-H		265	
Co-H		191	
Ni-H		177	

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

Cr-H	M-H ⁻	153	
Mn-H		137	
Fe-H		208	
Co-H		182	
Ni-H		217	

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

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Bond Enthalpy Terms (<i>E</i>)
Sc-H	M^+-H^-	762	
Ti-H		782	
V-H		750	
Cr-H		752	
Mn-H		771	
Fe-H		878	
Co-H		876	
Ni-H		907	
Cu-H		928	
Zn-H		919	
Mo-H		820	
Ru-H		863	
Rh-H		902	
Pd-H		966	
Ag-H		874	
Cd-H		864	
Au-H		1109	
Pt-H		1110	
Yb-H		689	

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

Sc-H	M^--H^+	1496	
Ti-H		1501	
V-H		1433	
Cr-H		1419	
Mn-H		>1438	
Fe-H		1488	
Co-H		1438	
Ni-H		1443	
Cu-H		1448	
Zn-H		>1398	
Mo-H		1448	
Ru-H		1445	
Rh-H		1449	
Pd-H		1492	
Ag-H		1402	
Cd-H		>1380	
Au-H		1381	
Pt-H		1458	

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

Cd-H		49	
Au-H		>113	
Hg-H		6	

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

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Bond Enthalpy Terms (<i>E</i>)
ScH ₂	M ⁺ -H	244	239
YH ₂		272	261
LaH ₂		266	243
LuH ₂		207	204
CoH ₂		209	195
Sc(H)Me	M ⁺ -Me	263	M ⁺ -H 239
V(H)Me		188	202
Co(H)Me		182	195

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

		Proton Affinity (kJ/mol)		
Ni(Cp) ⁺ -L	L = PH ₃	M(Cp ⁺)-L	190.4	-58.2
	L = MeOH		190.8	-84.1
	L = NO		192.0	-78
	L = Me ₂ O		196.2	-49.8
	L = MeCHO		196.7	-67.4
	L = MeSH		197.1	-68.6
	L = EtOH		198.7	-61.5
	L = HCN		199.2	-109.2
	L = EtCHO		201.3	-56.9
	L = <i>i</i> -PrCHO		205.4	-49.0
	L = C ₂ H ₃ CHO		206.3	-59.8
	L = <i>i</i> -PrOH		207.1	-43.9
	L = <i>t</i> -BuCHO		207.5	-52.3
	L = Me ₂ CO		212.1	-32.6
	L = <i>i</i> -BuOH		212.5	-41.8
	L = MeOAc		213.0	-41.4
	L = Et ₂ O		213.0	-19.2
	L = Me ₂ S		213.8	-18.0
	L = NH ₃		218.8	0
	L = MeCN		222.6	-59.0
	L = MeNH ₂		231.0	38.1
	L = NMe ₃		236.0	80.8
	L = Me ₂ NH		237.7	64.9
	L = AsMe ₃		239.3	36.4
	L = MeNC		241.0	-26.4
	L = PMe ₃		241.0	86.6

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

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Electron Affinity
Mn-Mn		159	
Mn-H		245	
R ⁺ -H	R = V(CO) ₆	R ⁺ -H	220
	R = Cr(CO) ₆		230
	R = Cr(CO) ₂ (Cp)NO		207
	R = Cr(CO) ₃ (Cp)Me		244
	R = Cr(CO) ₃ Bz		221
	R = Mo(CO) ₆		260
	R = W(CO) ₆		257
	R = Mn(CO) ₅ H		349
	R = Mn(CO) ₅ Me		267
	R = Cr(CO) ₃ (MeC ₅ H ₄)		283
	R = Mn(CO) ₁₀		204
	R = Re(CO) ₅ Me		294
	R = Re ₂ (CO) ₁₀		246
	R = MnRe(CO) ₁₀		<267
	R = Fe(CO) ₅		299
	R = Fe(Cp) ₂		215, 198, 202
	R = Fe(CO) ₂ (Cp)Me		210
	R = Ru(Cp) ₂		271
	R = Co(CO) ₂ (Cp)		245
	R = Rh(CO) ₂ (Cp)		287
	R = Ni(CO) ₄		248
	R = Ni(Cp) ₂		215
	R = Ni(Cp)NO		315
Mn(CO) ₅ H		L _n M ⁻ -H ⁺	1331
Fe(CO) ₄ H ₂			1334
Co(CO) ₄ H			≤1314
Fe(CO) ₄ H			≥1335
			≤245
			232
			≥227
			232

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

(kcal/mol)

pyCo(dimethylglyoxime) ₂	Co-I	34.6
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Toscano, P. J.; Seligson, A. L.; Curran, M. T.; Skrobitt, A. T.; Sonnenberger, D. *Inorg. Chem.* **1989**, *28*, 166-168

Compound		Bond Dissociation Enthalpy (kJ/mol)		
		Bond (C-Y)	Energy	Theory Level
M-O	M = Sc	M-O	681	
	M = Ti		672	
	M = V		625	
	M = Cr		429	
	M = Mn		403	
	M = Fe		390	
	M = Co		384	
	M = Ni		381	
	M = Cu		270	
	M = Zn		271	
	M = Y		719	
	M = Zr		776	
	M = Nb		769	
	M = Mo		560	
	M = Tc		548	
	M = Ru		528	
	M = Rh		405	
	M = Pd		381	
	M = Ag		221	
	M = Cd		236	
	M = La		801	
	M = Hf		801	
	M = Ta		799	
	M = W		672	
	M = Re		627	
	M = Os		598	
	M = Ir		414	
	M = Pt		391	
	M = Au		223	
	M = Hg		213	

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

(Resultant Radical)

H ₂ O	OH	O-H	499	463.5
H ₂ CO	HCO		372	423.4
MeOH			438	451.2
MeC(O)H			359	426.6
EtOH	EtO		436	451.2
	MeCHOH		389	401.7
EtC(O)H			366	426.6
MeC(O)CH ₃			411	410.8
PrOH			432	451.2
<i>i</i> -PrOH			438	451.2
PrC(O)H			366	426.6
BuOH			430	451.2
<i>s</i> -BuOH			443	451.2
<i>i</i> -BuOH			440	451.2
<i>t</i> -BuOH			440	451.2

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

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	O-O	27.2	DFT-AM1
		37.6	Experimental
		35.0	DFT-AM1
		46.3	Experimental
		31.0	DFT-AM1
		37.9	Experimental
		29.7	DFT-AM1
		37.7	Experimental
		24.3	DFT-AM1
		38.0	Experimental
		21.1	DFT-AM1
		35.5	Experimental
		21.6	DFT-AM1
		30.4	Experimental
	N-N	66.5	DFT-AM1
		70.8	Experimental
		63.6	DFT-AM1
		64.8	Experimental
		59.5	DFT-AM1
		62.7	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
H-H	H-H	79.5	HF
		95.8	MP2
		106.4	B3LYP
		104.2	Experimental

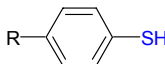
Korth, H.-G.; Sicking, W. *J. Chem. Soc. Perkin Trans. 2* **1997**, 715-719

H-F	136.25
H-Cl	103.15
H-Br	87.54
H-I	71.32

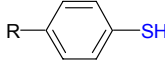
Blanksby, S. J.; Ellison, G. B. *Acc. Chem. Res.* **2003**, 36, 255

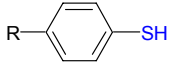
M-H	M = Y	M-H	70.0
	M = Zr		58.8
	M = Nb		63.0
	M = Mo		54.0
	M = Tc		52.1
	M = Ru		62.4
	M = Rh		68.2
	M = Pd		53.4
	M = H		H-H

Siegbahn, P. E. *M.J. Phys. Chem.* **1995**, 99, 12723-12729

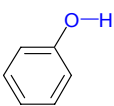
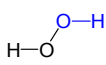
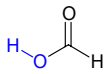
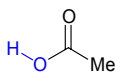


4-methoxythiophenol 	R = OMe	S-H heterol. heterolysis	31.92	
			27.85	9-Phenylxanthylum (rxn)
			27.67	xanthylum (rxn)
			21.90	triphenylcyclopropenylum
			21.61	triopylium (rxn)
			23.80	perinaphthenium (rxn)
			29.24	4,4'-dimethoxydiphenylmethyl
			11.47	triphenylpyrylium (rxn)
			30.24	9,9-dimethyl-10-phenyl- 9,10-dihydroanthracenium
		homolysis	77.3	
			23.51	9-Phenylxanthylum (rxn)
			23.22	xanthylum (rxn)
			39.52	triphenylcyclopropenylum
			23.56	triopylium (rxn)
			11.65	perinaphthenium (rxn)
			27.16	4,4'-dimethoxydiphenylmethyl
			16.77	triphenylpyrylium (rxn)
			20.85	9,9-dimethyl-10-phenyl- 9,10-dihydroanthracenium

Venimadhavan, S.; Amarnath, K.; Harvey, N.G.; Cheng, J.-P.; Arnett, E.M.J. *Am. Chem. Soc.*, **1992**, 114(1), 221-229

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
4-nitrothiophenol R = NO ₂ 	S-H heterol. heterolysis	23.34	
		18.33	9-Phenylxanthylum (rxn)
		21.66	xanthylum (rxn)
		14.44	triphenylcyclopropenylium
		12.95	triopylium (rxn)
		16.19	perinaphthenium (rxn)
		19.09	4,4'-dimethoxydiphenylmethyl
		22.60	9,9-dimethyl-10-phenyl- 9,10-dihydroanthracenium
		81.6	
		26.10	9-Phenylxanthylum (rxn)
		29.32	xanthylum (rxn)
		44.16	triphenylcyclopropenylium
		26.95	triopylium (rxn)
		27.42	4,4'-dimethoxydiphenylmethyl
24.32	9,9-dimethyl-10-phenyl- 9,10-dihydroanthracenium		
4-bromothiophenol R = Br	heterolysis	26.87	
		23.05	9-Phenylxanthylum (rxn)
		24.70	xanthylum (rxn)
		17.80	triphenylcyclopropenylium
		17.85	triopylium (rxn)
		18.50	triopylium (rxn)
		23.50	4,4'-dimethoxydiphenylmethyl
		24.75	9,9-dimethyl-10-phenyl- 9,10-dihydroanthracenium
		80.2	
		24.71	9-Phenylxanthylum (rxn)
		26.25	xanthylum (rxn)
		41.41	triphenylcyclopropenylium
		25.74	triopylium (rxn)
		12.34	perinaphthenium (rxn)
27.42	4,4'-dimethoxydiphenylmethyl		
21.36	9,9-dimethyl-10-phenyl- 9,10-dihydroanthracenium		
4-chlorothiophenol R = Cl	heterolysis	27.53	
		24.36	9-Phenylxanthylum (rxn)
		25.87	xanthylum (rxn)
		13.09	triphenylcyclopropenylium
		18.38	triopylium (rxn)
		20.37	perinaphthenium (rxn)
		23.88	4,4'-dimethoxydiphenylmethyl
		25.32	9,9-dimethyl-10-phenyl- 9,10-dihydroanthracenium
		78.4	
		23.71	9-Phenylxanthylum (rxn)
		25.11	xanthylum (rxn)
		39.40	triphenylcyclopropenylium
		23.96	triopylium (rxn)
		11.91	perinaphthenium (rxn)
25.49	4,4'-dimethoxydiphenylmethyl		
19.62	9,9-dimethyl-10-phenyl- 9,10-dihydroanthracenium		

Compound		Bond Dissociation Enthalpy (kcal/mol)			
		Bond (C-Y)	Energy	Theory Level	
thiophenol  R = H	S-H	heterol.	29.25		
		heterolysis	26.11	9-Phenylxanthylum (rxn)	
			26.43	xanthylum (rxn)	
			20.14	triphenylcyclopropenylum	
			20.37	triopylium (rxn)	
			22.42	perinaphthenium (rxn)	
			26.47	4,4'-dimethoxydiphenylmethyl	
			9.05	triphenylpyrylium (rxn)	
			27.08	9,9-dimethyl-10-phenyl- 9,10-dihydroanthracenium	
			homolysis	78.5	
				24.29	9-Phenylxanthylum (rxn)
		24.49		xanthylum (rxn)	
		40.27		triphenylcyclopropenylum	
		24.57		triopylium (rxn)	
		12.78		perinaphthenium (rxn)	
		26.91		4,4'-dimethoxydiphenylmethyl	
		16.87		triphenylpyrylium (rxn)	
		20.21		9,9-dimethyl-10-phenyl- 9,10-dihydroanthracenium	
		4-methylthiophenol R = Me	S-H	heterolysis	29.90
26.94	9-Phenylxanthylum (rxn)				
27.16	xanthylum (rxn)				
20.75	triphenylcyclopropenylum				
20.75	triopylium (rxn)				
22.98	perinaphthenium (rxn)				
27.90	4,4'-dimethoxydiphenylmethyl				
10.45	triphenylpyrylium (rxn)				
28.85	9,9-dimethyl-10-phenyl- 9,10-dihydroanthracenium				
homolysis	77.8				
	23.64			9-Phenylxanthylum (rxn)	
	23.75			xanthylum (rxn)	
	39.38			triphenylcyclopropenylum	
	39.52			triopylium (rxn)	
	11.87			perinaphthenium (rxn)	
	26.86			4,4'-dimethoxydiphenylmethyl	
	16.79			triphenylpyrylium (rxn)	
	20.50			9,9-dimethyl-10-phenyl- 9,10-dihydroanthracenium	

Venimadhavan, S.; Amarnath, K.; Harvey, N.G.; Cheng, J.-P.; Arnett, E.M.J. *Am. Chem. Soc.*, **1992**, *114*(1), 221-229

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
H ₂ N—H	N-H	110.6	DFT-AM1
		110.0	Experimental
ON—H		48.5	DFT-AM1
		49.5	Experimental
F ₂ N—H		73.5	DFT-AM1
		75.7	Experimental
N ₃ —H		89.7	DFT-AM1
		87.0	Experimental
HO—H	O-H	116.8	DFT-AM1
		119.0	Experimental
MeO—H		102.7	DFT-AM1
		104.4	Experimental
		85.9	DFT-AM1
		88.0	Experimental
		89.5	DFT-AM1
		87.2	Experimental
		110.0	DFT-AM1
		110.0	Experimental
		107.0	DFT-AM1
		106.0	Experimental
		76.8	DFT-AM1
		78.3	Experimental
		100.0	DFT-AM1
		101.2	Experimental
HS—H	S-H	90.9	DFT-AM1
		90.5	Experimental
MeS—H		87.8	DFT-AM1
		88.0	Experimental