
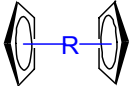
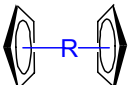
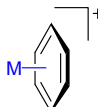
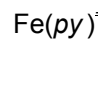
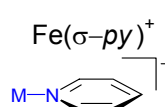
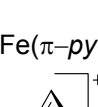







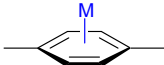
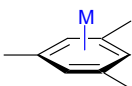
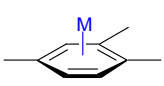
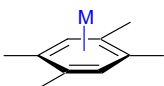
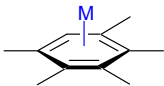
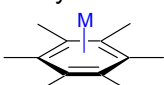
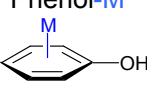
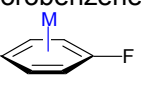
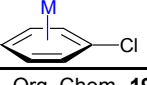
Compound	Bond Dissociation Enthalpy (kcal/mol)			
	Bond (C-Y)	Energy	Theory Level	
	R = Li	R-Cp	82.3	CCSD(T)/B//BP86/A
			79.0	BP86/A
	R = Na		58.6	CCSD(T)/B//BP86/A
			54.4	BP86/A
	R = K		57.9	CCSD(T)/B//BP86/A
			50.4	BP86/A
	R = Rb		55.3	CCSD(T)/B//BP86/A
			50.4	BP86/A
	R = Cs		60.0	CCSD(T)/B//BP86/A
			56.1	BP86/A
	R = B		87.3	CCSD(T)/B//BP86/A
			94.5	BP86/A
R = Al		87.4	CCSD(T)/B//BP86/A	
		88.4	BP86/A	
R = Ga		78.3	CCSD(T)/B//BP86/A	
		79.2	BP86/A	
R = In		78.0	CCSD(T)/B//BP86/A	
		76.7	BP86/A	
R = Tl		66.0	CCSD(T)/B//BP86/A	
		67.0	BP86/A	
	R = Be (D _{5d})	R-(Cp) ₂	153.9	CCSD(T)/B//BP86/A
			146.6	BP86/A
	R = Be (C _s)		154.0	CCSD(T)/B//BP86/A
			146.3	BP86/A
	R = Mg (D _{5d})		121.1	CCSD(T)/B//BP86/A
			112.5	BP86/A
R = Mg (D _{5h})		121.0	CCSD(T)/B//BP86/A	
		112.5	BP86/A	
R = Ca (D _{5d})		154.9	CCSD(T)/B//BP86/A	
		155.2	BP86/A	
	R = Sr (C ₁)	R-(Cp) ₂	149.3	CCSD(T)/B//BP86/A
			145.3	BP86/A
	R = Ba (C _s)		161.1	CCSD(T)/B//BP86/A
			154.3	BP86/A
	R = Zn (C _s)		69.6	CCSD(T)/B//BP86/A
			60.9	BP86/A
	R = Si (C ₂)		124.3	CCSD(T)/B//BP86/A
			131.0	BP86/A
R = Ge (C _s)		117.4	CCSD(T)/B//BP86/A	
		123.4	BP86/A	
R = Sn (C _s)		111.3	CCSD(T)/B//BP86/A	
		116.0	BP86/A	
R = Pb (C ₁)		106.2	CCSD(T)/B//BP86/A	
		107.9	BP86/A	

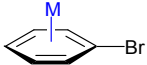
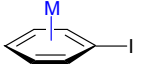
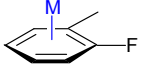
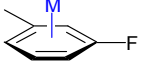
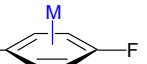
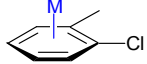
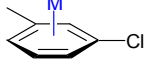
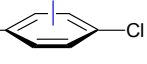
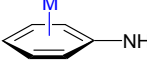
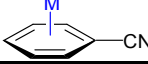
Compound	Bond Dissociation Enthalpy (kcal/mol)			
	Bond (C-Y)	Energy	Theory Level	
$\text{Fe}(\text{bz})^+$ 	M = Fe	<i>Arene-M⁺</i>	207.5 239.2 235.8	Threshold-CID <i>m</i> -PW1PW91 B3LYP
$\text{Fe}(\text{py})^+$ 	M = Fe		223.7 209.2 206.7	Threshold-CID Kinetics Method Kinetics Method
$\text{Fe}(\sigma\text{-py})^+$ 	M = Fe		228.6 255.1	<i>m</i> -PW1PW91 B3LYP
$\text{Fe}(\pi\text{-py})^+$ 	M = Fe		186.0 185.7	<i>m</i> -PW1PW92 B3LYP

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Benzene- <i>M</i> 	M = Cr+ M = Fe+ M = Co+	<i>Arene-M</i>	40.6 49.6 61.1	
Toluene- <i>M</i> 	M = Cr+ M = Fe+ M = Co+		42.6 51.8 63.4	
Ethylbenzene- <i>M</i> 	M = Cr+ M = Fe+ M = Co+		43.5 52.9 64.2	
<i>o</i> -xylene- <i>M</i> 	M = Cr+ M = Fe+ M = Co+		44.3 53.6 65.2	
<i>m</i> -xylene- <i>M</i> 	M = Cr+ M = Fe+ M = Co+		44.3 53.9 65.3	

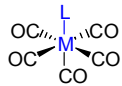
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Compound		Bond Dissociation Enthalpy (kcal/mol)		
		Bond (C-Y)	Energy	Theory Level
p -xylene-M	M = Cr+ M = Fe+ M = Co+	Arene-M	44.3	
			53.8	
			65.3	
Mesitylene-M	M = Cr+ M = Fe+ M = Co+		45.9	
			55.2	
			66.8	
1,2,4-trimethylbenzene-M	M = Cr+ M = Fe+ M = Co+		45.7	
			55.3	
			66.9	
Durene-M	M = Cr+ M = Fe+ M = Co+		47.1	
			56.6	
			68.2	
Penta-methylbenzene-M	M = Cr+ M = Fe+ M = Co+		48.2	
			57.8	
			69.7	
Hexa-methylbenzene-M	M = Cr+ M = Fe+ M = Co+		49.0	
			58.9	
			70.9	
Phenol-M	M = Cr+ M = Fe+ M = Co+		41.0	
			50.0	
			61.0	
Fluorobenzene-M	M = Cr+ M = Fe+ M = Co+		36.2	
			45.1	
			56.2	
Chlorobenzene-M	M = Cr+ M = Co+		37.1	
			57.4	

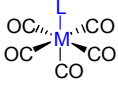
Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
Bromobenzene-M 	M = Co+	<i>Arene-M</i> 58.4	
Iodobenzene-M 	M = Co+		60.1
<i>o</i> -fluorotoluene-M 	M = Cr+ M = Fe+ M = Co+		38.8 47.8 58.8
<i>m</i> -fluorotoluene-M 	M = Cr+ M = Fe+ M = Co+		38.5 47.4 58.6
<i>p</i> -fluorotoluene-M 	M = Cr+ M = Fe+ M = Co+		38.5 47.7 58.6
<i>o</i> -chlorotoluene-M 	M = Co+		59.7
<i>m</i> -chlorotoluene-M 	M = Co+		59.6
<i>p</i> -chlorotoluene-M 	M = Co+		59.6
Aniline-M 	M = Cr+ M = Fe+ M = Co+		44.8 54.0 64.8
Benzonitrile-M 	M = Cr+ M = Fe+ M = Co+		47.0 47.8 57.8

Compound	Bond Dissociation Enthalpy (kcal/mol)			
	Bond (C-Y)	Energy	Theory Level	
F ₃ B—R	R = CO	M-R	2.5	MP2/II+//MP2/II
	R = C(NH ₂) ₂		39.8	
Cl ₃ B—R	R = CO		1.8	MP2/II+//MP2/II
	R = C(NH ₂) ₂		56.7	
F ₃ Al—R	R = CO		13.7	MP2/II+//MP2/II
	R = C(NH ₂) ₂		55.5	
Cl ₃ Al—R	R = CO		12.8	MP2/II+//MP2/II
	R = C(NH ₂) ₂		59.1	
F ₃ Ga—R	R = CO		11.3	MP2/II+//MP2/II
	R = C(NH ₂) ₂		56.8	
Cl ₃ Ga—R	R = CO		8.6	MP2/II+//MP2/II
	R = C(NH ₂) ₂		55.1	
F ₃ In—R	R = CO		13.0	MP2/II+//MP2/II
	R = C(NH ₂) ₂		57.5	
Cl ₃ In—R	R = CO		10.9	MP2/II+//MP2/II
	R = C(NH ₂) ₂		55.4	
F ₄ Ti—R	R = CO		35.7	MP2/II+//MP2/II
	R = C(NH ₂) ₂		21.2	
Cl ₄ Ti—R	R = CO		2.9	MP2/II+//MP2/II
	R = C(NH ₂) ₂		39.0	

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		(kJ/mol)			
	Cr(CO) ₅ L	L = OH ₂	Cr-CO _{ax}	242	
			L = OC	Cr-CO _{ax}	230
			L = CO	Cr-L	183
				Cr-CO _{ax}	183
			L = NH ₃		233
			L = PH ₃		213
			L = PMe ₃		214
			L = N ₂		205
	(staggered C _{2v})		L = CF ₂	Cr-L	211
				Cr-CO _{ax}	177
(staggered C _{2v})		L = CCl ₂	Cr-L	223	
			Cr-CO _{ax}	166	
		L = CS	Cr-L	249	
			Cr-CO _{ax}	167	
(staggered C _{2v})		L = CH ₂	Cr-L	344	
			Cr-CO _{ax}	164	
(eclipsed C _{2v})		L = CH ₂	Cr-L	341	
			Cr-CO _{ax}	166	
		L = NO ⁺	Cr-CO _{ax}	150	
Mo(CO) ₅ L		L = OH ₂	Mo-CO _{ax}	253	
		L = OC		242	
		L = NH ₃		231	
		L = PH ₃		199	
		L = PMe ₃		194	
		L = N ₂		202	
		L = CO	Mo-L	163	
			Mo-CO _{ax}	163	

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Compound		Bond Dissociation Enthalpy (kJ/mol)				
		Bond (C-Y)	Energy	Theory Level		
	Mo(CO) ₅ L	L = CF ₂	(staggered C _{2v})	Mo-L	191	
				Mo-CO _{ax}	153	
		L = CCl ₂	(staggered C _{2v})	Mo-L	205	
				Mo-CO _{ax}	142	
		L = CS		Mo-L	228	
				Mo-CO _{ax}	142	
		L = CH ₂	(staggered C _{2v})	Mo-L	321	
				Mo-CO _{ax}	128	
		L = NO ⁺		Mo-CO _{ax}	140	
		L = OH ₂		W-CO _{ax}	293	
W(CO) ₅ L		L = OC		W-CO _{ax}	278	
		L = NH ₃		W-CO _{ax}	269	
		L = PH ₃		W-CO _{ax}	233	
		L = PMe ₃		W-CO _{ax}	227	
		L = N ₂		W-CO _{ax}	233	
		L = CO		W-L	193	
				W-CO _{ax}	193	
		L = CF ₂	(staggered C _{2v})	W-L	224	
				W-CO _{ax}	184	
		L = CCl ₂	(staggered C _{2v})	W-L	239	
				W-CO _{ax}	173	
		L = CS		W-L	264	
				W-CO _{ax}	173	
		L = CH ₂	(staggered C _{2v})	W-L	362	
				W-CO _{ax}	159	
	L = NO ⁺		W-L	456		
			W-CO _{ax}	165		
Cr(CO) ₅ L		L = CH ₂		Cr-L	344	
					351	
					353	QR-DFT CCSD(T)//MP2
		L = CF ₂			211	
					180	MP2
				223		
	L = CCl ₂			223		
Mo(CO) ₅ L		L = CH ₂		Mo-L	321	
					335	
					353	QR-DFT CCSD(T)//MP2
		L = CF ₂			191	
					162	MP2
	L = CCl ₂			228		
W(CO) ₅ L		L = CH ₂		W-L	362	
					380	
					380	QR-DFT CCSD(T)//MP2
		L = CF ₂			224	
					199	MP2
	L = CCl ₂			239		

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
		ΔH°	
ZnMe ₂	Zn-C	374	
ZnEt ₂		312	
ZnPr ₂		337	
ZnBu ₂		334	

Smith, D. W. *J. Organomet. Chem.* **1999**, 585, 150-153

U(η^5 -C ₅ Me ₅) ₂ R ₂	R = Me	U-R _n	300
	R = CH ₂ Ph		244
	R = CH ₂ SiMe ₃		307
U(η^5 -C ₅ Me ₅) ₂ R(Cl)	R = Me		312
	R = CH ₂ Ph		263
	R = Ph		358
U(η^5 -C ₅ Me ₅) ₂ (OSi ^t BuMe ₂)(R)	R = Me		317
	R = H		342
U{ η^5 -C ₅ H ₄ (SiMe ₃) ₃ } ₃ R	R = Me		185
	R = Bu		152
	R = CH ₂ SiMe ₃		168
	R = CH ₂ Ph		149
	R = CHCH ₂		223
	R = C \equiv C-Ph		363
	R = I		262, 265.6
	R = SEt		266
	R = S ^t Bu		158
	R = H		253.7
U(η^5 -C ₅ H ₄ ^t Bu) ₃ R	R = H		251.6
	R = I		246.3
	R = SEt		252
U(C ₉ H ₇) ₃ R	R = Me		195
	R = OCH ₂ CF ₃		301
	R = I		267

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				(kcal/mol)
Ta(CH ₂ SiMe ₃) ₅		Ta-C		44
(alkylidene formation)	D ₁	Ta-C		67
		Ta=C		126

Luo, L.; Li, L.; Marks, T.J. *J. Am. Chem. Soc.* **1997**, 119, 8574-8575

TaMe ₅	Ta-C	261	237
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Simões, J.A.M.; Beauchamp, J.L. *Chem. Rev.* **1990**, 90, 629-688

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
U(C ₉ H ₆ Et) ₃ R	R = Me	U-R _n	187
U(C ₉ H ₆ SiMe ₃) ₃ R	R = SEt		158
U(η ⁵ -C ₅ H ₅) ₃ R	R = SiPh ₃		156
	R = GePh ₃		163
	R = SnPh ₃		156
	R = Fe(CO) ₂ (cp)		129
	R = Ru(CO) ₂ (cp)		169
	R = Cp		299
	UR ₂	R = C ₈ H ₈	
			442
			190
UR ₄	R = C ₈ H ₇ Bu		417
	R = MeCO ₂		517
UCl ₂ R(Tp ^{Me2}) ₃	R = Cl		422.6
	R = CH(SiMe ₃) ₂		295
	R = Cp		362
	R = O ^t Bu		460.5
	R = OCM ₂ CH ₂ COMe		484.2
	R = N(SiMe ₃) ₂		334
	R = (3,5-Me ₂ pz		293
UCl ₂ R(Tp ^{Me2}) ₃ .thf	R = Thf		21.5

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

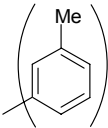
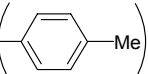
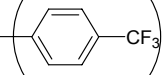
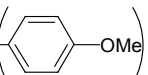
Compound		Bond Dissociation Enthalpy (kcal/mol)		
		Bond (C-Y)	Energy	Theory Level
RMe ₃	R = Si	C-Me	70.62	HF and NR
			70.46	HF and RESC
			89.30	B3LYP and NR
			89.12	B3LYP and RESC
			86.37	BOP and NR
			86.19	BOP and RESC
	R = Ge		62.99	HF and NR
			62.20	HF and RESC
			80.73	B3LYP and NR
			77.78	B3LYP and RESC
			77.67	BOP and NR
			76.55	BOP and RESC
	R = Sn		53.22	HF and NR
			51.30	HF and RESC
			71.41	B3LYP and NR
			68.84	B3LYP and RESC
			68.91	BOP and NR
			66.15	BOP and RESC
	R = Pb		46.09	HF and NR
			39.87	HF and RESC
			64.57	B3LYP and NR
			56.32	B3LYP and RESC
			62.28	BOP and NR
			53.49	BOP and RESC

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	M = Ru	110.2	GGA-BP86 XC
	M = Rh	114.6	GGA-BP86 XC
	M = Pd	113.9	GGA-BP86 XC
	M = Ru	67.1	GGA-BP86 XC
	M = Rh	67.4	GGA-BP86 XC
	M = Pd	58.2	GGA-BP86 XC

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Compound	Bond Dissociation Enthalpy (kcal/mol)			
	Bond (C-Y)	Energy	Theory Level	
	MC Bond Distance (Å)	M-C	BDE	
Cu—C(2)	1.799		90.3	
Ni—C(1)	1.624		141.4	
Ni—C(3)	1.625		131.2	
Fe—C(3)	1.565		155.6	
Fe—C(5)	1.628		138.0	
Ti—C(3)	1.679		148.6	
Ti—C(5)	1.829		126.7	
	MC (Å)	CO (Å)	M-C BDE	C-O BDE
Cu—CO(2)	1.903	1.160	15.4	228.2
Ni—CO(1)	1.661	1.167	61.4	223.1
Ni—CO(3)	1.861	1.164	27.5	199.5
Fe—CO(3)	1.698	1.173	47.1	194.6
Fe—CO(5)	1.864	1.166	39.6	204.7
Ti—CO(3)	2.013	1.171	27.7	182.2
Ti—CO(5)	2.034	1.171	44.4	220.7
		MC (Å)	M-C BDE	
Cu ₅ C(2)(5,0)		1.750	93.7	
Cu ₅ C(2)(4,1)		0.05	157.4	
Ni ₅ C(1)(5,0)		1.625	145.8	
Ni ₅ C(1)(4,1)		-	183.8	
Ni ₅ C(3)(5,0)		1.65	149.3	
Ni ₅ C(3)(4,1)		-	189.4	
Fe ₅ C(3)(4,1)		0.50	186.0	
Fe ₅ C(5)(4,1)		0.40	189.9	
Ti ₇ C(3)(7,0)		1.82	129.9	
Ti ₇ C(5)(7,0)		1.79	139.5	
	MC (Å)	CO (Å)	M-C BDE	C-O BDE
Cu ₅ CO(2)(5,0)	1.975	1.160	6.03	215.3
Cu ₅ CO(2)(4,1)	1.70	1.15	3.03	148.6
Ni ₅ CO(1)(5,0)	1.70	1.17	22.55	179.7
Ni ₅ CO(1)(4,1)	.0.02	1.23	26.16	145.3
Ni ₅ CO(3)(5,0)	1.75	1.17	28.02	181.6
Ni ₅ CO(3)(4,1)	0.05	1.22	13.65	127.2
Fe ₅ CO(3)(4,1)	1.05	1.22	17.86	134.8
Fe ₅ CO(5)(4,1)	0.90	1.25	46.24	159.3
Ti ₇ CO(3)(7,0)	2.00	1.16	33.16	206.3
Ti ₇ CO(5)(7,0)	2.05	1.19	40.95	204.4

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
Ti(Cp) ₂ R ₂	R = Me	Ti-Cp	298
	R = Ph		331
	R = 		342
	R = 		341
	R = 		340
	R = 		349
	R = Fe		331
Mo(Cp) ₂ R ₂	R = H	Mo-Cp	251
	R = Me		166
W(Cp) ₂ R ₂	R = H		305
	R = Me		221

Calhorda, M. J.; Dias, A. R.; da Piedade, M. E. M.; Salema, M. S.; Simoes, J. A. M *Organometallics* **1987**, 6, 734-738

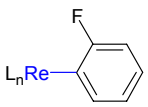
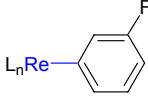
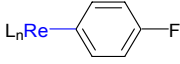
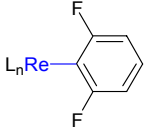
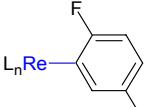
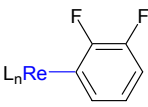
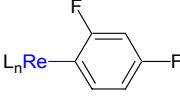
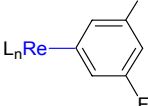
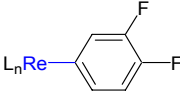
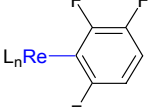
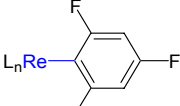
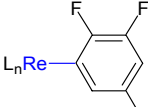
M(CO) ₄	M	Bond (M-CO)	All ZPE corrected	
			(kcal/mol)	
M(CO) ₄	M = Ni	M-CO	26.3	BP86/II
			27.0	BP86/TZP
			25 ± 2	Experimental
M(CO) ₄	M = Pd		12.9	BP86/II
			11.7	BP86/TZP
M(CO) ₄	M = Pt		14.2	BP86/II
			13.5	BP86/TZP

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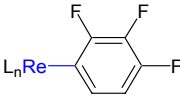
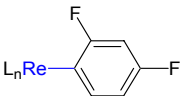
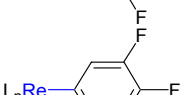
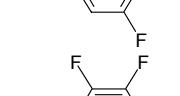
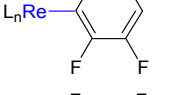
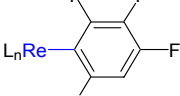
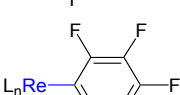
Compound		Bond Dissociation Enthalpy (kcal/mol)			
		Bond (C-Y)	Energy	Theory Level	
All singlet states, ZPE corrected					
Fe(CO) ₄ R	R = CO	Fe-R	D _{3h}	39.0	B3LYP/III//B3LYP/II
				45.1	CCSD(T)/III//B3LYP/II
	R = CS	axial	C _{3v}	55.8	B3LYP/III//B3LYP/II
				64.2	CCSD(T)/III//B3LYP/II
	equatorial	C _{2v}	55.4	B3LYP/III//B3LYP/II	
			64.2	CCSD(T)/III//B3LYP/II	
R = N ₂	axial	C _{2v}		16.5	B3LYP/III//B3LYP/II
				22.9	CCSD(T)/III//B3LYP/II
	equatorial	C _{2v}		15.3	B3LYP/III//B3LYP/II
				22.4	CCSD(T)/III//B3LYP/II
R = NO ⁺	axial	C _{3v}		79.2	B3LYP/III//B3LYP/II
				84.8	CCSD(T)/III//B3LYP/II
	equatorial	C _{2v}		92.4	B3LYP/III//B3LYP/II
				105.1	CCSD(T)/III//B3LYP/II
R = CN ⁻	axial	C _{3v}		87.0	B3LYP/III//B3LYP/II
				96.5	CCSD(T)/III//B3LYP/II
	equatorial	C _{2v}		81.0	B3LYP/III//B3LYP/II
				89.9	CCSD(T)/III//B3LYP/II
R = NC ⁻	axial	C _{3v}		70.7	B3LYP/III//B3LYP/II
				78.6	CCSD(T)/III//B3LYP/II
	equatorial	C _{2v}		64.2	B3LYP/III//B3LYP/II
				72.7	CCSD(T)/III//B3LYP/II
R = η ² -C ₂ H ₄	axial	C _s		18.3	B3LYP/III//B3LYP/II
				30.6	CCSD(T)/III//B3LYP/II
	equatorial	C _{2v}		25.9	B3LYP/III//B3LYP/II
				39.2	CCSD(T)/III//B3LYP/II
R = η ² -C ₂ H ₂	axial	C _s		16.9	B3LYP/III//B3LYP/II
				26.9	CCSD(T)/III//B3LYP/II

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Compound		Bond Dissociation Enthalpy (kcal/mol)		
		Bond (C-Y)	Energy	Theory Level
All singlet states, ZPE corrected				
Fe(CO) ₄ R	R = η^2 -C ₂ H ₂ equatorial	Fe-R C _{2v}	25.4	B3LYP/III//B3LYP/II
			37.3	CCSD(T)/III//B3LYP/II
R = CCH ₂	axial	C _s	64.7	B3LYP/III//B3LYP/II
			75.7	CCSD(T)/III//B3LYP/II
	equatorial	C _{2v}	70.3	B3LYP/III//B3LYP/II
			83.8	CCSD(T)/III//B3LYP/II
R = CH ₂	axial	C _s	69.1	B3LYP/III//B3LYP/II
			79.6	CCSD(T)/III//B3LYP/II
	equatorial	C _{2v}	75.1	B3LYP/III//B3LYP/II
			87.4	CCSD(T)/III//B3LYP/II
R = CF ₂	axial	C _s	52.2	B3LYP/III//B3LYP/II
			59.8	CCSD(T)/III//B3LYP/II
	equatorial	C _{2v}	55.2	B3LYP/III//B3LYP/II
			64.3	CCSD(T)/III//B3LYP/II
R = NH ₃	axial	C _s	29.9	B3LYP/III//B3LYP/II
			39.1	CCSD(T)/III//B3LYP/II
	equatorial	C _s	23.7	B3LYP/III//B3LYP/II
			33.1	CCSD(T)/III//B3LYP/II
R = NF ₃	axial	C _s	15.3	B3LYP/III//B3LYP/II
			23.5	CCSD(T)/III//B3LYP/II
	equatorial	C _s	12.2	B3LYP/III//B3LYP/II
			20.9	CCSD(T)/III//B3LYP/II
R = PH ₃	axial	C _{3v}	26.8	B3LYP/III//B3LYP/II
			38.9	CCSD(T)/III//B3LYP/II
	equatorial	C _s	25.9	B3LYP/III//B3LYP/II
			36.5	CCSD(T)/III//B3LYP/II
R = PF ₃	axial	C _{3v}	34.1	B3LYP/III//B3LYP/II
			45.2	CCSD(T)/III//B3LYP/II
	equatorial	C _s	34.5	B3LYP/III//B3LYP/II
			44.1	CCSD(T)/III//B3LYP/II
R = η^2 -H ₂	axial	C _s	10.3	B3LYP/III//B3LYP/II
			16.5	CCSD(T)/III//B3LYP/II
	equatorial	C _{2v}	12.8	B3LYP/III//B3LYP/II
			18.5	CCSD(T)/III//B3LYP/II

Compound	Bond Dissociation Enthalpy (kJ/mol)			
	Bond (C-Y)	Energy	Theory Level	
$\text{Re}(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2(\text{H})(\text{R})$	R = Phenyl	Re-R Re-H	252.0 489.8	ALL using Hybrid DFT B3PW91
	R = 	Re-R Re-H	276.9 500.5	
	R = 	Re-R Re-H	253.5 490.6	
	R = 	Re-R Re-H	255.3 494.3	
	R = 	Re-R Re-H	300.0 512.0	
	R = 	Re-R Re-H	278.7 501.2	
	R = 	Re-R Re-H	278.1 500.3	
	R = 	Re-R Re-H	279.9 504.6	
	R = 	Re-R Re-H	255.4 492.0	
	R = 	Re-R Re-H	256.1 494.5	
	R = 	Re-R Re-H	301.2 511.8	
	R = 	Re-R Re-H	302.7 515.5	
	R = 	Re-R Re-H	280.4 501.7	


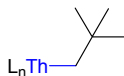
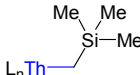
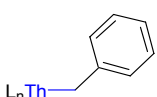
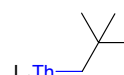
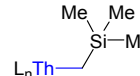
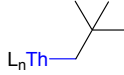
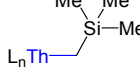
Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level

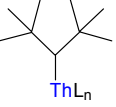
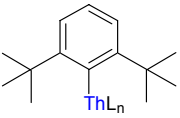
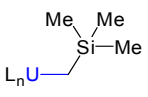
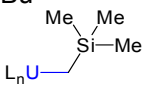
$\text{Re}(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2(\text{H})(\text{R})$	R = 	Re-R Re-H	280.8 503.6	ALL using Hybrid DFT B3PW91
	R = 	Re-R Re-H	281.0 504.8	
	R = 	Re-R Re-H	257.4 495.0	
	R = 	Re-R Re-H	304.7 512.4	
	R = 	Re-R Re-H	304.0 514.7	
	R = 	Re-R Re-H	283.0 504.4	
	R = 	Re-R Re-H	306.7 514.7	

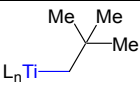
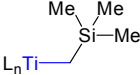
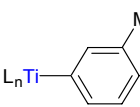
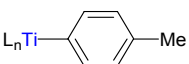
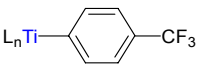

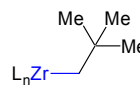
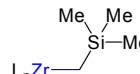
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$\text{Cr}(\text{CO})_6$	First Dissociation Enthalpy	M-CO	154
	Mean Dissociation Enthalpy	M(CO) ₆	107
$\text{Mo}(\text{CO})_6$		M-CO	170
		M(CO) ₆	152
$\text{W}(\text{CO})_6$		M-CO	192
		M(CO) ₆	178
$\text{Fe}(\text{CO})_5$		M-CO	174
		M(CO) ₅	118

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Compound	Bond Dissociation Enthalpy (kJ/mol)			
	Bond (C-Y)	Energy	Bond Enthalpy Terms	
$\text{Th}(\text{Cp}^*)_3\text{R}$	R = Me	Th-C	375	351
	R = 		350	351
	R = 		333	326
	R = 		369	365
	R = 		315	358
$\text{Th}(\text{Cp}^*)_2\text{R}_2$	R = Me		339	315
	R = Et		318	308
	R = Bu		307	300
	R = 		302	295
	R = 		335	331
	R = Ph		372	328
$\text{Th}(\text{Cp}^*)_2(\text{O}^t\text{Bu})\text{R}$	R = Me		349	326
	R = Et		330	320
	R = Bu		316	309
	R = 		321	314
	R = 		345	341
	R = Ph		387	343
$\text{Th}(\text{Cp}^*)_2[\text{OCH}(t\text{-Bu})_2]\text{Bu}$			347	340

Compound	Bond Dissociation Enthalpy (kJ/mol)			
	Bond (C-Y)	Energy	Bond Enthalpy Terms	
$\text{Th}(\text{Cp}^*)_2(\text{Cl})\text{R}$	R = Et	Th-C	313	303
	R = Ph		374	330
	R = Bz		285	328
$\text{Th}(\text{Cp}^*)_2[(\text{CH}_2)_2\text{CMe}_2]$			274	
$\text{Th}(\text{Cp}^*)_2[(\text{CH}_2)_2\text{SiMe}_2]$			318	
$\text{Th}(\text{Cp}^*)_2(\text{C}_4\text{H}_6)$			209	
$\text{Th}(\text{Cp}^*)_2[\text{CH}_2(\text{CMe})_2\text{CH}_2]$			188	
$\text{Th}(\text{Cp}^*)_2(\text{CHCH}_2\text{CH}_2)_2$			368	
$\text{Th}(\text{Cp}^*)_2(\text{OR})[\text{C}(\text{O})\text{H}]$	R = 		345	396
	R = 		351	402
$\text{U}(\text{Cp}^*)_2[\text{OSi}(t\text{-Bu})\text{Me}_2]\text{R}$	R = H	U-C	342	
	R = Me		317	293
$\text{U}(\text{Cp}^*)_2\text{R}_2$	R = Me		300	276
	R = Bz		244	287
	R = 		307	303
$\text{U}(\text{Cp}^*)_2(\text{Cl})\text{R}$	R = Me		312	288
	R = Ph		358	314
	R = Bz		263	306
$\text{U}(\text{Me}_3\text{SiC}_5\text{H}_4)_3\text{R}$	R = Me		185	161
	R = Bu		152	145
	R = 		168	164
	R = Bz		149	192
	R = CHCH ₂		223	185
	R = CPh		363	

Compound	Bond Dissociation Enthalpy (kJ/mol)			
	Bond (C-Y)	Energy	Bond Enthalpy Terms	
TiR_4	R = 	Ti-C	198	191
	R = 		253	249
	R = Bz		201	244
$Ti(Cp)_2R_2$	R = Me		298	274
	R = Ph		332	288
	R = 		343	299
	R = 		342	298
	R = 		341	297
	R = 		350	306
	R = $(\eta^5-C_5H_4)Fe(\eta^5-C_5H_5)$		-	278
$Ti(Cp)_2Bz_2$			237	280
$Ti(Cp)_2(Cl)R$	R = Me		-	293
	R = Ph		-	291
$Ti(Cp)_2(Cl)Et$			150	
$Ti(Cp^*)_2R_2$	R = Me		281	257
	R = Ph		280	236
ZrR_4	R = 	Zr-C	249	242
	R = 		310	306
	R = Bz		263	306
$Zr(Cp)_2Me_2$			285	261
$Zr(Cp)_2Ph_2$			300	256
$Zr(Cp^*)_2R_2$	R = Me		284	260
	R = Ph		312	268
$Zr(Cp^*)_2CH_2(CHEt)_2CH_2$			261	-
$Zr(Cp^*)_2CH_2CH_2C_6H_4-o$			282	-
$Zr(Cp^*)_2Me_3$			276	252
$Zr(Cp^*)(OC_6F_5)Me_2$			289	265
$Zr(Cp^*)(OC_6F_5)_2Me$			310	286

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Bond Enthalpy Terms
Hf(Cp*)(CH ₂ CMe ₃) ₄	Hf-R	266	259
Hf(Cp*) ₂ R ₂	R = H	346	346
	R = Me	306	282
	R = Bu	274	267
Hf(Cp*) ₂ H ₂		326	326
Hf(Cp*)(H)Ph		350	306
Hf(Cp*)Me ₃		294	270
Hf(Cp*)(OC ₆ F ₅)Me ₂		300	276
Hf(Cp*)(OC ₆ F ₅) ₂ Me		309	285
Hf(Cp*)(C ₅ Me ₄ CH ₂ CH ₂ CH ₂)H		243	-
Hf(Cp*)(C ₅ Me ₄ CH ₂ C ₆ H ₄ -o)H		320	-
Hf(Cp*) ₂ (Me)C(O)Me		298	366

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Mo(Cp) ₂ R ₂	R = H	Mo-R	257	-
	R = Me		166	142
	R = Et		156	146
	R = Bu		154	147
Mo(Cp) ₂ (C ₂ H ₄)			59	-
Mo(Cp) ₂ (C ₂ Ph ₂)			120	-
Mo(Cp)(CO) ₃ H			273	-
Mo(Cp)(CO) ₃ R	R = H		282	282
	R = Me		203	179
	R = Et		185	175
	R = C ₃ H ₅		147	195
	R = Bz		154	197

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WMe ₆		W-Cl		347.3
		W-R	160	136
W(Cp) ₂ R ₂	R = H		311	311
	R = Me		221	197
W(Cp) ₂ (I)H				273
W(Cp) ₂ (CO) ₃ H			339	339
W(CO) ₃ [P(c-C ₆ H ₁₁) ₃] ₂ (H ₂)			40	
W(CO) ₅ [C(OMe)Ph]			359	

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Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Bond Enthalpy Terms
$\text{Mn}(\text{CO})_5\text{R}$	R = H	Mn-Mn 159	
	R = Me	Mn-R 245	245
	R = Ph	187, 192	163, 168
	R = Bz	207	163
	R = CH ₂ F	129	172
	R = CHF ₂	139	130
	R = CF ₃	144	141
		182, 203	156, 177
$\text{Mn}(\text{CO})_5\text{C}(\text{O})\text{R}$	R = Me	160, 182, 185	228, 250, 253
	R = Ph	127, 131	193, 197
	R = CF ₃	176	222
	R = Et	181	242
	R = Pr	175	236
$\text{Mn}(\text{CO})_4(\text{P}(\text{C}_6\text{H}_4\text{OMe-}p)_3(\text{CH}_2\text{C}_6\text{H}_4\text{OMe-}p))$		105	
$\text{Re}(\text{CO})_5\text{Me}$	Re-Re	187	
	Re-C	220	196

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$\text{Fe}(\text{CO})_4\text{H}_2$	Fe-H	272	244
$\text{Fe}(\text{CO})_4(\text{C}_2\text{H}_4)$	Fe-C	152	96
$\text{Fe}(\text{CO})(1,3-\text{C}_4\text{H}_6)_2$			178
$\text{Fe}(\text{CO})(1,3\text{-}c\text{-C}_4\text{H}_6)_2$			194
$\text{Fe}(\text{CO})_3(1,3-\text{C}_4\text{H}_6)$			200
$\text{Fe}(\text{CO})_3(\text{I})(\text{C}_3\text{H}_5)$			170
$\text{Fe}(\text{CO})_3(1,3,5,7\text{-cyclooctatetraene})$			179
$\text{Fe}(\text{CO})_3(\text{C}_2\text{H}_4)_2$		113	
$\text{Ru}(2,3,7,8,12,13,17,18\text{-octaethylporphyrinato anion})\text{Et}_2$	Ru-C	91	

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Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Bond Enthalpy Terms
Co(CO) ₄ H	Co-C	227	227
Co ₃ (CO) ₉ (CCl)			114
Co ₃ (CO) ₉ (CBr)			135
Co(dimethylglyoxime) ₂ (R)CH(Me)Ph			
R = pyridine		113, 117, <90, <89	
R = 4-methylpyridine		115	
R = 4-aminopyridine		120, <97	
R = 4-cyanopyridine		106, <84	
R = imidazole		118, <96	
R = methylpyridine		91	
R = PMe ₂ Ph		100	
R = PBu ₃		87	
R = PEtPh ₂		81	
R = PPh ₃		73	
R = P(CH ₂ CH ₂ CN) ₃		85	
Co(dimethylglyoxime) ₂ (R)Bz			
R = PMe ₂ Ph		128	171
R = PBu ₃		121	164
R = PEtPh ₂		113	156
R = PPh ₃		108	151
R = P(c-C ₆ H ₁₁) ₃		96	139
Co(octaethylporphyrine)(R)Bz			
R = PMe ₂ Ph		114	157
R = PBu ₃		123	166
R = PEtPh ₂		110	153
R = PPh ₃		100	143
R = P(c-C ₆ H ₁₁) ₃		124	167
Co(dimethylglyoxime) ₂ (R)CH(CH ₂ X)COOMe			
R = pyridine, X = H		120	
R = 4-methylpyridine, X = H		123	
R = 4-cyanopyridine, X = H		118	
R = pyridine, X = COOMe		139	
Co(dimethylglyoxime) ₂ (pyridine)R			
R = Me		138	114
R = <i>i</i> -Pr		98	99
R = Bz		136	179

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Bond Enthalpy Terms
Co (<i>N,N'</i> -bis(salicylidene)- <i>o</i> -phenylenediamine)(pyridine)R			
R = Pr	Co-C	105	98
R = <i>i</i> -Pr		83	84
R = CH ₂ CMe ₃		77	70
R = Bz		91	134
Co [11-hydroxyl-2,10-diethyl-3,9-dimethyl-1,4,8,11-tetraazaundeca-1,3,8,10-tetraen-1-olato](I)R			
R = CH ₂ CMe ₃		127	120
R = Bz		109	152
Co (dimethylglyoximeBF ₂) ₂ (H ₂ O)Bz		99	142
Co (1,4,8,11-tetraazacyclotetradecane) ₂ (H ₂ O)Bz ²⁺		98	141
[cobinamide]R	R = <i>i</i> -Pr	110	111
	R = CH ₂ CMe ₃	126	119
	R = Bz	105	148
	R = Adenosine	144	
B ₁₂ R	R = <i>i</i> -Pr	79	80
	R = <i>i</i> -Bu	104	95
	R = CH ₂ CMe ₃	90, 99	83, 92
	R = Bz	95	138
	R = CH ₂ C ₅ H ₉	99	
B ₁₂ Ado		112, 125, 131	
Rh (Cp)(C ₂ H ₄) ₂	Rh-C	<130	
Rh (octaethylporphyrine)R			
	R = H	259	259
	R = C(O)H	249	300
	R = CH(Bu)OH	187	
Rh (Cl)(B)[P(4-tolyl) ₃] ₂ H ₂		242	242
Rh (NC ₃ H ₃ C ₆ H ₃ CO)(Cl)(pyridine)C(Ph)(OMe)H		128	
Ir (R)(CO)(PPh ₃) ₂ H ₂	R = Cl	247	272
	R = Br	253	
	R = I	258	270
Ir (Cl)(CO)(PPh ₃) ₂ (R)H			
	R = Cl	245	271
	R = Br	237	262
Ir (Cl)(CO)(PMePh ₂) ₂ (Cl)H		266	291

Compound	Bond Dissociation Enthalpy (kJ/mol)			
	Bond (C-Y)	Energy	Bond Enthalpy Terms	
$\text{Ir}(\text{Cl})(\text{CO})(\text{PR}_3)_2\text{H}_2$	R = Et	Ir-C	243	268
	R = <i>c</i> -C ₆ H ₁₁		246	271
$\text{Ir}(\text{R})(\text{CO})(\text{X})_2\text{H}_2$	R = Cl, X = P(<i>i</i> -Pr) ₃		240	265
	R = Cl, X = PBuPh ₂		242	267
	R = Cl, X = PPh ₃		251	276
	R = Cl, X = P(<i>c</i> -C ₆ H ₁₁) ₃		240	265
	R = Cl, X = PBz ₄		249	274
	R = Cl, X = P(<i>p</i> -tolyl) ₃		246	271
	R = Cl, X = P(OPh) ₃		244	269
	R = Br, X = P(<i>i</i> -Pr) ₃		245	270
	R = Br, X = PPh ₃		235	260
	R = Br, X = P(<i>c</i> -C ₆ H ₁₁) ₃		244	269
	R = Br, X = P(OPh) ₃		238	263
	R = I, X = P(<i>i</i> -Pr) ₃		227	252
	R = I, X = PPh ₃		229	254
	R = I, X = P(<i>c</i> -C ₆ H ₁₁) ₃		256	281
R = I, X = P(OPh) ₃		224	249	
$\text{Ir}(\text{Cl})_2(\text{CO})(\text{R})_2\text{C}(\text{O})\text{Me}$	R = PMe ₃			>237
	R = PEt ₃			>241
$\text{Ir}(\text{Cp}^*)(\text{PMe}_3)\text{H}_2$			310	310
$\text{Ir}(\text{Cp}^*)(\text{PMe}_3)(\text{R})\text{H}$	R = Ph		337	293
	R = <i>c</i> -C ₆ H ₁₁		209	216
$\text{Ir}(\text{Cp}^*)(\text{PMe}_3)(\text{H})\text{R}$	R = <i>c</i> -C ₅ H ₉		215	
	R = <i>c</i> -C ₅ H ₁₁		244	
	R = Ph		321	277
	R = <i>c</i> -C ₆ H ₁₁		218	225
	R = 2,3-Me ₂ Bu		240	237
	R = CH ₂ CMe ₂ Et		<233	
$\text{Ir}(\text{Cp}^*)(\text{PMe}_3)\text{Me}_2$			243	219
$\text{Ir}(\text{Cp}^*)(\text{PMe}_3)(\text{Br})\text{C}_2\text{H}_3$			326	288

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Bond Enthalpy Terms
Ir(R)(CO)(PPh ₃) ₂ X	R = F, X = C ₂ F ₄	Ir-X	79
	R = F, X = C ₄ F ₆		99
	R = Cl, X = C ₂ F ₄		67
	R = Cl, X = C ₄ F ₆		96
	R = Br, X = C ₂ F ₄		41
	R = Br, X = C ₄ F ₆		79
	R = I, X = C ₂ F ₄		57
	R = I, X = C ₄ F ₆		82

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Ni(cod) ₂	Ni-C	209	-
[Pd(C ₃ H ₅)Cl] ₂	Pd-C	-	262
<i>cis</i> -Pd(Cl) ₂ (cod)		-	344
Pd(I)(bipy)Me ₃		136	-
Pt(Cp)Me ₃	Pt-C	163	195
Pt(Cp) ₂ Me ₂		-	195
<i>trans</i> -Pt(PEt ₃) ₂ Ph ₂		-	159
<i>cis</i> -Pt(PEt ₃) ₂ Me ₂		269	245
<i>cis</i> -Pt(PEt ₃) ₂ (<i>o</i> -tolyl) ₂		298	254
<i>cis</i> -Pt(PEt ₃) ₂ (Cl)Me		251	227
<i>cis</i> -Pt(PEt ₃) ₂ (Cl)(<i>o</i> -tolyl)		300	256
<i>trans</i> -Pt(PPh ₃) ₂ (Cl)H		307	307
<i>cis</i> -Pt(PPh ₃) ₂ (I)Me		242	218
<i>trans</i> -Pt(PEt ₃) ₂ (Cl)Et		206	196
Pt(PPh ₃) ₂ (Cl)C(O)Ph		>232	>288
Pt(PMe ₂ Ph) ₂ (Cl)(Me) ₂ C(O)Me		306	
Pt(R) ₂ CH ₂ CH ₂ CH ₂	R = Cl	120	
	R = Br	122	
Pt(Cl) ₂ (R)CH ₂ CH ₂ CH ₂	R = (py) ₂	117	
	R = (4-Mepy) ₂	113	
	R = bipy	121	
Pt(Br) ₂ (R)CH ₂ CH ₂ CH ₂	R = (py) ₂	1117	
	R = (4-Mepy) ₂	114	
	R = bipy	124	
Pt(PPh ₃) ₂ (dpcb)		150	217, 217

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Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Bond Enthalpy Terms
Pt(PPh ₃) ₂ R	R = C ₂ H ₄	Pt-C	152
	R = PhCHCH ₂		169
	R = <i>cis</i> -C ₂ H ₂ Ph ₂		194
	R = <i>trans</i> -C ₂ H ₂ Ph ₃		210
	R = C ₂ Ph ₂		181
	R = C ₂ (CN) ₄		277
	R = pcbd		177
Pt(Cl) ₂ (cod)			398
Pt(AsMe ₃)(X)(Me)R	X = Cl, R = C ₂ F ₄		52
	X = Br, R = C ₂ F ₄		48
	X = Cl, R = C ₄ F ₆		69
	X = Br, R = C ₄ F ₆		61
Pt(AsMe ₂ Ph)(X)(Me)R	X = Cl, R = C ₄ F ₆		73
	X = Br, R = C ₄ F ₆		80

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Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Bond Enthalpy Terms
Sc-Me	M^+-L	247	
Ti-Me		226	
V-Me		207	
Cr-Me		126	
Mn-Me		213	
Fe-Me		242	
Co-Me		205	
Ni-Me		188	
Cu-Me		124	
Zn-Me		296	
Y-Me		249	
Ru-Me		226	
Rh-Me		198	
Pd-Me		247	
Cd-Me		228	
La-Me		231	
Hg-Me		285	
Lu-Me		190	

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Sc-CH ₂	M^+-L	412	
Ti-CH ₂		391	
V-CH ₂		335	
Cr-CH ₂		226	
Mn-CH ₂		297	
Fe-CH ₂		347	
Co-CH ₂		326	
Ni-CH ₂		314	
Cu-CH ₂		268	
Y-CH ₂		398	
Nb-CH ₂		456	
Rh-CH ₂		381	
La-CH ₂		411	
Lu-CH ₂		≥240	

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Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
Ti-CH	M ⁺ -L	508	
V-CH		481	
Cr-CH		314	
Fe-CH		426	
Co-CH		426	
Nb-CH		610	
Rh-CH		431	
La-CH		524	

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V-C	M ⁺ -C	383	
Fe-C		397	
Co-C		384	
Nb-C		600	
Rh-C		686	
La-C		427	

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Sc-Me	M-Me	134	
Ti-Me		192	
V-Me		155	
Cr-Me		172	
Mn-Me		126	
Fe-Me		155	
Co-Me		191	
Ni-Me		231	
Cu-Me		243	
Zn-Me		80	

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Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Theory Level
ScMe ₂	M ⁺ -Me	238	247
TiMe ₂		268	226
VMe ₂		203	207
FeMe ₂		>160	242
RuMe ₂		>176	226
CoMe ₂		255	205
RhMe ₂		>205	198
NiMe ₂		>214	188
PdMe ₂		>155	247
ZnMe ₂		115	296
CdMe ₂		109	228
HgMe ₂		96	285
Sc(H)Me	M ⁺ -Me	263	M ⁺ -H 239
V(H)Me		188	202
Co(H)Me		182	195

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ScL ⁺	L = C ₂ H ₂	M-L ⁺	326
	L = C ₂ H ₄		≥147, 167
	L = C ₆ H ₆		222
YL ⁺	L = C ₂ H ₄		>138
	L = C ₃ H ₄		>297
	L = C ₃ H ₆		>126
	L = C ₄ H ₆		>238
LaL ⁺	L = C ₂ H ₄		>138
	L = C ₃ H ₄		>297
	L = C ₃ H ₆		>126
	L = C ₄ H ₆		>238
TiC ₆ H ₆ ⁺			>205

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Compound		Bond Dissociation Enthalpy (kJ/mol)		
		Bond (C-Y)	Energy	Theory Level
VL ⁺	L = C ₂	V-L ⁺	≥527	
	L = C ₂ H		497	
	L = C ₂ H ₂		212	
	L = C ₂ H ₃		≥367	
	L = C ₂ H ₄		209	
	L = Et		234	
VC ₃ H ₅ ⁺			427	
VC ₆ H ₆ ⁺			260	
V(C ₆ H ₆) ₂ ⁺			239	
NbCH ₂ ²⁺		Nb-L ⁺	819	
NbC ₆ H ₆ ⁺			276	
TaC ₆ H ₆ ⁺		Ta-L ⁺	251 < D < 301	
CrC ₆ H ₆ ⁺		Cr-L ⁺	222	
MoL ⁺	L = C ₂ H ₂	Mo-L ⁺	≥312	
	L = C ₂ H ₄		≥137	
	L = 1,3-C ₄ H ₆		≥245	
	L = C ₆ H ₆		≥250	
FeC ₂ H ₄ ⁺		Fe-L ⁺	142, 174	
Fe(C ₃ H ₅) ₂ ⁺			232	
FeC ₃ H ₆ ⁺			155	
FeC ₄ H ₆ ⁺			201	
FeCp ⁺			>364	
Fe(c-C ₅ H ₆) ⁺			213	
FeC ₆ H ₄ ⁺			318	
FeC ₆ H ₆ ⁺			230	
RuC ₂ H ₄ ⁺		Ru-L ⁺	>159	
CoC ₂ H ₄ ⁺		Co-L ⁺	155, 192	
CoC ₃ H ₆ ⁺			201	
CoC ₄ H ₆ ⁺			<218	
Co(Cp)C ₄ H ₆ ⁺			>238	
CoCp ⁺			356	
Co(Cp) ₂ ⁺			513	
Co(C ₆ H ₆) ⁺			285	
Co(PhMe) ⁺			>201	
CoSiH ₂ ⁺			271	
RhC ₂ H ₄ ⁺		Rh-L ⁺	>159	
RhC ₄ H ₆ ⁺			>236	
RhC ₆ H ₆ ⁺			276	

Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Proton Affinity
NiC ₂ H ₄ ⁺	Ni-L ⁺	155	
Ni(C ₂ H ₄) ₂ ⁺		180	
NiC ₃ H ₅ ⁺		243	
NiC ₆ H ₆ ⁺		285	
NiCF ₂ ⁺		196	
NiSiH ₂ ⁺		271	
CuC ₆ H ₆ ⁺	Cu-L ⁺	209	

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Ni(Cp) ⁺ -L	L = PH ₃	Ni(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

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Mn(CO) ₅ L	L = H	Homolytic	Mn ⁺ -L	172
	L = Me			137, 132
	L = CH ₂ F			82
	L = CHF ₂			58
	L = CF ₃			72, 93
	L = Bz			153
	L = Mn(CO) ₅			166

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Compound	Bond Dissociation Enthalpy (kJ/mol)		
	Bond (C-Y)	Energy	Hydride/Electron Affinity
Cr(CO) ₆	D[M(CO) _{n-1} -CHO]	≤147	184 / ≤201
Mo(CO) ₆		≤172	184 / ≤192
W(CO) ₆		≤194	184 / ≤192
Fe(CO) ₅		187	235 / 232

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M-C	M = Sc	M-C	444
	M = Ti		423
	M = V		423
	M = Y		418
	M = Zr		561
	M = Nb		568
	M = Mo		482
	M = Tc		564
	M = Ru		648
	M = Rh		580
	M = Pd		436
	M = La		463
	M = Hf		540
	M = Os		649
	M = Ir		631
	M = Pt		610

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M-C ₂	M = Sc	M-C ₂	572
	M = Ti		573
	M = V		578
	M = Cr		451
	M = Y		638
	M = Zr		581
	M = Nb		656
	M = Mo		500
	M = Ru		519
	M = Rh		433
	M = La		659
	M = Hf		674


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

pyCo(dimethylglyoxime) ₂ CH ₃	Co-C	33.1
pyCo(dimethylglyoxime) ₂ CH ₂ C ₆ H ₅		31.2
pyCo(dimethylglyoxime) ₂ CH(CH ₃) ₂		21.3


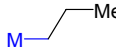

Toscano, P. J.; Seligson, A. L.; Curran, M. T.; Skrobitt, A. T.; Sonnenberger, D. *Inorg. Chem.* **1989**, *28*, 166-168

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Hydride/Electron Affinity
CH ₃ Co(Salen)H ₂ O	Co-C	168	
CH ₃ Co(Salen)imidazole		152	
CH ₃ Co(Salen)benzimidazole		136	
CH ₃ Co(Salen)pyridine		127	
C ₂ H ₅ Co(Salen)H ₂ O		125	
<i>n</i> -C ₄ H ₉ Co(Salen)H ₂ O		107	
<i>n</i> -C ₄ H ₉ Co(Salen)		108	
<i>i</i> -C ₄ H ₉ Co(Salen)H ₂ O		90	
<i>i</i> -C ₃ H ₇ Co(Salen)H ₂ O		81	
<i>i</i> -C ₃ H ₇ Co(Saloph)pyridine		84	
<i>i</i> -C ₃ H ₇ Co(DH) ₂ pyridine		89	

Li, G.; Zhang, F. F.; Chen, H.; Yin, H. F.; Chen, H. L.; Zhang, S. Y. *Chem. Soc. Dalton Trans.* **2002**, 105-110

M-CH ₃	M = Y	M-C	66.9	
	M = Zr		58.6	
	M = Nb		56.6	
	M = Mo		45.3	
	M = Tc		47.7	
	M = Ru		48.5	
	M = Rh		52.0	
	M = Pd		41.6	
	M = H		M-H	102.7
			M = Y	M-C
M = Zr		67.1		
M = Nb		67.3		
M = Mo		55.3		
M = Tc		54.9		
M = Ru		58.9		
M = Rh		62.4		
M = Pd		50.3		
M = H		M-H	108.3	
M≡C-H		M = Y	M-C	
	M = Zr	102.9		
	M = Nb	102.6		
	M = Mo	89.4		
	M = Tc	81.8		
	M = Ru	89.1		
	M = Rh	92.3		
	M = Pd	76.1		
	M = H	M-H		127.3

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

Compound	Bond Dissociation Enthalpy (kcal/mol)		
	Bond (C-Y)	Energy	Theory Level
	M = Y	M-C	61.6
	M = Zr		54.7
	M = Nb		53.3
	M = Mo		42.2
	M = Tc		44.9
	M = Ru		46.5
	M = Rh		50.3
	M = Pd		40.9
	M = H	M-H	99.8
	M = Y	M-C	62.9
	M = Zr		55.9
	M = Nb		54.6
	M = Mo		43.6
	M = Tc		46.1
	M = Ru		47.7
	M = Rh		51.8
	M = Pd		42.0
	M = H	M-H	100.6
	M = Y	M-C	58.3
	M = Zr		51.7
	M = Nb		51.0
	M = Mo		40.6
	M = Tc		43.2
	M = Ru		45.7
	M = Rh		50.3
	M = Pd		41.1
	M = H	M-H	98.2

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