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METAL–CARBON "BOND STRENGTHS" IN $Cr(CO)_6$, $Cr(\eta\text{-}C_6H_6)_2$, AND $Cr(CO)_3(\eta\text{-}C_6H_6)$

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Summary

Cr–CO and $Cr–C_6H_6$ bond enthalpy terms in the complexes $Cr(CO)_6$, $Cr(\eta\text{-}C_6H_6)_2$ and $Cr(CO)_3(\eta\text{-}C_6H_6)$ were obtained from thermochemical data by using extended Hückel molecular orbital calculations. The results show that E(Cr–CO) increases from $Cr(CO)_6$ to $Cr(CO)_3(\eta\text{-}C_6H_6)$ and $E(Cr–C_6H_6)$ is smaller in $Cr(CO)_3(\eta\text{-}C_6H_6)$ than in $Cr(\eta\text{-}C_6H_6)_2$.

Introduction

The importance of quantitative information about transition metal–ligand "bond strengths" in organometallic complexes has been stressed in several recent reviews [1–6]. These surveys show that a large majority of the available bond enthalpy data has been obtained from the values of the gaseous enthalpies of formation of the organometallic compounds.

The knowledge of $\Delta H_f^\circ(ML_n, g)$, ML_n being a molecule containing only one type of ligand, enables the calculation of the so-called "mean bond dissociation enthalpy", $\bar{D}$(M–L), defined as

$$\bar{D}(\text{M–L}) = 1/n\left[\Delta H_f^\circ(\text{M, g}) + n\,\Delta H_f^\circ(\text{L, g}) - \Delta H_f^\circ(\text{ML}_n, \text{g})\right] \quad (1)$$

This quantity is clearly not as useful as the partial bond dissociation enthalpies, $D_1,\ldots,D_i,\ldots,D_n$, where

$$D_i(\text{M–L}) = \Delta H_f^\circ(\text{ML}_{n-i}, \text{g}) + \Delta H_f^\circ(\text{L, g}) - \Delta H_f^\circ(\text{ML}_{n-i+1}, \text{g}) \quad (2)$$

and

$$\bar{D}(\text{M–L}) = \left(\sum_{i=1}^{n} D_i\right)/n \quad (3)$$

but unfortunately these values are only available for a very limited number of molecules. It is important to notice that $\bar{D}$(M–L) cannot be regarded as the average metal–ligand bond strength because eq. 1 contains the enthalpy of formation of the polyatomic free radical L, whose structure is eventually different from the structure

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it presents when bonded to the metal atom. In other words, $\bar{D}$(M–L) contains the reorganization enthalpy of L, ER_{L}, a quantity which should not be included in a correct calculation of the bond strength. Due to this reason it seems preferable to define another parameter, called "bond enthalpy term", E(M–L), which does not contain ER_{L} (Scheme 1).

$$\begin{tikzcd}
\text{ML}_n(\text{g}) \arrow[r, "nE(\text{M}-\text{L})"] \arrow[dr, "n\bar{D}(\text{M}-\text{L})"'] & \text{M(g)} \arrow[d, "0"] & + & nL^{*}(\text{g}) \arrow[d, "nER_{\text{L}}"] \\
 & \text{M(g)} & + & n\text{L(g)}
\end{tikzcd}$$

SCHEME 1

When a molecule has at least two different types of ligands (L and L′) bonded to the central metal atom the evaluation of one metal ligand bond strength, say M–L′, is usually more difficult than in the preceding example because it implies the knowledge of M–L bond strength in the molecule $\text{ML}_p\text{M}'_q$. The normal procedure in these cases simply consists in transferring $\bar{D}$(M–L) from the molecule ML_n to the molecule $\text{ML}_p\text{L}'_q$. This assumption, summarized by eq. 4, is however rather questionable as it neglects several reorganization enthalpies, which can significantly contribute to M–L′ bond strength.

$$\bar{D}(\text{M–L})\ (\text{in ML}_n) = \bar{D}(\text{M–L})\ (\text{in ML}_p\text{L}'_q) \qquad (4)$$

If it is accepted that ML bond strengths are similar in both complexes, then a better approximation will be not to consider identical mean bond dissociation enthalpies but to assume similar bond enthalpy terms:

$$E(\text{M–L})\ (\text{in ML}_n) = E(\text{M–L})\ (\text{in ML}_p\text{L}'_q) \qquad (5)$$

The ideas outlined above have been applied to the evaluation of metal–ligand bond enthalpies in $\text{M}(\eta\text{-C}_5\text{H}_5)_2\text{L}_2$ complexes [7–9] and have been extensively used to discuss thermochemical data of organometallic compounds containing transition metal–carbon and –hydrogen σ-bonds [6]. Their value is also evidenced, for example, in the calculation of metal–metal bond strengths [1].

Unfortunately the estimation of E values is often hindered by the lack of molecular structures of the complexes, which provide the necessary input data for the evaluation of reorganization enthalpies. An interesting set of molecules for which molecular structures and gaseous enthalpies of formation are available is Cr(CO)_6, $\text{Cr}(\eta\text{-C}_6\text{H}_6)_2$, and $\text{Cr(CO)}_3(\eta\text{-C}_6\text{H}_6)$. The aim of the present paper is to illustrate the usefulness of the bond enthalpy term concept by discussing the thermochemical data for those complexes [10]. Extended Hückel MO calculations were used to estimate the several reorganization enthalpies involved in the calculation of E values.

Calculations

The extended Hückel MO calculations were made by using the ICON8 program, developed by Hoffmann et al. [11–13]. The basis set for the chromium atom

TABLE 1

ORBITAL EXPONENTS AND PARAMETERS USED FOR THE EXTENDED HÜCKEL MOLECULAR ORBITAL CALCULATIONS

Orbital	Slater exponent	$-H_{ii}$(eV) [a]	Ref.
H 1*s*	1.300	13.60	12,13
C 2*s*	1.625	21.40	12,13
C 2*p*	1.625	11.40	12,13
O 2*s*	2.275	32.30	14
O 2*p*	2.275	14.80	14
Cr 4*s*	1.700	8.66	15,16
Cr 4*p*	1.700	5.24	15,16
Cr 3*d*	4.950 [b]	11.22	15,16

[a] 1 eV = 96.4845 kJ mol^{-1}. [b] $C_1 = 0.4876$, $\xi_2 = 1.600$, and $C_2 = 0.7205$.

consisted of 3*d*, 4*s*, and 4*p*-orbitals. The *s* and *p*-orbitals were described by single Slater-type wavefunctions and the *d*-orbitals were taken as contracted linear combinations of two Slater-type wavefunctions. The orbital exponents and the parameters for the extended Hückel calculations are collected in Table 1.

All calculations were performed by using the modified Wolfsberg-Helmholz method [17].

Results and discussion

The question of the transferability of metal–ligand bond enthalpies in several chromium molecules, including $Cr(CO)_6$, $Cr(\eta\text{-}C_6H_6)_2$, and $Cr(CO)_3(\eta\text{-}C_6H_6)$, has been discussed by Connor et al. by using available thermochemical, structural, and spectroscopic data for the complexes [10]. If the assumption defined by eq. 4 holds, then the enthalpy change associated with the reaction

$$Cr(CO)_6\ (g) + Cr(\eta\text{-arene})_2(g) \rightarrow 2\ Cr(CO)_3(\eta\text{-arene})\ (g) \qquad (6)$$

will be close to zero.

The standard enthalpies of formation of the arene complexes in reaction 6 are known for arene = 1,2,3,4,4a,8a-naphthalene, 1,3,5-trimethylbenzene, hexamethyl-

TABLE 2

STANDARD ENTHALPIES OF FORMATION AND ENTHALPY CHANGES OF REACTION 6 (kJ mol^{-1}) FOR SOME CHROMIUM-ARENE COMPLEXES [a]

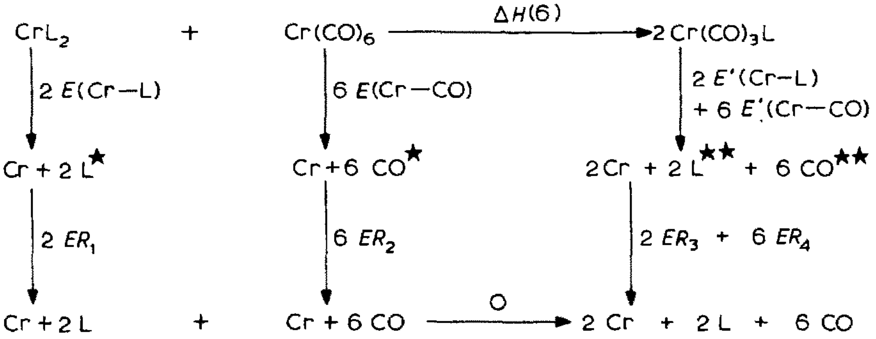
Complex	ΔH_f°(g)	$\Delta H(6)$ [b]
$Cr(\eta\text{-}C_6H_6)_2$	219.6 ± 8.0	−12 ± 21
$Cr(CO)_3(\eta\text{-}C_6H_6)$	−350.0 ± 9.4	
$Cr(\eta\text{-}1,3,5\text{-}Me_3\text{-}C_6H_3)_2$	63.5 ± 12.0	−88 ± 23
$Cr(CO)_3(\eta\text{-}1,3,5\text{-}Me_3C_6H_3)$	−466.3 ± 9.5	
$Cr(\eta\text{-}C_6Me_6)_2$	−88.0 ± 11.7	−100 ± 28
$Cr(CO)_3(\eta\text{-}C_6Me_6)$	−548.0 ± 12.6	
$Cr(\eta\text{-}C_{10}H_8)_2$	406.7 ± 10.8	−15 ± 19
$Cr(CO)_3(\eta\text{-}C_{10}H_8)$	−258.0 ± 7.6	

[a] See ref. 1. [b] $\Delta H_f^\circ[Cr(CO)_6, g] = -907.7 \pm 4.7$ kJ mol^{-1} [1].

benzene, and benzene and allow the calculation of ΔH (6) (Table 2). In a first approximation the results indicate that assumption 4 is reasonable for benzene and naphthalene complexes but starts to fail when hydrogen atoms of the benzene ring are replaced by methyl groups. On the other hand, the exothermicity of reaction 6 may suggest that Cr–CO bond strength is greater in $Cr(CO)_3(\eta\text{-arene})$ complexes than in $Cr(CO)_6$. This point has been made by Connor et al. and it is supported, for example, by infrared studies on $Cr(CO)_3(\eta\text{-arene})$ molecules, which show that the Cr–CO bond in these complexes has a greater multiple π-bonding character than in chromium hexacarbonyl [18].

As mentioned before, the structures of the molecules involved in reaction 6 are available in the case of benzene. A selection of these structural data is presented in Table 3, each value corresponding to an average of several results reported by different authors. The agreement between the indicated literature sources (Table 3) is, however, usually satisfactory.

In the absence of limiting factors, such as angular strain, bond lengths correlate with bond enthalpy terms [1,28,29]. Therefore, as shown in Table 3, the fact that Cr–CO bond length is shorter in $Cr(CO)_3(\eta\text{-}C_6H_6)$ than in $Cr(CO)_6$ suggests that Cr–CO bond strength is greater in the former complex. Inversely, it may be expected a weaker $Cr\text{–}C_6H_6$ bond in $Cr(CO)_3(\eta\text{-}C_6H_6)$ as compared with $Cr(\eta\text{-}C_6H_6)_2$, since the Cr–C bond length is about 10 pm longer in the mixed molecule. These bond enthalpy terms can be calculated if the reorganization enthalpies involved in



SCHEME 2

$$\Delta H(6) = [2\,E(\text{Cr–L}) + 2\,ER_1] + [6\,E(\text{Cr–CO}) + 6\,ER_2]$$
$$- [2\,E'(\text{Cr–L}) + 2\,ER_3 + 6\,E'(\text{Cr–CO}) + 6\,ER_4] \quad (7)$$

where

$$2\,E(\text{Cr–L}) + 2\,ER_1 = 2\,\bar{D}(\text{Cr–L}) = 2 \times (171.4 \pm 4.5)\ \text{kJ mol}^{-1} \quad (8)$$

$$6\,E(\text{Cr–CO}) + 6\,ER_2 = 6\,\bar{D}(\text{Cr–CO}) = 6 \times (106.9 \pm 1.1)\ \text{kJ mol}^{-1} \quad (9)$$

$$2\,E'(\text{Cr–L}) + 2\,ER_3 + 6\,E'(\text{Cr–CO}) + 6\,ER_4 = 2\,\bar{D}'(\text{Cr–L}) + 6\,\bar{D}'(\text{Cr–CO}) =$$
$$2 \times (497.9 \pm 10.3)\ \text{kJ mol}^{-1} \quad (10)$$

Schemes 2 and 3 are available ($L = \eta\text{-}C_6H_6$). In these cycles one star means that the fragments retain the structure they have when bonded to the chromium atom in CrL_2 or in $Cr(CO)_6$; two stars indicate the same structure as in $Cr(CO)_3L$. All the species are in the gaseous state.

$$\begin{tikzcd}
Cr(CO)_3^{\star} \arrow[r, "ER_5"] \arrow[d, "3\,E(Cr{-}CO)"] & Cr(CO)_3^{\star\star} \arrow[d, "3\,E'(Cr{-}CO)"] \\
Cr + 3\,CO^{\star} \arrow[d, "3\,ER_2"] & Cr + 3\,CO^{\star\star} \arrow[d, "3\,ER_4"] \\
Cr + 3\,CO \arrow[r, "0"] & Cr + 3\,CO
\end{tikzcd}$$

SCHEME 3

$$E'(\text{Cr–CO}) = E(\text{Cr–CO}) + ER_2 - ER_4 - ER_5/3 = \bar{D}(\text{Cr–CO}) - ER_4 - ER_5/3 \tag{11}$$

The values of the mean bond dissociation enthalpies shown in eqs. 8–10 were obtained from the data in Table 2 and also from $\Delta H_f^\circ(C_6H_6, g) = 82.9 \pm 0.3$ kJ mol^{-1} [30], $\Delta H_f^\circ(CO, g) = -110.53 \pm 0.17$ kJ mol^{-1} [31], and $\Delta H_f^\circ(Cr, g) = 396.6 \pm 4.2$ kJ mol^{-1} [1].

ER_1 and ER_3, the reorganization enthalpies of benzene from the complexes $Cr(\eta\text{-}C_6H_6)_2$ and $Cr(CO)_3(\eta\text{-}C_6H_6)$, respectively, were estimated as 4 kJ mol^{-1} and -24 kJ mol^{-1} from the energy values of C_6H_6 fragments and free benzene displayed in Table 4.

TABLE 3

SELECTED STRUCTURAL DATA FOR $Cr(CO)_6$, $Cr(\eta\text{-}C_6H_6)_2$, AND $Cr(CO)_3(\eta\text{-}C_6H_6)$

Bond length [a] or angle	$Cr(CO)_6$ [b]	$Cr(\eta\text{-}C_6H_6)_2$ [c]	$Cr(CO)_3(\eta\text{-}C_6H_6)$ [d]
Cr–CO	191.6		184.5
C–O	114.0		115.8
Cr–C		213.5	223.0
C–C		142.0	141.6
C–H		109	110.9
Cr–C–O	179.5		178.3
OC–Cr–CO	90.0		88.2

[a] In pm. [b] Values from refs. 19–21. [c] Values from refs. 22–24. [d] Values from refs. 25–27.

TABLE 4

ENERGY OF C_6H_6

Parent molecule	C–H (pm)	C–C (pm)	$-E$ (eV)
C_6H_6 [a]	108.4	139.7	535.08
$Cr(\eta\text{-}C_6H_6)_2$	109	142.0	535.12
$Cr(CO)_3(\eta\text{-}C_6H_6)$	110.9	141.6	534.83

[a] Bond lengths from ref. 32.

The result obtained for ER_1 seems rather surprising since, on the basis of C–H and C–C bond lengths in C_6H_6 and in $Cr(\eta\text{-}C_6H_6)_2$, a negative value for that reorganization enthalpy could be expected. This matter was further investigated by calculating the energy of C_6H_6 as a function of C–H and C–C bond lengths and also by looking for the molecular orbitals which have the largest contribution to the total energy changes. As shown in Fig. 1, it was found that the total energy increases when C–H bond lengths increase but it decreases with longer C–C bonds. The calculations also predict that the energy is less sensitive to changes in C–C bond lengths (a difference of 1 pm corresponds to 4–5 kJ mol^{-1} in the range of interest) than to changes in C–H bond lengths (1 pm corresponds to about 14 kJ mol^{-1}).

The destabilization of C_6H_6 with increasing C–H bond lengths is primarily due to the destabilization of three of the molecular orbitals **a**, **b**, and **c**, represented in Fig. 2 (refer also to Fig. 3). These essentially bonding σ-orbitals are involved in C–C and/or C–H bonds. On the other hand the stabilization of benzene with longer C–C bonds follows the stabilization (Fig. 3) of the five molecular orbitals shown in Fig. 2. The orbitals **d** and **e** are involved in C–C and in C–H σ-bonding.

These conclusions suggest that the positive value found for ER_1 may well be a result of basic assumptions of the extended-Hückel calculations, particularly the fact that only valence orbitals are considered [33]. It is likely that the carbon 1*s*-orbital participates in the σ-bonds.

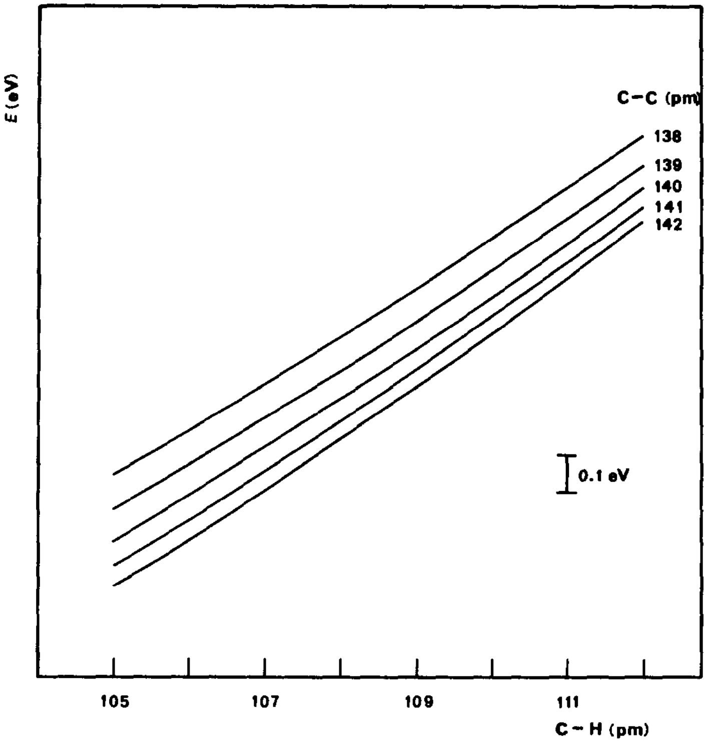


Fig. 1. Total energy of benzene as a function of C–H and C–C bond lengths.

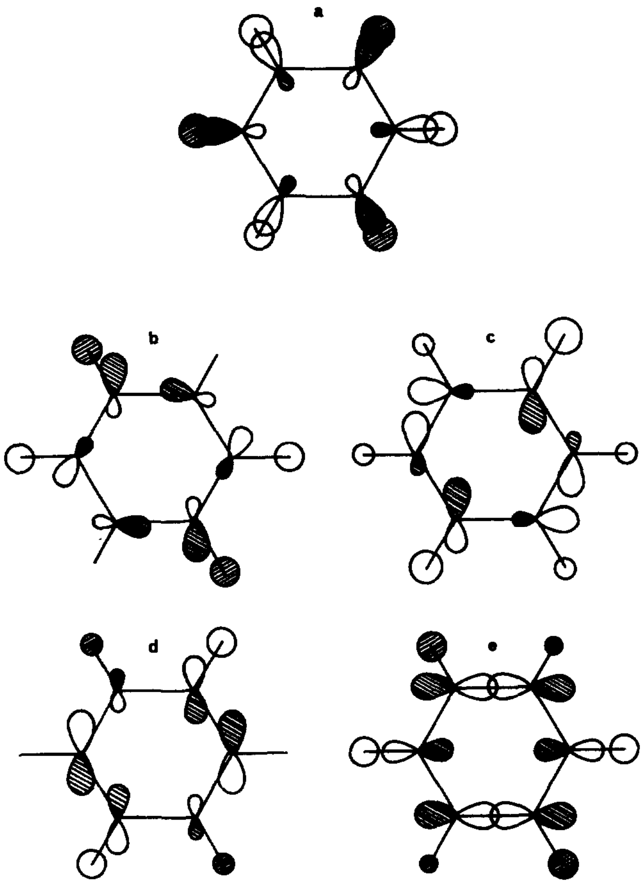


Fig. 2. Molecular orbitals of C_6H_6 (plane xy) involved in C–H (a, b, and d) and in C–C (b, c, and e) σ-bonding.

ER_2 and ER_4, the reorganization enthalpies of CO, were evaluated as -8 kJ mol^{-1} and -18 kJ mol^{-1}, respectively. The energies of CO fragments and free CO are presented in Table 5. An error of 1 pm in C–O bond length corresponds to a difference of about 6 kJ mol^{-1}.

The energies of Cr(CO)$_3^*$ (-677.19 eV) and Cr(CO)$_3^{**}$ (-677.94 eV) yield $ER_5 \sim -72$ kJ mol^{-1}, showing that this moiety is stabilized by the presence of the arene. The computed value is not very sensitive to a small error in Cr–C or C–O bond lengths, as evidenced by the results in Table 6. A change in the angles has also a small effect on ER_5. For example, the energy of Cr(CO)$_3^{**}$ calculated with C–Cr–C = 90° is about 7 kJ mol^{-1} smaller than the value quoted above.

Introducing the values of the reorganization enthalpies in eqs. 8–11 we are led to

$$E(\text{Cr–CO}) \sim 115 \text{ kJ mol}^{-1} \quad E'(\text{Cr–CO}) \sim 149 \text{ kJ mol}^{-1}$$

$$E(\text{Cr–C}_6\text{H}_6) \sim 167 \text{ kJ mol}^{-1} \quad E'(\text{Cr–C}_6\text{H}_6) \sim 129 \text{ kJ mol}^{-1}.$$

These results are consistent with the structural data (bond lengths) given in Table 3, i.e., $E(\text{Cr–CO}) < E'(\text{Cr–CO})$ and $E(\text{Cr–C}_6\text{H}_6) > E'(\text{Cr–C}_6\text{H}_6)$. However it is

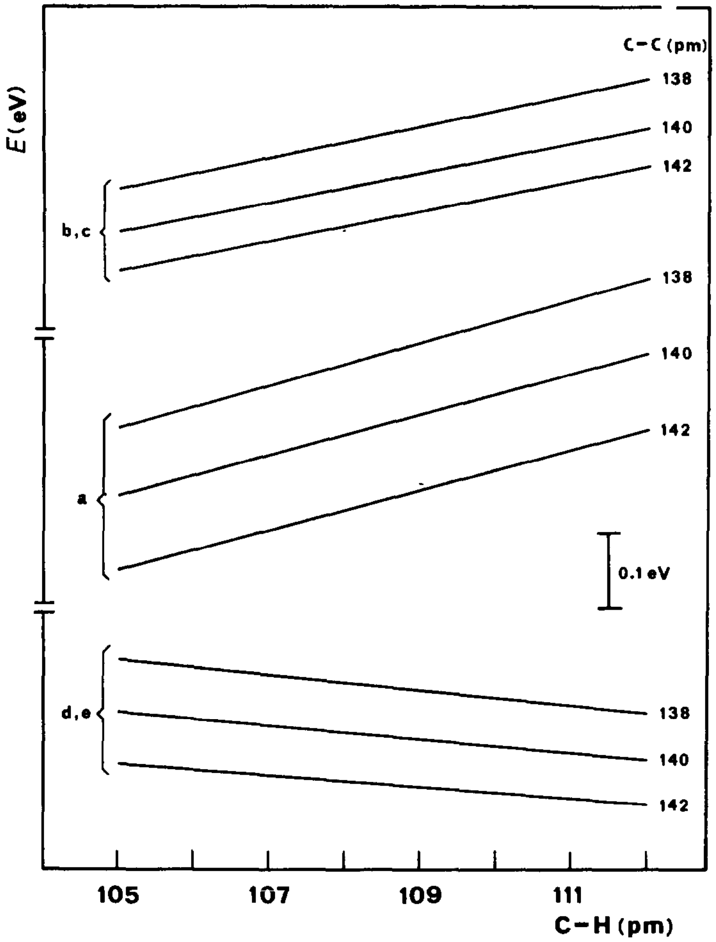


Fig. 3. Energy change of the molecular orbitals, a, b, c, d, and e (see Fig. 2) as a function of C–H and C–C bond lengths.

obvious that the reliability of quantitative predictions made by the extended Hückel calculations can be questioned [34]. Nevertheless it seems reasonable to assume that the errors associated with the computation of ER_2 and ER_4 will cancel and so the difference

$$E'(\mathrm{Cr{-}CO}) - E(\mathrm{Cr{-}CO}) = ER_2 - ER_4 - ER_5/3 = 10 - ER_5/3 \tag{12}$$

is only affected by the error in ER_5. If it is accepted that the Hückel calculations are at least qualitatively correct, i.e., the moiety $Cr(CO)_3$ is stabilized in $Cr(CO)_3(\eta\text{-}C_6H_6)$, then ER_5 will be negative and $E'(\mathrm{Cr{-}CO}) > E(\mathrm{Cr{-}CO})$.

If it is assumed that the errors in ER_1 and ER_2 are also identical, the difference

$$E(\mathrm{Cr{-}C_6H_6}) - E'(\mathrm{Cr{-}C_6H_6}) = -6 - ER_1 + ER_3 - ER_5 = -34 - ER_5 \tag{13}$$

depends once again upon the value of ER_5, but in this case the relationship $E(\mathrm{Cr{-}C_6H_6}) > E'(\mathrm{Cr{-}C_6H_6})$ will not hold if $ER_5 \gtrsim -34$ kJ mol^{-1}. However,

TABLE 5

ENERGY OF CO AS A FUNCTION OF C–O BOND LENGTH

C–O (pm)	$-E$ (eV)
112.8	198.10 [a]
113.6	198.05
114.0	198.02 [b]
114.1	198.02
115.2	197.95
115.8	197.91 [c]
116.0	198.90

[a] Energy of free CO (bond length from ref. 32). [b] Energy of CO in $Cr(CO)_6$. [c] Energy of CO in $Cr(CO)_3(\eta\text{-}C_6H_6)$.

TABLE 6

ENERGY OF $Cr(CO)_3$ MOIETY AS A FUNCTION OF Cr–C AND C–O BOND LENGTHS [a]

C–O 114 pm		Cr–C 191.6 pm	
Cr–C (pm)	$-E$ (eV)	C–O (pm)	$-E$ (eV)
184	678.28	114.0	677.19
186	678.00	114.4	677.15
188	677.72	114.8	677.10
190	677.43	115.2	677.05
192	677.13	115.6	677.01

[a] Cr–C–O = 180° and C–Cr–C = 90°.

accepting this value would be equivalent to consider an error of more than 100% in the Hückel calculations, which we do not consider likely, since a reorganization enthalpy is itself a *difference* between two energies calculated for the same type of fragments.

In conclusion, we believe that the trends obtained for the bond enthalpy terms are at least qualitatively reliable and furthermore we hope to have shown that the use of simple theoretical calculations, together with experimental thermochemical data can provide useful insights into metal–ligand "bond strengths".

References

1 G. Pilcher and H.A. Skinner, in F.R. Hartley and S. Patai, (Eds.), The Chemistry of the Metal-Carbon Bond, Wiley, New York, 1982.
2 J. Halpern, Acc. Chem. Res., 15 (1982) 238.
3 J.U. Mondal and D.M. Blake, Coord. Chem. Rev., 47 (1982) 205.
4 M. Mansson, Pure Appl. Chem., 55 (1983) 417.
5 P.M. Burkinshaw and C.T. Mortimer, Coord. Chem. Rev., 48 (1983) 101.
6 J.A. Martinho Simões and J.L. Beauchamp, Chem. Rev., to be published.
7 A.R. Dias, M.S. Salema and J.A. Martinho Simões, J. Organomet. Chem., 222 (1981) 69.
8 A.R. Dias, M.S. Salema and J.A. Martinho Simões, Organometallics, 1 (1982) 971.
9 M.J. Calhorda, R. Gomes da Costa, A.R. Dias and J.A. Martinho Simões, J. Chem. Soc., Dalton Trans., (1982) 2327.
10 J.A. Connor, J.A. Martinho Simões, H.A. Skinner and M.T. Zafarani-Moattar, J. Organomet. Chem., 179 (1979) 331.

11 R. Hoffmann and W.N. Lipscomb, J. Chem. Phys., 36 (1962) 2179.
12 R. Hoffmann, J. Chem. Phys., 39 (1963) 1397.
13 R. Hoffmann, J. Chem. Phys., 40 (1964) 2745.
14 R. Hoffmann, M.M.L. Chen, M. Elian, A.R. Rossi and D.M.P. Mingos, Inorg. Chem., 13 (1974) 2666.
15 T.A. Albright, P. Hofmann and R. Hoffmann, J. Am. Chem. Soc., 99 (1977) 7546.
16 J.W. Richardson, W.C. Nieuwpoort, R.R. Powell and W.E. Edgell, J. Chem. Phys., 36 (1962) 1057.
17 J.H. Ammeter, H.-B. Bürgi, J.C. Thibeault and R. Hoffmann, J. Am. Chem. Soc., 100 (1978) 3686.
18 See [10] and references cited therein.
19 L.O. Brockway, R.V.G. Ewens and M.W. Lister, Trans. Faraday Soc., 34 (1938) 1350.
20 A. Jost, B. Rees and W.B. Yelon, Acta Crystallogr., B31 (1975) 2649.
21 B. Rees and A. Mitschler, J. Am. Chem. Soc., 98 (1976) 7918.
22 A. Haaland, Acta Chem. Scand., 19 (1965) 41.
23 E. Keulen and F. Jellinek, J. Organomet. Chem., 5 (1966) 490.
24 E. Förster, G. Albrecht, W. Dürselen and E. Kurras, J. Organomet. Chem., 19 (1969) 215.
25 B.R. Rees and P. Coppens, J. Organomet. Chem., 42 (1972) C102.
26 B.R. Rees, Acta Crystallogr., B29 (1973) 2516.
27 N.-S. Chiu, L. Schäfer and R. Seip, J. Organomet. Chem., 101 (1975) 331.
28 H.A. Skinner, Trans. Faraday Soc., 41 (1945) 645.
29 C.E. Housecroft, M.E. O'Neill, K. Wade and B.C. Smith, J. Organomet. Chem., 213 (1981) 35.
30 J.B. Pedley and J. Rylance, Sussex-N.P.L. Computer Analysed Thermochemical Data: Organic and Organometallic Compounds, University of Sussex, Brighton, 1977.
31 CODATA Recommended Key Values for Thermodynamics, 1977; J. Chem. Thermodyn., 10 (1978) 903.
32 L.E. Sutton (Ed.), Tables of Interatomic Distances and Configuration in Molecules and Ions, Special Publication No. 18, Chemical Society, London, 1965.
33 D.M.P. Mingos, Adv. Organomet. Chem. 15 (1977) 1.
34 R. Hoffmann, T.A. Albright and D.L. Thorn, Pure Appl. Chem., 50 (1978) 1.