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BENZENECHROMIUM TRICARBONYL
III*. MEAN AMPLITUDES OF VIBRATION AND RELATED QUANTITIES FOR $C_6H_6Cr(CO)_3$

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SUMMARY

The results of a normal coordinate analysis of the whole molecule of benzenechromium tricarbonyl are reported. The calculations have revealed similar kinematic coupling phenomena to those previously described for transition metal sandwich complexes. Mean amplitudes of vibration (u), perpendicular amplitude correction coefficients (K) and selected shrinkage effects (δ) for $C_6H_6Cr(CO)_3$ are given which were calculated on the basis of this normal coordinate analysis. The u and δ values are compared with the corresponding quantities in related molecules, *viz.* free benzene, bis(benzene)chromium and chromium hexacarbonyl.

INTRODUCTION

This is a continuation of a series of studies concerning the vibrational properties of benzenechromium tricarbonyl[1,2]. In the present work a normal coordinate analysis for the whole complex was performed in a similar way as done previously for bis(benzene)chromium[3] and ferrocene[4].

STRUCTURAL AND SPECTRAL DATA

The structural parameters were taken from the recent X-ray work[5]. The molecular model has an overall symmetry of C_{3v}. For the benzene ligand a local sixfold symmetry was assumed as established by the X-ray study[5], which is in contrast to a qualitative spectroscopic analysis[6].

Experimental frequencies from infrared[6] and Raman[1] were employed. The normal modes of A_1+E are active in both infrared and Raman, while the A_2 modes are inactive. The more recent Raman values[1] were used for all the active frequencies for which they were available; *cf.* Table 1.

The wave numbers of the inactive A_2 normal modes had to be chosen in an

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* For Part II see ref. 2.

approximate way during the course of force constant calculations described in the subsequent section. The final complete assignment is shown in Table 1. While most of the inactive A_2 modes could be related to free C_6H_6 values, the two lowest A_2 frequencies are very uncertain, and especially the value of 100 cm^{-1} had to be chosen rather arbitrarily.

HARMONIC FORCE FIELD

(*a*). *Initial approximate force field*

The initial force constant calculations were based on the physical symmetry coordinates described in the previous paper[2]. These coordinates may be classified into three types which will be referred to as (A) chromium-tricarbonyl internal vibrations, (B) benzene internal vibrations, and (C) complex vibrations. In the initial force constant matrix all interaction terms between coordinates belonging to two different types were assumed to vanish.

All force constants for the benzene internal vibrations were transferred from free benzene. The force field adopted here has previously been used in recalculations of mean amplitudes of vibration[7], and in the normal coordinate analysis of bis(benzene)chromium[3]. It was developed in terms of the tentatively standardized symmetry coordinates specified elsewhere[9]. It is essentially equivalent to other published free benzene force fields (see for example Duinker and Mills[11]), and it is consistent with the vibrational assignment of Brodersen and Langseth[10]. (Calculated free benzene frequencies are given in Table 1.)

For the chromium tricarbonyl internal vibrations it is not so easy to estimate the force constants. In the present work a tentative starting set was produced from the force field of chromium hexacarbonyl[12]. This force field was formulated in terms of a valence coordinate compliance matrix, which had to be singular because of the presence of redundancies. After removing all elements not belonging to the $Cr(CO)_3$ part of $Cr(CO)_6$ the singularity disappeared, and the resulting matrix could be inverted to yield the usual valence coordinate force constant matrix. From this matrix the symmetry force constants appropriate to the $Cr(CO)_3$ part were obtained in the usual way.

The remaining force constants, classified as belonging to the complex vibrations, were chosen in what seemed to be the approximate order of magnitude. Qualitative comparisons are possible with the constants of similar modes in bis(benzene)-chromium[3] and ferrocene[4].

Table 1 shows the calculated frequencies from the initial approximate force field in the column headed "Approx." In these calculations none of the experimental frequencies for $C_6H_6Cr(CO)_3$ have been utilized so far.

(*b*). *Final force filed*

The above force field was modified so as to reproduce exactly the experimental frequencies of the active species A_1 and E. The proper adjustments were found in several cycles using the relative insensitivity of the eigenvectors and keeping as many of the off-diagonal force constants as possible equal to zero. This refinement was found to affect very much most of the force constant values pertaining to the coordinate types (A) and (C), while those of the type (B), *i.e.* pertaining to the benzene

TABLE 1

APPROXIMATE CALCULATED AND FINAL VIBRATIONAL FREQUENCIES (cm^{-1}) IN BENZENECHROMIUM TRICARBONYL ALONG WITH THE FREQUENCIES OF FREE BENZENE

Species of C_{3v}	No.[a]	$C_6H_6Cr(CO)_3$ Approx.	$C_6H_6Cr(CO)_3$ Final	C_6H_6	Species of D_{6h}
A_1[a]	2	3073	3090	3073	a_{1g}
	29	2083	1943		
	14	1307	1317	1309	b_{2u}
	15	1141	1152	1146	b_{2u}
	1	993	980	993	a_{1g}
	11	989	800	673	a_{2u}
	31	602	664		
	25	411	535		
	26	329	486		
	21	99	298		
A_2[b]	13	3057	3057	3057	b_{1u}
	3	1347	1350	1350	a_{2g}
	12	1010	1010	1010	b_{1u}
	5	987	990	990	b_{2g}
	4	706	707	707	b_{2g}
	32	395	465		
	22	95	100		
E[a]	7	3065	3076	3064	e_{1u}
	20	3056	3023	3056	e_{2g}
	30	2044	1865		
	8	1598	1631	1599	e_{2g}
	19	1481	1451	1482	e_{1u}
	9	1171	1158	1178	e_{2g}
	18	1042	1017	1037	e_{1u}
	17	965	965	967	e_{2u}
	10	858	902	846	e_{1g}
	33	607	644		
	6	529	614	606	e_{2g}
	34	444	543		
	16	418	426	398	e_{2u}
	23	396	332		
	27	298	306		
	24	146	132		
	28	80	110		

[a] Values for the active species A_1 and E from ref. 1. [b] Values for the inactive species A_2 were chosen as described in the text.

internal vibrations, were affected to a much smaller degree.

For complex molecules like benzenechromium tricarbonyl the result of a force field refinement in the absence of exhaustive isotopic data is imperfect to the extent of nearly rendering valence force symmetry constants physically meaningless. For one thing, the number of unknowns is so much larger than the number of observables that there are for each set of symmetry coordinates infinitely many sets of force constants which reproduce exactly the experimental frequencies. Secondly, because of internal couplings, several different assignments of closely neighbored frequencies will yield an acceptable potential energy distribution which shows in many cases an equivalent contribution of several internal coordinates to one frequency.

The first imperfection of force fields in general does not affect appreciably the values of the calculated, physically meaningful quantities (*e.g.* amplitudes of yibration), if the force constant values are chosen within the right order of magnitude.

The second imperfection, however, may influence the values of calculated physical quantities. In the present work we have proceeded by choosing a reasonable potential energy distribution which, at the same time, produced acceptable values for the calculated mean amplitudes of vibration and related quantities. The obtained values are accepted now on the basis of a comparison with the corresponding values of similar molecules [benzene, bis(benzene)chromium and chromium hexacarbonyl]. In a future work[8] we plan to make these calculated results self-consistent with the values obtained by an anticipated electron diffraction study.

In the inactive species A_2 the (A) type force constant, *viz.* $F_{11}(A_2)$, was taken to be equal to $F_{55}(E) = 0.282$ mdyne/Å because the corresponding coordinates are both composed of the same type of Cr–C–O linear bendings. This is a somewhat poor justification for the chosen value, but it is the best one can do without other experimental evidence. The (C) type force constant of A_2 was adjusted to the rather arbitrarily chosen frequency of 100 cm^{-1}.

The frequencies calculated for the species A_1, A_2 and E from our final force field are given in Table 1 under the heading "Final". The final force field was also transformed to our conventional symmetry coordinates[2], especially in order to study the influence of the different coordinate systems on kinematic coupling.

KINEMATIC COUPLING

Fig. 1 shows a mapping of the G matrix in terms of the applied physical sym-

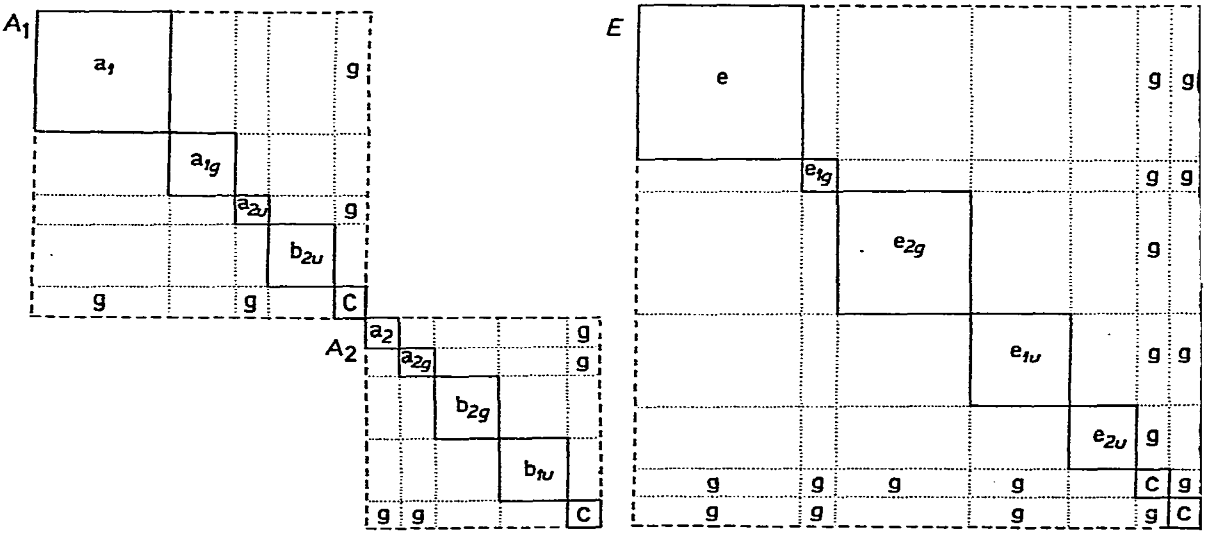

Fig. 1. Mapping of the G matrix. The different diagonal blocks pertain to: (A) chromium–tricarbonyl internal vibrations $4a_1+a_2+5e$; (B) benzene internal vibrations $2a_{1g}+a_{2u}+2b_{2u}+a_{2g}+2b_{2g}+2b_{1u}+e_{1g}+4e_{2g}+3e_{1u}+2e_{2u}$; (C) complex vibrations; C. Nonvanishing interaction terms between blocks of different types are indicated by "g".

metry coordinates[2]. There are no elements of direct coupling between coordinates of the types (A) and (B), but both of these types display coupling with the coordinates of complex vibrations (C). This type of coupling is referred to as kinematic coupling[3,4,13,14]. It can, at least partly, explain some frequency shifts from free to complexed molecules which were sometimes explained by a potential energy change alone. The magnitude of the off-diagonal coupling G matrix elements depends on the choice of the symmetry coordinates. The coupling phenomena are observed in this case for both natural systems which we investigated: our physical system[2] which preserves the identity of the individual groups in the molecule as far as possible; and the conventional system[2] which emphasizes the structural features of the complex as a whole.

TABLE 2

MEAN AMPLITUDES (Å) IN $C_6H_6Cr(CO)_3$
Lowest A_2 frequency assumed to be 100 cm^{-1}.

Distance				$u[C_6H_6Cr(CO)_3]$	
No.	Type	(R_{ij})	i–j	$T=0$°K	298°K
	Benzene				
1	C–H	(1.100)	4–14	0.077	0.077
2	C–C	(1.400)	4–5	0.046	0.046
3	C–C	(2.425)	4–6	0.054	0.055
4	C–C	(2.800)	4–7	0.057	0.059
5	C–H	(2.170)	4–15	0.100	0.100
6	C–H	(3.422)	4–16	0.096	0.097
7	C–H	(3.900)	4–17	0.092	0.093
8	H–H	(2.500)	14–15	0.158	0.159
9	H–H	(4.330)	14–16	0.133	0.134
10	H–H	(5.000)	14–17	0.117	0.118
	Cr-benzene				
11	Cr–H	(3.037)	10–14	0.115	0.124
12	Cr–C	(2.221)	4–10	0.059	0.070
	Cr–tricarbonyl				
13	Cr–C	(1.840)	1–10	0.050	0.057
14	C–O	(1.150)	1–11	0.036	0.036
15	Cr–O	(2.990)	10–11	0.049	0.056
16	C–C	(2.556)	1–2	0.072	0.097
17	C–O	(3.456)	1–12	0.080	0.122
18	O–O	(4.154)	11–12	0.093	0.166
	Tricarbonyl–benzene				
19	C–C	(2.920)	1–4	0.077	0.103
20	C–C	(3.479)	1–6	0.077	0.107
21	C–C	(3.960)	1–7	0.070	0.087
22	C–H	(3.163)	1–14	0.156	0.180
23	C–H	(4.049)	1–16	0.143	0.173
24	C–H	(4.774)	1–17	0.125	0.139
25	O–C	(3.770)	4–11	0.088	0.136
26	O–C	(4.475)	4–13	0.084	0.131
27	O–C	(5.084)	4–12	0.071	0.093
28	O–H	(3.733)	11–14	0.171	0.223
29	O–H	(4.931)	11–16	0.154	0.207
30	O–H	(5.891)	11–17	0.126	0.145

MEAN AMPLITUDES OF VIBRATION

(*a*). *Presentation of results*

The calculated mean amplitudes of vibration (u) for the thirty different distances in $C_6H_6Cr(CO)_3$ are given in Table 2. The u values are shown at the temperatures of absolute zero and 298° K. The interatomic distances (in Å) are given in parentheses in order to facilitate the identification of the different atom pairs. They are all calculated values from the adopted structural data[5]. The numbers i–j, which are included for further identification, correspond to the numbering of atoms as given in the theoretical part[2].

(*b*). *Influence of the lowest A_2 frequency*

In order to investigate the influence of the unknown lowest A_2 frequency two other runs were executed in addition to the one with 100 cm^{-1}. In these two runs the A_2 force constants were adjusted to fit a lowest frequency of 50 and 200 cm^{-1}, respectively, in addition to all the other frequencies unchanged. As might be expected these different choices of the lowest A_2 frequency affected only the twelve mean amplitudes pertaining to the tricarbonyl–benzene distances (Nos. 19–30 in Table 2). They are the distances which depend on the angle of rotation of the benzene and $Cr(CO)_3$ groups relative to each other around the three-fold axis of symmetry. The calculated values of mean amplitudes at 298° K for the corresponding distances are given in Table 3. The mean amplitude values for a given distance increase with decreasing frequency, and the shifts increase towards the lower range of frequencies. Specifically, the Table displays for every distance the difference u (50 cm^{-1})–u (100 cm^{-1}) to be larger than u (100 cm^{-1})–u (200 cm^{-1}).

TABLE 3

MEAN AMPLITUDES (Å) FOR $C_6H_6Cr(CO)_3$ AT 298°K FOR DISTANCES DEPENDING ON ANGLE OF INTERNAL ROTATION

Three different lowest A_2 frequencies.

Distance No.[a]	50 cm^{-1}	100 cm^{-1}	200 cm^{-1}
19	0.113	0.103	0.100
20	0.133	0.107	0.099
21	0.093	0.087	0.085
22	0.196	0.180	0.176
23	0.210	0.173	0.162
24	0.148	0.139	0.137
25	0.149	0.136	0.133
26	0.165	0.131	0.121
27	0.103	0.093	0.090
28	0.247	0.223	0.217
29	0.262	0.207	0.191
30	0.160	0.145	0.141

[a] See Table 2.

(*c*). *Influence of different assignments*

Because of the mentioned uncertainties in the force field determination of the type which always are present in analyses of molecules with so many atoms, it was decided to investigate the influence of changes in the force field on mean amplitudes. If (L) represents the normal-coordinate matrix, and if (λ) represents the diagonal matrix of eigenvalues to GF, then the F matrix is given by:

$$F = \tilde{L}^{-1} \cdot \lambda \cdot L^{-1}$$

Different force fields were produced by using the above relation without changing the L matrix, but permuting the elements of λ. This procedure produces new force fields, which all are consistent with the same set of vibrational frequencies, but the assignments (reflected by the potential energy distribution) are effectively altered.

In the present investigation we maintained the original assignment of frequencies in the inactive species A_2 (with 100 cm^{-1} as the lowest frequency). In two runs we interchanged the sequence of two frequencies in each of the A_1 and E species, for which different assignments really seemed to be reasonable: (*i*) 535/486 cm^{-1} in A_1 along with 332/306 cm^{-1} in E; (*ii*) 664/535 cm^{-1} in A_1 and 664/543 cm^{-1} in E. In a third run (*iii*) more drastic changes were made which included some of the relatively high frequencies: 980/800 cm^{-1} were interchanged in A_1, and the ten (out of seventeen) lowest frequencies were chosen in the sequence 902, 965, 644, 426, 332, 543, 614, 306, 132, 110 cm^{-1}.

The following conclusions were drawn: In the cases (*i*) and (*ii*) most of the mean amplitudes were practically not affected by the changed assignments. For some of the distances an influence was detected, but never exceeding some few thousandths of an Ångström. In case (*iii*), where rather drastic changes in the assignment were made, also some of the mean amplitudes changed substantially. This was especially the case for many of the benzene mean amplitudes and for the Cr–benzene u(Cr–C). In the former group No. 4, *viz.* one of the u(C–C), came out with 0.071 Å, and the u(Cr–C) value became 0.119 Å, both results at 298°K. These values are highly improbable when compared with the corresponding mean amplitudes in related molecules (see the next paragraph), We are therefore convinced that the potential energy distribution employed to produce the data presented in the Tables is a reasonable one. In case of serious discrepancies between these and the anticipated electron diffraction results, however, we may try different distributions in order to reduce the differences between observed and calculated mean amplitudes, as soon as the experimental values will be available.

(*d*). *Comparison with related molecules*

In Table 4 the calculated mean amplitudes for $C_6H_6Cr(CO)_3$ at 298°K are compared with corresponding data for bis(benzene)chromium[15], free benzene[15,16], and chromium hexacarbonyl[12,16,17]. The benzene ligand mean amplitudes are found to be very close to the corresponding ones in free benzene, as also observed in the case of bis(benzene)chromium[15,18]. The Cr–benzene mean amplitudes of $C_6H_6Cr(CO)_3$ are found to be remarkably close to the corresponding ones in $(C_6H_6)_2Cr$. The Cr–tricarbonyl mean amplitudes are very similar to the $Cr(CO)_6$ values of bonded (Cr–C and C–O) distances and the (linear) Cr–O distance. The u(C–C),

TABLE 4

MEAN AMPLITUDES (Å) FOR $C_6H_6Cr(CO)_3$ AT 298°K COMPARED WITH CORRESPONDING QUANTITIES IN RELATED MOLECULES

Distance[a]	$C_6H_6Cr(CO)_3$[b]	$(C_6H_6)_2Cr$[c]	C_6H_6[d]	$Cr(CO)_6$	
1	0.077	0.079	0.077		
2	0.046	0.047	0.046		
3	0.055	0.056	0.055		
4	0.059	0.059	0.059		
5	0.100	0.101	0.100		
6	0.097	0.098	0.097		
7	0.093	0.095	0.093		
8	0.159	0.160	0.158		
9	0.134	0.135	0.133		
10	0.118	0.120	0.118		
11	0.124	0.124			
12	0.070	0.073			
13	0.057			0.0556[e]	0.0577[f]
14	0.036			0.0350	0.0346
15	0.056			0.0571	0.0571
16	0.097			0.1498	0.136
17	0.122			0.1790	0.180
18	0.166			0.2373	0.262

[a] See Table 2. [b] This work. [c] Ref. 15. [d] Ref. 16; see also ref. 15. [e] Ref. 7 quoted in ref. 16. [f] Ref. 12.

u(C–O) and u(O–O) values in $C_6H_6Cr(CO)_3$ were found to be significantly smaller than the corresponding values in $Cr(CO)_6$.

PERPENDICULAR AMPLITUDE CORRECTION COEFFICIENTS

The calculated perpendicular amplitude corrections of K values[16] for C_6H_6-$Cr(CO)_3$ are shown in Table 5. Data for free C_6H_6 from ref. 15 are included for comparison. The K values, in contrast to the u values, are seen to be subjected to substantial shifts from free to complexed benzene. The same feature was observed in the case of bis(benzene)chromium[15,19] and for ferrocene in comparison with the cyclopentadienide anion[19]. In the present case the shifts go in the same direction as was reported for bis(benzene)chromium[15,19], but there are significant quantitative differences between the K values in the two complexed molecules in question.

SHRINKAGE EFFECTS

It is possible to calculate the Bastiansen–Morino shrinkage effects[16] for the benzene part and for the linear Cr–carbonyl chains from the harmonic vibrational analysis of benzenechromium tricarbonyl. For all the other distances the shrinkages cannot be obtained from spectroscopical data without a detailed analysis of anharmonicity. Table 6 shows the calculated results for $C_6H_6Cr(CO)_3$ at absolute zero and 298° K. For precise definitions of shrinkage effect values we refer to Cyvin[16]. Here it is recalled that the shrinkage effects (δ values) may be obtained as linear combinations of appropriate K values.

TABLE 5

PERPENDICULAR AMPLITUDE CORRECTION COEFFICIENTS (Å) IN $C_6H_6Cr(CO)_3$ ALONG WITH DATA FOR FREE C_6H_6

Lowest A_2 frequency in benzenechromium tricarbonyl assumed to be 100 cm^{-1}.

Distance No.[a]	$K[C_6H_6Cr(CO)_3]$		$K[C_6H_6]$
	$T=0°K$	298°K	298°K
(Benzene)			
1	0.0169	0.0193	0.017
2	0.0033	0.0058	0.003
3	0.0026	0.0061	0.001
4	0.0023	0.0062	0.001
5	0.0101	0.0142	0.009
6	0.0075	0.0127	0.006
7	0.0068	0.0125	0.004
8	0.0134	0.0184	0.013
9	0.0101	0.0167	0.008
10	0.0092	0.0164	0.006
(Cr–benzene)			
11	0.0066	0.0107	
12	0.0019	0.0048	
(Cr–tricarbonyl)			
13	0.0023	0.0043	
14	0.0055	0.0109	
15	0.0022	0.0073	
16	0.0023	0.0045	
17	0.0023	0.0068	
18	0.0023	0.0079	
(Tricarbonyl–benzene)			
19	0.0020	0.0045	
20	0.0015	0.0030	
21	0.0012	0.0023	
22	0.0056	0.0100	
23	0.0046	0.0070	
24	0.0041	0.0059	
25	0.0018	0.0056	
26	0.0013	0.0037	
27	0.0010	0.0029	
28	0.0047	0.0099	
29	0.0037	0.0063	
30	0.0032	0.0052	

[a] See Table 2.

TABLE 6

SHRINKAGE EFFECTS (Å) IN $C_6H_6Cr(CO)_3$

Lowest A_2 frequency 100 cm^{-1}

Distance		$\delta[C_6H_6Cr(CO)_3]$	
No.[a]	Type	$T=0°K$	298°K
	Benzene		
3	C–C	0.0031	0.0039
4	C–C	0.0042	0.0054
5	C–H	0.0069	0.0070
6	C–H	0.0140	0.0152
7	C–H	0.0167	0.0185
8	H–H	0.0068	0.0068
9	H–H	0.0250	0.0268
10	H–H	0.0312	0.0338
	Cr–tricarbonyl		
15	Cr–O	0.0056	0.0079

[a] See Table 2.

TABLE 7

SHRINKAGE EFFECTS (Å) FOR $C_6H_6Cr(CO)_3$ AT 298°K ALONG WITH DATA FOR FREE C_6H_6 AND $Cr(CO)_6$

Distance No.[a]	$C_6H_6Cr(CO)_2$[b]	C_6H_6[c]	$Cr(CO)_6$
3	0.0039	0.00342	
4	0.0054	0.00485	
5	0.0070	0.00714	
6	0.0152	0.01483	
7	0.0185	0.01807	
8	0.0068	0.00695	
9	0.0268	0.02626	
10	0.0338	0.03340	
15	0.0079		0.0052[d] 0.010[e]

[a] See Table 2. [b] This work. [c] Ref. 16. [d] Ref. 7 quoted in ref. 16. [e] Ref. 12.

The calculations were performed with the three choices for the lowest A_2 frequency (see above). The influence on the shrinkage effects was found to be entirely negligible, in spite of the fact that the K values for absolutely all distances were largely affected. Also, in contrast to the K values, the δ values for the benzene ligand were found to be similar to those of free benzene[16]. The shrinkages of $C_6H_6Cr(CO)_3$ and C_6H_6 are compared in Table 7. No conclusion can be drawn from the comparison of the calculated linear Cr–O shrinkage in the $Cr(CO)_3$ part (see Table 7) with the corresponding quantity in chromium hexacarbonyl because of great discrepancies between the two available independent calculations of shrinkage effects in chromium hexacarbonyl[12,17].

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