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## QUANTITATIVE STUDY OF STRUCTURAL PARAMETERS OF SPECIFIC ADSORPTION OF ALKENES ON ZINC IONS USING GAS-SOLID CHROMATOGRAPHY AND TOPOLOGICAL DATA-PROCESSING TECHNIQUES

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(First received December 18th, 1983; revised manuscript received February 13th, 1984)

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### SUMMARY

Gas-solid chromatography can provide information on the adsorption processes involved in heterogeneous catalysis. Retention indices of a set of 44 alkenes on the zinc form of a sulfonated porous polymer are analyzed to evaluate the polar and steric contributions to adsorption on this metal ion. DARC/PELCO topological analysis is used to evaluate the effect of each carbon atom in the environment of the double bond on the overall retention of a compound by adsorption.

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### INTRODUCTION

Gas chromatographic (GC) columns have been used as efficient catalytic reactors<sup>1</sup>. Phillips<sup>2</sup>, for example, has shown that a large variety of reactions of saturated and unsaturated hydrocarbons can occur on columns of silica or alumina coated with salts of metal ions such as Cd<sup>2+</sup> or Ni<sup>2+</sup>. These gas-solid chromatographic (GSC) systems can be used as models of a large-scale catalytic reactor and can serve as a powerful technique for studying the process of adsorption on a metal catalyst surface. The latter use of GSC would be quite valuable for elucidating at a molecular level the nature of the interactions between the substrate and catalyst in, for example, petrochemistry. Thanks to progress in data-processing techniques in recent years, it is now possible to extract precise information on structural effects on specific adsorption from large sets of GC data. This paper reports on the use of GSC to study the interaction of alkenes with Zn<sup>2+</sup> at the level of the individual carbon atoms as a complement to information obtained by other methods of studying such interactions.

Despite the use of powerful spectroscopic techniques (NMR, IR, Raman) for

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the study of adsorbed species, the information obtained has been relatively limited. For example, NMR needs homogeneous samples to obtain fine detail about adsorption of species; the NMR spectra of molecules adsorbed on solids show broad bands so only small molecules or molecules with a high degree of symmetry can be studied<sup>3</sup>. Ali and Gay<sup>4</sup> have described the use of <sup>13</sup>C NMR to study adsorption of alkenes on ZnO. The study was limited to molecules of uncomplicated structure (ethylene, propene, butenes and simple cycloalkenes) and was carried out at 28°C, rather than at a temperature at which the metal would show significant catalytic activity.

Raman spectroscopy provides more extensive information about adsorption on metals<sup>5</sup>. However, the conditions of measurement are again quite different from those at which catalysis would be carried out. Emphasis in many Raman studies has been on the nature of the spectroscopic effect (surface-enhanced Raman scattering) rather than the study of catalysis *per se*<sup>6</sup>.

The strength of adsorption of an unsaturated molecule on a catalyst site is a combination of the energy of charge-transfer complexation and the hindrance to complexation posed by steric factors. The latter depend both on the nature of the catalyst and the structure of the substrate. The reactivity of alkenes and the product composition are influenced, for instance, by the extent of crowding at the metal atom site<sup>7</sup>.

The contribution of the structure of the alkene to catalytic reactivity is also a major factor, and this is what we intend to explore. The competition between the steric and polar effects is a major interest of ours, in both homogeneous<sup>8,9</sup> and heterogeneous<sup>10,11</sup> systems. This work has required new approaches and techniques of experimentation and data processing. For crowded alkenes, information on non-specific adsorption can be obtained, for example, on graphitized carbon black<sup>12</sup>. The specific alkene-metal ion interaction can best be studied using the appropriate metal ion forms of the sulfonated porous polymer we have developed. It is also essential to use an efficient experimental design so that a maximum of information can be obtained from the studies. For this purpose we have applied Correspondence Factor Analysis (CFA)<sup>13</sup> to elucidate the main trends, and DARC\* Topological Analysis (DTA)<sup>14</sup> to define the contributions of the individual carbon atoms of alkenes adsorbed onto Ni<sup>2+</sup>.

We will show how one can determine the molecular structural factors which influence the strength of specific adsorption on a metal ion site. The present report deals with the adsorption of a wide variety of linear and branched C<sub>2</sub>-C<sub>8</sub> alkenes on Zn<sup>2+</sup>, chosen because of its particular selectivity in adsorption of branched alkenes and because of its known catalytic activity<sup>15-17</sup>. DTA is used to analyze the experimental data and a brief description of this technique is included.

## EXPERIMENTAL

The details of the preparation of the zinc form of sulfonated divinylbenzene-ethylvinylbenzene copolymer have been published previously, along with the conditions used for GC study of this column packing material<sup>13</sup>. The present work was

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\* DARC stands for Description, Acquisition, Restitution and Computer-aided design.

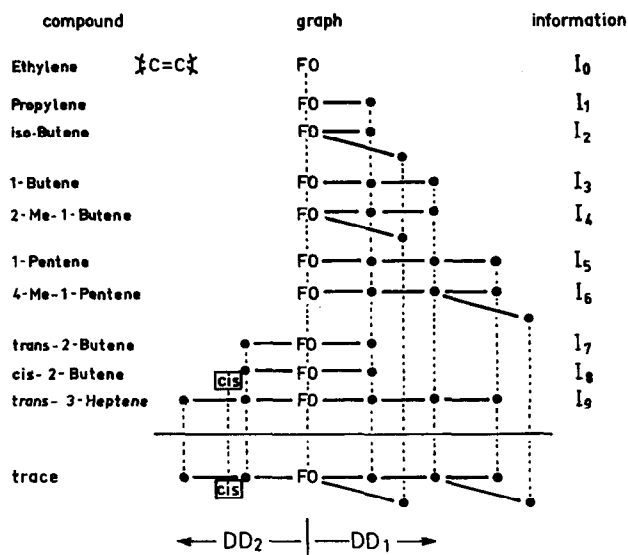


Fig. 1. Principle of superposition of the elementary graphs of ten alkenes to give the characteristic trace of the population studied (the C=C group is taken as the focus FO).

carried out on a packing containing 2.3%  $\text{Zn}^{2+}$ . Measurements were made using ultra-high-purity nitrogen (AGL Welding Supply, Clifton, NJ, U.S.A.), specially deoxygenated in the laboratory, as the carrier gas. The Varian Model 200 chromatograph was operated at 175°C and with a carrier gas flow-rate of 40 ml/min. The sample sizes injected were about 25 ng, and it was determined that such quantities were well within the linear isotherm of this adsorbent, *i.e.*, well below the level of monolayer coverage of the active sites. The retention times obtained experimentally were converted into Kováts retention index units (I.U.).

#### DATA PROCESSING

Topological analysis offers the possibility of calculating the contribution of every heavy atom (usually the carbon atoms) of the skeleton of the molecule. This involves the calculation of a set of parameters equal in size to the number of unique heavy atom positions, and hence requires selection of a homogeneous set of compounds larger in number than the number of parameters. The analysis calculates the contribution of each topological site to the experimentally determined property of the molecules. The DARC/PELCO\* procedure developed by Dubois and co-workers has been described elsewhere with respect to applications in chromatography<sup>14</sup>, pharmacology<sup>18</sup>, spectroscopy<sup>19</sup> and reactivity<sup>20</sup>.

The organization of the series of compounds is done by starting at the active site or focus of the molecules, and writing the graph of the carbon atom skeleton leading away from this active site for each compound. The graphs are then superimposed for the set, producing the trace of the series. This is illustrated in Fig. 1 for

















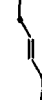


\* PELCO stands for Perturbation of an Environment that is Limited, Concentric and Ordered.

TABLE I  
 TOPOLOGICAL ANALYSIS OF THE BEHAVIOR OF ALKENES ON THE UNSULFONATED SUPPORT AND ON THE ZINC FORM OF THE CATION-EXCHANGE RESIN

Experimental (1 and 3) and calculated Kováts retention indices at 175°C and Kováts retention index increments,  $\Delta I$ . Correlation 3 (calculation (5)) is done with seven supplementary interaction parameters.

No.	Compound	Graph	Unsulphonated support			Zinc form of resin			$\Delta I$ (3)-(1)	B.p. (°C)
			Exptl. (1)	Calc. (2)	Diff. (1)-(2)	Exptl. (3)	Calc. (4)	Diff. (3)-(4)		
				1(2)		2(4)		3(5)		
				44		44		44		
				19		19		25		
				0.9997		0.988		0.999		
				4.8		28.7		10.2		
				2.6		14.6		4.1		
				0.001		0.02		0.005		
1	Ethylene		200	200	0	220	220	0	20	-103.7
2	Propylene		304	306	-2	387	433	-46	83	-47.7
3	1-Butene		404	399	5	513	529	-16	109	-6.3
4	<i>trans</i> -2-Butene		410	409	1	508	528	-20	98	0.9
5	<i>cis</i> -2-Butene		418	412	6	516	527	-11	98	3.7
6	Isobutene		398	402	-4	596	562	34	198	-6.9
7	2-Methyl-1-butene		493	495	-2	697	658	39	204	31.2
8	2-Methyl-2-butene		507	506	1	698	657	41	191	38.6
9	1-Pentene		493	495	-2	613	615	-2	120	30.0
10	<i>trans</i> -2-Pentene		502	502	0	615	623	-8	113	36.4

## GSC OF ALKENES

11	<i>cis</i> -2-Pentene		507	505	2	616	622	-6	616	0	109	36.9
12	2,3-Dimethyl-1-butene		577	570	7	746	787	-41	746	0	169	55.6
13	3,3-Dimethyl-1-butene		550	559	-9	730	691	39	730	0	180	41.2
14	2-Ethyl-1-butene		593	593	0	763	742	21	758	5	170	64.7
15	2-Methyl-1-pentene		590	591	-1	751	744	7	759	-8	161	62.1
16	3-Methyl-1-pentene		574	570	4	761	744	17	758	3	187	54.2
17	4-Methyl-1-pentene		573	574	-1	740	708	32	739	1	167	53.9
18	2-Methyl-2-pentene		596	598	-2	749	747	2	763	-14	153	67.3
19	3-Methyl- <i>trans</i> -2-pentene		601	599	2	770	752	18	766	4	169	70.4
20	3-Methyl- <i>cis</i> -2-pentene		601	601	0	770	751	19	769	1	169	67.7
21	4-Methyl- <i>trans</i> -2-pentene		573	577	-4	763	752	11	763	0	190	58.6
22	4-Methyl- <i>cis</i> -2-pentene		573	580	-7	763	751	12	766	-3	190	56.4
23	1-Hexene		590	595	-5	703	712	-9	702	1	113	63.5
24	<i>trans</i> -2-Hexene		602	598	4	707	709	-2	710	-3	105	67.9
25	<i>cis</i> -2-Hexene		602	601	1	707	708	-1	713	-6	105	68.9
26	<i>trans</i> -3-Hexene		593	595	-2	702	713	-11	701	1	103	67.1
27	2,4-Dimethyl-1-pentene		664	670	-6	778	837	-59	778	0	114	81.6
28	2,3,3-Trimethyl-1-butene		661	655	6	778	820	-42	778	0	117	77.9
29	2,3-Dimethyl-2-pentene		697	697	0	792	792	0	792	0	95	97.4

(Continued on p. 6) 5

TABLE I (continued)

No.	Compound	Graph	Unsulphonated support		Zinc form of resin		AI (3)-(1)	B.p. (°C)			
			Exptl. (1)	Calc. Diff. (1)-(2)	Exptl. (3)	Calc. Diff. (3)-(4)			Calc. Diff. (5)-(3)		
30	4-Methyl-1-hexene		680	7	831	805	26	832	-1	151	86.7
31	1-Heptene		692	2	802	803	-1	797	5	110	93.6
32	trans-2-Heptene		692	-6	789	807	-18	803	-14	97	97.9
33	trans-3-Heptene		693	2	802	799	3	797	5	109	95.7
34	cis-3-Heptene		693	-1	802	798	4	800	2	109	95.8
35	3-Ethyl-2-pentene		695	-1	816	837	-21	829	-13	121	96.0
36	4,4-Dimethyl-cis-2-pentene		665	3	788	785	3	788	0	123	80.4
37	2-Methyl-cis-3-heptene		767	0	927	927	0	927	0	160	112.0
38	1-Octene		796	0	896	896	0	896	0	100	121.3
39	trans-2-Octene		794	0	898	898	0	899	-1	104	124.9
40	cis-2-Octene		794	-2	898	897	1	902	-4	104	125.6
41	trans-3-Octene		794	3	897	896	1	891	6	103	123.3
42	2-Ethyl-1-hexene		789	1	925	925	0	917	8	136	120
43	2,4,4-Trimethyl-1-pentene		750	0	822	822	0	822	0	72	101.5
44	2,4,4-Trimethyl-2-pentene		747	0	823	823	0	823	0	76	104.9

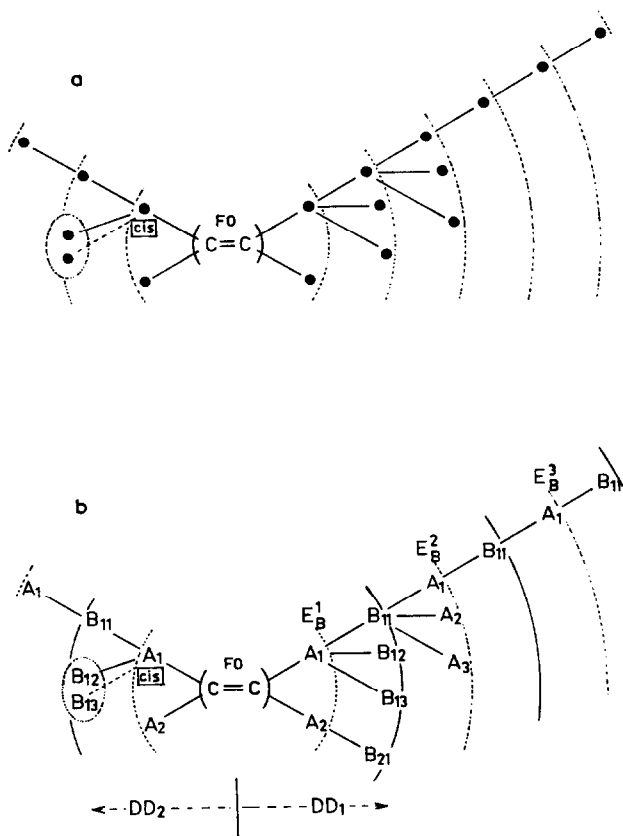


Fig. 2. Characteristic trace (a) of the population of 44 alkenes listed in Table I, and topological site ordering (b) of the molecular environment by the ELCO concept for the superposition of the elementary graphs. Environment is organized in concentric layers of two rows of atoms ( $A_i$ ,  $B_{ij}$ ) labelled  $E_B^1$  for the first,  $E_B^2$  for the second and  $E_B^3$  for the third layer.

a set of ten alkenes, where the  $C=C$  group is taken as the focus. The individual compounds are ordered according to a set of rules involving chain lengths and branching, to ensure that each alkene contributes in a unique way to the trace. Note that there are two development directions,  $DD_1$  and  $DD_2$ , for this set, and that each position in the trace is coded ( $A_i$ ,  $B_{ij}$ ) according to its topological site in the environment of the focus. The  $I$  values are the experimental data for the compounds.

The influence of each topological site is interpreted as a perturbation term,  $P$ . For example, the term  $A_2$  in the first environment in  $DD_1$  is formally equivalent to the difference in behavior of 2-methylpropene and propene. Since this site also appears in several other compounds in this set, its perturbation term is actually the average value obtained by a multiple regression program that takes into account the information from all of the compounds containing this site in the set.

These perturbation terms are the components of a vector,  $\vec{I}(m)$ , that characterizes the information for an experimental population made up of  $m$  compounds. This vector is defined by the basic topology-information relationship

$$\vec{I}(\varepsilon) = \langle \vec{T}(\varepsilon) / \vec{I}(m) \rangle$$

where  $\vec{T}(\varepsilon)$  is the contribution from the environment and  $\vec{T}(\varepsilon)$  is the topological vector of the environment.  $\vec{T}(\varepsilon) = X_1, X_2, \dots, X_j, \dots, X_n$ ; thus  $X_j = 1$  when the  $j$ th site of the environment is occupied and  $X_j = 0$  when it is not.

The set of 44 alkenes used in this work is listed, along with the experimental data, in Table I. The trace of this population is shown in Fig. 2. For practical reasons, sites  $B_{12}$  and  $B_{13}$  in  $DD_2$  have been grouped together as they are simultaneously either present or absent in the series. Only one *cis* parameter is given (relative to the *trans* isomer which is taken as standard for each site for which *cis-trans* isomerization is possible, obviously only in  $DD_2$ ).

## RESULTS AND DISCUSSION

The experimental results are given in Table I. The data for the unsulfonated copolymer (UnS) were published previously<sup>14</sup>. The difference between the retention index on the  $Zn^{2+}$  and on the UnS packing represents the specific interaction,  $\Delta I$ , of the substrate with  $Zn^{2+}$ .

The contrast in behavior of the alkenes on the two packings is shown in Fig. 3, which gives the Kováts retention indices as a function of boiling point. The reten-

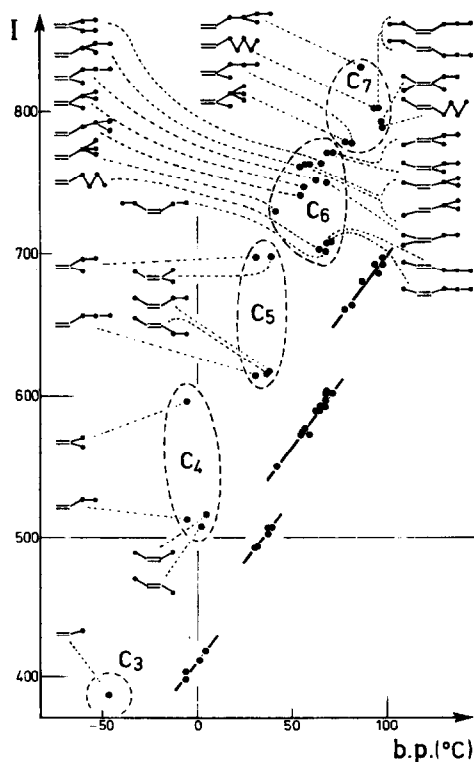


Fig. 3. Retention indices of alkenes on the zinc form of the ion exchanger (-----) and on the corresponding unsulfonated copolymer matrix (——) as a function of the boiling point of the alkene ( $C_3$ – $C_7$ ).



tion data on the UnS packing show a linear relationship with boiling point for each carbon atom subclass. The "roof-tiling" effect<sup>21</sup> seen when the entire set of data is considered is evidence for a specific interaction, nevertheless quite weak, between the alkene double bond and the aromatic groups in the copolymer. The plot of retention index vs. boiling point is a continuous curve only with alkanes on a non-polar, non-specific packing such as graphitized carbon black<sup>12</sup>. The specific interaction with the UnS packing observed in our work is very weak in comparison with the interactions with  $Zn^{2+}$ . As we will emphasize the difference between packings,  $\Delta I$ , this weak contribution of specific interaction with the copolymer matrix is more or less completely eliminated.

The specific interaction between an alkene and  $Zn^{2+}$  is the vertical displacement of this compound from its position on the plot for the UnS packing. It ranges from 100 to 200 I.U. for the  $C_4$ ,  $C_5$  and  $C_6$  compounds. The increase is approximately twice as large for branched alkenes as it is for the linear isomers. This confirms our previous analysis of trends using a smaller set (fifteen compounds) of alkenes and the factor analysis data reduction technique<sup>13</sup>. The branched/linear effect is smallest for the  $C_6$  set, and disappears entirely in the  $C_7$  and  $C_8$  sets.

For the moment, it can be pointed out that the branched/linear distinction found with the lower-molecular-weight alkenes is mainly due to a strong increase in the electronic (inductive) effect with increase of the degree of substitution on the carbon-carbon double bond. This produces a greater net  $\pi$ -charge density on the double bond and hence a stronger charge-transfer interaction between the double bond and the  $Zn^{2+}$ . As the molecular weight increases, this interaction is reduced by the steric interaction of the additional carbon atoms with the surface of the packing, which reduces the ease of overlapping of the  $sp^2$  carbon orbitals and the vacant orbitals of the metal ion. We will now characterize these effects in a quantitative way using topological analysis.

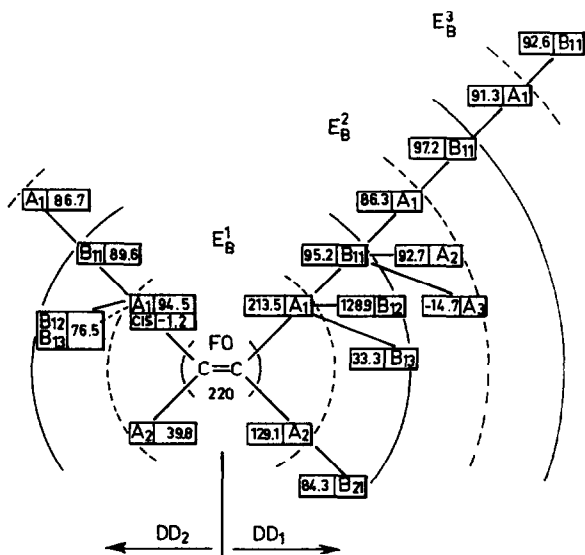


Fig. 4. Topological information diagram for retention on  $Zn^{2+}$ , giving the average contributions of the topological sites.

Alkenes :		2-Methyl-1-Pentene	2-Methyl-2-Pentene	cis-4,4-diMethyl-2-Pentene
Graph				
Topographic information				
Kovats retention index	calc. exp.	744 751	747 749	785 788

Fig. 5. Calculation of predicted retention index on  $Zn^{2+}$ , using the information in Fig. 4.

Fig. 4 gives the results of the topological analysis of the retention of the alkenes on  $Zn^{2+}$ . The contribution of each topological site in the imprint is given in this diagram. These contributions can be added together to give an estimate of the retention of any compound fitting onto the imprint. Fig. 5 shows some examples of the calculations for compounds in the set of alkenes studied. The deviations between the experimental and calculated Kovats indices are given in Table I. In general the agreement is quite good, within the range of experimental uncertainty.

But the main interest of Fig. 4 is to give a quantification of structural effects as an average contribution of the topological sites.

The contribution of the focus ( $C=C$ ) is 220 I.U., somewhat higher than the 200 units expected in the absence of specific interactions (and observed on the UnS column). Much more significant is the 213 I.U. contribution from the first substitution on the double bond (as opposed to 100 I.U. normally for addition of a methylene group). This is due to the increase in  $\pi$ -electron density on the double bond by induction from the methyl group. Further chain lengthening results in retention increments somewhat less than 100 I.U. per methylene group; the average increment is about 90 I.U.

The effect of branching is more complicated. A second substitution on the same side of the double bond gives an enhanced retention of 129 I.U., well above 100 but much less than the contribution of the initial substitution. The increase in  $\pi$ -electron density by induction from this substituent results in stronger adsorption onto  $Zn^{2+}$ , but this factor is counterbalanced by increased steric hindrance of the approach of the double bond to the active site.

Branching one carbon atom away from the double bond (site  $B_{12}$ ) contributes an enhanced  $\pi$ -electron density by induction, but of course less than a substituent directly on the double bond. At the same time, steric hindrance of the adsorption process by this latter substituent is much greater. Hence the overall effect on adsorption of substitution in site  $B_{12}$  is about the same as that for site  $A_2$ . It is interesting to note that site  $B_{12}$  contributes 46 I.U. more to adsorption onto  $Zn^{2+}$  than onto  $Ni^{2+}$  (ref. 14). This underlines the enhancement of adsorption onto  $Zn^{2+}$  produced by chain branching, which we pointed out earlier.

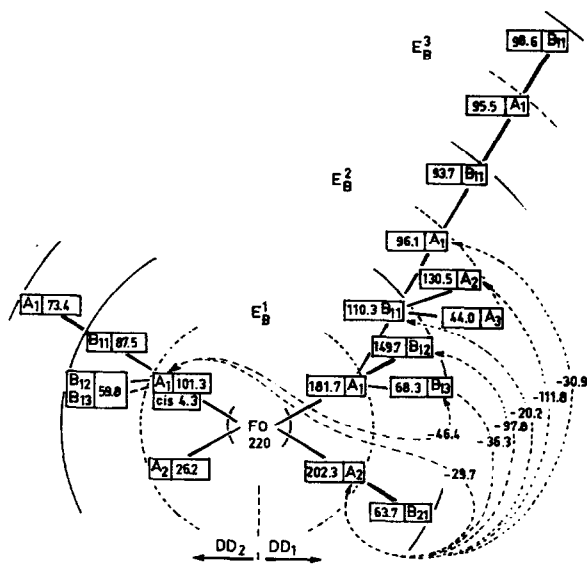


Fig. 6. Topological information diagram on  $Zn^{2+}$  showing seven interaction parameters. The presence of branching at the  $A_1$  and  $B_{11}$  positions greatly reduces the enhancement of retention by the inductive effect of carbon groups attached directly to the double bond. (This diagram corresponds to correlation no. 3 in Table I.)

The influence on adsorption of branching at a still more distant point ( $A_2$  in the second environment) is of the same magnitude as chain lengthening; the inductive effect weakens with distance from the focus of the molecule.

A second branch at a particular point in the chain gives a very small increase in adsorption. This indicates that the steric effect of the *tert.*-butyl group overwhelms the electronic effect of the added carbon atom. The effect is still larger with a second branching located one carbon atom farther from the double bond.

The importance of the steric effect on adsorption is underlined by the results for the third and fourth substituents on the double bond (in direction  $DD_2$ ). The contributions are only 95 and 40 I.U., respectively, a reflection of the difficulty of adsorption of a highly crowded double bond onto  $Zn^{2+}$ , even with the considerably increased  $\pi$ -electron density that these substituents provide.

A continuation of chain lengthening in the  $DD_2$  direction from the focus produces retention increments the same as those observed in the  $DD_1$  direction away from the double bond, about 90 I.U. Branching to produce a *tert.*-butyl group in  $DD_2$  (2,4,4-trimethyl-2-pentene) gives a contribution of only 76 I.U. for the two sites  $B_{12}$  and  $B_{13}$  combined. This illustrates an important deviation from additivity of the effects of individual sites, in  $DD_1$  the same groups produced a retention increment twice this value.

This deviation from additivity is clearly shown in Fig. 6, which gives the supplementary contributions due to the simultaneous presence of various pairs of sites. These interactions were mainly calculated with  $A_2$  as one of the sites in each pair. All of these parameters of interaction have a negative contribution to retention, an indication of the steric influence of multiple branching on the specific adsorption of

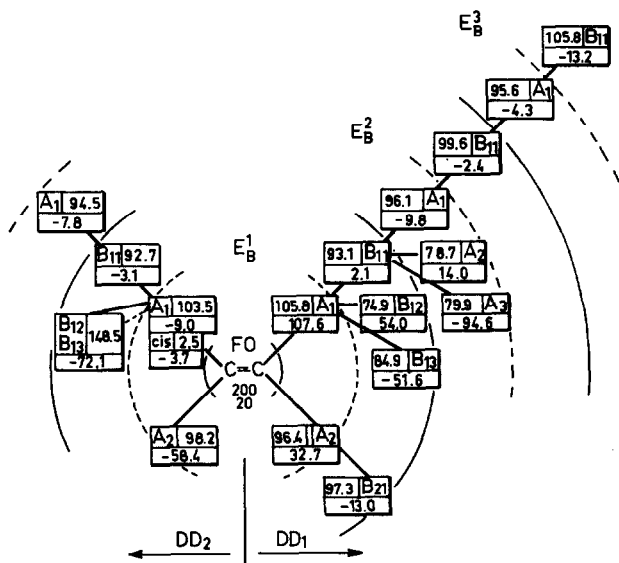


Fig. 7. Extent of specific interaction with  $Zn^{2+}$ . The lower values represent the difference between the contribution on  $Zn^{2+}$  (Fig. 4) and that on the unsulfonated packing (upper values for each position).

the alkenes. Notice the interaction contribution of  $-98$  I.U. for the presence of  $A_2$  and  $B_{12}$  together; much of the positive inductive effect on adsorption of the individual substitutions is counteracted by the crowding when both are present. Likewise, the crowding effect of  $-112$  I.U. when  $A_2$  in the first environment ( $E_B^1$ ) and  $A_2$  in the second environment ( $E_B^2$ ) are both present is quite substantial.

This diagram also gives the reciprocal influence of simultaneous substitution in  $DD_1$  and  $DD_2$ :  $-46$  and  $-30$  I.U. for  $A_1$  in  $DD_2$  paired with  $A_1$  and  $A_2$  in  $DD_1$ , respectively. This steric effect is less than that noticed with disubstitution on the same side of the double bond due to the distance between the two groups and the planarity of the ethylenic system.

Fig. 7 shows the separated contributions of the unsulfonated copolymer matrix and the specific adsorption on  $Zn^{2+}$ . The latter corresponds to the topological analysis of the  $\Delta I$  values given in Table I. They can be compared with the results for  $Ni^{2+}$  previously published (Fig. 8 of ref. 14).

Fig. 7 shows clearly the positive contribution of a monosubstitution on ethylene ( $+108$  I.U.) and also the somewhat smaller contribution ( $+33$  I.U.) for disubstitution on ethylene. It also shows the positive influence of the first step of branching ( $54$  and  $14$  I.U. for  $B_{12}$  and  $A_2$  in the second environment). This also confirms the negative contribution to adsorption of chain lengthening after  $B_{11}$  (after butene-1) in  $DD_1$  or in the second development direction. Chain branching corresponding to a third methyl group also results in a substantial negative specific interaction of  $-52$  and  $-95$  I.U. in the cases studied in the first development direction, and an equally strong negative contribution in  $DD_2$ . It is also interesting to note the trend in the specific interaction with  $Zn^{2+}$  with increasing substitution on the double bond:  $+108$ ,  $+33$ ,  $-9$  and  $-58$  respectively for the four degrees of substitution.

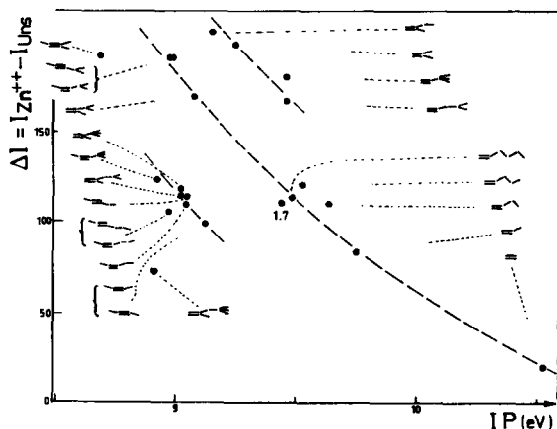


Fig. 8. Net contribution of  $Zn^{2+}$  ( $\Delta I = I_{Zn} - I_{Uns}$ ) as a function of the ionization potential (IP) of the alkene. The competition between the steric effect of branching (creating isopropyl and isobutyl-like groups) and the polar effect is brought out by comparisons of  $\Delta I$  values at constant IP.

The unique behavior of  $Zn^{2+}$  is also brought out in Fig. 8, which shows the specific retention due to  $Zn^{2+}$  as a function of the ionization potential of the alkene. In the absence of geometric and steric effects, the ionization potential and strength of the  $Zn^{2+}$ -alkene interaction should show a consistent inverse relationship. In fact, the data show considerable scatter, giving a range of  $\Delta I$  values for a particular ionization potential. The compounds with the smallest  $\Delta I$  are either 2-alkenes (rather than 1-alkenes) or are highly branched. Both cases involve more steric resistance to formation of the charge transfer between the  $\pi$  bond of alkenes and the empty orbitals of the  $Zn^{2+}$  than when the double bond is exposed at the end of the hydrocarbon chain and is not protected by extensive branching.

## CONCLUSIONS

We have demonstrated the utility of DARC topological analysis for the quantitative study of adsorption. This data-processing technique allows calculation of contributions from individual structural units in a molecule to its specific interactions with an adsorbent. While our example has involved a series of alkenes, the technique is quite general and could be applied equally well to data for any set of compounds of sufficient size to allow adequate statistical precision. In this work 44 compounds were used to obtain 19 structural parameters and 7 interaction parameters; with careful selection, a smaller number of compounds would have been sufficient.

The GSC method offers several advantages for studying adsorption onto metal ions. Data can be obtained rapidly and for much more complicated molecules than are conveniently studied by many other methods, such as the spectroscopic methods usually used in catalysis studies, and are readily converted into a form (Kováts retention indices) to which powerful means of extracting information (such as topological analysis) can be easily applied.

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