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ELECTRONIC STRUCTURE OF ORGANOMETALLIC COMPOUNDS

XV *. LITHIUM AS LIGAND IN TRANSITION METAL COMPOUNDS; AN INDO MO INVESTIGATION

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Summary

The electronic structures of transition metal-olefin complexes with lithium containing ligands have been investigated by means of semiempirical MO calculations of the INDO-type. It is shown that the olefinic ligands are bonded to the 3*d* center (Ni/Fe) via a metal to ligand charge transfer. Lithium acts as an electron rich partner due to electron transfer from ethylenediamine. The charge excess at the Li side is transferred partially to the π^* acceptor orbitals of the olefinic system but is also used in an electron rich Li—M—Li moiety (polarized as $M^{\delta+}$ (M = Ni, Fe) and $Li^{\delta-}$) coupled by means of electrostatic Coulomb interaction. A detailed investigation of the MO wave functions shows an enhanced metal olefin interaction and significant olefin Li coupling. The relevance with other ligands with donor properties is discussed. Additionally the bonding capability of the Li-ethylenediamine moiety in compounds without 3*d* centers is discussed and compared with that in the transition metal Li complexes.

Introduction

Recently new synthetic routes for the preparation of olefinic transition metal complexes with lithium containing ligands have been published [2]. Four examples of these new species are: $[Li(TMEDA)]_2Ni(nor)_2$ (**1**), $[Li(TMEDA)]_2$-Ni(CDT) (**2**), $[Li(TMEDA)][\pi\text{-}C_5H_5]Fe(C_2H_4)_2$ (**3**) and $[Li(TMEDA)]_2Fe$-$(C_2H_4)_4$ (**4**). In these formulas TMEDA denotes *N,N,N',N'*-tetramethylethylenediamine, CDT denotes all-*trans*-1,5,9-cyclododecatriene and nor represents norbornene. The main structural features of **1**—**4** [2] are given in Fig. 1.

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* For part XIV see ref. 1.

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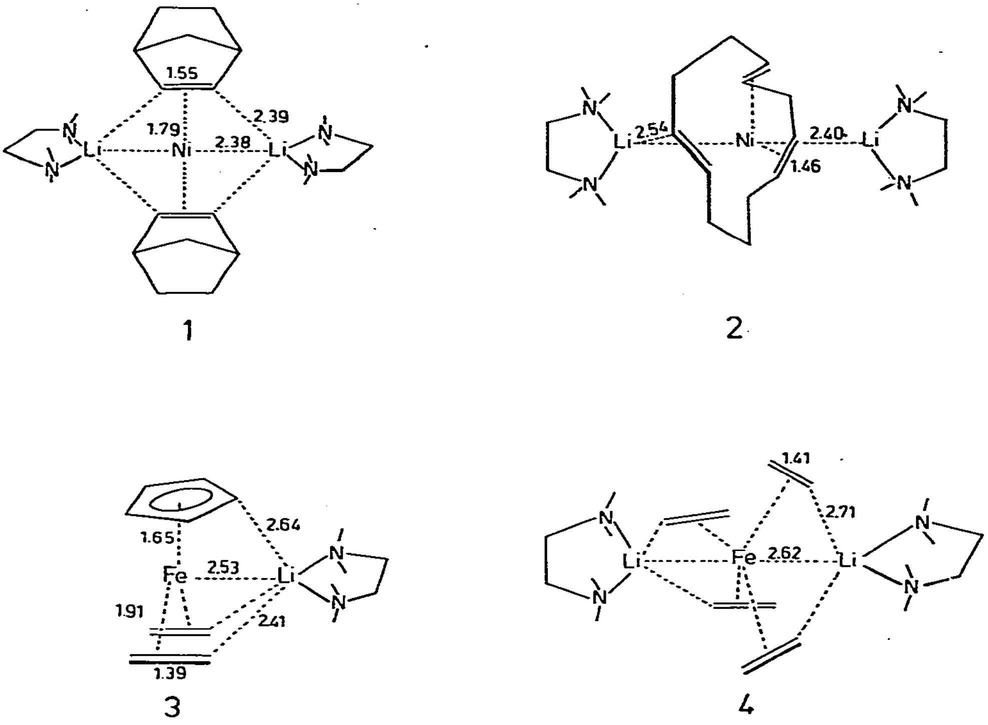
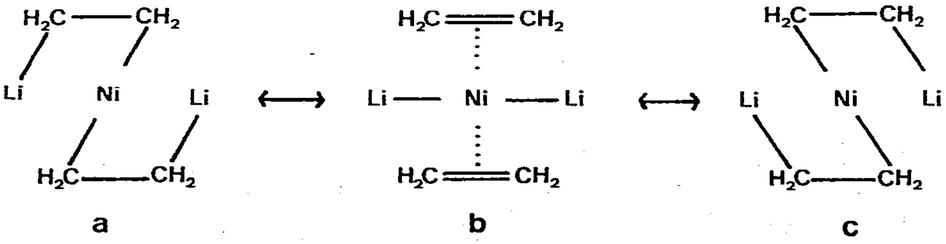


1 2

3 4

Fig. 1. The most important geometrical features in the Li complexes **1—4**.

The complexes have been described as non-polar because of their solubility in benzene and toluene. The bond between Ni and Li has been regarded as covalent but strongly polarized, with a surplus of positive charge at Li and a δ^- charge at Ni. Of special interest is the finding of Li—Ni and Li—Fe distances between 2.4 and 2.6 Å, a lengthening of the C—C double bond to 1.4—1.55 Å, and a distance of 2.4—2.7 Å between the π-ligands and Li. These findings [2] led to the following valence bond formulation for **1**:



In view of the electron rich nature of the ligands on Li such a polarization of the Li—Ni bond seemed to us peculiar. We have therefore investigated the electronic structure of some of the above-mentioned transition metal Li complexes (**1—4**) by means of quantum chemical calculations. As the computational framework we used a recently developed INDO Hamiltonian for the valence electrons [3] suitable for use with transition metal complexes. The calculated atomic

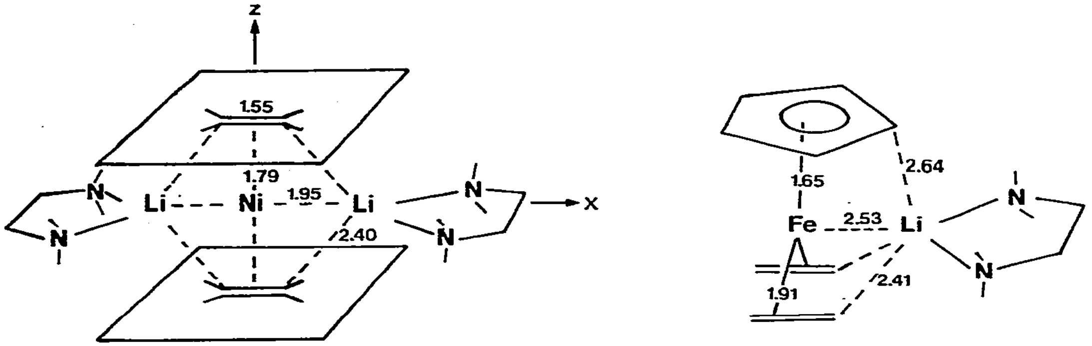


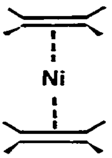
Fig. 2. Geometrical parameters in the model systems **5** and **6**.

populations and net charges derived by our INDO model are usually close to the values derived by ab initio calculations of high sophistication (double-zeta quality).

To save computer time we selected diethylenenickel-bis(lithiumethylenediamine) (**5**) as the model system for the norbornene complex **1** and diethylenecyclopentadienyliron-lithiumethylenediamine (**6**). The latter compound corresponds to **3** with H atoms instead of CH_3 groups. The most important geometrical parameters used for **5** and **6** are shown in Fig. 2.

Model calculations on 5

To understand the nature of the bonding in **5** we first consider the electronic structure of the molecular fragments **7** to **9**. The interaction in **7** has been analyzed by Rösch and Hoffmann using the extended Hückel method [4].



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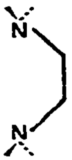

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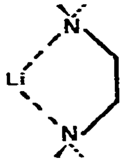
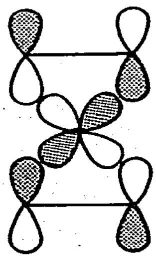
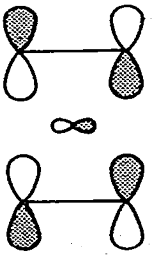


9

These authors showed that a $3d_{xz} - b_{2g}(\pi^*)$ interaction (see below) leading to a charge transfer from the metal to the ligand is essential for the bonding in **7**. For symmetry reasons the corresponding $b_{3u}(\pi^*)$ linear combination has no $3d$ partner to interact with, and thus yields the lowest unoccupied MO of **7**.



b_{2g}



b_{3u}

TABLE 1

CALCULATED NET CHARGES IN DIETHYLENENICKEL (7), ETHYLENEDIAMINE (8), LITHIUMETHYLENEDIAMINE (9) AND WATER AS INDICATED BY THE INDO METHOD

Compound	Atom	Net charge
7	Ni	0.51258
	C	−0.35852
	H	0.11519
8	N	−0.42477
	C	−0.07615
	H_N	0.17631
	H_C	0.07415
9	Li	−0.66497
	N	−0.15834
	C	−0.10718
	H_N	0.19504
	H_C	0.10396
H_2O	O	−0.65279
	H	0.32639

The metal to ligand charge transfer in **7** is exemplified in the calculated net charges according to Mulliken [5] and the Wiberg bond indices [6] listed in Tab. 1 and 2. We predict a positive charge of 0.51 for the metal, which means that 0.13 electrons have been transferred to each of the carbon atoms of the two ethylene moieties. This donor acceptor interaction between Ni and the ligands results in a Ni—C bond index of 0.24 (see Table 2).

A comparison between calculated net charges and bond indices of the uncomplexed ethylenediamine system (**8**) and the corresponding lithium complex (**9**) indicates predominantly a charge drift from the N centers to the Li atom. According to the INDO calculation 0.66 *e* are transferred from the diamine to

TABLE 2

CALCULATED WIBERG BOND INDICES IN DIETHYLENENICKEL (7), ETHYLENEDIAMINE (8), LITHIUMETHYLENEDIAMINE (9) AND WATER AS INDICATED BY THE INDO METHOD

Compound	Bond	Bond index
7	NiC	0.2412
	CC	1.7090
8	NC	0.9974
	CC	0.9881
	CH	0.9894
	NH	0.9660
9	LiN	0.4585
	NC	0.9928
	CC	0.9871
	CH	0.9766
	NH	0.9269
H_2O	OH	0.8934

TABLE 3

CALCULATED NET CHARGES IN DIETHYLENENICKEL-BIS(LITHIUMETHYLENEDIAMINE) (5) AND THE DIHYDRATE OF DIETHYLENENICKEL (10) AS INDICATED BY THE INDO METHOD

Compound	Atom	Net charge
5	Ni	0.77597
	$C_{ethylene}$	−0.57144
	$H_{ethylene}$	0.16071
	Li	−0.56619
	N	−0.16127
	$C_{diamine}$	−0.10899
	H_N	0.19761
	H_C	0.10664
10	Ni	0.54459
	$C_{ethylene}$	−0.37898
	$H_{ethylene}$	0.10728
	O	−0.61283
	H_{H_2O}	0.33474

the metal (Li) site leading to a negative net charge at Li (Table 1).

Similar effects have been encountered in various complexes with Li [7,8]. In the system CH_3Li/CH_3NH_2 a charge transfer of 0.27 *e* from the amine part to CH_3Li has been calculated [9]. This result is in line with our findings, in that in **9** there are two NH_2 fragments which transfer approximately twice the amount of electron density to the Li center.

The calculated net charges and Wiberg bond indices of our model system **5** are collected in Tables 3 and 4. It is seen that the Li atoms also show a remarkable charge excess in the Ni complex **5** (net charge −0.56 *e*) while the electron density at the Ni center is reduced (net charge 0.78) compared with that in **7**. A comparison of the calculated net charges for **5** and **9** in Tables 1 and 3

TABLE 4

CALCULATED WIBERG BOND INDICES IN DIETHYLENENICKEL-BIS(LITHIUMETHYLENEDIAMINE) (5) AND THE DIHYDRATE OF DIETHYLENENICKEL (10) AS INDICATED BY THE INDO METHOD

Compound	Bond	Bond index
5	NiC	0.2671
	NiLi	0.0381
	$CC_{ethylene}$	1.0728
	$LiC_{ethylene}$	0.2599
	LiN	0.4512
	NC	0.9935
	$CC_{diamine}$	0.9868
	CH	0.9757
	NH	0.9319
10	NiC	0.2478
	NiO	0.0280
	CC	1.3727
	OC	0.0212
	OH	0.8854

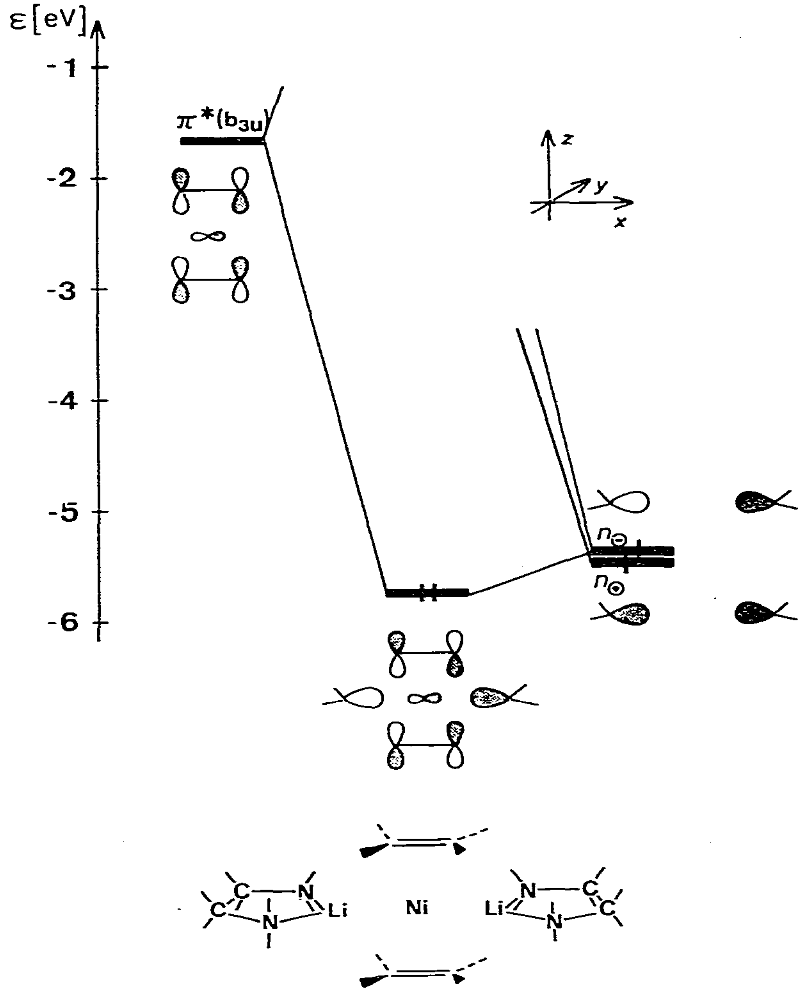


Fig. 3. Qualitative interaction diagram between the b_{3u} acceptor of **7** and the lithiumethylenediamine ligands. *The $n(+)$ combination is destabilized by the occupied $\pi(a_{1g})$ linear combination.*

reveals that electron density has been transferred from the Li atoms to the carbon atoms. The net charge at the C centers has been increased from —0.36 in **7** to —0.57 in **5**. The indicated charge transfer can be traced back to an interaction between the LUMO of **7**, the $b_{3u}(\pi^*)$ orbital, localized at the ethylene fragments and the $b_{3u}(n(-))$ linear combination centered at the Li atoms (see Fig. 3). As a result of this interaction we predict a Li—C bond index of 0.26, which is close to that found for the Ni—C bond, and we find a decrease of the C—C bond index from 1.71 for the uncomplexed double bond to 1.07.

A comparison between the atomic populations at the Li center in **9** and **5** (Table 5) indicates significant charge reorganization due to the interaction between **9** and **7**. While the electron density of $2s$ and $2p_x$ is reduced due to the charge transfer into the $b_{3u}(\pi^*)$ acceptor orbital, the $2p_z$ AO of Li shows an increase of electron density caused by a transfer from the occupied π-orbitals

TABLE 5

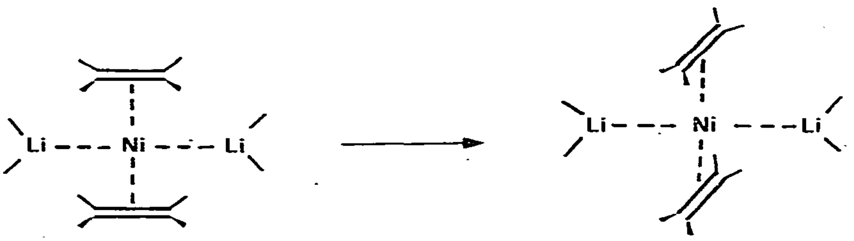
ATOMIC POPULATIONS OF Li IN LITHIUMETHYLENEDIAMINE (9) AND THE DILITHIUM DERIVATIVE OF DIETHYLENENICKEL (5)

AO	9	5
$2s$	0.7944	0.4217
$2p_x$	0.5595	0.4190
$2p_y$	0.2616	0.3682
$2p_z$	0.0495	0.3573

of the olefinic part to the empty $2p_z$ orbital of Li (see Table 5).

A comparison of the Ni—carbon bond indices between **5** and **7** (Tables 2 and 4) confirms that the covalent interaction is increased because of the lithiumethylenediamine moieties. This increased interaction has its origin in the lowering of the ethylene $b_{2g}(\pi^*)$ orbital of the Li complex **5** as the charge transfer from Li to ethylene results in a stabilization of the π^* orbitals (the CC distances are enlarged). Thus the interaction between Li and the ethylene ligands in **5** causes an enhanced interaction between the Ni $3d$ orbitals and the ethylene part, accompanied by a charge transfer from the transition metal center to the π ligands. This is apparent from the Ni net charges calculated for **5** and **7** (see Tables 1 and 3). The bond index between Li and Ni is predicted to be 0.04 (see Table 4), a relatively small value. The stabilizing interaction between Ni and Li is therefore dominated by an electrostatic attraction. A similar situation was encountered in the case of hydrogen bonds [10] and in the half sandwich CpNiNO [11,12].

The Ni coordination in the model system **5** is square planar with respect to the ethylene moieties. This arrangement is stabilized by two Li atoms. The four carbon centers of the ethylene ligands and the Li atoms form a planar coordination sphere in **5**. The well known octahedral symmetry for Ni [13] could be achieved by rotating the olefinic ligands by 90° as indicated below. Here the carbon centers are in equatorial positions in the complex while the two Li atoms occupy the axial ones. However, this rotation would lead to the loss of bonding interaction between Li and the olefin.



planar

octahedral

Examples of NiL_4 complexes coordinated by two electron rich ligands L′ (L′ = pyridine, ethanol, H_2O) are legion in the chemistry of Ni [13]. If our bonding model for **1** and **5** is valid, diethylenenickel derivatives with two donor groups should show a similar behaviour to **5** with respect to calculated net

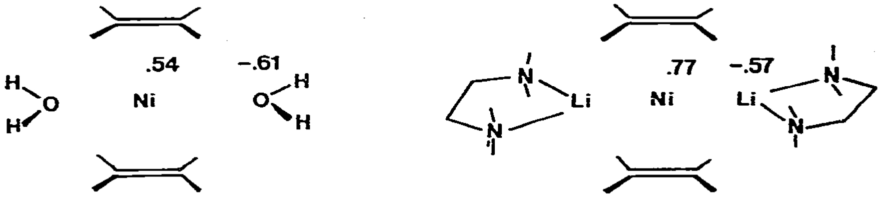
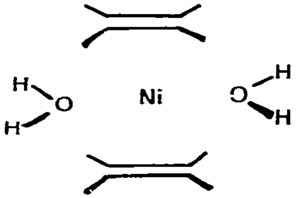


Fig. 4. Net charges at the 3*d* center and the heteroligand (O or Li) in **5** and **10** according to an INDO calculation.

charges and bond indices. The INDO results for the dihydrate **10**, collected in Tables 1 to 4 confirm this assumption. There is a charge transfer from the water ligands to the olefin π-units, while the interaction between Ni and O is mainly electrostatic. As a result of the larger energy gap between the donor functions of H_2O and the $b_{3u}(\pi^*)$ acceptor, the interaction is reduced compared to that in model **5**. The INDO calculation predicts that each H_2O group transfers 0.06 *e* to the ethylene fragments. The calculated bond index for the olefinic double bond in **10** (1.37) is predicted to lie in between the double bond in **7** (1.71) and **5** (1.01). The Wiberg bond indices for the Ni—Li and Ni—O bond are predicted to be of similar size (0.04 and 0.03, respectively) as well as the calculated net charges shown in Fig. 4.



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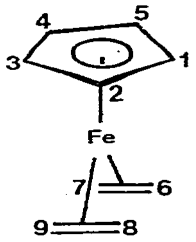
Model calculations on 6

To study the influence of Li(TMEDA) upon the fragment π-cyclopentadienyl-iron-diethylene (**11**) we compared the calculated net charges and Wiberg bond indices of **6** and **11** in Tables 6 and 7. The results for the hydrate **12** are also given. It is evident that the gross features derived for **5**, **7** and **10** are also valid



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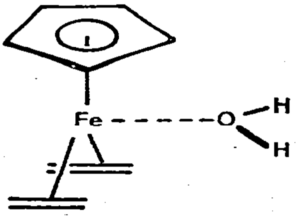

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TABLE 6

CALCULATED NET CHARGES IN DIETHYLENECYCLOPENTADIENYLIRON (11), THE CORRESPONDING LITHIUMETHYLENEDIAMINE (6) AND THE MONOHYDRATE (12), AS INDICATED BY THE INDO METHOD [a]

Compound	Atom	Net charge
11	Fe	0.53950
	C(1)	−0.24252
	C(2)=C(5)	−0.15213
	C(3)=C(4)	−0.20198
	C(6)=C(8)	−0.35829
	C(7)=C(9)	−0.33813
6	Fe	0.35896
	C(1)	−0.17991
	C(2)=C(5)	−0.16312
	C(3)=C(4)	−0.18303
	C(6)=C(8)	−0.39336
	C(7)=C(9)	−0.36767
	Li	−0.53266
	N	−0.19057
	$C_{diamine}$	−0.10700
12	Fe	0.56685
	C(1)	−0.18132
	C(2)=C(5)	−0.18886
	C(3)=C(4)	−0.20522
	C(6)=C(8)	−0.33294
	C(7)=C(9)	−0.37535
	O	−0.62926
	H_{H_2O}	0.33863

[a] The numbering refers to **11**.

in the case of the iron system. In contrast to the Ni complex **5**, however, in the iron complexes the charge deficiency at the metal center is not increased by adding the ethylenediaminelithium ligand (see Table 6), and is, in fact, lowered from 0.54 to 0.36. The net charges and bond indices in Table 6 and Table 7 indicate that Li acts as a bridge, allowing a charge transfer from the cyclopentadienyl unit to the two ethylene molecules. The electron density at the carbon atoms is reduced in C_5H_5 but increased in both C_2H_4 fragments. This redistribution leads to a smaller bond index for the olefinic bond in **6** (1.27) compared to that in **11** (1.35). As in the case of **5** the bond index between the metal and the carbon atoms is increased in the presence of the diaminelithium ligand. This enhanced interaction is predominantly between Fe and the carbon centers of the ethylene units. The bond indices for the bonds Li—C(1), Li—C(6) and Li—C(8) are considerable, and thus justify describing the coordination number of Li in **3** as 5. In a situation analogous to that with the Ni complex, there is a small bond index for Li—Fe and a δ^+ charge for Fe and a δ^- polarization for Li.

Discussion of the results

The various bonding interactions derived in detail for **5** and **6** can be extended in a straightforward manner to the more complex organometallics **1** to **4**. Each Li center exhibits a roughly tetrahedral (**1**, **2**) or a fivefold (**3**, **4**)

TABLE 7

CALCULATED WIBERG BOND INDICES IN DIETHYLENECYCLOPENTADIENYLIRON (11), THE CORRESPONDING LITHIUMETHYLENEDIAMINE (6) AND THE MONOHYDRATE (12), AS INDICATED BY THE INDO METHOD [a]

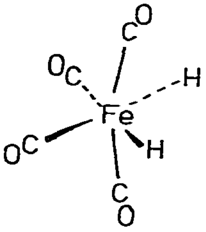
Compound	Bond	Bond index
11	FeC(1)	0.1324
	FeC(2)=FeC(5)	0.2329
	FeC(3)=FeC(4)	0.1643
	FeC(6)=FeC(8)	0.3713
	FeC(7)=FeC(9)	0.3714
	C(1)C(2)=C(1)C(5)	1.3270
	C(2)C(3)=C(4)C(5)	1.2668
	C(3)C(4)	1.3676
	C(6)C(7)=C(8)C(9)	1.3487
6	FeC(1)	0.1819
	FeC(2)=FeC(5)	0.2535
	FeC(3)=FeC(4)	0.2035
	FeC(6)=FeC(8)	0.4597
	FeC(7)=FeC(9)	0.5009
	FeLi	0.0449
	C(1)C(2)=C(1)C(5)	1.2608
	C(2)C(3)=C(4)C(5)	1.3092
	C(3)C(4)	1.3137
	C(6)C(7)=C(8)C(9)	1.2711
	LiC(1)	0.2656
	LiC(6)=LiC(8)	0.2143
	LiN	0.4076
	NC	0.9936
	CC_{diamine}	0.9855
12	FeC(1)	0.1243
	FeC(2)=FeC(5)	0.2287
	FeC(3)=FeC(4)	0.1596
	FeC(6)=FeC(8)	0.3654
	FeC(7)=FeC(9)	0.3657
	FeO	0.0441
	C(1)C(2)=C(1)C(5)	1.3317
	C(2)C(3)=C(4)C(5)	1.2438
	C(3)C(4)	1.3902
	C(6)C(7)=C(8)C(9)	1.3372
	OC(1)	0.0099
	OC(6)=OC(8)	0.0102
	OH	0.8784

[a] The numbering refers to **11**.

coordination due to the Li—C interaction. The strong covalent coupling between Li and N on one side and Li and C on the other is caused by a transfer of electron density from the diamine ligand via Li to the π^* acceptor orbitals of the olefinic ligand. Each Li atom carries a significant excess of electrons leading to the formation of an electron rich transition metal—lithium arrangement stabilized mainly by electrostatic forces. The Li ligands furthermore lead to an enlargement of the covalent interaction between the 3*d* center and the olefinic ligand. In terms of the valence bond structures **a** to **c** presented for **1** and **2** in the beginning, this means that structure **b** plays a minor role.

The interaction derived for **5** and **6** must be carefully distinguished from the stabilization in ionic Ni^0 π-systems where Li$^+$ atoms are tetrahedrally coordinated by complexing groups. In these cases the separation between the transition metal and Li is in the order of 7 Å [2,14] and typical ionic properties are reported for these species.

The complexes **1**—**4** and simplified models **5** and **6** are reminiscent of the hydride analogues Fe(CO)$_4$H$_2$ (**13**) and CpCr(CO)$_3$H (**14**). The analogy between



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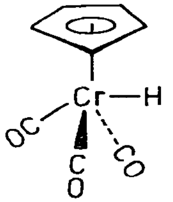

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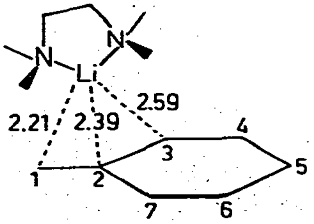
5 and **13** as well as **6** and **14** must remain only qualitative. Its limitations are evident upon comparing the gross structural features of both pairs: in **5** the Li ligands occupy axial positions *trans* to each other while in **13** the H atoms are found *cis* to each other [15]. In case of **14** a further CO ligand is needed to compensate for the lower number of 3*d* electrons in the case of Cr compared with Fe in **6**. According to our INDO model a net charge of —0.15 is predicted for the H centers of **13** while for the 3*d* center a positive charge of 0.23 is calculated. For **14** INDO predicts a charge of 0.02 for the H center.

Investigations on related systems

Recently the system Li$^+$—H$_2$O was investigated by high quality ab initio calculations [16]. It was found that 0.06 *e* are transferred from the H$_2$O donor to the Li acceptor. This result must be compared with that of an INDO calculation which indicates that 0.21 *e* are transferred. This comparison suggests that INDO overestimates the absolute values, but the direction of the charge transfer is correctly reproduced.

Our prediction of a significant Li—C interaction in all investigated species is substantiated by ab initio calculations of Schleyer and coworkers [17].

In connection with our analysis the results on the lithium salt of benzyl anion associated with one TMEDA (**15**) unit might be of interest. In this example the distance between Li and three atoms of the benzylic moiety is found between 2.2 and 2.6 Å [18,19]. The calculated net charges in the benzylanion (**16**) and **9**$^+$ are listed in Table 8, together with the INDO charges in **15**.



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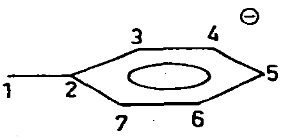

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TABLE 8

CALCULATED NET CHARGES IN THE LITHIUMETHYLENEDIAMINE CATION (9^+), THE BENZYL ANION (16) AND THE 1/1 ADDUCT (15) AS INDICATED BY THE INDO METHOD

Compound	Atom	Net charge
9^+	Li	0.35740
	N	−0.25425
	C	−0.10456
16	C(1)	−0.73133
	C(2)	0.25479
	C(3)=C(7)	−0.36260
	C(4)=C(6)	−0.02285
	C(5)	−0.40088
15	C(1)	−0.51867
	C(2)	0.25373
	C(3)	−0.26874
	C(4)	0.00795
	C(5)	−0.31014
	C(6)	−0.00999
	C(7)	−0.28675
	Li	−0.49360
	N_{av} [a]	−0.16542
	C_{av}	−0.10960

[a] av means averaged net charges in the lithiumethylenediamine fragment.

It is seen that Li has a significant charge deficit in the cationic ethylenediaminelithium arrangement. This deficit is removed by complexation of the benzyl anion **16**. As a result of the charge transfer to the Li atom a surplus of 0.49 *e* is calculated. For **15**, INDO predicts a charge excess of about 0.17 *e* in the benzyl fragment and the corresponding deficit in the diaminelithium part. As Li is nearly tetrahedrally coordinated by electron rich centers (diamine N-atoms, C(1)C(3)), a strong charge transfer to Li takes place. The Li—C bond indices to C(1), C(2) and C(3) of 0.53, 0.11 and 0.29, respectively, indicate a covalent interaction between the carbon centers of the organic π-system and the alkali atom. The Wiberg indices show that Li acts as bridge between the allylic subunit C(1)/C(3), while the coupling to the central C(2)-atom is less important. In the 3*d* complexes the function of Li is threefold. It acts as donor for the organometallic residue, has a bridging function for the complexed ligands and leads to an electrostatic Coulomb stabilization in an electron rich arrangement. In **15** Li has typical acceptor properties, resulting in a covalent interaction between both fragments. In a situation analogous to that in the transition metal complexes, Li forms multi-center bonds to the coordinated carbon centers.

Calculations

The INDO model used is described in detail in a separate publication [3]. The geometrical parameters used for **5** and **6** are shown in Fig. 2. The bond lengths and angles for the other systems were taken from the literature [2,15, 18,19,20] or are standard values [21].

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