formation, anion formation, ionization potentials, and other properties of these small-ring systems. They have provided useful insights into the structures and charge distributions of small-ring compounds and the ions derived from them. They have also provided an impetus for futher experimental studies.

We are in the process of examining substituent effects on the bicyclo[1.1.1]pentyl 1-cation (**2**) and the bicyclo[1.1.1]pentyl 1-radical (**5**) both experimentally and theoretically. In the case of the radical, we are especially interested in the effect of substituents on the spin density distribution. We also are studying the transition states for the ring opening of both the cation and the radical.

Calculations

The ab initio calculations at Yale (HF and MP2 optimizations, MP3 larger basis set) were carried out using GAUSSIAN 90 and a Trace 7/200 computer, and those at Erlangen (MP4) were carried out using GAUSSIAN 88 and a Convex computer. The atoms in molecules charge distributions were obtained using PROAIM; the natural population analysis was carried out using a modified GAUSSIAN 88 program, Convex version, installed by Dr. Alan Reed, and the NMR chemical shifts were estimated using the IGLO program, Convex version, as supplied by Dr. Michael Schindler.

Acknowledgment. The investigation at Yale was supported by a grant from the National Science Foundation. Financial support at Erlangen was provided by the Deutsche Forschungsgemeinschaft, the Fonds der Chemischen Industrie, and the Convex Computer Corp. C.M.H. gratefully acknowledges the Fannie and John Hertz Foundation for a predoctoral fellowship.

Registry No. 1, 311-75-1; **2**, 22907-79-5; **3**, 141398-00-7; **4**, 37908-33-1; **5**, 71490-77-2; **6**, 141398-01-8; **7**, 141435-29-2; cyclopropane, 75-19-4; cyclopropane anion, 2417-82-5; cyclopropane radical cation, 34496-93-0; cyclobutane, 287-23-0; cyclobutane cation, 19067-43-7; cyclobutane radical, 4548-06-5; bicyclo[1.1.0]butane, 157-33-5; bicyclo-[1.1.0]butane 1-anion, 96666-81-8; bicyclo[1.1.0]butane 1-radical, 95694-51-2; bicyclo[1.1.0]butane radical cation, 85915-57-7; [1.1.1]-propellane, 35634-10-7; [1.1.1]propellane radical cation, 141398-02-9; isobutane, 75-28-5; *tert*-butyl cation, 14804-25-2; *tert*-butyl radical, 1605-73-8; methane, 74-82-8; methyl cation, 14531-53-4; methyl ion, 15194-58-8; methyl radical, 2229-07-4; hydrogen, 12385-13-6; hydride ion, 12184-88-2.

Supplementary Material Available: MP2/6-31G*-optimized geometries in Z-matrix format (4 pages). Ordering information is given on any current masthead page.

An Energy Criterion for Determining Relative σ and π Contributions in Transition Metal–Carbonyl Bonding

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Received November 20, 1991

Abstract: In this paper a new criterion is presented for determining the contribution of a particular class or group of orbitals to a chemical bond. The new criterion is the diatomic energy contribution of particular orbitals in a particular bond (any diatomic atom pair) to the total molecular energy. It is a unique feature of NDO (neglect of diatomic overlap) type procedures that the total energy can be divided entirely into monatomic and diatomic energy terms. Here this method is applied to determining the contribution of σ and π orbitals to the cohesive energy of CO adsorbed on a cluster of 12 iron atoms. While recent theoretical calculations have tended to downplay the role of the σ orbitals in metal–CO bonding, the results here show that the largest contribution to the stability of the metal–carbon bond is provided by the σ electrons.

Introduction

There is great interest in the adsorption and reaction of CO on transition metal surfaces. In addition, the hydrogenation of CO to hydrocarbon and alcohol fuels is of considerable commercial interest. Iron in various forms is one of the most commonly used Fischer–Tropsch catalysts and so is chosen for this work. Because CO adsorbs strongly on many clean metal surfaces, it is readily studied by many physical techniques, so there is a wealth of data for chemisorbed CO. It has been shown that a simple molecular orbital model would qualitatively explain variations in adsorbed C–O stretching frequencies from one metal to another and the effect of other adsorbates on the chemisorbed CO.[1,2]

The adsorption of carbon monoxide on a metal surface is a classical case of CO σ donation and metal π back-bonding. The CO σ orbitals form a covalent bond with the σ orbitals of the metal. The 2π* orbital in gas-phase carbon monoxide is empty but it is a fairly low lying orbital and therefore the metal π orbitals can donate charge to it. Charge donation from the metal to the CO 2π orbitals weakens the CO bond, strengthens the metal–carbon bond, and thereby shifts the C-O stretching frequency to a lower value. The relative amounts of σ donation and π back-bonding vary from metal to metal. The strength of the metal–CO bond increases as one moves to the left and to the top of the transition metals. This correlates well with the above description of the metal–CO bonding, since the dπ electrons are held less tightly by the metals on the left side of the periodic table. As one moves to the left, the ratio of the size of the d orbitals to the sp orbitals increases. These two contributions increase metal to CO back-bonding, and therefore the metal–CO bond strength increases as one moves to the left of the periodic chart.[3]

The published[4] calculational results using MINDO/SR show that the breakdown of the adsorption energy into monatomic and diatomic terms indicates a complex interaction in which a large Fe–C diatomic energy term of 325 kcal/mol for CO in an on-top site is needed to obtain a net adsorption energy of 23 kcal/mol because adsorption destabilizes the C–O bond and the Fe–Fe bonds in Fe_{12}. The cluster d band is shifted by adsorbate–adsorbent charge transfer even though the d orbitals overlap only very weakly with the adsorbate. While the interaction of CO with its nearest neighbor dominates the interaction energy, the energy for the interaction with the other cluster atoms is necessary for a quan-

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Table I. Calculated Properties for CO Adsorbed at an On-Top Site of Fe_{12}[a]

Charges (e)

C	O	CO	Fe_{12}	$Fe(7)/Fe_{12}CO$	$Fe(7)/Fe_{12}$
0.23	−0.59	−0.36	+0.36	−0.02	+0.10

Orbital Populations

atom	s	p_x	p_y	p_z	$\sum sp$	σ	π	$\sum d$
Fe(7)	0.531	0.089	0.095	0.309	1.024	0.840	0.184	6.999
$(Fe(7)/Fe_{12})$[b]	(0.659)	(0.092)	(0.077)	(0.073)	(0.901)	(0.732)	(0.169)	(6.998)
C	1.408	0.452	1.113	0.795	3.768	2.203	1.565	
O	1.849	1.532	1.788	1.423	6.591	3.272	3.320	
C + O						5.475	4.885	

Bond Orders and Lengths

	bond order	*R* (Å)		bond order	*R* (Å)
C–O	1.57 (66% σ)	1.22	C–Fe(7)	1.10	2.07
$C–Fe_{12}$	1.45				

[a] CO adsorption energy = 22.2 kcal/mol. [b] The values in this line are for Fe(7) in the bare cluster Fe_{12} whereas all other values in this table are for the cluster $Fe_{12}CO$.

titative account of adsorption and can be as large as the net adsorption energy. The calculated binding energies, which vary from 14 to 28 kcal/mol for different surface sites, compare well with the experimental adsorption energies for CO on the Fe(100) face, which vary from 13 to 26 kcal/mol.[5]

One of the most common ways of discussing chemical bonding is in terms of the Mulliken bond order.[6] Although a numerical index is produced, bond orders are generally regarded as a qualitative measure of bonding. It has been pointed out that, in dealing with complex many-electron systems, there is generally no single unique way to analyze the bonding.[7] In a paper with the partial title "A clear-cut analysis", it was pointed out that all population analysis for carbonyls is intrinsically unclear because, with the large overlap between metal and CO orbitals, "the assignment of charge to one or the other of these sets of orbitals is quite arbitrary".[8] One approach to associating definite energies with the contribution of various types of orbitals in bond formation is the CSOV (constrained-space orbital variation) method.[8] Starting with metal and ligand charge distributions frozen at values for the isolated components, the energy lowering obtained by reorganizing the charge distribution for various types of orbitals (σ, π, metal, ligand) as bonds are formed is calculated to determine the energetic importance of various types of interaction. These results have established $d\pi$ interactions as among the most important for Fe, Ni, and Cu interactions with CO.[8-11]

In this paper, a new criterion is presented for determining the contribution of a particular class or group of orbitals to a chemical bond. The new criterion is the diatomic energy contribution of particular orbitals in a particular bond (any diatomic atom pair) to the total molecular energy. It is a unique feature of NDO (neglect of diatomic overlap) type procedures that the total energy can be divided entirely into monatomic and diatomic energy terms.[12] Here this method is applied to determining the contribution of σ and π orbitals to the cohesive energy of CO adsorbed on a cluster of 12 iron atoms. This paper does not address the question of energy changes as bonds are formed but rather addresses the problem of clarifying the σ and π orbital contributions to the total molecular energy for the electronic state of the final molecule, $Fe_{12}CO$ in this case.

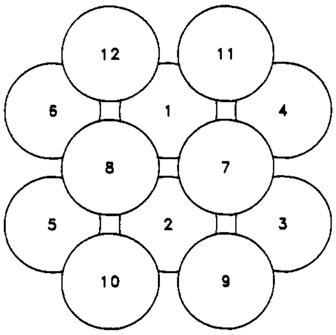

Figure 1. Top view of the Fe_{12} cluster.

Calculational Procedure

The MINDO/SR (modified intermediate neglect of differential overlap/SR) procedure used here is parametrized to give bond energies and lengths for selected reference compounds in agreement with experimental values. The MINDO/SR semiempirical SCF method explicitly includes electron–electron repulsions. Its ability to handle a wide variety of compounds, including large metal clusters, has been described previously.[4,13-16] The decomposition of the total energy into monatomic and diatomic energy terms has been used to put the effect of one adsorbate on another on a firm quantitative basis.[4] Specific expressions for this partitioning have been given.[12]

The computer program used was obtained by modifying QCPE Program 290 by Rinaldi with the changes by Schmidling[17] to incorporate MINDO/3. Automatic geometry optimization is done with analytically calculated gradients. The inclusion of transition metals, symmetry,[18] and selective molecular orbital filling further enhances MINDO/SR.

Parameters selected to give reasonable properties to FeH, FeO, $Fe(CO)_5$, $HFe(CO)_4^-$, $(CO)_3FeCHO^-$, $CH_3Fe(CO)_4^-$, $(CO)_3FeC(O)CH_3^-$, HFe_{12}, $COFe_{12}$, and OFe_{12} have been reported.[4] The Clementi and Roetti[19] double-ζ basis for the Fe 3d orbitals and the de Brouckere[20] d orbital energy and the Slater–Condon parameters are used. Small adjustments in the literature parameter values were made to obtain better agreement between calculated and experimental properties for the above compounds. The s, p, and d orbitals all use the same β parameters.

The geometric arrangement of the atoms is shown in Figure 1. Calculations were done with the Fe cluster atom positions fixed as in the bulk[21] with a nearest neighbor distance of 2.48 Å and a next nearest

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Table II. Properties of Gas-Phase CO (Optimized in MINDO/2 for Free CO)

Populations and Bond Orders

	σ	% σ	π	% π	tot.
population	6.00	60	4.00	40	10.00
bond order	1.08	54	0.91	46	1.99

Diatomic Energies (au)

	$\epsilon_{\mu\mu}$						
μ on	s	p_x	p_y	p_z		$\sum\sigma$	$\sum\pi$
C	−3.6045	−0.9987	−0.9987	−1.6000		−5.2045	−1.9974
O	−2.3324	−1.9220	−1.9220	−1.9614		−4.2938	−3.8440
					totals	−9.4983	−5.8414

	$\epsilon_{\mu\nu}$							
	C s	C p_x	C p_y	C p_z		$\sum\sigma$	$\sum\sigma\pi$	$\sum\pi$
O s	1.0033	0.3001	0.3001	0.1736		1.1769	0.6002	
O p_x	0.8924	−0.1056	0.2473	0.3961			1.2285	0.1417
O p_y	0.8924	0.2473	−0.1056	0.3961			1.2885	0.1417
O p_z	0.7712	0.2523	0.2523	0.0759		0.8471	0.5046	
					totals	2.0240	3.6818	0.2834
					$\epsilon_{\mu\nu}(\sigma + {}^1/_2\sigma\pi)$	3.8649		
					$\epsilon_{\mu\nu}(\pi + {}^1/_2\sigma\pi)$			2.2143

	σ	% σ	π	% π
$\epsilon_{\mu\mu} + \epsilon_{\mu\nu}$	−5.6334	61	−3.7171	40

Table III. Diatomic Energies for C–O On-Top Fe_{12}

	$\epsilon_{\mu\mu}$ (au)						
μ on	s	p_x	p_y	p_z		$\sum\sigma$	$\sum\pi$
C	−2.6358	−0.8468	−2.0823	−1.4872		−4.1230	−2.9291
O	−2.3074	−1.9115	−2.2307	−1.7739		−4.0813	−4.1422
					totals	−8.2043	−7.0713

	$\epsilon_{\mu\nu}$ (au)							
	C s	C p_x	C p_y	C p_z		$\sum\sigma$	$\sum\sigma\pi$	$\sum\pi$
O s	0.7712	0.2610	0.6418	0.2269		0.9981	0.9028	
O p_x	0.6370	−0.0699	0.5317	0.3797			1.0167	0.4618
O p_y	0.7854	0.2523	0.4848	0.4431			1.2285	0.7371
O p_z	0.4443	0.2007	0.4934	0.0127		0.4570	0.6941	
					totals	1.4551	3.8421	1.1989
					$\epsilon_{\mu\nu}(\sigma + {}^1/_2\sigma\pi)$	3.3762		
					$\epsilon_{\mu\nu}(\pi + {}^1/_2\sigma\pi)$			3.1200

	σ	% σ	π	% π
$\epsilon_{\mu\mu} + \epsilon_{\mu\nu}$	−4.8282	55	−3.9514	45

distance of 2.86 Å. The atoms on the top layer are next nearest neighbors to each other and nearest neighbors to bottom layer atoms. In order to obtain a cluster large enough that it represents several types of binding sites on an Fe(100) plane and small enough that calculations could be done in a reasonable length of time, a 12-atom cluster was chosen. A state with multiplicity 39 was found to give the lowest energy. The multiplicity 39 corresponds to a d^7 configuration with three unpaired electrons per atom. No magnetic data for small iron clusters are available. The atomic magnetic moment of bulk Fe is 2.22 μ_B,[22] so a state of such high multiplicity is expected.

An on-top site has an atom or molecule adsorbed directly over atom 7. For CO in an on-top site, the Fe(7)–C–O group is linear with the axis perpendicular to the plane of the top layer of atoms.

Results

The general results for calculated properties of CO adsorbed at an on-top site of Fe_{12} are shown in Table I. The bond lengths are calculated equilibrium positions. The configuration for all of the Fe atoms in the cluster is essentially s^1d^7. The atom Fe(7) has this s^1d^7 configuration before and after CO adsorption. The calculated CO adsorption energy of 22 kcal/mol compares well with the experimental adsorption energies for CO on the Fe(100) face, which vary from 13 to 26 kcal/mol.[5] The calculated binding energy compares well with the α_2-state binding energies of −20.3 and −18.0 kcal/mol from the TDS of Benziger and Madix and of Moon et al.,[5] respectively. In a review of experimental metal–CO bond distances, the metal–C distance varies from 1.70 to 2.03 Å for various transition metals and crystal faces.[23] The optimized Fe–C bond distance of 2.07 Å may be a little too long, as judged by comparisons to metal carbonyls. The calculated C–O bond length is in fair agreement with the results of Rhodin et al.,[24] who used angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) to obtain a C–O bond length of 1.27 Å for CO chemisorbed on an Fe(110) surface.

The diatomic energies and bond orders for gas-phase CO are given in Table II. The term $\epsilon_{\mu\mu}$ is the attraction of the electronic charge in atomic orbital μ on atom A for the core of atom B. The term $\epsilon_{\mu\nu}$ contains the repulsion of the electronic charge in orbital μ on atom A against the electronic charge in orbital ν on atom B, and it also contains the attractive resonance term, which is usually relatively small. Division of the $\epsilon_{\mu\nu}$ terms into σ and π parts results in cross terms where one orbital is a σ type and the other a π type. These cross terms are divided in half and one half

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Table IV. Diatomic Energies for Fe–C in CO On-Top Fe_{12}

	$\epsilon_{\mu\mu}$ (au)						
μ on	s	p_x	p_y	p_z		$\sum\sigma$	$\sum\pi$
Fe	−0.4747	−0.0742	−0.0791	−0.2580		−0.7327	−0.1533
C	−2.5159	−0.7894	−1.9411	−1.3864		−3.9023	−2.7303
					$\epsilon_{\mu\mu}(\text{Fe} + {}^1/_8\text{C})$	−1.2205	−0.4946

	$\epsilon_{\mu\nu}$ (au)							
	Fe s	Fe p_x	Fe p_y	Fe p_z		$\sum\sigma$	$\sum\sigma\pi$	$\sum\pi$
C s	−0.0479	0.0261	0.0278	−0.2379		−0.2858	0.0539	
C p_x	0.0524	−0.0045	0.0087	0.0284			0.0808	0.0042
C p_y	0.1288	0.0201	−0.0142	0.0699			0.1987	0.0059
C p_z	0.0625	0.0144	0.0153	0.0303		0.0928	0.0297	
					totals	−0.1930	0.3631	0.0101
					$\epsilon_{\mu\nu}(\sigma + {}^1/_2\sigma\pi)$	−0.0112		
					$\epsilon_{\mu\nu}(\pi + {}^1/_2\sigma\pi)$			0.1916

	σ	% σ	π	% π
$\epsilon'_{\mu\mu} + \epsilon_{\mu\nu}$	−1.2317	80	−0.3027	20

is added to the σ total and the other half is added to the π total. Thus the total $\epsilon_{\mu\nu}$ term for σ orbitals is given by the entirely σ terms plus half of the $\sigma\pi$ cross terms. Likewise, the π $\epsilon_{\mu\nu}$ term is given by ($\pi + 1/2\sigma\pi$). The diatomic energy term, exclusive of the core repulsion term, is then given by $\epsilon_{\mu\mu} + \epsilon_{\mu\nu}$. The results in Table II indicate that, for gas-phase CO, 60% of the diatomic energy comes from electrons in σ orbitals and 40% from electrons in π orbitals. The more qualitative bond order measure gives a similar result of 54% σ.

When CO is adsorbed at an on-top site on the cluster, the molecular cluster in the C_s point group does not contain σ or π irreducible representations. Here the σ and π designations are defined with respect to the C–O axis and will be kept in order to simplify the discussion even though in the strictest sense they do not exist. The diatomic energies for CO adsorbed at an on-top site of Fe_{12} are given in Table III. These results indicate that the σ contribution to the C–O bond decreases upon adsorption and that the π contribution increases in both magnitude and percentage. The σ energies are still the largest at 55%.

The diatomic energies for the Fe–C bond are given in Table IV. The calculations performed include the valence shell d electrons. Previous work[25] shows that the d electrons make only a very small net contribution to the diatomic energy of the Fe–C bond. The d orbital occupations and contributions to bonding are thoroughly discussed in ref 25 and are therefore totally removed from further consideration here. In Table IV the $\epsilon_{\mu\mu}$ term for the attraction of an electron in a carbon orbital to the Fe core is for an Fe +8 core because the Fe atom includes the d electrons. if the seven d electrons are removed, the carbon orbital electrons should be attracted to an Fe +1 core. Since the $\epsilon_{\mu\mu}$ term is directly proportional to the core charge, a new term, $\epsilon'_{\mu\mu}$, is defined as the sum of the Fe orbital terms plus one-eighth of the carbon orbital terms. As before, the $\epsilon_{\mu\nu}$ $\sigma\pi$ cross-term energies are equally divided between the $\epsilon_{\mu\nu}$ σ and π energies. For the Fe–C bond the total diatomic energy ($\epsilon'_{\mu\mu} + \epsilon_{\mu\nu}$) is given in Table IV, broken into its σ and π parts. The results indicate that 80% of the diatomic energy making up the Fe–C bond is due to σ electrons.

The monatomic energies for the Fe(7), C, and O atoms as parts of $Fe_{12}CO$ may also be divided into σ and π parts. These are included here for completeness of the σ and π terms, since the total energy is the sum of the monatomic terms, the diatomic terms, and the core repulsion terms. The core–core repulsion terms, of course, cannot be divided into σ and π parts. The monatomic terms for electrons in a particular orbital consist of core attraction terms, electron–electron repulsion terms, and relatively small electron-exchange terms. The values given in Table V indicate that the σ contribution is larger than the π contribution of the Fe(7), C, and O atoms to the total energy of the $Fe_{12}CO$ cluster.

Table V. Monatomic Energies (au) in $Fe_{12}CO$

	σ	% σ	π	% π	tot.
Fe(sp)	−1.4299	85.7	−0.2378	14.3	−1.6677
C	−2.4879	64.8	−1.3512	35.2	−3.8391
O	−5.8888	53.5	−5.1089	46.5	−10.9977

Discussion

Recent theoretical calculations have tended to downplay the role of the σ orbitals in metal–CO bonding.[8-11,26-29] The results of the calculations by Koutecky et al. on PdCO and RhCO[26] indicated that low occupancy of the metal 5s orbital is necessary for PdCO and RhCO to be more stable than the metal and CO at infinite separation. Furthermore, density contour maps showed that the metal σ orbitals polarize away from the CO σ orbitals. Hermann and Bagus have been by far the strongest proponents of π bonding between the metal and CO.[8-11,27-29] Their constrained-space orbital variation method (CSOV) allows for quantitative determination of the energy changes which follow from allowing σ and π populations to vary. In the first CSOV step, the metal and CO orbitals are frozen. When the molecule is held fixed in its equilibrium geometry, charge superposition of the frozen fragments causes a large repulsion, which is mainly due to interactions between the CO and metal orbitals of σ symmetry. The initial frozen-orbital repulsion is a large destabilization term and must be offset by other stabilizing terms in order for the molecule to be stable. The second CSOV step allows the metal orbitals to reorganize. In the third step, the CO orbitals are allowed to relax. The fourth CSOV step allows for charge transfer from the metal to the CO. This step can be broken into two separate steps; one allows for metal σ donation, and the other allows for metal π donation. It turns out that the metal σ donation is very small. The metal π donation results in a very large energy stabilization. The fifth CSOV step allows for CO to metal charge transfer, which is indicative of the CO σ donation. The general result is that the metal π electron reorganization and donation step makes the largest contribution to the stabilization of the M–CO bond. This paper does not disagree with this conclusion as it, indeed, does not even address the question of charge reorganization at all.

Several recent publications have considered metal–carbonyl bonding using much larger basis sets and more extensive electron correlation than previously.[30-33] For the linear FeCO triatomic

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molecule, the σ charge donated from the carbon atom was found to be larger than the π charge accepted,[31] thus affirming the importance of the σ electron charge.

The nature of the bonding of atoms together into a molecular unit is examined in this paper from the viewpoint of the final electronic structure. While interesting and important from other views, changes in charges and bonding as bonds are formed are not relevant to the viewpoint here and so are not considered. The question considered here is, What are the energy contributions (σ and π) to the total electronic energy of the molecule in its stable molecular state?

The main point of this paper is to point out the importance of the σ electrons to the stability of the metal-carbon bond of transition metal carbonyls, including chemisorbed CO. In the consideration of the relative roles of σ and π electrons, the π electrons have received the most attention. This occurs because the π electrons generally have the highest energies and therefore are the most readily shifted. The π electron shifts produced by changing the surface site of chemisorbed CO (on-top vs bridge bonding) and the effect of other adsorbents on CO are reflected in large shifts in the C-O infrared stretching frequency and adsorption binding energies. There is a large amount of literature in this area. The importance of the CSOV approach is that it shows that charge reorganization is necessary to form a stable bond between CO and a metal and that, of the various types of reorganization, the shifting of the π electrons makes the largest contribution to stability. The importance of the separation of the total calculated energy into monatomic and diatomic energy terms presented here is that it shows that after the charge reorganization has occurred, the largest contribution to the stability of the metal-carbon bond is provided by the σ electrons. It is the attraction of the σ electrons to the metal and carbon atoms that provides the largest share of the glue (cohesive energy) that constitutes the metal-carbon bond. This is shown using, for the first time, an energy criterion rather than the more qualitative bond order criterion.

Acknowledgment is made to the donors of the Petroleum Research Fund, administered by the American Chemical Society, for partial support of this research and to the University of Arkansas for a computing time grant.

Registry No. CO, 630-08-0; Fe, 7439-89-6.

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Ziegler-Natta Catalysis. A Theoretical Study of the Isotactic Polymerization of Propylene

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Abstract: The stereotacticity of *ansa*-zirconium metallocene Ziegler-Natta propylene polymerization catalysts is studied using a combination of ab initio electronic structure techniques and empirical force field molecular mechanics techniques. The experimental observation of isotacticity for the *rac*-(1,2-ethylenebis(η^5-indenyl)zirconium and *rac*-(1,2-ethylenebis(η^5-tetrahydroindenyl)zirconium based catalysts is computationally reproduced, and an explanation for the reduced rate of reaction and the atacticity for the *meso*-(1,2-ethylenebis(η^5-indenyl))zirconium catalysts is provided. In addition, modified *rac*-(1,2-ethylenebis(η^5-tetrahydroindenyl))zirconium catalysts with predicted increased isotacticity and decreased isotacticity (despite the presence of a chiral metal center), respectively, are proposed. Further, a new catalyst is proposed which should yield syndiotactic polypropylene.

I. Introduction

Homogeneous catalysts are actively being studied as useful reagents for the stereospecific Ziegler-Natta polymerization of propylene. Isotactic polypropylene has been produced using active catalysts derived from chiral, *ansa*-metallocene compounds of group 4 transition metal elements and methylaluminoxane ($[Al(CH_3)-O]_n$) (MAO) cocatalysts.[1] The discovery of a highly isotactic (ethylenebis(tetrahydroindenyl))$ZrCl_2$/MAO, catalytic system (Figure 1, A) by Kaminsky, Brintzinger, and co-workers[2] and a highly syndiotactic isopropyl(cyclopentadienyl-1-fluorenyl)$ZrCl_2$/MAO catalytic system (Figure 1, B) by Ewen and co-workers[3] has prompted further research into the effects of ligand on stereoregulation.[4]

In general, Ziegler-Natta catalysts produce syndiotactic, isotactic, or atactic polypropylenes. These three types of polymer have differing relative orientations of the chiral centers which occur at alternate positions along the polymer chain (Figure 2). Isotactic polypropylene has the same relative configuration at all of the chiral centers (the methine carbons) and is commercially important owing to its greater tensile strength.[6] Syndiotactic polypropylene has a regular alternation of configuration at adjacent chiral centers along the polymer chain, and atactic polypropylene has a ster-

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