hydrolysis. A relatively small ratio of propane:propene (30:70) was found after 5 min, suggesting that besides from **1a**, **7** is also formed by alternative modes of reaction between *tert*-butyllithium and **5a**.[11] Even when the reaction was carried out at −60 °C, **1a** was accompanied by considerable amounts of **7**. In light of these results, it would appear that the synthesis of **1a** from lithium and 1,3-dichloropropane, claimed in the patent literature[12] but supported by little experimental evidence, is highly unlikely.

It could be expected that a 1,3-dilithium compound not containing β hydrogen would be (more) stable. We therefore prepared 1,3-dilithio-2,2-dimethylpropane (**1b**) by an analogous route (Scheme I). Slow addition (2 days) of 1,3-dibromo-2,2-dimethylpropane (**2b**)[13] to magnesium in diethyl ether yielded 1,3-bis(bromomagnesio)-2,2-dimethylpropane (**3b**, 18% yield), practically free from any organometallic impurities and completely stable in solution. Addition of a solution of $HgBr_2$ in THF to the solution of **3b** in THF gave **4b**.[14] When a suspension of **4b** in pentane was treated with 2 equiv of *tert*-butyllithium, a solution of **5b**[15] and a precipitate of LiBr were formed, which were separated by filtration. On addition of 2 more equiv of *tert*-butyllithium to the clear filtrate, **1b** gradually deposited during 1 week at room temperature. After shorter periods of time, unreacted **5b** was still present. Therefore, we conclude that the essential step of this reaction, i.e., the addition of *tert*-butyllithium to **5b** to form an unstable -ate compex, is retarded by extreme steric hindrance in the adduct. **1b** was collected in pure form by decanting and washing with pentane as a white powder (70–80% yield); it was characterized by its NMR spectrum (vide infra) and by reaction with trimethylchlorostannane to give **6b**[16] as the sole product (Scheme II).

It turned out that **1b** was indeed a rather stable compound. Not only did it not show signs of decomposition in the solid state, but also it was soluble in diethyl ether. Somewhat to our surprise, these solutions were found (NMR) to be fairly stable at room temperature for several weeks ($t_{1/2}$ = 70 days), a finding quite exceptional for a primary alkyllithium.[17] The ^1H NMR spectrum in Et_2O-d_{10} was in agreement with the proposed structure: at room temperature, broad ^1H resonances were found at δ −0.74 (s, 4 H, CH_2) and 1.15 (s, 6 H, CH_3). As the solution cooled, complicated, reversible dynamic effects were observed in the ^1H NMR spectrum (cf. ref 6 for similar phenomena with **3a**); they are presently under investigation.

Registry No. **1a**, 13439-59-3; **1b**, 83528-95-4; **2a**, 109-64-8; **2b**, 5434-27-5; **3a**, 62934-64-9; **3b**, 83528-98-7; **4a**, 82773-71-5; **4b**, 83528-96-5; **5a**, 83542-61-4; **5b**, 83542-62-5; **6a**, 35434-81-2; **6b**, 83528-97-6; **7**, 3052-45-7; **8**, 762-73-2; Me_3SnCl, 1066-45-1; *t*-BuLi, 594-19-4; $HgBr_2$, 7789-47-1.

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(11) We thank a referee for valuable comments on this possibility.

(12) Eberly, K. C. *U.S. Patent* **1960**, 2 947 793; *Chem. Abstr.* **1961**, *55*, 382.

(13) Shortridge, R. W.; Craig, R. A.; Greenlee, K. W.; Derfner, J. M.; Board, C. E. *J. Am. Chem. Soc.* **1948**, *70*, 946.

(14) **4b**: mp 171 °C dec ($CHCl_3$); ^1H NMR (250 MHz, Me_2SO-d_6) δ 1.15 (s, $^4J_{HgH}$ = 18.1 Hz, 6 H, CH_3), 2.07 (s, $^2J_{HgH}$ = 211.2 Hz, 4 H, CH_2); ^{13}C NMR (62.89 MHz, Me_2SO-d_6) δ 56.5 (t, $^1J_{CH}$ = 132.0 Hz, $^1J_{HgC}$ = 1656.3 Hz, $^3J_{HgC}$ = 148.9 Hz, CH_2), 38.6 (s, $^2J_{HgC}$ = 61.6 Hz, quaternary C), 36.5 (q, $^1J_{CH}$ = 123.3 Hz, $^3J_{HgC}$ = 163.6 Hz, CH_3). Anal. $C_5H_{10}Br_2Hg_2$: C, H, Hg.

(15) **5b**: colorless liquid obtained by GLC; slowly disproportionates under polymerization; ^1H NMR (250 MHz, $CDCl_3$) δ 1.04 (s, 6 H, C(2)–CH_3), 1.24 (s, 4 H, CH_2), 1.29 (s, $^3J_{HgH}$ = 106 Hz, 18 H, *t*-Bu); ^{13}C NMR (62.89 MHz, $CDCl_3$) δ 30.87 (q of sept, $^1J_{CH}$ = 124.5 Hz, $^3J_{CH}$ = 6.1 Hz, $^2J_{HgC}$ = 20.1 Hz, CH_3 of *t*-Bu), 39.6 (s, quaternary C of *t*-Bu), 40.0 (q, $^1J_{CH}$ = 119.5 Hz, $^3J_{HgC}$ = 62.9 Hz, C(2)–CH_3), 60.9 (s, C(2)), 65.6 (t, $^1J_{CH}$ = 124.5 Hz, $^1J_{HgC}$ = 540.8 Hz, $^3J_{HgC}$ = 74.2 Hz, CH_2).

(16) **6b**: colorless liquid obtained by GLC; ^1H NMR (250 MHz, $CDCl_3$) δ 0.10 (s, $^2J_{SnH}$ = 49 and 51.5 Hz, 18 H, Sn–CH_3), 1.04 (s, 6 H, C–CH_3), 1.10 (s, $^2J_{SnH}$ = 53.5 Hz, 4 H, CH_2); ^{13}C NMR (62.89 MHz, $CDCl_3$) δ −8.2 (q, $^1J_{CH}$ = 128.2 Hz, $^1J_{SnC}$ = 301.5 and 316.2 Hz, Sn–CH_3), 33.5 (t, $^1J_{CH}$ = 124.5 Hz, $^1J_{SnC}$ = 349.2 and 366.2 Hz, $^3J_{SnC}$ = 41.5 Hz, CH_2), 34.6 (q, $^1J_{CH}$ = 124.5 Hz, $^3J_{SnC}$ = 31.7 Hz, (C–CH_3), 35.9 (s, $^3J_{SnC}$ = 20.8 Hz, quaternary C). Anal. $C_{11}H_{28}Sn_2$: C, H, Sn.

(17) **Note Added in Proof**: Prof. P. von R. Schleyer has informed us that ab initio calculations (3-21G) reveal symmetrical double lithium 1,3-bridging to stabilize **1b** by 24.6 kcal mol^{-1} relative to the open extended form, which may explain the unusual stability of **1b** (or an oligomeric cluster derived thereof).

Experimental Observations of Large Interactions of π^* Orbitals through Four Bonds

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Received September 13, 1982

Analysis of orbital interactions (OI) in terms of through-space (TS) and through-bond (TB) components has contributed significantly to our understanding of the nature of interactions between remote groups in molecules.[1,2] One expects OITB to diminish with increasing number of intervening σ bonds and that these interactions are of longer range than OITS.[1] However, only two systematic experimental studies of this attenuation have been reported; one on the σ-type lone-pair splittings along a series of diiodopolyacetylenes[3] and the other on the π,π interactions in the series of "norbornylogues".[4,5] From these limited data it appears that OIT-*n*-B are attenuated more slowly with increasing number, *n*, of intervening σ bonds than expected on the basis of theoretical predictions. In fact, the latter study showed that π,π interactions may be even larger for OIT-4-B than for OIT-3-B.[4]

To date, no experimental studies of through-bond-*dominated* π^*,π^* interactions (π^*-OIT-*n*-B) have been reported.[6] Such a study would be timely in light of the suggestion that OITB involving π^* MO's is responsible for the enhanced reactivity of the double bonds in nonconjugated dienes toward Birch reduction.[2a,7] We have therefore embarked on a systematic study of π^*-OIT-*n*-B by using electron transmission spectroscopy (ETS)[8] as a probe of the anion states and report in Figure 1 ET spectra for the series of compounds **2**–**8**, the structures of which are indicated in the figure. The vertical attachment energies (−EA) are indicated by vertical lines. The details of the method and the assumptions inherent in the association of the structure with the vertical EA's are discussed elsewhere.[8,9]

The EA's and the IP's of compounds **2**–**8**, together with those of ethylene,[10] *cis*-2-butene,[10] cyclohexene,[6] norbornene, and norbornadiene[6] (**1**) are summarized in Table I, and these data

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[‖] NSW Institute of Technology.

[§] John Simon Guggenheim Memorial Fellow.

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(5) The first two members of the "norbornylogue" series are norbornadiene and compound **3**.

(6) The splitting between the π^* orbitals of 1,4-cyclohexadiene and norbornadiene have been determined, but for these systems both through-space and through-bond interactions are important. Jordan, K. D.; Michejda, J. A.; Burrow, P. D. *Chem. Phys. Lett.* **1976**, *42*, 227.

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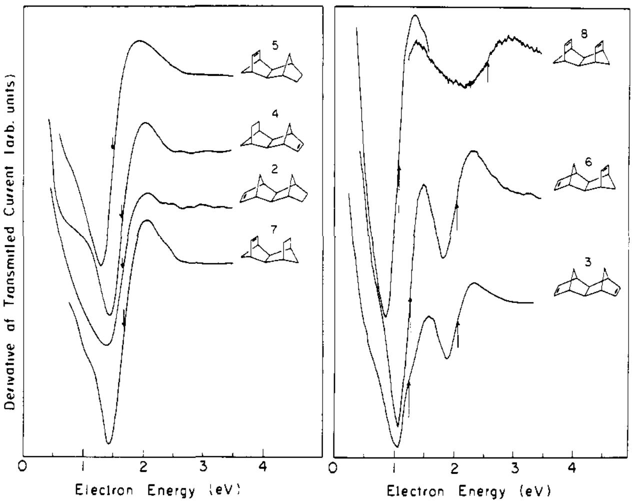

Figure 1. Derivative of transmitted current as a function of electron energy in compounds **2**–**8**.

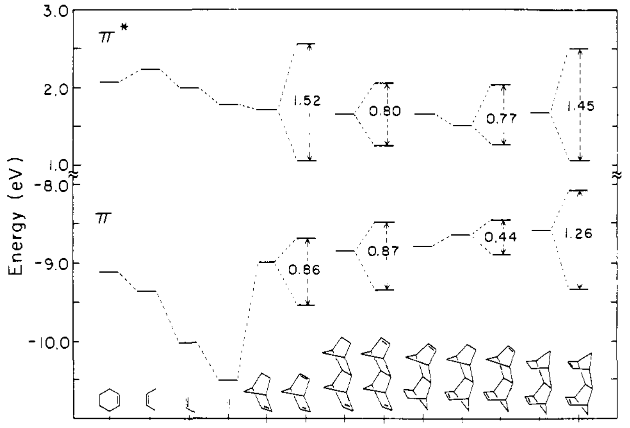

Figure 2. Correlation diagram of the vertical IP's and EA's of **2**–**8** and ethylene, cyclohexene, *cis*-2-butene, norbornene, and norbornadiene.

were used to construct the correlation diagram shown in Figure 2. It is noteworthy that the π^* level in each of the monoenes **2**, **4**, **5**, **7**, and norbornene lies below that of ethylene, whereas the opposite is true for 2-butene and cyclohexene. In the latter two molecules the dominant mixing is between the π^* MO and the pseudo π orbitals of the alkyl groups, with a resultant destablization of the former.[11] In the monoenes **2**, **4**, **5**, and **7**, the π^* MO is well aligned to mix with the appropriate C–C σ and σ^* MO's. It thus appears that the π^*,σ^* mixing predominates, resulting in a depression of the π^* level.

Each of the dienes forms two anion states in the range 1.0–2.5 eV. The data in Table I reveal a satisfactory correlation between the measured differences in the EA's of the dienes and values calculated at a STO-3G SCF level (in conjunction with Koopmans' theorem). In all cases the calculations place the $\pi^* - \pi^*$ level above the $\pi^* + \pi^*$ level. The large splittings observed for the π and the π^* levels of **8** and norbornadiene are due to the combined presence of both OITS and OIT-4-B.[12,13] However, the large separation (ca. 4.5 Å) between the double bonds in **3** and **6** precludes appreciable TS interactions, and the splittings in the π and π^* levels of these compounds must be due almost exclusively to TB interactions.[14]

Table I. Experimental Vertical Electron Affinities and Ionization Potentials

compound	IP, eV	$\pi \pm \pi^a$ splittings, eV	EA, eV	$\pi^* \pm \pi^{*a}$ splittings, eV
cyclohexene	9.12^b		-2.07^i	
cis-2-butene	9.36^c		-2.22^i	
ethylene	10.51^d		-1.78^i	
norbornene	8.97^e		-1.70^j	
norbornadiene	8.69^e		-1.04^i	
	9.55	0.86 (0.80)	−2.56	1.52 (1.70)
2	8.85^f		-1.65^j	
3	8.48^f		-1.25^j	
	9.35	0.87 (0.89)	−2.05	0.80 (0.81)
4	8.78^f		-1.65^j	
5	8.65^f		-1.51^j	
6	8.46^f		-1.26^j	
	8.90	0.44 (0.52)	−2.03	0.77 (0.54)
7	8.60^g		-1.68^j	
8	8.80^h		-1.05^j	
	9.34	1.26 (1.17)	−2.50	1.45 (0.98)

[a] The orbital splittings obtained from STO-3G calculations are given in parentheses. STO-3G optimized geometries were utilized for norbornene and norbornadiene, and the partially optimized geometries of ref 4a were used for 3, 6, and 8. [b] Reference 19. [c] Reference 20. [d] Reference 21. [e] Reference 22. [f] Reference 4. [g] Reference 12. [h] Reference 23. [i] Reference 8b. [j] Present study.

To learn more about the interactions responsible for the splittings in the π^* orbitals, we utilize in an extended form a model recently employed in an analysis[4] of π-OITB in nonconjugated dienes. In that work it was found that the basis[15] π MO of the monoenes **2**, **4**, and **5** and the basis $\pi \pm \pi$ MO's in the dienes **3** and **6** are all raised through mixing with the two high-lying σ orbitals of the correct symmetry.[16] The splittings between the $\pi - \pi$ and $\pi + \pi$ symmetry-adapted orbitals of the dienes result from the fact that this mixing is much larger for the former.

To explain the π^*-OITB-4-B, it is necessary to allow for mixing with both the σ and σ^* framework orbitals. A simplified model,[17] including only the mixing of the π^* MO's with the higher σ orbital (σ') and the lower σ^* orbital (σ'^*),[18] suffices to explain the qualitative trends. In the monenes **2**, **4**, **5**, **7**, and norbornene, the ethylenic π^* MO mixes with both the σ' and σ'^* orbitals. The former mixing elevates the π^* level by an amount y, whereas the latter mixing tends to depress the π^* level by an amount x. The net effect will shift the level by $x - y$, the sign of which, if positive (negative), corresponds to an overall depression (elevation) of the π^* level. The $\pi^* + \pi^*$ level in the diene is lowered by an amount $2x$ through mixing with the symmetric σ'^* MO, and the $\pi^* - \pi^*$ level is raised by $2y$ through mixing with the antisymmetric σ' MO.

The reasonableness of this model may be checked by employing the values of x and y calculated from the EA values of ethylene

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(11) Libit, L.; Hoffmann, R. *J. Am. Chem. Soc.* **1974**, *96*, 1370.

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(13) STO-3G and 3-21G calculations on two ethylenes separated by the distance of the ethylenic groups of **8** give splittings of 1.0–2.0 eV between the two π and the two π^* orbitals. Similar calculations on the two ethylenes separated the appropriate distance for norbornadiene gave splittings of over 3 eV, while calculations on two ethylenes arranged as in compounds **3** and **6** give essentially no splitting between the π or π^* orbitals.

(14) Although TS interactions may be much more important for π^* MO's than π MO's [For example: Burrow, P. D.; Jordan, K. D. *J. Am. Chem. Soc.* **1982**, *104*, 5247], the distances between the double bonds in **3** and **6** are too large for appreciable TS interaction even allowing for the more extended nature of the anion wave functions.

(15) The MO's from SCF calculations on **3**–**8** of course are not of pure π or σ symmetry. The *basis* MO's utilized in our analysis are not the SCF MO's but rather π-type ethylenic MO's and C–C MO's formed from sp^3 hybrids; see ref 4.

(16) Note that mixing of π levels with σ^* levels in negligible because of the large difference in their energies.

(17) We will present a more complete analysis allowing for the interactions of the π^* and orbitals with two σ and two σ^* orbitals in a future publication.

(18) The σ orbitals that mix with the π^* orbitals are distinct from those that mix with the π orbitals due to the presence of an additional nodal plane.

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and the diene **3** to predict the difference, ΔEA, between the E_A's of ethylene and the monoene **2**. This procedure yields $x = 0.27$ eV and $y = 0.14$ eV, or $x - y = +0.13$ eV, in agreement with experiment. The σ'^*,π^* and σ',π^* interactions are significantly smaller than the σ,π interactions in the same systems on account of the large energy gap between the $\pi^* - \pi^*$ MO and the σ' MO and the relatively poor overlap between the $\pi^* + \pi^*$ MO and the σ'^* MO.

The present study indicates two salient features of π^*-OITB: (1) these interactions result from the mixing of the $\pi^* \pm \pi^*$ symmetry-adapted orbitals with both σ and σ^* frontier MO's, with the latter predominating (i.e., $x > y$); (2) the net splitting in the π^* manifolds is nearly the same as in the π manifolds. This follows because the $\pi^* \pm \pi^*$ combinations are shifted in *opposite* directions through mixing with the σ and σ^* MO's, while the $\pi \pm \pi$ combinations are shifted in the *same* direction through mixing with the occupied σ orbitals.

Acknowledgment. This research was supported by the National Science Foundation (P.D.B. and K.D.J.) and the Australian Research Grants Scheme (M.N.P.R.). We thank K. N. Houk for valuable discussions and L. Ng for assistance with the experiments.

Registry No. 2, 1076-12-6; **3**, 83602-18-0; **4**, 36012-52-9; **5**, 15914-93-9; **6**, 15914-94-0; **7**, 1076-12-6; **8**, 1076-13-7; norbornene, 498-66-8.

Diprotonated Methane, CH_6^{2+}, and Diprotonated Ethane, $C_2H_8^{2+}$

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Received July 2, 1982

The stabilization of the *pentacoordinate* CH_5^+ ion[1] finds its origin in the interaction of the electron-deficient carbon with two ligands (three center, two electron (3c-2e)). The size of this effect is reflected in the heat of hydrogenation of CH_3^+, experimentally deduced as 40 kcal/mol[2a] and calculated as 34.5 kcal/mol by ab initio molecular orbital theory (MP3/6-31G** + ZPE).[2b] The 3c-2e stabilization is a common phenomenon in larger systems, like the norbornyl cation,[3] although its magnitude reduces as illustrated by the heats of hydrogenation of $C_2H_5^+$ (11.8 kcal/mol) and $C_3H_7^+$ (2.3 kcal/mol).[2a]

Table I. Total (hartrees) and Relative Energies (kcal/mol) Using the 6-31G** Basis and HF/6-31G* Geometries and Zero-Point Energies (kcal/mol)

geometry	HF	MP3	zero point
1, C_{2v}	−40.30397 (0)	−40.49674 (0)	37.9
2, C_{2v}	−40.29730 (4.2)	−40.49264 (2.6)	35.8
3, C_2	−79.45620 (0)	−79.80097 (0)	58.1[a]
4, D_{4d}	−79.44122 (9.4)	−79.79618 (3.0)	55.8[a]
7, C_{2v}	−78.27287 (5.9)	−78.56410 (3.5)	43.2[a]
8, C_s	−78.28234 (0)	−78.56969 (0)	44.4[a]
5, D_{2d}	−77.09538	−77.32626	30.1[a]

[a] Zero-point vibrational energy obtained with the 3-21G basis.

Scheme I

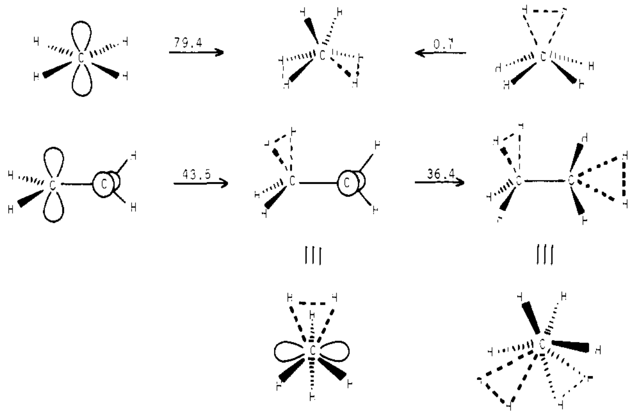
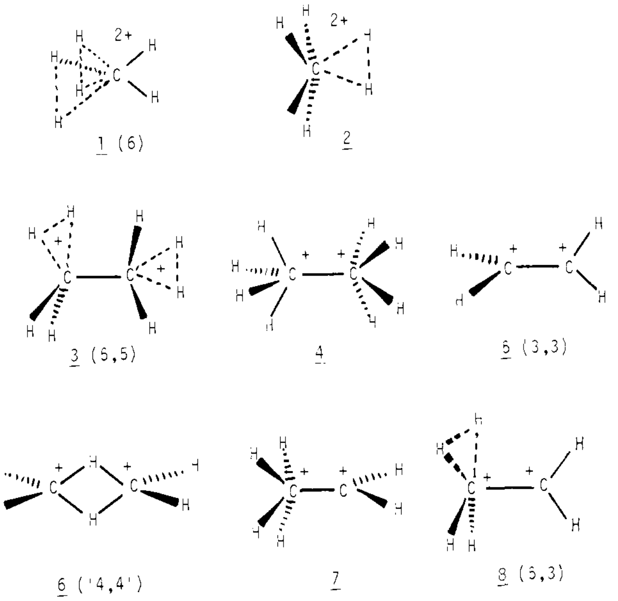


Chart I



The concept of hypercoordination of electron-deficient species can also be applied to dications. From our ab initio theoretical[4] studies on small carbocations, the prototypes of new unprecedented types of hypercoordinate ions emerged, i.e., diprotonated methane, CH_6^{2+}, and diprotonated ethane, $C_2H_8^{2+}$. In the context of pentacoordinate carbon stabilization we also restudied the ethane dication, $C_2H_6^{2+}$.

In order to describe these hypercoordinate species, we have used single-point calculations with the flexible 6-31G** basis set, which has polarization functions on both hydrogen and carbon, for geometries optimized within the Hartree–Fock limit at the 6-31G* (d functions) level.[5] Furthermore, at this level we have included electron correlation corrections with the Møller–Plesset perturbation theory[6,7] to the third order with frozen core (MP3/6-

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