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Tuning Reactivities of *tert*-Butyllithium by the Addition of Stoichiometric Amounts of Tetrahydrofuran

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In alkyllithium chemistry the highest reactivity has historically been linked to the smallest degree of aggregation possible. Since *tert*-butyllithium is known to form a monomer in tetrahydrofuran solution, using just stoichiometric amounts of the LEWIS base to selectively form a dimeric species seemed irrational. In this study, we showed a considerable increase of the reactivity of *t*-BuLi when using stoichiometric amounts of THF in the non-polar solvent *n*-pentane in order to enable the deprotonation of simple methyl silanes and other low C–H–acidic substrates. In this context, we were able to obtain the corresponding aggregates of *t*-BuLi with the ligand THF in suspension and as crystalline solids and investigate them by single crystal X-ray structural analysis, *in situ* FTIR spectroscopy and quantum chemical calculations. Furthermore, we were able to explain the enhanced reactivity of *t*-BuLi with stoichiometric amounts of THF on the basis of structural features of the bridged dimer obtained under these conditions. With these findings, we present a new target in the aggregation of alkyllithium reagents: the selectively formed *"frustrated"* aggregates!

In the fields of organic and inorganic chemistry, the use of metal alkyl reagents has become widely accepted as one of the most used BRØNSTED bases[1] and carbon nucleophiles.[2] In particular, GRIGNARD[3] reagents and alkyllithium compounds implemented by SCHLENK[4] are widely used in both fields.[5] Due to the need for some kind of coordinating side on the educt, as shown in the Complex Induced Proximity Effect (CIPE) by SNIECKUS and BEAK,[6] the scope of these reactions is somewhat limited. It is well known, that LEWIS basic solvents like diethyl ether and tetrahydrofuran (THF) increase the reactivity and reduce the stability of alkyllithium compounds significantly. In these solvents the tetrameric *tert*-butyllithium (*t*-BuLi) aggregate as shown by WEST,[7] THOMAS[8] and STALKE[9] is separated and deaggregated into a dimer in diethylether as described by THOMAS[10] and STALKE[9] or even a monomer in the presence of THF. These types of monomeric aggregates are also known from diamine or triamine ligands as a LEWIS basic donor.[11] The formed structures could be identified via NMR spectroscopy and validated via X-ray crystal structures in the case of the tetramer and the formed dimer in ether. BAUER[12] showed with a wide range of NMR measurements that a monomer in THF solution should be present and did not identify any other structure in his findings. The validation via single crystal X-ray diffraction is still missing to this day.

Only pure solvents were used in the structure determination due to better solubility of the alkyllithium compounds and an easier evaluation of the analytical data.[9,10,12] Nevertheless, in a variety of reactions solvent mixtures of a non-polar solvent and THF seemed to have a positive effect on the yield and selectivity in these compounds.[13] Since the effects of solvent mixtures on alkyllithium aggregation have not been extensively evaluated, we started our research with a stoichiometric use of THF as a ligand in the non-polar solvent *n*-pentane. We used the equimolar ratios of *t*-BuLi to THF of 1:2, 1:1 and 2:1 (*t*-BuLi:THF). All of these approaches led to the formation of pale-yellow suspensions at and below 0 °C.

In the first case (*t*-BuLi:THF = 1:2) we obtained fine yellow crystals at −80 °C, which turned out to be extremely sensitive and led to gas emission upon decomposition. After we repeated the crystallization under equal conditions various times, we were finally able to determine a molecular structure of the aggregate of *tert*-butyllithium with tetrahydrofuran as a donor using single crystal X-ray diffraction (see Figure 1).

To our surprise we did not observe a monomeric structure as predicted by BAUER *et al.*[12] or a classic dimer, which was quantum chemically proposed by PRATT *et al.*[14] The bridged dimeric structure **1** of *t*-BuLi includes three THF molecules, with one capping the two lithium centers. Thus, each cation has a closed coordination sphere with three strong (Li1–O1 and both Li1–C5) and one weak contact (Li1–O2) based on the length of these contacts. The strong ionic contacts between the lithium cations and the carbanionic centers form a four membered ring. The distances between O2 of the bridging THF and the lithium centers are with 2.1826(18) Å significantly longer compared to usual O–Li distances of monodentate coordinating ether molecules (see Scheme 1).[9,15]

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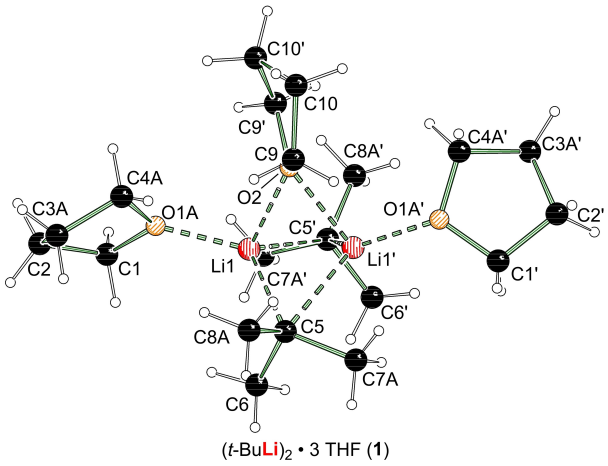
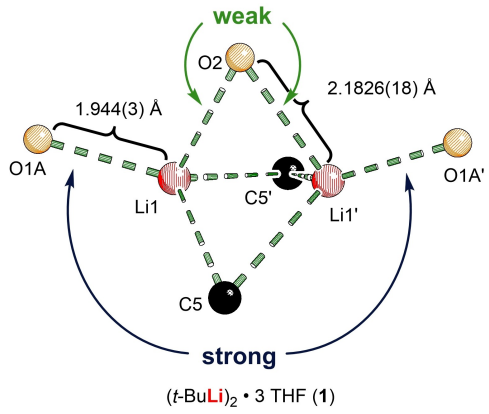


Figure 1. Molecular structure of [*t*-BuLi]$_2$ · 3 THF (**1**) in the crystal. Symmetry operation: 1−x, +y, 3/2−z. Minor disorder has been omitted for clarity. Small selection of bond lengths [Å] and angles [°]: O1A-Li1 1.944(3), O2–Li1 2.1826(18), C5-Li1 2.2241(17), C5′-Li1 2.3250(17), Li1-O2-Li1′ 58.98(8). For further information on selected bond lengths and angles see SI Figure S1.



Scheme 1. Cutout from the molecular structure of [(*t*-BuLi)$_2$ · 3 THF] (**1**) in the crystal. THF molecules are represented by their respective oxygen atom and *t*-Bu groups are represented by the respective carbanionic center.

The weak coordination of the bridging THF indicates a tendency towards the opening of this structure and tilting towards one of the lithium centers. Following quantum chemical calculations, tilting of the bridging THF molecule to one of the lithium cations should be within the range of possibilities ($\Delta H = 10$ kJ mol^{-1}, see SI). Thus, leading to the opening of a coordination spot, which should be accessible for even very weak coordinating reagents. In a previous work we were able to show a similar mechanism to open a coordination spot in a ferrocene-based LOCHMANN-SCHLOSSER base.[16]

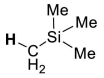
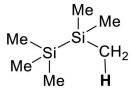
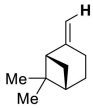
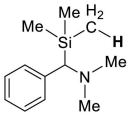
One example for a weak coordinating reagent could be tetramethylsilane (TMS). Because of the difference in electronegativity of silicon and carbon, all methyl groups in TMS carry a slightly negative charge ($q_{(nbo;\ Me)} = -0.43$ eV). Therefore, the methyl groups at a silicon center are able to coordinate to a lithium cation as shown in molecular structures published by our own research group in cooperation with J. O. BAUER[17] determined by X-ray analysis. The proximity of the carbanionic centers and the TMS molecules should be enough in these postulated structures to lead to a metalation.

Quantum chemical calculations verified this proposed reaction mechanism and showed a deprotonation barrier of around 60 kJ mol^{-1} starting from the bridged dimer **1** and TMS. After multiple experimental screenings with different temperatures it could be shown that the mixture of *t*-BuLi and THF in a ratio of 1:2 in *n*-pentane is actually able to deprotonate the rather negative methyl groups of TMS at 0 °C in a couple of hours. These findings are remarkable and show the potential of this simple reaction mixture. Most of the observed side products occur due to the decomposition of THF, which on this timescale starts at around −40 °C.[18] A selection of examples is shown in Table 1 below.

In each case a significant increase in the reactivity of *t*-BuLi could be shown by using stoichiometric amounts of THF. The reactive mixture of *t*-BuLi:THF (1:2) in *n*-pentane especially showed potential for synthetic use with toluene and silylamine **6**. In addition, the formation of a suspension could be observed in every reaction showcasing a solubility issue of the polar reactive species in *n*-pentane, which should not be a hindrance as long as the substrate is decently soluble in the non-polar solvent.

With the molecular structure, experimental findings and a mechanism hypothesis in line, we needed proof that the bridged dimer **1** is actually present in our reactions. Since the

Table 1. Experimental investigations of the enhanced reactivity of *t*-BuLi when used with THF in a ratio of 1:2 in *n*-pentane at 0 °C for 3 h (Entries end with b) in comparison to *t*-BuLi in THF solution at 0 °C for 3 h (Entries end with a).

Entry	Substrate[a]	Conversion [%][b]
1a		0[c]
1b	TMS (**2**)	10
2a		15
2b	hexamethyldisilane (**3**)	30
3a		0[c]
3b	(−)-β-pinene (**4**)	5
4a		5
4b	toluene (**5**)	65
5a		0[c]
5b	silylamine **6**	80[e]

[a] Abstracted protons are written bold. [b] Conversion determined via GC/EI-MS analysis after electrophilic work-up with $PhMe_2SiCl$ or Me_3SiCl. [c] no traces were detectable. [d] traces were detectable. [e] yield of isolated crystals of the lithiated product (SI).

formation of a suspension was observed in the experimental studies, NMR measurements proved problematic. After the crystals of **1** were added to *n*-pentane-*d*12, suspensions were formed even in small concentrations. In the NMR measurements, only insufficient traces of *t*-BuLi-containing aggregates could be detected at the temperature range of −60 °C to −40 °C (prior work of STANETTY and MIHOVILOVIC[18] showed a good stability of THF and *t*-BuLi at these temperatures for several hours). The use of more polar NMR solvents would lead to side reactions within the NMR tube or cause a different aggregation. In order to prove the existence of **1** a better solubility in the suspensions is required, which could be realized by heavy stirring of the mixture. However, this rules out NMR studies for validation.

Thus, an alternative *in situ* spectrometric method was explored: *in situ* FTIR, which not only allows but also requires the probe to be heavily stirred. In the FTIR experiment *tert*-butyllithium was dissolved in *n*-pentane, and 0.5 equivalents of tetrahydrofuran were added every twelve minutes. The resulting yellow suspension was stirred heavily during the whole experiment (see Figure 2). To work around potential side reactions the whole probe was held under −60 °C at any time (SI).

Starting with the addition of the first portion of THF, the amount of tetrameric *t*-BuLi (blue) drops, and another species (green) is formed. The proposed amount of species 2 (green) rises until 1.5 equivalents of THF have been added to the probe and stays at about the same concentration until the amount of THF added rose to 2.5 equivalents. At this point a third species (red) is formed. We strongly believe that species 3 (red) is the monomer postulated by BAUER and coworkers.[12] This leads to the assumption that species 2 is actually the observed structure from the singe crystal X-ray diffraction, which should be in line with the conditions for the crystal formation. Since NMR measurements were impossible, the only possible clue for species 2 remained via characterization of species 3. In this context, we removed the *n*-pentane from the commercially available *tert*-butyllithium solution at −60 °C and added about 3 equivalents of THF to the precipitate leading to yellow colored crystals of **7** (see Figure 3).

Monomer **7** corresponds to the NMR findings of BAUER *et al.*[12] **7** also shows that the formation of the bridged dimer **1** is not related to crystallization-specific effects, such as packing, and should be linked to the amount of THF used. Besides the direct addition of THF to the crystalline *tert*-butyllithium leading to recrystallization, as described previously, the isolation of the crystalline compound **7** from *n*-pentane suspension was also achieved under the exact same conditions as in the *in situ* FTIR measurements. Therefore, we were able to derive the aggregation of *tert*-butyllithium with different amounts of THF as shown in Scheme 2.

To further support these results, quantum chemical calculations were performed showing a preference of $\Delta H = -14\ kJ\,mol^{-1}$ of the bridged dimer **1** over the separated aggregates when using 1.5 equivalents of THF. In an excess of THF the monomer **7** showed to be preferred over **1** by $\Delta H = -50\ kJ\,mol^{-1}$, which matches our experimental findings in the *in situ* FTIR study. For a better understanding of the enhanced reactivity we observed, we carried out additional quantum chemical calculations for the deprotonation of the simple silanes TMS and **3** starting from the respective aggregates **1** and **7** of *t*-BuLi with THF. According to our mechanistic assumptions based on the CIPE, we calculated the pre-reaction complex based on **1** in combination with the tilting of the bridging THF. In case of monomer **7**, the pre-reaction complexes and transition states were calculated with and without the release of one THF molecule. The quantum chemical calculations of the reaction pathways (see SI) result in a clear barrier lowering effect starting from the bridged dimer **1** in both reactions. Looking at hexamethyldisilane specifically, the deprotonation starting from **1** is preferred by about 40 $kJ\,mol^{-1}$, representing a significant reactivity enhancement

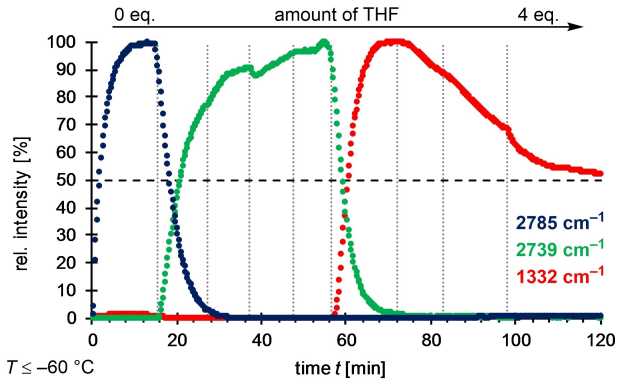
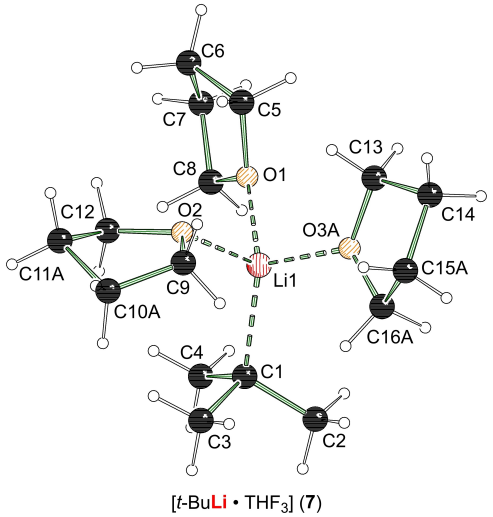
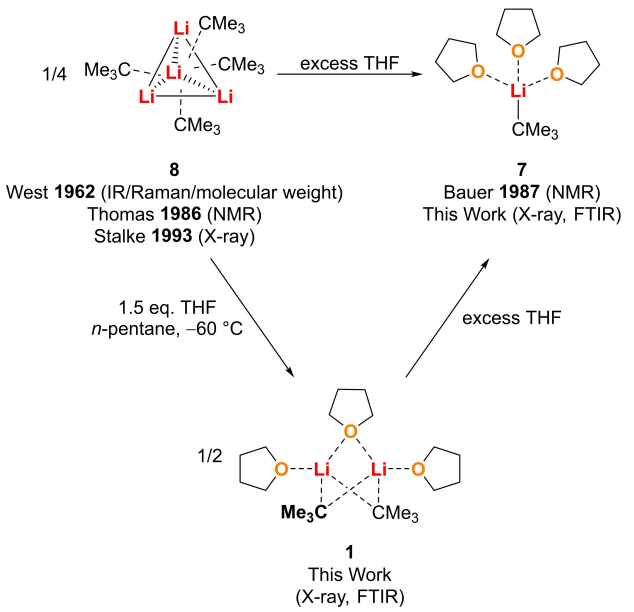


Figure 2. Plot of the normalized intensities of selected bands against the measurement time of the *in situ* FTIR experiment of *t*-BuLi with stepwise addition of 0.5 equivalents of THF in *n*-pentane. The three selected bands indicate three different species: Blue: 2785 cm^{-1} can be assigned to $\nu(CH_3)$; Green: 2739 cm^{-1} can be assigned to $\nu(CH_3)$; Red: 1332 cm^{-1} can be assigned to $\delta(CH_3)$.



[*t*-BuLi • THF_3] (**7**)

Figure 3. Molecular structure of [*t*-BuLi · 3 THF] (**7**) in the crystal. Minor disorder has been omitted for clarity. Small selection of bond lengths [Å]: O1-Li1 2.0145(12), O2-Li1 2.0376(12), O3A-Li1 1.9722(13), C1-Li1 2.1678(12). For further information on selected bond lengths and angles see SI Figure S2.



Scheme 2. The aggregation of *tert*-butyllithium with different amounts of THF in *n*-pentane.[7–9,12]

shown in the quantum chemical calculations. In case of TMS, the deprotonation based on aggregate **1** is preferred by at least 16 kJ mol^{-1}. A comparable effect could be seen in the reactivity studies performed.

To conclude our findings, we updated the aggregation of *tert*-butyllithium with THF as LEWIS-donor in non-polar suspension by determining the molecular structure of the aggregates **1** and **7** via single crystal X-ray diffraction. Due to the weak coordination of the bridging THF ligand in **1** we proposed a significant increase in the reactivity of *t*-BuLi when using 1.5 equivalents of THF in *n*-pentane. Through the deprotonation of TMS and other low C–H–acidic substrates, the increase in reactivity could be showcased and quantum chemically calculated. Since the usage of stoichiometric amounts of THF and *t*-BuLiK in *n*-pentane resulted in the formation of a suspension, no NMR measurements were possible to identify **1** in the suspension. The combination of an *in situ* FTIR study with quantum chemical calculations and the already mentioned X-ray diffraction data lead to the conclusion that **1** is very likely present in the suspension. **1** is a novel kind of alkyllithium aggregate, which contains formally saturated lithium cations with three strong and one weak contact. Due to the high reactivity, which is related to this specific structural feature, we decided to call these type of aggregates *"frustrated"* ones.

With this contribution, we would like to enlargen the understanding of alkyllithium aggregation and the structure reactivity relation. We also hope to help scientists in all chemical fields using alkyllithium reagents optimize their reaction conditions by deliberatly using lower quantities of ligands, which could also show promising results. Lastly, we would like to inspire the chemical community to enlargen the focus on the investigation of selectively formed solvent mixtures.

Supporting Information

The authors have cited additional references within the Supporting Information.[20–27] Material and methods, synthetic chemistry and compound characterization, single crystal X-ray data, GC/EI-MS data, IR spectra, NMR spectra, general information on the quantum chemical calculations are located in the SI.pdf file. All cartesian coordinates are included in a SI.xyz file.

Deposition Numbers 2304161 (for 1), 2304163 (for 7), and 2304162 (for 9) contain the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service.

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Conflict of Interests

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available in the supplementary material of this article.

Keywords: Alkyllithium chemistry · Lewis bases · Lithium · Aggregation · X-ray diffraction

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