Electronic Supplementary Information

Computational study of structural properties of lithium cation complexes with carbamate-modified disiloxanes

Steffen Jeschke,* Hans-Dieter Wiemhöfer and Christian Mück-Lichtenfeld

Institute of Inorganic and Analytical Chemistry, University Münster, Corrensstr. 28/30, 48149 Münster, Germany

*e-mail: s.jeschke@wwu.de

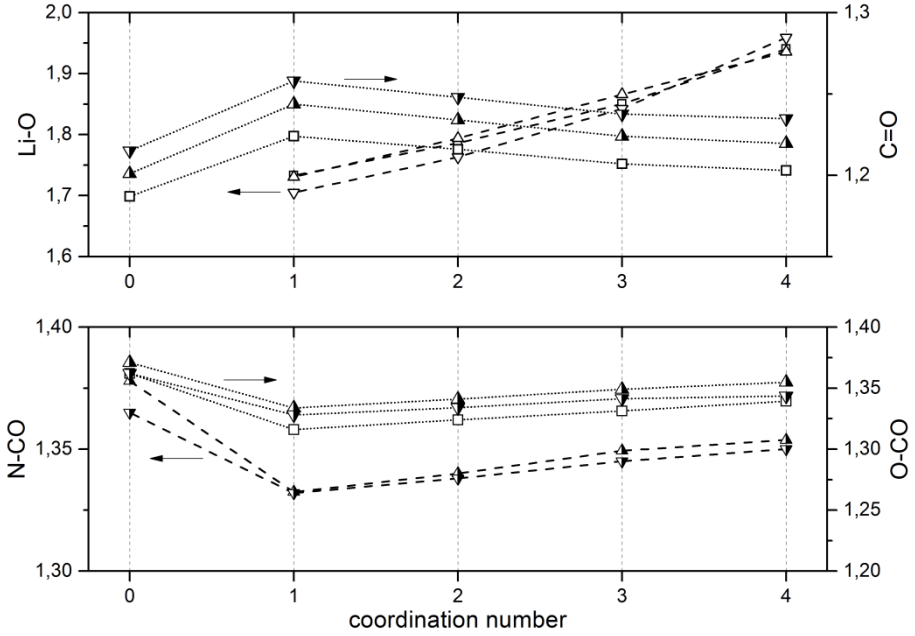

Figure S1 Examples of various bond length for solvents **1** (□), **3** (△) and **4** (▽); identical values for carbamate-modified disiloxanes and simplified carbamates are denoted as ◭ for **3**/**5** and ▼ for **4**/**6** [in Å].

Table T1 Atomic NBO charges of carbonyl functionalities in isolated solvents **1** - **6**.

	1	**2**	**3**	**4**	**5**	**6**
C=**O**	-0.56	-0.64	-0.61	-0.67	-0.63	-0.68
C=O	1.02	1.04	0.93	0.94	0.94	0.94
O–CO	-0.55	-0.54	-0.55	-0.58	-0.55	-0.57
N–CO	–	–	-0.51	-0.48	-0.52	-0.49

Table T2 Radius *r* and volume *V* of spherical cavities for solvation structure $[Li(\mathbf{S})_4]^+$ of solvents **1** - **6**.

	1	**2**	**3**	**4**	**5**	**6**
$r[Li(\mathbf{S})_4]^+$/Å	5.52	5.79	5.63	6.35	8.14	8.76
$V[Li(\mathbf{S})_4]^+$ /Å^3	705	813	748	1074	2259	2816

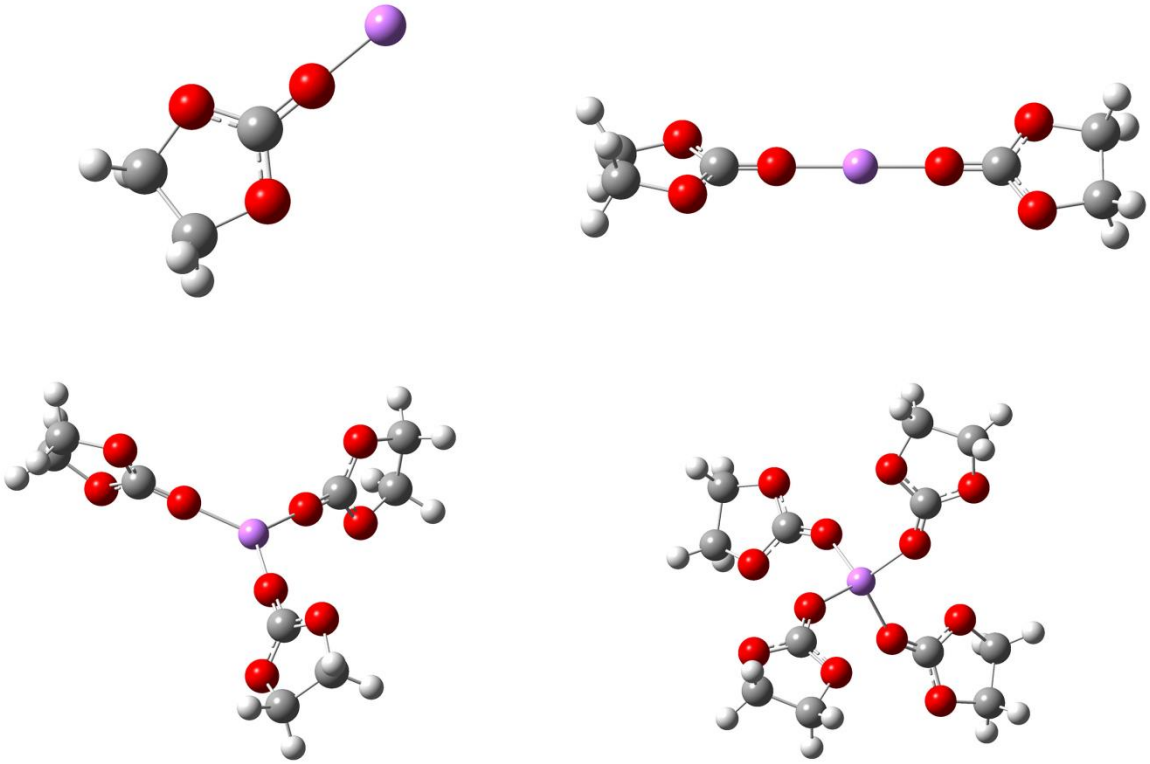

Figure S2 Geometries of solvation structures $[Li(\mathbf{1})_{n=1-4}]^+$ optimized at B3LYP/6-311G(d,p) level of theory.

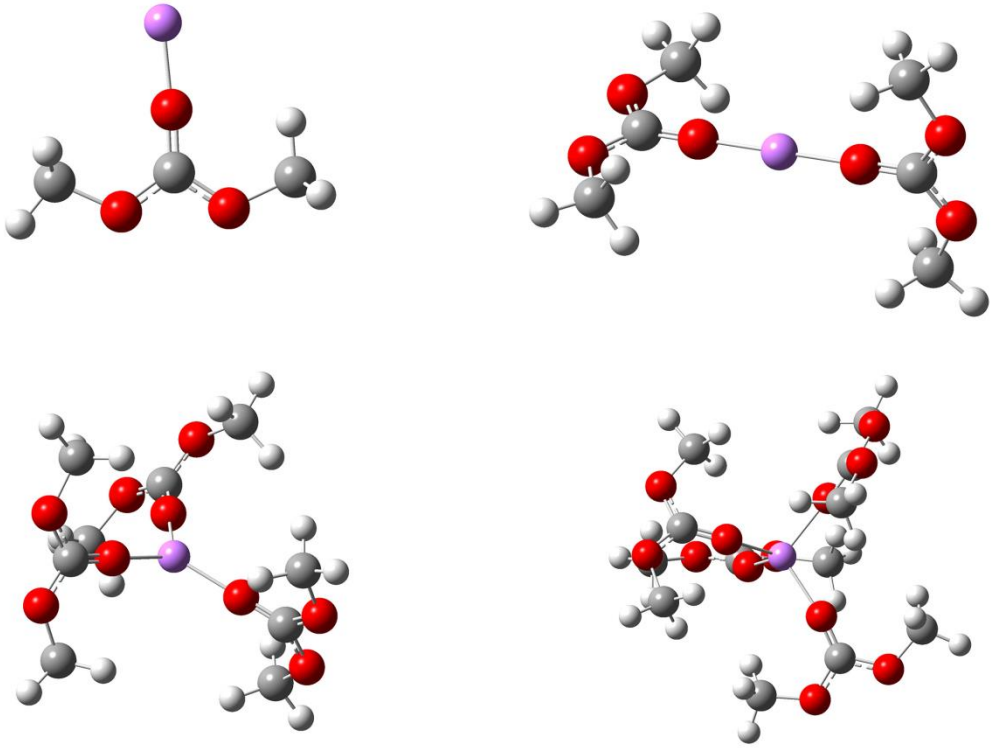

Figure S3 Geometries of solvation structures $[Li(\mathbf{2})_{n=1-4}]^+$ optimized at B3LYP/6-311G(d,p) level of theory.

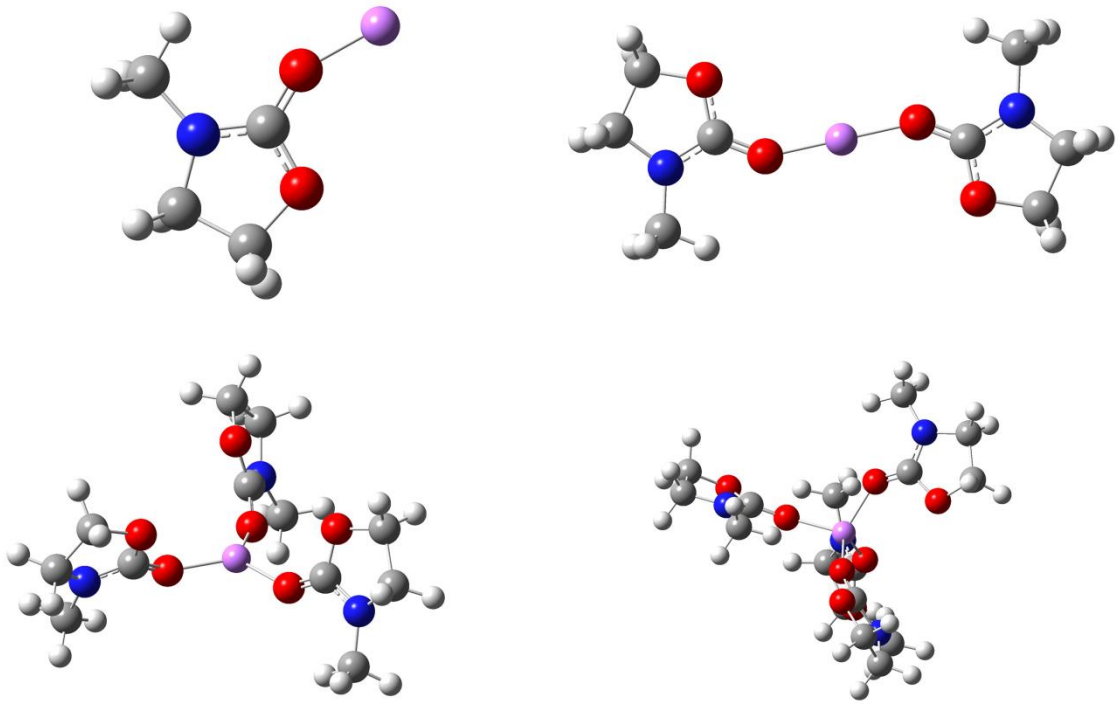

Figure S4 Geometries of solvation structures $[Li(\mathbf{3})_{n=1\text{-}4}]^+$ optimized at B3LYP/6-311G(d,p) level of theory.

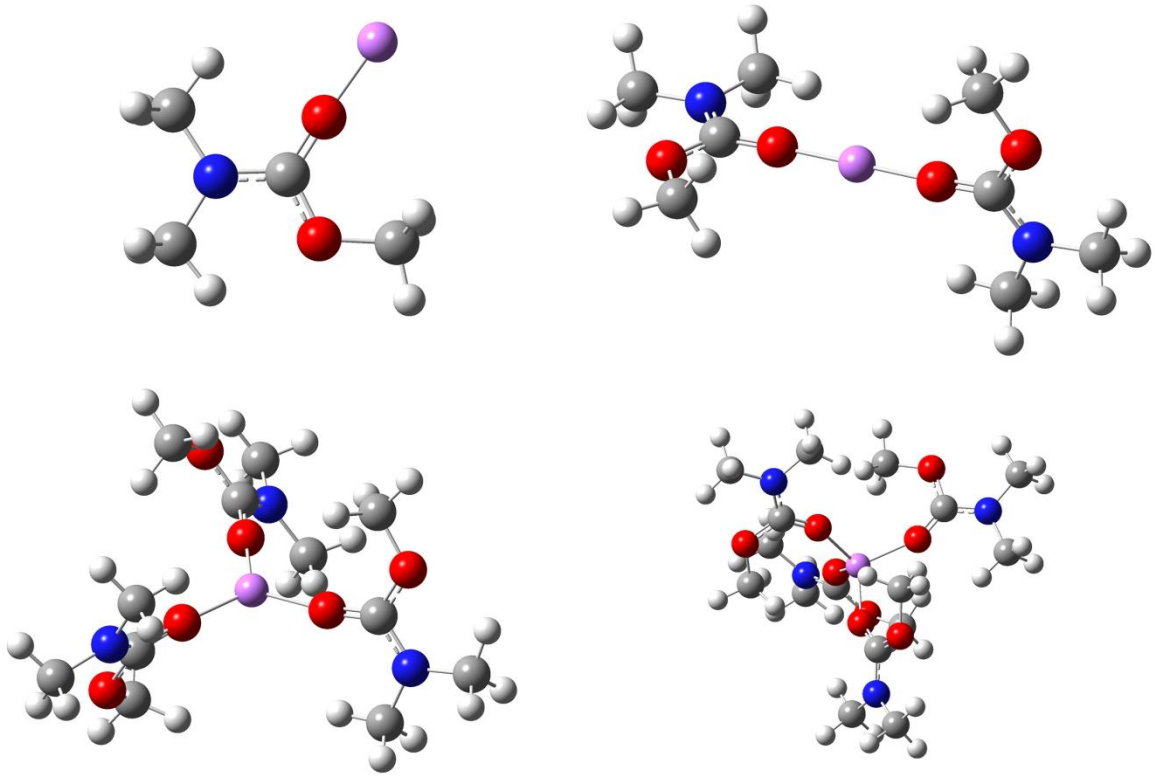

Figure S5 Geometries of solvation structures $[Li(\mathbf{4})_{n=1\text{-}4}]^+$ optimized at B3LYP/6-311G(d,p) level of theory.

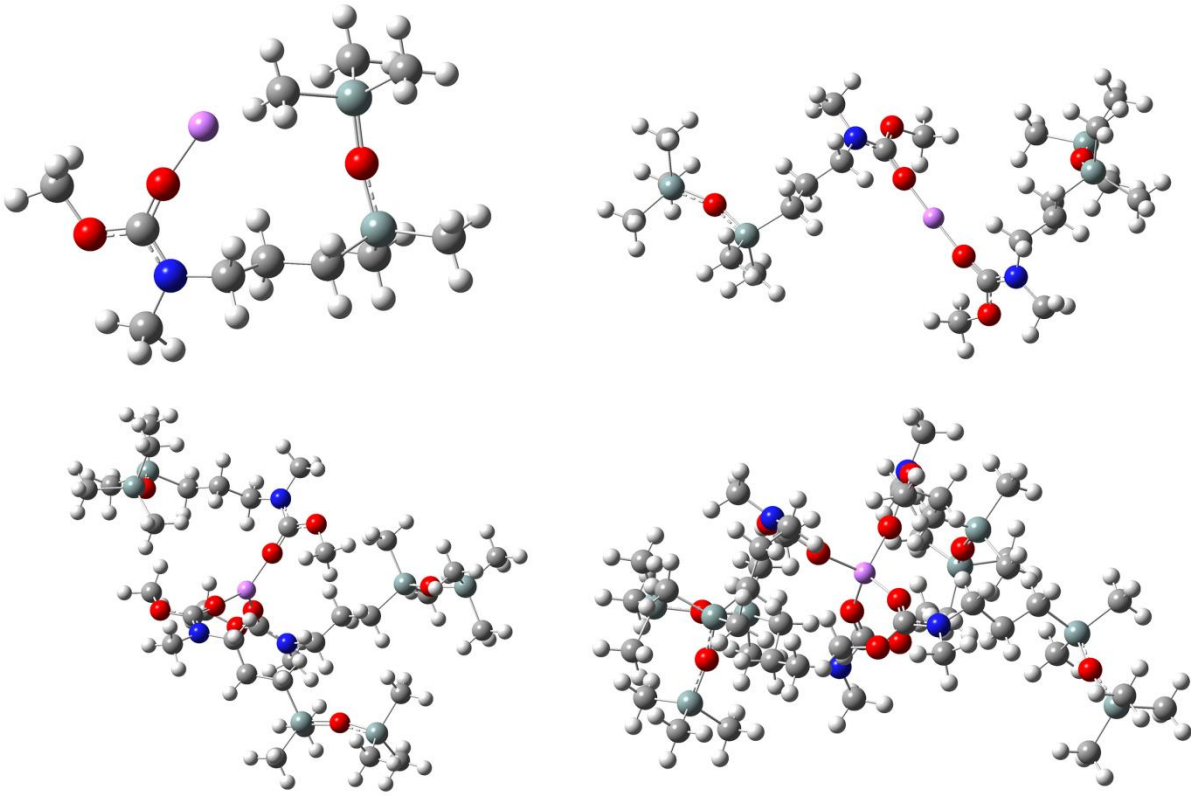

Figure S6 Geometries of solvation structures $[Li(\mathbf{6})_{n=1\text{-}4}]^+$ optimized at B3LYP/6-311G(d,p) level of theory.