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Supplemental Material

Lithiated Sulfoxides: α-Sulfinyl Functionalized Carbanions

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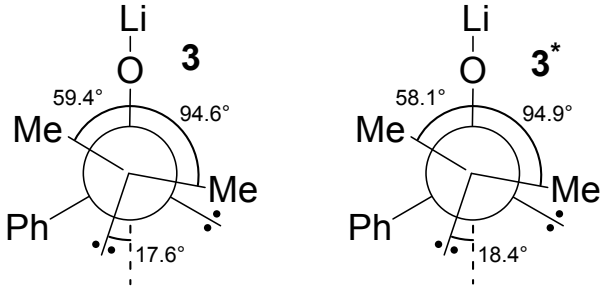
Table S1 Comparison of selected distances (in Å) and angles (in °) of the lithiated sulfoxides of the type $[Li_2\{CRR'S(O)Ar\}_2(TMEDA)_2]$ (**1**–**4**; experimental results and **1***–**4***; calculated results).

	R/R'	Ar	Li–O	Li···Li'	Li···C_α	O–Li–O'	O–Li···Li–O'
1	H/H	Ph	1.878(8)/1.882(8)/1.909(8)/1.900(8)	2.614(1)	3.775(1)/3.889(9)	90.9(3)/90.8(3)	159.1(5)
1*	H/H	Ph	1.941/1.936/1.937/1.938	2.685	3.995/3.978	87.7/87.7	157.2
2	H/H	*p*-Tol	1.843(1)/1.878(9)/1.917(9)/1.878(9)	2.558(1)	4.039(2)/4.007(1)	93.9(5)/91.9(9)	163.9(6)
2*	H/H	*p*-Tol	1.937/1.939/1.939/1.937	2.688	3.985/3.985	87.8/87.8	158.2
3	Me/Me	Ph	1.890(4)/1.914(4)/1.890(4)/1.914(4)	2.609(7)	4.144(4)/4.144(4)	92.0(2)/92.0(2)	162.4(2)
3*	Me/Me	Ph	1.925/1.946/1.948/1.925	2.648	4.224/4.226	86.3/86.2	159.5
4	H/Ph	Ph	1.903(6)/1.902(6)/1.909(6)/1.911(5)	2.646(8)	3.888(6)/3.769(7)	91.0(3)/90.5(3)	162.7(3)
4*	H/Ph	Ph	1.956/1.959/1.959/1.956	2.742	3.874/3.874	88.9/88.9	158.7

Table S2 Comparison of selected distances (in Å) and angles (in °) at the carbanionic C atom of the lithiated sulfoxides of the type $[Li_2\{CRR'S(O)Ar\}_2(TMEDA)_2]$ (**1**–**4**, experimental results; **1***–**4***, calculated results).

	R/R'	Ar	S–C_α	S–O	S–C_i	$\sum^a$	Δd^b	$\Delta\measuredangle^c$
1	H/H	Ph	1.660(5)/1.606(7)	1.576(3)/1.574(3)	1.809(5)/1.817(5)	-	-	-
1*	H/H	Ph	1.681/1.681	1.624/1.624	1.829/1.829	347.0/347.2	0.260/0.260	17.5/17.5
2	H/H	*p*-Tol	1.572(1)/1.665(7)	1.583(4)/1.581(4)	1.844(4)/1.821(3)	-	-	-
2*	H/H	*p*-Tol	1.681/1.681	1.625/1.625	1.827/1.827	347.0/347.0	0.260/0.260	17.3/17.3
3	Me/Me	Ph	1.646(2)/1.646(2)	1.583(1)/1.583(1)	1.809(2)/1.809(2)	355.0/355.0	0.208/0.208	17.6/17.6
3*	Me/Me	Ph	1.677/1.677	1.649/1.649	1.834/1.834	354.6/354.7	0.211/0.210	18.3/18.4
4	H/Ph	Ph	1.641(3)/1.666(5)	1.565(2)/1.573(2)	1.795(3)/1.826(5)	-	-	-
4*	H/Ph	Ph	1.687/1.687	1.614/1.614	1.826/1.826	359.5/359.5	0.060/0.058	16.4/16.4

a) Sum of angles around the α-C atom. b) Deviation of the α-C atom from the plane spanned by its substituents (S, C/H, C/H) c) Deviation of the lone pair at the carbanionic C atom from the antiperiplanar position to the S–O bond.



Graphical illustration of the structure of the carbanionic C atom in **3** (left) representing the structure in the solid state and **3*** (calculated parameters). The Newman projection is shown along the C–S vector.

Table S3 Comparison of the Wiberg bond indices of the lithium compounds of the type $[Li_2\{CRR'S(O)Ar\}_2(TMEDA)_2]$ (**1***–**4***) and the corresponding sulfoxides (**A***–**D***).

	R/R'	Ar	S–C_α	S–O	S–C_i	C_i–C_o	C_o–C_m
1*	H/H	Ph	1.35/1.35	0.84/0.84	0.91/0.91	1.41/1.41	1.44/1.44
A*	H/H	Ph	0.91	1.23	0.90	1.40	1.44
2*	H/H	*p*-Tol	1.35/1.35	0.83/0.83	0.91/0.91	1.41/1.39	1.42/1.45
B*	H/H	*p*-Tol	0.91	1.23	0.90	1.40	1.44
3*	Me/Me	Ph	1.35/1.35	0.79/0.79	0.89/0.89	1.40/1.41	1.44/1.42
C*	Me/Me	Ph	0.86	1.23	0.90	1.40	1.44
4*	H/Ph	Ph	1.24/1.24	0.87/0.87	0.91/0.91	1.40/1.41	1.44/1.42
D*	H/Ph	Ph	0.85	1.24	0.90	1.40	1.44

Table S4 Crystallographic data, data collection parameters, and refinement parameters for **1**, **2**, **3** and **4**·Et_2O.

	1[1)]	**2**[2)]	**3**[3)]	**4**·Et_2O[4)]
Empirical formula	$C_{26}H_{46}Li_2N_4O_2S_2$	$C_{28}H_{50}Li_2N_4O_2S_2$	$C_{30}H_{54}Li_2N_4O_2S_2$	$C_{42}H_{64}Li_2N_4O_3S_2$
M_r	524.67	552.72	580.77	750.97
Crystal System	triclinic	monoclinic	monoclinic	monoclinic
Space group	*P*–1	$P2_1/c$	*C*2/c	*C*2/c
a / Å	9.359(2)	19.731(3)	18.1825(1)	32.7559(2)
b / Å	17.329(3)	9.308(1)	10.4665(4)	14.9684(8)
c / Å	21.126(4)	19.687(3)	19.3943(9)	19.0716(1)
α / °	112.47(1)			
β / °	93.93(2)	112.117(2)	100.665(5)	96.636(4)
γ / °	90.27(2)			
V / Å^3	3156.7(1)	3349.7(8)	3627.1(3)	9288.2(9)
Z	4	4	4	8
D_{cal} / g·cm^{-3}	1.104	1.096	1.607	1.074
μ(Mo/Cu-Kα) / mm^{-1}	0.195 (Mo)	1.648 (Cu)	1.064 (Mo)	0.152 (Mo)
F(000)	1136	1200	1264	3248
θ range / °	2.09–25.00	4.85–60.00	2.96–25.00	2.61–25.00
Rfln collected	39931	14683	6938	21650
Rfln observed [$I > 2\sigma(I)$]	7252	2417	2362	3809
Rfln independent	10941 (R_{int} = 0.1746)	4817 (R_{int} = 0.0792)	3193 (R_{int} = 0.0344)	8090 (R_{int} = 0.0752)
Data/restraints/parameters	10941/400/707	4817/382/404	3193/98/181	8090/184/553
Types of restraints used	DFIX/DANG DELU/SIMU/ISOR	DFIX/DANG/EADP DELU/SIMU/ISOR	DFIX/SIMU/ ISOR	DFIX/DANG DELU/SIMU/ISOR
Goodness-of-fit on F^2	1.037	0.976	1.007	0.812
*R*1, *wR*2 [$I > 2\sigma(I)$]	0.0987, 0.2546	0.0996, 0.2687	0.0484, 0.0949	0.0587, 0.1185
*R*1, *wR*2 (all data)	0.1357, 0.2823	0.1520, 0.3157	0.0763, 0.1028	0.1424, 0.1628
Largest diff. peak and hole/ e Å^{-3}	1.752 and –0.372	0.344 d –0.351	0.379 and –0.224	0.444 and –0.174

1) Comments for **1**:

Crystals of **1**, approximately plate-like (ca. 0.5 × 0.5 × 0.1 mm^{-3}), suitable for X-ray crystallographic studies, could be grown from concentrated solutions at ca. –7 degree °C only. Crystallization at lower temperatures gave extremely tiny crystals, not suitable for crystallographic studies. During the crystal selection under the optical microscope at about 0 °C the original formed crystals were covered with further material which could not be completely removed. The data integration revealed that the crystals were (slightly) twinned with more than 2 additional individual domains. As the additional minor domains overlapped to a very high extend with the major domain it was tried to perform the measurement at longer crystal-to-detector distances. Therefore, however, unusual large exposure times for the measurement of individual frames were required, leading to an icing of the crystal at poor data set completeness. Due to that the reported data refer to a measurement at a short distance, intensities and/or positions of individual reflections could be read poorly only, which is expressed by a poor R_{int} value.

A comparatively large residual density peak of 1.75 e $Å^{-3}$ is observed at a distance of 1.11 Å from the sulfur atom S3. The next three highest peaks of 1.11, 1.11 and 0.85 e $Å^{-3}$ are also located at distances of up to 1.3 Å away from the sulfur atoms S2, S3 and S4, respectively. This may indicate a disorder of the $PhSCH_2$ fragments. Trials to apply a model of disorder (either for individual S atoms or for the $PhSCH_2$ fragments) gave, however, non-reliable results.

The carbon atoms C17/18 and C49/50 were refined disordered on two positions with occupancy factors of 0.56 *vs.* 0.44 and 0.46 *vs.* 0.54, respectively. The thereby used constraints are given below:

```
DELU    0.010   0.010 C47 C48 C49' C50' C51 C52 N7 N8 LI4
SIMU    0.040   0.080   1.700 C47 C48 C49' C50' C51 C52 N7 N8 LI4
ISOR    0.100 C47 C48 C49' C50' C51 C52 N7 N8 LI4
DELU    0.010   0.010 C47 C48 C49 C50 C51 C52 N7 N8 LI4
SIMU    0.040   0.080   1.700 C47 C48 C49 C50 C51 C52 N7 N8 LI4
ISOR    0.100 C47 C48 C49 C50 C51 C52 N7 N8 LI4
DFIX    1.450   0.020 N2 C17
DFIX    1.450   0.020 C17 C18
DFIX    1.450   0.020 C18 N1
DFIX    1.450   0.020 N2 C17'
DFIX    1.450   0.020 C17' C18'
DFIX    1.450   0.020 C18' N1
DELU    0.010   0.010 C15 C16 C17' C18' C19 C20 N2 LI1
SIMU    0.040   0.080   1.700 C15 C16 C17' C18' C19 C20 N2 LI1
ISOR    0.100 C15 C16 C17' C18' C19 C20 N2 LI1
DELU    0.010   0.010 C15 C16 C17 C18 C19 C20 N1 N2 LI1
```

```
SIMU    0.040   0.080   1.700 C15 C16 C17 C18 C19 C20 N1 N2 LI1
ISOR    0.100 C15 C16 C17 C18 C19 C20 N1 N2 LI1
DANG    2.850   0.040 LI4 C50'
DANG    2.250   0.040 C19 C18'
DANG    2.40   0.040 C17' C16
DANG    2.40   0.040 C47 C49'
DANG    2.300   0.040 C15 C17
```

2) Comments for **2**:

Crystals of **2** were all weakly diffractive, which forced the use of "sealed-tube" Cu Kα radiation and a measurement at 110 K. Even in that case exposure times were comparatively large and the crystal did start to ice, for which reason data collection was limited to 120° in 2θ only. Most likely an intrinsic disorder is responsible for the weak diffractive properties. Eventually, data integration did reveal the presence of several domains, at least four individual ones, which did significantly overlap. Trials to increase the crystal-to-detector distance gave, however, no reasonable 'incoming' intensities. Therefore, the original data set as reported here was used for refinement, taking thereby reflections of the 'major' domain (ca. 40 % of all reflections). No absorption correction was applied, although overlapping reflections were (partially) removed by finalizing the data set.

A number of atoms/group could be refined disordered over two positions with occupancy factors as following: S1/C1 with 0.78 *vs.* 0.22; S2/C9 with 0.91 *vs.* 0.09; C19/20 with 0.36 *vs.* 0.64 and C23–26/N3 with 0.77 *vs.* 0.23. The thereby required restraints are given below. Trials to refine further atoms or even fragments as disordered gave, however, non-reliable results:

```
DFIX    1.580   0.020 S1 O1
DFIX    1.550   0.020 S1 C1
DFIX    1.800   0.020 S1 C2
DANG    3.300   0.040 S1 LI2
DANG    3.100   0.040 S1 LI1
DANG    2.800   0.040 S1 C3
DANG    2.800   0.040 S1 C7
DFIX    1.580   0.020 S1' O1
DFIX    1.550   0.020 S1' C1
DFIX    1.800   0.020 S1' C2
DANG    3.300   0.040 S1' LI2
DANG    3.100   0.040 S1' LI1
DANG    2.800   0.040 S1' C3
DANG    2.800   0.040 S1' C7
DFIX    1.580   0.020 S2 O2
DFIX    1.600   0.020 S2 C9
DFIX    1.800   0.020 S2 C10
DANG    2.780   0.040 S2 C15
DANG    2.780   0.040 S2 C11
DANG    3.300   0.040 S2 LI1
DANG    3.100   0.040 LI2 S2
```

```
DFIX    1.580   0.020 S2' O2
DFIX    1.600   0.020 S2' C9
DFIX    1.800   0.020 S2' C10
DANG    2.780   0.040 S2' C15
DANG    2.780   0.040 S2' C11
DANG    3.300   0.040 S2' LI1
DANG    3.100   0.040 LI2 S2'
DANG    2.750   0.040 C1 C2
DANG    2.750   0.040 C1 O1
DANG    2.750   0.040 C1' C2
DANG    2.750   0.040 C1' O1
EADP S2 S2'
DANG    2.800   0.040 C9 O2
DANG    2.750   0.040 C9 C10
DANG    2.800   0.040 C9' O2
DANG    2.750   0.040 C9' C10
EADP C9 C9'
DFIX    1.480   0.020 N1 C19
DFIX    1.450   0.020 C19 C20
DFIX    1.480   0.020 C20 N2
DANG    2.450   0.040 C19 C17
DANG    2.450   0.040 C19 C18
DANG    2.450   0.040 C20 C21
DANG    2.450   0.040 C20 C22
DFIX    1.480   0.020 N1 C19'
DFIX    1.450   0.020 C19' C20'
DFIX    1.480   0.020 C20' N2
DANG    2.450   0.040 C19' C17
DANG    2.450   0.040 C19' C18
DANG    2.450   0.040 C20' C21
DANG    2.450   0.040 C20' C22
DANG    3.000   0.040 C19' LI1
EADP C19 C19'
DFIX    2.150   0.020 LI2 N3
DFIX    1.500   0.020 N3 C24
DFIX    1.450   0.020 N3 C23
DFIX    1.450   0.020 N3 C25
DFIX    1.450   0.020 C25 C26
DFIX    1.480   0.020 C26 N4
DANG    2.420   0.040 C28 C26
DANG    2.440   0.040 C27 C26
DANG    2.490   0.040 N4 C25
DANG    2.460   0.040 C26 N3
DANG    2.420   0.040 C25 C23
DANG    2.440   0.040 C25 C24
DFIX    2.150   0.020 LI2 N3'
DFIX    1.500   0.020 N3' C24'
DFIX    1.450   0.020 N3' C23'
DFIX    1.450   0.020 N3' C25'
DFIX    1.450   0.020 C25' C26'
DFIX    1.480   0.020 C26' N4
DANG    2.420   0.040 C28 C26'
DANG    2.440   0.040 C27 C26'
DANG    2.490   0.040 N4 C25'
DANG    2.460   0.040 C26' N3'
DANG    2.420   0.040 C25' C23'
DANG    2.440   0.040 C25' C24'
DELU    0.010   0.010 C23 C24 C25 C26 N3
SIMU    0.040   0.080   1.700 C23 C24 C25 C26 N3
ISOR    0.100 C23 C24 C25 C26 N3
DELU    0.010   0.010 C23' C24' C25' C26' N3'
```

```
SIMU     0.040   0.080   1.700 C23' C24' C25' C26' N3'
ISOR     0.100 C23' C24' C25' C26' N3'
DELU     0.010   0.010 C19' C20' C21 C22 N1 N2 LI1
SIMU     0.040   0.080   1.700 C19' C20' C21 C22 N1 N2 LI1
ISOR     0.100 C19' C20' C21 C22 N1 N2 LI1
DELU     0.010   0.010 C2 S1' C1' LI2
SIMU     0.040   0.080   1.700 C2 S1' C1' LI2
ISOR     0.100 C2 S1' C1' LI2
DELU     0.010   0.010 C21 C22 N2 O1 O2 LI1 LI2
SIMU     0.040   0.080   1.700 C21 C22 N2 O1 O2 LI1 LI2
ISOR     0.100 C21 C22 N2 O1 O2 LI1 LI2
```

3) Comments for **3**:

Restraints were applied in order to refine a part of the molecule anisotropically, which was otherwise not possible.

```
DELU     0.010   0.010 LI1 C10 C11 C12 C13 N1 N2 O1
SIMU     0.040   0.080   1.700 LI1 C10 C11 C12 C13 N1 N2 O1
ISOR     0.100 LI1 C10 C11 C12 C13 N1 N2 O1
```

4) Comments for **4**:

One PhSCHPh fragment including S2A, C14A–26A was refined disordered over two positions with occupancy factors of 0.79 *vs.* 0.21. Additionally, one diethyl ether molecule as packing solvent was refined disordered over two positions, whereby here non-hydrogen atoms were refined isotropically only. The following restraints were applied:

```
DFIX  1.470 0.020 O3A C41A
DFIX  1.500 0.020 C41A C42A
DANG  2.450 0.040 O3A C42A
DFIX  1.450 0.020 O3A C39A
DFIX  1.500 0.020 C39A C40A
DANG  2.450 0.040 O3A C40A
DANG  2.450 0.040 C39A C41A
DFIX  1.470 0.020 O3B C41B
DFIX  1.500 0.020 C41B C42B
DANG  2.450 0.040 O3B C42B
DFIX  1.450 0.020 O3B C39B
DFIX  1.500 0.020 C39B C40B
DANG  2.450 0.040 O3B C40B
DANG  2.450 0.040 C39B C41B
FREE C41B C39B
DFIX     1.690   0.020 S2B C21B
DFIX     1.720   0.020 S2A C21A
DELU     0.010   0.010 C15B C16B C17B C18B C19B C20B
SIMU     0.040   0.080   1.700 C15B C16B C17B C18B C19B C20B
ISOR     0.100 C15B C16B C17B C18B C19B C20B
DELU     0.010   0.010 C21B C22B C23B C24B C25B C26B
SIMU     0.040   0.080   1.700 C21B C22B C23B C24B C25B C26B
ISOR     0.100 C21B C22B C23B C24B C25B C26B
```

Table S5 Crystallographic data, data collection parameters, and refinement parameters for **3a'**, **4a'** and **4b'**.

	3a'	**4a'**	**4b'**
Empirical formula	$C_{16}H_{18}O_2S$	$C_{20}H_{18}O_2S$	$C_{26}H_{22}O_2S$
M_r	274.36	322.40	398.50
Crystal System	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a / Å	8.965(6)	11.211(4)	8.699(3)
b / Å	11.926(7)	6.441(3)	11.456(6)
c / Å	13.283(9)	24.169(9)	20.803(9)
β / °	100.343(6)	108.848(3)	105.316(3)
V / Å^3	1397.1(2)	1651.63(11)	1999.61(2)
Z	4	4	4
D_{cal} / g·cm^{-3}	1.304	1.297	1.324
μ(Mo -Kα) / mm^{-1}	0.227	0.203	0.182
F(000)	584	680	840
θ range / °	2.87–26.00	3.01–26.00	2.70–25.99
Rfln collected	8902	21236	20417
Rfln observed [$I > 2\sigma(I)$]	2284	2836	3053
Rfln independent	2736	3228	3922
	(R_{int} = 0.0229)	(R_{int} = 0.0305)	(R_{int} = 0.0309)
Data/restraints/parameters	2736/0/177	3228/0/212	2922/0/265
Goodness-of-fit on F^2	1.038	1.061	0.926
$R1$, $wR2$ [$I > 2\sigma(I)$]	0.0267, 0.0680	0.0284, 0.0776	0.0295, 0.0709
$R1$, $wR2$ (all data)	0.0334, 0.0693	0.0327, 0.0793	0.0428, 0.0740
Largest diff. peak and hole/ e Å^{-3}	0.262 and –0.278	0.215 and –0.234	0.219 and –0.236

Figures

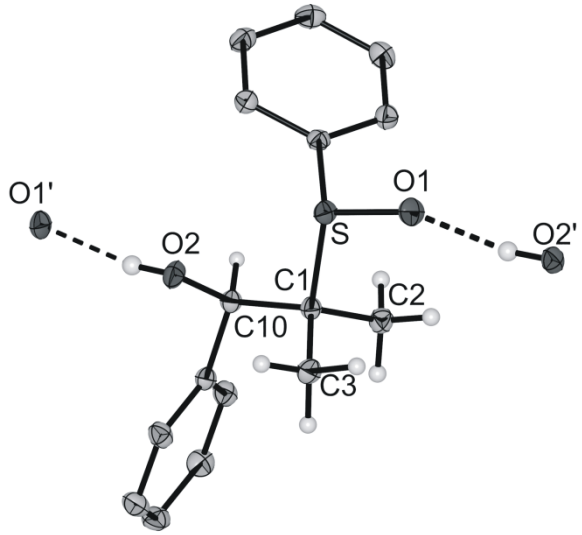


Fig. S1 Structure of $PhS(O)CMe_2CHPhOH$ in crystals of **3a'**; hydrogen bonds are shown by dashed lines (thermal ellipsoids at 30%; aromatic H atoms are not shown). Selected distances (in Å) and angles (in °): S–C1 1.876(1), S–O1 1.502(9), O1–S–C1 105.5(5), O1–S–C4 105.1(6), C1–S–C4 101.5(5). O2–H···O1': O2···O1' 2.727(1), O2–H 0.84, O1···H' 1.98, O2–H···O1' 170.

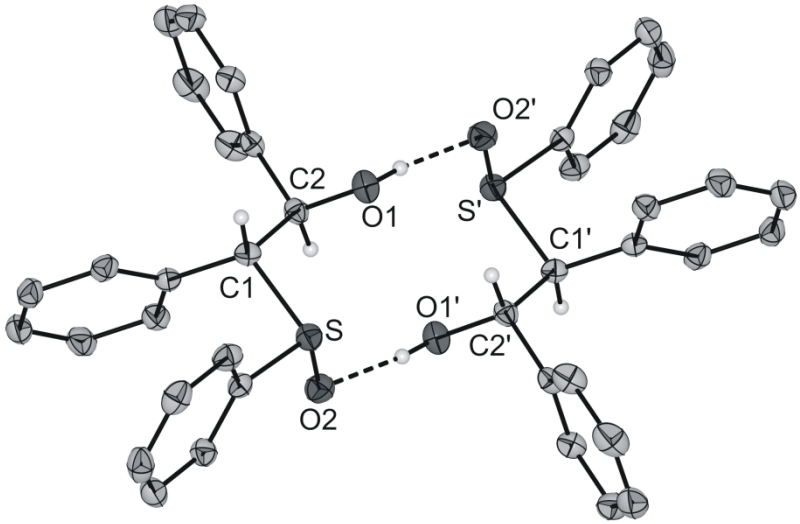


Fig. S2 Dinuclear structure of PhS(O)CHPhCHPhOH in crystals of **4a'**; hydrogen bonds are shown by dashed lines (thermal ellipsoids at 30%; aromatic H atoms are not shown). Selected distances (in Å) and angles (in °): S–C1 1.860(1), S–O2 1.507(1), O2–S–C1 105.9(5), O2–S–C15 106.2(5), C1–S–C15 99.2(5). O1–H···O2': O2···O1' 2.710(1), O1–H 0.91, O2···H' 1.88, O1–H···O2' 170.

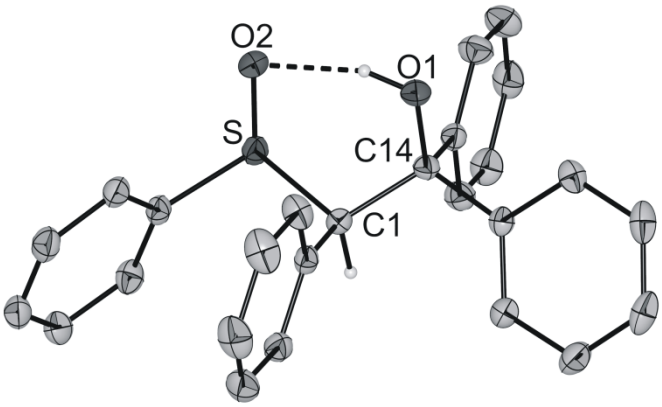


Fig. S3 Molecular structure of $PhS(O)CHPhCPh_2OH$ in crystals of **4b'**; hydrogen bond is shown by a dashed line (thermal ellipsoids at 30%; aromatic H atoms are not shown). Selected distances (in Å) and angles (in °): S–C1 1.879(1), S–O2 1.508(1), O2–S–C1 106.3(6), O2–S–C8 107.2(6), C1–S–C8 98.3(6), O1–H···O2': O2···O1' 2.710(1), O1–H 0.87, O2–H 1.88, O1–H···O2' 158.

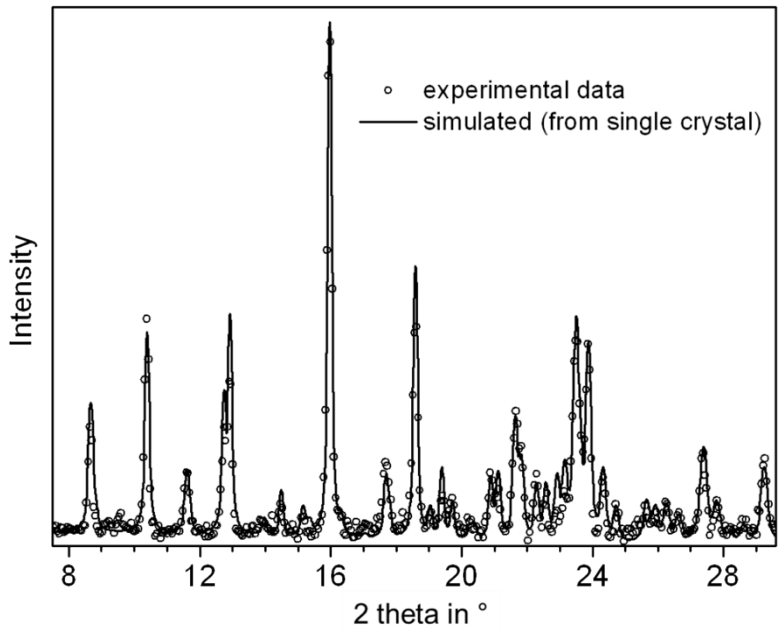


Fig. S4 X-ray powder diffraction measurement and simulated diffraction pattern (from X-ray single crystal measurements data) of **4b**. Refinement of the cell parameters led to: a = 8.799 Å, b = 11.512 Å, c = 21.087 Å, β = 105.21 °. Small deviations from the single crystal results are due to different measuring temperatures (200 K for single crystal and 300 K for powder).

Protocol of the Quantum Chemical Calculations

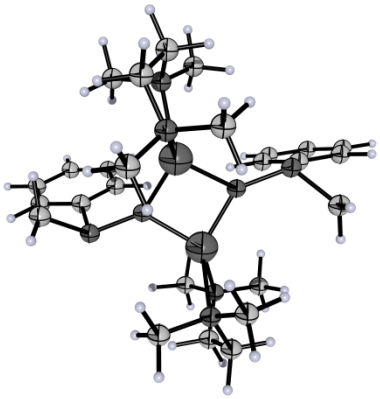
The following section contains potential energies, Gibbs free energies (298.15 K) with consideration of solvent effects (THF) and Cartesian coordinates of all structures calculated within this work.

Equilibrium Structure of $[Li_2\{CH_2S(O)Ph\}_2(TMEDA)_2]$ (1^*)

(file: P.ISS.log)

E(RB3LYP) –2199.42264094 a.u.

Sum of electronic and thermal Free Energies –2198.742470 a.u.



S	2.76420000	-1.11100000	-0.55210000
O	1.29330000	-0.42490000	-0.48930000
Li	-0.43470000	-1.24650000	-0.79700000
Li	0.42890000	1.29470000	-0.70680000
C	-0.82310000	-4.13270000	-0.94940000
N	-0.97000000	-3.17340000	0.16370000
N	-0.70780000	-2.35920000	-2.71020000
O	-1.30250000	0.45180000	-0.46350000
H	-1.28330000	3.31400000	-2.30810000
C	1.35640000	3.76280000	-2.00410000
C	0.80100000	4.19480000	-0.64600000
N	0.68560000	2.56160000	-2.53880000
N	0.95590000	3.15590000	0.39190000
H	-1.32080000	-5.09100000	-0.71320000
H	0.24340000	-4.35310000	-1.05990000
C	-1.38060000	-3.59680000	-2.26910000
C	-0.07630000	-3.53860000	1.27230000
C	-2.35820000	-3.12500000	0.64900000
C	0.61750000	-2.64510000	-3.28050000
C	-1.53010000	-1.65730000	-3.70570000

S	-2.77100000	1.14530000	-0.45140000
C	-0.64170000	2.88710000	-3.08220000
H	2.42340000	3.53610000	-1.91400000
H	1.27310000	4.60990000	-2.70940000
H	-0.26680000	4.41810000	-0.73640000
H	1.29540000	5.13500000	-0.34030000
C	1.50830000	1.94300000	-3.58810000
C	0.06570000	3.43510000	1.52790000
C	2.34630000	3.07670000	0.86680000
H	-1.30070000	-4.38720000	-3.03790000
H	-2.44680000	-3.37530000	-2.15910000
H	-0.18430000	-2.81250000	2.08320000
H	0.96330000	-3.52370000	0.93270000
H	-0.30310000	-4.54300000	1.67290000
H	-2.43560000	-2.39370000	1.45760000
H	-2.69110000	-4.10880000	1.02660000
H	-3.03550000	-2.81230000	-0.14930000
H	1.10170000	-1.70640000	-3.56330000
H	0.54460000	-3.29020000	-4.17490000
H	1.25720000	-3.13880000	-2.54550000
H	-1.02160000	-0.73960000	-4.01610000
H	-2.49200000	-1.38150000	-3.26530000
H	-1.70870000	-2.27520000	-4.60450000
H	-1.12090000	1.97290000	-3.44300000
H	-0.57320000	3.60510000	-3.91970000
H	2.46910000	1.62980000	-3.17030000
H	1.68920000	2.63260000	-4.43270000
H	0.99880000	1.05510000	-3.97400000
H	0.17790000	2.65080000	2.28200000
H	-0.97510000	3.44350000	1.19180000
H	0.29190000	4.40740000	2.00160000
H	2.43000000	2.28760000	1.61840000
H	2.67770000	4.03090000	1.31490000
H	3.02120000	2.82660000	0.04460000
C	4.00020000	-0.32570000	-1.37650000
C	-4.02250000	0.43190000	-1.31770000
H	4.21380000	0.71410000	-1.12190000
H	4.01920000	-0.58140000	-2.43490000
C	3.27610000	-0.90150000	1.19110000
C	2.32250000	-0.61120000	2.17190000
C	4.60920000	-1.12580000	1.55760000
C	2.70620000	-0.52250000	3.51490000
H	1.29440000	-0.44390000	1.87120000
C	4.98680000	-1.03830000	2.90090000
H	5.34150000	-1.34820000	0.78850000
C	4.03770000	-0.73550000	3.88380000
H	1.96210000	-0.28570000	4.27190000
H	6.02510000	-1.20440000	3.17790000
H	4.33380000	-0.66740000	4.92750000
C	-3.25830000	0.80270000	1.27800000
C	-4.58700000	0.98890000	1.67990000

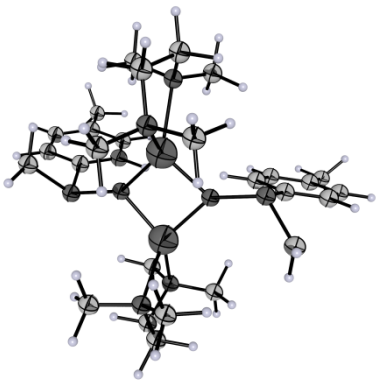
C	-2.28810000	0.44900000	2.22130000
C	-4.94360000	0.80060000	3.01860000
H	-5.33260000	1.26170000	0.94060000
C	-2.65050000	0.26010000	3.55980000
H	-1.26360000	0.31160000	1.89470000
C	-3.97760000	0.43510000	3.96290000
H	-5.97860000	0.93770000	3.32200000
H	-1.89310000	-0.02480000	4.28630000
H	-4.25710000	0.28930000	5.00320000
H	-4.05200000	0.76950000	-2.35280000
H	-4.23510000	-0.62470000	-1.14440000

Equilibrium Structure [Li_2{$CH_2S(O)$*p*-Tol}$_2$(TMEDA)$_2$] (2*)

(file: P.TolSSopt.log)

E(RB3LYP) –2278.05938201 a.u.

Sum of electronic and thermal Free Energies –2276.840405 a.u.



S	2.79480000	-0.81310000	1.06540000
S	-2.79480000	-0.81320000	-1.06530000
C	-0.01550000	1.12140000	3.47240000
N	-0.90920000	-0.00820000	3.17960000
H	1.02600000	0.78800000	3.44880000
H	-0.22190000	1.56660000	4.46250000
H	-0.14600000	1.89730000	2.71250000
C	-2.30160000	0.46540000	3.14160000
H	-2.97990000	-0.35140000	2.88300000
H	-2.40280000	1.23790000	2.37520000
H	-2.61410000	0.88620000	4.11460000
C	-0.73270000	-1.07460000	4.18580000
C	-1.29070000	-2.42230000	3.72470000
H	0.33910000	-1.16730000	4.38790000
H	-1.21170000	-0.79760000	5.14270000
N	-0.63580000	-2.92050000	2.49940000
H	-2.36110000	-2.32920000	3.51610000

H	-1.19290000	-3.15060000	4.55050000
C	0.69750000	-3.46860000	2.79070000
H	1.34190000	-2.70560000	3.23310000
H	1.16650000	-3.79870000	1.85990000
H	0.64110000	-4.32810000	3.48330000
C	-1.46320000	-3.95340000	1.86000000
H	-2.43110000	-3.53110000	1.57560000
H	-1.62920000	-4.82090000	2.52450000
H	-0.96550000	-4.30720000	0.95190000
C	0.01540000	1.12100000	-3.47260000
N	0.90920000	-0.00870000	-3.17960000
H	-1.02600000	0.78760000	-3.44900000
H	0.22200000	1.56600000	-4.46270000
H	0.14590000	1.89690000	-2.71280000
C	2.30160000	0.46490000	-3.14160000
H	2.97980000	-0.35180000	-2.88290000
H	2.40270000	1.23760000	-2.37530000
H	2.61410000	0.88560000	-4.11470000
C	0.73270000	-1.07520000	-4.18570000
C	1.29070000	-2.42280000	-3.72440000
H	-0.33910000	-1.16790000	-4.38790000
H	1.21170000	-0.79830000	-5.14270000
N	0.63570000	-2.92090000	-2.49910000
H	2.36110000	-2.32970000	-3.51580000
H	1.19280000	-3.15120000	-4.55020000
Li	0.40550000	-1.06130000	-1.28120000
C	-0.69770000	-3.46890000	-2.79040000
H	-1.34200000	-2.70590000	-3.23290000
H	-1.16670000	-3.79890000	-1.85960000
H	-0.64130000	-4.32850000	-3.48300000
C	1.46310000	-3.95380000	-1.85950000
H	0.96530000	-4.30740000	-0.95150000
H	2.43090000	-3.53140000	-1.57520000
H	1.62900000	-4.82130000	-2.52400000
Li	-0.40550000	-1.06110000	1.28130000
O	1.30740000	-0.79670000	0.41210000
O	-1.30740000	-0.79680000	-0.41200000
C	4.02180000	-1.65500000	0.28290000
H	4.20570000	-1.43900000	-0.77130000
H	4.05540000	-2.70340000	0.57660000
C	-4.02190000	-1.65490000	-0.28270000
H	-4.20580000	-1.43870000	0.77150000
H	-4.05560000	-2.70330000	-0.57620000
C	3.27720000	0.92470000	0.77450000
C	4.60960000	1.32400000	0.94380000
C	2.30840000	1.88470000	0.47550000
C	4.96210000	2.66580000	0.79140000
H	5.36340000	0.57890000	1.17610000
C	2.67370000	3.22750000	0.32320000
H	1.27780000	1.57200000	0.35000000
C	4.00270000	3.64340000	0.47650000

H	6.00320000	2.95790000	0.91750000
H	1.90790000	3.96160000	0.07990000
C	4.40060000	5.09180000	0.30470000
H	4.94140000	5.46450000	1.18340000
H	5.06450000	5.22190000	-0.55980000
H	3.52470000	5.73090000	0.15190000
C	-3.27720000	0.92470000	-0.77460000
C	-4.60950000	1.32410000	-0.94400000
C	-2.30830000	1.88470000	-0.47570000
C	-4.96200000	2.66590000	-0.79170000
H	-5.36340000	0.57900000	-1.17620000
C	-2.67350000	3.22750000	-0.32360000
H	-1.27780000	1.57190000	-0.35020000
C	-4.00250000	3.64350000	-0.47690000
H	-6.00300000	2.95800000	-0.91800000
H	-1.90770000	3.96160000	-0.08040000
C	-4.40030000	5.09190000	-0.30510000
H	-4.94350000	5.46390000	-1.18260000
H	-5.06210000	5.22240000	0.56100000
H	-3.52430000	5.73140000	-0.15480000

Equilibrium Structure $[Li_2\{CMe_2S(O)Ph\}_2(TMEDA)_2]$ (3^*)

(file: P.ISOSSopt2.log)

E(RB3LYP) –2356.66773793 a.u.

Sum of electronic and thermal Free Energies –2355.375813 a.u.

Li	-0.23270000	-0.47740000	1.35210000
O	-1.37310000	-0.37980000	-0.19610000
O	1.37060000	-0.32760000	0.25550000
N	-0.35040000	-2.22270000	2.75660000
N	-0.37670000	0.74390000	3.25600000
Li	0.23000000	-0.72960000	-1.24260000
C	4.18730000	-1.04260000	0.20800000
C	4.51250000	-2.36990000	0.86310000
C	4.61700000	-0.89840000	-1.23320000

S	2.89510000	-0.20440000	0.87080000
H	4.18880000	-2.40230000	1.91150000
H	5.60110000	-2.54140000	0.85320000
H	4.06130000	-3.24490000	0.35620000
H	4.40090000	0.09770000	-1.63600000
H	4.14730000	-1.63570000	-1.91280000
H	5.70350000	-1.05710000	-1.32230000
C	3.25120000	1.52800000	0.38650000
C	2.25100000	2.35360000	-0.13320000
C	4.52410000	2.05450000	0.64110000
C	2.52910000	3.69560000	-0.42120000
H	1.26820000	1.93270000	-0.31230000
C	3.80070000	4.22100000	-0.17620000
H	1.74840000	4.32910000	-0.83630000
C	4.79730000	3.39550000	0.35850000
H	4.01430000	5.26390000	-0.39680000
H	5.78980000	3.79450000	0.55360000
H	5.29610000	1.40500000	1.04320000
C	0.97820000	-2.83640000	2.89250000
H	1.28660000	-3.25390000	1.93050000
H	0.97710000	-3.64540000	3.64600000
H	1.72080000	-2.08980000	3.18130000
C	-1.31780000	-3.23810000	2.31990000
H	-0.98440000	-3.67690000	1.37500000
H	-2.29480000	-2.77610000	2.15560000
H	-1.42870000	-4.05120000	3.06030000
C	-0.78750000	-1.60440000	4.02310000
C	-0.09810000	-0.26640000	4.29560000
H	-0.60470000	-2.28120000	4.87800000
H	-1.87090000	-1.45880000	3.96750000
H	-0.40670000	0.09800000	5.29290000
H	0.98610000	-0.41060000	4.33700000
C	0.60390000	1.83600000	3.33240000
H	1.61270000	1.44090000	3.18560000
H	0.56560000	2.35780000	4.30590000
H	0.40210000	2.56510000	2.54240000
C	-1.73210000	1.29650000	3.39830000
H	-1.91510000	2.02250000	2.60180000
H	-1.86510000	1.80020000	4.37340000
H	-2.48260000	0.50820000	3.31020000
S	-2.90090000	-0.37890000	-0.81670000
C	-4.18820000	-1.07850000	-0.00120000
C	-3.25930000	1.41340000	-0.66960000
C	-4.50780000	-2.50870000	-0.38750000
C	-4.61510000	-0.66320000	1.38730000
C	-2.25710000	2.32480000	-0.32700000
C	-4.53610000	1.87960000	-1.00850000
H	-4.18480000	-2.74160000	-1.41040000
H	-5.59550000	-2.68010000	-0.34250000
H	-4.05180000	-3.26720000	0.27810000
H	-4.40250000	0.39230000	1.59200000

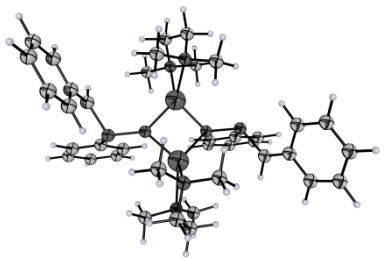
H	-4.14130000	-1.25580000	2.19380000
H	-5.70080000	-0.80590000	1.50800000
H	-1.27170000	1.94740000	-0.07860000
C	-2.53650000	3.69670000	-0.29990000
C	-4.81070000	3.24960000	-0.98610000
H	-5.30970000	1.16390000	-1.27080000
H	-1.75410000	4.39910000	-0.02160000
C	-3.81180000	4.16370000	-0.62940000
H	-5.80620000	3.60250000	-1.24460000
H	-4.02640000	5.22930000	-0.61150000
C	0.81450000	-2.35500000	-3.63210000
C	0.10840000	-1.10840000	-4.16810000
N	0.37690000	-2.71840000	-2.27030000
N	0.36140000	0.09180000	-3.34670000
H	0.64790000	-3.19010000	-4.33740000
H	1.89520000	-2.18460000	-3.60100000
H	0.42250000	-0.94350000	-5.21520000
H	-0.97310000	-1.27560000	-4.18880000
C	-0.94760000	-3.35640000	-2.28750000
C	1.34880000	-3.62590000	-1.64580000
C	-0.63520000	1.13040000	-3.64410000
C	1.70970000	0.62800000	-3.58680000
H	-1.24960000	-3.59450000	-1.26420000
H	-0.94190000	-4.28940000	-2.88050000
H	-1.69710000	-2.68060000	-2.70450000
H	1.01510000	-3.87790000	-0.63500000
H	2.32280000	-3.13520000	-1.57180000
H	1.46600000	-4.56500000	-2.21680000
H	-1.63910000	0.75480000	-3.42910000
H	-0.59510000	1.45030000	-4.70130000
H	-0.45270000	2.00460000	-3.01240000
H	1.87340000	1.50150000	-2.95030000
H	1.84540000	0.92890000	-4.64190000
H	2.47110000	-0.11400000	-3.33710000

Equilibrium Structure [Li_2{CHPhS(O)Ph}$_2$(TMEDA)$_2$] (4*)

(file: P.BenzSSopt.log)

E(RB3LYP) –2661.56541099 a.u.

Sum of electronic and thermal Free Energies –2660.151108 a.u.



C	-4.05514700	-0.16753300	0.14448600
S	-2.83183100	0.26188100	-0.93438400
H	-4.24583700	0.50573300	0.97698900
C	4.05515400	-0.16813700	-0.14465300
S	2.83209400	0.26119300	0.93453700
H	4.24590500	0.50535900	-0.97695500
C	-0.62388000	-2.80995500	-2.42460800
N	0.53740500	-1.91669400	-2.53802600
H	-1.53630700	-2.26677700	-2.68558100
H	-0.71585900	-3.16147300	-1.39292000
H	-0.53495800	-3.69110600	-3.08501900
C	1.75245200	-2.63601800	-2.12241900
H	2.62516500	-1.98161200	-2.16503300
H	1.93722200	-3.51921800	-2.75989700
H	1.64227100	-2.97001500	-1.08723000
C	1.48050900	-0.11749500	-3.99508400
N	0.88477500	0.98323600	-3.20961100
C	0.66477900	-1.40848100	-3.91895000
Li	0.36525600	-0.06727700	-1.32129400
H	2.48866000	-0.29332000	-3.60590400
H	1.59372100	0.17278400	-5.05577800
C	1.85970200	2.07278100	-3.05226000
H	1.42278500	2.87195500	-2.44653900
H	2.16240800	2.49840100	-4.02574400
H	2.75152800	1.70147300	-2.54045000
H	-0.34276500	-1.23422400	-4.30857800
H	1.12893200	-2.16413200	-4.57749700
C	-0.32838700	1.50811500	-3.85717000
H	-0.73008700	2.33160700	-3.26157100
H	-1.09910700	0.73640800	-3.92284000
H	-0.11667200	1.88025600	-4.87571900
C	-1.75389200	-2.63699400	2.12267300
N	-0.53840900	-1.91823100	2.53797500
H	-2.62629400	-1.98218900	2.16548800
H	-1.93891300	-3.52009200	2.76021700
H	-1.64413000	-2.97107000	1.08746700
C	0.62242500	-2.81206200	2.42433500
H	1.53519100	-2.26929300	2.68498800
H	0.71393900	-3.16377700	1.39266800
H	0.53327200	-3.69308700	3.08488300
C	-1.85834900	2.07206500	3.05281900
N	-0.88393400	0.98205200	3.21006200
H	-2.75021700	1.70129300	2.54068700

H	-1.42093300	2.87121900	2.44743500
H	-2.16109600	2.49752600	4.02635900
C	0.32934100	1.50619600	3.85800300
H	1.09978600	0.73419000	3.92336600
H	0.11763800	1.87790500	4.87671300
H	0.73137500	2.32984700	3.26286300
C	-1.48032200	-0.11856500	3.99522300
C	-0.66524000	-1.40994100	3.91892000
Li	-0.36513900	-0.06895700	1.32135500
H	-2.48852100	-0.29379600	3.60590200
H	-1.59350500	0.17155300	5.05596700
H	-1.12960500	-2.16538800	4.57755400
H	0.34247100	-1.23616800	4.30833400
O	1.32287100	0.19027500	0.36804600
O	-1.32270300	0.19063800	-0.36767200
C	-4.72500000	-1.44794000	0.11651000
C	-5.71229200	-1.72885000	1.10162100
C	-4.50157400	-2.46849100	-0.84792500
C	-6.42659300	-2.92604100	1.11292700
H	-5.91822400	-0.97854800	1.86356300
C	-5.22295700	-3.66128600	-0.83402500
H	-3.75153800	-2.31901900	-1.62048000
C	-6.19541100	-3.91200900	0.14424900
H	-7.17331000	-3.09011900	1.88806400
H	-5.01750300	-4.41012600	-1.59725000
H	-6.75060300	-4.84629000	0.15333000
C	-3.08316200	2.06790900	-1.03174500
C	-4.32761600	2.55492000	-1.44985200
C	-2.03503700	2.94949100	-0.76441600
C	-4.52187300	3.93161800	-1.58539700
H	-5.13964800	1.86253300	-1.65173200
C	-2.23925000	4.32910300	-0.88939500
H	-1.07650700	2.54841500	-0.45499800
C	-3.47952600	4.82284200	-1.30167200
H	-5.48946700	4.30789300	-1.90750300
H	-1.42537900	5.01516000	-0.66739600
H	-3.63485100	5.89374300	-1.40308900
C	3.08375500	2.06713000	1.03226800
C	2.03571100	2.94895500	0.76540500
C	4.32837300	2.55382600	1.45024800
C	2.24016200	4.32849700	0.89076500
H	1.07704000	2.54814100	0.45608300
C	4.52286500	3.93045800	1.58617700
H	5.14034900	1.86126600	1.65174900
C	3.48059400	4.82192400	1.30295500
H	1.42635200	5.01475200	0.66915800
H	5.49058800	4.30647500	1.90819500
H	3.63608800	5.89276900	1.40469100
C	4.72464200	-1.44874600	-0.11727300
C	5.71179300	-1.72950300	-1.10257900
C	4.50093900	-2.46967300	0.84668700

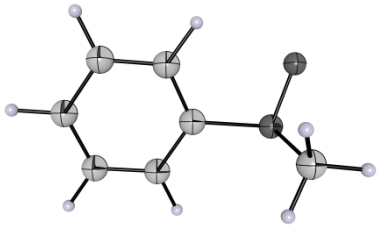
C	6.42570000	-2.92691300	-1.11449200
H	5.91791400	-0.97889900	-1.86417200
C	5.22196300	-3.66268700	0.83220300
H	3.75096000	-2.32033800	1.61932800
C	6.19426900	-3.91325700	-0.14624600
H	7.17231300	-3.09088300	-1.88975200
H	5.01631600	-4.41181900	1.59508900
H	6.74916100	-4.84771200	-0.15581200

Equilibrium Structure of PhS(O)CH$_3$ (A*)

(file: P.PhSOMe.log)

E(RB3LYP) –744.950910640 a.u.

Sum of electronic and thermal Free Energies –744.852281 a.u.



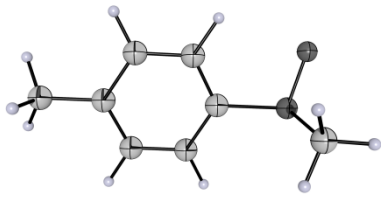
C	-2.30326900	-1.10192400	-0.23278700
C	-0.92098800	-1.19294700	-0.41969800
C	-0.12790100	-0.06538900	-0.18607700
C	-0.69055900	1.15246000	0.19583800
C	-2.07540700	1.23485400	0.37449800
C	-2.87983000	0.10996200	0.16466000
H	-2.92851100	-1.97335900	-0.40721900
H	-0.47441800	-2.12968900	-0.74572500
H	-0.05012600	2.01773300	0.34096600
H	-2.52435200	2.17831600	0.67343700
H	-3.95562600	0.17858200	0.30147000
S	1.67357400	-0.16944500	-0.45992600
C	2.12469800	-0.89724100	1.16169200
H	1.65214300	-1.87832400	1.26098700
H	3.21265700	-1.00230300	1.16988000
H	1.79716400	-0.22215400	1.95667700
O	2.21667700	1.26295900	-0.44255200

Equilibrium Structure of *p*-TolS(O)CH$_3$ (B*)

(file: P.TolSOMe.log)

E(RB3LYP) –784.269810332 a.u.

Sum of electronic and thermal Free Energies –784.146796 a.u.



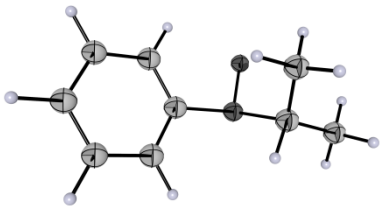
C	-1.82165400	-1.15329500	-0.33031800
C	-0.43353300	-1.22112300	-0.46698900
C	0.33481400	-0.08196700	-0.21184700
C	-0.27133200	1.12309300	0.14095200
C	-1.66204000	1.17651500	0.26660300
C	-2.45815700	0.04246900	0.04154700
H	-2.41898500	-2.04049900	-0.52787200
H	0.03660400	-2.15254200	-0.77485100
H	0.33995600	2.00660900	0.30156200
H	-2.13504200	2.11755300	0.53851700
S	2.14265200	-0.15273600	-0.42600400
C	2.56071500	-0.85382800	1.21621100
H	2.10664300	-1.84420700	1.31067600
O	2.65748900	1.29085200	-0.40856700
H	2.19384600	-0.17896700	1.99405700
H	3.64998000	-0.93479400	1.25922600
C	-3.95864300	0.10138700	0.21003200
H	-4.24624400	-0.15479600	1.23868500
H	-4.34537000	1.10478700	0.00321000
H	-4.46474900	-0.60570300	-0.45575200

Equilibrium Structure of PhS(O)CH(CH_3)$_2$ (C*)

(file: P.PhSOCHMe2.log)

E(RB3LYP) –823.582511428 a.u.

Sum of electronic and thermal Free Energies –823.430649 a.u.



C	-2.68277300	-1.31262300	-0.32308400
C	-1.34487400	-1.12882400	-0.68205100
C	-0.71249200	0.07795200	-0.36363500
C	-1.40227600	1.10925900	0.27405000

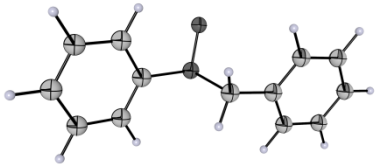
C	-2.74293700	0.91778800	0.62500400
C	-3.38160900	-0.29097200	0.33101700
H	-3.18027900	-2.24855400	-0.56262300
H	-0.80986200	-1.91647900	-1.20797800
H	-0.89068800	2.04377200	0.48508000
H	-3.28709200	1.71465700	1.12504900
H	-4.42401500	-0.43501800	0.60202700
S	1.01145800	0.35158700	-0.88878800
C	1.88316300	-0.74348500	0.36742600
H	1.39865900	-1.71850000	0.23348500
O	1.35799300	1.80427400	-0.53944600
C	1.69407500	-0.23281600	1.79202700
H	0.64224000	-0.23619900	2.09393400
H	2.24772200	-0.88101500	2.48183600
H	2.08372100	0.78534800	1.89519700
C	3.35353600	-0.82929000	-0.05008800
H	3.88147300	-1.51773300	0.61990500
H	3.46595800	-1.20093000	-1.07466100
H	3.84201300	0.14913900	0.02091900

Equilibrium Structure of PhS(O)CH_2Ph (D^*)

(file: P.PhSOCH2Ph.log)

E(RB3LYP) –976.011837902 a.u.

Sum of electronic and thermal Free Energies –975.839557 a.u.



C	-3.92427400	1.45429600	-0.16862500
C	-2.61824700	1.28608500	0.29982700
C	-2.05260000	0.00708700	0.29298200
C	-2.77527600	-1.10404300	-0.14276300
C	-4.08341700	-0.92612400	-0.60433800
C	-4.65569300	0.35012700	-0.62120000
H	-4.37210600	2.44432000	-0.17036500
H	-2.05667400	2.14134000	0.66898700
H	-2.31778700	-2.08859900	-0.10878100
H	-4.65500100	-1.78487100	-0.94616000
H	-5.67349500	0.48408200	-0.97740900
S	-0.36128200	-0.22140500	0.93519200
C	0.54233100	0.26145300	-0.64014400
H	0.18176300	1.26485300	-0.88683800
O	-0.14710500	-1.72636600	1.10759300
H	0.19334400	-0.44712800	-1.39737700

C	2.03096100	0.22183000	-0.45367500
C	2.75591000	-0.94718400	-0.73415700
C	2.72214800	1.34982200	0.01911300
C	4.14025100	-0.98789400	-0.54668900
H	2.23365700	-1.82632900	-1.10229500
C	4.10564300	1.31052100	0.20720500
H	2.17444500	2.26445600	0.23636500
C	4.81881500	0.14036900	-0.07528500
H	4.68772500	-1.89971300	-0.77073800
H	4.62639700	2.19314700	0.56943700
H	5.89578300	0.10978300	0.06784600