Lithium Di– and Trimethyl Dimolybdenum(II) Complexes with Mo–Mo Quadruple Bonds and Bridging Methyl Groups

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Supporting information

1. Selected NMR spectra of complexes

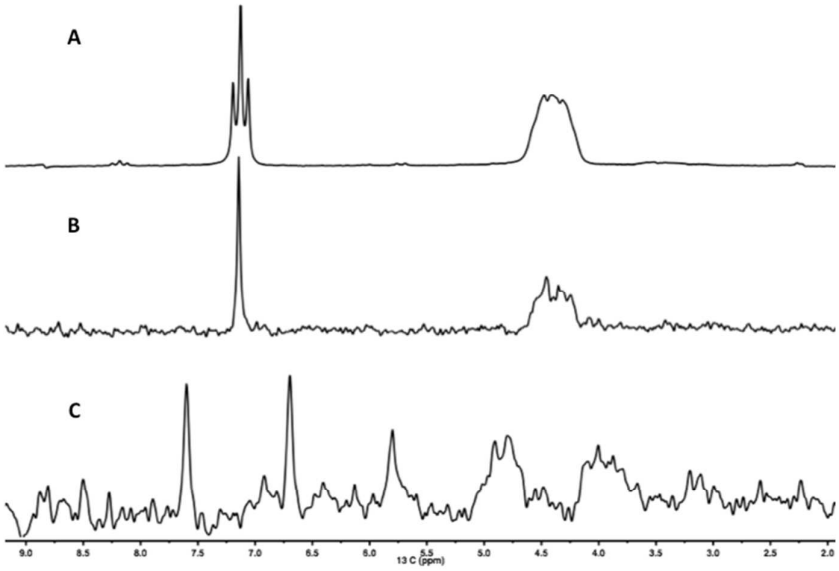


Figure S1. The ^{13}C NMR spectrum of complex **3c** recorded in C_6D_6 in the region corresponding to the metal-bound methyl groups. (A) Sample enriched in ^{13}C. (B) Sample with natural abundance. (C) Proton-coupled spectrum.

2. Schematic representation of the dihapto agostic interaction in 3b

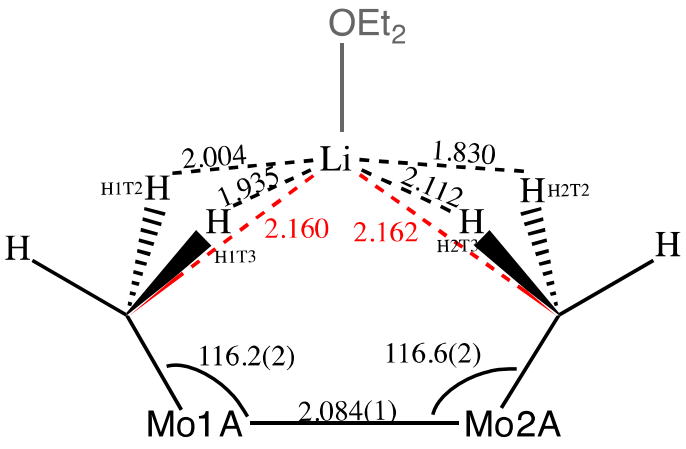


Figure S2. Schematic representation of the dihapto agostic interaction. Selected distances and angles shown in Å and °, respectively.

3. X–ray Crystal structures of complexes 3a, 3b and 4c.

A single crystal of suitable size, coated with dry perfluoropolyether, was mounted on a glass fiber and fixed in a cold nitrogen stream [T = 173(2) K for compounds 3a, 3b and 4c] to the goniometer head. Data collections were performed on a Bruker-Nonius X8APEX–II CCD diffractometer and a Bruker-AXSX8Kappa diffractometer equipped with a CCD area detector, using monochromatic radiation λ(Mo Kα1) = 0.71073 Å, by means of ω and ϕ scans in all cases. The data were reduced (SAINT)[1] and corrected for Lorentz polarisation effects and absorption by multiscan method applied by SADABS.[2] All structures were solved by direct methods and refined against all F^2 data by full-matrix least-squares techniques (SHELXTL–6.12).[3] The non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were included from calculated positions and refined riding on their respective carbon atoms with isotropic displacement parameters. A summary of the fundamental crystal and refinement data are given in Tables S1–S3. X–ray crystallographic data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

3.1 X–ray Crystal structure of 3a

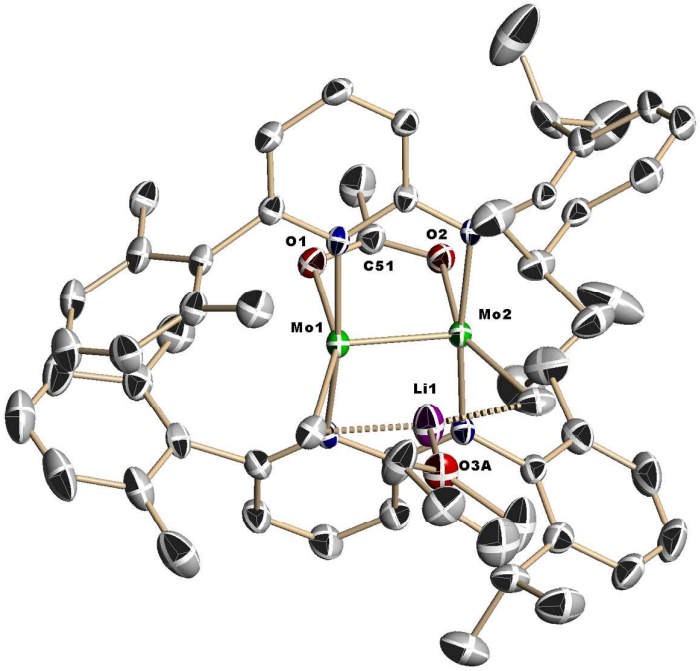


Figure S3. The solid-state molecular structure of **3a**, with thermal ellipsoids set at 30% probability. The molecule of solvent and all hydrogen atoms are omitted for clarity. Selected bond lengths (Å): Mo(1)–Mo(2), 2.107(1); Mo(1)–O(1), 2.156(3); Mo(1)–N(3), 2.191(4); Mo(1)–C(54), 2.218(5); Mo(1)–N(1), 2.220(4); Mo(2)–N(2), 2.133(4); Mo(2)–N(4), 2.150(4); Mo(2)–O(2), 2.154(3); Mo(2)–C(53) 2.207(5); C(54)–Li(1) 2.080(1); C(53)–Li(1) 2.143(3); O(3A)–Li(1) 1.93(2).

Table S1. Crystal data and structure refinement **3a**.

Empirical formula	$C_{58}H_{75}LiMo_2N_4O_3$	
Formula weight	1147.19	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.2509(6)Å	α = 90°.
	b = 14.4835(6) Å	β = 97.764(2)°
	c = 34.4912(16) Å	γ = 90°.
Volume	6063.9(5) $Å^3$	
Z	4	
Density (calculated)	1.257 Mg/m^3	
Absorption coefficient	0.46 mm^{-1}	
F(000)	2416	
Crystal size	0.40 x 0.19 x 0.14 mm^3	
Theta range for data collection	2.38 to 23.83°	
Index ranges	–14<=h<=14, –17<=k<=17, –41<=l<=41	
Reflections collected	60299	
Independent reflections	10909 [R(int) = 0.066]	
Completeness to theta = 26.4°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9385 and 0.8977	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10909 / 224 / 718	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0551, wR2 = 0.1227	
R indices (all data)	R1 = 0.0793, wR2 = 0.1315	
Largest diff. peak and hole	0.938 and –0.605 $e.Å^{-3}$	

3.2 X–ray Crystal structure of 3b

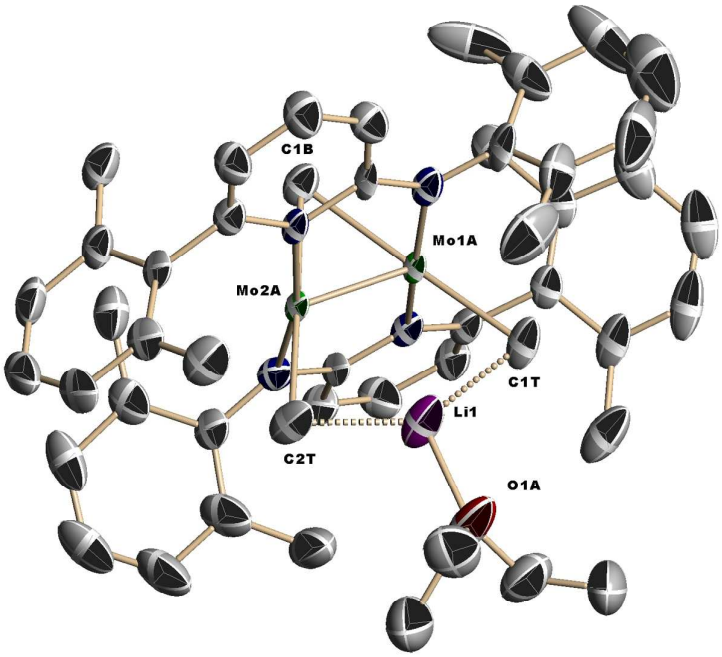
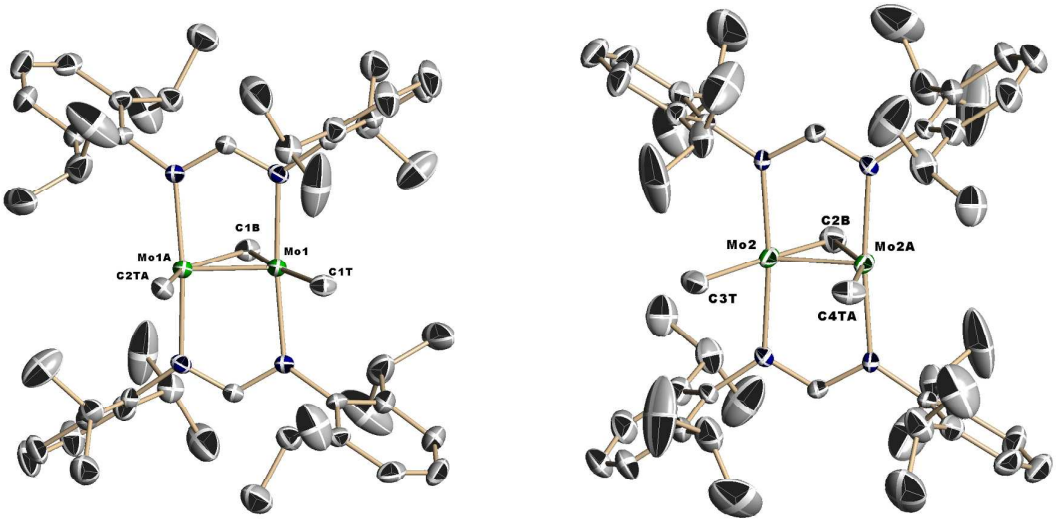


Figure S4. The solid-state molecular structure of **3b**, with thermal ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity. Selected bond lengths (Å): Mo(1)–Mo(2), 2.084(7); Mo(1A)–N(1), 2.111(6); Mo(1A)–N(3), 2.176(6); Mo(1A)–C(1T), 2.273(8); Mo(2A)–N(4), 2.117(7); Mo(2A)–N(2), 2.191(6); Mo(2)–C(2T), 2.251(7); Mo(2A)–C(1B), 2.411(7); C(2T)–Li(1), 2.162(6); C(1T)–Li(1), 2.160(5); O(1A)–Li(1) 1.954(2).

Table S2. Crystal data and structure refinement for **3b**.

Empirical formula	$C_{48}H_{66}LiMo_2N_4O$	
Formula weight	920,84	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P –1	
Unit cell dimensions	a = 10.2420 (13) Å	α = 79.420 (4)°.
	b = 10.8683 (15) Å	β = 80.038 (4)°.
	c = 22.381 (30) Å	γ = 70.732 (4)°.
Volume	2294.7 (5) $Å^3$	
Z	2	
Density (calculated)	1.333 Mg/m^3	
Absorption coefficient	0.59 mm^{-1}	
F(000)	959	
Crystal size	0.23 x 0.21 x 0.15 mm^3	
Theta range for data collection	0.93 to 25.25°.	
Index ranges	–12<=h<=10, –13<=k<=12, –26<=l<=26	
Reflections collected	36706	
Independent reflections	8073 [R(int) = 0.045]	
Completeness to theta = 25.25°	97.1 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.916 and 0.615	
Refinement method	Full–matrix least–squares on F^2	
Data / restraints / parameters	8073 / 1/ 556	
Goodness–of–fit on F^2	1.099	
Final R indices [I>2sigma(I)]	R1 = 0.0756, wR2 = 0.2347	
R indices (all data)	R1 = 0.0984, wR2 = 0.2566	
Largest diff. peak and hole	1.542 and –1.348 e.$Å^{-3}$	

3.3 X–ray Crystal structure of 4c



(B) **(C)**

Figure S5. The solid-state molecular structure of **4c**, with thermal ellipsoids set at 30% probability. All hydrogen atoms are omitted for clarity. Selected bond lengths (Å): **(B)**: Mo(1A)–Mo(1), 2.084(1); Mo(1A)–C(2TA), 2.396(1); Mo(1A)–C(2TA), 2.397(1); Mo(1A)–C(1B), 2.172(1); Mo(1)–C(1B), 2.411(7); Mo(1)–N1, 2.158(1) ; Mo(1)–N2, 2.172(2). **(C)**: Mo(2)–Mo(2A), 2.083(1); Mo(2)–C(3T), 2.429(1); Mo(2A)–C(4TA), 2.473(1); Mo(2)–C(2B), 2.328(1); Mo(2A)–C(2B), 2.157(7); Mo(2)–N3, 2.156(4) ; Mo(2)–N4, 2.159(2).

Table S3. Crystal data and structure refinement for **4c**.

Empirical formula	$C_{69}H_{111}Mo_2N_4O_4Li$	
Formula weight	1259,44	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 45.402(3) Å	α = 90°.
	b = 12.1781(15) Å	β = 114.171(1)°.
	c = 27.374(2) Å	γ = 90°.
Volume	13808.5(17) $Å^3$	
Z	8	
Density (calculated)	1.212 Mg/m^3	
Absorption coefficient	0.41 mm^{-1}	
F(000)	5376	
Crystal size	0.16 x 0.16 x 0.15 mm^3	
Theta range for data collection	1.52 to 26.40°.	
Index ranges	−52<=h<=51, −15<=k<=12, −34<=l<=33	
Reflections collected	60299	
Independent reflections	13662 [R(int) = 0.097]	
Completeness to theta = 23.8°	96.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.928 and 0.923	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13662 / 16 / 820	
Goodness-of-fit on F^2	1.138	
Final R indices [I>2sigma(I)]	R1 = 0.0783, wR2 = 0.1748	
R indices (all data)	R1 = 0.1338, wR2 = 0.2047	
Largest diff. peak and hole	0.564 and −1.132 e.$Å^{-3}$	

4. Computational studies.

- **QTAIM analyses of 3a$_c$ and 3b**

QTAIM analyses were performed with the Multiwfn[4] software on wavefunctions generated with the Gaussian 09 program.[5]

The value of the electron density at a bcp (ρ_b) has been associated with the bond strength, the value of the laplacian of the electron density at a bcp, $\nabla\rho_b$, is negative in covalent interactions (density of charge accumulates) and positive in *closed shell* or ionic interactions (the density of charge is depleted), also the total energy density (H_b) tends to be negative for covalent interactions and positive for ionic interactions. Another criterion to determine the nature of an interaction between two atoms is the ratio between the local Potential (V_b) and Kinetic (G_b) energies. A ratio $|V_b|/G_b < 1$ is found in ionic interactions whereas in covalent interactions $|V_b|/G_b > 2$ (intermediate interactions including metal-metal and metal-ligand interactions are characterized by positive values of $\nabla\rho_b$, by values of H_b close to zero and $1 < |V_b|/G_b < 2$).[6,7]

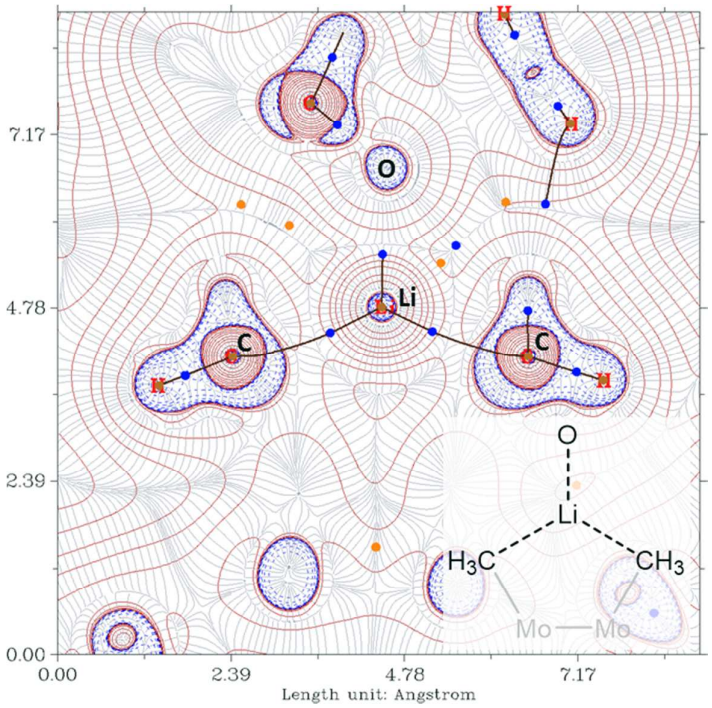


Figure S6. Plot of the laplacian of the electron density $\nabla^2\boldsymbol{\rho}$ of **3b** in the C_{Mo},C_{Mo},Li plane calculated with the M06 functional. The solid and dashed lines correspond to positive and negative values of $\nabla^2\boldsymbol{\rho}$ respectively. In plane bcps and bond paths of the electron density are superimposed. The O atom of the Et_2O fragment is out of the plane, but the bcp and part of the bond path connecting this atom and the Li is shown.

Tables S4–8. Selected properties of the electron density at relevant bcps. Results for MeLi are included for comparison purposes.

	bond	ρ[c]	G_b[d]	V_b[d]	H_b[d]	$\lvert V_b \rvert / G_b$	$\nabla^2\rho$[e]
3a$_C$[a]	**C–Li**[b]	0.0226	0.0274	−0.0241	0.0033	0.8800	0.1228
	Li–O	0.0267	0.0389	−0.0309	0.0080	0.7933	0.1879
	Mo–Mo	0.1796	0.2122	−0.3186	−0.1094	1.5012	0.4233
	Mo–C[b]	0.0840	0.0609	−0.0856	−0.0250	1.4056	0.1449

[a]calculations with the M06 functional, [b]average values, [c]e·bohr^{-3}, [d]hartree, [e]e·bohr^{-5}

	bond	ρ[c]	G_b[d]	V_b[d]	H_b[d]	$\lvert V_b \rvert / G_b$	$\nabla^2\rho$[e]
3a$_C$[a]	**C–Li**[b]	0.0241	0.0283	−0.0254	0.0030	0.8950	0.1253
	Li–O	0.0289	0.0416	−0.0333	0.0083	0.8008	0.1994
	Mo–Mo	0.1810	0.2112	−0.3204	−0.1123	1.5173	0.4078
	Mo–C[b]	0.0899	0.0645	−0.0935	−0.0295	1.4510	0.1415

[a]calculations with the PBE0–D3 functional, [b]average values, [c]e·bohr^{-3}, [d]hartree, [e]e·bohr^{-5}

	bond	ρ[c]	G_b[d]	V_b[d]	H_b[d]	$\lvert V_b \rvert / G_b$	$\nabla^2\rho$[e]
3b[a]	**C–Li**[b]	0.0212	0.0255	−0.0223	0.0032	0.8726	0.1151
	Li–O	0.0254	0.0366	−0.0290	0.0076	0.7921	0.1771
	Mo–Mo	0.1881	0.2249	−0.3396	−0.1183	1.5099	0.4410
	Mo–C[b]	0.0808	0.0602	−0.0831	−0.0233	1.3804	0.1489

[a]calculations with the M06 functional, [b]average values, [c]e·bohr^{-3}, [d]hartree, [e]e·bohr^{-5}

	bond	ρ^c	$G_b{}^d$	$V_b{}^d$	$H_b{}^d$	$\lvert V_b \rvert / G_b$	$\nabla^2\rho^e$
3b[a]	**C–Li**[b]	0.0230	0.0265	–0.0237	0.0028	0.8936	0.1171
	Li–O	0.0275	0.0390	–0.0312	0.0078	0.8007	0.1871
	Mo–Mo	0.1878	0.2209	–0.3368	–0.1194	1.5243	0.4204
	Mo–C[b]	0.0863	0.0634	–0.0903	–0.0272	1.4217	0.1463

[a]calculations with the PBE0–D3 functional, [b]average values, [c]e·bohr^{-3}, [d]hartree, [e]e·bohr^{-5}

	bond	ρ^c	$G_b{}^d$	$V_b{}^d$	$H_b{}^d$	$\lvert V_b \rvert / G_b$	$\nabla^2\rho^e$
MeLi[a]	**C–Li**[b]	0.0242	0.0257	–0.0235	0.0021	0.9175	0.1111
	C–H[b]	0.2524	0.0531	–0.2950	–0.2419	5.5581	–0.7554

[a]calculations with the M06 functional, [b]average values, [c]e·bohr^{-3}, [d]hartree, [e]e·bohr^{-5}

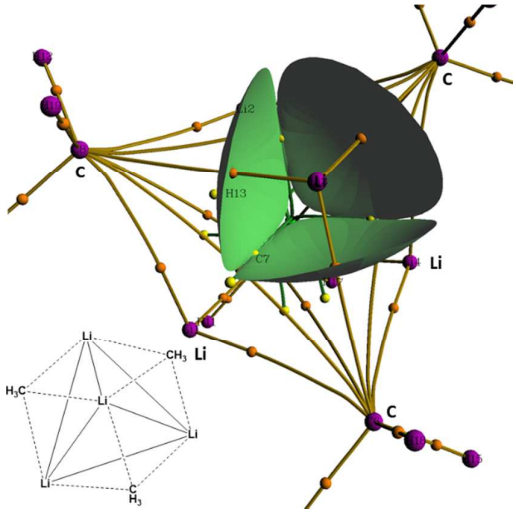
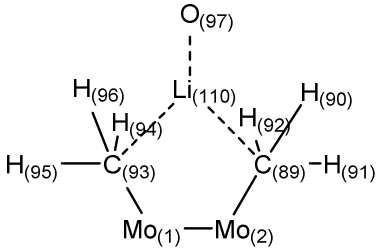


Figure S7. Molecular graph of Me_4Li_4 showing bcps as orange balls and interbasin surfaces for one of the lithium atoms.

Tables S9–17. Selected localization λ(A) and delocalization δ(A,B) indices.

3a$_C$[a]	**Atom**	**λ(A) (electrons)**
	Mo_1[b]	9.84
	Mo_2[b]	9.74
	C_{89}	4.57
	C_{93}	4.54
	Li_{110}	1.97
	O_{97}	7.88



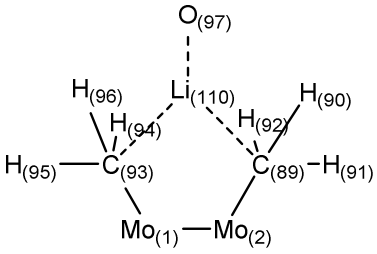
[a]calculations with the M06 functional, [b]14 electrons considered explicitly by the Electron Core Potential

δ(A,B) (electrons)

3a$_C$[a]	**Interacting atoms**	**Mo_1**	**Mo_2**	**C_{89}**	**C_{93}**	**Li_{110}**	**O_{97}**
	Mo_1		2.974082	0.068955	0.681118		
	Mo_2	2.974082		0.6661648	0.079216		
	C_{89}	0.068955	0.66616			0.058248	
	C_{93}	0.681118	0.079216			0.057099	
	Li_{110}			0.058248	0.057099		0.064921
	O_{97}					0.064921	

[a]calculations with the M06 functional

3a$_C$[a]	**Atom**	**λ(A) (electrons)**
	Mo_1[b]	9.83
	Mo_2[b]	9.71
	C_{89}	4.60
	C_{93}	4.58
	Li_{110}	1.96
	O_{97}	7.89



[a]calculations with the PBE0–D3 functional, [b]14 electrons considered explicitly by the Electron Core Potential

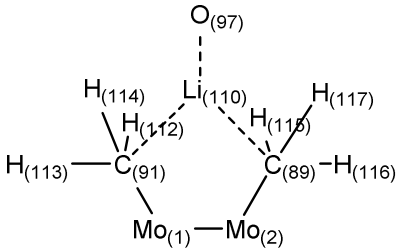
δ(A,B) (electrons)

3a$_C$[a]	**Interacting atoms**	**Mo_1**	**Mo_2**	**C_{89}**	**C_{93}**	**Li_{110}**	**O_{97}**
	Mo_1		2.910659	0.070016	0.709613		
	Mo_2	2.910659		0.695064	0.079216		
	C_{89}	0.070016	0.695064			0.060758	
	C_{93}	0.709613	0.079216			0.061361	
	Li_{110}			0.060758	0.061361		0.071632
	O_{97}					0.071632	

[a]calculations with the PBE0–D3 functional

3b[a]

Atom	**λ(A) (electrons)**
Mo_1[b]	9.84
Mo_2[b]	9.76
C_{91}	4.53
C_{92}	4.59
Li_{108}	1.97
O_{93}	8.04



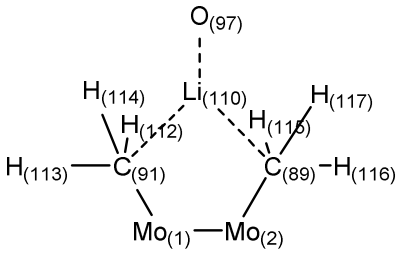
[a]calculations with the M06 functional, [b]14 electrons considered explicitly by the Electron Core Potential.

δ(A,B) (electrons)

3b[a]	**Interacting atoms**	**Mo_1**	**Mo_2**	**C_{91}**	**C_{92}**	**Li_{108}**	**O_{93}**
	Mo_1		3.000470	0.690512	0.064853		
	Mo_2	3.000470		0.077875	0.610258		
	C_{91}	0.690512	0.077875			0.050841	
	C_{92}	0.064853	0.610258			0.056852	
	Li_{108}			0.050841	0.056852		0.062085
	O_{93}					0.062085	

[a]calculations with the M06 functional

3b[a]	**Atom**	**λ(A) (electrons)**
	Mo_1[b]	9.74
	Mo_2[b]	9.84
	C_{91}	4.55
	C_{92}	4.63
	Li_{108}	1.96
	O_{93}	7.91



[a]calculations with the PBE0–D3 functional, [b]14 electrons considered explicitly by the Electron Core Potential.

δ(A,B) (electrons)

3b[a]	**Interacting atoms**	**Mo_1**	**Mo_2**	**C_{91}**	**C_{92}**	**Li_{108}**	**O_{93}**
	Mo_1		2.946416	0.727958	0.064428		
	Mo_2	2.946416		0.077875	0.630294		
	C_{91}	0.727958	0.077875			0.054372	
	C_{92}	0.064428	0.630294			0.062630	
	Li_{108}			0.054372	0.062630		0.067418
	O_{93}					0.067418	

[a]calculations with the PBE0–D3 functional.

δ(A,B) (electrons)[b]

MeLi[a]		**Li**	**C**
λ(Li) = 1.972	**Li**		0.077894
λ(C) = 4.925	**C**	0.077894	

[a]calculations with the M06 functional. [b]average values

NBO analysis of $3a_C$ and 3b.

Natural bonding orbital analyses of **$3a_C$** and **3b** were carried out with the NBO 3.0[8] program incorporated in the Gaussian 09 package. The analyses were performed on the DFT optimized geometries with the M06 functional.

				2nd order perturbation theory analysis (delocalization energies)		
NBO	***Type***	***Occupation (e)***	***E(a.u.)***	***Acceptor orbital (j)***	***Type (occupation)***	$\Delta E_{i,j}$ ***(kcal·mol^{-1})***
1	π_{Mo-Mo}	1.93493	–0.22435			
2	π_{Mo-Mo}	1.96845	–0.23110			
3	σ_{Mo-Mo}	1.87119	–0.20529	→ 231 → 232	LP* Li (0.16385) LP* Li (0.08019)	137.50 51.62
4	δ_{Mo-Mo}	1.75354	–0.14609			
5	σ_{Mo-C}	1.89394	–0.23078	→ 231 → 232		43.59 20.41
6	σ_{Mo-C}	1.90774	–0.25452	→ 231 → 234	 LP* Li (0.05739)	27.14 17.15
229	$LP_{O(thf)}$	1.94154	–0.61036	→ 232		13.64

Table S18. Relevant NBOs and donor-acceptor interactions in **$3a_C$**

LP = lone pair, *antibonding/empty

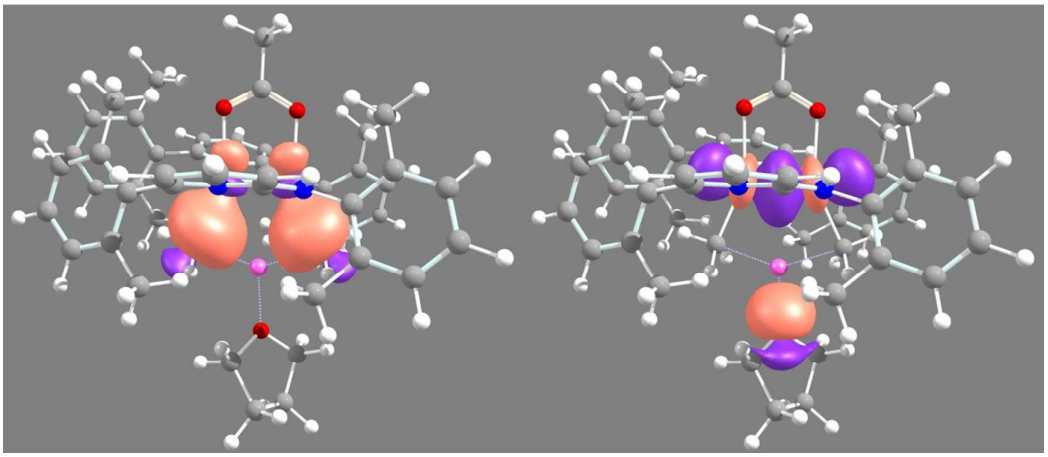


Figure S8. Selected natural bonding orbitals of **3a$_C$** which donate electron density to empty orbitals of lithium.

Table S19. Relevant NBOs and donor-acceptor interactions in **3b**

				2nd order perturbation theory analysis (delocalization energies)		
NBO	***Type***	***Occupation (e)***	***E(a.u.)***	***Acceptor orbital (j)***	***Type (occupation)***	$\Delta E_{i,j}$ ***(kcal·mol^{-1})***
1	π_{Mo-Mo}	1.90941	–0.23257			
2	π_{Mo-Mo}	1.95950	–0.23210			
3	σ_{Mo-Mo}	1.82560	–0.10917	→ 219	LP* Li (0.16775)	232.19
				→ 220	LP* Li (0.08361)	104.45
6	σ_{Mo-C}	1.90260	–0.24079	→ 219		36.34
				→ 220		17.98
				→ 222	LP* Li (0.05998)	18.24
9	σ_{Mo-C}	1.83477	–0.25521	→ 219		55.57
				→ 220		10.58
				→ 222		12.55
217	$LP_{O(Et2O)}$	1.94185	–0.61089	→ 220		10.75

LP = lone pair, *antibonding/empty

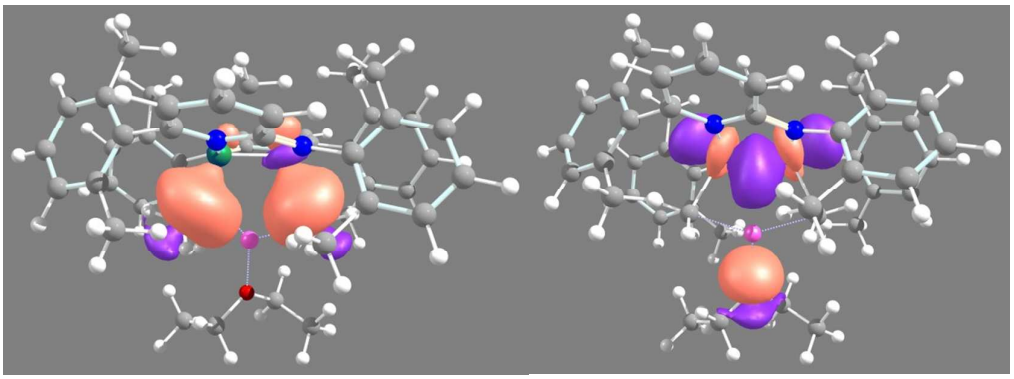


Figure S9. Selected natural bonding orbitals of **3b** which donate electron density to empty orbitals of lithium.

Tables S20–21. Selected Wiberg indices for **3a**$_C$ and **3b** at the M06 level.

Wiberg bond indices

3a$_C$[a]		**Mo$_1$**	**Mo$_2$**	**C$_{89}$**	**C$_{93}$**	**Li$_{110}$**	**O$_{97}$**
	Mo$_1$		3.1850		0.5989		
	Mo$_2$	3.1850		0.6354			
	C$_{89}$		0.6354			0.0956	
	H$_{90}$					0.0125	
	H$_{92}$					0.0166	
	H$_{91}$					0.0040	
	C$_{93}$	0.5989				0.1119	
	H$_{96}$					0.0162	
	H$_{94}$					0.0203	
	H$_{95}$					0.0037	
	Li$_{110}$			0.0953	0.1119		0.0832
	O$_{97}$					0.0832	

[a]calculations with the m06 functional

Wiberg bond indices

3b[a]		**Mo_1**	**Mo_2**	**C_{91}**	**C_{92}**	**Li_{108}**	**O_{93}**
	Mo_1		3.2370	0.6322			
	Mo_2	3.2370			0.5645		
	C_{91}	0.6322				0.0942	
	H_{114}					0.0139	
	H_{112}					0.0187	
	H_{113}					0.0036	
	C_{92}		0.5645			0.0956	
	H_{115}					0.0135	
	H_{117}					0.0196	
	H_{116}					0.0041	
	Li_{108}			0.0942	0.0956		0.0798
	O_{93}					0.0798	

[a]calculations with the m06 functional

Tables of the optimized geometries (Cartesian coordinates, in Angstroms) for the calculated species.

Gas phase potential energies (in Hartrees) in parenthesis:

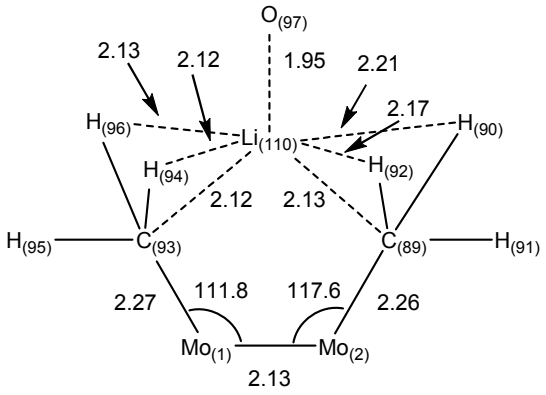


Table S22. 3a$_C$ (M06) (–2527.99498564)

42	0.763540000	0.037410000	−0.239875000	1	2.128861000	−4.832296000	−1.874942000
42	−1.278936000	0.522711000	−0.598967000	6	1.450170000	−2.959482000	−1.124047000
8	1.319890000	0.493213000	−2.297406000	6	2.711653000	−2.771739000	−0.360248000
8	−0.778306000	1.134763000	−2.640266000	6	3.856160000	−2.222787000	−0.960865000
7	1.246622000	2.203937000	0.148101000	6	5.039236000	−2.187424000	−0.223619000
7	−1.049206000	2.553112000	0.003889000	1	5.931933000	−1.771057000	−0.686573000
7	0.461640000	−2.026539000	−1.000571000	6	5.088337000	−2.658025000	1.081638000
7	−1.750007000	−1.421975000	−1.346455000	1	6.018343000	−2.599322000	1.644543000
6	0.184438000	3.084319000	0.121657000	6	3.954942000	−3.211004000	1.661309000
6	0.389977000	4.485686000	0.203850000	1	3.992103000	−3.603743000	2.676942000
1	−0.482851000	5.131955000	0.159231000	6	2.764416000	−3.299229000	0.941548000
6	1.657591000	4.990055000	0.312689000	6	3.828954000	−1.721996000	−2.374728000
1	1.824231000	6.063996000	0.359853000	1	3.544992000	−2.518883000	−3.074270000
6	2.734814000	4.095824000	0.355355000	1	4.815213000	−1.348535000	−2.672339000
1	3.760470000	4.440485000	0.461787000	1	3.100672000	−0.910723000	−2.507582000
6	2.496523000	2.737437000	0.270422000	6	1.585464000	−4.015513000	1.535038000
6	3.697388000	1.864445000	0.398164000	1	0.637161000	−3.512595000	1.304580000
6	4.108071000	1.484230000	1.687427000	1	1.684636000	−4.090004000	2.624809000
6	5.339091000	0.845355000	1.844375000	1	1.503781000	−5.035826000	1.135977000
1	5.652901000	0.540136000	2.842447000	6	−3.097178000	−1.837777000	−1.505105000
6	6.170774000	0.633470000	0.755174000	6	−3.672623000	−2.697506000	−0.546339000
1	7.136629000	0.149132000	0.892427000	6	−5.030612000	−2.999392000	−0.637203000
6	5.769910000	1.036259000	−0.512329000	1	−5.474754000	−3.653573000	0.113009000
1	6.426671000	0.881144000	−1.368606000	6	−5.812490000	−2.487642000	−1.665147000
6	4.536065000	1.653856000	−0.712652000	1	−6.871519000	−2.729067000	−1.720752000
6	3.312361000	1.857327000	2.905536000	6	−5.224886000	−1.685742000	−2.634269000
1	2.246403000	1.978989000	2.690298000	1	−5.819289000	−1.312398000	−3.467652000
1	3.670322000	2.812885000	3.313568000	6	−3.869272000	−1.357900000	−2.578454000
1	3.420400000	1.102100000	3.692558000	6	−2.843614000	−3.316810000	0.540093000
6	4.157182000	2.151748000	−2.075560000	1	−2.119021000	−2.603543000	0.954382000
1	4.885728000	1.824978000	−2.825599000	6	−3.240918000	−0.560277000	−3.681089000
1	4.116330000	3.248462000	−2.099529000	1	−2.291062000	−1.007975000	−4.000789000
1	3.168394000	1.784547000	−2.372814000	6	0.408127000	0.959483000	−3.044275000
6	−2.156720000	3.309925000	0.459559000	6	0.735755000	1.306182000	−4.466735000
6	−3.161730000	3.705682000	−0.438406000	1	0.239308000	0.594036000	−5.135708000
6	−4.299568000	4.342963000	0.057254000	1	1.813528000	1.268256000	−4.642185000
1	−5.075863000	4.649001000	−0.643513000	1	0.348463000	2.300395000	−4.707901000
6	−4.447573000	4.594054000	1.415347000	6	−2.732448000	0.259898000	1.110183000
1	−5.342498000	5.087818000	1.787404000	1	−3.097640000	−0.746494000	1.370684000
6	−3.441622000	4.212374000	2.294441000	1	−3.584022000	0.734104000	0.593863000
1	−3.547493000	4.404350000	3.362191000	1	−2.641788000	0.840471000	2.045921000
6	−2.289405000	3.573370000	1.838793000	6	1.124344000	−0.537823000	1.921366000
6	−3.011959000	3.445463000	−1.905515000	1	0.860476000	0.163787000	2.736306000
1	−3.131924000	2.379505000	−2.147834000	1	2.225488000	−0.527648000	1.903124000
6	−1.223755000	3.158604000	2.809616000	1	0.880283000	−1.554471000	2.277422000
6	−0.768696000	−2.324980000	−1.545821000	8	−1.671629000	−1.598305000	3.523519000
6	−0.969039000	−3.527016000	−2.273934000	6	−2.939981000	−1.342478000	4.148324000
1	−1.950221000	−3.705043000	−2.707287000	1	−3.746675000	−1.573406000	3.434986000
6	0.060918000	−4.415584000	−2.433053000	1	−2.990308000	−0.275602000	4.391705000
1	−0.081966000	−5.329119000	−3.006060000				
6	1.295682000	−4.135141000	−1.829331000				

6	−2.973667000	−2.265239000	5.349046000
1	−3.991045000	−2.471111000	5.693704000
1	−2.408582000	−1.829446000	6.183014000
6	−2.254854000	−3.492412000	4.799831000
1	−1.863917000	−4.159282000	5.573573000
1	−2.934177000	−4.073770000	4.162701000
6	−1.152482000	−2.865620000	3.961883000
1	−0.239314000	−2.681523000	4.545893000
1	−0.885574000	−3.462243000	3.079455000
3	−0.992284000	−0.567953000	2.007761000
1	−0.814266000	2.171466000	2.551120000
1	−0.369940000	3.851263000	2.803550000
1	−1.617111000	3.124473000	3.832154000
1	−3.763095000	3.999247000	−2.478919000
1	−2.013443000	3.721674000	−2.264385000
1	−3.480849000	−3.685084000	1.354053000
1	−2.257800000	−4.168315000	0.163873000
1	−3.910758000	−0.508381000	−4.546225000
1	−2.993955000	0.464651000	−3.382268000

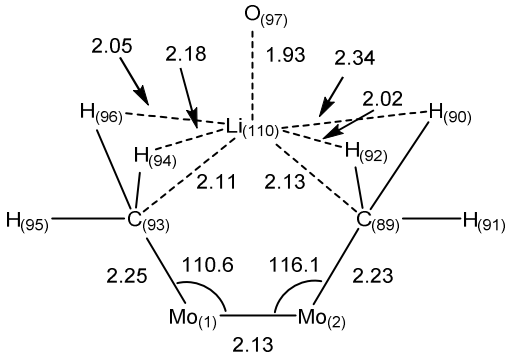


Table S23. 3a$_C$ (PBE0–D3) (−2526.95129357)

42	0.717202000	0.035720000	−0.299244000
42	−1.378843000	0.287445000	−0.583392000
8	1.133065000	0.330874000	−2.403049000
8	−1.034750000	0.718507000	−2.677025000
7	0.999187000	2.247019000	−0.103787000
7	−1.328938000	2.365270000	−0.195040000
7	0.583247000	−2.104094000	−0.835330000
7	−1.695342000	−1.736465000	−1.123058000
6	−0.146618000	3.017299000	−0.150784000
6	−0.081981000	4.435019000	−0.174223000
1	−1.013196000	4.986393000	−0.236501000
6	1.129406000	5.072797000	−0.146130000
1	1.186865000	6.157168000	−0.181457000
6	2.290860000	4.293978000	−0.078714000
1	3.275707000	4.746225000	−0.036258000
6	2.192142000	2.914049000	−0.060469000
6	3.497209000	2.192701000	0.058037000
6	4.042203000	1.997211000	1.341143000
6	5.344545000	1.506062000	1.458079000
1	5.763597000	1.349017000	2.449031000
6	6.111927000	1.254026000	0.329658000
1	7.129946000	0.887947000	0.433881000
6	5.580810000	1.484319000	−0.933639000
1	6.189139000	1.311864000	−1.818513000
6	4.277437000	1.958353000	−1.092484000
6	3.296495000	2.411988000	2.580587000
1	2.218389000	2.282992000	2.475754000
1	3.476820000	3.472667000	2.795388000
1	3.630989000	1.835966000	3.448251000
6	3.758450000	2.275914000	−2.466741000
1	4.513898000	2.052843000	−3.225289000
1	3.495425000	3.336255000	−2.550351000
1	2.857766000	1.697751000	−2.691668000
6	−2.500362000	3.086760000	0.157003000
6	−3.510478000	3.319042000	−0.796221000
6	−4.686276000	3.958818000	−0.397358000
1	−5.460589000	4.140402000	−1.139246000
6	−4.873827000	4.370424000	0.915783000
1	−5.795769000	4.864320000	1.209384000
6	−3.867320000	4.151029000	1.848536000
1	−4.001902000	4.473552000	2.878710000
6	−2.676417000	3.518048000	1.491623000
6	−3.337482000	2.898262000	−2.227113000
1	−3.566132000	1.834827000	−2.365843000
6	−1.601469000	3.322120000	2.523380000
6	−0.637399000	−2.559690000	−1.290931000
6	−0.760201000	−3.828802000	−1.914171000
1	−1.735791000	−4.122392000	−2.285710000
6	0.336556000	−4.638504000	−2.053835000
1	0.254239000	−5.602107000	−2.548856000
6	1.560903000	−4.204637000	−1.526650000
1	2.445979000	−4.830993000	−1.555233000
6	1.641388000	−2.964971000	−0.921742000
6	2.929852000	−2.634143000	−0.245540000
6	4.002118000	−2.078920000	−0.965020000
6	5.233031000	−1.932515000	−0.322062000
1	6.065597000	−1.504823000	−0.872276000
6	5.402492000	−2.321729000	0.999973000
1	6.365999000	−2.192518000	1.485496000
6	4.342373000	−2.888529000	1.696671000
1	4.478749000	−3.216495000	2.724573000
6	3.103146000	−3.070419000	1.082159000
6	3.856321000	−1.706303000	−2.414689000
1	3.748600000	−2.601744000	−3.038303000
1	4.736743000	−1.158406000	−2.761003000
1	2.974199000	−1.083862000	−2.590683000
6	2.008701000	−3.801980000	1.811339000
1	1.026149000	−3.357595000	1.632749000
1	2.198376000	−3.811341000	2.889002000
1	1.948994000	−4.844180000	1.474683000
6	−2.998404000	−2.301018000	−1.204933000
6	−3.454323000	−3.144998000	−0.167591000
6	−4.771690000	−3.605036000	−0.193770000
1	−5.122065000	−4.241992000	0.615446000
6	−5.629673000	−3.268477000	−1.233089000
1	−6.653828000	−3.630583000	−1.238385000
6	−5.157768000	−2.484139000	−2.277805000
1	−5.809214000	−2.248021000	−3.116003000
6	−3.847661000	−1.999982000	−2.288793000
6	−2.536854000	−3.595492000	0.933722000
1	−1.830295000	−2.810112000	1.215102000
6	−3.350436000	−1.222940000	−3.473448000
1	−2.377432000	−1.596839000	−3.806647000
6	0.141276000	0.622201000	−3.137777000
6	0.355163000	0.862143000	−4.606383000
1	−0.214175000	0.127111000	−5.183169000
1	1.411632000	0.788318000	−4.865159000
1	−0.024790000	1.851250000	−4.877154000
6	−2.689871000	0.062169000	1.218635000
1	−2.973377000	−0.948271000	1.548203000
1	−3.603726000	0.461697000	0.755258000
1	−2.560373000	0.692574000	2.113711000
6	1.244191000	−0.290851000	1.854362000
1	0.953109000	0.459702000	2.610804000
1	2.334979000	−0.193437000	1.776390000

1	1.107208000	−1.282281000	2.314404000	1	0.208197000	−0.323341000	5.080599000
8	−1.207352000	−1.209138000	3.863017000	1	0.582975000	−1.979038000	4.557803000
6	−2.516593000	−1.468521000	4.400900000	3	−0.835226000	−0.543555000	2.051514000
1	−2.813469000	−2.491078000	4.133628000	1	−1.054459000	2.389780000	2.354132000
1	−3.216374000	−0.768130000	3.939866000	1	−0.860212000	4.130086000	2.484397000
6	−2.367331000	−1.308539000	5.903283000	1	−2.028255000	3.310087000	3.530928000
1	−3.134213000	−1.853010000	6.459726000	1	−4.011653000	3.462655000	−2.878118000
1	−2.426511000	−0.250520000	6.181896000	1	−2.309271000	3.035947000	−2.568403000
6	−0.955398000	−1.844885000	6.127125000	1	−3.106897000	−3.896022000	1.818102000
1	−0.501656000	−1.506209000	7.061736000	1	−1.934784000	−4.456136000	0.616720000
1	−0.962343000	−2.940385000	6.129846000	1	−4.057802000	−1.301585000	−4.303967000
6	−0.216359000	−1.318561000	4.904060000	1	−3.200711000	−0.163168000	−3.252000000

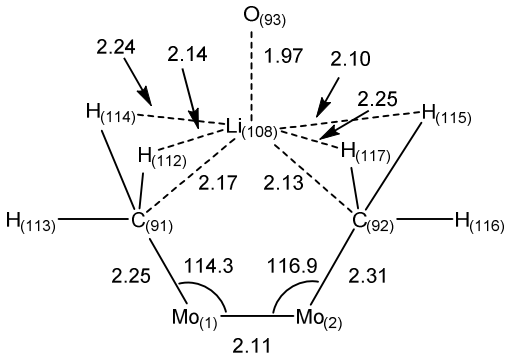


Table S24. 3b (M06) (−2340.62623369)

42	1.095624000	0.080251000	−0.360332000	1	−5.679138000	1.824168000	1.996169000
42	−0.990481000	0.365635000	−0.359998000	6	−5.753954000	1.706080000	−0.153063000
7	1.471228000	2.129205000	0.079603000	1	−6.732225000	1.230468000	−0.173339000
7	−0.804818000	2.534787000	−0.004271000	6	−5.101255000	2.001364000	−1.343153000
7	0.910339000	−1.921119000	−1.280668000	1	−5.579586000	1.782244000	−2.297583000
7	−1.368122000	−1.601716000	−1.096470000	6	−3.834316000	2.588142000	−1.340864000
6	0.476090000	3.035900000	0.074471000	6	−3.282493000	2.996155000	2.417337000
6	0.698600000	4.438158000	0.131598000	1	−3.362613000	4.077361000	2.592526000
1	1.723897000	4.795201000	0.190987000	1	−2.216050000	2.744850000	2.457942000
6	−0.362124000	5.302332000	0.084470000	1	−3.786876000	2.484514000	3.244554000
1	−0.196244000	6.377004000	0.114581000	6	−3.180889000	2.980068000	−2.634691000
6	−1.666458000	4.785832000	−0.012462000	1	−2.176674000	2.552677000	−2.745049000
1	−2.539624000	5.433066000	−0.044196000	1	−3.066030000	4.069609000	−2.700896000
6	−1.843764000	3.421656000	−0.053116000	1	−3.781033000	2.652362000	−3.490656000
6	−3.217865000	2.853149000	−0.105419000	6	2.769865000	2.531888000	0.485338000
6	−3.895708000	2.615947000	1.101409000				
6	−5.162206000	2.032689000	1.060180000				
6	3.023239000	2.781924000	1.847941000	1	−6.346955000	−3.197996000	−0.309995000
6	4.332619000	3.045238000	2.248619000	6	−4.279857000	−3.473907000	0.225210000
1	4.531595000	3.226638000	3.304702000	1	−4.494939000	−4.212104000	0.998214000
6	5.372838000	3.083972000	1.327601000	6	−2.953496000	−3.107722000	−0.002408000
1	6.388855000	3.288227000	1.658164000	6	−3.395717000	−0.689612000	−2.915122000
6	5.102676000	2.882315000	−0.019947000	1	−2.934545000	0.246647000	−2.575950000
6	3.806320000	2.614141000	−0.460324000	1	−4.300371000	−0.438408000	−3.480262000
6	1.908694000	2.802113000	2.850850000	1	−2.674377000	−1.149125000	−3.604422000
1	2.295259000	2.676197000	3.868257000	6	−1.850365000	−3.756318000	0.779289000
1	1.168332000	2.016365000	2.653549000	1	−1.323225000	−4.514991000	0.183912000
1	1.363018000	3.756007000	2.817128000	1	−2.240025000	−4.249463000	1.677989000
6	3.513140000	2.442200000	−1.919213000	1	−1.090880000	−3.027163000	1.090406000
1	3.269486000	1.398922000	−2.162265000	6	3.310291000	−2.152612000	−1.344967000
1	4.379157000	2.725537000	−2.528694000	6	3.976116000	−1.250654000	−2.193670000
1	2.652080000	3.046495000	−2.232330000	6	5.179762000	−0.691656000	−1.761337000
6	−0.364827000	−2.365693000	−1.560399000	1	5.691418000	0.026291000	−2.402450000
6	−0.559962000	−3.560727000	−2.302673000	6	5.725074000	−1.037936000	−0.530564000
1	−1.580438000	−3.867470000	−2.521728000	1	6.652840000	−0.577354000	−0.198645000
6	0.519878000	−4.284311000	−2.735595000	6	5.093149000	−1.983563000	0.266790000
1	0.374166000	−5.194101000	−3.313750000	1	5.529909000	−2.275672000	1.221098000
6	1.818969000	−3.834204000	−2.431893000	6	3.885280000	−2.557388000	−0.130455000
1	2.704300000	−4.383253000	−2.743485000	6	3.435723000	−0.939377000	−3.560253000
6	1.967288000	−2.667462000	−1.719618000	1	3.547460000	−1.803621000	−4.227982000
6	−2.676456000	−2.134623000	−0.983816000	1	3.970952000	−0.098172000	−4.014342000
6	−3.711976000	−1.611701000	−1.777732000	1	2.365696000	−0.696363000	−3.546220000
6	−5.025728000	−1.999069000	−1.515840000	6	3.234775000	−3.611120000	0.719064000
1	−5.827340000	−1.575217000	−2.120917000	1	3.583446000	−3.549544000	1.757465000
6	−5.316730000	−2.911865000	−0.509740000				

1	3.467656000	−4.617241000	0.345018000
1	2.140958000	−3.520771000	0.716755000
6	−0.041445000	0.869875000	−2.435498000
6	1.943841000	−0.572207000	1.622630000
6	−2.108943000	−0.129078000	1.594564000
8	−0.342380000	−2.136872000	3.547436000
6	−2.511441000	−2.925959000	4.354152000
1	−2.998953000	−2.715415000	3.394555000
1	−3.249177000	−2.782628000	5.151084000
1	−2.212656000	−3.981067000	4.366312000
6	−1.333984000	−2.002001000	4.567445000
1	−0.865421000	−2.167846000	5.549978000
1	−1.658995000	−0.955456000	4.532210000
6	0.554142000	−3.233366000	3.731362000
1	0.000950000	−4.089578000	4.145864000
1	0.887372000	−3.526964000	2.726118000
6	1.734629000	−2.860167000	4.597861000
1	2.298850000	−2.040279000	4.138511000
1	2.405107000	−3.718831000	4.715055000
1	1.418003000	−2.544240000	5.598543000
3	−0.162595000	−0.890092000	2.030838000
1	−0.187731000	1.925884000	−2.707776000
1	−0.435888000	0.218980000	−3.229657000
1	1.070984000	0.750726000	−2.534370000
1	1.718021000	−0.002177000	2.543562000
1	3.001612000	−0.340016000	1.417077000
1	1.940445000	−1.641857000	1.890903000
1	−2.234254000	−1.186635000	1.886698000
1	−3.122291000	0.169663000	1.287638000
1	−1.908184000	0.450467000	2.517323000
1	5.905137000	2.943341000	−0.755453000

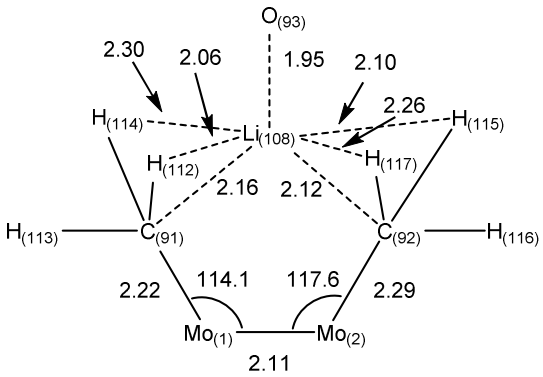


Table S25. 3b (PBE0–D3) (–2339.68452278)

42	1.091201000	0.014241000	−0.316721000
42	−1.005684000	0.240790000	−0.380155000
7	1.404820000	2.095380000	−0.076656000
7	−0.888197000	2.425298000	−0.218846000
7	0.986441000	−2.053159000	−1.002549000
7	−1.314197000	−1.790482000	−0.897096000
6	0.380855000	2.966924000	−0.166334000
6	0.569767000	4.375154000	−0.216304000
1	1.583267000	4.759169000	−0.183333000
6	−0.509310000	5.211245000	−0.323369000
1	−0.369020000	6.287551000	−0.371148000
6	−1.798840000	4.655534000	−0.380659000
1	−2.682997000	5.278305000	−0.462910000
6	−1.946223000	3.285753000	−0.328827000
6	−3.327613000	2.720629000	−0.375532000
6	−4.080907000	2.651673000	0.810555000
6	−5.379162000	2.140929000	0.756974000
1	−5.958504000	2.069462000	1.674224000
6	−5.932675000	1.726855000	−0.448500000
1	−6.940294000	1.321441000	−0.474319000
6	−5.202256000	1.852014000	−1.624001000
1	−5.645620000	1.562365000	−2.573451000
6	−3.902116000	2.363003000	−1.610145000
6	−3.526318000	3.156270000	2.114391000
1	−3.599310000	4.248980000	2.171038000
1	−2.470802000	2.900304000	2.231735000
1	−4.080710000	2.739950000	2.960035000
6	−3.169442000	2.595318000	−2.903052000
1	−2.169807000	2.153646000	−2.892864000
1	−3.040858000	3.668493000	−3.085452000
1	−3.722784000	2.173827000	−3.746391000
6	2.697517000	2.603741000	0.227994000
6	2.994833000	3.010028000	1.545982000
6	4.295688000	3.414126000	1.850443000
1	4.526920000	3.715909000	2.869608000
6	5.286095000	3.444199000	0.875893000
1	6.293833000	3.761248000	1.129337000
6	4.972171000	3.085529000	−0.429304000
6	3.684714000	2.669402000	−0.773693000
6	1.926263000	3.063215000	2.600166000
1	2.356370000	2.961644000	3.600943000
1	1.180556000	2.279482000	2.448292000
1	1.390842000	4.020476000	2.562819000
6	3.357601000	2.325208000	−2.198259000
1	3.316007000	1.240929000	−2.348861000
1	4.122126000	2.718719000	−2.874677000
1	2.385616000	2.728348000	−2.496324000
6	−0.272348000	−2.578159000	−1.227208000
6	−0.420725000	−3.877524000	−1.783124000
1	−1.424483000	−4.247675000	−1.961208000
6	0.683767000	−4.625405000	−2.097115000
1	0.572406000	−5.615904000	−2.529143000
6	1.962101000	−4.084198000	−1.870846000
1	2.864150000	−4.635839000	−2.112551000
6	2.070468000	−2.816916000	−1.342725000
6	−2.612751000	−2.369655000	−0.857596000
6	−3.568255000	−2.027219000	−1.833761000
6	−4.863581000	−2.534749000	−1.721783000
1	−5.598353000	−2.266212000	−2.477094000
6	−5.218540000	−3.379051000	−0.676733000
1	−6.232473000	−3.761640000	−0.601241000
6	−4.260904000	−3.742091000	0.261684000
1	−4.523421000	−4.418197000	1.072390000
6	−2.953995000	−3.257104000	0.185150000
6	−3.194385000	−1.163571000	−3.002835000
1	−2.920175000	−0.151175000	−2.692218000
1	−4.026810000	−1.088408000	−3.708185000
1	−2.326614000	−1.569880000	−3.532645000
6	−1.929671000	−3.721354000	1.180497000
1	−1.323609000	−4.539262000	0.771014000
1	−2.408271000	−4.084299000	2.094688000
1	−1.235171000	−2.918556000	1.442045000
6	3.422660000	−2.219571000	−1.140476000
6	4.000392000	−1.461146000	−2.178540000
6	5.264237000	−0.901765000	−1.979413000
1	5.711026000	−0.307328000	−2.772526000

6	5.954606000	−1.104858000	−0.789807000	6	−1.348593000	−1.035083000	4.886994000
1	6.931509000	−0.652702000	−0.644032000	1	−0.890937000	−0.872629000	5.871294000
6	5.401521000	−1.902033000	0.204028000	1	−1.723626000	−0.071232000	4.533285000
1	5.953323000	−2.085680000	1.122775000	6	0.601224000	−2.371775000	4.470773000
6	4.140888000	−2.481110000	0.039669000	1	0.065728000	−3.115693000	5.073860000
6	3.315823000	−1.323174000	−3.512266000	1	1.008864000	−2.894344000	3.600336000
1	3.377398000	−2.264032000	−4.071786000	6	1.714630000	−1.719186000	5.265955000
1	3.788730000	−0.544578000	−4.116955000	1	2.273462000	−1.020755000	4.637635000
1	2.252965000	−1.085641000	−3.416232000	1	2.406096000	−2.484978000	5.632000000
6	3.610419000	−3.417718000	1.090621000	1	1.330996000	−1.176999000	6.135581000
1	3.974110000	−3.137138000	2.083445000	3	−0.199560000	−0.618512000	2.132666000
1	3.944580000	−4.443772000	0.893123000	1	−0.197599000	1.572805000	−2.859046000
1	2.518872000	−3.434252000	1.109707000	1	−0.373254000	−0.178583000	−3.198471000
6	−0.050339000	0.562130000	−2.456929000	1	1.072984000	0.469881000	−2.481983000
6	1.919224000	−0.444609000	1.696210000	1	1.697003000	0.210013000	2.554660000
6	−2.177651000	−0.019494000	1.565286000	1	2.981457000	−0.251350000	1.487539000
8	−0.334317000	−1.421848000	3.955112000	1	1.890299000	−1.482444000	2.059487000
6	−2.483621000	−2.036588000	4.967827000	1	−2.283872000	−1.022014000	2.011415000
1	−2.969133000	−2.145046000	3.994560000	1	−3.185026000	0.200264000	1.189047000
1	−3.231302000	−1.686602000	5.686802000	1	−2.031440000	0.693841000	2.394009000
1	−2.141759000	−3.021671000	5.299697000	1	5.732540000	3.136555000	−1.205209000

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