Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Computational Raman spectroscopy of organometallic reaction products in lithium and sodium-based battery systems

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Table S1. DFT/B3PW91/Sadlej optimized atomic coordinates (in Å) for $Li_2C_2O_4$ and $Na_2C_2O_4$ molecular dimers.

Atom	X	Y	Z		Atom	X	Y	Z
C	0.02572	3.79329	3.33621		C	-0.33570	5.03110	1.46227
C	0.20550	-0.49235	0.55215		C	0.36219	-0.05950	-0.56353
C	-1.22362	3.46338	4.23482		C	-1.78620	5.48124	0.98192
C	1.45512	-0.16310	-0.34637		C	1.81269	-0.50764	-0.08118
LI	-0.35914	5.70525	4.85447		NA	-0.72407	7.67663	2.51885
LI	0.58999	-2.40438	-0.96538		NA	0.75364	-2.70892	-1.61212
LI	-0.92533	1.38976	2.69746		NA	-1.48442	2.72710	-0.15090
LI	1.15696	1.91111	1.19052		NA	1.51026	2.24693	1.04764
O	-0.12559	0.39663	1.38299		O	-0.01786	1.09189	-0.21439
O	-0.35529	-1.59648	0.37502		O	0.04311	3.88007	1.11069
O	0.35706	2.90460	2.50511		O	-0.31114	-0.86323	-1.25240
O	0.58608	4.89761	3.51353		O	0.33912	5.83270	2.15213
O	-1.54317	4.35712	5.06234		O	-2.16701	6.62655	1.34052
O	-1.77033	2.35817	4.04178		O	2.19458	-1.65347	-0.43676
O	1.77462	-1.05721	-1.17355		O	-2.42901	4.66412	0.28841
O	2.00208	0.94203	-0.15360		O	2.45458	0.31144	0.61091

Table S2. DFT/B3PW91/Sadlej optimized atomic coordinates (in Å) for HCO_2Li and HCO_2Na molecular dimers.

Atom	X	Y	Z		Atom	X	Y	Z
C	2.23030	5.56204	1.37037		C	3.78710	5.49212	4.46497
C	5.76309	8.47929	1.35473		C	7.71389	8.81080	3.71166
H	1.40492	4.81849	1.36646		H	2.72645	5.33239	4.76394
H	6.58844	9.22289	1.35850		H	8.77442	8.97060	3.41225
LI	2.95868	8.21959	1.57511		NA	5.18333	8.60761	4.44913
LI	5.03467	5.82175	1.15020		NA	6.31786	5.69529	3.72820
O	1.90560	6.76602	1.52039		O	4.21673	6.68584	4.49208
O	3.39521	5.11365	1.22426		O	4.45807	4.49322	4.13164
O	4.59817	8.92765	1.50094		O	7.04288	9.80969	4.04493
O	6.08782	7.27531	1.20475		O	7.28445	7.61702	3.68504

Table S3. DFT/B3PW91/Sadlej optimized atomic coordinates (in Å) for CH_3CO_2Li and CH_3CO_2Na molecular dimers.

Atom	X	Y	Z		Atom	X	Y	Z
C	-2.33080	0.25480	-0.04289		C	5.73244	7.84716	5.63654
C	2.33725	-0.24308	0.04678		C	5.74354	13.60762	2.46909
C	-3.74841	-0.25461	-0.07101		C	5.98095	6.36019	5.77916
C	3.75490	0.26624	0.07510		C	5.99209	12.12071	2.61212
H	-3.89132	-0.89586	-0.95251		H	4.68734	13.83091	2.67865
H	3.89790	0.90697	0.95698		H	5.38377	5.81641	5.03204
H	-3.92839	-0.88289	0.81330		H	5.71942	6.00750	6.78219
H	3.93490	0.89501	-0.80886		H	6.00594	13.96027	1.46627
H	-4.46376	0.57320	-0.09072		H	6.33984	14.15160	3.21676
H	4.47018	-0.56163	0.09436		H	7.03688	6.13668	5.56854
LI	-0.25911	1.28762	0.00982		NA	5.24366	10.44181	5.49614
LI	0.26552	-1.27609	-0.00603		NA	6.48092	9.52614	2.75262
O	-1.38463	-0.60303	-0.03346		O	5.22955	8.48374	6.59299
O	1.39112	0.61477	0.03735		O	5.67533	11.57720	3.72301
O	-2.10907	1.49162	-0.02781		O	6.04916	8.39090	4.52573
O	2.11547	-1.47989	0.03159		O	6.49501	11.48395	1.65579

Table S4. DFT/B3PW91/Sadlej optimized atomic coordinates (in Å) for CH_3OCO_2Li and CH_3OCO_2Na molecular dimers.

Atom	X	Y	Z		Atom	X	Y	Z
C	2.22698	-0.68353	-0.05408		C	10.9970	3.9241	7.3136
C	-2.23700	0.68761	0.05174		C	12.8625	2.6977	8.0552
C	4.42101	-1.50939	-0.10505		C	5.1496	7.9921	4.9451
C	-4.43056	1.51475	0.10273		C	7.0157	6.7655	5.6848
H	4.24145	-2.14962	-0.97915		H	12.3564	2.3218	8.9556
H	-4.25056	2.15497	0.97677		H	12.7764	1.9357	7.2675
H	4.30082	-2.11436	0.80372		H	13.9193	2.8901	8.2740
H	-4.31000	2.11957	-0.80611		H	4.0925	7.7998	4.7273
H	5.43171	-1.08953	-0.14686		H	5.2365	8.7538	5.7329
H	-5.44152	1.09552	0.14461		H	5.6547	8.3684	4.0443
LI	0.03331	-1.27843	0.01663		NA	8.4521	3.8550	6.7006
LI	-0.04324	1.28235	-0.01903		NA	9.5606	6.8341	6.2968
O	1.45006	0.31857	-0.04667		O	10.3471	2.8574	7.3974
O	-1.46065	-0.31493	0.04436		O	10.5330	5.0407	6.9440
O	1.82870	-1.87231	-0.02409		O	12.3144	3.9393	7.6350
O	-1.83817	1.87623	0.02164		O	5.6981	6.7503	5.3643
O	3.53500	-0.39348	-0.09734		O	7.4799	5.6487	6.0537
O	-3.54522	0.39831	0.09508		O	7.6655	7.8322	5.6011

Table S5. DFT/B3PW91/Sadlej optimized atomic coordinates (in Å) for CH_3OLi and CH_3ONa molecular dimers.

Atom	X	Y	Z		Atom	X	Y	Z
C	-2.69096	-0.57842	0.00037		C	-2.92230	-0.54435	-0.03511
C	2.69099	0.57846	-0.00039		C	2.92439	0.54496	0.03572
H	3.00485	1.16989	-0.88746		H	-3.20941	-1.39482	-0.69872
H	-3.00504	-1.16917	0.88780		H	3.21188	1.39148	0.70420
H	3.00519	1.16965	0.88670		H	-3.33909	-0.80009	0.96846
H	-3.00522	-1.17016	-0.88634		H	3.34008	0.80694	-0.96670
H	-3.33118	0.32889	-0.00008		H	-3.53283	0.31884	-0.39135
H	3.33138	-0.32874	-0.00064		H	3.53560	-0.32017	0.38606
LI	-0.23622	1.09314	0.00074		NA	-0.25128	1.35948	-0.27483
LI	0.23625	-1.09335	-0.00085		NA	0.25340	-1.35913	0.27546
O	-1.34115	-0.28694	0.00007		O	-1.56980	-0.29300	-0.01877
O	1.34122	0.28672	-0.00018		O	1.57195	0.29328	0.01924

Table S6. DFT/PBE0/TZVPPD optimized atomic coordinates (in Å) for $Li_2C_2O_4$ and $Na_2C_2O_4$ molecular dimers.

Atom	X	Y	Z		Atom	X	Y	Z
C	-0.07039	3.74129	3.43271		C	-0.32365	5.02353	1.44679
C	0.30656	-0.40609	0.53411		C	0.35511	-0.05151	-0.54693
C	-1.30147	3.34239	4.32944		C	-1.77023	5.47570	0.96471
C	1.53782	-0.00712	-0.36244		C	1.80171	-0.50368	-0.06492
LI	-0.50042	5.58810	4.99927		NA	-0.70111	7.66622	2.48796
LI	0.73720	-2.25299	-1.03212		NA	0.73257	-2.69411	-1.58828
LI	-0.92237	1.34615	2.74072		NA	-1.48263	2.72365	-0.15111
LI	1.15815	1.98912	1.22600		NA	1.51408	2.24831	1.05104
O	-0.04935	0.44049	1.38978		O	-0.01352	1.09811	-0.20306
O	-0.21453	-1.51722	0.32994		O	0.04497	3.87387	1.10303
O	0.28524	2.89476	2.57690		O	-0.32128	-0.84869	-1.22709
O	0.45088	4.85233	3.63690		O	0.35273	5.82075	2.12692
O	-1.63654	4.19466	5.18393		O	-2.14518	6.61684	1.31739
O	-1.81514	2.23442	4.10592		O	2.17667	-1.64480	-0.41766
O	1.87319	-0.85944	-1.21676		O	-2.40973	4.66144	0.27776
O	2.05134	1.10092	-0.13891		O	2.44122	0.31056	0.62204

Table S7. DFT/PBE0/TZVPPD optimized atomic coordinates (in Å) for HCO_2Li and HCO_2Na molecular dimers.

Atom	X	Y	Z		Atom	X	Y	Z
C	2.21120	5.59969	1.38428		C	3.76395	5.50951	4.35248
C	5.78162	8.44322	1.34136		C	7.73710	8.79369	3.82428
H	1.37970	4.87283	1.38371		H	2.68337	5.36682	4.54584
H	6.61313	9.17007	1.34197		H	8.81768	8.93638	3.63089
LI	2.97741	8.24126	1.59990		NA	5.15849	8.61947	4.29884
LI	5.01543	5.80163	1.12570		NA	6.34256	5.68372	3.87802
O	1.90714	6.80059	1.54564		O	4.18846	6.69953	4.35550
O	3.36116	5.13615	1.22332		O	4.45788	4.50056	4.15168
O	4.63167	8.90677	1.50232		O	7.04315	9.80264	4.02502
O	6.08567	7.24232	1.17997		O	7.31260	7.60366	3.82136

Table S8. DFT/PBE0/TZVPPD optimized atomic coordinates (in Å) for CH_3CO_2Li and CH_3CO_2Na molecular dimers.

Atom	X	Y	Z		Atom	X	Y	Z
C	-2.33899	0.20913	-0.07161		C	5.64091	7.86586	5.63523
C	2.33925	-0.20583	0.07279		C	5.86268	6.38069	5.79766
C	-3.74211	-0.32741	-0.11695		C	6.07958	12.09867	2.61072
C	3.74248	0.33048	0.11751		C	5.85796	13.58386	2.44838
H	3.84347	1.02809	0.94985		H	6.91331	6.14347	5.62267
H	-3.84591	-1.01321	-0.95881		H	5.56559	6.04657	6.78884
H	-3.93321	-0.90354	0.79053		H	5.28331	5.84546	5.04255
H	3.93774	0.89332	-0.79749		H	6.15561	13.91813	1.45743
H	4.46525	-0.47594	0.21119		H	6.43687	14.11897	3.20392
H	-4.46578	0.47962	-0.19724		H	4.80722	13.82107	2.62278
LI	-0.27955	1.27933	0.01810		NA	5.18631	10.45189	5.46416
LI	0.27982	-1.27604	-0.01759		NA	6.53390	9.51259	2.78166
O	-1.38228	-0.62851	-0.06012		O	6.01206	8.39421	4.54038
O	1.38262	0.63187	0.06051		O	5.10718	8.50985	6.56003
O	-2.14007	1.44164	-0.04020		O	6.61347	11.45472	1.68598
O	2.14026	-1.43835	0.04169		O	5.70811	11.57024	3.70544

Table S9. DFT/PBE0/TZVPPD optimized atomic coordinates (in Å) for CH_3OCO_2Li and CH_3OCO_2Na molecular dimers.

Atom	X	Y	Z		Atom	X	Y	Z
C	2.21515	-0.71963	0.00001		C	11.01804	3.93032	7.30507
C	-2.21521	0.71953	-0.00002		C	12.90458	2.73873	8.03471
C	4.39298	-1.57899	0.00007		C	5.12715	7.92874	4.97676
C	-4.39304	1.57893	0.00001		C	7.01380	6.73701	5.70586
H	4.23496	-2.19271	0.88716		H	12.40626	2.34306	8.92076
H	4.23496	-2.19284	-0.88692		H	12.84270	1.99454	7.23943
H	-4.23499	2.19276	0.88701		H	13.94688	2.95799	8.25960
H	-4.23505	2.19266	-0.88707		H	4.08481	7.70953	4.75200
H	5.40171	-1.17194	0.00004		H	5.18915	8.67276	5.77219
H	-5.40177	1.17188	0.00006		H	5.62532	8.32461	4.09072
LI	0.01172	-1.29746	0.00006		NA	8.49000	3.83788	6.68313
LI	-0.01176	1.29737	-0.00012		NA	9.54190	6.82938	6.32754
O	1.46053	0.29224	-0.00007		O	10.39318	2.85572	7.37236
O	-1.46061	-0.29237	0.00002		O	10.53366	5.03723	6.94935
O	1.80051	-1.89628	0.00010		O	12.32700	3.96818	7.62985
O	-1.80054	1.89617	-0.00009		O	5.70479	6.69920	5.38126
O	3.52349	-0.45489	-0.00002		O	7.49824	5.63002	6.06125
O	-3.52355	0.45482	0.00004		O	7.63863	7.81164	5.63873

Table S10. DFT/PBE0/TZVPPD optimized atomic coordinates (in Å) for CH_3OLi and CH_3ONa molecular dimers.

Atom	X	Y	Z		Atom	X	Y	Z
C	2.68889	0.59921	-0.05115		C	-2.89805	-0.63556	-0.12715
C	-2.68896	-0.59913	0.05134		C	2.89878	0.62919	0.13780
H	2.92714	1.44082	-0.72244		H	3.11127	1.58954	0.64620
H	-2.92720	-1.44064	0.72275		H	-3.12281	-1.50219	-0.77846
H	3.07461	0.87750	0.94376		H	-3.34269	-0.88006	0.85638
H	-3.07469	-0.87758	-0.94353		H	3.37876	0.70897	-0.85623
H	3.30671	-0.24682	-0.39497		H	3.48452	-0.12845	0.69312
H	-3.30680	0.24695	0.39503		H	-3.50718	0.19581	-0.53137
LI	0.24467	-1.08682	0.03008		NA	-0.30494	1.34605	0.29440
LI	-0.24476	1.08692	-0.02994		NA	0.30575	-1.35397	-0.28126
O	1.34224	0.30096	-0.03120		O	-1.55707	-0.34238	-0.05620
O	-1.34232	-0.30085	0.03134		O	1.55791	0.33509	0.06867

Table S11. DFT/PBE0/TZVPPD vibrational frequencies for dimers of $Li_2C_2O_4$ and $Na_2C_2O_4$ and their respective band assignments. The reported vibrational frequencies were scaled by 0.9594 (see text for details).

$Li_2C_2O_4$				$Na_2C_2O_4$		
(cm^{-1})	(Å^4/amu)	Assignment		(cm^{-1})	(Å^4/amu)	Assignment
1694	0	ν(C=O)		1663	2	ν(C=O)
1678	0	ν(C=O)		1655	0	ν(C=O)
1647	23	ν(C=O)		1624	22	ν(C=O)
1635	0	ν(C=O)		1610	0	ν(C=O)
1428	62	ν(C-C) + ν(C-O)		1411	83	ν(C-C) + ν(C-O)
1427	0	ν(C-C) + ν(C-O)		1411	0	ν(C-C) + ν(C-O)
1321	1	ν(OCO)		1315	1	ν(OCO)
1319	0	ν(OCO)		1313	0	ν(OCO)
877	0	δ(OCO) + ν(C-C)		855	1	δ(OCO) + ν(C-C)
871	15	δ(OCO) + ν(C-C)		855	17	δ(OCO) + ν(C-C)
851	0	δ(OCO) out of plane		850	0	δ(OCO) out of plane
850	0	δ(COC) out of plane		850	0	δ(OCO) out of plane
803	0	δ(OCO)		764	0	δ(OCO)
787	0	δ(OCO)		763	0	δ(OCO)
651	0	ν(O-Li)		555	4	δ(OCO)
622	2	ν(O-Li)		554	0	δ(OCO)
592	11	δ(OCO) + δ(O-Li)		495	0	δ(OCO) out of plane
590	0	δ(OCO) + δ(O-Li)		493	0	δ(OCO) out of plane
577	5	δ(OCO) + ν(O-Li)		470	16	ν(C-C)
554	0	δ(OCO) + ν(O-Li)		467	0	ν(C-C)
516	2	δ(OCO) + δ(O-Li)				
516	0	δ(OCO) + δ(O-Li)				
490	0	δ(OCO) out of plane				
487	0	δ(OCO) out of plane				
449	0	ν(C-C)				
433	5	ν(C-C)				

Table S12. DFT/PBE0/TZVPPD vibrational frequencies for dimers of HCO_2Li and HCO_2Na and their respective band assignments. The reported vibrational frequencies were scaled by 0.9594 (see text for details).

HCO_2Li				HCO_2Na		
(cm^{-1})	(Ă^4/amu)	Assignment		(cm^{-1})	(Ă^4/amu)	Assignment
2868	324	ν(CH)		2836	386	ν(CH)
2866	0	ν(CH)		2835	0	ν(CH)
1643	0	ν(C=O)		1609	0	ν(C=O)
1601	1	ν(C=O)		1608	4	ν(C=O)
1377	27	ν(OCO)		1360	28	ν(OCO)
1376	0	ν(OCO)		1356	0	ν(OCO)
1346	0	δ(HCO)		1321	11	δ(HCO)
1346	10	δ(HCO)		1320	0	δ(HCO)
1046	0	τ(CH)		1038	0	τ(CH)
1046	1	τ(CH)		1038	1	τ(CH)
742	0	δ(OCO) + ν(O-Li)		760	0	δ(OCO)
740	1	δ(OCO)		759	2	δ(OCO)
690	0	ν(O-Li)				
673	0	ν(O-Li)				

Table S13. DFT/PBE0/TZVPPD vibrational frequencies for dimers of CH_3CO_2Li and CH_3CO_2Na and their respective band assignments. The reported vibrational frequencies were scaled by 0.9594 (see text for details).

CH_3CO_2Li				CH_3CO_2Na		
(cm^{-1})	(Å^4/amu)	Assignment		(cm^{-1})	(Å^4/amu)	Assignment
3051	71	$\nu(HCH_2)$		3044	104	$\nu(HCH_2)$
3051	31	$\nu(HCH_2)$		3044	6	$\nu(HCH_2)$
3011	41	$\nu(HCH_2)$		3006	31	$\nu(HCH_2)$
3011	52	$\nu(HCH_2)$		3006	62	$\nu(HCH_2)$
2944	175	$\nu(CH)_3$		2939	306	$\nu(CH)_3$
2944	169	$\nu(CH)_3$		2939	30	$\nu(CH)_3$
1589	0	ν(C=O)		1587	0	ν(C=O)
1578	8	ν(C=O)		1584	11	ν(C=O)
1445	15	ν(C-O) + $\delta(CH_3)$		1420	19	ν(C-O) + $\delta(CH_3)$
1433	0	ν(C-O) + $\delta(CH_3)$		1416	0	$\delta(HCH_2)$
1411	6	$\delta(HCH_2)$		1414	8	$\delta(HCH_2)$
1411	0	$\delta(HCH_2)$		1410	0	ν(C-O) + $\delta(CH_3)$
1394	1	$\delta(HCH_2)$		1395	14	$\delta(HCH_2)$
1394	13	$\delta(HCH_2)$		1395	0	$\delta(HCH_2)$
1313	1	$\delta(CH_3)$ + ν(C-O)		1308	2	$\delta(CH_3)$ + ν(C-O)
1312	0	$\delta(CH_3)$ + ν(C-O)		1307	0	$\delta(CH_3)$ + ν(C-O)
1026	0	$\tau(CH_3CO)$		1023	0	$\tau(CH_3CO)$
1026	0	$\tau(CH_3CO)$		1023	0	$\tau(CH_3CO)$
995	0	$\tau(CH_3CO)$		985	0	$\tau(CH_3CO)$
989	4	$\tau(CH_3CO)$		984	3	$\tau(CH_3CO)$
947	0	ν(C-C) + δ(OCO)		921	0	ν(C-C) + δ(OCO)
932	21	ν(C-C) + δ(OCO)		920	27	ν(C-C) + δ(OCO)
697	0	ν(O-Li)		645	2	δ(OCO) + ν(C-C)
697	0	ν(O-Li)		645	0	δ(OCO) + ν(C-C)
649	0	δ(OCO) + ν(C-C)		600	0	δ(CCO) out of plane
646	3	δ(OCO) + ν(C-C)		600	2	δ(CCO) out of plane
603	0	δ(CCO) out of plane		452	0	δ(CCO) in plane
601	2	δ(CCO) out of plane		443	0	δ(CCO) in plane
450	0	δ(CCO) in plane				
441	0	δ(OCO) in plane				

Table S14. DFT/PBE0/TZVPPD vibrational frequencies for dimers of CH_3OCO_2Li and CH_3OCO_2Na and their respective band assignments. The reported vibrational frequencies were scaled by 0.9594 (see text for details).

CH_3OCO_2Li				CH_3OCO_2Na		
(cm^{-1})	(Ă^4/amu)	Assignment		(cm^{-1})	(Ă^4/amu)	Assignment
3041	92	$\nu(HCH_2)$		3030	98	$\nu(HCH_2)$
3041	41	$\nu(HCH_2)$		3030	42	$\nu(HCH_2)$
3015	3	$\nu(HCH_2)$		3004	0	$\nu(HCH_2)$
3015	74	$\nu(HCH_2)$		3004	84	$\nu(HCH_2)$
2940	334	$\nu(CH)_3$		2933	346	$\nu(CH)_3$
2940	4	$\nu(CH)_3$		2933	1	$\nu(CH)_3$
1622	0	ν(C=O)		1628	6	ν(C=O)
1615	4	ν(C=O)		1627	0	ν(C=O)
1463	9	ν(C-O) + $\delta(CH_3)$		1440	10	ν(C-O) + $\delta(CH_3)$
1452	0	ν(C-O) + $\delta(CH_3)$		1438	0	ν(C-O) + $\delta(CH_3)$
1434	6	$\delta(HCH_2)$		1434	5	$\delta(HCH_2)$
1433	0	$\delta(HCH_2)$		1431	0	$\delta(HCH_2)$
1421	1	$\delta(HCH_2)$		1418	1	$\delta(HCH_2)$
1421	7	$\delta(HCH_2)$		1418	7	$\delta(HCH_2)$
1369	4	ν(C-O) + $\delta(CH_3)$		1348	8	ν(C-O) + $\delta(CH_3)$
1357	0	ν(C-O) + $\delta(CH_3)$		1337	0	ν(C-O) + $\delta(CH_3)$
1174	0	τ(HCOC)		1168	3	τ(HCOC)
1174	4	τ(HCOC)		1167	0	τ(HCOC)
1133	0	τ(HCOC)		1132	4	τ(HCOC)
1133	5	τ(HCOC)		1132	0	τ(HCOC)
1119	0	ν(C-O)		1110	1	ν(C-O)
1116	1	ν(C-O)		1109	0	ν(C-O)
958	0	ν(C-O)		936	0	ν(C-O)
947	29	ν(C-O)		935	30	ν(C-O)
811	0	$\delta(CO_3)$ out of plane		812	0	$\delta(CO_3)$ out of plane
810	0	$\delta(CO_3)$ out of plane		811	0	$\delta(CO_3)$ out of plane
733	1	δ(O-C=O) + ν(O-Li)		695	1	δ(O-C=O)
722	0	δ(O-C=O) + ν(O-Li)		695	0	δ(O-C=O)
681	0	δ(COO) + ν(O-Li)		587	4	δ(O-C-O)
638	1	δ(COO) + ν(O-Li)		584	0	δ(O-C-O)
580	4	δ(O-C-O)				
561	0	δ(O-C-O)				

Table S15. DFT/PBE0/TZVPPD vibrational frequencies for dimers of CH_3OLi and CH_3ONa and their respective band assignments. The reported vibrational frequencies were scaled by 0.9594 (see text for details).

CH_3OLi				CH_3ONa		
(cm^{-1})	(Å^4/amu)	Assignment		(cm^{-1})	(Å^4/amu)	Assignment
2847	0	$\nu(HCH_2)$		2790	80	$\nu(HCH_2)$
2847	215	$\nu(HCH_2)$		2790	241	$\nu(HCH_2)$
2845	0	$\nu(HCH_2)$		2787	19	$\nu(HCH_2)$
2845	239	$\nu(HCH_2)$		2786	303	$\nu(HCH_2)$
2815	453	$\nu(CH)_3$		2772	428	$\nu(CH)_3$
2811	0	$\nu(CH)_3$		2768	0	$\nu(CH)_3$
1437	11	$\delta(HCH_2)$		1430	12	$\delta(HCH_2)$
1436	0	$\delta(HCH_2)$		1429	1	$\delta(HCH_2)$
1434	16	$\delta(HCH_2)$		1428	7	$\delta(HCH_2)$
1434	0	$\delta(HCH_2)$		1427	9	$\delta(HCH_2)$
1428	10	$\delta(HCH_2)$		1423	9	$\delta(HCH_2)$
1425	0	$\delta(HCH_2)$		1420	0	$\delta(HCH_2)$
1160	1	ν(C-O)		1142	0	$\tau(OCH_3)$
1151	3	$\tau(OCH_3)$		1141	0	$\tau(OCH_3)$
1151	0	$\tau(OCH_3)$		1136	0	ν(C-O)
1142	0	ν(C-O)		1134	0	$\tau(OCH_3)$
1139	0	$\tau(OCH_3)$		1133	0	$\tau(OCH_3)$
1138	1	$\tau(OCH_3)$		1122	0	ν(C-O)
622	0	ν(O-Li)				
591	9	δ(LiOLi)				
549	0	ν(O-Li)				
527	0	δ(O-Li)				

Table S16. DFT/LDA vibrational frequencies for the crystalline structure of HCO_2Na and its respective band assignments.

HCO_2Na	
(cm^{-1})	Assignment
2830	ν(CH)
2829	ν(CH)
1577	ν(C=O)
1575	ν(C=O)
1353	ν(OCO)
1351	ν(OCO)
1319	δ(HCO)
1315	δ(HCO)
1026	τ(CH)
1021	τ(CH)
771	δ(OCO)
770	δ(OCO)

Table S17. DFT/B3PW91/Sadlej optimized atomic coordinates (in Å) for CH_3OLi and CH_3ONa molecular trimers.

Atom	X	Y	Z		Atom	X	Y	Z
C	-0.05093	3.86295	-0.22896		C	0.09782	4.21517	-0.11332
C	-2.78590	-1.13047	-0.04104		C	3.13872	-1.29645	0.09550
C	2.90749	-0.99471	0.12749		C	-3.16090	-1.17090	-0.12141
H	-0.54287	4.24571	-1.14790		H	-0.38396	4.65663	-1.01763
H	-0.57496	4.33878	0.62662		H	-0.39798	4.70589	0.75732
H	0.97265	4.29425	-0.23318		H	1.13796	4.61972	-0.11666
H	2.76905	-2.09485	0.19331		H	2.98531	-2.40174	0.10277
H	-2.87652	-1.83193	-0.89704		H	-3.29191	-1.84869	-0.99789
H	-2.93374	-1.73763	0.87682		H	-3.34981	-1.80552	0.77655
H	3.51152	-0.71349	1.01581		H	3.73905	-1.08457	1.01183
H	3.55665	-0.82515	-0.75730		H	3.82784	-1.10849	-0.76158
H	-3.67004	-0.46111	-0.10508		H	-4.03045	-0.47266	-0.16700
LI	0.08722	-1.02089	0.04662		NA	0.00578	-1.42837	-0.05186
LI	1.37558	1.43401	-0.05615		NA	-1.70692	1.59600	-0.10750
LI	-1.39468	1.32103	-0.13199		NA	1.75101	1.55647	0.00336
O	-0.05490	2.47639	-0.15632		O	0.03700	2.83631	-0.07553
O	-1.58155	-0.43961	-0.03900		O	-1.93646	-0.53339	-0.09702
O	1.70728	-0.30060	0.05319		O	1.96506	-0.57255	0.02714

Table S18. DFT/B3PW91/Sadlej optimized atomic coordinates (in Å) for CH_3OLi and CH_3ONa molecular tetramers.

Atom	X	Y	Z		Atom	X	Y	Z
C	0.73961	-0.80201	2.95312		C	0.86247	-0.63694	3.15075
C	-1.67122	2.65516	0.04496		C	-1.77670	2.96998	-0.17496
C	-1.69616	-2.27936	-1.31401		C	-1.88113	-2.49194	-1.34612
C	2.63153	0.43636	-1.64517		C	2.84386	0.41173	-1.96696
H	0.33432	-1.79421	3.24272		H	0.43394	-1.59788	3.51940
H	0.34812	-0.08256	3.70264		H	0.50534	0.13659	3.86997
H	-1.19204	3.48082	-0.52184		H	-1.31748	3.76840	-0.80304
H	-1.20735	-2.70053	-2.21759		H	-1.41634	-2.99665	-2.22494
H	1.83459	-0.85785	3.12772		H	-1.91445	3.43272	0.83004
H	-1.83998	3.04761	1.06973		H	1.95956	-0.71850	3.33124
H	-1.87443	-3.13982	-0.63538		H	-2.07839	-3.30748	-0.61194
H	-2.67967	2.52503	-0.40105		H	-2.80757	2.83814	-0.57876
H	-2.70029	-1.93796	-1.64235		H	-2.88780	-2.16486	-1.69604
H	2.71263	-0.24394	-2.51874		H	2.92223	1.41259	-2.45224
H	2.71617	1.46578	-2.05239		H	2.92833	-0.32374	-2.80053
H	3.54995	0.27037	-1.04384		H	3.78525	0.29738	-1.38066
LI	-0.34973	0.38926	-1.39091		NA	-0.44623	0.44088	-1.83775
LI	0.79572	-1.27036	-0.00548		NA	0.98626	-1.51993	-0.03268
LI	0.81955	1.09347	0.63937		NA	1.05360	1.44081	0.59268
LI	-1.25053	-0.20396	0.80499		NA	-1.50852	-0.12085	0.92744
O	0.41964	-0.44945	1.65093		O	0.53896	-0.35836	1.83688
O	-0.92279	1.48817	0.03237		O	-1.04254	1.80002	-0.14651
O	-0.95228	-1.27095	-0.72085		O	-1.11531	-1.46245	-0.83392
O	1.46850	0.23986	-0.91640		O	1.70023	0.25560	-1.20833