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Design, preparation and characterization of 7-hydroxy-4-methylcoumarin based deep eutectic solvents

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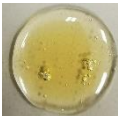




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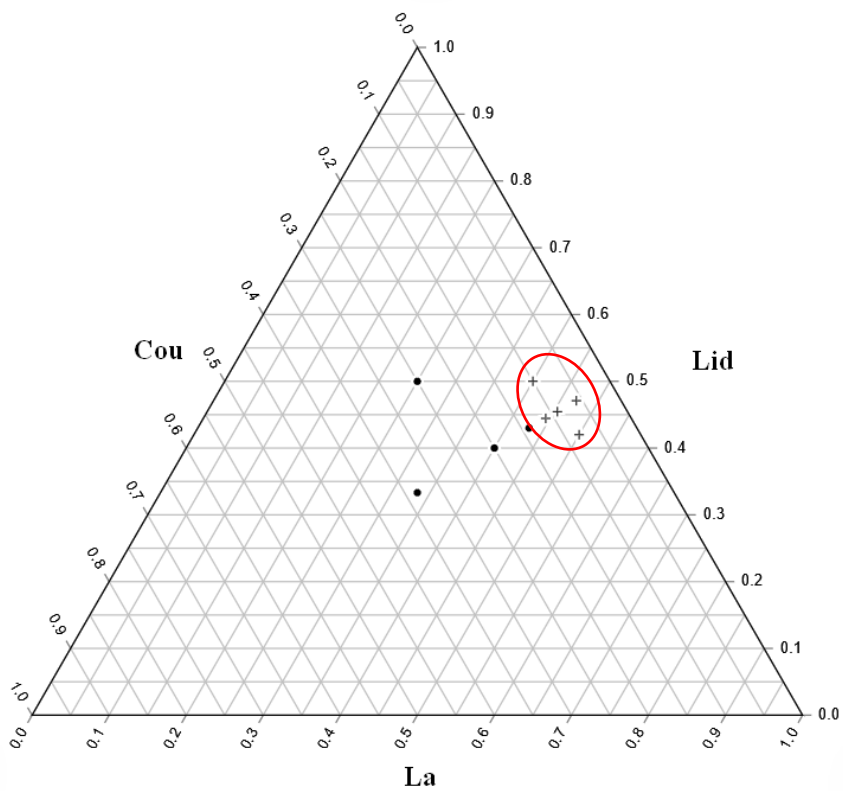
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Table S1. Appearance of pure compounds and their mixtures obtained in different mixing ratios.

Sample	Component 1	Component 2	Component 3	Molar ratio	Appearance
	lidocaine	-	-	-	Solid
	7-hydroxy-4 methylcoumarin	-	-	-	Solid
	lactic acid	-	-	-	Liquid
	levulinic acid	-	-	-	Liquid
	Mixed components				
	lidocaine	7-hydroxy-4 methylcoumarin	lactic acid	1:1:1	Opaque solid
	lidocaine	7-hydroxy-4 methylcoumarin	lactic acid	2:1:1	Transparent solid
	lidocaine	7-hydroxy-4 methylcoumarin	lactic acid	2:1:2	Transparent solid
	lidocaine	7-hydroxy-4 methylcoumarin	lactic acid	3:1:3	Transparent solid
	lidocaine	7-hydroxy-4 methylcoumarin	lactic acid	4:1:4	Viscous liquid

					
	lidocaine	7-hydroxy-4 methylcoumarin	lactic acid	5:1:4	Viscous liquid
	lidocaine	7-hydroxy-4 methylcoumarin	lactic acid	5:1:5	Viscous liquid
	lidocaine	7-hydroxy-4 methylcoumarin	lactic acid	5:1:6	Liquid
	lidocaine	7-hydroxy-4 methylcoumarin	lactic acid	8:1:8	Liquid
	lidocaine	7-hydroxy-4 methylcoumarin	levulinic acid	1:1:1	Opaque solid
	lidocaine	7-hydroxy-4 methylcoumarin	levulinic acid	2:1:1	Transparent solid
	lidocaine	7-hydroxy-4 methylcoumarin	levulinic acid	2:1:2	Transparent solid
	lidocaine	7-hydroxy-4 methylcoumarin	levulinic acid	3:1:3	Viscous liquid
	lidocaine	7-hydroxy-4 methylcoumarin	levulinic acid	4:1:4	Liquid

	lidocaine	7-hydroxy-4 methylcoumarin	levulinic acid	5:1:4	Liquid
	lidocaine	7-hydroxy-4 methylcoumarin	levulinic acid	5:1:5	Liquid
	lidocaine	7-hydroxy-4 methylcoumarin	levulinic acid	5:1:6	Liquid
	lidocaine	7-hydroxy-4 methylcoumarin	levulinic acid	8:1:8	Liquid



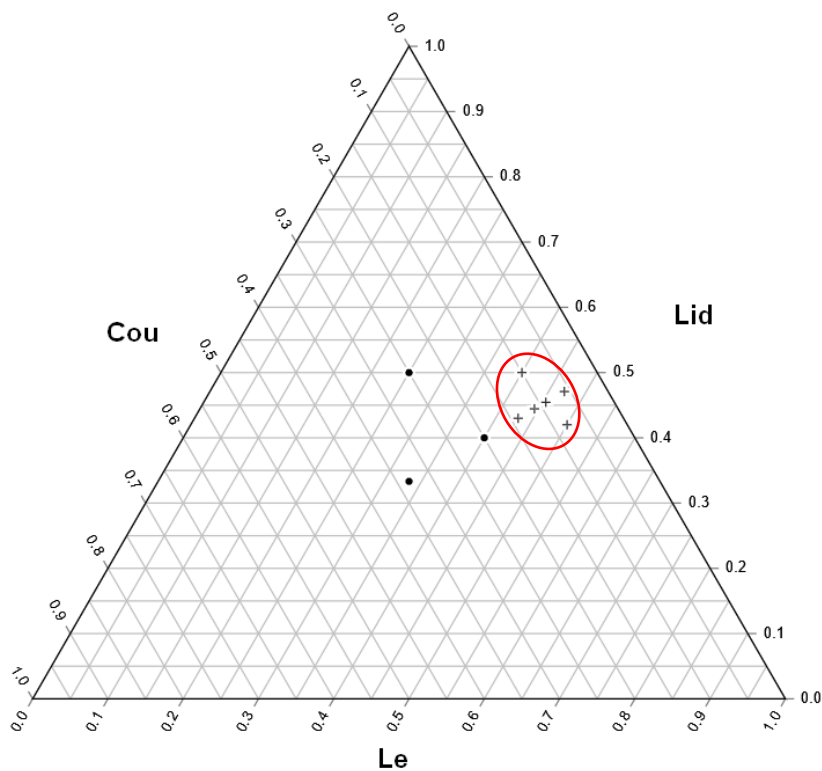


Fig. S1. Ternary solid-liquid phase diagram for (a) Lid:Cou:La and (b) Lid:Cou:La. Black dots represent the experimental points of the solid phase and black crosses represent points of the liquid phase. The red circle represents the area of liquid form at 298 K.

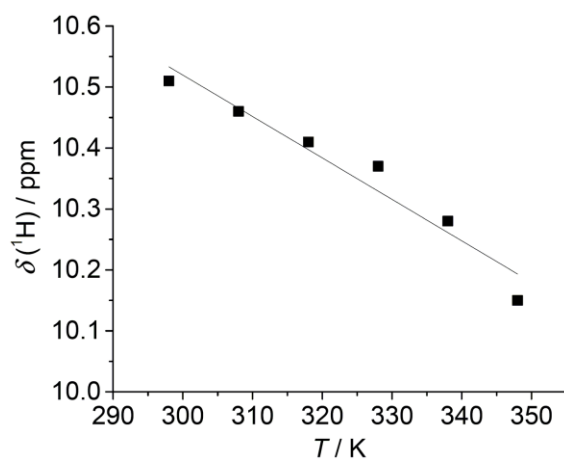
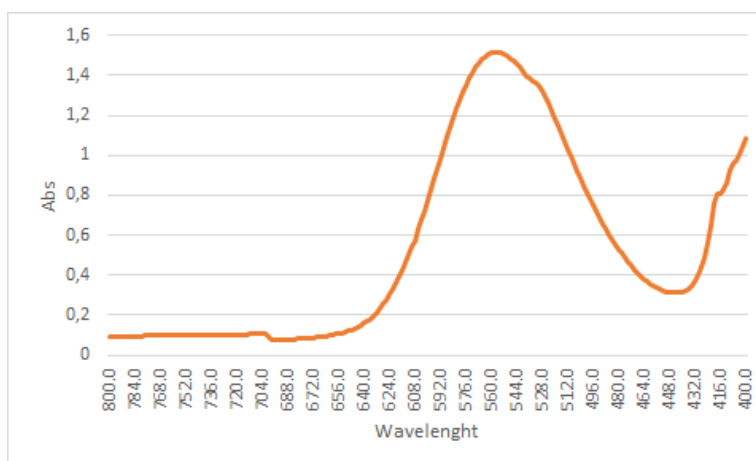


Fig. S2. Hydroxyl proton chemical shift of 7-hydroxy-4-methylcoumarin in DMSO- d_6 as a function of temperature.

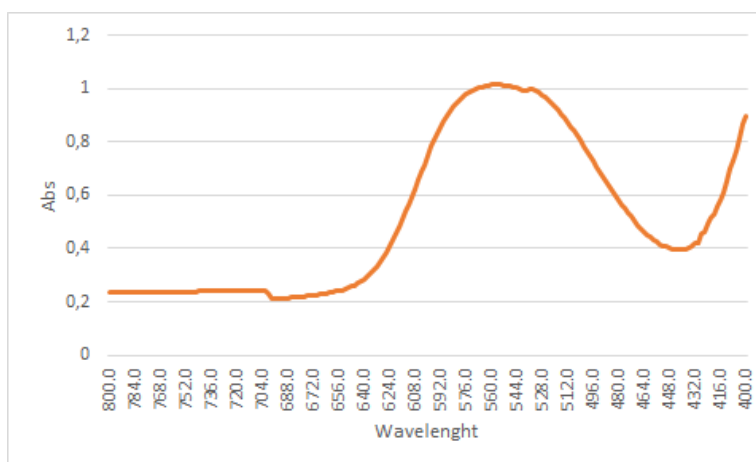
Table S2. Viscosity as a function of temperature for Lid:Cou:La and Lid:Cou:Le DESs.

Lid:Cou:La		Lid:Cou:Le	
<i>T</i> (°C)	η (mPa/s)	<i>T</i> (°C)	η (mPa/s)
59.57	3939.55	59.525	296.375
58.475	3587.25	58.41	285.46
57.14	3741.6	57.095	292.865
55.75	4105.8	55.71	308.775
54.385	4708.9	54.335	332.445
53.03	5506.25	52.975	368.38
51.635	6399.6	51.62	411.045
50.24	7557.65	50.245	457.98
48.86	9031.2	48.87	518.235
47.47	10835.2	47.495	582.72
46.09	13121.5	46.13	670.125
44.71	15967.5	44.735	755.84
43.325	19573.5	43.35	857.345
41.95	24156.5	41.955	974.71
40.56	29896.5	40.57	1112.75
39.18	37315	39.19	1275.35
37.8	46782.5	37.81	1467.15
36.42	59054	36.425	1695.15
35.04	75256	35.04	1967.4
33.65	96389	33.66	2290.5
32.27	123790	32.275	2679.4
30.89	160530	30.89	3144.55
29.51	210290	29.51	3706.25
28.13	276190	28.125	4384.9
26.75	366820	26.745	5220
25.37	483575	25.37	6242.85

23.99	607740	23.99	7489.7
22.605	826060	22.61	9021.7
21.225	1184400	21.23	10942.5
19.84	1695950	19.845	13326



a)



b)

Fig. S3. VIS spectra of Nile red with: a) Lid:Cou:La; b) Lid:Cou:Le DESs.

Table S3. ^1H and ^{13}C NMR chemical shifts of La and Le in DMSO- d_6 at 0.4 mol L^{-1} and $25 \text{ }^\circ\text{C}$.

Atom	La		La in Lid:Cou:La		Le		Le in Lid:Cou:Le	
	$\delta(^1\text{H})/\text{ppm}$	$\delta(^{13}\text{C})/\text{ppm}$	$\delta(^1\text{H})/\text{ppm}$	$\delta(^{13}\text{C})/\text{ppm}$	$\delta(^1\text{H})/\text{ppm}$	$\delta(^{13}\text{C})/\text{ppm}$	$\delta(^1\text{H})/\text{ppm}$	$\delta(^{13}\text{C})/\text{ppm}$
1		176.35		176.54		173.78		173.80
1OH	12.38		– ^a		12.07		10.70	
2	4.03	65.80	4.02	65.90	2.37	27.70	2.39	27.77
2OH	5.14		– ^a					
3	1.23	20.49	1.24	20.55	2.65	37.54	2.65	37.55
4						207.02		206.96
5					2.09	29.61	2.10	29.59

^a not observed

Table S4. ¹H NMR chemical shifts of Lid in DMSO-d₆ at different temperatures.

Atom	Lid			Lid in Lid:Cou:La			Lid in Lid:Cou:Le		
	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$
	298 K	348 K		298 K	348 K		298 K	348 K	
2	3.13	3.16	-0.03	3.19	3.19	0	3.15	3.17	-0.02
2'Me, 6'Me	2.13	2.16	-0.03	2.13	2.16	-0.03	2.13	2.16	-0.03
3'(5')	7.06	7.06	0	7.06	7.06	0	7.06	7.06	0
4'	7.06	7.06	0	7.06	7.06	0	7.06	7.06	0
NH	9.15	8.99	0.16	9.20	9.01	0.19	9.17	8.99	0.17
A(A')	2.62	2.66	-0.04	2.65	2.67	-0.02	2.63	2.67	-0.04
B(B')	1.07	1.09	-0.02	1.08	1.10	-0.02	1.07	1.09	-0.02

$$^a\Delta(^1\text{H})/\text{ppm} = \delta(^1\text{H}, 298 \text{ K})/\text{ppm} - \delta(^1\text{H}, 348 \text{ K})/\text{ppm}$$

Table S5. ¹H NMR chemical shifts of Cou in DMSO-d₆ at different temperatures.

Atom	Cou			Cou in Lid:Cou:La			Cou in Lid:Cou:Le		
	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$
	298 K	348 K		298 K	348 K		298 K	348 K	
3	6.12	6.08	0.04	6.12	6.09	0.03	6.12	6.09	0.03
4Me	2.36	2.37	-0.01	2.36	2.37	-0.01	2.36	2.37	-0.01
5	7.59	7.58	0.01	7.59	7.58	0.01	7.59	7.58	0.01
6	6.80	6.80	0	6.81	6.81	0	6.80	6.81	-0.01
7OH	10.51	10.15	0.36	_b	_b	_b	_b	_b	_b
8	6.70	6.70	0	6.71	6.71	0	6.71	6.70	0.01

$$^a\Delta(^1\text{H})/\text{ppm} = \delta(^1\text{H}, 298 \text{ K})/\text{ppm} - \delta(^1\text{H}, 348 \text{ K})/\text{ppm}$$

^b not observed

Table S6. ¹H NMR chemical shifts of La and Le in DMSO-d₆ at different temperatures.

Atom	La			La in Lid:Cou:La			Le			Le in Lid:Cou:Le		
	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$
	298 K	348 K		298 K	348 K		298 K	348 K		298 K	348 K	
1OH	12.43	12.16	0.27	_b	_b	_b	12.07	11.79	0.28	11.57	11.14	0.43
2	4.04	4.06	-0.02	4.02	4.06	-0.04	2.37	2.41	-0.04	2.38	2.41	-0.03
2OH	5.15	5.14	0.01	_b	_b	_b						
3	1.23	1.26	-0.03	1.23	1.26	-0.03	2.65	2.65	0	2.65	2.67	-0.02
4												
5							2.09	2.10	-0.01	2.09	2.10	-0.01

$$^a\Delta(^1\text{H})/\text{ppm} = \delta(^1\text{H}, 298 \text{ K})/\text{ppm} - \delta(^1\text{H}, 348 \text{ K})/\text{ppm}$$

^b not observed

Table S7. ¹H NMR chemical shifts of Lid in DMSO-d₆ at different concentrations.

Atom	Lid			Lid in Lid:Cou:La			Lid in Lid:Cou:Le		
	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$
	0.1 mol/L	0.4 mol/L		0.1 mol/L	0.4 mol/L		0.1 mol/L	0.4 mol/L	
2	3.13	3.14	-0.01	3.19	3.26	-0.07	3.15	3.17	-0.02
2'Me, 6'Me	2.13	2.15	-0.02	2.13	2.14	-0.01	2.13	2.14	-0.01
3'(5')	7.06	7.07	-0.01	7.06	7.06	0	7.06	7.06	0
4'	7.06	7.07	-0.01	7.06	7.06	0	7.06	7.06	0
NH	9.15	9.16	-0.01	9.20	9.27	-0.07	9.17	9.18	-0.01
A(A')	2.62	2.63	-0.01	2.65	2.69	-0.04	2.63	2.64	-0.01
B(B')	1.07	1.08	-0.01	1.08	1.09	-0.01	1.07	1.08	-0.01

$$^a\Delta(^1\text{H})/\text{ppm} = \delta(^1\text{H}, 0.1 \text{ mol/L})/\text{ppm} - \delta(^1\text{H}, 0.4 \text{ mol/L})/\text{ppm}$$

Table S8. ¹H NMR chemical shifts of Cou in DMSO-d₆ at different concentrations.

Atom	Cou			Cou in Lid: Cou:La			Cou in Lid: Cou:Le		
	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$
	0.1 mol/L	0.4 mol/L		0.1 mol/L	0.4 mol/L		0.1 mol/L	0.4 mol/L	
3	6.12	6.09	0.03	6.12	6.10	0.02	6.12	6.11	0.01
4Me	2.36	2.34	0.02	2.36	2.35	0.01	2.36	2.35	0.01
5	7.59	7.55	0.04	7.59	7.57	0.02	7.59	7.57	0.02
6	6.80	6.78	0.02	6.81	6.81	0	6.80	6.81	-0.01
7OH	10.51	10.51	0	- ^b	- ^b	- ^b	- ^b	- ^b	- ^b
8	6.70	6.68	0.02	6.71	6.72	-0.01	6.71	6.71	0

$$^a\Delta(^1\text{H})/\text{ppm} = \delta(^1\text{H}, 0.1 \text{ mol/L})/\text{ppm} - \delta(^1\text{H}, 0.4 \text{ mol/L})/\text{ppm}$$

^b not observed

Table S9. ¹H NMR chemical shifts of La and Le in DMSO-d₆ at different concentrations.

Atom	La			La in Lid: Cou:La			Le			Le in Lid: Cou:Le		
	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$	$\delta(^1\text{H})/\text{ppm}$		$\Delta(^1\text{H})/\text{ppm}^a$
	0.1 mol/L	0.4 mol/L		0.1 mol/L	0.4 mol/L		0.1 mol/L	0.4 mol/L		0.1 mol/L	0.4 mol/L	
1OH	12.43	12.38	0.05	- ^b	- ^b	- ^b	12.07	12.07	0	11.57	10.70	0.87
2	4.04	4.03	0.01	4.02	4.02	0	2.37	2.37	0	2.38	2.39	-0.01
2OH	5.15	5.14	0.01	- ^b	- ^b	- ^b						
3	1.23	1.23	0	1.23	1.24	-0.01	2.65	2.65	0	2.65	2.65	0
4												
5							2.09	2.09	0	2.09	2.10	-0.01

$$^a\Delta(^1\text{H})/\text{ppm} = \delta(^1\text{H}, 0.1 \text{ mol/L})/\text{ppm} - \delta(^1\text{H}, 0.4 \text{ mol/L})/\text{ppm}$$

^b not observed

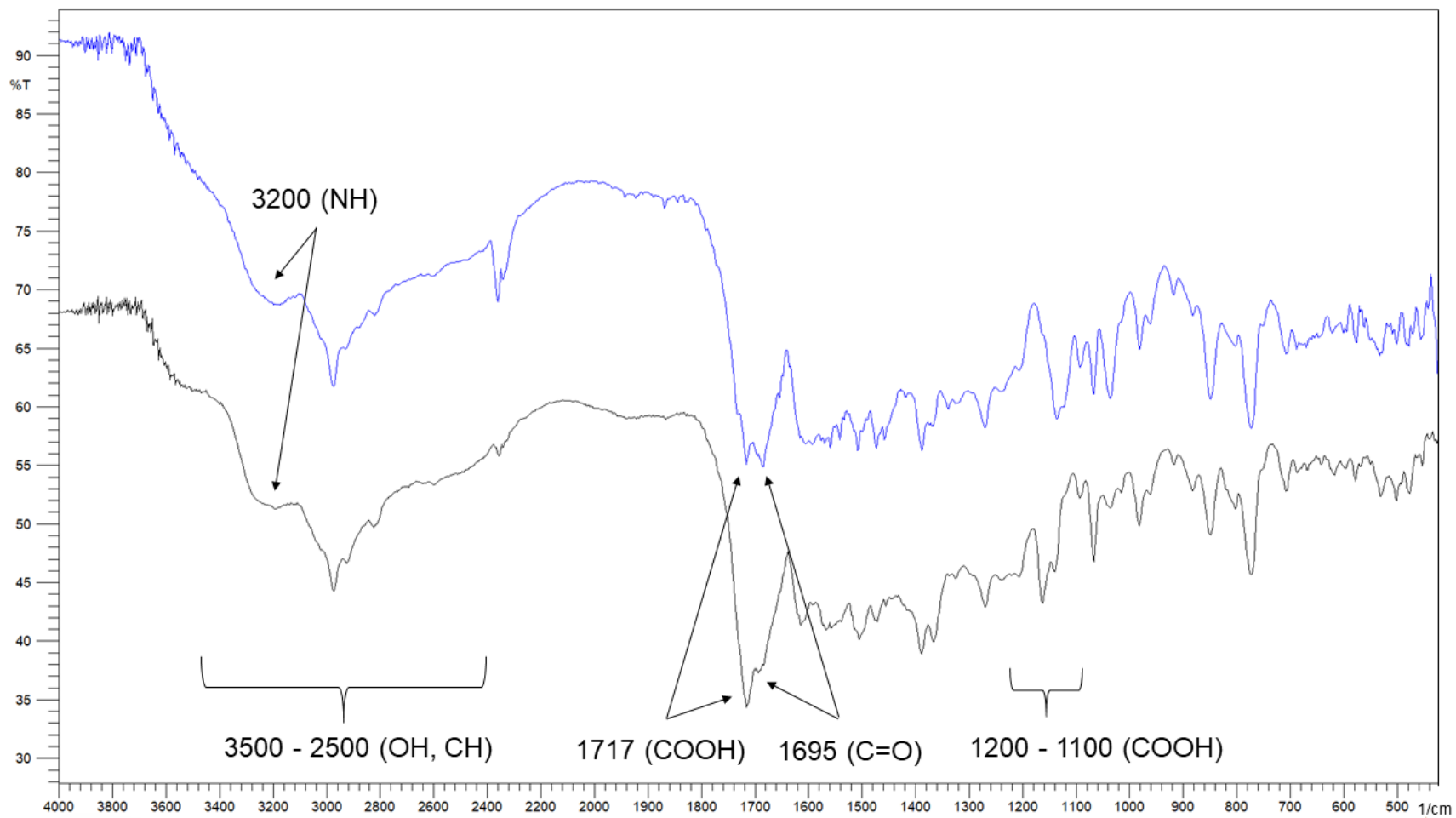


Fig. S4. IR spectra of Lid:Cou:La (blue) and Lid in Lid:Cou:Le (black).

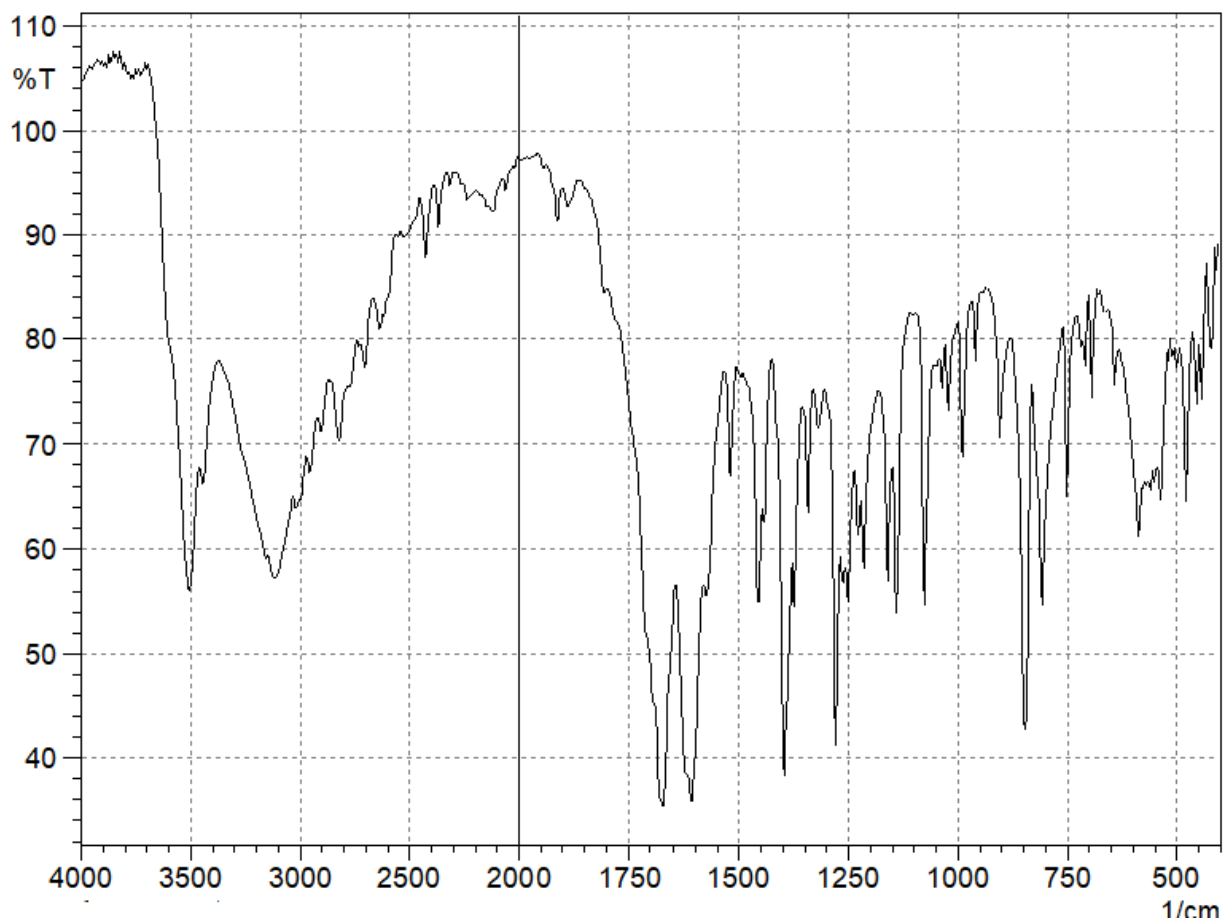


Fig. S5. IR spectrum of coumarin.

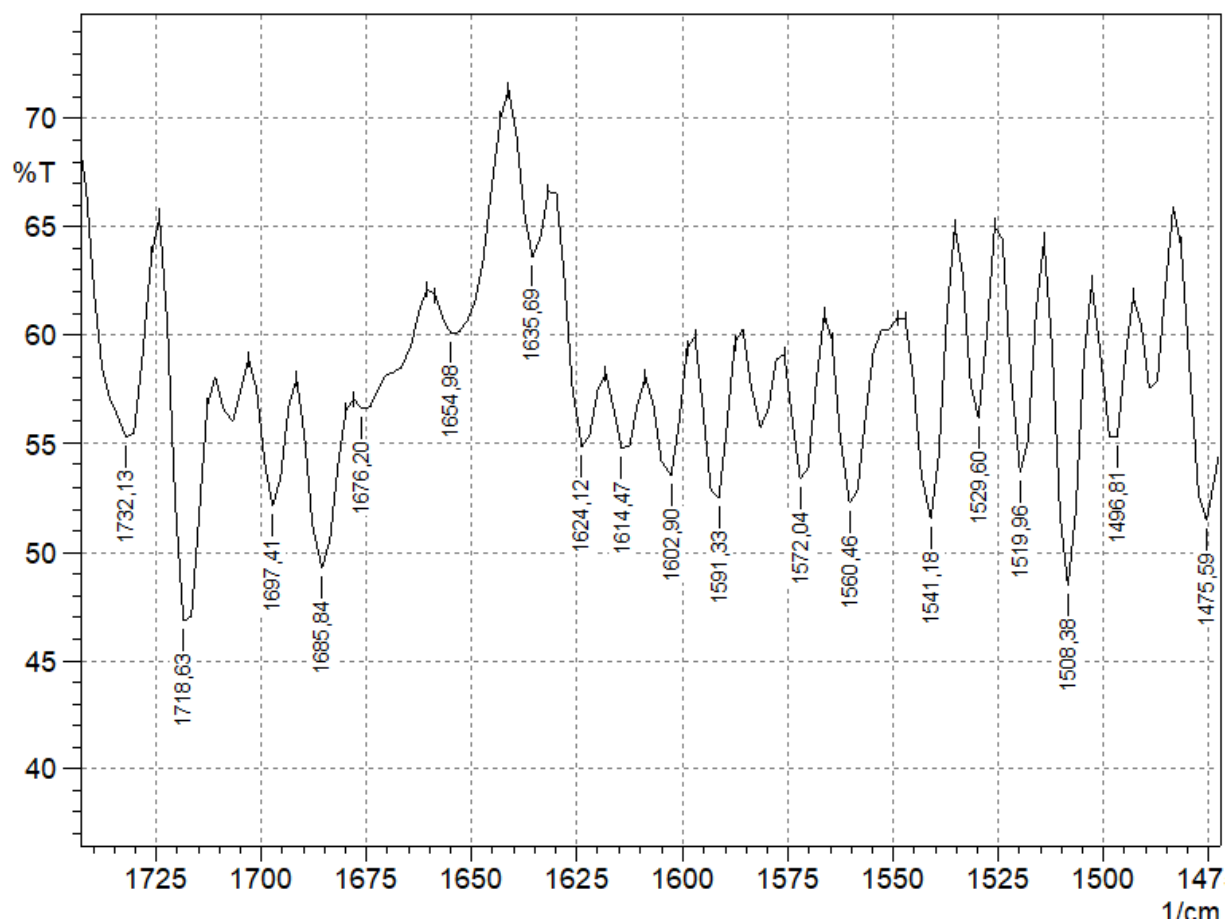


Fig S6. Deconvoluted IR spectrum of Lid:Cou:La.

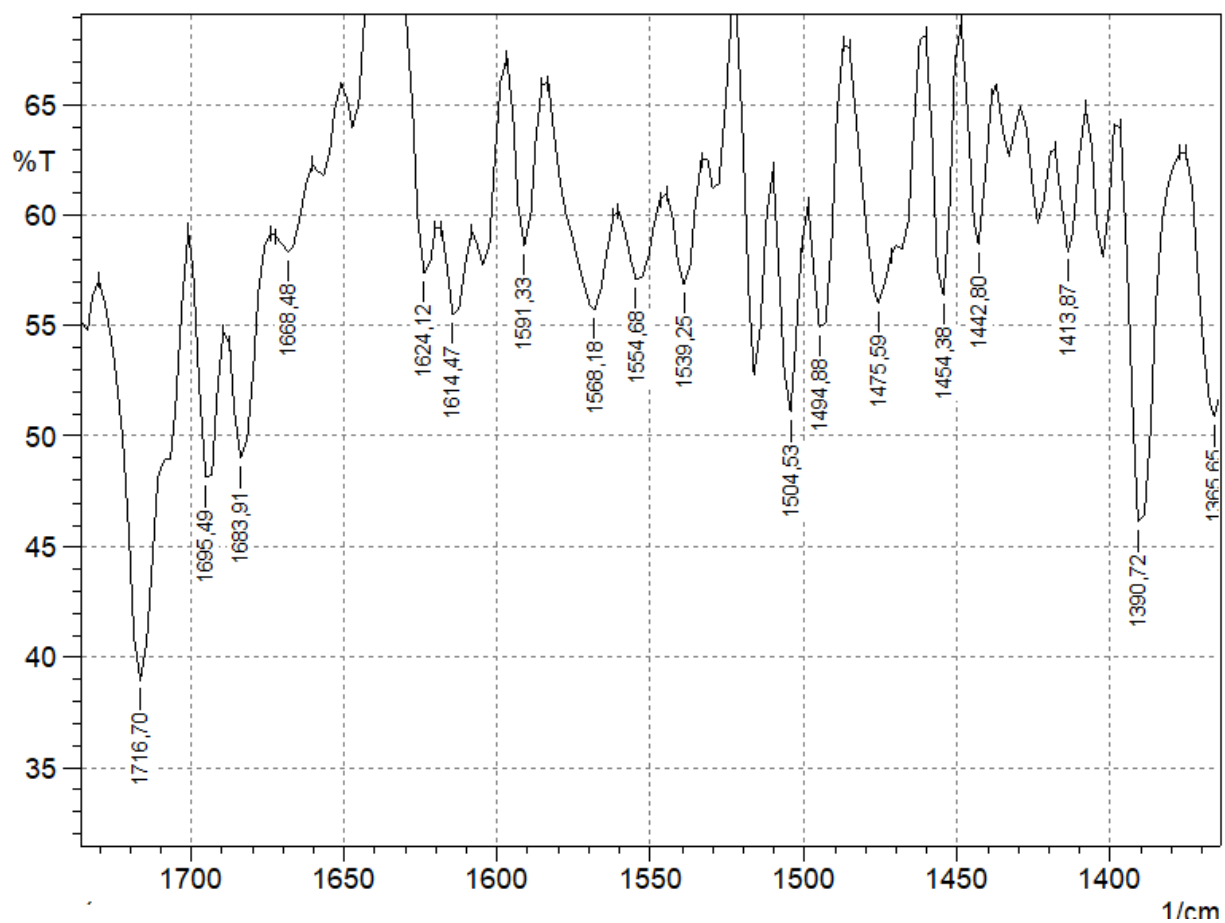


Fig. S7. Deconvoluted IR spectrum of Lid:Cou:Le.

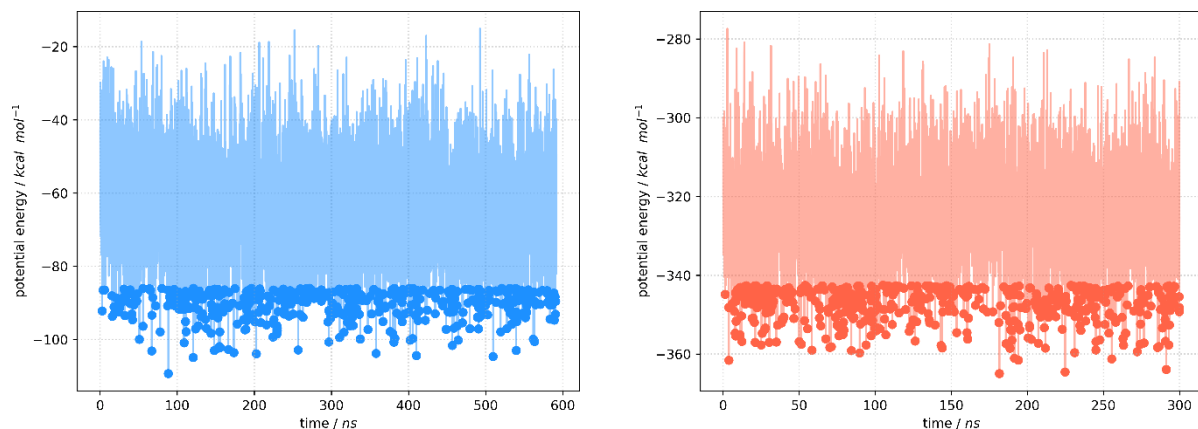


Fig. S8. Evolution of the potential energy of the Lid:Cou:La (left) and Lid:Cou:Le (right) clusters along MD simulation. Dots represent 500 lowest energy structures, which entered into the second phase of optimizations.

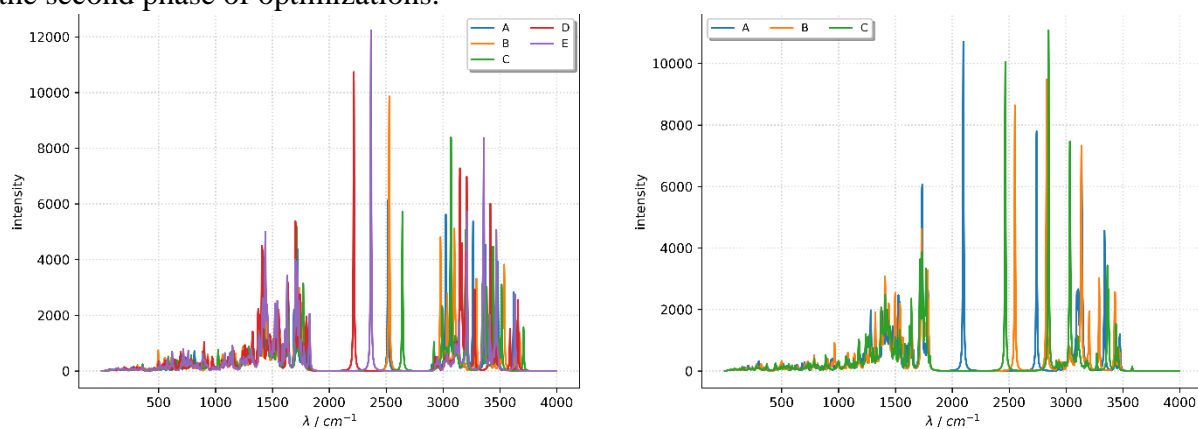


Fig. S9. IR spectra of the top structures of Lid:Cou:La (left) and Lid:Cou:Le (right).

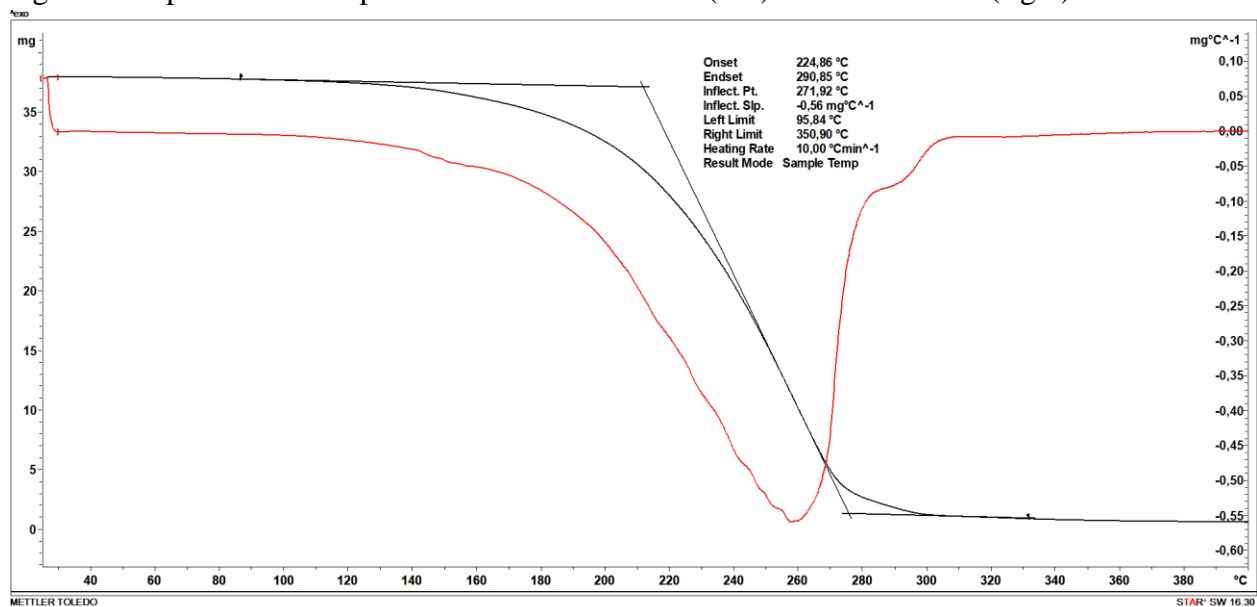


Fig. S10. TG (black) and dTG (red) curves of Lid:Cou:La

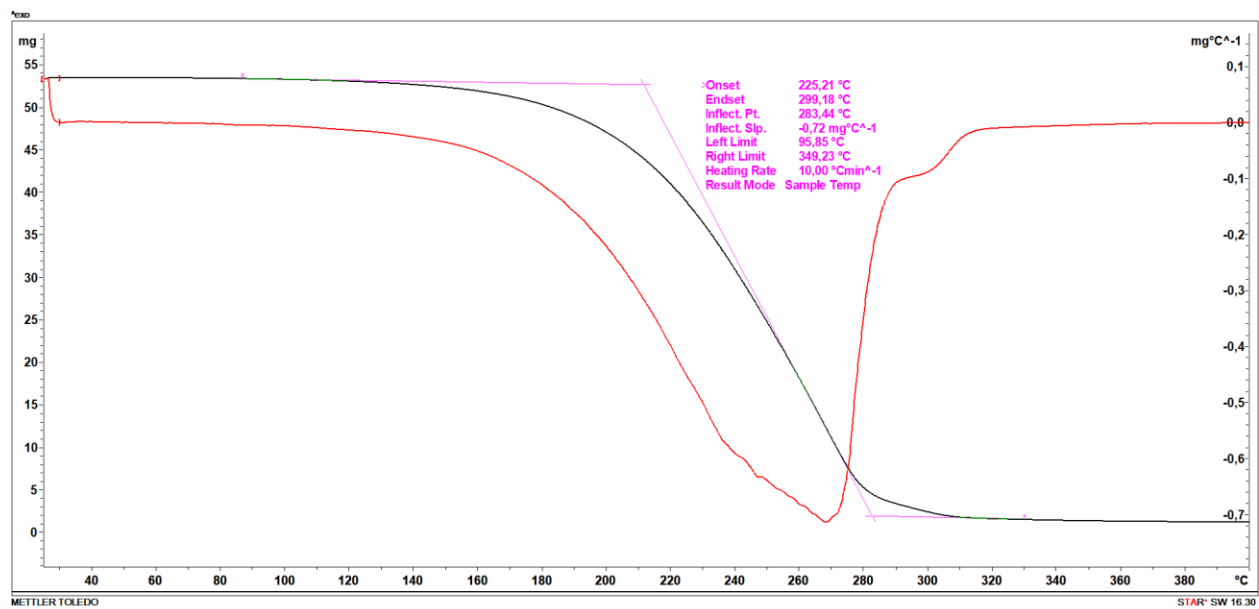


Fig S11. TG (black) and dTG (red) curves of Lid:Cou:Le

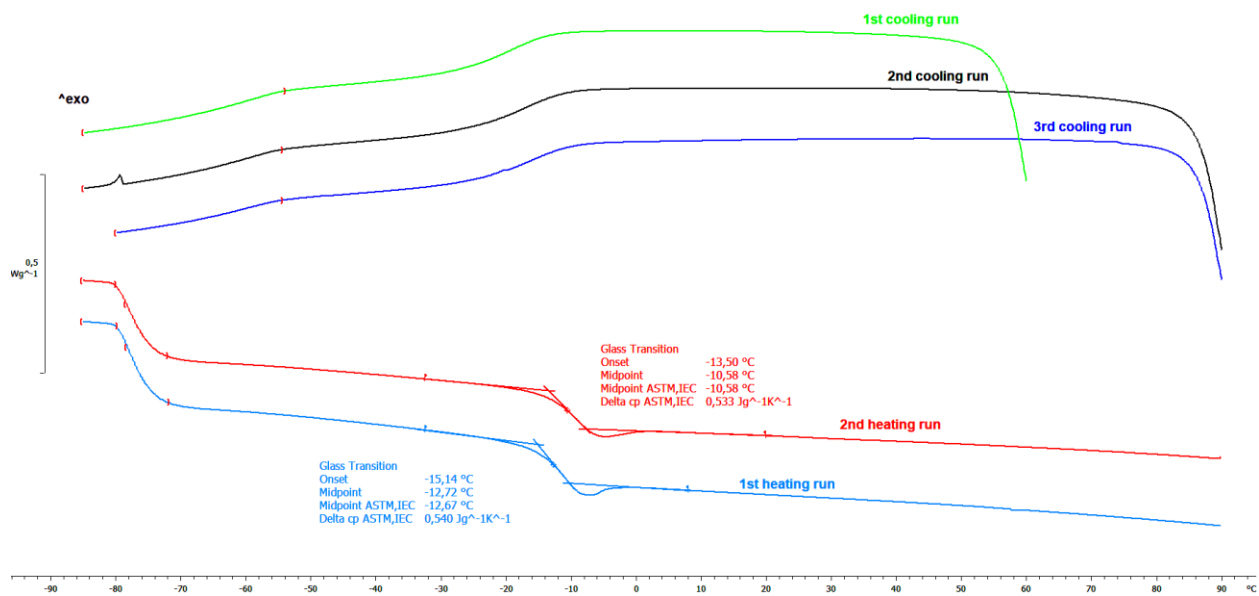


Fig S12. Low-temperature DSC curves of Lid:Cou:La.

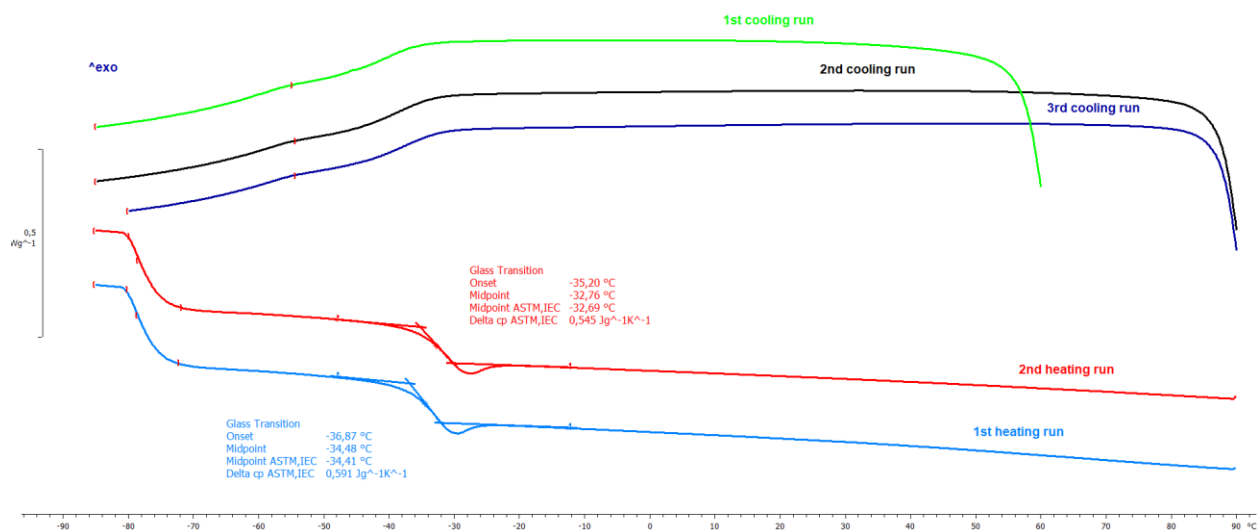


Fig S13. Low-temperature DSC curves of Lid:Cou:Le.

Table S10. B3LYP/aug-cc-pVDZ optimized geometry of Le.

16

C	2.586901	-1.056244	1.621691
C	1.793177	-0.058896	0.807625
O	2.237593	1.030955	0.522532
C	0.409255	-0.502256	0.369371
C	-0.331617	0.545937	-0.443253
C	-1.702632	0.092778	-0.870786
O	-2.209445	-0.972890	-0.625608
O	-2.336472	1.047337	-1.594341
H	3.555760	-0.638021	1.880103
H	2.044514	-1.318667	2.532422
H	2.723851	-1.981464	1.058046
H	0.507601	-1.433727	-0.194675
H	-0.162212	-0.780013	1.259168
H	-0.438492	1.476423	0.116965
H	0.230978	0.822820	-1.336496
H	-3.204761	0.692929	-1.835766

Table S11. B3LYP/aug-cc-pVDZ optimized geometry of Lid.

39

C	3.344639	2.395921	1.160599
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C	2.281810	1.415581	1.642920
N	2.568020	0.025810	1.278103
C	3.613940	-0.578752	2.103476
C	4.307515	-1.765472	1.442222
C	1.375724	-0.783981	1.224508
C	0.437523	-0.429181	0.061616
O	0.795309	0.153595	-0.939427
N	-0.842986	-0.891160	0.255034
C	-1.935919	-0.723362	-0.644223
C	-3.063999	-0.022293	-0.188750
C	-3.102681	0.571733	1.194912
C	-4.150789	0.122863	-1.046349
C	-4.118182	-0.404904	-2.329243
C	-2.999068	-1.100739	-2.759353
C	-1.893855	-1.285613	-1.928532
C	-0.716508	-2.084444	-2.411894
H	3.059920	3.414995	1.427434
H	4.321414	2.204160	1.605327
H	3.443971	2.334734	0.077651
H	2.139909	1.513436	2.733700
H	1.336172	1.689733	1.177410
H	4.361394	0.188604	2.297820
H	3.217655	-0.877147	3.090659
H	5.113296	-2.129452	2.081641
H	3.630597	-2.602658	1.269023
H	4.730907	-1.471370	0.482252
H	1.657825	-1.827571	1.074647
H	0.803480	-0.755740	2.172785
H	-1.072306	-1.179384	1.192273
H	-2.249979	1.229275	1.372509
H	-4.012463	1.151844	1.337687
H	-3.084677	-0.196143	1.974309
H	-5.023564	0.664843	-0.705870
H	-4.965684	-0.278895	-2.989502
H	-2.979690	-1.525228	-3.754731
H	0.128719	-1.434763	-2.640631
H	-0.379245	-2.791491	-1.652009
H	-0.978144	-2.646386	-3.307007

Table S12. B3LYP/aug-cc-pVDZ optimized geometry of LidH.

40

C	3.318184	2.458326	1.469690
C	2.366582	1.433828	2.058662
N	2.462611	0.080247	1.379335

C	3.731361	-0.668336	1.718869
C	4.059430	-1.753272	0.708908
C	1.216485	-0.723919	1.575214
C	0.329671	-0.444038	0.342744
O	0.853295	0.111116	-0.616200
N	-0.935386	-0.869998	0.422375
C	-1.934125	-0.738975	-0.610083
C	-3.056564	0.049884	-0.324756
C	-3.205721	0.762720	0.993476
C	-4.039729	0.159798	-1.303597
C	-3.904748	-0.491530	-2.521454
C	-2.788886	-1.274386	-2.773038
C	-1.781278	-1.424184	-1.820691
C	-0.595422	-2.302803	-2.109333
H	3.137887	3.415604	1.957120
H	4.365544	2.208539	1.627767
H	3.141904	2.594559	0.402459
H	2.542399	1.264009	3.120216
H	1.337280	1.761362	1.928224
H	4.526025	0.071242	1.749423
H	3.601929	-1.064561	2.725054
H	5.000925	-2.220089	0.994691
H	3.307335	-2.539960	0.669239
H	4.183790	-1.341146	-0.292493
H	1.471132	-1.780339	1.608551
H	0.746297	-0.447602	2.516088
H	-1.247138	-1.227656	1.313448
H	-2.364265	1.430180	1.190029
H	-4.112575	1.362780	1.002955
H	-3.274886	0.065684	1.833732
H	-4.914272	0.765325	-1.108259
H	-4.675586	-0.394189	-3.273251
H	-2.696454	-1.791381	-3.718501
H	0.292402	-1.707204	-2.327607
H	-0.359965	-2.953667	-1.265269
H	-0.793256	-2.937254	-2.970304
H	2.422999	0.267590	0.355926

Table S13. B3LYP/aug-cc-pVDZ optimized geometry of deCou.

20

C	0.480513	1.807961	2.320590
C	0.676891	0.710372	1.307824
C	1.919405	0.144680	1.158773
C	2.174139	-0.901475	0.215325

O	3.239613	-1.459844	0.015703
O	1.093878	-1.319354	-0.547308
C	-0.167661	-0.776788	-0.427358
C	-1.147207	-1.281387	-1.242583
C	-2.499860	-0.784929	-1.197381
O	-3.418009	-1.225301	-1.929875
C	-2.726680	0.277910	-0.228882
C	-1.732339	0.761874	0.570925
C	-0.404664	0.261734	0.514147
H	1.412901	2.026253	2.839687
H	0.130508	2.726708	1.844888
H	-0.268536	1.529467	3.065067
H	2.764386	0.465816	1.749979
H	-0.909262	-2.072199	-1.940757
H	-3.732522	0.675060	-0.168016
H	-1.959494	1.554445	1.274252

Table S14. B3LYP/aug-cc-pVDZ optimized geometry of La.

12

C	1.210592	1.452062	-0.467723
C	0.749209	0.225566	0.320414
H	0.756037	0.468714	1.389707
O	1.609714	-0.868176	0.087965
C	-0.676180	-0.168479	-0.025318
O	-0.978243	-1.238318	-0.494474
O	-1.571601	0.796004	0.253992
H	1.157549	1.259189	-1.539220
H	0.602156	2.323057	-0.229335
H	2.246724	1.663102	-0.209058
H	1.069046	-1.595832	-0.250298
H	-2.448001	0.463112	0.009348

Table S15. B3LYP/cc-pVDZ optimized geometry of Lid:Cou:La structure A.

225

C	0.805119	-2.195849	6.052705
C	0.877857	-1.495253	4.722769
C	0.933212	-0.121173	4.663946
C	0.998252	0.578221	3.417845
O	1.050532	1.808650	3.282834

O	1.011150	-0.156830	2.264533
C	0.953604	-1.535999	2.276247
C	0.969259	-2.161746	1.042267
C	0.917099	-3.579079	0.954962
O	0.933091	-4.204353	-0.188897
C	0.848378	-4.308750	2.189965
C	0.834717	-3.662274	3.407423
C	0.888068	-2.245486	3.501684
H	1.659653	-2.879374	6.185011
H	0.806112	-1.476522	6.882718
H	-0.108669	-2.807932	6.125504
H	0.923979	0.494683	5.562603
H	1.012022	-1.564658	0.132605
H	0.800563	-5.397874	2.131419
H	0.779621	-4.252454	4.324176
C	4.584565	0.347121	-3.499974
C	3.838132	1.614885	-3.108141
N	2.546446	1.368850	-2.362943
C	1.521996	0.563395	-3.139098
C	1.253458	1.093160	-4.537893
C	2.755053	0.747988	-1.013304
C	3.636312	1.637813	-0.129133
O	3.354070	2.818435	0.037519
N	4.706529	0.999031	0.427817
C	5.585667	1.594162	1.390293
C	6.383686	2.705366	1.043949
C	6.368629	3.301357	-0.340112
C	7.230655	3.238969	2.026752
C	7.300451	2.683253	3.303690
C	6.520568	1.570286	3.618993
C	5.651958	1.010274	2.673785
C	4.810110	-0.192114	3.021158
H	4.860944	-0.272746	-2.633747
H	4.010890	-0.274563	-4.204259
H	5.514540	0.645495	-4.009094
H	4.441229	2.255945	-2.453808
H	3.581522	2.230032	-3.980047
H	1.852724	-0.481650	-3.155427
H	0.609662	0.611637	-2.530754
H	0.973694	2.156185	-4.529673
H	2.113654	0.970926	-5.212181
H	0.423456	0.503844	-4.953608
H	1.767108	0.694933	-0.535178
H	3.152609	-0.265981	-1.140637
H	4.786918	-0.009898	0.274503
H	5.428786	3.841933	-0.531182

H	7.209777	3.996328	-0.475146
H	6.448389	2.515828	-1.109469
H	7.852225	4.101350	1.773296
H	7.968549	3.114798	4.052759
H	6.574301	1.127882	4.616706
H	3.759184	-0.043804	2.731116
H	5.161465	-1.096609	2.496964
H	4.847866	-0.397383	4.100318
H	2.093249	2.302938	-2.192729
C	-2.304810	2.999638	3.890727
C	-3.319972	3.773714	3.058484
N	-4.537418	3.013264	2.728583
C	-5.512716	3.834823	2.010475
C	-6.942056	3.294163	2.080882
C	-4.347053	1.687614	2.152009
C	-3.742633	1.642377	0.738903
O	-2.667546	2.223690	0.501091
N	-4.437739	0.938703	-0.182212
C	-4.040093	0.769167	-1.552101
C	-4.791561	1.432698	-2.544861
C	-5.967510	2.303507	-2.172532
C	-4.425303	1.254152	-3.884359
C	-3.346606	0.435072	-4.224825
C	-2.628149	-0.228918	-3.231247
C	-2.964205	-0.079485	-1.875485
C	-2.198591	-0.826339	-0.812087
H	-1.498195	3.672869	4.218246
H	-2.778532	2.555960	4.782766
H	-1.828092	2.199128	3.305535
H	-3.661329	4.649211	3.638300
H	-2.817702	4.167834	2.152483
H	-5.489455	4.832307	2.478954
H	-5.223176	3.997022	0.945673
H	-7.058408	2.333430	1.555579
H	-7.241264	3.147482	3.131837
H	-7.638537	4.012797	1.618358
H	-3.660976	1.117019	2.796517
H	-5.306556	1.151469	2.154466
H	-5.331356	0.524000	0.102737
H	-5.669901	3.119123	-1.493135
H	-6.419248	2.753872	-3.068288
H	-6.749429	1.727121	-1.650051
H	-4.995957	1.762851	-4.665512
H	-3.070827	0.302742	-5.273701
H	-1.800427	-0.884180	-3.510460
H	-2.852835	-1.107717	0.025631

H	-1.751595	-1.745766	-1.214477
H	-1.391582	-0.204909	-0.390386
C	-9.492724	-3.417904	3.636165
C	-10.468236	-2.346124	3.152989
N	-10.054793	-1.726526	1.884835
C	-11.168982	-1.171242	1.097629
C	-11.982918	-0.045648	1.750601
C	-8.913395	-0.820015	1.989935
C	-7.815235	-1.057188	0.942569
O	-6.915558	-0.223546	0.791417
N	-7.929017	-2.227541	0.277015
C	-7.071114	-2.727459	-0.755271
C	-7.611810	-2.881510	-2.048539
C	-9.038890	-2.488896	-2.346797
C	-6.789281	-3.404432	-3.053299
C	-5.466278	-3.755129	-2.781985
C	-4.948454	-3.603977	-1.495713
C	-5.744178	-3.097741	-0.456322
C	-5.190417	-2.981004	0.941684
H	-9.850371	-3.860672	4.579660
H	-9.391748	-4.223978	2.891808
H	-8.488134	-3.007146	3.828413
H	-11.452167	-2.811421	2.978287
H	-10.618403	-1.590874	3.953326
H	-10.748718	-0.815804	0.141700
H	-11.842043	-2.008378	0.843901
H	-12.762656	0.304541	1.054969
H	-12.486190	-0.385144	2.669831
H	-11.356982	0.823977	2.008695
H	-9.190598	0.246394	1.915823
H	-8.422237	-0.930894	2.969935
H	-8.798692	-2.716026	0.505295
H	-9.765488	-3.096879	-1.779232
H	-9.231735	-1.434800	-2.086877
H	-9.264685	-2.620901	-3.414550
H	-7.192429	-3.525821	-4.061737
H	-4.831383	-4.152075	-3.576442
H	-3.910757	-3.884952	-1.298278
H	-5.877566	-3.422570	1.682167
H	-4.221432	-3.492949	1.020097
H	-5.048497	-1.926857	1.227947
C	2.087965	7.155117	-4.955896
C	1.739260	6.076047	-3.931911
H	0.761328	5.629975	-4.180393
O	1.737997	6.625388	-2.623019
C	2.759261	4.928071	-3.999629

O	2.902264	4.199650	-4.961689
O	3.495204	4.808198	-2.888464
H	3.046644	7.630463	-4.692613
H	2.174699	6.715498	-5.960634
H	1.309705	7.932736	-4.962357
H	0.951046	6.277175	-2.132633
H	3.090408	5.469696	-2.270824
C	-2.177970	4.743979	-2.255134
C	-1.115736	4.649417	-1.157989
H	-1.605366	4.451656	-0.190532
O	-0.399230	5.865965	-1.103924
C	-0.185971	3.464541	-1.451749
O	0.868849	3.600974	-2.061371
O	-0.591394	2.259688	-1.077292
H	-2.853902	5.582814	-2.032191
H	-1.704114	4.929765	-3.232329
H	-2.763841	3.814866	-2.319002
H	0.021021	5.930874	-0.204243
H	-1.442466	2.274122	-0.537753
C	7.020846	-6.037470	-3.008471
C	5.969768	-4.929370	-3.000908
N	4.921842	-5.113148	-1.979059
C	3.945442	-6.148679	-2.368140
C	3.152587	-6.716879	-1.192923
C	4.285979	-3.836230	-1.651606
C	5.074291	-3.011107	-0.631361
O	4.870573	-1.799804	-0.487501
N	5.953526	-3.745269	0.095221
C	6.722951	-3.321991	1.220562
C	7.716984	-2.331607	1.079714
C	8.018174	-1.691140	-0.251209
C	8.450092	-1.969484	2.219621
C	8.224810	-2.584398	3.450367
C	7.255272	-3.582213	3.562564
C	6.487365	-3.964324	2.455975
C	5.431111	-5.035759	2.582335
H	6.591011	-7.024314	-3.240836
H	7.786226	-5.826212	-3.772563
H	7.523239	-6.109206	-2.030197
H	6.472966	-3.972102	-2.790452
H	5.515071	-4.824054	-4.010443
H	3.252150	-5.757429	-3.144801
H	4.510090	-6.964343	-2.843518
H	2.485469	-5.973226	-0.729259
H	2.518131	-7.547769	-1.543452
H	3.834709	-7.112929	-0.422343

H	4.100165	-3.194891	-2.534645
H	3.300965	-4.016114	-1.193966
H	5.902791	-4.739878	-0.140679
H	8.099609	-2.449361	-1.047080
H	7.217559	-0.998538	-0.553021
H	8.963899	-1.132463	-0.209573
H	9.216930	-1.196837	2.129331
H	8.811678	-2.290431	4.323421
H	7.080743	-4.070504	4.524500
H	5.677051	-5.930717	1.983572
H	5.329193	-5.361023	3.627533
H	4.446591	-4.681393	2.236497
C	3.120704	4.668600	3.160954
C	1.653497	5.070053	3.347116
H	1.595512	6.128401	3.640702
O	1.000857	4.342837	4.372634
C	0.912204	5.004575	2.003634
O	0.749797	6.011204	1.326877
O	0.445223	3.835104	1.571985
H	3.615821	5.325412	2.429239
H	3.641750	4.751186	4.126890
H	3.210436	3.635061	2.793706
H	1.126241	3.387710	4.210619
H	0.683740	3.068887	2.153367
C	-1.635996	-4.424366	-4.137976
C	-0.618524	-4.260116	-3.021975
H	0.083324	-5.121376	-3.037899
O	-1.306558	-4.221107	-1.775590
C	0.248341	-2.994389	-3.218829
O	0.177532	-2.290719	-4.211876
O	1.102394	-2.706291	-2.236044
H	-2.195581	-5.360399	-3.990851
H	-2.343772	-3.581719	-4.135942
H	-1.138977	-4.445881	-5.117735
H	-0.641489	-4.364206	-1.065136
H	1.026209	-3.331240	-1.411920

Table S16. B3LYP/cc-pVDZ optimized geometry of Lid:Cou:La structure B.

225

C	0.898771	3.386346	7.313837
C	0.533446	2.551762	6.115964
C	-0.449575	1.589403	6.215794
C	-0.814191	0.775040	5.103244
O	-1.680902	-0.117312	5.100180
O	-0.167075	0.978632	3.913581

C	0.830030	1.919929	3.769253
C	1.418370	2.010229	2.519337
C	2.457503	2.953666	2.279775
O	3.037243	3.056690	1.129034
C	2.833046	3.802277	3.380651
C	2.232180	3.690686	4.614828
C	1.203091	2.740264	4.864203
H	0.291001	3.116782	8.187914
H	1.960893	3.252474	7.576080
H	0.752712	4.459182	7.107791
H	-0.983579	1.403275	7.146805
H	1.091428	1.353549	1.712765
H	3.628141	4.529926	3.207270
H	2.557593	4.344094	5.426567
C	-0.463190	-4.340384	-1.462446
C	-0.655522	-2.830060	-1.476846
N	-0.361669	-2.202292	-0.128626
C	1.125421	-2.255225	0.194632
C	1.433693	-2.308801	1.682170
C	-0.829778	-0.787741	-0.061077
C	-2.347641	-0.635471	-0.147081
O	-3.120347	-1.582471	0.007930
N	-2.719388	0.651082	-0.362475
C	-4.071627	1.129795	-0.387472
C	-4.617754	1.580485	-1.606763
C	-3.899639	1.428609	-2.927549
C	-5.908272	2.135985	-1.586377
C	-6.641894	2.212778	-0.404358
C	-6.092910	1.735586	0.788582
C	-4.801259	1.194666	0.822157
C	-4.215244	0.697680	2.119255
H	-1.073007	-4.816891	-0.678291
H	-0.796390	-4.737293	-2.434079
H	0.588603	-4.634063	-1.331766
H	0.000744	-2.333670	-2.203982
H	-1.697364	-2.578663	-1.704250
H	1.536716	-3.133910	-0.312476
H	1.571698	-1.374187	-0.287712
H	1.068023	-1.430534	2.233566
H	1.006654	-3.210341	2.144997
H	2.527961	-2.362834	1.778153
H	-0.513808	-0.386418	0.910372
H	-0.353051	-0.231453	-0.878770
H	-1.993285	1.329143	-0.621742
H	-2.843982	1.152121	-2.817239
H	-4.392311	0.640760	-3.524714

H	-3.957947	2.359614	-3.513582
H	-6.343690	2.492626	-2.523258
H	-7.647116	2.640572	-0.410540
H	-6.669584	1.789550	1.715145
H	-4.110388	-0.398396	2.108570
H	-3.206408	1.103328	2.294815
H	-4.853055	0.975789	2.970348
H	-0.883171	-2.742240	0.606552
C	8.654932	-0.270395	3.188247
C	7.159474	-0.439645	2.929692
N	6.780502	-0.235901	1.521217
C	6.792229	1.186030	1.113624
C	7.130878	1.370414	-0.362863
C	5.501848	-0.877621	1.219537
C	5.615262	-2.334529	0.772546
O	4.608976	-3.052527	0.711206
N	6.869373	-2.715574	0.433485
C	7.261486	-3.953407	-0.160582
C	7.086994	-5.167255	0.536077
C	6.501978	-5.210243	1.924628
C	7.503439	-6.350215	-0.092585
C	8.091132	-6.330575	-1.356632
C	8.277418	-5.115676	-2.018158
C	7.864499	-3.910257	-1.436999
C	8.046775	-2.598817	-2.162698
H	9.240808	-0.981048	2.583061
H	9.008426	0.745455	2.951341
H	8.879349	-0.456842	4.250953
H	6.871168	-1.467917	3.202466
H	6.576011	0.233659	3.596250
H	5.818390	1.665107	1.340443
H	7.544808	1.708312	1.722840
H	7.002378	2.424943	-0.649899
H	8.166740	1.056251	-0.571223
H	6.463518	0.778806	-1.009652
H	4.789338	-0.845021	2.067563
H	5.001216	-0.355990	0.389087
H	7.526690	-1.931722	0.464111
H	5.424385	-4.985489	1.910249
H	6.650388	-6.199870	2.379908
H	6.974109	-4.456781	2.576554
H	7.371895	-7.299559	0.432226
H	8.412575	-7.263595	-1.824993
H	8.742811	-5.096018	-3.006634
H	7.085177	-2.076211	-2.290012
H	8.720715	-1.914160	-1.618029

H	8.484111	-2.762840	-3.157978
C	-0.613201	6.742280	3.226448
C	-1.005314	5.340407	2.765499
N	-2.000374	5.329918	1.675029
C	-3.351371	5.708758	2.127790
C	-4.256984	6.181481	0.992986
C	-1.984256	4.060091	0.946922
C	-1.136857	4.082134	-0.328307
O	-0.924812	3.025804	-0.954425
N	-0.710804	5.304637	-0.685222
C	0.033697	5.677675	-1.852417
C	1.341337	6.175921	-1.677023
C	1.980678	6.235264	-0.311151
C	2.039192	6.608982	-2.812177
C	1.460619	6.537985	-4.080076
C	0.168572	6.036169	-4.230410
C	-0.572670	5.602359	-3.122327
C	-1.976486	5.082343	-3.299039
H	0.182886	6.673169	3.984414
H	-0.230356	7.342540	2.384994
H	-1.452211	7.292915	3.679894
H	-0.104255	4.828661	2.394419
H	-1.367136	4.742196	3.630079
H	-3.831655	4.870014	2.676946
H	-3.238303	6.528007	2.852233
H	-3.816791	7.049704	0.476618
H	-4.439014	5.393232	0.244943
H	-5.239143	6.479788	1.393169
H	-1.621020	3.216855	1.563036
H	-3.000757	3.785099	0.624320
H	-0.979192	6.013877	0.005348
H	1.956005	5.255369	0.191292
H	3.034602	6.535317	-0.391345
H	1.471849	6.959118	0.349646
H	3.052623	6.998702	-2.693785
H	2.020007	6.876642	-4.954932
H	-0.285327	5.985038	-5.222804
H	-2.667409	5.523142	-2.562847
H	-2.354316	5.311300	-4.305497
H	-2.013041	3.990022	-3.160843
C	4.543703	3.644397	-3.221296
C	3.916175	3.252845	-1.893903
H	2.882365	3.647926	-1.849420
O	4.713145	3.794286	-0.846986
C	3.787818	1.723085	-1.752784
O	4.098750	0.961843	-2.670317

O	3.337014	1.240960	-0.609229
H	5.546821	3.204222	-3.321056
H	3.928074	3.300434	-4.063608
H	4.629568	4.739626	-3.264704
H	4.208054	3.736520	-0.008220
H	3.140815	1.970733	0.101033
C	0.770744	1.510184	-5.919487
C	1.238304	0.719900	-4.695124
H	2.291179	0.985112	-4.474800
O	1.086110	-0.645635	-4.976633
C	0.436739	1.135906	-3.458428
O	-0.344399	0.408782	-2.866021
O	0.687983	2.398140	-3.085993
H	0.855919	2.593059	-5.749534
H	1.385837	1.228618	-6.787062
H	-0.277612	1.259074	-6.147401
H	1.486179	-1.146839	-4.240951
H	0.114665	2.630562	-2.305196
C	-4.862641	-3.079065	-4.975820
C	-6.282656	-2.859123	-4.452627
N	-6.404188	-1.664492	-3.604140
C	-7.747805	-1.066214	-3.617565
C	-7.991824	-0.213515	-4.863796
C	-5.837829	-1.826127	-2.278647
C	-6.546251	-2.812645	-1.328105
O	-7.622062	-3.337719	-1.587671
N	-5.864742	-3.010539	-0.149719
C	-6.281558	-3.894049	0.892309
C	-7.472884	-3.644927	1.606545
C	-8.347318	-2.459936	1.288961
C	-7.826767	-4.530117	2.635559
C	-7.024055	-5.624124	2.957535
C	-5.846608	-5.853653	2.243828
C	-5.461232	-5.001643	1.200115
C	-4.202386	-5.269757	0.412121
H	-4.511088	-2.200992	-5.541029
H	-4.142262	-3.263783	-4.161889
H	-4.831857	-3.958182	-5.640524
H	-6.951790	-2.717956	-5.315442
H	-6.644878	-3.764435	-3.925962
H	-8.537586	-1.834288	-3.513986
H	-7.830976	-0.422998	-2.726450
H	-8.999793	0.233569	-4.832600
H	-7.249720	0.598254	-4.937708
H	-7.927503	-0.808134	-5.789925
H	-4.780002	-2.124206	-2.363041

H	-5.823735	-0.847661	-1.772381
H	-4.930197	-2.604972	-0.079286
H	-7.746514	-1.544516	1.163623
H	-8.879866	-2.620208	0.338256
H	-9.084323	-2.289178	2.087530
H	-8.747728	-4.346913	3.195216
H	-7.316810	-6.300369	3.764332
H	-5.219659	-6.716183	2.484184
H	-4.405350	-5.271714	-0.671110
H	-3.431873	-4.505518	0.603351
H	-3.772901	-6.244927	0.684623
C	-3.791109	-3.066957	4.568128
C	-2.311078	-3.405435	4.370516
H	-2.179710	-4.495857	4.322245
O	-1.493013	-2.955690	5.437334
C	-1.802745	-2.879654	3.019552
O	-1.597889	-3.613827	2.060067
O	-1.581012	-1.573214	2.901580
H	-3.940451	-1.975046	4.607556
H	-4.411248	-3.477247	3.755848
H	-4.132735	-3.495773	5.522363
H	-1.690545	-2.017622	5.610399
H	-1.673439	-1.055122	3.757125
C	3.281922	-4.729814	-3.642624
C	3.837241	-3.920585	-2.480312
H	4.936053	-4.013581	-2.440128
O	3.255400	-4.410294	-1.276432
C	3.490254	-2.431757	-2.643628
O	2.353300	-2.039697	-2.883139
O	4.523550	-1.621281	-2.466622
H	2.194023	-4.584479	-3.715668
H	3.738047	-4.418210	-4.595759
H	3.493308	-5.796652	-3.478147
H	3.792524	-4.063546	-0.530856
H	4.239959	-0.650616	-2.545205

Table S17. B3LYP/cc-pVDZ optimized geometry of Lid:Cou:La structure C.

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C	6.046978	1.119944	-4.637735
C	4.885009	0.899474	-3.707722
C	3.593070	1.038956	-4.162048
C	2.466467	0.826415	-3.305119
O	1.273310	0.920534	-3.629468
O	2.704492	0.464012	-2.010652
C	3.977679	0.347727	-1.503800

C	4.071773	0.027571	-0.159996
C	5.342796	-0.113725	0.449030
O	5.464146	-0.378354	1.726944
C	6.498878	0.050089	-0.382778
C	6.377305	0.372296	-1.719132
C	5.107550	0.544576	-2.333890
H	5.705735	1.389128	-5.646315
H	6.702053	1.924738	-4.266286
H	6.667594	0.212094	-4.712463
H	3.369900	1.314429	-5.192236
H	3.163912	-0.115699	0.424251
H	7.478825	-0.091178	0.077131
H	7.280041	0.497848	-2.319831
C	-2.409213	1.813119	3.141150
C	-1.788081	0.438741	2.944942
N	-1.091417	0.300673	1.600646
C	0.411091	0.498555	1.675130
C	0.845501	1.797974	2.331465
C	-1.357522	-1.025869	0.958759
C	-2.776313	-1.102486	0.391275
O	-3.683174	-0.388469	0.832083
N	-2.921510	-2.013208	-0.596959
C	-4.177122	-2.331477	-1.214687
C	-4.716432	-3.614262	-0.991682
C	-4.001536	-4.609799	-0.110428
C	-5.931255	-3.941764	-1.607422
C	-6.591825	-3.017780	-2.417756
C	-6.034543	-1.757150	-2.635295
C	-4.814176	-1.390190	-2.047783
C	-4.205904	-0.039801	-2.332415
H	-3.164009	2.004386	2.364584
H	-2.917205	1.833082	4.117320
H	-1.667493	2.623666	3.121864
H	-1.045466	0.186417	3.714102
H	-2.574808	-0.320596	2.970747
H	0.807846	-0.379171	2.200435
H	0.752814	0.476316	0.631709
H	1.945689	1.821077	2.331518
H	0.488682	2.671604	1.766809
H	0.526893	1.868648	3.380936
H	-0.622489	-1.179758	0.163003
H	-1.187808	-1.799530	1.721640
H	-2.098103	-2.574497	-0.854118
H	-4.584084	-5.537398	-0.015794
H	-3.009321	-4.871160	-0.514469
H	-3.835491	-4.205922	0.902015

H	-6.362823	-4.931702	-1.440673
H	-7.542025	-3.282558	-2.887276
H	-6.546628	-1.039213	-3.280060
H	-3.180759	-0.128129	-2.726676
H	-4.807293	0.507961	-3.071697
H	-4.144791	0.571706	-1.419230
H	-1.457899	1.035216	0.941243
C	6.694209	5.396730	-0.569546
C	5.631507	4.360556	-0.209425
N	4.621045	4.853629	0.744223
C	5.151145	4.983144	2.119143
C	4.373926	5.999272	2.953243
C	3.419854	4.015473	0.703443
C	2.369450	4.449366	-0.325921
O	1.476755	3.684558	-0.687602
N	2.501341	5.746245	-0.725479
C	1.646621	6.449112	-1.624511
C	2.205353	6.970840	-2.811559
C	3.664560	6.761480	-3.135642
C	1.377883	7.686063	-3.685463
C	0.025989	7.875356	-3.395370
C	-0.507688	7.362415	-2.213815
C	0.287241	6.650532	-1.302582
C	-0.305010	6.149919	-0.010045
H	7.379184	4.985224	-1.328488
H	6.233727	6.309669	-0.980434
H	7.307838	5.689733	0.296515
H	5.096935	4.070503	-1.128782
H	6.114686	3.434139	0.169683
H	5.164179	3.998782	2.629473
H	6.196120	5.317728	2.044720
H	3.314596	5.717206	3.069395
H	4.803799	6.069905	3.965464
H	4.408428	6.998711	2.490109
H	3.639447	2.946939	0.522327
H	2.911994	4.058962	1.678922
H	3.367224	6.174711	-0.391462
H	3.901212	7.141672	-4.139772
H	4.325176	7.285418	-2.422430
H	3.937908	5.694408	-3.098171
H	1.801505	8.090855	-4.607957
H	-0.610312	8.431284	-4.087594
H	-1.561690	7.526333	-1.976783
H	-1.266056	6.643162	0.195165
H	-0.469079	5.061220	-0.041640
H	0.372173	6.345179	0.836958

C	4.191295	-3.532402	-3.251266
C	4.096584	-4.526760	-2.096497
N	2.713995	-4.981103	-1.844557
C	2.662982	-6.268094	-1.122570
C	3.046182	-7.470456	-1.982677
C	1.908351	-3.966931	-1.153805
C	0.468583	-3.879207	-1.663294
O	-0.399824	-3.289257	-1.005723
N	0.275912	-4.447327	-2.874621
C	-0.936833	-4.454573	-3.632514
C	-1.573835	-5.690617	-3.867996
C	-1.007021	-6.974137	-3.311157
C	-2.746662	-5.699789	-4.633488
C	-3.274560	-4.514030	-5.145674
C	-2.624321	-3.303111	-4.911014
C	-1.441454	-3.247417	-4.159650
C	-0.729118	-1.935419	-3.950446
H	5.239483	-3.229733	-3.405553
H	3.817082	-3.978513	-4.187100
H	3.614282	-2.613376	-3.059414
H	4.694839	-5.413952	-2.350584
H	4.543028	-4.101157	-1.175688
H	3.295507	-6.232258	-0.210660
H	1.626999	-6.402650	-0.771606
H	2.924113	-8.399876	-1.403529
H	2.406702	-7.537284	-2.877905
H	4.094041	-7.432745	-2.319009
H	1.874631	-4.104545	-0.058443
H	2.338225	-2.966284	-1.321857
H	1.104968	-4.956133	-3.196616
H	-0.845555	-6.908420	-2.222958
H	-1.683973	-7.818117	-3.506136
H	-0.031187	-7.223304	-3.763673
H	-3.253050	-6.649944	-4.820224
H	-4.195165	-4.534195	-5.732783
H	-3.032264	-2.376792	-5.321438
H	-0.793043	-1.605780	-2.902156
H	0.342567	-2.016895	-4.191701
H	-1.160287	-1.142728	-4.577334
C	3.747186	1.542683	5.701932
C	4.165033	0.704479	4.506778
H	5.033717	0.071428	4.782739
O	4.510791	1.573124	3.429688
C	3.057326	-0.269231	4.062517
O	2.031369	-0.449600	4.710247
O	3.251094	-0.909941	2.918912

H	2.892564	2.185045	5.440526
H	3.446756	0.900369	6.541176
H	4.586477	2.181419	6.013664
H	5.030057	1.043985	2.785427
H	4.154374	-0.705281	2.469281
C	8.085039	-4.276500	2.160217
C	7.114248	-3.150020	1.803599
H	7.017948	-3.087332	0.701207
O	7.602852	-1.956177	2.357758
C	5.720950	-3.495646	2.336272
O	5.374122	-3.267184	3.493551
O	4.939663	-4.073668	1.434907
H	8.147518	-4.375977	3.254766
H	7.764300	-5.235668	1.724635
H	9.084713	-4.025201	1.775251
H	6.905130	-1.273762	2.218815
H	4.017677	-4.216711	1.821213
C	-6.579626	4.391840	-0.853521
C	-7.901608	3.727193	-0.465383
N	-7.938209	2.293104	-0.779771
C	-9.295011	1.729638	-0.835149
C	-9.391756	0.508204	-1.751425
C	-6.988702	1.488398	-0.035420
C	-7.188093	1.408864	1.494900
O	-8.153064	1.894202	2.072323
N	-6.173139	0.739724	2.141282
C	-6.159296	0.417536	3.532394
C	-6.140212	1.436284	4.509618
C	-6.162292	2.895866	4.136852
C	-6.091634	1.057733	5.860300
C	-6.050131	-0.283664	6.237820
C	-6.064560	-1.278027	5.258670
C	-6.128124	-0.946983	3.899430
C	-6.190679	-2.029672	2.848604
H	-6.330557	4.178522	-1.906112
H	-6.656740	5.484162	-0.727119
H	-5.735806	4.054660	-0.229896
H	-8.127018	3.928021	0.600980
H	-8.709048	4.195666	-1.051936
H	-9.684935	1.485975	0.171598
H	-9.948707	2.519313	-1.239962
H	-10.439682	0.173991	-1.829006
H	-9.025001	0.750760	-2.762409
H	-8.806445	-0.346968	-1.376097
H	-7.001632	0.456473	-0.424008
H	-5.965749	1.851781	-0.224639

H	-5.469426	0.278436	1.562657
H	-7.167516	3.191148	3.798998
H	-5.870629	3.524016	4.991573
H	-5.476848	3.104038	3.299601
H	-6.077588	1.838760	6.624947
H	-6.006575	-0.555045	7.295213
H	-6.041680	-2.331761	5.548480
H	-5.332110	-1.990164	2.158503
H	-6.207934	-3.025511	3.315183
H	-7.095369	-1.928344	2.226279
C	-2.415334	3.804106	-2.600918
C	-1.187843	2.905302	-2.633907
H	-0.271886	3.520194	-2.534493
O	-1.197446	2.173466	-3.852803
C	-1.145181	1.961592	-1.422900
O	-1.733879	2.187897	-0.370488
O	-0.423758	0.848343	-1.539831
H	-3.330360	3.204854	-2.727416
H	-2.482400	4.342811	-1.646635
H	-2.355064	4.529049	-3.424988
H	-0.283749	1.928144	-4.076595
H	0.131780	0.834162	-2.371023
C	-0.313483	-4.545076	3.021499
C	0.637510	-3.685700	3.835296
H	0.561596	-3.938763	4.910089
O	0.299744	-2.318320	3.623705
C	2.104072	-3.892455	3.436743
O	2.453807	-4.284747	2.319841
O	2.937327	-3.567151	4.399467
H	-0.225339	-4.307115	1.950770
H	-0.094892	-5.615162	3.160444
H	-1.347117	-4.354593	3.348016
H	0.931335	-1.735021	4.114464
H	3.887569	-3.517146	4.047851

Table S18. B3LYP/cc-pVDZ optimized geometry of Lid:Cou:La structure D.

225

C	-3.155245	-6.086210	5.665498
C	-2.822749	-4.933786	4.757366
C	-3.464054	-3.723724	4.905255
C	-3.182963	-2.616734	4.047291
O	-3.745956	-1.507314	4.091348
O	-2.231363	-2.768060	3.085456
C	-1.553416	-3.956088	2.906544
C	-0.613171	-3.979703	1.891546

C	0.105867	-5.170254	1.616024
O	0.993626	-5.235708	0.654110
C	-0.181632	-6.317879	2.425371
C	-1.113417	-6.265596	3.441023
C	-1.838544	-5.077667	3.724657
H	-3.920473	-5.806266	6.401899
H	-3.528820	-6.947012	5.087302
H	-2.259732	-6.429435	6.208584
H	-4.222921	-3.562050	5.669985
H	-0.446887	-3.088049	1.290113
H	0.373704	-7.234729	2.218517
H	-1.297538	-7.157277	4.042865
C	-0.286959	-0.185911	-3.335192
C	-0.445513	0.983644	-2.375677
N	-1.470793	0.705557	-1.291356
C	-1.010197	-0.324681	-0.277976
C	0.199909	0.091933	0.543583
C	-1.949319	1.946982	-0.601356
C	-2.850497	2.814512	-1.483746
O	-2.747744	2.857191	-2.704765
N	-3.715679	3.574953	-0.753400
C	-4.518883	4.629386	-1.287422
C	-3.911358	5.740733	-1.910018
C	-2.416135	5.849476	-2.058545
C	-4.743788	6.764905	-2.385854
C	-6.128616	6.702755	-2.239490
C	-6.709535	5.600961	-1.610204
C	-5.919244	4.549186	-1.131533
C	-6.553318	3.348062	-0.474686
H	0.507041	0.067716	-4.051608
H	0.022183	-1.117659	-2.839656
H	-1.219613	-0.376569	-3.889870
H	0.501963	1.241216	-1.883411
H	-0.826482	1.862348	-2.905582
H	-1.878803	-0.501983	0.370598
H	-0.827407	-1.248192	-0.840580
H	0.448368	-0.733793	1.226470
H	1.091922	0.277099	-0.070898
H	0.003787	0.983460	1.156697
H	-2.479807	1.636344	0.307224
H	-1.086015	2.554621	-0.293156
H	-3.859050	3.311533	0.224635
H	-2.122277	6.888735	-2.269278
H	-1.889981	5.507907	-1.153148
H	-2.065430	5.212675	-2.887134
H	-4.285861	7.631543	-2.869647

H	-6.756576	7.515389	-2.612506
H	-7.795004	5.545269	-1.494377
H	-6.261777	3.254958	0.584333
H	-7.650380	3.410435	-0.522748
H	-6.237503	2.415589	-0.971384
H	-2.310220	0.271691	-1.729613
C	-7.018707	-0.261729	0.886625
C	-6.676336	-1.693859	1.285289
N	-6.122286	-2.500310	0.183983
C	-6.128429	-3.936347	0.520873
C	-6.014172	-4.853726	-0.693768
C	-4.804883	-2.009987	-0.251042
C	-4.784545	-1.330711	-1.623381
O	-3.822318	-0.648698	-1.993975
N	-5.867180	-1.601481	-2.392311
C	-6.079427	-1.221741	-3.751513
C	-7.236112	-0.475069	-4.063751
C	-8.200547	-0.049770	-2.983700
C	-7.470376	-0.127624	-5.399115
C	-6.577798	-0.504740	-6.402994
C	-5.448192	-1.253502	-6.078455
C	-5.179076	-1.636941	-4.756034
C	-3.974256	-2.488015	-4.449729
H	-7.761113	-0.242692	0.074020
H	-7.446366	0.274608	1.749497
H	-6.134491	0.305252	0.557174
H	-5.980607	-1.682041	2.153686
H	-7.595640	-2.196908	1.625925
H	-5.325594	-4.178438	1.251732
H	-7.083693	-4.137770	1.032155
H	-6.832542	-4.663496	-1.407871
H	-5.052068	-4.738580	-1.212498
H	-6.086793	-5.905077	-0.369085
H	-4.369043	-1.301408	0.473390
H	-4.086745	-2.841824	-0.350989
H	-6.613985	-2.054052	-1.860386
H	-9.011265	0.562234	-3.404058
H	-8.668173	-0.913540	-2.478569
H	-7.695279	0.542759	-2.204095
H	-8.360605	0.455154	-5.648002
H	-6.767999	-0.220799	-7.440482
H	-4.757376	-1.564903	-6.865921
H	-4.211498	-3.288742	-3.732393
H	-3.581409	-2.947335	-5.368636
H	-3.175482	-1.889577	-3.985340
C	4.914706	5.575406	0.437155

C	3.483457	5.700463	-0.079147
N	2.575816	6.425845	0.832308
C	2.870600	7.865426	0.904948
C	2.319984	8.529933	2.165502
C	1.181529	6.160323	0.476141
C	0.587376	4.905543	1.126325
O	-0.424476	4.376392	0.669428
N	1.238546	4.505875	2.253199
C	0.920032	3.370283	3.055370
C	-0.339887	3.269735	3.682731
C	-1.373996	4.360811	3.571943
C	-0.609312	2.124261	4.449514
C	0.354977	1.132047	4.621064
C	1.610919	1.268208	4.026699
C	1.910859	2.378292	3.228509
C	3.252589	2.498818	2.549302
H	4.925161	5.160496	1.458038
H	5.474436	4.883996	-0.209861
H	5.451321	6.537568	0.455023
H	3.483352	6.177849	-1.085190
H	3.071487	4.689371	-0.220101
H	3.963897	7.981409	0.899467
H	2.498039	8.393821	-0.001072
H	1.221523	8.466774	2.228172
H	2.736202	8.055766	3.068776
H	2.586624	9.599240	2.180481
H	0.544745	6.995441	0.808760
H	1.023729	6.062672	-0.615094
H	2.128282	4.989241	2.384320
H	-0.904260	5.356355	3.614054
H	-1.915230	4.303125	2.615359
H	-2.101568	4.286870	4.393161
H	-1.592421	2.011794	4.913119
H	0.128756	0.250601	5.225894
H	2.369710	0.493806	4.163849
H	3.879755	1.624558	2.777336
H	3.147633	2.566355	1.454485
H	3.807583	3.394287	2.881110
C	-5.388855	2.857404	4.578719
C	-4.839305	1.507805	4.145386
H	-5.676365	0.786256	4.039150
O	-3.923867	1.053935	5.132487
C	-4.173332	1.583289	2.754286
O	-4.274291	2.555808	2.024731
O	-3.485108	0.512444	2.349867
H	-4.574511	3.591736	4.666253

H	-6.116150	3.240774	3.850027
H	-5.875287	2.750973	5.559129
H	-3.852075	0.084607	5.058880
H	-3.492664	-0.232225	3.015838
C	4.143485	-3.479337	-2.704308
C	3.047304	-3.822819	-1.708287
H	3.286183	-4.760864	-1.173590
O	1.796293	-3.975198	-2.397456
C	2.864849	-2.730163	-0.632676
O	3.424797	-1.636742	-0.725160
O	2.083652	-3.004715	0.380095
H	5.116503	-3.373124	-2.199410
H	4.221946	-4.279075	-3.456156
H	3.911749	-2.532206	-3.212638
H	1.518281	-4.923579	-2.369506
H	1.651896	-3.972093	0.410749
C	4.611480	-1.777221	2.776327
C	5.900468	-2.242221	2.088511
N	6.848879	-1.190549	1.671998
C	7.451664	-0.417081	2.770957
C	8.276571	-1.259096	3.740814
C	6.321311	-0.314095	0.626747
C	7.341439	0.009866	-0.469735
O	7.115864	0.873350	-1.333593
N	8.458612	-0.748240	-0.429584
C	9.517876	-0.793284	-1.385654
C	9.786431	-2.034407	-2.003057
C	8.956879	-3.254395	-1.681563
C	10.837051	-2.109054	-2.924673
C	11.599807	-0.981242	-3.231000
C	11.326471	0.232317	-2.602179
C	10.291005	0.352832	-1.663133
C	10.050307	1.667793	-0.967986
H	3.981850	-2.649464	3.013754
H	4.813535	-1.243206	3.719343
H	4.016537	-1.124799	2.118704
H	6.444720	-2.941852	2.742276
H	5.642133	-2.812436	1.181438
H	8.111527	0.332813	2.303888
H	6.684387	0.158201	3.331692
H	9.036639	-1.851185	3.204944
H	8.796180	-0.601842	4.455851
H	7.655663	-1.953481	4.327900
H	5.471475	-0.799988	0.119379
H	5.931447	0.648334	1.007308
H	8.395288	-1.462037	0.303275

H	7.880429	-3.060880	-1.820389
H	9.237569	-4.099016	-2.326632
H	9.090622	-3.583131	-0.635367
H	11.049975	-3.063551	-3.412089
H	12.413776	-1.051101	-3.955974
H	11.933831	1.111746	-2.829660
H	9.912023	1.526180	0.116447
H	10.899442	2.349536	-1.119563
H	9.134901	2.149667	-1.343859
C	4.076905	1.894114	-3.985385
C	4.032737	1.002221	-2.744137
H	5.005705	0.488023	-2.637090
O	2.984830	0.072239	-2.908775
C	3.821807	1.889626	-1.501443
O	2.726470	2.238237	-1.104843
O	4.936153	2.320445	-0.891458
H	3.124053	2.435916	-4.088754
H	4.897531	2.624888	-3.918487
H	4.227475	1.270186	-4.879062
H	3.042379	-0.550066	-2.155796
H	5.748657	1.807580	-1.177249
C	-1.776060	-7.114185	-1.441749
C	-0.959472	-5.977369	-2.053075
H	-1.040038	-6.030219	-3.154470
O	0.428241	-6.117633	-1.767072
C	-1.554233	-4.600224	-1.674606
O	-2.749298	-4.459090	-1.504078
O	-0.731537	-3.552776	-1.574690
H	-2.830133	-7.039781	-1.741164
H	-1.365473	-8.076769	-1.780025
H	-1.729196	-7.078131	-0.341381
H	0.583630	-5.955979	-0.791788
H	0.220647	-3.756475	-1.776715

Table S19. B3LYP/cc-pVDZ optimized geometry of Lid:Cou:La structure E.

225

C	8.476097	-1.985206	3.637168
C	7.297842	-1.729347	2.736398
C	7.456505	-1.742503	1.365747
C	6.363757	-1.491732	0.486565
O	6.433195	-1.467699	-0.757879
O	5.135908	-1.247737	1.025345
C	4.922915	-1.240129	2.389974
C	3.626594	-0.995343	2.812431
C	3.330303	-0.947464	4.205298

O	2.140174	-0.720749	4.664481
C	4.420109	-1.172904	5.117620
C	5.695658	-1.425468	4.670772
C	6.003156	-1.469732	3.282661
H	8.295776	-2.859967	4.282876
H	9.389984	-2.167791	3.055902
H	8.655399	-1.126435	4.304304
H	8.421398	-1.934594	0.897999
H	2.839291	-0.839617	2.073205
H	4.193292	-1.137625	6.184876
H	6.493188	-1.593856	5.396686
C	-1.795682	-1.311515	-3.160384
C	-1.554875	-1.552378	-1.676191
N	-1.938083	-0.376734	-0.809913
C	-1.862658	-0.704117	0.668282
C	-2.878724	-1.734630	1.135914
C	-1.111202	0.837055	-1.082303
C	-1.921075	2.088837	-0.736571
O	-3.150629	2.038825	-0.722364
N	-1.171834	3.195756	-0.530343
C	-1.697610	4.528067	-0.480434
C	-1.340482	5.409305	-1.523436
C	-0.457424	4.949764	-2.658539
C	-1.827320	6.721911	-1.478811
C	-2.647893	7.145361	-0.431928
C	-2.982570	6.259679	0.591454
C	-2.511565	4.938071	0.592805
C	-2.867232	4.001114	1.717206
H	-1.150183	-0.531664	-3.588007
H	-1.588025	-2.251945	-3.695141
H	-2.846156	-1.042320	-3.343666
H	-2.181578	-2.383408	-1.332580
H	-0.508216	-1.792915	-1.441041
H	-0.831388	-1.033625	0.854242
H	-2.020885	0.239226	1.204743
H	-3.911569	-1.424883	0.922675
H	-2.716589	-2.729530	0.694571
H	-2.759999	-1.834264	2.225801
H	-0.165155	0.765883	-0.530943
H	-0.870553	0.890980	-2.152117
H	-0.150023	3.083847	-0.555793
H	-0.820008	4.019125	-3.121782
H	-0.390978	5.721619	-3.439081
H	0.568680	4.732029	-2.317222
H	-1.563995	7.414010	-2.282797
H	-3.023952	8.171181	-0.412135

H	-3.615299	6.594755	1.417254
H	-1.998299	3.405242	2.036119
H	-3.237948	4.563533	2.587493
H	-3.645581	3.290897	1.398084
H	-2.934424	-0.142884	-1.030297
C	-8.686311	1.294563	-4.268302
C	-7.333390	1.461947	-3.579479
N	-7.400649	1.336279	-2.113069
C	-7.968031	2.537491	-1.470008
C	-8.614769	2.238534	-0.119709
C	-6.089610	0.986527	-1.560136
C	-5.791172	-0.510900	-1.606452
O	-4.639194	-0.954117	-1.509313
N	-6.900172	-1.287734	-1.712790
C	-6.980136	-2.705191	-1.564238
C	-6.355954	-3.560265	-2.495473
C	-5.595500	-3.020340	-3.678833
C	-6.482474	-4.944906	-2.310017
C	-7.220539	-5.467605	-1.248893
C	-7.853797	-4.604620	-0.353463
C	-7.744727	-3.215066	-0.491558
C	-8.425578	-2.286901	0.484887
H	-9.122762	0.308664	-4.040008
H	-9.411944	2.063792	-3.960087
H	-8.568435	1.374721	-5.361215
H	-6.654105	0.676104	-3.947531
H	-6.870515	2.430584	-3.870806
H	-7.190722	3.323240	-1.359704
H	-8.730397	2.950865	-2.147381
H	-9.003507	3.167920	0.328209
H	-9.456264	1.536440	-0.241205
H	-7.901900	1.796768	0.592249
H	-5.246942	1.522649	-2.032983
H	-6.054540	1.246082	-0.491134
H	-7.756655	-0.729006	-1.691128
H	-5.397840	-3.814375	-4.413638
H	-6.159048	-2.217074	-4.180730
H	-4.636385	-2.583342	-3.362867
H	-6.003316	-5.618469	-3.025171
H	-7.312432	-6.549293	-1.125535
H	-8.440270	-5.009830	0.474961
H	-9.206905	-1.679112	-0.005898
H	-8.917014	-2.860338	1.284492
H	-7.715034	-1.582940	0.945445
C	2.886214	-5.553415	4.099907
C	1.418166	-5.178231	4.289310

N	0.715913	-4.931795	3.015493
C	-0.746181	-5.062864	3.147494
C	-1.229495	-6.503464	3.300848
C	1.062377	-3.624492	2.450196
C	1.057666	-3.574326	0.919746
O	0.963967	-2.503949	0.317915
N	1.224347	-4.788935	0.325072
C	1.304882	-5.043316	-1.077624
C	0.338359	-5.891773	-1.660391
C	-0.766220	-6.496172	-0.827592
C	0.425693	-6.166281	-3.030848
C	1.444519	-5.611416	-3.807000
C	2.398632	-4.786389	-3.212516
C	2.355607	-4.490879	-1.841280
C	3.428700	-3.635575	-1.221092
H	3.354564	-5.754575	5.076881
H	2.981186	-6.457086	3.476505
H	3.464977	-4.746476	3.623234
H	0.907203	-6.008930	4.797470
H	1.331945	-4.296406	4.960217
H	-1.120948	-4.443176	3.992546
H	-1.194862	-4.636686	2.235442
H	-0.875566	-6.971376	4.232664
H	-2.330820	-6.529662	3.321196
H	-0.886502	-7.125865	2.458955
H	0.416257	-2.804397	2.815401
H	2.087210	-3.354108	2.747172
H	1.167228	-5.565484	0.985966
H	-0.376317	-7.213270	-0.083477
H	-1.321799	-5.726986	-0.266909
H	-1.481784	-7.040176	-1.460572
H	-0.319402	-6.820294	-3.490824
H	1.501278	-5.833338	-4.875195
H	3.213099	-4.371694	-3.811180
H	3.036106	-2.642384	-0.953429
H	3.800293	-4.086617	-0.286434
H	4.274954	-3.508972	-1.909911
C	1.936195	-0.758012	-4.839072
C	1.865364	0.601246	-5.528462
H	1.256766	0.509243	-6.448268
O	3.133697	1.134101	-5.899961
C	1.138297	1.649410	-4.663373
O	0.055564	1.478464	-4.142173
O	1.815454	2.801542	-4.567773
H	2.505356	-0.698065	-3.899023
H	0.924131	-1.120246	-4.613191

H	2.429972	-1.486210	-5.499469
H	3.859774	0.603279	-5.489102
H	2.640417	2.615028	-5.090141
C	7.222371	-2.272755	-5.256357
C	6.823156	-1.788896	-3.870316
H	7.645912	-1.177873	-3.443417
O	6.569052	-2.917984	-3.050194
C	5.602539	-0.848007	-3.933150
O	5.239940	-0.330309	-4.980335
O	4.951175	-0.598893	-2.799528
H	7.399813	-1.426334	-5.933158
H	8.134668	-2.881622	-5.178987
H	6.421802	-2.895080	-5.684480
H	6.700271	-2.646963	-2.121934
H	5.396127	-0.999205	-1.999295
C	5.143908	4.744443	-3.452731
C	5.713347	3.485801	-2.800459
N	5.085761	3.175825	-1.503543
C	5.935364	2.319797	-0.652885
C	7.102080	3.065947	-0.009298
C	3.746556	2.601715	-1.661799
C	2.739160	3.047171	-0.602178
O	1.618348	2.526914	-0.550631
N	3.178098	4.040694	0.205645
C	2.461524	4.665828	1.273824
C	2.210015	6.050892	1.187834
C	2.647277	6.844132	-0.020032
C	1.543536	6.672566	2.251071
C	1.136028	5.939228	3.366694
C	1.399890	4.571259	3.438167
C	2.070821	3.909974	2.398193
C	2.382248	2.441851	2.517542
H	5.656867	4.944319	-4.407468
H	4.067771	4.651420	-3.671412
H	5.279851	5.619561	-2.796979
H	5.630679	2.622471	-3.495604
H	6.788386	3.638236	-2.623064
H	5.294317	1.914609	0.145864
H	6.305117	1.442164	-1.223094
H	7.800089	3.480694	-0.753897
H	6.741901	3.898747	0.616430
H	7.678586	2.380197	0.632364
H	3.309954	2.906775	-2.623461
H	3.749344	1.495988	-1.673521
H	4.089216	4.402697	-0.085910
H	3.747696	6.911797	-0.093864

H	2.292247	6.384823	-0.956684
H	2.257854	7.871154	0.024812
H	1.335098	7.743666	2.193537
H	0.615129	6.438649	4.186948
H	1.103568	3.991160	4.315585
H	2.108207	2.069895	3.511941
H	1.828021	1.857023	1.767938
H	3.454158	2.245305	2.349041
C	-6.078832	-0.226949	4.888295
C	-5.062332	0.357313	3.908702
H	-4.352328	-0.424412	3.593124
O	-4.371031	1.449462	4.507653
C	-5.772002	0.848721	2.635822
O	-6.319079	0.118600	1.833904
O	-5.751375	2.178090	2.496420
H	-5.559488	-0.642452	5.764653
H	-6.767071	0.559877	5.236552
H	-6.665661	-1.020906	4.403416
H	-3.415375	1.353754	4.264950
H	-5.205065	2.489129	3.261000
C	-1.379115	1.830736	6.246984
C	-0.405139	0.869457	5.582973
H	-0.421091	-0.099967	6.126585
O	0.891166	1.440008	5.641061
C	-0.812479	0.522037	4.131173
O	-1.916620	0.812583	3.662198
O	0.054698	-0.133699	3.393838
H	-2.401676	1.429483	6.264043
H	-1.048464	2.017038	7.279076
H	-1.394096	2.791279	5.708946
H	1.540688	0.718864	5.477984
H	0.954054	-0.368862	3.877114

Table S20. B3LYP/cc-pVDZ optimized geometry of Lid:Cou:Le structure A.

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C	0.013496	-0.250209	-8.583838
C	0.164537	0.005964	-7.109875
C	-0.513548	1.030604	-6.504478
C	-0.403625	1.289680	-5.093919
O	-1.014594	2.165355	-4.480172
O	0.448314	0.502840	-4.362718
C	1.147327	-0.537192	-4.929380
C	1.956971	-1.271407	-4.070757
C	2.672378	-2.367223	-4.580328
O	3.450884	-3.132591	-3.806616

C	2.562340	-2.691810	-5.956197
C	1.763313	-1.935661	-6.792123
C	1.024868	-0.829229	-6.306548
H	-0.379941	-1.263214	-8.768545
H	-0.668918	0.475316	-9.046341
H	0.987608	-0.186441	-9.095629
H	-1.182729	1.689356	-7.057312
H	2.020026	-1.008239	-3.015786
H	3.121567	-3.548704	-6.333998
H	1.697403	-2.200937	-7.848132
C	-2.999577	0.609020	3.056949
C	-1.706491	1.382648	2.850057
N	-1.159516	1.351094	1.441744
C	0.127429	2.160438	1.331084
C	0.034342	3.581527	1.860838
C	-0.901557	-0.034169	0.937771
C	-2.151474	-0.688254	0.350661
O	-3.112585	-0.003404	-0.022371
N	-2.048921	-2.027417	0.231792
C	-2.978363	-2.841016	-0.495021
C	-3.746838	-3.791382	0.205696
C	-3.644716	-3.945021	1.705404
C	-4.624663	-4.603303	-0.530371
C	-4.735741	-4.472058	-1.914790
C	-3.944557	-3.541956	-2.592487
C	-3.042895	-2.722587	-1.900056
C	-2.127082	-1.780626	-2.642041
H	-2.871170	-0.474700	2.919576
H	-3.320348	0.767981	4.098473
H	-3.799567	0.955290	2.387865
H	-1.872498	2.442183	3.077913
H	-0.899836	0.999997	3.491142
H	0.896554	1.581127	1.855593
H	0.358740	2.168455	0.258677
H	-0.073675	3.621027	2.954820
H	0.983786	4.074199	1.607670
H	-0.787862	4.141240	1.390968
H	-0.170208	0.042037	0.121253
H	-0.422692	-0.614695	1.737382
H	-1.209047	-2.507009	0.616755
H	-2.612737	-3.819624	2.062861
H	-4.278374	-3.208684	2.229947
H	-3.995609	-4.941522	2.012594
H	-5.226535	-5.346725	-0.002254
H	-5.429207	-5.108032	-2.470218
H	-4.009820	-3.459044	-3.680251

H	-2.250999	-1.894348	-3.728748
H	-2.320975	-0.727859	-2.381177
H	-1.073401	-1.987571	-2.392974
H	-1.846498	1.811431	0.797861
C	-7.859363	-3.932359	1.843832
C	-8.097270	-2.531677	2.407961
N	-6.845252	-1.789286	2.641413
C	-6.924765	-0.831832	3.752396
C	-6.829524	-1.507741	5.120738
C	-6.249124	-1.230177	1.440503
C	-6.949825	-0.007703	0.818137
O	-8.130335	0.253419	1.011890
N	-6.126822	0.743547	0.004820
C	-6.604164	1.742286	-0.897038
C	-6.429218	1.525597	-2.282709
C	-5.765435	0.266176	-2.785474
C	-6.909608	2.486692	-3.181152
C	-7.562366	3.632669	-2.722129
C	-7.715999	3.837488	-1.351577
C	-7.233860	2.909652	-0.414365
C	-7.383917	3.179974	1.060124
H	-8.819207	-4.459838	1.714800
H	-7.368633	-3.903069	0.857211
H	-7.221936	-4.525658	2.519454
H	-8.782671	-1.960896	1.755697
H	-8.603730	-2.630673	3.380359
H	-6.076152	-0.134933	3.646813
H	-7.841359	-0.210631	3.693797
H	-7.666237	-2.203250	5.296526
H	-5.893001	-2.081600	5.208948
H	-6.857449	-0.753586	5.924861
H	-5.196461	-0.971624	1.637882
H	-6.215580	-2.007845	0.659116
H	-5.177695	0.393870	-0.143830
H	-4.732167	0.163004	-2.415053
H	-6.306252	-0.633675	-2.448556
H	-5.734648	0.252623	-3.884766
H	-6.787874	2.318593	-4.254442
H	-7.948891	4.366261	-3.433759
H	-8.217078	4.738779	-0.988697
H	-7.616950	4.239476	1.243085
H	-8.183825	2.555936	1.486605
H	-6.460125	2.924697	1.603588
C	6.079300	1.693862	3.708506
C	5.071710	0.853215	2.926713
N	4.605161	-0.341439	3.660161

C	5.615440	-1.417591	3.680828
C	5.390199	-2.427739	4.804841
C	3.307187	-0.795257	3.145627
C	2.121900	-0.259775	3.945083
O	0.976030	-0.230219	3.481473
N	2.443635	0.118008	5.210575
C	1.545264	0.567834	6.216846
C	1.755813	1.845438	6.781331
C	2.892420	2.718782	6.308106
C	0.890169	2.285336	7.789949
C	-0.164051	1.482101	8.227840
C	-0.350394	0.218544	7.668328
C	0.499169	-0.269907	6.663672
C	0.299543	-1.658331	6.112070
H	5.657209	2.024789	4.671623
H	7.013422	1.149158	3.921712
H	6.348811	2.590957	3.127600
H	4.194537	1.476041	2.694927
H	5.495518	0.560689	1.943676
H	5.653828	-1.928016	2.698378
H	6.596152	-0.940181	3.832646
H	4.425367	-2.948955	4.707835
H	6.182502	-3.194853	4.787021
H	5.416881	-1.933075	5.790177
H	3.153447	-0.551523	2.081408
H	3.221991	-1.890355	3.222175
H	3.458414	0.164929	5.344232
H	3.875513	2.297241	6.583550
H	2.891602	2.828939	5.211803
H	2.829769	3.721050	6.755911
H	1.044841	3.273935	8.229668
H	-0.834492	1.838085	9.013607
H	-1.162771	-0.419754	8.025503
H	1.256062	-2.183867	5.968908
H	-0.332446	-2.255981	6.785591
H	-0.173312	-1.626063	5.118016
C	7.052647	3.800727	-2.433792
C	6.028667	2.827467	-3.013136
N	4.667383	3.044212	-2.484096
C	3.626705	2.470000	-3.353563
C	3.410285	3.243386	-4.653334
C	4.517821	2.569751	-1.102630
C	3.663705	3.483871	-0.217307
O	3.229515	3.104237	0.870876
N	3.480478	4.733017	-0.729755
C	2.704868	5.770378	-0.129299

C	1.520263	6.187980	-0.771660
C	1.067236	5.551441	-2.063634
C	0.757090	7.203736	-0.179270
C	1.165522	7.791476	1.019039
C	2.345534	7.374414	1.635770
C	3.137116	6.361137	1.076611
C	4.414689	5.927384	1.748583
H	6.762250	4.845353	-2.632513
H	7.170132	3.676751	-1.345811
H	8.041328	3.622993	-2.887351
H	5.986229	2.972674	-4.102750
H	6.357998	1.785435	-2.832640
H	3.846082	1.402841	-3.579662
H	2.683007	2.473897	-2.784947
H	3.160356	4.296854	-4.448744
H	4.295312	3.226775	-5.308323
H	2.577076	2.798229	-5.220329
H	4.086618	1.553959	-1.036871
H	5.502945	2.492498	-0.619419
H	3.820779	4.820284	-1.689474
H	0.059409	5.896893	-2.328528
H	1.745782	5.797225	-2.900088
H	1.041475	4.452082	-1.986449
H	-0.179515	7.503131	-0.653781
H	0.560756	8.579579	1.474338
H	2.668733	7.842593	2.569210
H	5.244417	5.867805	1.025712
H	4.698464	6.630153	2.545454
H	4.302602	4.922400	2.186326
C	8.467401	-0.687077	0.741861
C	7.539153	-0.643332	-0.451610
O	7.060466	0.403326	-0.853312
C	7.269582	-1.970462	-1.149405
C	5.930330	-2.023066	-1.874335
C	4.741020	-2.073110	-0.910215
O	4.902093	-1.910105	0.300142
O	3.578815	-2.293452	-1.469689
H	8.748226	0.329661	1.046436
H	7.942381	-1.188620	1.572074
H	9.367875	-1.283931	0.520365
H	8.096923	-2.104259	-1.872944
H	7.357198	-2.790707	-0.420428
H	5.808364	-1.128798	-2.507455
H	5.880546	-2.890636	-2.550910
H	3.501289	-2.770115	-2.806751
C	-4.314089	6.750468	-0.462395

C	-3.411343	5.984314	-1.403995
O	-2.274187	6.350130	-1.645686
C	-4.007992	4.739785	-2.044793
C	-2.965687	3.772580	-2.587102
C	-2.225571	3.040658	-1.483255
O	-2.537774	3.132226	-0.302692
O	-1.204672	2.263605	-1.841790
H	-4.396532	6.179143	0.478628
H	-3.893799	7.741665	-0.247830
H	-5.333564	6.840618	-0.870675
H	-4.679457	4.239881	-1.331338
H	-4.656913	5.090887	-2.867570
H	-3.436494	3.010012	-3.229007
H	-2.228142	4.291139	-3.217786
H	-1.077572	2.241854	-2.836906
C	-1.329686	-6.800233	0.030400
C	-0.197371	-7.291199	-0.841710
O	0.844827	-7.707999	-0.368244
C	-0.422406	-7.239611	-2.349624
C	0.873816	-7.199009	-3.149427
C	1.560377	-5.851974	-3.038277
O	1.230608	-4.982620	-2.251431
O	2.576514	-5.728154	-3.900430
H	-1.195945	-5.711853	0.161306
H	-2.316176	-6.959333	-0.430509
H	-1.280709	-7.276246	1.019558
H	-0.999776	-8.147718	-2.606284
H	-1.070565	-6.382308	-2.590167
H	1.576840	-7.956230	-2.764333
H	0.710536	-7.424465	-4.214499
H	2.961838	-4.818483	-3.794641
C	0.941171	-5.867250	4.130741
C	1.800319	-4.936081	3.303408
O	2.234647	-3.892825	3.763630
C	2.112924	-5.392447	1.887282
C	2.394585	-4.265217	0.900963
C	1.203595	-3.359363	0.661167
O	0.105597	-3.551886	1.190251
O	1.381629	-2.328142	-0.142386
H	1.267195	-6.914209	4.018317
H	0.955757	-5.569963	5.187474
H	-0.092561	-5.809899	3.748146
H	3.015464	-6.028016	1.971272
H	1.324837	-6.063979	1.518251
H	3.237198	-3.633350	1.222867
H	2.675767	-4.679877	-0.079655

H 2.306130 -2.328924 -0.590113

Table S21. B3LYP/cc-pVDZ optimized geometry of Lid:Cou:Le structure B.

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C	1.580265	-7.667292	3.624445
C	1.719451	-6.187421	3.391125
C	1.805754	-5.319833	4.451180
C	1.943486	-3.901044	4.266642
O	2.017910	-3.061820	5.166955
O	1.999339	-3.429770	2.980160
C	1.911367	-4.263622	1.888597
C	1.962677	-3.652607	0.645643
C	1.854194	-4.424094	-0.536574
O	1.870432	-3.861001	-1.727377
C	1.712282	-5.838966	-0.387919
C	1.672876	-6.428801	0.861700
C	1.764321	-5.661177	2.051583
H	1.561468	-7.901617	4.697348
H	0.653798	-8.053330	3.168544
H	2.417054	-8.217516	3.163836
H	1.775156	-5.664388	5.484481
H	2.095891	-2.573202	0.588599
H	1.641970	-6.439455	-1.296825
H	1.567113	-7.512743	0.935901
C	-1.157189	-1.565209	2.284141
C	-0.840021	-0.098479	2.525983
N	-0.691422	0.735258	1.273701
C	0.498206	0.380107	0.400612
C	1.831290	0.295433	1.123581
C	-1.921934	0.748502	0.422059
C	-3.081519	1.416428	1.152562
O	-2.906440	2.466903	1.768557
N	-4.276055	0.781570	1.018037
C	-5.529285	1.314602	1.462039
C	-5.782669	1.500174	2.836754
C	-4.764834	1.142596	3.889348
C	-7.034569	2.013216	3.209396
C	-8.006124	2.315723	2.255900
C	-7.742150	2.103406	0.901766
C	-6.503059	1.603299	0.482540
C	-6.213074	1.379044	-0.981547
H	-0.378499	-2.073933	1.696823
H	-1.209127	-2.055500	3.268304
H	-2.124977	-1.712094	1.781856
H	-1.618390	0.388686	3.125570

H	0.093989	0.026499	3.082299
H	0.248033	-0.558982	-0.106267
H	0.514237	1.173514	-0.358407
H	2.599066	0.064709	0.368472
H	2.097498	1.241612	1.610496
H	1.866019	-0.498580	1.882740
H	-1.683961	1.365649	-0.455266
H	-2.144854	-0.270805	0.087622
H	-4.296034	-0.078551	0.461410
H	-5.229997	1.103160	4.885084
H	-4.304303	0.162722	3.687165
H	-3.943680	1.875806	3.913422
H	-7.247048	2.164789	4.270669
H	-8.974988	2.711930	2.569152
H	-8.502937	2.334225	0.152093
H	-5.303924	1.916663	-1.297548
H	-6.048285	0.311592	-1.204122
H	-7.051749	1.723702	-1.603021
H	-0.529249	1.698653	1.635953
C	6.308581	-4.084255	1.471863
C	6.397421	-2.619180	1.037957
N	7.737821	-2.236013	0.581795
C	8.679753	-2.071243	1.698543
C	10.118264	-1.807877	1.260648
C	7.715535	-1.148500	-0.397194
C	7.258197	0.222601	0.134122
O	7.882857	0.811045	1.011959
N	6.112911	0.713429	-0.446864
C	5.572612	2.012825	-0.207912
C	5.099650	2.379565	1.070605
C	5.157290	1.435166	2.242446
C	4.551698	3.662807	1.231697
C	4.468229	4.554347	0.162510
C	4.936675	4.173793	-1.097356
C	5.497383	2.906647	-1.300551
C	6.040659	2.513334	-2.654151
H	5.263597	-4.347543	1.703277
H	6.666425	-4.745628	0.665985
H	6.908047	-4.293279	2.372165
H	5.698308	-2.460296	0.201739
H	6.040470	-1.966354	1.866244
H	8.358181	-1.264154	2.388102
H	8.654228	-3.013173	2.270455
H	10.443316	-2.540266	0.502729
H	10.233450	-0.792730	0.852274
H	10.792058	-1.890181	2.128787

H	8.734775	-1.003276	-0.786754
H	7.085830	-1.462231	-1.243556
H	5.735956	0.196709	-1.246905
H	4.465280	1.744121	3.038742
H	4.897824	0.409186	1.939189
H	6.180662	1.391959	2.646480
H	4.171465	3.951954	2.214378
H	4.043228	5.550265	0.311888
H	4.889390	4.875099	-1.935090
H	5.502696	1.652860	-3.084913
H	5.969017	3.353231	-3.361077
H	7.099909	2.214491	-2.583184
C	2.864002	3.406710	-4.928750
C	1.577525	2.692924	-5.337150
N	0.392898	3.185661	-4.607471
C	-0.861243	2.930360	-5.337564
C	-1.091750	3.887320	-6.505703
C	0.319878	2.661429	-3.239078
C	-0.297139	3.639070	-2.231016
O	-0.629790	3.273306	-1.103447
N	-0.394290	4.915641	-2.696478
C	-0.803885	6.071568	-1.970160
C	-2.107937	6.165260	-1.440140
C	-3.115213	5.055877	-1.597814
C	-2.460758	7.344227	-0.765351
C	-1.560196	8.400054	-0.627550
C	-0.278827	8.293629	-1.171255
C	0.119590	7.133621	-1.846292
C	1.508855	7.020185	-2.426890
H	3.102994	3.262227	-3.863176
H	3.716502	3.015178	-5.506944
H	2.787491	4.490228	-5.116043
H	1.402764	2.872861	-6.408739
H	1.692545	1.595040	-5.219353
H	-0.901384	1.876235	-5.690858
H	-1.690123	3.044494	-4.621138
H	-1.126553	4.931878	-6.156241
H	-0.303496	3.813918	-7.271539
H	-2.050486	3.659548	-6.999432
H	-0.234286	1.706306	-3.165124
H	1.336691	2.458476	-2.867603
H	0.046368	5.022708	-3.612989
H	-3.088836	4.636273	-2.616291
H	-2.898765	4.228253	-0.904301
H	-4.132999	5.422515	-1.400432
H	-3.470188	7.432621	-0.355735

H	-1.859150	9.310934	-0.103863
H	0.429991	9.118936	-1.068291
H	1.493166	6.971957	-3.530483
H	2.121323	7.889454	-2.147878
H	2.022584	6.110460	-2.075474
C	-2.659603	-6.144468	-3.078027
C	-2.355532	-6.175117	-1.581905
N	-3.292305	-5.358894	-0.784754
C	-3.413285	-5.840948	0.603341
C	-4.270245	-7.098026	0.737167
C	-2.947032	-3.936860	-0.812354
C	-4.151377	-3.018341	-0.593801
O	-4.015345	-1.860028	-0.186338
N	-5.335374	-3.589994	-0.932077
C	-6.602341	-2.940431	-1.043387
C	-7.250020	-2.439512	0.104307
C	-6.651151	-2.592889	1.479452
C	-8.496370	-1.817870	-0.061906
C	-9.090768	-1.717912	-1.319642
C	-8.446014	-2.246486	-2.438989
C	-7.193672	-2.863260	-2.323004
C	-6.502066	-3.444021	-3.533199
H	-2.608061	-5.127396	-3.495203
H	-1.932453	-6.769060	-3.623206
H	-3.668604	-6.542151	-3.276200
H	-2.433828	-7.213109	-1.225533
H	-1.307244	-5.861830	-1.392156
H	-2.408323	-6.009623	1.048390
H	-3.878640	-5.035975	1.194465
H	-5.290017	-6.918977	0.359906
H	-3.851244	-7.952677	0.182737
H	-4.342337	-7.397191	1.795415
H	-2.164721	-3.656084	-0.081443
H	-2.559768	-3.670934	-1.808248
H	-5.214433	-4.533323	-1.306821
H	-7.372727	-2.299292	2.254640
H	-6.350166	-3.637390	1.664366
H	-5.747691	-1.975475	1.596399
H	-9.006304	-1.415562	0.816257
H	-10.064431	-1.234213	-1.426830
H	-8.914424	-2.176797	-3.423982
H	-6.484948	-4.548658	-3.497243
H	-7.031643	-3.161438	-4.454990
H	-5.453722	-3.116266	-3.617945
C	4.551724	-0.461522	-6.883231
C	3.899426	-1.249765	-5.768213

O	2.773492	-0.992441	-5.375695
C	4.727147	-2.373152	-5.160566
C	4.192149	-2.865630	-3.821768
C	4.310668	-1.800171	-2.736431
O	5.122792	-0.884853	-2.828008
O	3.539123	-1.929898	-1.675465
H	5.088026	-1.121760	-7.583635
H	3.803747	0.138419	-7.417871
H	5.303810	0.212751	-6.437457
H	4.746683	-3.197058	-5.898018
H	5.766637	-2.023743	-5.057968
H	3.153964	-3.217001	-3.893476
H	4.782923	-3.732578	-3.478214
H	2.880496	-2.724488	-1.745884
C	-3.431348	-1.126404	-5.824300
C	-2.505653	-2.017833	-5.027283
O	-2.934325	-2.843633	-4.237426
C	-1.014719	-1.827570	-5.266445
C	-0.139785	-2.302967	-4.112870
C	-0.465837	-1.553487	-2.829589
O	-1.143626	-0.538921	-2.813804
O	0.025188	-2.061009	-1.700760
H	-4.461403	-1.504348	-5.791701
H	-3.401294	-0.121183	-5.368641
H	-3.091680	-1.020689	-6.867224
H	-0.764823	-2.383827	-6.189440
H	-0.821901	-0.766629	-5.487889
H	-0.245762	-3.383693	-3.935296
H	0.919889	-2.112214	-4.352896
H	0.699792	-2.815816	-1.827946
C	-1.721100	2.232589	6.834867
C	-0.881512	1.025088	6.489295
O	-1.180796	0.271004	5.577971
C	0.369037	0.789341	7.329799
C	1.322854	-0.229853	6.714185
C	2.050446	0.344302	5.505625
O	2.237752	1.548106	5.391734
O	2.497647	-0.502245	4.591522
H	-2.769501	2.052598	6.559267
H	-1.642129	2.505434	7.898462
H	-1.362008	3.090514	6.236951
H	0.878493	1.753023	7.488135
H	0.026182	0.450221	8.324778
H	2.096332	-0.520946	7.445886
H	0.794207	-1.147886	6.424031
H	2.293427	-1.457867	4.818305

C	-3.160088	5.376152	3.292873
C	-1.678077	5.137492	3.471660
O	-1.192440	4.857634	4.556297
C	-0.815277	5.226179	2.223545
C	0.674439	5.081062	2.520583
C	1.022822	3.739509	3.125402
O	0.450640	2.693250	2.837795
O	2.048983	3.790082	3.963397
H	-3.572210	4.536614	2.708220
H	-3.655150	5.426254	4.271807
H	-3.346976	6.300944	2.723080
H	-1.157931	4.439895	1.529529
H	-1.014388	6.181844	1.710166
H	1.244449	5.160355	1.578808
H	1.035608	5.870199	3.194463
H	2.187645	2.888487	4.366482

Table S22. B3LYP/cc-pVDZ optimized geometry of Lid:Cou:Le structure C.

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C	2.923164	-0.352859	7.014160
C	2.500472	-0.902954	5.678892
C	1.630276	-1.965160	5.607645
C	1.203002	-2.507950	4.352866
O	0.412898	-3.450494	4.209024
O	1.706178	-1.951923	3.207385
C	2.572011	-0.879827	3.229773
C	2.984734	-0.393684	1.997982
C	3.830373	0.744465	1.931447
O	4.181350	1.270662	0.784359
C	4.287608	1.302918	3.171211
C	3.881635	0.782995	4.382301
C	2.994771	-0.322930	4.461560
H	4.017743	-0.404296	7.133014
H	2.641243	0.708457	7.109523
H	2.458991	-0.909421	7.839485
H	1.218612	-2.437448	6.499029
H	2.647686	-0.889767	1.087814
H	4.958236	2.163216	3.132368
H	4.242910	1.242276	5.304176
C	-0.475271	-0.040035	0.788574
C	-1.365504	0.186303	-0.423097
N	-1.384800	-0.981741	-1.388896
C	-0.012579	-1.248904	-1.972323
C	-0.020824	-2.220588	-3.142490
C	-2.030860	-2.188581	-0.788631

C	-2.834926	-2.934667	-1.851835
O	-3.347061	-2.311525	-2.782663
N	-2.959846	-4.263352	-1.616653
C	-3.761605	-5.159599	-2.394607
C	-5.160478	-4.987040	-2.451043
C	-5.850937	-3.867661	-1.715177
C	-5.907409	-5.906713	-3.201888
C	-5.293774	-6.972254	-3.858881
C	-3.910245	-7.133883	-3.777100
C	-3.121217	-6.231372	-3.052731
C	-1.620912	-6.394488	-3.002666
H	-0.644627	0.786037	1.495356
H	-0.707406	-0.977467	1.316014
H	0.589837	-0.037455	0.526179
H	-2.408474	0.332415	-0.113564
H	-1.033390	1.047642	-1.014378
H	0.372155	-0.269427	-2.282360
H	0.612139	-1.629968	-1.155239
H	-0.350999	-3.229031	-2.850254
H	-0.637032	-1.863598	-3.980016
H	1.015113	-2.308769	-3.506034
H	-1.273725	-2.816264	-0.308072
H	-2.744981	-1.844293	-0.023669
H	-2.325250	-4.664109	-0.914189
H	-5.498731	-3.795767	-0.673744
H	-5.645115	-2.896063	-2.192235
H	-6.939001	-4.026269	-1.699566
H	-6.992276	-5.785605	-3.254698
H	-5.895109	-7.682343	-4.431335
H	-3.425628	-7.967938	-4.290670
H	-1.236831	-6.446589	-1.972202
H	-1.313480	-7.307084	-3.533609
H	-1.116284	-5.539208	-3.484387
H	-1.986386	-0.679713	-2.179823
C	10.422092	0.651289	-2.412103
C	8.975499	0.254387	-2.696887
N	8.020412	0.668249	-1.658254
C	6.629626	0.365712	-2.028891
C	6.072474	1.266174	-3.132503
C	8.353853	0.220068	-0.300589
C	8.430647	-1.304480	-0.107940
O	9.430994	-1.947719	-0.399631
N	7.273094	-1.885212	0.378712
C	7.105056	-3.250639	0.753358
C	7.293771	-4.293542	-0.180910
C	7.673467	-4.030157	-1.614519

C	7.091853	-5.613018	0.255551
C	6.694669	-5.897353	1.561779
C	6.492155	-4.851920	2.464500
C	6.699660	-3.521604	2.081134
C	6.505546	-2.400582	3.073667
H	10.848769	0.055478	-1.592098
H	11.037675	0.468822	-3.307634
H	10.499007	1.721759	-2.158395
H	8.651818	0.736778	-3.632161
H	8.931238	-0.842381	-2.875593
H	6.512548	-0.699697	-2.331945
H	6.009044	0.504583	-1.129972
H	6.589535	1.127731	-4.095201
H	5.008836	1.025733	-3.293491
H	6.141111	2.326114	-2.843961
H	9.345302	0.608372	-0.029997
H	7.623737	0.676132	0.384738
H	6.577856	-1.237345	0.735011
H	7.088780	-3.195004	-2.033459
H	8.731118	-3.735755	-1.687367
H	7.501117	-4.922517	-2.234242
H	7.243746	-6.428515	-0.456264
H	6.544985	-6.932623	1.877271
H	6.184814	-5.066390	3.491161
H	7.402441	-1.763184	3.141821
H	5.662027	-1.741105	2.802540
H	6.294420	-2.800266	4.075819
C	-6.114618	2.433464	5.219020
C	-6.755447	2.732025	3.865552
N	-6.703478	1.584264	2.937796
C	-7.712934	1.691990	1.862945
C	-9.142884	1.437993	2.334666
C	-5.367459	1.423552	2.352355
C	-4.979153	-0.028687	2.065880
O	-4.070620	-0.303703	1.277296
N	-5.679271	-0.938097	2.794558
C	-5.509054	-2.354971	2.774831
C	-6.600077	-3.156846	2.376052
C	-7.911542	-2.532311	1.965856
C	-6.439129	-4.547872	2.366814
C	-5.223242	-5.129222	2.731010
C	-4.160287	-4.322700	3.135145
C	-4.285372	-2.926121	3.183127
C	-3.147528	-2.078847	3.692020
H	-6.612034	1.580848	5.709136
H	-5.042155	2.195761	5.130870

H	-6.197387	3.311541	5.879563
H	-7.814303	2.979478	4.029200
H	-6.289885	3.627915	3.405051
H	-7.636559	2.675979	1.356194
H	-7.455097	0.936916	1.102280
H	-9.230712	0.454494	2.824251
H	-9.496401	2.201015	3.045738
H	-9.829737	1.455416	1.473131
H	-5.239291	2.007372	1.424484
H	-4.609035	1.796002	3.059463
H	-6.460794	-0.512824	3.299333
H	-8.399561	-2.007135	2.805800
H	-7.773423	-1.789958	1.163082
H	-8.614119	-3.297833	1.606586
H	-7.276597	-5.178216	2.057617
H	-5.107401	-6.215150	2.705659
H	-3.208764	-4.772733	3.423716
H	-2.687814	-1.501420	2.875421
H	-3.505875	-1.347323	4.435107
H	-2.370990	-2.699613	4.158901
C	-4.497120	5.691588	-3.732470
C	-5.507840	4.697152	-3.162603
N	-4.928050	3.408291	-2.766064
C	-5.995883	2.423774	-2.503630
C	-5.500012	1.039589	-2.092550
C	-3.884032	3.507217	-1.755004
C	-4.278980	4.130749	-0.403269
O	-5.420162	4.049457	0.049623
N	-3.247864	4.753581	0.252974
C	-3.336316	5.284793	1.578550
C	-4.179461	6.382763	1.851156
C	-5.016267	7.025250	0.775569
C	-4.213225	6.882550	3.161784
C	-3.426943	6.326131	4.169891
C	-2.589026	5.248485	3.879190
C	-2.533900	4.708403	2.587868
C	-1.649292	3.522145	2.289146
H	-3.912696	5.244262	-4.553425
H	-5.025849	6.572933	-4.129572
H	-3.791437	6.057655	-2.969659
H	-6.060907	5.170619	-2.323182
H	-6.259322	4.475193	-3.939208
H	-6.708268	2.797630	-1.742938
H	-6.557576	2.332577	-3.450772
H	-5.118287	1.013306	-1.060229
H	-6.335727	0.322884	-2.143491

H	-4.698933	0.676628	-2.754673
H	-3.501103	2.496723	-1.546907
H	-3.028344	4.058887	-2.172705
H	-2.309643	4.651307	-0.144057
H	-5.388305	8.007546	1.101484
H	-4.435621	7.162458	-0.150882
H	-5.874488	6.384974	0.518484
H	-4.860924	7.734454	3.384044
H	-3.461244	6.736775	5.181736
H	-1.968952	4.809631	4.665017
H	-0.884327	3.754719	1.531171
H	-1.134815	3.180718	3.199302
H	-2.240037	2.678659	1.892801
C	6.917742	7.979790	-1.087974
C	7.186692	6.746095	-0.247661
O	6.877829	6.689986	0.926494
C	7.870120	5.581449	-0.955283
C	7.818703	4.283893	-0.160716
C	6.421681	3.697544	-0.096991
O	5.515910	4.044080	-0.842718
O	6.313167	2.740989	0.818278
H	6.611946	8.815709	-0.445211
H	7.800763	8.258958	-1.685997
H	6.105623	7.754434	-1.800985
H	7.411615	5.450988	-1.948803
H	8.918850	5.882374	-1.135719
H	8.446500	3.510907	-0.636187
H	8.186206	4.426450	0.865496
H	5.410354	2.267541	0.761360
C	-0.291491	5.612528	-2.854205
C	0.295939	4.833128	-1.701017
O	-0.401258	4.424075	-0.781241
C	1.795730	4.604562	-1.735402
C	2.307513	3.415135	-0.932489
C	1.926553	2.087035	-1.557384
O	1.082421	2.000850	-2.451855
O	2.514733	1.000456	-1.104956
H	-0.457770	4.903068	-3.684558
H	-1.254773	6.059004	-2.573953
H	0.400307	6.388498	-3.216431
H	2.125713	4.544102	-2.784742
H	2.246812	5.533344	-1.336358
H	3.402131	3.473702	-0.827944
H	1.890159	3.428478	0.088594
H	3.210621	1.159042	-0.346908
C	3.541675	-4.293590	-1.328029

C	2.444071	-4.273296	-0.291787
O	1.851038	-3.249858	0.010973
C	2.098451	-5.597165	0.375410
C	1.148504	-5.430520	1.558883
C	-0.207756	-4.882151	1.141593
O	-0.736014	-5.201954	0.081742
O	-0.828506	-4.067950	1.980716
H	4.510207	-4.462029	-0.825651
H	3.398985	-5.126781	-2.035335
H	3.576466	-3.337550	-1.866224
H	1.642744	-6.243217	-0.395419
H	3.032455	-6.096139	0.684681
H	0.963316	-6.413958	2.024242
H	1.589004	-4.785096	2.330009
H	-0.273529	-3.841418	2.792045
C	-3.475467	-2.026252	-6.190497
C	-2.750526	-0.709057	-6.038711
O	-1.537852	-0.621629	-6.126459
C	-3.604046	0.507935	-5.708399
C	-2.790612	1.773756	-5.448553
C	-1.807491	1.611755	-4.312294
O	-2.000539	0.876793	-3.352674
O	-0.735571	2.394185	-4.422166
H	-2.843128	-2.744770	-6.729134
H	-3.670122	-2.414696	-5.174418
H	-4.446438	-1.910360	-6.697200
H	-4.309236	0.674171	-6.542195
H	-4.229115	0.249490	-4.837765
H	-2.245346	2.101199	-6.344163
H	-3.474380	2.584030	-5.139655
H	-0.119937	2.223677	-3.661191

Table S23. B3LYP/cc-pVDZ//B3LYP-GD3BJ/6-311++g(d,p) counterpoise corrected interaction energies (in kcal mol⁻¹) of Lid:Cou:La and Lid:Cou:Le.

Structure	Lid:Cou:La	Lid:Cou:Le
A	-276.2	-314.1
B	-275.5	-254.7
C	-273.9	-252.4
D	-267.2	-
E	-251.6	-