Electronic Supplementary Material (ESI) for RSC Advances.

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Supporting information for

Light-induced synthesis of triazine N-oxide-based cross-linked polymers for effective photocatalytic degradation of methyl orange

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Contents

1. Characterization figure

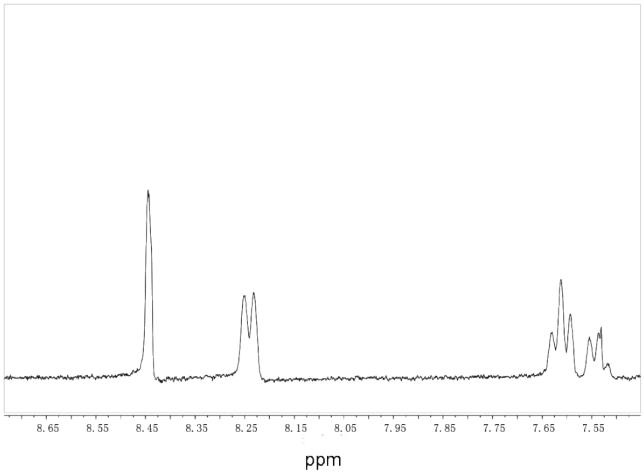

Figure S1. ^{1}H NMR spectrum for BPTB.

2. TGA curves

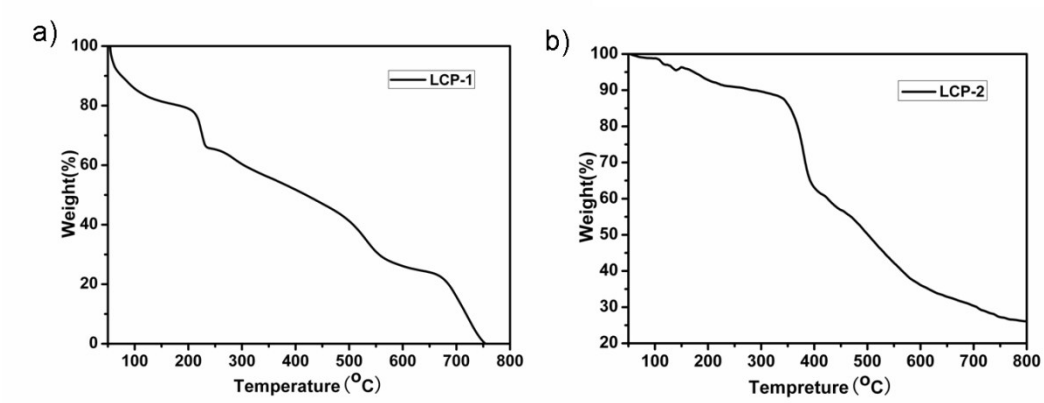

Figure S2. TGA curves of LCP-1(a) and LCP-2 (b).

3. FTIR spectra

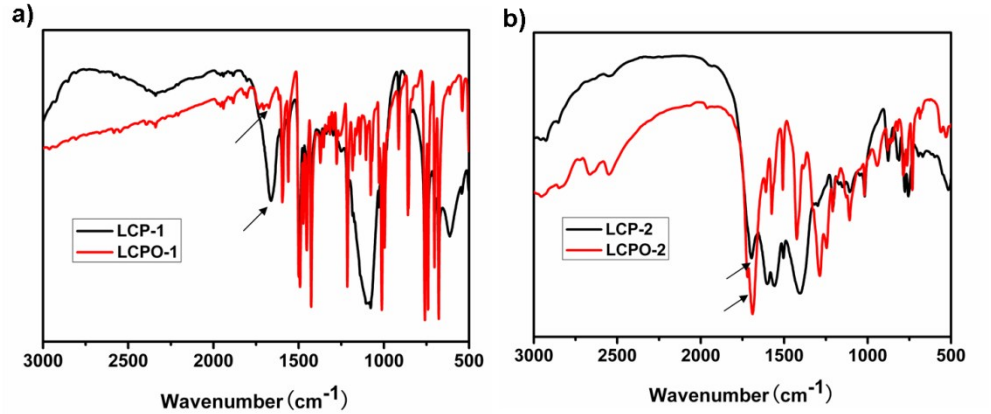

Figure S3. FT-IR spectra of LCP-1(a) and LCP-2 (b).

4. SEM and TEM images

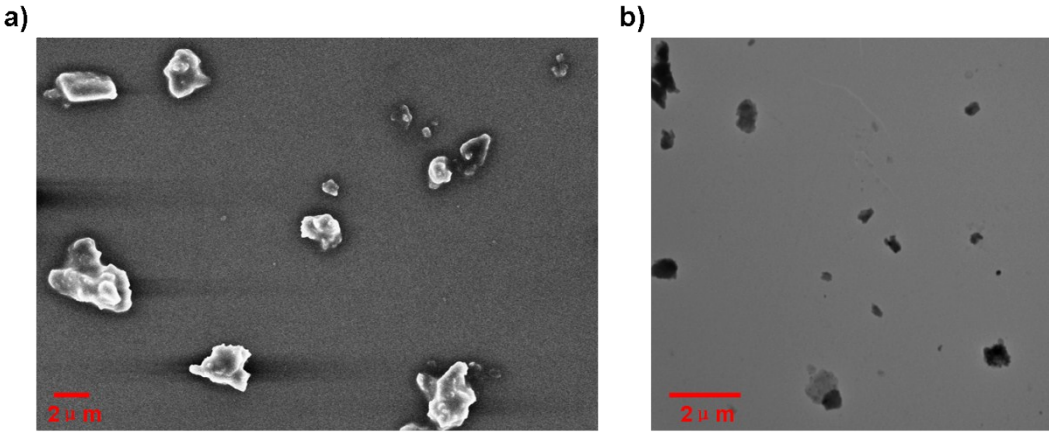

Figure S4. SEM image (a) and TEM image (b) of LCPO-1.

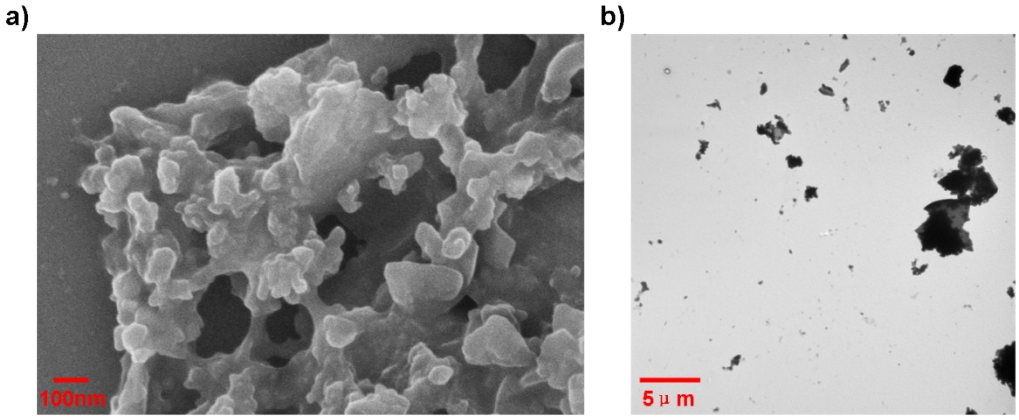

Figure S5.SEM image (a) and TEM image (b) of LCPO-2.

5. Photo images

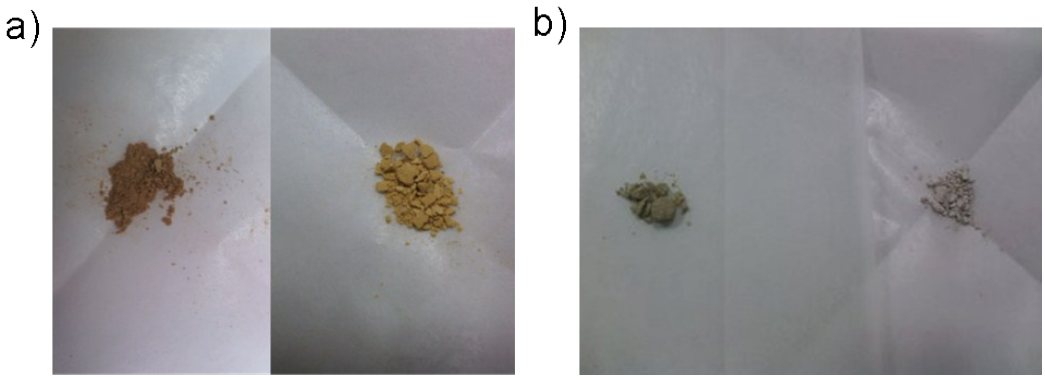

Figure S6. Photo images of LCP and LCPO polymers. (a) LCP-1 (left) and LCPO-1 (right); (b) LCP-2 (left) and LCPO-2 (right).

6. HOMO-LUMO calculation

Computational details: Density functional theory (DFT) calculations have been performed with Gaussian09[S1] suite of program with a tight self-consistent field convergence threshold at B3LYP/6-31G(d) level of theory in gas phase, [S2, S3] which has been reported as good balance between accuracy and computational efficiency. [S4, S5] The crystal structure coordinates are used as the initial configuration to complete the geometry optimization calculation. As the large size and complexity in spatial conformation, symmetry constraints are switched off in all calculations. Visualization of the optimized geometrical structures and frontier molecular orbitals are performed by GaussView version 5.0.9.

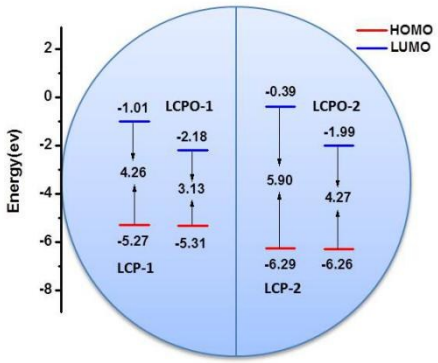

Figure S7. Frontier molecular orbital energy level diagrams for LCP polymers and LCPO polymers.

The final coordinates are extracted from G09 output files with open Babel application, and presented here in xyz format.

Ground state geometry for LCP-1, B3LYP/6-31G(d) level of theory.

```
234
LCP-1.log    Energy: -4007442.0661778
C        -0.27983      -0.23808      -0.88379
N         0.58364       0.71710      -1.23641
C         0.26824       1.92339      -0.75596
C        -1.55979       1.18667       0.27678
N        -1.36970      -0.07966      -0.12745
N        -0.78602       2.23212       0.00638
O        -2.62722       1.46846       1.03252
O         0.02082      -1.45109      -1.35142
O         1.06424       2.95610      -1.03559
C        -3.48629       0.36824       1.43201
C        -4.69855       0.90921       2.10693
H        -2.91766      -0.30176       2.08377
H        -3.78219      -0.19123       0.54272
C        -5.95468       1.11931       1.57732
N        -4.79478       1.20592       3.44885
C        -6.76741       1.53595       2.66195
```

H	-6.23592	0.97797	0.54378
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C	-8.96240	1.82189	1.49249
C	-8.82790	2.31279	3.84668
C	-10.31330	2.15453	1.50067
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C	-10.17506	2.64496	3.85489
H	-8.24413	2.37710	4.75898
C	-10.94650	2.57143	2.68107
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H	-10.65151	2.97054	4.77369
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C	-13.28611	2.97600	1.60859
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H	-13.11335	2.74839	0.56822
N	-14.27149	3.51807	3.50518
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H	-16.64421	3.17664	2.12933
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H	5.25346	-17.17864	5.50349
C	9.03322	-20.29594	1.73631
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H	8.27973	-20.86599	2.27593
H	4.22982	-17.68002	7.67310
H	4.00506	-16.33106	8.91787
C	-3.80414	1.11013	4.46841
C	-4.17166	0.59379	5.71658
C	-2.49526	1.54528	4.23697
C	-3.21895	0.50177	6.72794
H	-5.19702	0.28074	5.87649
C	-1.54711	1.43176	5.25534
H	-2.23077	1.99152	3.28483
C	-1.90249	0.91183	6.49997
H	-3.50567	0.10183	7.69663
H	-0.53140	1.77248	5.07484
H	-1.16195	0.83415	7.29105

Ground state geometry for LCPO-1, B3LYP/6-31G(d) level of theory.

237

LCPO-1.log Energy: -4148869.6005839

C	0.83221	-2.08537	-1.63432
N	0.76807	-0.85148	-1.01720
C	-0.46640	-0.29910	-0.74202
C	-1.54374	-2.20433	-1.67877
N	-0.31847	-2.73593	-1.99800
N	-1.60932	-0.99343	-1.03985
O	-2.62715	-2.90304	-1.93251
O	2.02137	-2.52036	-1.98167
O	-0.48893	0.83099	-0.07421
C	-3.59338	-2.33190	-2.91355
C	-4.80852	-3.17517	-2.93920
H	-3.08427	-2.30385	-3.87982
H	-3.83476	-1.32764	-2.56821
C	-5.97393	-3.02026	-2.21542
N	-5.01322	-4.25250	-3.77492
C	-6.84904	-4.03486	-2.67484
H	-6.15306	-2.26327	-1.46572
N	-6.25162	-4.76741	-3.62460
C	-8.22401	-4.33366	-2.24925
C	-8.85702	-3.57773	-1.25146
C	-8.94401	-5.38926	-2.83707
C	-10.16029	-3.86208	-0.85626
H	-8.33008	-2.75576	-0.77514
C	-10.24368	-5.67295	-2.44274
H	-8.46529	-5.98506	-3.60719
C	-10.87955	-4.91346	-1.44420
H	-10.62173	-3.25443	-0.08336
H	-10.78747	-6.49176	-2.90205
C	-12.25820	-5.21613	-1.03316
C	-13.03229	-4.60611	-0.01008
N	-12.95467	-6.18039	-1.64146
C	-14.24720	-5.25240	-0.03272
H	-12.76852	-3.78846	0.64247
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H	-15.54679	-5.66725	1.65571
H	-16.39098	-5.12773	0.20675
C	-16.01590	-7.75678	-0.60105
C	-15.24950	-7.35696	-2.86797
C	-16.32452	-3.20929	2.09345

C	-16.99065	-8.62761	-1.09040
H	-15.90905	-7.61100	0.46850
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H	-14.56169	-6.85704	-3.53977
N	-17.31533	-4.03926	2.42831
N	-16.15489	-1.95009	2.50239
C	-17.09458	-8.87303	-2.45922
H	-17.65724	-9.12609	-0.39235
H	-16.28452	-8.43103	-4.40984
C	-18.20311	-3.49224	3.26494
C	-17.11266	-1.53478	3.32782
H	-17.85043	-9.55627	-2.83578
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O	-16.97469	-0.27828	3.75034
C	-20.20187	-3.79422	4.52824
C	-17.96151	0.24680	4.66887
C	-21.15216	-4.91350	4.82033
H	-20.70922	-2.93552	4.07763
H	-19.69530	-3.44643	5.43647
C	-17.53505	1.63437	5.03545
H	-18.00121	-0.40848	5.54753
H	-18.94929	0.23521	4.19760
C	-22.47414	-4.81272	4.69110
H	-20.70011	-5.83540	5.18335
C	-18.33237	2.69828	4.95384
H	-16.51762	1.73191	5.41117
H	-23.13745	-5.63208	4.95303
H	-22.94607	-3.90396	4.32327
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C	-0.14484	6.59335	1.19019
C	-1.39350	2.34874	3.81130
C	-2.76899	1.31348	2.10318

C	0.49108	7.29128	0.15279
C	-0.37346	7.27085	2.40135
C	-1.85589	1.41964	4.73987
H	-0.68840	3.12138	4.09257
C	-3.21103	0.37839	3.03938
H	-3.14645	1.26384	1.09075
C	0.88536	8.61524	0.31694
H	0.68791	6.79713	-0.79447
C	0.02068	8.59105	2.56539
H	-0.86620	6.74346	3.21153
C	-2.76163	0.42701	4.35874
H	-1.49786	1.46853	5.76457
H	-3.91832	-0.38453	2.72707
C	0.65856	9.29092	1.52532
H	1.37350	9.12682	-0.50740
H	-0.15942	9.10201	3.50543
H	-3.11428	-0.30056	5.08438
C	1.07422	10.68963	1.70438
C	1.79322	11.52219	0.80537
N	0.79118	11.34620	2.83287
C	1.92898	12.73017	1.45072
H	2.14681	11.29798	-0.18907
N	1.31869	12.58768	2.67652
C	2.55806	14.00084	0.96728
C	1.13557	13.54571	3.71061
O	2.54919	13.93761	-0.46913
H	3.59343	14.11598	1.30801
H	2.00849	14.88467	1.30677
C	2.15119	14.44842	4.04251
C	-0.07729	13.56262	4.41046
C	3.12379	14.94530	-1.13375
C	1.93821	15.38812	5.05223
H	3.11215	14.40138	3.54160
C	-0.27113	14.49337	5.42758
H	-0.84418	12.84303	4.14893
N	3.65210	15.95560	-0.43882
N	3.09504	14.80838	-2.46122
C	0.72955	15.41519	5.74734
H	2.73034	16.08787	5.30320
H	-1.21378	14.50349	5.96776
C	4.19289	16.90309	-1.21144
C	3.66566	15.82427	-3.10415
H	0.56970	16.14375	6.53702
N	4.23339	16.90617	-2.54596

O	4.72774	17.92187	-0.53801
O	3.64916	15.71934	-4.43286
C	5.34715	18.98736	-1.29768
C	4.26800	16.77109	-5.20991
C	5.94766	19.94505	-0.31615
H	4.59785	19.47054	-1.93250
H	6.10940	18.54816	-1.95216
C	4.17911	16.37234	-6.65033
H	5.31006	16.87619	-4.88431
H	3.75961	17.72123	-5.01820
C	5.70898	21.25557	-0.32202
H	6.63419	19.51056	0.40905
C	3.69094	17.16072	-7.60658
H	4.57158	15.38576	-6.89215
H	6.19556	21.92758	0.37911
H	5.02096	21.70928	-1.03243
H	3.28605	18.14625	-7.38572
H	3.68087	16.85452	-8.64873
C	2.44899	-3.86054	-1.54401
C	3.83930	-4.10483	-2.01068
H	1.71734	-4.57741	-1.91605
H	2.44372	-3.87311	-0.45089
C	4.91362	-4.44855	-1.21791
N	4.30281	-4.09208	-3.31043
C	6.00600	-4.63041	-2.10311
H	4.89642	-4.55363	-0.14267
N	5.62192	-4.39748	-3.36057
C	3.66700	-3.69910	-4.52856
C	7.38990	-5.01930	-1.79659
C	4.44511	-3.07293	-5.51050
C	2.31079	-3.94433	-4.75934
C	7.83015	-5.15810	-0.47197
C	8.31251	-5.26258	-2.82986
C	3.86039	-2.69193	-6.71552
H	5.49621	-2.89844	-5.31688
C	1.73404	-3.54166	-5.96447
H	1.69227	-4.43400	-4.01974
C	9.14145	-5.52658	-0.18843
H	7.14565	-4.97207	0.35090
C	9.62041	-5.62906	-2.54704
H	7.98468	-5.16024	-3.85906
C	2.50211	-2.91889	-6.94799
H	4.47079	-2.20638	-7.47199
H	0.67609	-3.72740	-6.12840

C	10.06184	-5.76960	-1.21889
H	9.44887	-5.62726	0.84841
H	10.32273	-5.81251	-3.35341
H	2.04797	-2.61328	-7.88645
C	11.44825	-6.16105	-0.92552
C	12.08770	-6.28097	0.33729
N	12.29692	-6.45558	-1.91430
C	13.37821	-6.67228	0.06131
H	11.67326	-6.13229	1.32229
N	13.47318	-6.76136	-1.30905
C	14.49612	-6.99720	1.00360
C	14.57362	-7.16499	-2.11388
O	13.88435	-7.35989	2.25421
H	15.16586	-6.14665	1.17445
H	15.11400	-7.82313	0.63730
C	15.87775	-6.76807	-1.80035
C	14.33078	-7.95562	-3.24385
C	14.70174	-7.63127	3.27711
C	16.94027	-7.19132	-2.60031
H	16.06371	-6.10874	-0.95932
C	15.39721	-8.35667	-4.04401
H	13.31091	-8.23708	-3.47835
N	16.01523	-7.57011	3.09197
N	14.06215	-7.94550	4.41338
C	16.70571	-7.98551	-3.72231
H	17.95087	-6.88169	-2.34966
H	15.20488	-8.97044	-4.91966
C	16.72187	-7.86896	4.19642
C	14.88595	-8.21978	5.42164
H	17.53443	-8.30795	-4.34614
N	16.22883	-8.20296	5.38436
O	18.04189	-7.81168	4.02576
O	14.38032	-8.54798	6.60929
C	18.88017	-8.10570	5.17124
C	12.93706	-8.60626	6.73287
C	20.30060	-7.89084	4.75083
H	18.70104	-9.13293	5.50283
H	18.59232	-7.43638	5.99036
C	12.62680	-9.06654	8.12297
H	12.55438	-9.30334	5.97823
H	12.51054	-7.62088	6.52236
C	21.26460	-8.79561	4.91419
H	20.52426	-6.91648	4.31854
C	11.79813	-8.42494	8.94530

H	13.10168	-9.99703	8.43090
H	22.29454	-8.58888	4.63745
H	21.06259	-9.77712	5.33799
H	11.31851	-7.49084	8.66017
H	11.56110	-8.81086	9.93269
C	-4.15338	-4.80577	-4.76936
C	-4.71325	-5.20861	-5.98804
C	-2.78564	-4.96432	-4.52623
C	-3.89505	-5.76332	-6.96852
H	-5.77918	-5.08925	-6.14433
C	-1.97664	-5.50947	-5.52586
H	-2.34828	-4.69438	-3.57160
C	-2.52313	-5.91025	-6.74503
H	-4.33126	-6.07715	-7.91283
H	-0.91586	-5.63793	-5.33045
H	-1.88808	-6.34244	-7.51331
O	-2.76652	-0.50262	-0.73099
O	1.83168	-0.22971	-0.71352
O	-0.25008	-3.85949	-2.62891

Ground state geometry for LCP-2, B3LYP/6-31G(d) level of theory.

180

LCP-2.log Energy: -3012916.6086839

C	-0.49391	-4.20996	3.31883
N	-0.35545	-3.58352	2.14041
C	-1.38716	-3.77078	1.31465
C	-2.47921	-5.05530	2.77647
N	-1.52273	-4.95901	3.70496
N	-2.48186	-4.49378	1.56487
O	-1.36826	-3.19982	0.10909
O	0.47967	-4.09379	4.22456
O	-3.52412	-5.80060	3.14213
C	-4.60715	-5.95644	2.20701
C	-5.65008	-6.80677	2.90827
H	-4.25269	-6.44986	1.29591
H	-5.01096	-4.97805	1.93013
C	-6.56141	-6.14776	3.95836
H	-5.19317	-7.74665	3.24674
O	-6.77421	-7.05711	2.02881
C	-7.72197	-6.64785	3.05397
H	-6.47564	-5.05855	3.99495
H	-6.52129	-6.55375	4.97124
C	-8.75499	-5.66122	2.57711

H	-8.22086	-7.53131	3.47784
C	-9.93892	-5.48350	3.30476
C	-8.54351	-4.88010	1.43624
C	-10.87837	-4.53393	2.91043
H	-10.12340	-6.08690	4.19155
C	-9.49338	-3.94329	1.03020
H	-7.63681	-5.02715	0.85832
C	-10.67084	-3.75902	1.76200
H	-11.78592	-4.39985	3.49597
H	-9.32103	-3.33214	0.15001
C	-11.72654	-2.78339	1.31100
C	-12.75368	-3.25600	0.24304
H	-12.20338	-2.32274	2.18741
O	-11.22807	-1.75462	0.41014
C	-12.22924	-2.07251	-0.58888
H	-13.80678	-3.20613	0.53165
H	-12.53643	-4.23973	-0.17742
C	-13.16312	-0.88946	-0.78028
H	-11.76989	-2.33946	-1.54872
O	-14.12708	-1.29678	-1.76858
H	-12.61093	-0.01063	-1.12786
H	-13.66970	-0.62361	0.15322
C	-15.06698	-0.42157	-2.13264
N	-15.07146	0.78894	-1.56899
N	-15.91882	-0.88402	-3.05236
C	-16.05539	1.57613	-2.01295
C	-16.84587	0.00429	-3.40060
N	-16.97793	1.25259	-2.92322
O	-16.07841	2.79084	-1.46279
O	-17.71345	-0.42934	-4.31658
C	-17.10020	3.71620	-1.90251
C	-18.74197	0.48144	-4.76784
C	-16.84674	5.02167	-1.21463
H	-18.08987	3.31459	-1.66300
H	-17.03294	3.81478	-2.99262
C	-19.51735	-0.21813	-5.84089
H	-18.25978	1.39067	-5.14700
H	-19.37991	0.76758	-3.92559
C	-17.77470	5.68942	-0.53098
H	-15.84267	5.42797	-1.32753
C	-20.84500	-0.32616	-5.84308
H	-18.92732	-0.62390	-6.66135
H	-17.56684	6.65577	-0.08054
H	-18.78133	5.29804	-0.39888

H	-21.45298	0.06394	-5.02935
H	-21.37738	-0.80458	-6.66019
C	-0.23102	-2.39233	-0.24681
C	-0.49393	-1.89206	-1.65530
H	0.68487	-2.99147	-0.21276
H	-0.12479	-1.56055	0.45639
C	-1.48233	-0.73028	-1.85679
H	-0.67296	-2.74662	-2.32190
O	0.61545	-1.08623	-2.12158
C	-0.28066	-0.01799	-2.53784
H	-1.80061	-0.25437	-0.92556
H	-2.35338	-0.92766	-2.48500
C	0.12617	1.34981	-2.05646
H	-0.37389	-0.01364	-3.63338
C	-0.43206	2.49034	-2.64939
C	1.02556	1.51397	-0.99874
C	-0.11182	3.76175	-2.18114
H	-1.12893	2.38235	-3.47844
C	1.36303	2.78901	-0.54367
H	1.47406	0.63464	-0.54792
C	0.79787	3.92628	-1.12792
H	-0.56616	4.63548	-2.64454
H	2.05644	2.91245	0.28197
C	1.18020	5.31222	-0.67592
C	2.41745	5.98249	-1.33748
H	0.29196	5.95954	-0.67756
O	1.82613	5.34755	0.62684
C	2.96978	6.06406	0.09649
H	2.23927	6.94013	-1.83335
H	2.97710	5.32408	-2.00453
C	3.05557	7.44274	0.72920
H	3.90431	5.51695	0.27144
O	4.17996	8.09600	0.11219
H	3.20524	7.36710	1.81065
H	2.14197	8.02009	0.55317
C	4.49608	9.32776	0.51819
N	3.76779	9.89344	1.48394
N	5.54343	9.86147	-0.11715
C	4.18031	11.12222	1.80730
C	5.84105	11.08789	0.30334
N	5.20459	11.78254	1.26031
O	3.46763	11.70595	2.77181
O	6.88067	11.64992	-0.31576
C	3.85984	13.03206	3.19741

C	7.28534	12.97545	0.09632
C	2.97480	13.41294	4.34334
H	3.76691	13.73112	2.36025
H	4.91513	13.00320	3.49431
C	8.50898	13.33241	-0.68950
H	7.48996	12.95785	1.17373
H	6.46892	13.68363	-0.07741
C	2.28676	14.55212	4.40019
H	2.94124	12.70428	5.16960
C	8.64191	14.46584	-1.37653
H	9.32351	12.61080	-0.64817
H	1.68777	14.81421	5.26765
H	2.29910	15.27075	3.58323
H	7.83756	15.19606	-1.43795
H	9.56112	14.71122	-1.90075
C	1.63515	-3.30408	3.89192
C	2.55111	-3.36762	5.10031
H	1.34154	-2.26964	3.68440
H	2.12529	-3.70755	3.00052
C	3.39627	-4.63333	5.32555
H	2.00487	-3.03504	5.99336
O	3.73589	-2.56376	4.87986
C	4.60543	-3.65804	5.28377
H	3.37273	-5.33600	4.48840
H	3.23576	-5.17224	6.26157
C	5.73348	-3.93382	4.32465
H	5.01051	-3.46335	6.28726
C	6.82579	-4.70801	4.73825
C	5.70197	-3.46555	3.00744
C	7.85057	-5.02105	3.84904
H	6.87056	-5.07623	5.76147
C	6.73877	-3.76210	2.12256
H	4.86710	-2.85068	2.68727
C	7.82380	-4.54311	2.53214
H	8.68379	-5.63590	4.18406
H	6.70591	-3.40431	1.09842
C	8.97189	-4.83762	1.60162
C	10.11712	-3.79085	1.49645
H	9.34032	-5.85740	1.78073
O	8.64667	-4.65939	0.19490
C	9.75830	-3.74894	0.00053
H	11.12130	-4.15100	1.73461
H	9.92374	-2.86301	2.03810
C	10.75656	-4.35324	-0.97226

H	9.42001	-2.77480	-0.37365
O	11.83123	-3.40256	-1.08666
H	10.29314	-4.52251	-1.94920
H	11.13956	-5.31230	-0.60843
C	12.83628	-3.68410	-1.91897
N	12.80144	-4.82963	-2.60433
N	13.78805	-2.74735	-1.96541
C	13.85594	-4.99899	-3.40671
C	14.77671	-3.04720	-2.80343
N	14.87951	-4.15401	-3.55700
O	13.84146	-6.13715	-4.10195
O	15.74475	-2.13151	-2.87026
C	14.93619	-6.38891	-5.01395
C	16.84524	-2.36696	-3.77795
C	14.63439	-7.66772	-5.73163
H	15.87615	-6.44641	-4.45603
H	15.00998	-5.54363	-5.70870
C	17.73465	-1.16360	-3.72226
H	16.43893	-2.52093	-4.78503
H	17.37656	-3.27928	-3.48878
C	15.48688	-8.68788	-5.81504
H	13.66400	-7.71551	-6.22362
C	19.04935	-1.22494	-3.51686
H	17.24444	-0.20605	-3.89167
H	15.25040	-9.58441	-6.38096
H	16.45797	-8.66478	-5.32470
H	19.55743	-2.17017	-3.33698
H	19.67064	-0.33393	-3.52521

Ground state geometry for LCPO-2, B3LYP/6-31G(d) level of theory.

183

LCPO-2.log Energy: -3154344.1211523

C	1.62821	2.24357	1.26442
N	1.66918	3.59080	1.51441
C	1.59987	4.48620	0.47782
C	1.45687	2.68521	-1.06583
N	1.60178	1.79224	-0.03303
N	1.41314	4.03787	-0.81100
O	1.68427	5.77552	0.69868
O	1.63001	1.37503	2.24649
O	1.44091	2.27996	-2.31500
C	0.32154	1.44370	-2.75422
C	0.80980	0.69294	-3.97761

H	-0.51424	2.10517	-3.00319
H	0.04986	0.75234	-1.95585
C	1.72190	-0.52527	-3.75452
H	1.17592	1.40614	-4.72828
O	-0.25121	-0.13599	-4.50790
C	0.60592	-1.31425	-4.49531
H	1.84349	-0.79303	-2.70311
H	2.69663	-0.49810	-4.24618
C	-0.00794	-2.51581	-3.82561
H	0.89609	-1.57215	-5.52370
C	0.55661	-3.78303	-4.02237
C	-1.11297	-2.39702	-2.97717
C	0.03927	-4.89922	-3.37012
H	1.41391	-3.89613	-4.68328
C	-1.64343	-3.51840	-2.33961
H	-1.56465	-1.42091	-2.83379
C	-1.07385	-4.78155	-2.52750
H	0.50023	-5.87315	-3.52350
H	-2.49434	-3.41903	-1.67313
C	-1.66169	-6.00822	-1.88029
C	-2.87108	-6.69709	-2.57442
H	-0.85763	-6.71291	-1.62602
O	-2.47027	-5.72108	-0.70481
C	-3.60520	-6.44286	-1.24587
H	-2.73489	-7.74587	-2.85083
H	-3.26768	-6.14331	-3.42749
C	-3.91075	-7.65227	-0.37850
H	-4.49387	-5.80333	-1.31402
O	-5.04205	-8.30341	-0.98499
H	-4.15301	-7.34523	0.64389
H	-3.05925	-8.33884	-0.33324
C	-5.52037	-9.40771	-0.40739
N	-4.92565	-9.86527	0.69719
N	-6.57685	-9.93751	-1.03086
C	-5.49260	-10.97288	1.18366
C	-7.03853	-11.03490	-0.43737
N	-6.54770	-11.61211	0.67137
O	-4.91206	-11.44995	2.28550
O	-8.09413	-11.58818	-1.03705
C	-5.47651	-12.63748	2.88975
C	-8.67244	-12.77329	-0.44383
C	-4.69588	-12.91852	4.13599
H	-5.42866	-13.47089	2.18185
H	-6.53355	-12.44515	3.10989

C	-9.88220	-13.13066	-1.25065
H	-8.93447	-12.54925	0.59732
H	-7.93491	-13.58217	-0.43653
C	-4.14757	-14.10037	4.41352
H	-4.61881	-12.09272	4.84172
C	-10.10272	-14.34367	-1.75491
H	-10.61114	-12.33315	-1.38687
H	-3.62345	-14.28133	5.34760
H	-4.20603	-14.93608	3.71912
H	-9.38366	-15.15193	-1.63814
H	-11.01232	-14.57854	-2.30029
C	0.57078	6.43297	1.38846
C	0.48618	7.83652	0.81506
H	0.77925	6.43152	2.45963
H	-0.35357	5.88146	1.19229
C	-0.07548	7.97677	-0.60933
H	1.42626	8.37107	1.00137
O	-0.64538	8.53360	1.38966
C	-1.24908	8.72752	0.07849
H	-0.32904	7.03373	-1.09772
H	0.52907	8.58103	-1.28846
C	-2.63634	8.14562	-0.04731
H	-1.27177	9.79922	-0.16278
C	-3.33072	8.27055	-1.25903
C	-3.24704	7.46775	1.01086
C	-4.59802	7.71556	-1.40915
H	-2.87089	8.79343	-2.09550
C	-4.52562	6.92558	0.86461
H	-2.71595	7.37646	1.95265
C	-5.21475	7.04244	-0.34505
H	-5.11488	7.80677	-2.36263
H	-4.99192	6.38969	1.68518
C	-6.60835	6.49371	-0.50969
C	-7.80687	7.39080	-0.08935
H	-6.72346	6.07544	-1.51951
O	-6.96948	5.50040	0.49027
C	-8.16539	6.23295	0.85874
H	-8.54005	7.61278	-0.86909
H	-7.51551	8.31576	0.41192
C	-9.39828	5.41288	0.51878
H	-8.17058	6.48425	1.92653
O	-10.53127	6.22111	0.88603
H	-9.40519	4.47171	1.07731
H	-9.43710	5.17311	-0.54884

C	-11.75280	5.71157	0.71087
N	-11.86953	4.47868	0.21171
N	-12.74463	6.53086	1.07203
C	-13.13720	4.07622	0.08565
C	-13.95194	6.00229	0.89067
N	-14.22638	4.78174	0.40246
O	-13.27721	2.84674	-0.41150
O	-14.96438	6.79864	1.23798
C	-14.61820	2.32376	-0.56099
C	-16.31133	6.29361	1.09122
C	-14.49561	0.91369	-1.04900
H	-15.18296	2.94951	-1.25921
H	-15.11947	2.37201	0.41321
C	-17.24105	7.34734	1.60843
H	-16.39844	5.36278	1.66490
H	-16.50707	6.05825	0.04031
C	-15.13656	0.44291	-2.11762
H	-13.85912	0.26119	-0.45310
C	-18.28441	7.81311	0.92375
H	-17.03387	7.70694	2.61523
H	-15.05697	-0.59786	-2.41827
H	-15.77071	1.07910	-2.73171
H	-18.50407	7.47384	-0.08649
H	-18.96297	8.54819	1.34707
C	2.85770	1.22111	3.03226
C	2.91305	-0.23889	3.44603
H	2.80615	1.89685	3.88761
H	3.72086	1.47798	2.41100
C	3.26612	-1.26044	2.35246
H	2.03163	-0.48758	4.05049
O	4.14218	-0.50065	4.16533
C	4.55379	-1.49885	3.18838
H	3.41244	-0.83460	1.35777
H	2.59165	-2.11585	2.28105
C	5.88664	-1.20646	2.54263
H	4.57904	-2.49019	3.66166
C	6.39352	-2.08354	1.57310
C	6.63005	-0.07145	2.87648
C	7.60663	-1.81946	0.94440
H	5.82845	-2.97205	1.29770
C	7.85493	0.18427	2.25657
H	6.24486	0.60618	3.63134
C	8.35685	-0.68491	1.28470
H	7.97559	-2.50217	0.18125

H	8.42183	1.07455	2.50962
C	9.69188	-0.44322	0.62954
C	10.96827	-0.97922	1.33793
H	9.64100	-0.73165	-0.42972
O	10.16789	0.92586	0.75531
C	11.42994	0.48882	1.31889
H	11.58055	-1.67928	0.76353
H	10.78500	-1.38582	2.33439
C	12.56539	0.84774	0.37551
H	11.60846	0.93888	2.30329
O	13.77380	0.36901	0.99580
H	12.61963	1.93087	0.22749
H	12.43539	0.37897	-0.60513
C	14.92610	0.56147	0.34897
N	14.91490	1.18017	-0.82590
N	16.00108	0.08395	0.99620
C	16.13637	1.30802	-1.37165
C	17.14087	0.28080	0.33930
N	17.28455	0.88499	-0.85160
O	16.13961	1.92473	-2.55289
O	18.28587	-0.14489	0.87299
C	17.41875	2.12294	-3.20378
C	18.21941	-0.82384	2.15101
C	17.16440	2.89981	-4.45785
H	17.88179	1.15293	-3.40884
H	18.07620	2.66641	-2.51502
C	19.60552	-1.27859	2.48671
H	17.52590	-1.66790	2.05823
H	17.81616	-0.14441	2.90811
C	17.60185	2.52714	-5.65964
H	16.61219	3.83037	-4.33415
C	20.20728	-1.02211	3.64719
H	20.10540	-1.87471	1.72446
H	17.43629	3.13827	-6.54237
H	18.14929	1.59839	-5.80682
H	19.72950	-0.42324	4.41980
H	21.19805	-1.40579	3.87360
O	1.23081	4.86573	-1.76345
O	1.76758	4.01463	2.72166
O	1.67351	0.53341	-0.28071

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