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Supporting Information for Carbon dots analysis of charge transfer intrinsic capacity based on the analytic calculation of chemical reactivity descriptors

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Table 1: Cartesian coordinates of the structure DOH0

Atom	X	Y	Z
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.221324
O	1.147829	0.000000	-0.743778
H	1.887782	-0.036655	-0.099578
C	-1.250283	0.014187	-0.894328
N	-2.456890	0.501151	-0.221795
H	-2.720535	-0.160702	0.514953
H	-2.249005	1.381648	0.260303
C	-1.485101	-1.380135	-1.464311
C	-1.701589	-1.549757	-2.834773
C	-1.519387	-2.489163	-0.608067
C	-1.777054	-3.774147	-1.114722
C	-1.957993	-2.820559	-3.384223
C	-1.997772	-3.955812	-2.514040
C	-2.252754	-5.249117	-3.052939
C	-2.474454	-5.430965	-4.452002
C	-2.721691	-6.717918	-4.959476
C	-2.755518	-7.825632	-4.105471
C	-2.546657	-7.655633	-2.731110
C	-2.290589	-6.384567	-2.182806
C	-2.182688	-3.016358	-4.785028
C	-2.431173	-4.263952	-5.299929
O	-2.654208	-4.496313	-6.636964
H	-2.601506	-3.645858	-7.110684
C	-2.071725	-6.188403	-0.780837
C	-1.824256	-4.940709	-0.265921
O	-1.607341	-4.706036	1.071342
H	-1.659949	-5.555390	1.547147
H	-2.880502	-6.846537	-6.030132
C	-2.981347	-9.221058	-4.679087
N	-1.719868	-9.965759	-4.725833
H	-1.348165	-10.058210	-3.775227
H	-1.896728	-10.922292	-5.049245
H	-1.336655	-2.369503	0.461099
C	-4.088295	-9.923653	-3.878769
O	-3.909711	-10.713987	-2.963546
O	-5.332353	-9.560736	-4.314075
H	-5.970695	-10.025974	-3.730789
H	-1.678021	-0.679822	-3.495638
H	-2.591566	-8.519914	-2.062762
H	-2.153631	-2.145596	-5.446573
H	-2.104794	-7.058918	-0.119088
H	-3.353045	-9.106318	-5.708999
H	-1.025669	0.689775	-1.735371

Table 2: Cartesian coordinates of the structure DOHN1

Atom	X	Y	Z
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.221956
O	1.148498	0.000000	-0.741861
H	1.887457	-0.035034	-0.096451
C	-1.251520	0.006432	-0.893977
N	-2.443179	0.548674	-0.235001
H	-2.710108	-0.067507	0.538927
H	-2.214106	1.449289	0.197751
C	-1.507892	-1.408784	-1.395754
C	-1.635026	-1.652590	-2.754105
C	-1.656784	-2.459673	-0.456187
C	-1.934693	-3.769073	-0.863078
C	-1.900084	-2.968901	-3.212360
C	-2.028844	-4.038251	-2.272607
C	-2.324199	-5.346279	-2.703063
N	-2.562760	-5.628169	-4.021368
N	-2.498786	-6.405341	-1.788099
C	-2.436022	-6.120499	-0.448934
C	-2.177250	-4.861316	0.037016
O	-2.621711	-7.226597	0.330891
C	-2.394549	-4.603042	-4.947917
C	-2.086873	-3.313208	-4.579773
O	-1.949144	-2.303669	-5.502127
H	-2.114474	-2.659564	-6.394296
H	-2.481311	-6.959305	1.257698
C	-2.239889	-7.755329	-2.279006
C	-2.523642	-7.987150	-3.585322
C	-2.932174	-6.918515	-4.435435
H	-1.785979	-8.444856	-1.575901
H	-2.539008	-4.904006	-5.983902
C	-2.307567	-9.355614	-4.216680
N	-1.005029	-9.414887	-4.888495
H	-0.267947	-9.378628	-4.176896
H	-0.901183	-10.318292	-5.361120
C	-2.518932	-10.456970	-3.170197
O	-1.639980	-10.955688	-2.482680
O	-3.826831	-10.848254	-3.101117
H	-3.869919	-11.522067	-2.388070
H	-1.552536	-0.843295	-3.478599
H	-2.192229	-4.688011	1.113354
H	-1.563319	-2.248363	0.611711
H	-2.996862	-7.043920	-5.512303
H	-3.092371	-9.484749	-4.979889
H	-1.018576	0.637196	-1.765964

Table 3: Cartesian coordinates of the structure DOHN2

Atom	X	Y	Z
C	-0.635629	4.817325	-1.227847
O	-0.635629	4.817325	-0.006683
O	0.506111	4.817325	-1.973675
H	1.245686	4.782011	-1.329253
C	-1.885925	4.791643	-2.105127
N	-2.998951	5.365913	-1.338427
H	-3.879818	4.955315	-1.657018
H	-2.881977	5.117525	-0.350202
C	-2.117195	3.369927	-2.598979
C	-2.144003	3.126573	-3.934520
N	-2.393014	1.829892	-4.444330
C	-2.416125	1.598295	-5.806715
C	-2.650490	0.360410	-6.334966
O	-2.676311	0.109564	-7.690631
C	-2.621059	0.750331	-3.557097
C	-2.862902	-0.517796	-4.090360
N	-3.083784	-1.599042	-3.204311
C	-3.047762	-1.371407	-1.841263
C	-2.810474	-0.134161	-1.312823
O	-2.768764	0.113206	0.042496
C	-3.359902	-2.889998	-3.709243
C	-3.380991	-3.135555	-5.045781
H	-2.491096	0.936401	-8.171872
H	-2.921282	-0.719958	0.524461
C	-2.583903	1.023203	-2.151184
C	-2.343567	2.297598	-1.662056
C	-2.892752	-0.793392	-5.495575
C	-3.133592	-2.068717	-5.979830
C	-3.635928	-4.538953	-5.576641
N	-2.362728	-5.230848	-5.811450
H	-1.909011	-5.407246	-4.909428
H	-2.535568	-6.147679	-6.235827
H	-3.126718	-2.261808	-7.049806
C	-4.590092	-5.291833	-4.645241
O	-4.256895	-5.931683	-3.655366
O	-5.891999	-5.192548	-5.055532
H	-6.422226	-5.684317	-4.391080
H	-3.540350	-3.647903	-2.949810
H	-1.972920	3.890192	-4.691186
H	-2.314949	2.477737	-0.589739
H	-2.232611	2.472412	-6.431644
H	-3.222500	-2.248382	-1.217764
H	-4.146051	-4.432872	-6.546426
H	-1.674748	5.425995	-2.982621

Table 4: Cartesian coordinates of the structure DOHN3

Atom	X	Y	Z
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.221830
O	1.141576	0.000000	-0.745014
H	1.881546	-0.034652	-0.100948
C	-1.249389	-0.034799	-0.875454
N	-2.347240	0.600760	-0.135366
H	-3.240474	0.236994	-0.476333
H	-2.269928	0.349391	0.855658
C	-1.511882	-1.476770	-1.299037
C	-1.580842	-1.763368	-2.625175
C	-1.722166	-2.499611	-0.313951
C	-1.991860	-3.797813	-0.722987
C	-2.201607	-4.901331	0.174392
C	-2.467977	-6.164267	-0.278948
N	-2.553240	-6.467309	-1.619049
O	-2.677486	-7.243787	0.531670
C	-2.078044	-4.129941	-2.120190
C	-2.351033	-5.420278	-2.563730
C	-2.434071	-5.753491	-3.960242
C	-2.704627	-7.052132	-4.364496
C	-2.913302	-8.075385	-3.382108
C	-2.841626	-7.788746	-2.055514
C	-2.213018	-4.653001	-4.859491
C	-1.945148	-3.390391	-4.405817
N	-1.868495	-3.084670	-3.066862
O	-1.726292	-2.312545	-5.218203
H	-1.792928	-2.620865	-6.140270
H	-2.589331	-6.942530	1.454312
C	-3.184465	-9.497113	-3.855191
N	-1.923767	-10.157506	-4.214409
H	-1.366649	-10.287535	-3.363679
H	-2.114441	-11.095429	-4.580895
H	-1.423369	-1.038855	-3.415998
H	-2.977632	-8.512589	-1.260265
C	-4.012981	-10.264204	-2.820053
O	-3.558162	-10.926742	-1.897897
O	-5.357001	-10.149908	-3.055108
H	-5.798777	-10.649932	-2.334626
H	-2.738529	-7.303752	-5.424085
H	-1.654513	-2.262063	0.747637
H	-2.257888	-4.829510	-5.934985
H	-2.147973	-4.726701	1.249871
H	-3.798907	-9.424606	-4.766778
H	-1.030952	0.550499	-1.783444

Table 5: Cartesian coordinates of the structure LOH0

Atom	X	Y	Z
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.221320
O	1.148072	0.000000	-0.743612
H	1.887795	0.036589	-0.099111
C	-1.250510	-0.014775	-0.894506
N	-2.457501	-0.498417	-0.220454
H	-2.717771	0.163347	0.517627
H	-2.251360	-1.380002	0.260453
C	-1.484443	1.378107	-1.468581
C	-1.708051	1.543769	-2.838240
C	-1.513866	2.489949	-0.615571
C	-1.774630	3.773393	-1.124633
C	-1.967946	2.812766	-3.390028
C	-2.003963	3.950578	-2.523174
C	-2.265008	5.241722	-3.064268
C	-2.495601	5.419018	-4.462515
C	-2.750887	6.703607	-4.971993
C	-2.785734	7.813247	-4.120498
C	-2.567205	7.647715	-2.747082
C	-2.301233	6.379356	-2.197161
C	-2.200817	3.004093	-4.789998
C	-2.454796	4.249650	-5.307109
O	-2.686876	4.477402	-6.643443
H	-2.635598	3.625250	-7.114381
C	-2.071277	6.188137	-0.796343
C	-1.817254	4.942653	-0.279348
O	-1.589579	4.713055	1.057082
H	-1.639716	5.564338	1.529784
H	-2.917503	6.828772	-6.041957
C	-3.024280	9.205886	-4.695999
N	-1.767600	9.957793	-4.754187
H	-1.390782	10.057225	-3.806284
H	-1.952320	10.911672	-5.081081
C	-4.130334	9.903998	-3.890390
O	-3.950834	10.703528	-2.983476
O	-5.375002	9.526911	-4.312375
H	-6.012279	9.991415	-3.727272
H	-1.326245	2.373515	0.453167
H	-1.687883	0.671862	-3.496775
H	-2.611212	8.513502	-2.080521
H	-2.174348	2.131328	-5.449125
H	-2.101300	7.060687	-0.136998
H	-3.403232	9.086155	-5.722874
H	-1.026850	-0.693656	-1.733269

Table 6: Cartesian coordinates of the structure LOHN1

Atom	X	Y	Z
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.221147
O	1.141660	0.000000	-0.745893
H	1.881382	0.035595	-0.101682
C	-1.250311	0.026324	-0.877282
N	-2.362827	-0.549219	-0.111222
H	-3.244431	-0.140021	-0.429303
H	-2.246041	-0.302226	0.877319
C	-1.481071	1.448896	-1.368945
C	-1.499945	1.695395	-2.704110
N	-1.745048	2.993299	-3.212453
C	-1.759836	3.228144	-4.574442
C	-1.987314	4.467927	-5.101056
O	-2.004704	4.722078	-6.456309
C	-1.975210	4.071531	-2.323948
C	-2.210032	5.341565	-2.855653
N	-2.433796	6.421410	-1.968491
C	-2.409191	6.189963	-0.605831
C	-2.178579	4.950779	-0.078875
O	-2.148515	4.699609	1.276152
C	-2.699537	7.715057	-2.472112
C	-2.711628	7.963800	-3.808268
H	-1.819180	3.895848	-6.938493
H	-2.303387	5.531623	1.759356
C	-1.947757	3.795054	-0.918526
C	-1.712655	2.519157	-0.431098
C	-2.230830	5.620486	-4.260313
C	-2.464246	6.897760	-4.743026
C	-2.956568	9.369912	-4.336410
N	-1.679296	10.060330	-4.552118
H	-1.235358	10.229617	-3.643912
H	-1.845142	10.980487	-4.972085
H	-2.450869	7.092935	-5.812589
C	-3.920821	10.119605	-3.412724
O	-3.598415	10.756173	-2.417121
O	-5.218210	10.020752	-3.836926
H	-5.755915	10.509542	-3.176315
H	-2.881250	8.471954	-1.711922
H	-1.323649	0.933655	-3.461465
H	-1.691147	2.336392	0.640911
H	-1.575612	2.355002	-5.200530
H	-2.587335	7.065503	0.018721
H	-3.455163	9.269355	-5.312796
H	-1.039045	-0.606347	-1.755947

Table 7: Cartesian coordinates of the structure LOHN2

Atom	X	Y	Z
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.222097
O	1.148537	0.000000	-0.741999
H	1.887440	0.035393	-0.096465
C	-1.251078	-0.006865	-0.894242
N	-2.443067	-0.550063	-0.236310
H	-2.712914	0.067658	0.535393
H	-2.213485	-1.449405	0.198863
C	-1.509908	1.407854	-1.396410
C	-1.649119	1.648472	-2.754292
C	-1.651521	2.460866	-0.457880
C	-1.933753	3.769136	-0.865420
C	-1.919154	2.963640	-3.213195
C	-2.040110	4.035023	-2.274676
C	-2.339644	5.341950	-2.705511
N	-2.590922	5.620677	-4.022100
N	-2.505561	6.403462	-1.791666
C	-2.431122	6.121797	-0.452589
C	-2.168849	4.863582	0.034095
O	-2.609299	7.229975	0.326059
C	-2.430003	4.593807	-4.948185
C	-2.117876	3.304884	-4.579872
O	-1.986875	2.293240	-5.501241
H	-2.160816	2.646659	-6.392769
H	-2.461556	6.964520	1.252293
C	-2.249503	7.751742	-2.288991
C	-2.547183	7.980519	-3.592388
C	-2.965208	6.909788	-4.435364
H	-1.785997	8.441923	-1.592755
H	-2.582932	4.892606	-5.983577
C	-2.335968	9.346443	-4.230653
N	-1.048654	9.394974	-4.931917
H	-0.295719	9.354303	-4.237379
H	-0.948839	10.296630	-5.408667
C	-2.515648	10.451702	-3.182380
O	-1.617737	10.946543	-2.517187
O	-3.818762	10.851610	-3.084159
H	-3.840761	11.528486	-2.373001
H	-1.572787	0.837590	-3.477677
H	-2.174473	4.692989	1.110960
H	-1.549717	2.251495	0.609644
H	-3.041690	7.032336	-5.511777
H	-3.136884	9.479382	-4.976333
H	-1.016972	-0.637048	-1.766356

Table 8: Cartesian coordinates of the structure LOHN3

Atom	X	Y	Z
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.223199
O	1.152393	0.000000	-0.739202
H	1.887485	0.042994	-0.089584
C	-1.248336	-0.027292	-0.887885
N	-2.365924	-0.790580	-0.321375
H	-2.608019	-0.392079	0.591539
H	-2.074099	-1.757274	-0.145960
C	-1.698444	1.388729	-1.221362
C	-1.494906	2.401565	-0.337984
N	-1.948674	3.716063	-0.633084
C	-1.756960	4.750368	0.254967
C	-2.170099	6.028654	-0.004165
O	-1.118877	4.365693	1.399945
C	-2.608073	3.994925	-1.864753
C	-3.035831	5.289339	-2.144121
H	-1.036362	5.151084	1.971139
N	-3.701940	5.565788	-3.374020
C	-3.901571	4.529803	-4.256451
C	-3.486974	3.251647	-3.998642
O	-4.548251	4.911915	-5.398901
C	-4.145771	6.884831	-3.669724
C	-3.936753	7.897917	-2.790188
H	-4.652209	4.119876	-5.957120
C	-2.834422	6.381065	-1.229435
C	-3.266679	7.662124	-1.542615
C	-2.809691	2.903045	-2.778805
C	-2.369478	1.625807	-2.465433
C	-4.387843	9.304457	-3.169377
N	-3.303354	10.284624	-3.305433
H	-2.459120	9.814806	-3.640544
H	-3.094814	10.679266	-2.382356
H	-4.652813	6.996467	-4.621286
H	-1.003167	2.292368	0.621935
H	-2.546534	0.798246	-3.151715
H	-3.677576	2.474626	-4.740146
H	-1.988253	6.803821	0.741461
H	-3.110924	8.480888	-0.840272
C	-5.363875	9.814863	-2.111679
O	-5.073009	10.570493	-1.196420
O	-6.616352	9.307659	-2.288938
H	-7.152537	9.651367	-1.542090
H	-4.946347	9.237256	-4.117756
H	-0.956186	-0.508234	-1.834827

Table 9: Cartesian coordinates of the structure DSH0

Atom	X	Y	Z
S	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.355372
C	1.778316	0.000000	-0.168294
C	2.619203	0.012909	0.918231
C	4.042781	0.010600	0.772931
C	4.899226	0.021285	1.889779
C	6.286972	0.018903	1.735104
C	6.842379	0.007462	0.448516
C	6.029656	-0.008138	-0.699459
C	4.606831	-0.005382	-0.541150
C	3.740147	-0.016603	-1.669992
C	2.317287	-0.014987	-1.512165
C	1.505707	-0.027058	-2.660897
C	2.059338	-0.044940	-3.945865
C	3.449065	-0.051560	-4.101720
C	4.304186	-0.033334	-2.983916
C	5.727792	-0.037659	-3.129725
C	6.568861	-0.023789	-2.043433
S	8.347069	-0.027131	-2.210553
H	8.346314	-0.052345	-3.565878
H	0.418919	-0.017325	-2.554681
C	7.192099	-0.018470	2.961727
N	7.695836	-1.376567	3.178090
H	8.213681	-1.680628	2.347514
H	8.377312	-1.373005	3.943755
C	1.146107	-0.014332	-5.167418
N	1.101565	1.335640	-5.735250
H	2.043151	1.605956	-6.036560
H	0.526836	1.333913	-6.583968
H	7.929696	0.017917	0.336574
C	1.596468	-1.094358	-6.163105
O	2.322409	-0.908527	-7.128671
O	1.080591	-2.318851	-5.844010
H	1.441651	-2.948524	-6.505456
C	8.294995	1.042982	2.820925
O	9.448019	0.825971	2.483431
O	7.830558	2.291105	3.129185
H	8.582722	2.905365	2.983973
H	4.466379	0.024197	2.892996
H	3.887049	-0.079862	-5.103026
H	2.210867	0.024567	1.931321
H	6.135169	-0.051411	-4.143210
H	0.130771	-0.283742	-4.837905
H	6.586610	0.269120	3.835943

Table 10: Cartesian coordinates of the structure DSHN1

Atom	X	Y	Z
S	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.355992
C	1.774028	0.000000	-0.179204
C	2.624652	0.005993	0.892685
N	3.993738	0.006138	0.760244
C	4.825193	0.010418	1.908075
C	6.177530	0.016121	1.797420
C	4.569522	0.002853	-0.533977
C	3.715399	-0.005483	-1.640137
N	4.289323	-0.004002	-2.934256
C	5.658599	0.017743	-3.068420
C	6.509205	0.029118	-1.996458
C	3.463469	-0.045971	-4.083075
C	2.110076	-0.043724	-3.974240
C	6.000437	0.015093	-0.636916
C	6.797537	0.018024	0.498749
C	2.284748	-0.006340	-1.538567
C	1.492277	-0.011250	-2.677305
S	8.282797	0.060297	-2.175641
H	8.281989	0.043765	-3.531600
C	7.030619	-0.016704	3.060965
N	7.914996	-1.178790	3.181745
H	7.482190	-1.996281	2.746882
H	8.793928	-0.983061	2.692077
C	1.227168	-0.048150	-5.214760
N	0.861892	1.325341	-5.579178
H	1.699414	1.817313	-5.906446
H	0.202632	1.315891	-6.363672
H	0.406268	0.017145	-2.602218
C	1.905008	-0.831674	-6.343449
O	2.704763	-0.366284	-7.145121
O	1.497851	-2.136635	-6.377373
H	1.996373	-2.557399	-7.111627
H	3.999626	-0.071668	-5.029115
H	4.293691	0.019247	2.857648
H	7.883873	0.026157	0.418926
H	2.266710	0.011780	1.921187
H	6.014474	0.024401	-4.097594
C	7.893659	1.243390	3.103089
O	9.068762	1.299064	2.777405
O	7.183274	2.325959	3.529323
H	7.796844	3.089990	3.471293
H	0.302526	-0.586391	-4.955228
H	6.350803	0.030467	3.928537

Table 11: Cartesian coordinates of the structure DSHN2

Atom	X	Y	Z
S	-5.876905	0.110532	-1.570983
H	-5.876905	0.110532	-0.211035
C	-4.095732	0.110532	-1.647658
C	-3.258024	-0.053643	-0.562935
N	-3.597736	0.247128	-2.920392
C	-2.224023	0.386870	-3.105325
N	-1.802233	0.801061	-4.340258
C	-0.437873	0.897647	-4.569154
C	0.502666	0.690652	-3.584189
C	-1.314714	0.203758	-2.044407
C	0.092151	0.349208	-2.257694
C	0.969724	0.176729	-1.158059
C	0.466473	-0.128334	0.101771
C	-0.922032	-0.250504	0.316635
C	-1.836992	-0.061133	-0.731756
C	-4.423657	-0.063321	-4.080994
C	-3.982350	0.440491	-5.277702
C	-2.737950	1.090172	-5.362607
S	2.249002	0.847114	-3.909202
H	2.116826	1.157278	-5.222238
H	-5.133873	-0.880036	-3.968763
H	-0.179205	1.166231	-5.590609
C	-4.759296	0.203142	-6.568337
N	-4.218374	-0.952908	-7.291321
H	-4.436168	-1.803265	-6.761455
H	-4.699932	-1.050202	-8.190729
C	-6.258995	0.097284	-6.261977
O	-6.860422	-0.944125	-6.044966
O	-6.868597	1.319234	-6.281514
H	-7.806362	1.158707	-6.037929
H	2.043853	0.308290	-1.295802
H	-3.681178	-0.159684	0.434570
C	1.418838	-0.278626	1.282900
N	1.324013	0.883085	2.170007
H	0.361989	0.968510	2.512477
H	1.899877	0.725065	3.003078
C	1.141777	-1.619814	1.983734
O	0.500716	-1.761591	3.014164
O	1.713220	-2.664026	1.312314
H	1.464243	-3.474773	1.807105
H	-1.301598	-0.477242	1.315565
H	-2.300126	1.407232	-6.303653
H	-4.619521	1.096991	-7.197322
H	2.444872	-0.330266	0.886561

Table 12: Cartesian coordinates of the structure DSHN3

Atom	X	Y	Z
S	-6.137114	0.038409	-4.046383
H	-6.137114	0.038409	-2.691731
C	-4.354597	0.038409	-4.148410
C	-3.549885	0.011745	-3.038565
N	-3.819406	0.062714	-5.423988
C	-4.646119	0.150504	-6.576976
C	-4.117796	0.118055	-7.829720
C	-2.403620	0.014003	-5.577293
C	-1.580345	-0.010247	-4.451962
N	-0.163940	-0.069791	-4.607064
C	0.366072	-0.138267	-5.881751
C	-0.438517	-0.119555	-6.991958
C	0.663640	-0.054002	-3.450002
C	0.135678	-0.020720	-2.198438
C	-2.116530	0.006913	-3.119452
C	-1.282930	0.001692	-2.007763
C	-1.869095	-0.026589	-6.909417
C	-2.705261	0.010358	-8.017598
S	2.145253	-0.259143	-5.986919
H	2.146379	-0.245555	-7.341196
C	1.082033	0.042923	-1.003997
N	0.987562	1.270758	-0.205200
H	0.756195	2.058727	-0.815069
H	0.225597	1.168613	0.473377
H	1.733496	-0.063828	-3.637853
H	-5.710709	0.248335	-6.383907
C	-5.026738	0.163745	-9.051525
N	-5.336752	-1.199408	-9.495462
H	-5.916172	-1.656296	-8.783934
H	-5.899609	-1.168092	-10.351302
C	-6.262404	1.022362	-8.763163
O	-7.312729	0.611949	-8.288374
O	-6.070840	2.329093	-9.120192
H	-6.896915	2.799976	-8.874418
H	-2.290510	-0.047321	-9.023293
H	0.016267	-0.185087	-7.979306
H	-4.007931	-0.012444	-2.050769
H	-1.704803	0.008762	-1.003020
C	0.799348	-1.146017	-0.088217
O	0.104527	-1.105589	0.915615
O	1.397612	-2.284361	-0.537620
H	1.119253	-2.996087	0.078581
H	2.112177	-0.072323	-1.379768
H	-4.466558	0.664249	-9.856557

Table 13: Cartesian coordinates of the structure LSH0

Atom	X	Y	Z
S	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.355163
C	1.778617	0.000000	-0.166832
C	2.618429	-0.003341	0.920601
C	4.042121	-0.000400	0.776675
C	4.897282	-0.001610	1.894644
C	6.285085	-0.000613	1.741510
C	6.841767	0.001478	0.455335
C	6.030461	0.010413	-0.693722
C	4.607515	0.007099	-0.536992
C	3.741945	0.009798	-1.666702
C	2.319087	0.005432	-1.510068
C	1.508536	0.006312	-2.659609
C	2.062696	0.018349	-3.944117
C	3.452777	0.030315	-4.099005
C	4.307113	0.020654	-2.980488
C	5.731042	0.026269	-3.124638
C	6.571064	0.018757	-2.037366
S	8.349503	0.019866	-2.202828
H	8.349238	0.043104	-3.557933
H	0.421784	-0.005848	-2.553905
C	7.189957	0.041546	2.968082
N	7.723053	1.392099	3.159828
H	8.253236	1.667274	2.326976
H	8.399026	1.389091	3.930359
C	1.151952	-0.016921	-5.167260
N	1.163541	-1.349534	-5.775704
H	2.113606	-1.568471	-6.091775
H	0.582990	-1.347162	-6.620460
C	1.558100	1.111079	-6.128931
O	2.289031	0.984222	-7.099781
O	0.996286	2.304104	-5.769746
H	1.332075	2.968551	-6.410255
H	7.929192	-0.011211	0.344838
C	8.269357	-1.046506	2.846490
O	9.425505	-0.862016	2.497658
O	7.780641	-2.276705	3.188899
H	8.518614	-2.910338	3.054172
H	4.463002	0.001712	2.897249
H	3.891560	0.057680	-5.100061
H	2.209027	-0.007272	1.933328
H	6.139651	0.034443	-4.137721
H	0.126216	0.200344	-4.831642
H	6.578202	-0.217007	3.846877

Table 14: Cartesian coordinates of the structure LSHN1

Atom	X	Y	Z
S	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.355917
C	1.774043	0.000000	-0.179716
C	2.624429	-0.013385	0.892090
N	3.993565	-0.013459	0.759759
C	4.824925	-0.019020	1.907661
C	6.177131	-0.021747	1.797688
C	4.569292	-0.002518	-0.534435
C	3.715356	0.012470	-1.640532
N	4.289505	0.018389	-2.934427
C	5.658733	-0.003843	-3.068746
C	6.509281	-0.022342	-1.997194
C	3.463677	0.063513	-4.083269
C	2.110241	0.063224	-3.974333
C	6.000313	-0.013913	-0.637470
C	6.797117	-0.020040	0.498855
C	2.284570	0.014299	-1.539063
C	1.492184	0.027138	-2.677511
S	8.282646	-0.055377	-2.177404
H	8.280897	-0.047869	-3.533373
C	7.027923	0.019011	3.060836
N	7.873595	1.210971	3.193621
H	7.419725	2.007668	2.740800
H	8.762920	1.043936	2.711182
C	1.226609	0.070759	-5.214087
N	0.839094	-1.300248	-5.564529
H	1.668078	-1.808859	-5.888063
H	0.178101	-1.288778	-6.347486
H	0.406126	-0.000709	-2.602998
C	1.913770	0.832174	-6.352082
O	2.708165	0.348276	-7.148258
O	1.522238	2.141612	-6.401270
H	2.024989	2.547412	-7.141031
H	4.000311	0.087657	-5.029014
H	4.292407	-0.027453	2.856609
H	7.883526	-0.033450	0.418664
H	2.266506	-0.025230	1.920501
H	6.014412	-0.004821	-4.097982
C	7.929173	-1.214274	3.092907
O	9.104297	-1.230115	2.761828
O	7.256198	-2.321177	3.516693
H	7.894708	-3.064138	3.453799
H	0.310856	0.626352	-4.959136
H	6.350446	-0.052732	3.928260

Table 15: Cartesian coordinates of the structure LSHN2

Atom	X	Y	Z
S	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.359971
C	1.781050	0.000000	-0.077061
C	2.619029	0.168069	1.006897
N	2.278568	-0.141444	-1.349377
C	3.652159	-0.282028	-1.534269
N	4.073920	-0.700074	-2.767957
C	5.438133	-0.797781	-2.996752
C	6.378891	-0.588063	-2.012613
C	4.561737	-0.095981	-0.474127
C	5.968462	-0.242888	-0.687132
C	6.846414	-0.068157	0.411849
C	6.343508	0.240342	1.670925
C	4.955261	0.365117	1.885387
C	4.039880	0.173690	0.837721
C	1.451310	0.162260	-2.510853
C	1.893305	-0.344841	-3.706190
C	3.138380	-0.992392	-3.789654
S	8.125073	-0.746022	-2.337364
H	7.992546	-1.058934	-3.649521
H	0.738870	0.977311	-2.400634
H	5.696374	-1.069339	-4.017532
C	1.114178	-0.114703	-4.996761
N	1.645062	1.045339	-5.720695
H	1.419233	1.894138	-5.191710
H	1.162210	1.137423	-6.619993
C	-0.386211	-0.021954	-4.689379
O	-0.998592	1.014907	-4.480166
O	-0.982167	-1.250911	-4.696384
H	-1.921019	-1.098791	-4.451660
H	7.920394	-0.200926	0.274223
H	2.196081	0.277776	2.004103
C	7.295476	0.394163	2.851846
N	7.188447	-0.756569	3.751641
H	6.226189	-0.826658	4.096902
H	7.767721	-0.596028	4.581887
C	7.028896	1.745784	3.536731
O	6.387791	1.904703	4.564385
O	7.612692	2.776793	2.855754
H	7.370438	3.595282	3.340895
H	4.575650	0.595955	2.883358
H	3.576576	-1.313701	-4.729066
H	1.260701	-1.008055	-5.624946
H	8.322599	0.432188	2.456827

Table 16: Cartesian coordinates of the structure LSHN3

Atom	X	Y	Z
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.221310
O	1.138880	0.000000	-0.747219
H	1.881573	0.034294	-0.106184
C	-1.252118	0.029568	-0.874135
N	-2.354040	-0.581461	-0.121342
H	-3.245468	-0.208801	-0.456917
H	-2.263004	-0.325069	0.867278
C	-1.500096	1.465736	-1.324268
C	-1.554907	1.734634	-2.654967
C	-1.728073	2.502050	-0.362489
C	-2.056319	3.777536	-0.805174
C	-2.312376	4.884846	0.072232
C	-2.668366	6.127047	-0.386959
N	-2.798708	6.382682	-1.740336
C	-2.141478	4.078517	-2.207377
C	-2.496194	5.345173	-2.668631
C	-2.542093	5.657487	-4.069780
C	-2.921280	6.918983	-4.508788
C	-3.299767	7.912394	-3.553044
C	-3.243617	7.643978	-2.221386
C	-2.145852	4.591196	-4.946966
C	-1.804427	3.345184	-4.486746
N	-1.824288	3.045779	-3.137481
C	-3.739177	9.284385	-4.048632
N	-2.564105	10.130429	-4.285287
H	-2.855547	11.028898	-4.682806
H	-2.120479	10.341059	-3.385445
C	-4.764329	9.896990	-3.089069
O	-4.495455	10.584268	-2.113296
O	-6.048571	9.606670	-3.459746
S	-2.982391	7.505083	0.704210
S	-1.296394	2.022360	-5.574694
H	-6.625420	10.015436	-2.777855
H	-1.423366	0.972441	-3.417876
H	-3.537983	8.358760	-1.458247
H	-2.102746	4.793572	-6.016206
H	-2.211243	4.723970	1.144636
H	-2.926281	7.155168	-5.572252
H	-1.658934	2.290319	0.704233
H	-4.248847	9.134576	-5.013095
H	-1.038268	-0.575267	-1.770734
H	-1.519290	2.749800	-6.695124
H	-2.779466	6.766279	1.821321

Table 17: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for DOH0.

Atom	f^-	f^+	f^0	f^d	Charge
C	0.006	0.010	0.008	0.003	0.365
O	0.024	0.026	0.025	0.002	-0.384
O	0.002	0.002	0.002	0.000	-0.352
H	0.016	0.016	0.016	0.000	0.325
C	0.011	0.007	0.009	-0.004	-0.129
N	0.006	0.006	0.006	0.000	-0.366
H	0.003	0.004	0.003	0.001	0.204
H	0.025	0.026	0.026	0.000	0.178
C	-0.006	-0.006	-0.006	0.000	0.154
C	0.072	0.082	0.077	0.010	-0.146
C	0.081	0.080	0.080	-0.001	-0.213
C	0.000	0.013	0.007	0.013	0.037
C	0.003	0.003	0.003	0.000	0.099
C	0.013	0.010	0.011	-0.003	-0.014
C	0.013	0.010	0.011	-0.003	-0.016
C	0.000	0.012	0.006	0.011	0.022
C	0.081	0.081	0.081	-0.001	-0.156
C	-0.006	-0.006	-0.006	0.000	0.148
C	0.071	0.081	0.076	0.009	-0.195
C	0.003	0.005	0.004	0.002	0.113
C	0.062	0.051	0.057	-0.011	-0.225
C	0.039	0.040	0.039	0.001	0.178
O	0.035	0.023	0.029	-0.012	-0.367
H	0.028	0.029	0.029	0.000	0.303
C	0.063	0.051	0.057	-0.012	-0.227
C	0.038	0.039	0.039	0.000	0.178
O	0.035	0.022	0.029	-0.013	-0.366
H	0.028	0.028	0.028	0.000	0.301
H	0.024	0.025	0.025	0.001	0.109
C	0.010	0.007	0.009	-0.003	-0.132
N	0.004	0.004	0.004	0.000	-0.364
H	0.005	0.005	0.005	0.000	0.201
H	0.026	0.026	0.026	0.000	0.176
H	0.020	0.020	0.020	0.000	0.115
C	0.008	0.009	0.008	0.001	0.365
O	0.022	0.023	0.023	0.001	-0.389
O	0.003	0.004	0.004	0.001	-0.350
H	0.016	0.016	0.016	0.000	0.326
H	0.024	0.025	0.024	0.001	0.077
H	0.020	0.020	0.020	0.000	0.081
H	0.025	0.025	0.025	0.000	0.076
H	0.025	0.024	0.025	0.000	0.078
H	0.011	0.012	0.012	0.001	0.094
H	0.012	0.012	0.012	0.001	0.088

Table 18: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for DOHN1.

Atom	f^-	f^+	f^0	f^d	Charge
C	0.009	0.02	0.014	0.011	0.386
O	0.024	0.035	0.029	0.011	-0.396
O	0.003	0.009	0.006	0.006	-0.354
H	0.016	0.019	0.017	0.003	0.327
C	0.02	0.026	0.023	0.006	-0.129
N	0.025	0.026	0.026	0.001	-0.365
H	-0.001	0.002	0.001	0.003	0.184
H	0.009	0.01	0.009	0.001	0.203
C	0.002	0.026	0.014	0.024	0.065
C	0.049	0.063	0.056	0.014	-0.090
N	0.007	-0.018	-0.006	-0.024	-0.123
C	0.024	0.045	0.034	0.021	-0.152
C	0.043	0.026	0.035	-0.017	0.167
O	0.018	0.017	0.018	-0.001	-0.365
C	0.030	0.024	0.027	-0.006	0.090
C	0.033	0.026	0.029	-0.007	0.068
N	0.006	-0.014	-0.004	-0.021	-0.110
C	0.022	0.051	0.037	0.029	-0.166
C	0.042	0.024	0.033	-0.018	0.170
O	0.018	0.016	0.017	-0.002	-0.364
C	0.052	0.053	0.053	0.001	-0.113
C	-0.003	0.025	0.011	0.028	0.139
H	0.028	0.025	0.026	-0.003	0.294
H	0.027	0.025	0.026	-0.002	0.293
C	0.003	0.039	0.021	0.036	0.093
C	0.099	0.034	0.067	-0.065	-0.194
C	0.004	0.032	0.018	0.028	0.069
C	0.100	0.047	0.073	-0.053	-0.154
C	0.015	0.019	0.017	0.004	-0.114
N	0.001	0.000	0.000	-0.001	-0.374
H	0.010	0.011	0.010	0.001	0.202
H	0.028	0.028	0.028	0.000	0.175
H	0.027	0.024	0.026	-0.003	0.106
C	0.016	0.016	0.016	0.001	0.354
O	0.027	0.026	0.027	-0.001	-0.399
O	0.010	0.010	0.010	0.000	-0.352
H	0.017	0.017	0.017	0.000	0.327
H	0.017	0.014	0.016	-0.002	0.061
H	0.027	0.022	0.025	-0.005	0.076
H	0.025	0.023	0.024	-0.002	0.121
H	0.023	0.022	0.023	-0.001	0.078
H	0.023	0.024	0.023	0.001	0.082
H	0.014	0.014	0.014	0.001	0.097
H	0.012	0.015	0.013	0.003	0.089

Table 19: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for DOHN2.

Atom	f^-	f^+	f^0	f^d	Charge
C	0.009	0.019	0.014	0.011	0.367
O	0.023	0.034	0.029	0.011	-0.389
O	0.003	0.007	0.005	0.004	-0.351
H	0.015	0.019	0.017	0.004	0.325
C	0.014	0.02	0.017	0.006	-0.127
N	0.003	0.004	0.004	0.001	-0.362
H	0.004	0.006	0.005	0.003	0.198
H	0.024	0.026	0.025	0.003	0.176
C	0.007	0.028	0.018	0.021	0.160
C	0.051	0.047	0.049	-0.004	-0.177
C	0.067	0.030	0.048	-0.037	-0.229
C	0.001	0.034	0.017	0.033	0.155
C	0.028	0.029	0.028	0.001	0.042
C	0.010	0.016	0.013	0.006	-0.076
C	0.032	0.049	0.041	0.017	0.355
N	-0.014	0.008	-0.003	0.022	-0.060
N	0.005	-0.003	0.001	-0.008	-0.155
C	0.013	0.029	0.021	0.017	0.201
C	0.073	0.032	0.052	-0.041	-0.306
O	0.013	0.017	0.015	0.004	-0.361
C	0.036	0.033	0.035	-0.002	-0.193
C	0.034	0.039	0.037	0.005	0.184
O	0.023	0.021	0.022	-0.002	-0.362
H	0.024	0.025	0.025	0.001	0.302
H	0.025	0.025	0.025	0.000	0.303
C	0.092	0.057	0.074	-0.035	-0.109
C	-0.005	0.025	0.010	0.030	0.136
C	0.114	0.049	0.082	-0.066	-0.205
H	0.026	0.020	0.023	-0.005	0.113
H	0.019	0.024	0.021	0.005	0.083
C	0.010	0.020	0.015	0.010	-0.095
N	-0.004	-0.007	-0.005	-0.004	-0.387
H	0.011	0.011	0.011	0.000	0.203
H	0.032	0.029	0.030	-0.003	0.173
C	0.008	0.011	0.009	0.003	0.369
O	0.024	0.024	0.024	0.000	-0.392
O	0.006	0.007	0.007	0.001	-0.353
H	0.017	0.016	0.017	-0.001	0.326
H	0.023	0.024	0.024	0.001	0.105
H	0.025	0.023	0.024	-0.002	0.079
H	0.020	0.021	0.020	0.001	0.080
H	0.033	0.023	0.028	-0.010	0.067
H	0.017	0.014	0.016	-0.003	0.091
H	0.011	0.014	0.013	0.003	0.094

Table 20: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for DOHN3.

Atom	f^-	f^+	f^0	f^d	Charge
C	0.009	0.025	0.017	0.016	0.382
O	0.023	0.038	0.030	0.015	-0.400
O	0.004	0.012	0.008	0.008	-0.350
H	0.016	0.020	0.018	0.004	0.326
C	0.019	0.027	0.023	0.008	-0.128
N	0.026	0.027	0.027	0.001	-0.366
H	0.000	0.003	0.002	0.003	0.183
H	0.009	0.009	0.009	0.001	0.201
C	-0.001	0.027	0.013	0.028	0.060
C	0.060	0.070	0.065	0.010	-0.139
C	0.099	0.029	0.064	-0.070	-0.172
C	-0.002	0.037	0.018	0.039	0.152
C	0.056	0.026	0.041	-0.030	-0.274
C	0.015	0.039	0.027	0.024	0.288
N	0.004	-0.008	-0.002	-0.013	-0.133
O	0.016	0.020	0.018	0.004	-0.362
C	0.033	0.022	0.027	-0.011	0.065
C	0.035	0.026	0.031	-0.008	0.046
C	-0.001	0.029	0.014	0.031	0.126
C	0.101	0.044	0.073	-0.057	-0.131
C	-0.005	0.028	0.011	0.033	0.130
C	0.062	0.056	0.059	-0.006	-0.175
C	0.057	0.028	0.042	-0.029	-0.277
C	0.016	0.035	0.025	0.019	0.292
N	0.005	-0.012	-0.004	-0.017	-0.138
O	0.017	0.018	0.017	0.001	-0.368
H	0.023	0.025	0.024	0.002	0.290
H	0.023	0.025	0.024	0.001	0.284
C	0.015	0.019	0.017	0.004	-0.099
N	0.000	-0.001	-0.001	-0.001	-0.379
H	0.010	0.010	0.010	0.001	0.203
H	0.028	0.027	0.028	-0.001	0.173
H	0.028	0.022	0.025	-0.006	0.129
H	0.019	0.016	0.017	-0.003	0.125
C	0.011	0.013	0.012	0.002	0.351
O	0.026	0.026	0.026	0.000	-0.390
O	0.008	0.009	0.008	0.001	-0.354
H	0.017	0.017	0.017	0.000	0.326
H	0.027	0.021	0.024	-0.006	0.074
H	0.026	0.020	0.023	-0.006	0.084
H	0.022	0.024	0.023	0.002	0.078
H	0.022	0.023	0.022	0.001	0.079
H	0.014	0.014	0.014	0.001	0.092
H	0.012	0.015	0.013	0.003	0.095

Table 21: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for LOH0.

Atom	f^-	f^+	f^0	f^d	Charge
C	0.006	0.010	0.008	0.003	0.365
O	0.024	0.026	0.025	0.002	-0.384
O	0.002	0.002	0.002	0.000	-0.352
H	0.016	0.016	0.016	0.000	0.325
C	0.011	0.007	0.009	-0.004	-0.129
N	0.006	0.006	0.006	0.000	-0.366
H	0.003	0.004	0.003	0.001	0.204
H	0.025	0.026	0.026	0.000	0.178
C	-0.006	-0.006	-0.006	0.000	0.155
C	0.072	0.082	0.077	0.010	-0.146
C	0.081	0.080	0.080	-0.001	-0.213
C	0.000	0.013	0.007	0.013	0.037
C	0.003	0.003	0.003	0.000	0.099
C	0.013	0.010	0.011	-0.003	-0.014
C	0.013	0.010	0.011	-0.003	-0.016
C	0.000	0.012	0.006	0.011	0.022
C	0.082	0.081	0.081	-0.001	-0.156
C	-0.006	-0.006	-0.006	0.000	0.149
C	0.071	0.081	0.076	0.009	-0.195
C	0.003	0.005	0.004	0.002	0.113
C	0.063	0.052	0.058	-0.011	-0.225
C	0.038	0.039	0.039	0.001	0.178
O	0.035	0.023	0.029	-0.012	-0.367
H	0.028	0.029	0.029	0.000	0.303
C	0.064	0.051	0.058	-0.012	-0.227
C	0.038	0.039	0.039	0.000	0.178
O	0.035	0.023	0.029	-0.013	-0.366
H	0.028	0.028	0.028	0.000	0.301
H	0.024	0.025	0.024	0.001	0.109
C	0.010	0.007	0.008	-0.003	-0.133
N	0.004	0.004	0.004	0.000	-0.364
H	0.005	0.005	0.005	0.000	0.201
H	0.026	0.026	0.026	0.000	0.176
C	0.008	0.009	0.008	0.001	0.365
O	0.022	0.023	0.023	0.001	-0.389
O	0.003	0.004	0.003	0.001	-0.350
H	0.016	0.016	0.016	0.000	0.326
H	0.020	0.020	0.020	0.000	0.115
H	0.024	0.025	0.024	0.001	0.077
H	0.020	0.020	0.020	0.000	0.081
H	0.024	0.024	0.024	0.000	0.076
H	0.024	0.024	0.024	0.000	0.077
H	0.011	0.012	0.012	0.001	0.093
H	0.012	0.012	0.012	0.001	0.088

Table 22: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for LOHN2.

Atom	f^-	f^+	f^0	f^d	Charge
C	0.009	0.019	0.014	0.011	0.367
O	0.023	0.034	0.029	0.011	-0.389
O	0.003	0.007	0.005	0.004	-0.351
H	0.015	0.019	0.017	0.004	0.325
C	0.014	0.020	0.017	0.006	-0.126
N	0.003	0.004	0.004	0.001	-0.362
H	0.004	0.006	0.005	0.002	0.198
H	0.024	0.026	0.025	0.003	0.176
C	0.007	0.028	0.018	0.021	0.160
C	0.051	0.047	0.049	-0.004	-0.176
C	0.067	0.030	0.048	-0.037	-0.230
C	0.001	0.034	0.017	0.033	0.155
C	0.028	0.029	0.028	0.001	0.042
C	0.010	0.016	0.013	0.006	-0.076
C	0.032	0.049	0.041	0.017	0.356
N	-0.014	0.008	-0.003	0.022	-0.060
N	0.005	-0.003	0.001	-0.008	-0.155
C	0.012	0.029	0.021	0.017	0.200
C	0.073	0.032	0.053	-0.041	-0.306
O	0.013	0.017	0.015	0.004	-0.361
C	0.036	0.034	0.035	-0.002	-0.193
C	0.034	0.039	0.036	0.005	0.184
O	0.023	0.021	0.022	-0.002	-0.362
H	0.024	0.025	0.025	0.001	0.302
H	0.025	0.025	0.025	0.000	0.303
C	0.092	0.057	0.074	-0.035	-0.109
C	-0.005	0.025	0.010	0.030	0.135
C	0.114	0.049	0.082	-0.066	-0.204
H	0.026	0.021	0.023	-0.005	0.112
H	0.018	0.024	0.021	0.005	0.084
C	0.010	0.020	0.015	0.010	-0.094
N	-0.004	-0.007	-0.006	-0.003	-0.388
H	0.011	0.011	0.011	0.000	0.203
H	0.032	0.029	0.030	-0.003	0.173
C	0.007	0.011	0.009	0.003	0.368
O	0.024	0.024	0.024	0.000	-0.393
O	0.006	0.007	0.007	0.001	-0.353
H	0.017	0.016	0.017	-0.001	0.326
H	0.023	0.024	0.024	0.001	0.105
H	0.024	0.023	0.024	-0.002	0.079
H	0.020	0.021	0.020	0.001	0.081
H	0.033	0.023	0.028	-0.010	0.067
H	0.017	0.014	0.016	-0.003	0.091
H	0.011	0.015	0.013	0.003	0.094

Table 23: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for LOHN3.

Atom	f^-	f^+	f^0	f^d	Charge
C	0.011	0.014	0.012	0.002	0.353
O	0.026	0.026	0.026	0.000	-0.391
O	0.008	0.009	0.008	0.001	-0.353
H	0.017	0.017	0.017	0.000	0.326
C	0.014	0.018	0.016	0.004	-0.106
N	0.000	0.000	0.000	-0.001	-0.377
H	0.009	0.010	0.010	0.001	0.203
H	0.028	0.027	0.028	-0.001	0.174
C	-0.005	0.028	0.012	0.033	0.136
C	0.063	0.057	0.06	-0.006	-0.173
N	0.004	-0.008	-0.002	-0.013	-0.131
C	0.015	0.039	0.027	0.024	0.286
C	0.055	0.026	0.041	-0.03	-0.274
O	0.016	0.020	0.018	0.004	-0.363
C	0.035	0.026	0.031	-0.008	0.044
C	0.033	0.022	0.027	-0.011	0.066
H	0.023	0.025	0.024	0.001	0.284
N	0.005	-0.012	-0.004	-0.017	-0.138
C	0.016	0.035	0.026	0.019	0.293
C	0.057	0.027	0.042	-0.03	-0.277
O	0.017	0.018	0.017	0.001	-0.368
C	0.060	0.069	0.064	0.009	-0.138
C	-0.001	0.027	0.013	0.028	0.062
H	0.023	0.025	0.024	0.002	0.290
C	-0.002	0.037	0.018	0.039	0.151
C	0.099	0.030	0.064	-0.069	-0.173
C	-0.002	0.030	0.014	0.031	0.127
C	0.099	0.043	0.071	-0.057	-0.135
C	0.019	0.027	0.023	0.008	-0.129
N	0.026	0.026	0.026	0.001	-0.365
H	0.000	0.003	0.002	0.003	0.184
H	0.009	0.010	0.009	0.001	0.201
H	0.028	0.022	0.025	-0.006	0.129
H	0.019	0.016	0.018	-0.003	0.125
H	0.029	0.023	0.026	-0.006	0.074
H	0.022	0.024	0.023	0.002	0.078
H	0.022	0.023	0.023	0.001	0.078
H	0.026	0.020	0.023	-0.006	0.084
C	0.009	0.024	0.017	0.015	0.383
O	0.024	0.038	0.031	0.014	-0.400
O	0.003	0.011	0.007	0.008	-0.350
H	0.016	0.020	0.018	0.004	0.326
H	0.012	0.015	0.013	0.003	0.095
H	0.014	0.015	0.014	0.001	0.091

Table 24: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for DSH0.

Atom	f^-	f^+	f^0	f^d	Charge
S	0.121	0.088	0.105	-0.033	0.123
H	0.026	0.023	0.025	-0.003	-0.038
C	0.001	0.016	0.009	0.015	-0.385
C	0.048	0.048	0.048	0.000	-0.133
C	-0.001	0.005	0.002	0.006	0.087
C	0.069	0.077	0.073	0.007	-0.136
C	-0.003	-0.005	-0.004	-0.002	0.161
C	0.060	0.068	0.064	0.008	-0.085
C	0.008	0.008	0.008	0.000	0.305
C	0.015	0.012	0.014	-0.003	0.026
C	0.015	0.011	0.013	-0.004	-0.012
C	0.005	0.003	0.004	-0.002	0.253
C	0.065	0.073	0.069	0.008	-0.088
C	-0.005	-0.008	-0.007	-0.003	0.177
C	0.071	0.077	0.074	0.006	-0.124
C	0.001	0.009	0.005	0.007	0.086
C	0.051	0.049	0.050	-0.003	-0.125
C	0.002	0.016	0.009	0.014	-0.357
S	0.126	0.087	0.106	-0.039	0.126
H	0.027	0.023	0.025	-0.004	-0.039
H	0.017	0.021	0.019	0.004	0.024
C	0.010	0.007	0.008	-0.003	-0.129
N	0.006	0.005	0.005	-0.001	-0.367
H	0.002	0.004	0.003	0.002	0.204
H	0.024	0.025	0.024	0.001	0.179
C	0.009	0.007	0.008	-0.002	-0.131
N	0.003	0.003	0.003	0.000	-0.363
H	0.005	0.006	0.005	0.000	0.203
H	0.024	0.025	0.025	0.001	0.178
H	0.013	0.018	0.015	0.004	0.006
C	0.007	0.008	0.008	0.002	0.366
O	0.020	0.022	0.021	0.002	-0.387
O	0.003	0.004	0.003	0.001	-0.350
H	0.014	0.015	0.015	0.001	0.327
C	0.006	0.008	0.007	0.003	0.364
O	0.019	0.022	0.021	0.002	-0.383
O	0.003	0.003	0.003	0.000	-0.351
H	0.014	0.015	0.015	0.001	0.327
H	0.020	0.023	0.022	0.003	0.080
H	0.015	0.017	0.016	0.002	0.081
H	0.020	0.020	0.020	0.000	0.059
H	0.020	0.020	0.020	-0.001	0.061
H	0.009	0.012	0.011	0.002	0.087
H	0.012	0.012	0.012	0.001	0.090

Table 25: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for DSHN1.

Atom	f^-	f^+	f^0	f^d	Charge
S	0.074	0.070	0.072	-0.004	0.123
H	0.024	0.020	0.022	-0.004	-0.038
C	0.028	0.010	0.019	-0.018	-0.385
C	0.015	0.045	0.030	0.030	-0.133
N	0.006	-0.015	-0.004	-0.021	0.087
C	0.053	0.058	0.056	0.005	-0.136
C	0.001	0.030	0.015	0.029	0.161
C	0.030	0.025	0.027	-0.005	-0.085
C	0.032	0.026	0.029	-0.006	0.305
N	0.005	-0.012	-0.003	-0.017	0.026
C	0.014	0.051	0.032	0.037	-0.012
C	0.027	0.008	0.018	-0.019	0.253
C	0.056	0.050	0.053	-0.007	-0.088
C	-0.004	0.028	0.012	0.033	0.177
C	0.003	0.034	0.019	0.031	-0.124
C	0.082	0.022	0.052	-0.06	0.086
C	0.004	0.028	0.016	0.024	-0.125
C	0.083	0.034	0.058	-0.049	-0.357
S	0.074	0.068	0.071	-0.005	0.126
H	0.024	0.021	0.023	-0.003	-0.039
C	0.018	0.025	0.021	0.007	0.024
N	0.024	0.025	0.024	0.001	-0.129
H	0.001	0.003	0.002	0.002	-0.367
H	0.008	0.009	0.009	0.001	0.204
C	0.013	0.017	0.015	0.003	0.179
N	-0.001	-0.001	-0.001	-0.001	-0.131
H	0.010	0.011	0.010	0.001	-0.363
H	0.027	0.027	0.027	0.000	0.203
H	0.027	0.022	0.024	-0.005	0.178
C	0.012	0.014	0.013	0.001	0.006
O	0.025	0.025	0.025	0.000	0.366
O	0.009	0.009	0.009	0.000	-0.387
H	0.016	0.016	0.016	0.000	-0.350
H	0.016	0.013	0.014	-0.002	0.327
H	0.025	0.02	0.023	-0.005	0.364
H	0.025	0.019	0.022	-0.005	-0.383
H	0.020	0.019	0.019	-0.001	-0.351
H	0.020	0.02	0.02	0.000	0.327
C	0.009	0.019	0.014	0.010	0.080
O	0.022	0.033	0.027	0.011	0.081
O	0.003	0.008	0.006	0.005	0.059
H	0.015	0.018	0.016	0.003	0.061
H	0.013	0.014	0.013	0.001	0.087
H	0.011	0.014	0.013	0.003	0.090

Table 26: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for DSHN2.

Atom	f^-	f^+	f^0	f^d	Charge
S	0.071	0.079	0.075	0.007	0.128
H	0.030	0.027	0.029	-0.003	-0.043
C	0.000	0.016	0.008	0.016	-0.139
C	0.060	0.023	0.042	-0.037	-0.139
N	0.007	0.003	0.005	-0.004	-0.114
C	0.016	0.051	0.033	0.035	0.369
N	-0.013	0.01	-0.002	0.023	-0.073
C	0.025	0.020	0.023	-0.005	-0.104
C	0.019	0.023	0.021	0.004	-0.173
C	0.008	0.014	0.011	0.006	-0.061
C	0.017	0.028	0.022	0.011	0.202
C	0.047	0.036	0.042	-0.011	-0.130
C	0.004	0.03	0.017	0.026	0.176
C	0.066	0.027	0.046	-0.039	-0.233
C	0.002	0.039	0.020	0.037	0.151
C	0.097	0.036	0.066	-0.061	-0.153
C	-0.008	0.028	0.010	0.036	0.164
C	0.116	0.034	0.075	-0.082	-0.207
S	0.077	0.076	0.077	-0.001	0.122
H	0.018	0.022	0.02	0.004	-0.045
H	0.031	0.019	0.025	-0.012	0.088
H	0.015	0.022	0.018	0.006	0.073
C	0.008	0.018	0.013	0.010	-0.097
N	-0.003	-0.006	-0.004	-0.003	-0.386
H	0.011	0.010	0.010	-0.001	0.203
H	0.031	0.027	0.029	-0.004	0.174
C	0.005	0.009	0.007	0.004	0.375
O	0.022	0.021	0.022	-0.001	-0.393
O	0.007	0.007	0.007	0.000	-0.354
H	0.016	0.014	0.015	-0.001	0.326
H	0.021	0.022	0.021	0.001	0.036
H	0.021	0.021	0.021	0.000	0.066
C	0.010	0.019	0.015	0.009	-0.127
N	0.002	0.003	0.003	0.001	-0.361
H	0.004	0.006	0.005	0.003	0.200
H	0.023	0.026	0.024	0.003	0.178
C	0.008	0.018	0.013	0.010	0.368
O	0.021	0.032	0.027	0.011	-0.386
O	0.002	0.006	0.004	0.004	-0.350
H	0.014	0.018	0.016	0.004	0.326
H	0.017	0.020	0.018	0.003	0.085
H	0.031	0.021	0.026	-0.010	0.077
H	0.017	0.014	0.016	-0.003	0.091
H	0.010	0.013	0.012	0.004	0.090

Table 27: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for DSHN3.

Atom	f^-	f^+	f^0	f^d	Charge
S	0.072	0.078	0.075	0.006	0.150
H	0.018	0.021	0.020	0.002	-0.033
C	-0.005	0.020	0.007	0.025	-0.104
C	0.049	0.022	0.036	-0.027	-0.109
N	0.005	-0.007	-0.001	-0.012	-0.089
C	0.058	0.049	0.054	-0.009	-0.083
C	-0.004	0.031	0.013	0.035	0.165
C	0.032	0.025	0.029	-0.007	0.078
C	0.031	0.023	0.027	-0.008	0.088
N	0.005	-0.010	-0.002	-0.015	-0.100
C	-0.005	0.018	0.007	0.023	-0.085
C	0.050	0.024	0.037	-0.027	-0.111
C	0.057	0.056	0.056	-0.001	-0.082
C	-0.001	0.030	0.015	0.032	0.085
C	-0.002	0.034	0.016	0.036	0.162
C	0.096	0.029	0.062	-0.067	-0.165
C	-0.002	0.029	0.014	0.031	0.139
C	0.098	0.040	0.069	-0.058	-0.134
S	0.073	0.076	0.075	0.003	0.139
H	0.018	0.021	0.020	0.003	-0.029
C	0.017	0.024	0.020	0.008	-0.122
N	0.025	0.026	0.025	0.000	-0.364
H	0.000	0.002	0.001	0.002	0.184
H	0.009	0.009	0.009	0.001	0.202
H	0.021	0.015	0.018	-0.005	0.001
H	0.012	0.009	0.011	-0.003	-0.035
C	0.012	0.015	0.014	0.004	-0.109
N	0.001	0.000	0.001	-0.001	-0.376
H	0.009	0.010	0.009	0.001	0.204
H	0.027	0.027	0.027	0.000	0.176
C	0.013	0.014	0.013	0.001	0.355
O	0.024	0.023	0.023	0.000	-0.394
O	0.009	0.009	0.009	0.000	-0.352
H	0.016	0.016	0.016	0.000	0.327
H	0.026	0.021	0.024	-0.005	0.075
H	0.019	0.021	0.020	0.002	0.059
H	0.019	0.020	0.020	0.002	0.060
H	0.025	0.020	0.022	-0.005	0.086
C	0.009	0.019	0.014	0.010	0.382
O	0.022	0.033	0.028	0.011	-0.398
O	0.003	0.008	0.006	0.005	-0.349
H	0.016	0.018	0.017	0.002	0.327
H	0.012	0.014	0.013	0.002	0.087
H	0.013	0.015	0.014	0.001	0.093

Table 28: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for LSH0.

Atom	f^-	f^+	f^0	f^d	Charge
S	0.121	0.088	0.105	-0.033	0.124
H	0.026	0.023	0.025	-0.003	-0.038
C	0.001	0.016	0.009	0.015	-0.385
C	0.048	0.048	0.048	0.000	-0.131
C	-0.002	0.004	0.001	0.006	0.087
C	0.070	0.077	0.073	0.007	-0.137
C	-0.003	-0.005	-0.004	-0.002	0.160
C	0.060	0.068	0.064	0.008	-0.084
C	0.008	0.008	0.008	0.000	0.305
C	0.015	0.012	0.014	-0.003	0.025
C	0.015	0.011	0.013	-0.004	-0.012
C	0.005	0.003	0.004	-0.002	0.254
C	0.065	0.072	0.068	0.007	-0.088
C	-0.004	-0.008	-0.006	-0.003	0.176
C	0.071	0.077	0.074	0.006	-0.121
C	0.001	0.008	0.005	0.007	0.088
C	0.051	0.049	0.05	-0.003	-0.127
C	0.002	0.016	0.009	0.014	-0.357
S	0.126	0.087	0.106	-0.039	0.127
H	0.027	0.023	0.025	-0.004	-0.039
H	0.017	0.022	0.019	0.004	0.023
C	0.010	0.007	0.008	-0.003	-0.131
N	0.005	0.005	0.005	-0.001	-0.366
H	0.002	0.004	0.003	0.002	0.204
H	0.024	0.025	0.024	0.001	0.179
C	0.009	0.007	0.008	-0.002	-0.134
N	0.002	0.003	0.003	0.000	-0.361
H	0.005	0.005	0.005	0.000	0.203
H	0.024	0.025	0.025	0.001	0.178
C	0.007	0.009	0.008	0.002	0.367
O	0.021	0.022	0.022	0.002	-0.387
O	0.002	0.003	0.003	0.001	-0.350
H	0.014	0.015	0.015	0.001	0.328
H	0.013	0.018	0.015	0.004	0.007
C	0.006	0.009	0.007	0.003	0.365
O	0.019	0.022	0.021	0.003	-0.383
O	0.004	0.003	0.003	0.000	-0.352
H	0.014	0.015	0.015	0.001	0.327
H	0.020	0.023	0.021	0.003	0.079
H	0.016	0.017	0.017	0.002	0.082
H	0.020	0.020	0.02	0.000	0.059
H	0.020	0.020	0.020	-0.001	0.061
H	0.009	0.012	0.010	0.002	0.087
H	0.011	0.012	0.012	0.001	0.090

Table 29: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for LSHN1.

Atom	f^-	f^+	f^0	f^d	Charge
S	0.074	0.070	0.072	-0.004	0.112
H	0.024	0.020	0.022	-0.004	-0.051
C	0.028	0.010	0.019	-0.018	-0.172
C	0.015	0.045	0.030	0.030	-0.075
N	0.006	-0.015	-0.004	-0.021	-0.126
C	0.053	0.058	0.056	0.005	-0.099
C	0.000	0.029	0.015	0.029	0.081
C	0.030	0.025	0.027	-0.005	0.093
C	0.032	0.026	0.029	-0.006	0.073
N	0.005	-0.012	-0.003	-0.017	-0.116
C	0.014	0.051	0.032	0.037	-0.089
C	0.027	0.008	0.018	-0.019	-0.175
C	0.056	0.050	0.053	-0.007	-0.121
C	-0.004	0.028	0.012	0.033	0.159
C	0.003	0.034	0.019	0.031	0.222
C	0.082	0.023	0.053	-0.059	-0.109
C	0.004	0.028	0.016	0.024	0.204
C	0.083	0.034	0.058	-0.049	-0.098
S	0.074	0.068	0.071	-0.005	0.116
H	0.024	0.021	0.023	-0.003	-0.050
C	0.018	0.025	0.021	0.007	-0.131
N	0.025	0.026	0.025	0.001	-0.365
H	0.000	0.002	0.001	0.002	0.185
H	0.008	0.009	0.009	0.001	0.203
C	0.014	0.018	0.016	0.004	-0.115
N	-0.001	-0.002	-0.001	-0.001	-0.373
H	0.010	0.011	0.01	0.001	0.203
H	0.027	0.027	0.027	0.000	0.177
H	0.027	0.022	0.024	-0.005	0.034
C	0.012	0.014	0.013	0.001	0.355
O	0.025	0.024	0.025	0.000	-0.396
O	0.009	0.009	0.009	0.000	-0.351
H	0.016	0.016	0.016	0.000	0.328
H	0.016	0.013	0.014	-0.002	0.066
H	0.025	0.021	0.023	-0.004	0.082
H	0.024	0.019	0.022	-0.005	0.028
H	0.020	0.019	0.019	-0.001	0.067
H	0.020	0.020	0.020	0.000	0.071
C	0.009	0.018	0.014	0.009	0.385
O	0.022	0.032	0.027	0.011	-0.395
O	0.003	0.009	0.006	0.005	-0.353
H	0.015	0.018	0.016	0.003	0.329
H	0.013	0.014	0.013	0.001	0.095
H	0.012	0.014	0.013	0.003	0.091

Table 30: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for LSHN2.

Atom	f^-	f^+	f^0	f^d	Charge
S	0.071	0.079	0.075	0.007	0.128
H	0.031	0.027	0.029	-0.003	-0.043
C	0.000	0.015	0.008	0.016	-0.139
C	0.060	0.023	0.041	-0.037	-0.139
N	0.006	0.003	0.005	-0.003	-0.114
C	0.016	0.051	0.033	0.035	0.368
N	-0.013	0.01	-0.002	0.023	-0.073
C	0.025	0.020	0.022	-0.005	-0.104
C	0.019	0.023	0.021	0.004	-0.173
C	0.008	0.014	0.011	0.006	-0.061
C	0.017	0.028	0.022	0.011	0.202
C	0.047	0.035	0.041	-0.012	-0.130
C	0.004	0.03	0.017	0.026	0.176
C	0.066	0.027	0.046	-0.039	-0.232
C	0.002	0.039	0.020	0.037	0.152
C	0.097	0.036	0.066	-0.061	-0.153
C	-0.009	0.028	0.009	0.036	0.164
C	0.115	0.034	0.074	-0.082	-0.206
S	0.077	0.076	0.077	-0.001	0.122
H	0.018	0.022	0.02	0.004	-0.045
H	0.031	0.019	0.025	-0.012	0.087
H	0.015	0.022	0.019	0.007	0.073
C	0.007	0.017	0.012	0.010	-0.097
N	-0.003	-0.006	-0.004	-0.003	-0.385
H	0.011	0.010	0.010	-0.001	0.203
H	0.031	0.027	0.029	-0.004	0.174
C	0.005	0.009	0.007	0.004	0.375
O	0.022	0.021	0.022	-0.001	-0.393
O	0.007	0.007	0.007	0.000	-0.354
H	0.016	0.014	0.015	-0.001	0.326
H	0.021	0.022	0.021	0.001	0.035
H	0.021	0.021	0.021	0.000	0.066
C	0.010	0.019	0.014	0.009	-0.128
N	0.002	0.003	0.003	0.001	-0.361
H	0.004	0.007	0.005	0.003	0.200
H	0.023	0.026	0.024	0.003	0.178
C	0.008	0.018	0.013	0.010	0.368
O	0.021	0.032	0.027	0.011	-0.386
O	0.002	0.006	0.004	0.004	-0.350
H	0.014	0.018	0.016	0.004	0.326
H	0.017	0.020	0.018	0.003	0.085
H	0.032	0.021	0.026	-0.010	0.077
H	0.017	0.014	0.016	-0.003	0.090
H	0.010	0.014	0.012	0.004	0.090

Table 31: Mulliken condensed Fukui functions, dual descriptor, and Mulliken atomic charge for LSHN3.

Atom	f^-	f^+	f^0	f^d	Charge
C	0.009	0.019	0.014	0.010	0.382
O	0.022	0.033	0.028	0.011	-0.398
O	0.003	0.008	0.005	0.006	-0.349
H	0.016	0.018	0.017	0.003	0.327
C	0.017	0.025	0.021	0.008	-0.123
N	0.025	0.025	0.025	0.000	-0.364
H	0.000	0.002	0.001	0.002	0.184
H	0.009	0.009	0.009	0.001	0.202
C	-0.002	0.030	0.014	0.032	0.085
C	0.057	0.057	0.057	0.000	-0.084
C	0.095	0.028	0.062	-0.066	-0.166
C	-0.002	0.035	0.017	0.036	0.163
C	0.049	0.022	0.035	-0.027	-0.109
C	-0.005	0.020	0.008	0.025	-0.105
N	0.005	-0.007	-0.001	-0.012	-0.090
C	0.030	0.023	0.027	-0.008	0.089
C	0.032	0.025	0.029	-0.007	0.081
C	-0.001	0.029	0.014	0.030	0.138
C	0.096	0.039	0.068	-0.058	-0.133
C	-0.004	0.031	0.013	0.035	0.162
C	0.058	0.049	0.053	-0.009	-0.084
C	0.051	0.025	0.038	-0.027	-0.110
C	-0.005	0.018	0.006	0.022	-0.087
N	0.005	-0.010	-0.002	-0.015	-0.103
C	0.012	0.016	0.014	0.003	-0.108
N	0.001	0.000	0.000	-0.001	-0.376
H	0.027	0.027	0.027	0.000	0.176
H	0.009	0.010	0.010	0.001	0.204
C	0.012	0.014	0.013	0.001	0.355
O	0.023	0.023	0.023	0.000	-0.394
O	0.009	0.009	0.009	0.000	-0.352
S	0.072	0.079	0.075	0.007	0.151
S	0.073	0.076	0.074	0.003	0.137
H	0.016	0.016	0.016	0.000	0.328
H	0.021	0.015	0.018	-0.006	0.007
H	0.012	0.009	0.011	-0.003	-0.033
H	0.019	0.021	0.020	0.002	0.060
H	0.019	0.021	0.020	0.001	0.060
H	0.027	0.022	0.024	-0.006	0.076
H	0.025	0.020	0.022	-0.005	0.086
H	0.013	0.015	0.014	0.001	0.094
H	0.011	0.014	0.013	0.002	0.088
H	0.018	0.022	0.020	0.003	-0.031
H	0.018	0.021	0.020	0.002	-0.034