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

Electronic supplementary information (ESI)

Exploring function activated chlorins using MCD spectroscopy and DFT methods: design of a chlorin with a remarkably intense, red Q band

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Table S1. Atomic coordinates of the geometry optimized **Syn3**.

	Syn3-Ni				Syn3-Zn		
Atom	**x**	**y**	**z**	**Atom**	**x**	**y**	**z**
C	1.790319	5.137188	-0.4075	C	1.815902	5.231368	0.000226
C	-1.31513	5.44111	0.504556	C	-1.41224	5.528561	0.00019
NI	-0.29451	0.012647	-0.00188	ZN	-0.31677	0.012986	0.000253
C	-0.09044	-4.17479	0.225697	C	-0.04096	-4.2662	0.000084
C	-1.36943	-4.04785	-0.20334	C	-1.39249	-4.1364	0.000135
C	-1.62711	-2.62308	-0.30243	C	-1.6741	-2.70599	0.000198
C	0.443896	-2.82714	0.314697	C	0.505517	-2.91358	0.000105
N	-0.49907	-1.89276	0.004347	N	-0.49822	-1.99497	0.000203
C	1.772497	-2.55179	0.548134	C	1.861477	-2.62288	0.000022
C	2.322377	-1.31265	0.311978	C	2.438484	-1.35814	-0.00004
C	3.822434	-1.11173	0.268381	C	3.942538	-1.14756	-0.00016
C	3.914296	0.298212	-0.25895	C	4.033417	0.366812	-0.00019
C	2.564967	0.792071	-0.30169	C	2.673303	0.851635	-2.8E-05
N	1.634955	-0.19697	0.013447	N	1.773822	-0.20059	0.000044
C	-2.86267	-2.08658	-0.52675	C	-2.93957	-2.16161	0.000187
C	2.27105	2.116745	-0.48497	C	2.334089	2.18977	0.000059
C	1.02136	2.659631	-0.26441	C	1.055113	2.740918	0.000126
C	-3.13978	-0.74215	-0.31872	C	-3.25727	-0.7976	0.000088
C	-4.48043	-0.21413	-0.23595	C	-4.60449	-0.2604	-0.00013
C	-4.35583	1.07967	0.166815	C	-4.47702	1.09826	-0.0002
C	-2.93995	1.337099	0.264742	C	-3.05409	1.376236	-0.00007
N	-2.20517	0.204823	-0.02701	N	-2.34402	0.202025	0.000128
C	-2.40089	2.577421	0.481569	C	-2.48278	2.633306	-6.8E-05
C	-1.05956	2.863011	0.300939	C	-1.12031	2.940203	0.000028
C	-0.53042	4.198052	0.229975	C	-0.58662	4.281242	0.000158
C	0.771279	4.07138	-0.15941	C	0.775887	4.156603	0.000213
N	-0.1031	1.925676	0.012366	N	-0.10765	2.022892	0.000011
C	0.691828	-5.41119	0.526953	C	0.787767	-5.5093	-3.4E-05
C	-2.38041	-5.10814	-0.49462	C	-2.43981	-5.20182	0.000161
S	5.308073	1.086603	-0.65415	S	5.434737	1.235682	-0.00036
C	4.4148	-1.176	1.690232	C	4.595155	-1.73452	1.261988
C	4.529132	-2.11806	-0.64915	C	4.595015	-1.73463	-1.26232
C	-5.71981	-1.00118	-0.518	C	-5.84902	-1.08907	-0.00039
C	-5.42268	2.092554	0.431379	C	-5.54756	2.141457	-0.0006
H	2.43483	-3.37246	0.789498	H	2.540531	-3.46733	-3.5E-05
H	-3.68531	-2.75201	-0.75509	H	-3.77188	-2.85606	0.000169
H	3.100592	2.775743	-0.70804	H	3.17146	2.878485	0.000054
H	-3.07259	3.398134	0.701626	H	-3.16463	3.476949	-0.00014
H	3.918227	-0.4704	2.360542	H	4.128579	-1.34292	2.169101
H	5.477533	-0.92704	1.649065	H	5.655124	-1.47188	1.277331

H	4.303283	-2.18232	2.100784	H	4.50369	-2.8231	1.268827
H	4.465109	-3.12834	-0.23982	H	4.503551	-2.82322	-1.26904
H	4.088857	-2.12043	-1.64889	H	4.128341	-1.34312	-2.16942
H	5.582569	-1.84546	-0.7362	H	5.654983	-1.47199	-1.27781
H	-6.61172	-0.38023	-0.42325	H	-6.74366	-0.46458	0.001908
H	-5.71084	-1.4132	-1.53176	H	-5.90001	-1.73552	-0.88233
H	-5.82844	-1.84306	0.173156	H	-5.89796	-1.73911	0.879006
H	-5.32729	2.520819	1.433611	H	-5.47503	2.789114	0.878728
H	-6.41614	1.648597	0.355247	H	-6.54183	1.692447	0.001709
H	-5.37529	2.9214	-0.28195	H	-5.47764	2.785756	-0.88262
H	1.348242	6.131452	-0.32893	H	1.362354	6.223655	0.001687
H	2.227911	5.048459	-1.40634	H	2.4617	5.165294	-0.88094
H	2.613033	5.083515	0.312374	H	2.463502	5.163523	0.879919
H	-1.75155	5.42687	1.507877	H	-2.06018	5.581694	0.880804
H	-2.13885	5.563389	-0.20597	H	-2.05956	5.582143	-0.88086
H	-0.68518	6.328878	0.432875	H	-0.7844	6.42078	0.000625
H	0.076683	-6.30511	0.415972	H	0.164196	-6.40435	0.00053
H	1.551559	-5.51417	-0.14264	H	1.435664	-5.55667	-0.88102
H	1.078121	-5.39913	1.55077	H	1.436585	-5.55621	0.880292
H	-3.22977	-5.05024	0.193236	H	-3.08489	-5.1262	0.881053
H	-2.77748	-5.01046	-1.50941	H	-3.08546	-5.12568	-0.88027
H	-1.94645	-6.10453	-0.4023	H	-1.99524	-6.19793	-0.00028

Table S2. Atomic coordinates of the geometry optimized **Syn6**.

Syn6-Ni				Syn6-Zn			
Atom	**x**	**y**	**z**	**Atom**	**x**	**y**	**z**
C	2.961591	-1.461717	2.065499	C	3.304453	-1.788404	1.629666
NI	-1.739156	0.046778	-0.218211	ZN	-1.798303	0.029335	-0.109081
C	3.448392	-2.220343	3.124762	C	3.899163	-2.777923	2.405003
C	4.817874	-2.328356	3.363474	C	5.286014	-2.917137	2.454939
C	-2.00165	-5.288215	-1.679383	C	-1.638645	-5.510224	-1.078462
C	-3.484717	-2.75475	-0.759993	C	-3.316127	-3.003834	-0.391459
N	-3.547944	-0.482973	0.122392	N	-3.720464	-0.638933	0.052367
C	-4.147391	-1.678767	-0.192604	C	-4.150643	-1.929931	-0.079914
C	-5.511845	-1.70629	0.243653	C	-5.573006	-2.006481	0.13
C	-5.739677	-0.508066	0.865904	C	-5.995286	-0.726179	0.388284
C	-4.523518	0.241704	0.749363	C	-4.822602	0.107259	0.326507
C	-0.025846	-2.302387	-0.682818	C	0.114806	-2.246583	-0.692301
C	1.153861	-1.593407	-0.465423	C	1.252512	-1.427083	-0.608934
C	-4.412282	1.594019	1.066122	C	-4.808578	1.502979	0.483396
N	0.090433	0.581265	-0.468269	N	0.183202	0.712217	-0.20728
C	1.197323	-0.234511	-0.352209	C	1.294967	-0.084275	-0.317328
C	2.446056	0.535043	-0.426906	C	2.52787	0.726171	-0.278608
C	2.033901	1.825127	-1.129467	C	2.051658	2.149266	-0.576499
C	0.536069	1.812453	-0.813302	C	0.55616	2.002433	-0.263897
C	-0.234599	2.939864	-0.852041	C	-0.287549	3.086582	-0.14416
N	-2.223371	1.872359	0.049526	N	-2.420306	1.925185	0.138763
C	-1.523166	2.968656	-0.327112	C	-1.668638	3.047675	0.079719
C	-3.358702	2.365116	0.673068	C	-3.719039	2.333904	0.380896
C	-3.34054	3.811188	0.692769	C	-3.764777	3.782286	0.482115
C	-2.216403	4.18989	0.028931	C	-2.493449	4.227886	0.286552
C	1.137381	-4.554266	-1.257538	C	1.416881	-4.437055	-1.235302
C	-6.446075	-2.859557	0.054767	C	-6.382757	-3.263049	0.064893
C	-6.992996	-0.008475	1.512835	C	-7.380149	-0.236829	0.67473
C	2.69988	3.087442	-0.571941	C	2.69305	3.218296	0.315437
C	2.156369	1.726189	-2.667522	C	2.126081	2.49681	-2.08195
C	5.718453	-1.648981	2.553118	C	6.095085	-2.034607	1.751892
C	5.231473	-0.887931	1.497567	C	5.498967	-1.042154	0.982835
C	5.950659	-0.03321	0.556577	C	6.116272	0.056078	0.245687
C	7.317357	0.153799	0.399493	C	7.461102	0.322561	0.026867
C	7.772188	0.992179	-0.61147	C	7.815417	1.432974	-0.729678
C	6.86041	1.612008	-1.462632	C	6.823729	2.249377	-1.267406
C	5.490755	1.420261	-1.306627	C	5.475932	1.976544	-1.05299
C	3.854772	-0.809182	1.215011	C	4.101085	-0.92877	0.870913
C	5.012864	0.618238	-0.270488	C	5.098428	0.88456	-0.270814
C	3.644687	0.156787	0.092709	C	3.772567	0.28397	0.056817
C	-4.406289	4.660905	1.305385	C	-5.005512	4.573313	0.744439
C	-1.710641	5.563868	-0.271488	C	-1.976898	5.63059	0.279394
N	-1.269237	-1.766213	-0.602151	N	-1.160807	-1.842443	-0.485037
C	-0.067955	-3.686898	-1.081606	C	0.163839	-3.667346	-0.960418
C	-1.38447	-3.991808	-1.263209	C	-1.124458	-4.118465	-0.891209

C	-2.125613	-2.803258	-0.926559	C	-1.948211	-2.97067	-0.586166
H	-6.52919	-3.141127	-0.999488	H	-6.315719	-3.734871	-0.920732
H	-7.449479	-2.61764	0.408665	H	-7.438047	-3.068254	0.26311
H	-6.816132	0.303018	2.546923	H	-7.441182	0.251546	1.652653
H	-7.763053	-0.781375	1.531165	H	-8.100838	-1.056334	0.672899
H	-7.407294	0.85465	0.981446	H	-7.712386	0.493276	-0.070491
H	2.35767	3.972955	-1.112255	H	2.298001	4.207566	0.073103
H	3.782757	3.052696	-0.659733	H	3.773625	3.261075	0.200732
H	2.452466	3.215771	0.483918	H	2.476714	3.015201	1.366702
H	1.623501	0.848041	-3.040546	H	1.570608	1.760972	-2.669049
H	3.193732	1.648517	-2.992942	H	3.147597	2.513153	-2.459174
H	1.718648	2.614058	-3.130601	H	1.679868	3.478519	-2.258438
H	-4.062265	-3.640058	-0.999279	H	-3.793126	-3.974049	-0.485246
H	2.087292	-2.138445	-0.472689	H	2.202981	-1.916157	-0.773082
H	-5.256237	2.076432	1.544484	H	-5.764442	1.976074	0.681772
H	0.215223	3.875436	-1.153242	H	0.158494	4.070525	-0.216464
H	1.892887	-1.391202	1.915581	H	2.226794	-1.700698	1.626012
H	2.74687	-2.732518	3.775224	H	3.269883	-3.446546	2.983426
H	5.178288	-2.929038	4.192106	H	5.731679	-3.699406	3.06054
H	6.784471	-1.699017	2.751854	H	7.176187	-2.105612	1.818971
H	8.021651	-0.356454	1.049011	H	8.225288	-0.33164	0.434664
H	8.836736	1.150666	-0.748468	H	8.861421	1.65782	-0.909825
H	7.218077	2.247742	-2.265837	H	7.099711	3.109449	-1.868555
H	4.821718	1.897774	-2.006945	H	4.745406	2.62917	-1.504858
H	-4.149886	5.71983	1.250548	H	-4.794426	5.642451	0.795196
H	-4.558431	4.409925	2.359461	H	-5.471384	4.281732	1.690877
H	-5.366972	4.525462	0.79853	H	-5.750717	4.419366	-0.042332
H	-1.552295	5.706342	-1.345175	H	-1.514276	5.882314	-0.680539
H	-0.753954	5.75792	0.224296	H	-1.216215	5.781645	1.05204
H	-2.415928	6.326902	0.061253	H	-2.776493	6.351153	0.458056
H	-2.618362	-5.713931	-0.881343	H	-2.166134	-5.865785	-0.187765
H	-1.239289	-6.025724	-1.934542	H	-0.827506	-6.21083	-1.282342
H	-2.646562	-5.161477	-2.554085	H	-2.342789	-5.56813	-1.914478
H	0.856084	-5.570489	-1.538147	H	1.210909	-5.500889	-1.364154
H	1.724552	-4.617951	-0.335845	H	2.13693	-4.337118	-0.416737
H	1.802001	-4.167958	-2.036905	H	1.914427	-4.085468	-2.145062
H	-6.10971	-3.746742	0.600979	H	-6.041429	-4.000554	0.798373

Table S3. Atomic coordinates of the geometry optimized **Lie95**.

Lie95-Ni				Lie95-Zn			
Atom	**x**	**y**	**z**	**Atom**	**x**	**y**	**z**
N	-2.521961	-0.054069	-0.374101	N	-2.638338	0.050956	-0.287244
N	-1.910677	2.599226	-0.111687	N	-1.797474	2.825758	-0.044479
N	0.745629	2.000349	-0.289887	N	0.968961	2.068733	-0.463854
N	0.132639	-0.6328	-0.515632	N	0.126407	-0.675767	-0.699714
C	-3.775534	0.46489	-0.613879	C	-3.846441	0.660059	-0.065615
C	-2.649996	-1.396408	-0.199613	C	-2.805347	-1.279261	-0.436708
C	-4.093021	-1.867031	-0.21873	C	-4.267072	-1.691126	-0.332477
C	-4.791263	-0.596235	-0.655447	C	-4.925974	-0.34531	-0.060251
C	-3.243623	2.793964	-0.327946	C	-3.130461	3.017601	0.145275
C	-3.641814	4.145815	-0.041409	C	-3.422202	4.413312	0.365803
C	-2.515881	4.769942	0.395866	C	-2.220792	5.054853	0.303641
C	-1.447927	3.824139	0.321119	C	-1.213581	4.067336	0.050064
C	-4.13159	1.773787	-0.653405	C	-4.087875	1.991512	0.131044
C	0.910977	3.302274	0.129011	C	1.160257	3.41803	-0.319091
C	1.992008	1.604002	-0.685153	C	2.192052	1.528827	-0.695797
C	2.949944	2.668616	-0.552732	C	3.205886	2.558295	-0.707832
C	2.274018	3.723296	-0.004585	C	2.555741	3.741348	-0.465695
C	-0.121411	4.14387	0.484889	C	0.142692	4.332136	-0.077868
C	-0.295089	-1.908755	-0.337114	C	-0.4301	-1.907678	-0.780905
C	0.766315	-2.865364	-0.560673	C	0.590926	-2.918201	-1.011856
C	1.855047	-2.145572	-0.935235	C	1.779143	-2.259388	-1.073281
C	1.46436	-0.752407	-0.876003	C	1.483555	-0.846998	-0.881226
C	2.324519	0.295487	-1.024875	C	2.422206	0.156717	-0.89203
C	-1.611899	-2.276775	-0.099462	C	-1.793815	-2.189082	-0.663801
C	-4.525012	-2.218322	1.232872	C	-4.478392	-2.655562	0.860055
C	-4.355981	-3.003595	-1.209519	C	-4.790617	-2.255608	-1.661408
C	-6.018184	-2.360303	1.427554	C	-5.911525	-2.800456	1.323101
O	-6.716439	-1.541779	1.979862	O	-6.325818	-2.410089	2.390299
O	-6.485635	-3.514046	0.935405	O	-6.673104	-3.450185	0.433982
O	-5.965223	-0.484799	-0.950934	O	-6.115612	-0.157162	0.111667
C	-7.8998	-3.711968	1.061637	C	-8.05341	-3.591295	0.791101
C	0.624304	-4.346726	-0.42228	C	0.322171	-4.382599	-1.14255
C	-5.024851	4.69486	-0.181293	C	-4.776684	4.996712	0.611447
C	2.801049	5.076467	0.353509	C	3.141073	5.114048	-0.365901
NI	-0.886227	0.978675	-0.325444	ZN	-0.814031	1.082805	-0.380694
C	3.226832	-2.646937	-1.267992	C	3.15338	-2.826546	-1.254932
C	4.092763	-2.829931	-0.019621	C	3.893946	-2.991778	0.074652
C	5.519563	-3.17338	-0.353547	C	5.33164	-3.396331	-0.113222
O	5.974826	-3.293266	-1.469114	O	5.889436	-3.545122	-1.177728
O	6.257055	-3.3361	0.756444	O	5.948103	-3.57706	1.065001
C	7.633353	-3.667742	0.541091	C	7.327004	-3.954823	0.988843
C	4.399443	2.63879	-0.94897	C	4.676463	2.378423	-0.95736
C	5.382108	2.501905	0.221206	C	5.533065	2.270082	0.312374
C	5.468979	1.097412	0.761764	C	5.498667	0.89874	0.939147
O	5.305483	0.092145	0.101352	O	5.369295	-0.139817	0.323953

O	5.79499	1.078478	2.056158	O	5.676903	0.946198	2.261548
C	5.934861	-0.216916	2.656113	C	5.700068	-0.317201	2.940197
H	-2.404495	5.798963	0.711331	H	-2.033824	6.114421	0.421947
H	-5.176033	2.000061	-0.829743	H	-5.126032	2.260785	0.293146
H	0.120401	5.148238	0.812337	H	0.43419	5.372782	0.021846
H	3.35324	0.086902	-1.284427	H	3.453421	-0.139063	-1.037652
H	-1.833674	-3.327019	0.038207	H	-2.083543	-3.22897	-0.762719
H	-4.036083	-3.15275	1.519588	H	-4.101125	-3.644214	0.583711
H	-4.195501	-1.432433	1.914345	H	-3.911408	-2.304402	1.72319
H	-3.937256	-2.761921	-2.188996	H	-4.56214	-1.573534	-2.484141
H	-3.909151	-3.938726	-0.865439	H	-4.324577	-3.219528	-1.878456
H	-5.429766	-3.157284	-1.315979	H	-5.870208	-2.394779	-1.608725
H	-8.19056	-3.71668	2.113127	H	-8.151671	-4.157448	1.718409
H	-8.440923	-2.919527	0.542833	H	-8.511884	-2.609569	0.918607
H	-8.10598	-4.677709	0.605113	H	-8.520196	-4.126347	-0.033272
H	-0.164526	-4.737991	-1.072297	H	-0.382556	-4.589602	-1.954092
H	0.370104	-4.63241	0.603428	H	-0.112379	-4.793529	-0.225599
H	1.553181	-4.855382	-0.686224	H	1.238737	-4.937071	-1.350362
H	-5.732197	4.178541	0.475249	H	-5.238008	4.580114	1.512421
H	-5.398721	4.591231	-1.204523	H	-5.459061	4.797614	-0.220831
H	-5.043223	5.755473	0.076196	H	-4.712496	6.078963	0.739302
H	3.819966	5.211063	-0.014183	H	4.169926	5.134045	-0.730584
H	2.81977	5.228116	1.437694	H	3.154394	5.471427	0.669245
H	2.189151	5.875294	-0.074793	H	2.568917	5.839583	-0.950843
H	3.153589	-3.59792	-1.802837	H	3.0967	-3.793325	-1.761369
H	3.731692	-1.958744	-1.949449	H	3.746231	-2.180746	-1.907921
H	3.691273	-3.612133	0.632315	H	3.403673	-3.733676	0.712579
H	4.118542	-1.909064	0.567116	H	3.90284	-2.052141	0.6326
H	7.719774	-4.608072	-0.005835	H	7.437821	-4.894875	0.445873
H	8.133448	-2.879428	-0.023834	H	7.908388	-3.181202	0.484475
H	8.074836	-3.763579	1.531109	H	7.661553	-4.070053	2.017969
H	4.633907	3.569293	-1.474488	H	5.04017	3.23326	-1.534132
H	4.589728	1.832549	-1.660223	H	4.858662	1.494893	-1.573359
H	5.139445	3.185063	1.037106	H	5.247257	3.0145	1.057725
H	6.39258	2.760236	-0.117049	H	6.583812	2.458839	0.062341
H	6.417229	-0.048938	3.61691	H	6.044143	-0.105231	3.950408
H	6.5343	-0.874534	2.026961	H	6.370365	-1.014675	2.437824
H	4.951016	-0.666554	2.804643	H	4.696437	-0.745981	2.966904

Table S4. Atomic coordinates of the geometry optimized **M1** and **M2**.

M1				M2			
Atom	**x**	**y**	**z**	**Atom**	**x**	**y**	**z**
C	-0.046193	-0.073811	-0.166063	C	5.877395	-1.492466	0.863706
ZN	5.460032	-1.106522	0.068414	C	-0.505521	-1.36163	-1.547084
C	-1.245019	-0.736324	-0.378654	C	0.379557	-0.382016	-2.014225
C	-2.476589	-0.06316	-0.348576	C	5.56007	-0.394586	0.060528
C	3.065909	-4.626806	3.743435	C	6.460017	0.694565	-0.271519
C	-2.379488	6.891909	0.630331	C	5.747701	1.535107	-1.139959
C	-2.146364	8.20011	0.303844	C	4.440042	0.937397	-1.307091
C	5.350188	-4.065269	1.735388	N	4.367743	-0.209082	-0.562695
N	6.636236	-2.766716	0.120606	C	3.414001	1.426038	-2.102165
C	6.414792	-3.901973	0.850096	C	10.836828	0.401398	-0.688491
C	7.447623	-4.871377	0.588494	C	7.653561	2.973615	-1.274336
C	8.303774	-4.290992	-0.313412	C	6.355756	2.689401	-1.643694
C	7.779956	-2.975918	-0.581338	N	9.698036	2.467081	-0.037944
C	3.066652	-1.382268	1.914583	C	10.653933	1.445667	0.214208
C	2.512058	-0.152843	1.522379	C	10.077357	3.823225	0.146707
C	8.383941	-2.012284	-1.406164	C	2.070427	-4.465219	1.037947
N	4.265381	0.62522	0.035747	C	0.994053	-3.864988	0.412573
C	3.022418	0.736797	0.606475	C	-0.353456	-4.572301	0.217392
C	2.40092	2.024596	0.256871	C	-1.215799	-3.386576	-0.218237
C	3.568637	2.89242	-0.216638	C	-0.245361	-2.365996	-0.641366
C	4.601386	1.798001	-0.525335	N	1.007398	-2.653552	-0.16058
C	5.761884	2.043105	-1.230357	C	11.767625	-0.604811	-0.447992
N	6.803062	-0.166577	-1.097435	C	12.552885	-0.560016	0.702263
C	6.767305	1.116008	-1.526257	C	12.384957	0.491453	1.606598
C	7.951019	-0.726596	-1.626294	C	11.4408	1.474312	1.370598
C	8.654682	0.26279	-2.424956	C	9.265972	4.705745	0.869513
C	7.925968	1.410142	-2.356226	C	11.277058	4.300346	-0.374271
C	1.177523	-1.99545	3.600383	C	11.674532	5.619977	-0.178925
C	7.526295	-6.228914	1.212466	C	9.641549	6.024608	1.047706
C	9.549818	-4.856076	-0.91928	C	10.851895	6.492623	0.529773
C	3.259433	3.725732	-1.464674	O	13.49833	-1.482316	1.029304
C	4.184015	3.736519	0.923754	O	11.136585	7.80153	0.770034
C	-2.475788	1.314336	-0.116571	C	13.711119	-2.560915	0.137214
C	-1.275029	1.972582	0.098617	C	12.352456	8.320516	0.263651
C	-1.020806	3.401381	0.257145	C	-0.821801	-5.235251	1.517357
C	-1.924027	4.446805	0.358026	C	7.766879	0.989416	0.118625
C	-1.458007	5.75295	0.530432	C	8.372876	2.135025	-0.387224
C	-0.073456	5.958233	0.615815	C	-1.343453	0.800303	-3.568396
C	0.828246	4.909015	0.510617	C	4.402786	-4.562744	1.973303
C	-0.041808	1.29428	0.115016	C	5.469697	-3.71747	1.941869
C	0.372484	3.60662	0.30316	C	5.063709	-2.565131	1.157899
C	1.062783	2.291166	0.24756	C	3.34075	-3.917407	1.219564
C	9.936272	0.007971	-3.15041	N	3.760558	-2.719261	0.737069
C	8.197882	2.738553	-2.985298	C	-8.802736	-8.295114	-0.07596
N	4.210684	-1.917317	1.424336	C	2.144643	0.888304	-2.261916

C	2.449587	-2.279365	2.865987	C	1.110676	1.455575	-3.093588
C	3.245888	-3.38925	2.923292	C	0.00789	0.66047	-2.941711
C	4.341213	-3.159086	2.009421	N	1.676188	-0.23749	-1.6275
C	-3.267793	9.049522	0.526561	C	4.277645	-5.896075	2.637271
C	-4.343978	8.379845	1.02043	C	6.818897	-3.885466	2.562678
S	-4.005275	6.701319	1.227881	C	-2.569675	-3.226113	-0.138247
S	-5.24286	-0.238053	0.029306	C	-3.635854	-4.262765	-0.127903
C	-3.720287	-0.799697	-0.594969	C	-3.303781	-1.933767	-0.002204
C	-6.103522	-1.570797	-0.689064	C	-3.618251	-5.649191	-0.288054
C	-3.891353	-1.961199	-1.303599	C	-4.805523	-6.365305	-0.335649
C	-5.235619	-2.396846	-1.357388	C	-6.053517	-5.733933	-0.235648
C	-7.537129	-1.698023	-0.547128	C	-6.08176	-4.343136	-0.10442
C	-8.406937	-0.841842	0.100848	C	-4.894281	-3.630969	-0.060399
C	-9.745562	-1.257823	0.046313	C	-4.686173	-2.191263	0.057119
C	-9.924338	-2.44161	-0.645794	C	-5.614817	-1.185122	0.273272
S	-8.388983	-3.037042	-1.230109	C	-0.121965	-5.589792	-0.924774
C	-11.099972	-3.193444	-0.937701	S	-8.787313	-5.857597	-0.855685
C	-12.394795	-2.948043	-0.603377	C	-9.628318	-7.337902	-0.578626
C	-12.821563	-1.820555	0.152664	C	-7.466416	-7.833403	0.096741
C	-13.431172	-3.919364	-1.058181	C	-7.287333	-6.529103	-0.276247
N	-13.230433	-0.924054	0.764467	C	1.270474	2.682522	-3.933828
O	-13.163809	-4.90936	-1.698204	C	-5.178517	0.127779	0.465545
O	-14.704004	-3.65711	-0.729582	C	-3.7974	0.380843	0.460646
H	7.600993	-6.166729	2.302898	ZN	2.712216	-1.441599	-0.402471
H	8.396872	-6.781874	0.855952	C	-2.872079	-0.628558	0.245903
H	9.491861	-4.879365	-2.012218	O	-15.577184	7.501777	0.558073
H	9.730659	-5.877204	-0.579379	O	-13.645745	8.316147	1.253771
H	10.431368	-4.262195	-0.656528	N	-15.182084	4.217765	-0.422728
H	4.143782	4.283523	-1.78071	C	-14.267121	7.37753	0.813332
H	2.46361	4.447153	-1.293025	C	-14.462085	5.02009	0.005157
H	2.953331	3.078768	-2.289821	C	-13.638717	6.054238	0.532359
H	4.463067	3.096733	1.764718	C	-12.313215	5.90892	0.797479
H	3.497779	4.494397	1.299813	S	-9.782302	4.918676	1.064159
H	5.085102	4.240091	0.565611	C	-11.469021	4.771802	0.632581
H	5.304384	-5.011377	2.264945	C	-11.735287	3.494982	0.172957
H	1.567771	0.111954	1.979292	C	-10.610776	2.656022	0.178207
H	9.306295	-2.305713	-1.895934	C	-9.465024	3.27441	0.64082
H	5.905481	3.045091	-1.614764	C	-7.053002	3.231969	1.430909
H	0.87366	-0.639293	-0.213318	C	-5.914144	2.394381	1.383682
H	-1.226881	-1.804915	-0.561686	C	-8.142576	2.706294	0.78399
H	-3.40528	1.874378	-0.147251	C	-6.124167	1.222961	0.702417
H	-2.990338	4.252858	0.295133	S	-7.751352	1.156792	0.092934
H	0.304383	6.958818	0.793965	H	-1.590068	-0.065369	-4.19161
H	10.266779	0.89079	-3.699498	H	-2.130155	0.886369	-2.812051
H	9.831163	-0.810228	-3.86959	H	-1.398708	1.687014	-4.201851
H	10.737243	-0.271768	-2.458878	H	2.062908	2.558344	-4.67863
H	8.291584	3.526844	-2.231267	H	0.350494	2.920948	-4.469658
H	7.389476	3.034901	-3.661398	H	1.533257	3.554154	-3.326

H	9.123214	2.724513	-3.563219	H	5.203234	-6.179188	3.140728
H	2.987623	-5.517993	3.11277	H	3.624505	2.335936	-2.654612
H	2.161777	-4.573791	4.351775	H	0.589258	-6.353624	-0.601368
H	3.910842	-4.784723	4.421025	H	-1.039067	-6.088312	-1.235147
H	0.889744	-2.833442	4.237255	H	0.293462	-5.088055	-1.802386
H	0.348837	-1.806616	2.910279	H	-0.832814	-4.50877	2.332996
H	1.270215	-1.112	4.24036	H	-1.822074	-5.653822	1.430694
H	6.639494	-6.828822	0.984424	H	-0.148915	-6.049143	1.796841
H	-14.794094	-2.83709	-0.220629	H	8.310572	0.34722	0.802049
H	1.879644	5.132537	0.607022	H	8.144898	3.855101	-1.669166
H	-1.206268	8.545282	-0.108685	H	5.832291	3.35231	-2.325557
H	-3.269665	10.112374	0.318701	H	10.237888	0.368535	-1.592106
H	-5.317679	8.771081	1.278127	H	11.878552	-1.403444	-1.170118
H	-3.078423	-2.476308	-1.79891	H	12.99949	0.511812	2.499897
H	-5.551591	-3.28807	-1.886738	H	11.310417	2.2805	2.084173
H	-8.083791	0.063892	0.598477	H	8.331961	4.349959	1.290345
H	-10.556205	-0.703589	0.49923	H	11.916295	3.628951	-0.937181
H	-10.970654	-4.10525	-1.515959	H	12.616819	5.953043	-0.594645
				H	9.013996	6.711771	1.604525
				H	12.807319	-3.168364	0.017993
				H	14.497213	-3.171615	0.579853
				H	14.039233	-2.209548	-0.847091
				H	12.391563	8.258843	-0.829355
				H	12.385762	9.366998	0.564691
				H	13.21859	7.797307	0.683374
				H	3.479428	-5.897403	3.386363
				H	4.041398	-6.683089	1.913789
				H	7.609594	-3.887896	1.805804
				H	7.04197	-3.071043	3.258928
				H	6.889024	-4.822447	3.116942
				H	-15.966989	6.684607	0.212017
				H	-11.852413	6.810027	1.19513
				H	-12.71447	3.169885	-0.151068
				H	-10.637081	1.619851	-0.134836
				H	-7.071731	4.184161	1.947954
				H	-4.976214	2.636773	1.866638
				H	-10.682066	-7.412112	-0.805842
				H	-9.131364	-9.29666	0.172626
				H	-2.694192	-6.196832	-0.388635
				H	-4.764347	-7.439374	-0.478412
				H	-7.031332	-3.822581	-0.027332
				H	-6.672038	-1.424009	0.334409
				H	-3.441487	1.393191	0.616301
				H	-1.820119	-0.380409	0.265241
				H	1.912554	-5.454471	1.449344
				H	6.879597	-1.513862	1.277674
				H	-1.514182	-1.312839	-1.935135
				H	-6.670785	-8.442586	0.507819

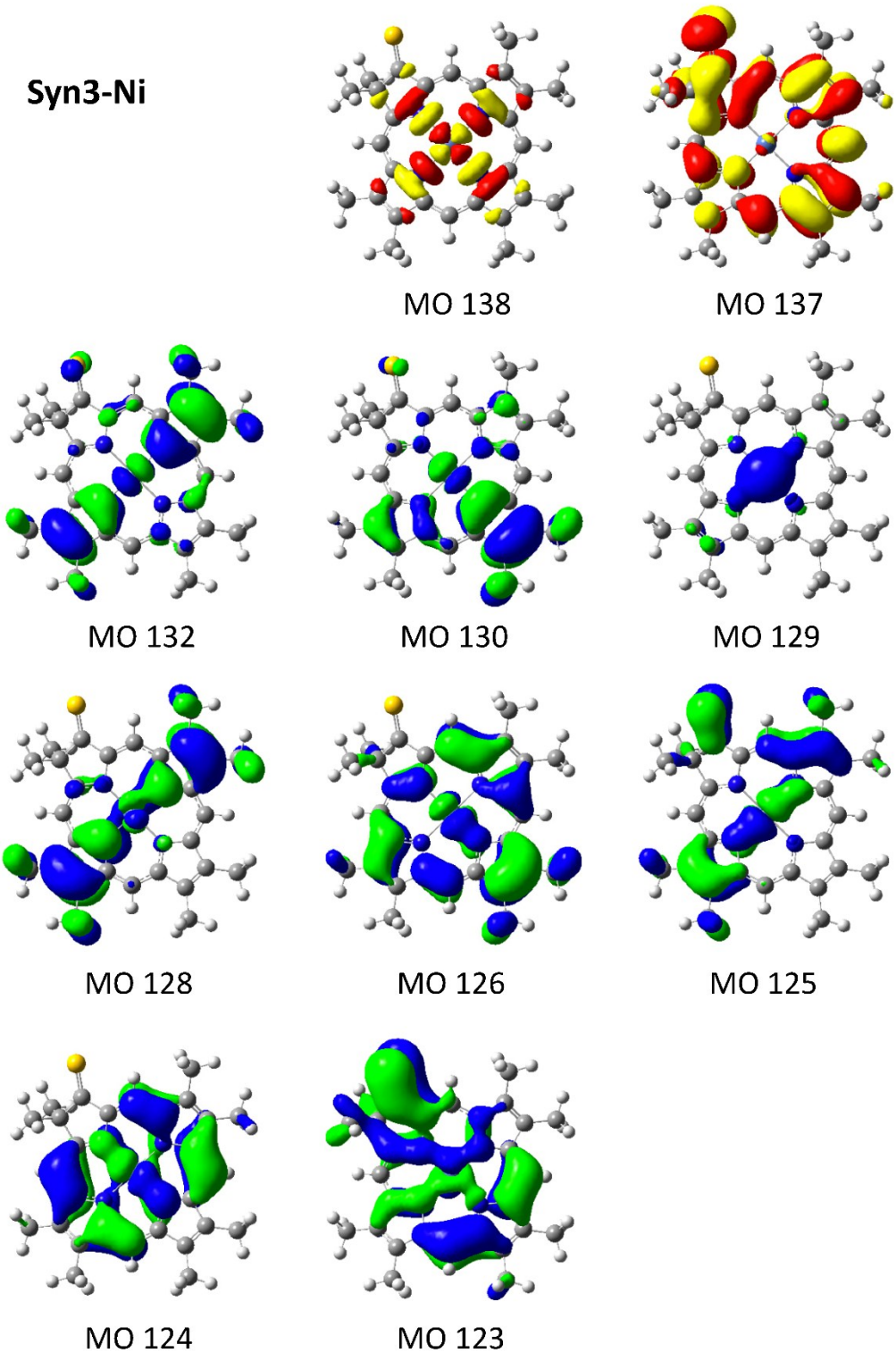

Figure S1. Electron density surfaces for non-Gouterman MOs of Ni-coordinated **Syn3**.

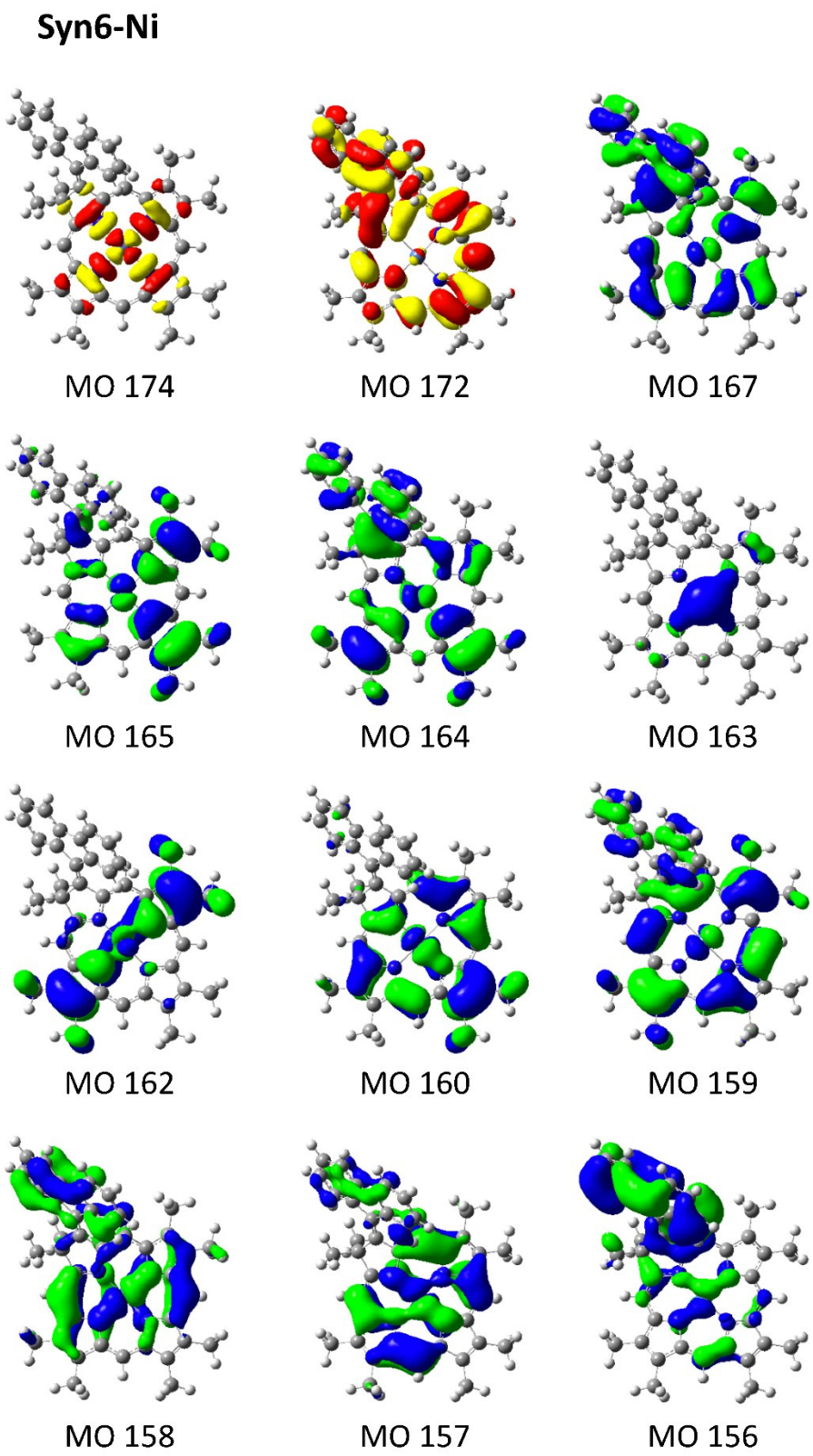

Figure S2. Electron density surfaces for non-Gouterman MOs of Ni-coordinated **Syn6**.

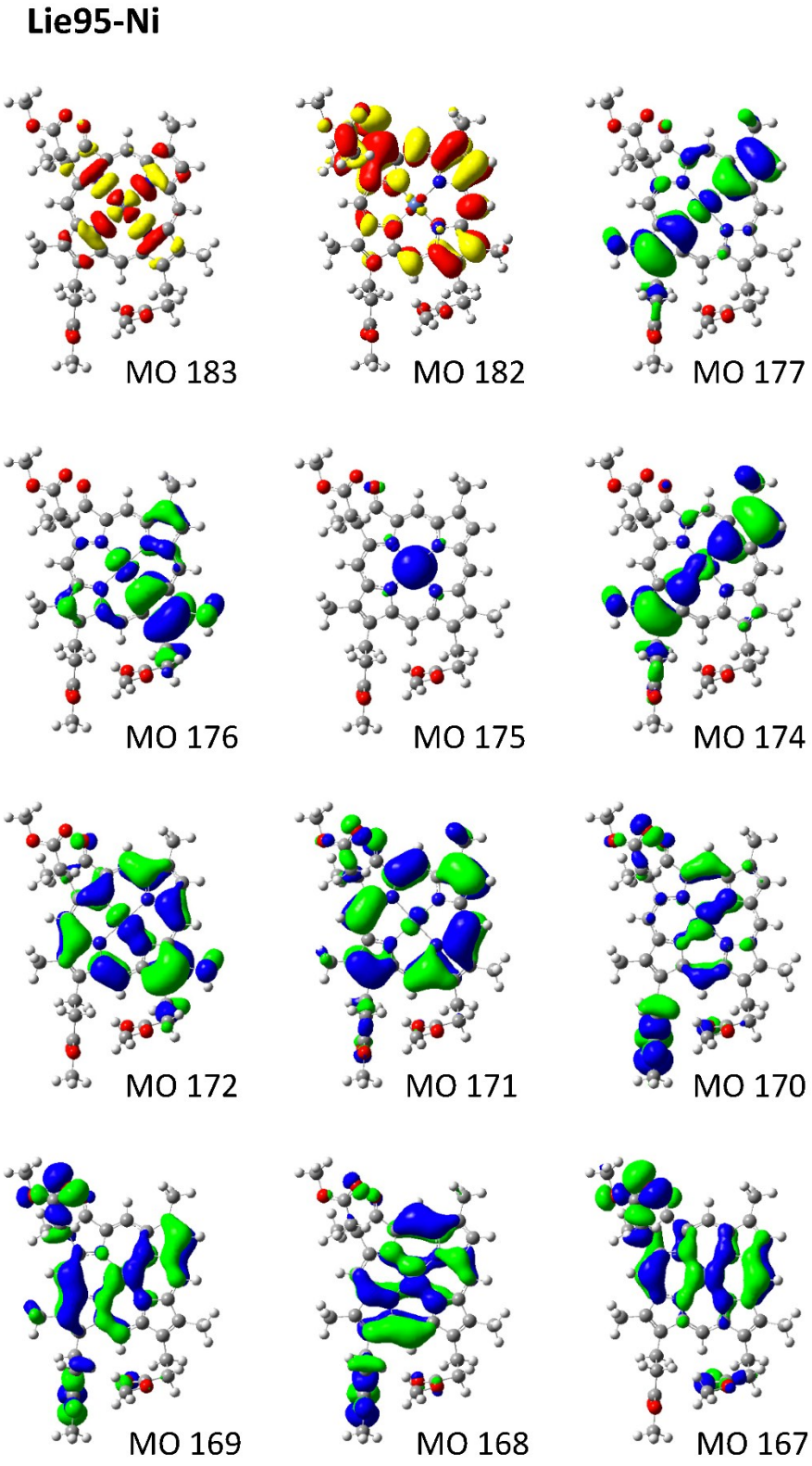

Figure S3. Electron density surfaces for non-Gouterman MOs of Ni-coordinated **Lie95**.

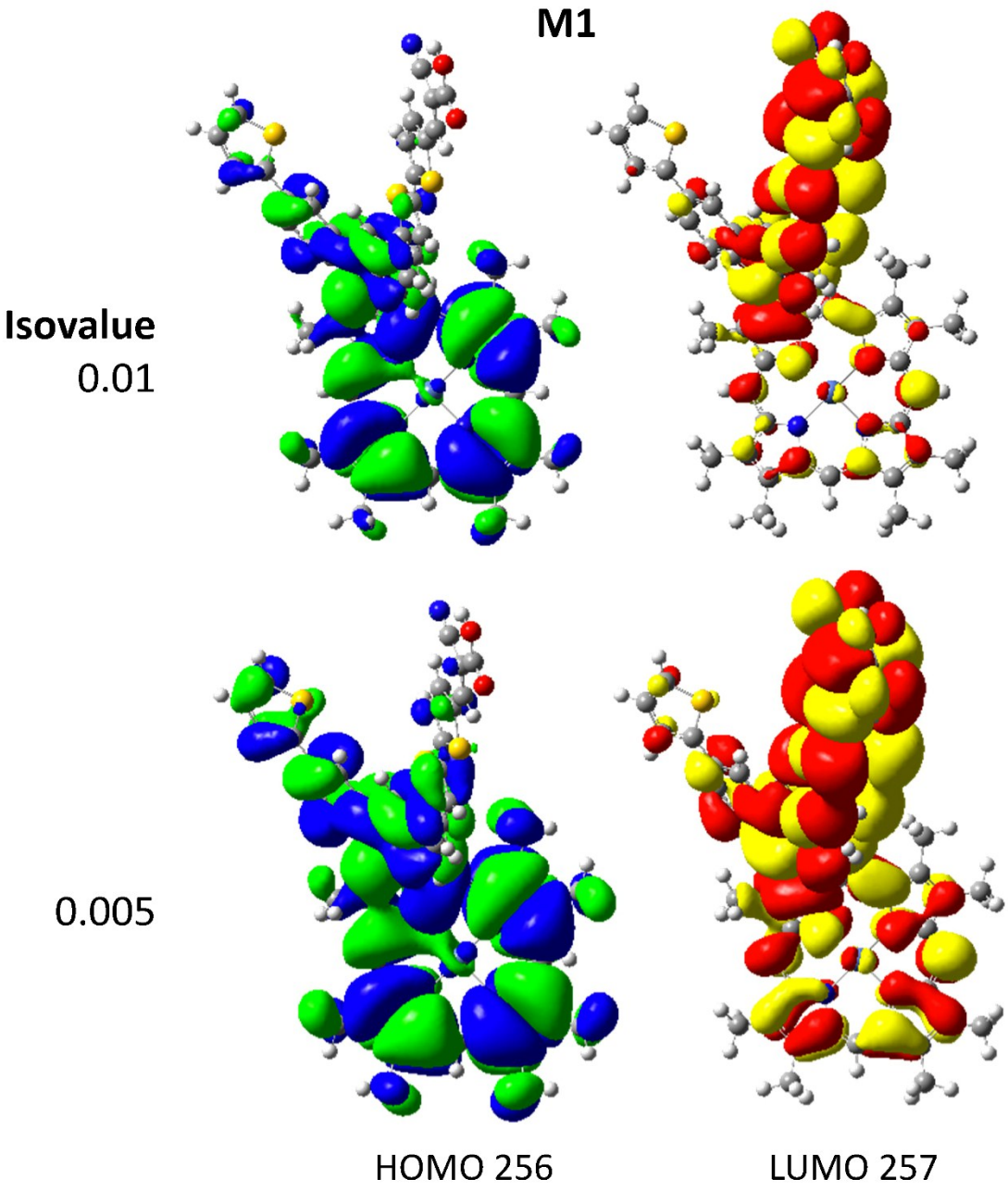

Figure S4. HOMO and LUMO electron density surfaces for **M1** with different isovalues.