

Supplementary material:

The aromatic character of thienopyrrole-modified 20 π -electron porphyrinoids

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1 Equilibrium geometries and frequencies of tautomers

The equilibrium geometries (in Å) and harmonic frequencies (in cm^{-1}) of the electronic ground state of the investigated tautomers optimized at the B3LYP/TZVP level of theory.

C	-3.23388	-1.98604	0.01372
H	-1.01789	5.48404	0.01470
H	1.66816	5.57232	0.00859
H	3.61965	3.63940	-0.00941
H	-2.76974	3.67999	-0.00260
H	5.54271	1.80073	-0.00709
H	5.59975	-0.88146	-0.00261
H	-4.91663	2.34657	-0.01952
H	-5.55754	-0.25978	-0.01024
H	-4.20205	-2.49012	0.02059
H	3.75011	-2.81647	-0.00143
H	1.87113	-4.80177	-0.00632
H	-3.23629	-4.84909	0.00749
H	-1.35708	0.10041	0.01745
H	0.47149	1.52966	-0.01387

1.1 1-2 tautomer

1.1.1 Cartesian coordinates

Atom	X	Y	Z
C	-2.14951	-2.89522	0.00904
C	-0.79701	-2.81523	0.00552
C	-2.27051	-4.35675	0.00616
C	-0.19413	-4.02304	0.00107
N	-1.08631	-5.06194	0.00126
S	0.22601	-1.55077	0.00668
C	1.61475	-2.61431	-0.00043
C	1.20425	-3.95095	-0.00247
C	2.94273	-2.09039	-0.00253
C	3.40072	-0.66275	-0.00566
N	2.59092	0.40118	-0.00898
C	3.35640	1.49048	-0.00884
C	4.68949	1.13471	-0.00752
C	4.71853	-0.25315	-0.00514
C	2.83666	2.88575	-0.00866
C	1.50749	3.38232	-0.00377
N	0.40148	2.54119	-0.00656
C	-0.74831	3.30244	0.00085
C	-0.34984	4.63180	0.00814
C	1.05327	4.68190	0.00473
C	-2.08546	2.82645	-0.00137
C	-2.84088	1.62560	-0.00258
N	-2.33796	0.34262	0.00767
C	-3.38150	-0.57122	0.00490
C	-4.55715	0.15403	-0.00615
C	-4.22148	1.51627	-0.01118

1.1.2 Harmonic frequencies

cm^{-1}	Intensity
39.31	0.09389
48.58	0.27449
58.64	0.04465
93.76	1.04062
100.66	4.01629
119.45	0.34117
125.71	1.42473
145.95	0.45240
165.86	0.14700
174.12	0.16702
243.60	0.37383
251.57	3.10533
261.22	1.73597
266.00	0.50667
286.94	2.78132
289.89	0.86778
311.95	4.63866
346.25	5.84586
363.29	0.58377
372.11	0.84128
394.10	1.17995
403.50	4.37431
454.04	1.23845
463.71	6.39676

474.12	0.86404	1101.69	27.90678
501.67	7.81497	1145.74	29.56294
542.19	12.07009	1160.43	29.39941
555.79	2.75222	1173.19	36.63675
565.20	41.28797	1197.81	6.28382
616.21	19.29830	1211.40	27.41611
648.49	13.86093	1216.89	4.03517
656.96	0.49166	1233.97	9.14365
659.38	0.29356	1254.68	19.27883
663.48	8.94710	1291.81	91.54965
688.93	14.00481	1307.56	1.28677
690.65	6.99337	1316.29	20.60764
695.54	2.61845	1324.01	103.41631
710.69	9.14617	1349.97	25.97369
714.89	7.44539	1355.69	29.44665
726.87	5.27746	1369.04	56.42747
735.34	4.11723	1387.79	42.30209
738.14	10.16819	1389.47	93.73395
753.51	16.62218	1413.93	124.74489
765.14	32.64415	1428.35	5.36274
781.89	0.86599	1435.97	76.25880
793.84	19.42740	1454.71	18.44607
798.96	10.30539	1463.54	269.99707
811.55	1.67716	1470.07	2.36456
817.63	7.44650	1482.59	81.62841
829.25	1.50466	1505.81	8.55843
831.67	12.45923	1534.48	17.75813
844.70	93.55295	1559.33	10.50562
850.80	2.04061	1573.19	36.55652
869.71	1.00350	1592.15	40.51950
881.96	2.89852	1598.38	13.95662
894.14	12.86516	1632.54	200.38752
917.29	19.48751	1634.47	305.71876
935.07	0.05116	1658.75	468.18572
938.12	20.53822	3149.37	5.15173
948.38	11.46380	3161.17	3.78070
961.40	63.86198	3172.84	2.99192
979.39	28.06313	3176.76	16.03438
999.91	48.84992	3184.89	4.65373
1019.70	0.18577	3208.51	1.69063
1024.88	13.97688	3214.73	2.34660
1040.11	93.76147	3229.68	0.02748
1070.53	70.00996	3234.44	13.11466
1077.90	55.13473	3234.95	2.43884
1098.02	87.80270	3248.02	3.35967

3250.41	1.71925
3558.39	27.89292
3587.72	86.22011

1.2 1-3 tautomer

1.2.1 Cartesian coordinates

Atom	X	Y	Z
C	-2.22621	-2.84900	0.00039
C	-0.84943	-2.69697	-0.00010
C	-2.31332	-4.31189	-0.00005
C	-0.21971	-3.88107	-0.00006
N	-1.09455	-4.95036	0.00002
S	0.19613	-1.43033	-0.00016
C	1.60497	-2.47270	-0.00024
C	1.19443	-3.80567	0.00003
C	2.95316	-1.99957	-0.00129
C	3.46208	-0.67906	-0.00132
N	2.61040	0.41659	-0.02282
C	3.42245	1.53813	-0.00133
C	4.74498	1.15430	0.00152
C	4.77330	-0.24878	0.00148
C	2.87418	2.83665	-0.00127
C	1.45056	3.24973	-0.00010
N	0.40300	2.40247	-0.00038
C	-0.68661	3.16968	0.00010
C	-0.34679	4.51243	0.00002
C	1.03300	4.56440	0.00005
C	-2.10443	2.75070	0.00066
C	-2.84671	1.56467	0.00010
N	-2.28185	0.30870	0.02679
C	-3.38630	-0.57444	0.00372
C	-4.57426	0.14167	-0.00129
C	-4.22052	1.48541	-0.00180
C	-3.32857	-1.99190	0.00233
H	-1.03482	5.35037	0.00001
H	1.65132	5.45663	-0.00001
H	3.59663	3.65162	0.00005
H	-2.76098	3.61217	-0.00008
H	5.60289	1.82070	0.00073
H	5.66537	-0.87466	0.00072

H	-4.88511	2.34307	-0.00085
H	-5.59773	-0.24879	-0.00088
H	-4.33169	-2.46857	-0.00004
H	3.73703	-2.76706	0.00006
H	1.90236	-4.62586	-0.00000
H	-3.26178	-4.87448	0.00001
H	-1.24680	0.18872	0.08759
H	1.57858	0.39954	-0.08221

1.2.2 Harmonic frequencies

cm ⁻¹	Intensity
38.26	0.12022
50.12	0.17792
58.10	0.16915
100.17	5.12995
104.63	1.77072
118.55	0.34730
128.75	0.18231
143.29	1.21133
161.73	0.14565
193.34	0.07104
234.39	0.90116
238.74	1.57942
256.97	0.69059
273.79	0.79602
283.11	1.94904
290.90	4.38252
309.93	5.95891
346.19	5.59579
358.02	0.63814
377.23	0.96412
398.72	1.56921
406.96	4.12733
451.39	0.88632
461.43	6.32599
476.78	2.21135
554.76	11.19442
562.98	0.45079
590.43	2.01763
611.94	16.20315
618.18	7.89886
655.30	0.33183
658.95	10.36247

664.34	1.32455	1260.92	91.39493
669.74	25.78635	1283.00	30.44163
678.93	6.46239	1305.34	63.67899
697.75	5.43319	1316.17	68.44842
702.49	10.67707	1333.30	19.51533
717.91	3.92634	1346.07	32.76067
721.85	10.59761	1361.81	16.35127
723.71	3.22640	1380.47	8.55114
734.60	13.39817	1384.21	31.62544
742.24	1.02009	1394.85	24.38850
751.67	14.60189	1419.33	108.26508
765.92	12.98774	1423.26	103.79771
788.45	34.00733	1440.06	0.69366
797.53	4.46614	1449.35	46.64371
800.79	9.99540	1463.95	107.58333
810.83	12.96986	1473.85	120.10502
817.62	1.48086	1485.42	55.84075
820.58	28.42581	1515.41	16.77978
827.43	9.06463	1531.96	28.22083
834.11	23.55298	1562.78	183.15955
858.86	1.38653	1565.99	4.76630
867.86	64.44479	1577.80	153.45082
874.46	3.57259	1616.99	64.06905
888.90	21.82012	1631.79	2.22595
919.07	0.89554	1634.23	276.52108
929.12	0.63747	1661.73	491.83939
935.98	28.47552	3149.45	5.41686
947.45	65.84584	3163.48	3.82118
956.35	17.99143	3173.03	2.32036
991.22	19.56306	3179.07	14.82640
998.82	16.71267	3191.79	3.72123
1015.43	1.40298	3210.61	1.65861
1028.65	7.32884	3214.51	2.24233
1037.26	52.12434	3230.23	0.17592
1071.91	77.38744	3235.49	5.75796
1085.07	31.65425	3235.58	9.05999
1090.83	4.82714	3248.29	3.56453
1096.56	59.34113	3251.09	1.75088
1135.96	50.03064	3513.21	40.49851
1151.74	59.48727	3567.48	61.09707
1162.79	17.89016		
1194.84	35.83197		
1213.70	4.70043		
1219.37	51.06354		
1227.60	26.71744		

1.3 1-4 tautomer

1.3.1 Cartesian coordinates

H	-3.28085	-4.94040	0.00379
H	-1.34097	0.12114	0.01627
H	-0.96261	-5.98800	-0.07288

1.3.2 Harmonic frequencies

Atom	X	Y	Z	cm ⁻¹	Intensity
C	-2.19718	-2.98543	0.01107	35.10	0.92004
C	-0.80018	-2.80039	0.00751	52.79	1.29748
C	-2.37180	-4.35613	0.00350	60.10	0.19492
C	-0.18611	-4.01939	-0.00634	95.12	3.10340
N	-1.15489	-4.99395	-0.02767	107.67	0.19225
S	0.31595	-1.51831	0.00944	116.36	0.63971
C	1.64041	-2.61610	0.00059	125.54	0.95401
C	1.23341	-3.94291	-0.00353	140.79	0.11917
C	2.96847	-2.09656	-0.00215	158.22	0.25293
C	3.42967	-0.66867	-0.00566	184.79	0.47114
N	2.63705	0.39747	-0.00921	243.14	15.21871
C	3.38285	1.49410	-0.00894	245.17	0.42124
C	4.71192	1.13495	-0.00768	264.09	1.98655
C	4.74184	-0.25514	-0.00531	265.62	9.07299
C	2.86405	2.88821	-0.00819	286.58	0.03359
C	1.44437	3.34207	-0.00371	291.52	7.23046
N	0.37308	2.53530	-0.00527	315.22	38.70851
C	-0.71032	3.29542	0.00057	335.31	30.43113
C	-0.34508	4.63427	0.00756	352.08	5.15894
C	1.04088	4.66362	0.00432	379.63	1.31204
C	-2.13082	2.84326	-0.00056	382.27	10.04628
C	-2.86128	1.62581	-0.00251	394.48	16.92639
N	-2.33426	0.34238	0.00725	399.36	4.92559
C	-3.37260	-0.58801	0.00530	450.40	0.70260
C	-4.55361	0.13980	-0.00631	467.60	5.95334
C	-4.23708	1.50541	-0.01143	470.68	2.31704
C	-3.24216	-2.01519	0.01583	518.47	1.81935
H	-1.01077	5.48751	0.01439	553.82	101.47782
H	1.66554	5.54973	0.00830	561.54	2.69642
H	3.61891	3.66436	-0.00875	616.15	0.28771
H	-2.78240	3.71257	-0.00169	618.68	11.27453
H	5.56051	1.80224	-0.00725	652.46	3.67271
H	5.61632	-0.88730	-0.00280	655.03	67.69331
H	-4.93128	2.33509	-0.01968	673.07	0.01089
H	-5.55297	-0.27440	-0.01021	692.11	0.01608
H	-4.21983	-2.49555	0.02115	694.47	0.03432
H	3.76787	-2.82555	-0.00149	710.45	1.95691
H	1.90193	-4.79420	-0.00835		

712.76	0.48726	1335.61	19.26408
718.53	0.09652	1352.88	29.31217
720.31	81.22601	1364.85	73.53571
737.61	2.03145	1383.47	3.90245
739.33	40.31571	1402.77	100.29424
742.00	3.15421	1417.00	76.21870
761.20	2.06214	1423.92	123.57572
771.49	7.54891	1442.99	85.03104
784.61	14.25086	1454.38	148.03911
797.55	0.39395	1464.60	262.68843
800.14	0.57254	1473.45	910.96093
801.61	79.77052	1518.74	52.28102
810.67	64.65355	1530.11	142.23311
815.44	9.39279	1552.65	476.16569
828.83	12.06834	1561.67	274.45479
831.28	5.52414	1575.59	296.69006
858.46	7.98966	1585.35	519.91480
878.93	3.77154	1608.87	382.30198
894.81	8.09955	1619.49	169.04706
908.61	1.90183	1647.88	596.58379
914.84	0.39506	1662.82	24.65892
927.11	0.01701	3152.92	4864.81412
941.59	292.80664	3156.83	4193.39778
954.14	315.09144	3163.95	4760.28719
963.33	205.59238	3178.57	4524.16938
994.57	1.78388	3205.30	6610.23541
1001.10	55.11827	3210.17	779.62949
1022.83	1.87481	3210.41	1747.74666
1073.06	54.62912	3227.27	1318.59117
1078.07	96.47225	3231.57	13710.70549
1082.15	52.54634	3231.94	15068.24195
1096.11	83.76942	3246.51	14112.88462
1110.54	0.41441	3250.04	9023.76797
1138.81	70.00198	3530.96	576.90359
1148.74	269.42327	3657.13	14992.67815
1160.15	290.83074		
1173.07	25.16563		
1193.11	3.97190		
1207.61	128.92928		
1234.06	153.63336		
1245.76	102.73457		
1263.07	65.48680		
1303.74	54.79542		
1313.99	114.02724		
1327.77	198.93329		

1.4 2-3 tautomer

1.4.1 Cartesian coordinates

Atom	X	Y	Z
C	-2.16677	-2.91780	0.00965

C	-0.80735	-2.81610	0.00561	39.45	0.11969
C	-2.27760	-4.37683	-0.00141	50.04	0.37845
C	-0.19669	-4.01873	-0.00758	65.83	0.53117
N	-1.08599	-5.06667	-0.01693	95.13	1.54668
S	0.22180	-1.54706	0.01199	112.91	0.49221
C	1.62013	-2.59386	-0.00048	119.31	1.20388
C	1.20747	-3.93568	-0.00590	123.11	0.61684
C	2.95671	-2.06620	-0.00340	143.66	0.11669
C	3.47165	-0.73455	-0.00518	170.58	0.10488
N	2.66525	0.37891	-0.02760	195.78	3.13832
C	3.40093	1.53614	-0.01024	229.87	0.55038
C	4.72948	1.14596	-0.00449	240.93	1.44083
C	4.77121	-0.26724	-0.00186	261.51	0.99047
C	2.82549	2.83597	-0.01293	273.99	4.06648
C	1.49390	3.34360	-0.00592	285.40	3.04955
N	0.35958	2.54601	-0.02755	289.18	6.72310
C	-0.76840	3.33691	-0.00052	310.94	5.03534
C	-0.34419	4.64794	0.01111	344.40	6.54426
C	1.06051	4.65757	0.00750	359.26	4.63124
C	-2.10846	2.87371	-0.00413	367.99	5.68792
C	-2.83968	1.57136	-0.00319	406.48	2.33694
N	-2.32050	0.34144	0.00366	409.31	5.83402
C	-3.34350	-0.52550	0.00609	458.04	41.51633
C	-4.54702	0.15448	-0.00524	463.49	18.84711
C	-4.22519	1.49892	-0.01070	475.27	15.01967
C	-3.25923	-2.02057	0.01586	477.26	35.28080
H	-1.00170	5.50609	0.01693	559.42	2.59575
H	1.68492	5.54202	0.01075	571.56	8.99108
H	3.57918	3.63128	-0.00927	603.53	25.98120
H	-2.81567	3.69981	-0.00262	605.80	25.53361
H	5.58092	1.81307	-0.00523	636.43	1.58546
H	5.65394	-0.88916	-0.00069	657.29	19.92461
H	-4.92531	2.32645	-0.01943	660.64	6.28670
H	-5.54385	-0.27179	-0.00963	665.11	0.54911
H	-4.24135	-2.48867	0.02096	676.79	1.29655
H	3.74012	-2.82564	-0.00176	680.29	113.75601
H	1.87828	-4.78500	-0.01047	693.30	72.62283
H	-3.23995	-4.88256	0.00239	704.06	24.71466
H	0.34392	1.54268	-0.08557	719.23	82.98402
H	1.65887	0.31621	-0.07615	725.61	25.24556
				729.51	19.74381
				740.77	2.81794
				756.37	19.14618
				761.01	15.24487
				778.98	25.90242

1.4.2 Harmonic frequencies

cm⁻¹ Intensity

794.10	41.21234
800.87	116.35834
809.48	59.07456
813.42	7.41443
824.94	63.52503
831.08	15.95816
840.15	7.89653
869.07	0.50417
875.27	11.04655
882.36	38.03148
894.58	5.41916
927.23	118.69607
929.48	6.04588
937.80	407.18898
951.61	21.98634
973.81	249.64433
982.94	32.72610
998.11	20.50531
1001.75	2.22918
1015.05	11.11856
1040.77	16.07435
1069.30	161.70396
1076.53	62.83243
1093.59	47.04845
1101.48	65.11842
1150.07	77.13690
1155.73	187.92072
1171.06	41.97598
1173.61	13.16286
1192.66	75.05991
1218.57	28.68116
1238.02	0.93189
1269.00	229.57696
1272.93	5.57417
1301.92	59.33970
1311.38	48.18227
1327.91	46.67605
1342.10	60.39111
1370.09	25.22809
1387.37	7.15888
1394.24	72.93113
1401.91	77.74138
1411.99	29.79205
1418.37	12.13738
1429.03	5.15967

1441.20	63.47304
1455.94	53.09725
1475.68	132.17801
1493.31	340.39032
1498.63	273.23816
1518.45	14.97725
1543.39	102.82797
1549.37	8.36174
1563.52	203.92755
1580.85	42.08421
1630.29	545.61500
1655.71	248.90203
1668.23	164.68813
3140.56	11.61355
3154.34	4.21621
3170.25	1.83637
3177.29	18.44265
3194.63	1.98785
3207.05	2.66153
3213.20	2.54190
3229.62	0.13359
3232.39	14.44867
3233.90	2.04753
3246.94	2.61608
3250.57	1.75041
3586.92	10.46230
3597.86	36.41222

1.5 2-4 tautomer

1.5.1 Cartesian coordinates

Atom	X	Y	Z
C	-2.16677	-2.91780	0.00965
C	-0.80735	-2.81610	0.00561
C	-2.27760	-4.37683	-0.00141
C	-0.19669	-4.01873	-0.00758
N	-1.08599	-5.06667	-0.01693
S	0.22180	-1.54706	0.01199
C	1.62013	-2.59386	-0.00048
C	1.20747	-3.93568	-0.00590
C	2.95671	-2.06620	-0.00340

C	3.47165	-0.73455	-0.00518	152.82	0.08265
N	2.66525	0.37891	-0.02760	173.47	0.01002
C	3.40093	1.53614	-0.01024	184.95	2.03436
C	4.72948	1.14596	-0.00449	236.32	5.06283
C	4.77121	-0.26724	-0.00186	249.84	0.73422
C	2.82549	2.83597	-0.01293	266.65	13.96461
C	1.49390	3.34360	-0.00592	266.96	0.82581
N	0.35958	2.54601	-0.02755	285.15	0.00552
C	-0.76840	3.33691	-0.00052	293.09	29.58383
C	-0.34419	4.64794	0.01111	310.06	21.18509
C	1.06051	4.65757	0.00750	347.06	21.67672
C	-2.10846	2.87371	-0.00413	362.00	0.10362
C	-2.83968	1.57136	-0.00319	373.78	2.52265
N	-2.32050	0.34144	0.00366	389.21	5.78391
C	-3.34350	-0.52550	0.00609	399.24	3.46006
C	-4.54702	0.15448	-0.00524	413.18	19.75287
C	-4.22519	1.49892	-0.01070	453.81	1.70082
C	-3.25923	-2.02057	0.01586	471.15	3.41435
H	-1.00170	5.50609	0.01693	476.78	10.96758
H	1.68492	5.54202	0.01075	561.59	0.01555
H	3.57918	3.63128	-0.00927	564.61	112.44462
H	-2.81567	3.69981	-0.00262	590.26	5.91687
H	5.58092	1.81307	-0.00523	622.00	2.16411
H	5.65394	-0.88916	-0.00069	622.02	11.08259
H	-4.92531	2.32645	-0.01943	649.99	52.08956
H	-5.54385	-0.27179	-0.00963	661.95	4.39115
H	-4.24135	-2.48867	0.02096	685.66	0.01214
H	3.74012	-2.82564	-0.00176	690.92	0.03760
H	1.87828	-4.78500	-0.01047	695.38	0.03510
H	-3.23995	-4.88256	0.00239	704.51	0.12880
H	0.34392	1.54268	-0.08557	710.99	0.43543
H	-0.90578	-6.06890	-0.11260	718.23	1.52636

1.5.2 Harmonic frequencies

cm ⁻¹	Intensity		
38.93	0.59134	723.21	45.32804
54.76	0.86035	736.53	34.51833
68.45	2.10527	745.83	3.54688
94.61	0.54150	748.03	1.90397
101.93	0.14371	760.15	7.40791
109.62	1.40188	771.24	14.45468
126.75	0.09279	785.07	0.00468
		792.93	8.34983
		798.10	1.26553
		800.38	14.17691
		814.25	32.92327
		822.91	20.86194
		831.97	16.20202

833.43	4.37294
852.18	16.10344
888.64	4.83099
895.28	2.62455
906.83	1.84295
916.17	1.33099
929.52	0.00166
953.78	248.91855
960.60	549.32918
971.74	65.86679
979.12	56.37995
1007.19	3.98514
1022.62	0.05158
1072.24	61.00142
1078.15	108.09634
1081.44	55.21281
1097.65	46.87577
1115.46	4.53306
1139.10	192.70139
1156.58	216.10478
1170.40	15.75570
1177.14	110.25820
1184.39	12.54359
1208.98	59.49147
1230.62	212.63308
1266.34	134.53172
1267.08	117.97762
1295.78	50.37696
1321.12	7.90261
1325.95	5.32086
1343.69	87.99762
1361.51	1.77765
1366.13	5.56076
1380.39	124.04802
1401.04	6.60395
1417.38	143.01263
1429.15	86.09586
1440.09	289.55145
1457.11	189.16081
1460.93	277.54077
1484.83	45.75542
1514.12	273.02024
1521.87	186.19599
1560.09	619.54134
1565.04	26.43650

1579.75	949.11781
1592.08	528.14492
1619.04	130.64660
1621.07	116.28342
1640.66	0.82237
1652.66	728.29180
3147.46	4872.27769
3156.03	4358.14651
3162.20	3886.20569
3183.88	5168.32214
3203.48	6266.62933
3210.26	1052.08356
3212.10	1237.39871
3228.78	734.18704
3231.24	14396.33283
3232.31	14716.22891
3247.20	14716.40105
3251.19	9214.80191
3566.45	671.49891
3654.54	14843.19351

1.6 3-4 tautomer

1.6.1 Cartesian coordinates

Atom	X	Y	Z
C	-2.20123	-3.00368	0.01003
C	-0.80496	-2.79741	0.00731
C	-2.35544	-4.37531	-0.00052
C	-0.17935	-4.01246	-0.00941
N	-1.13397	-5.00103	-0.03504
S	0.30678	-1.50197	0.01369
C	1.63758	-2.58505	-0.00094
C	1.23766	-3.91767	-0.00653
C	2.96809	-2.06314	-0.00490
C	3.48537	-0.72959	-0.00742
N	2.66709	0.39184	-0.03795
C	3.43480	1.53870	-0.01228
C	4.75171	1.14207	-0.00364
C	4.78507	-0.27038	-0.00089
C	2.85690	2.83837	-0.01300
C	1.43932	3.31926	-0.00948

N	0.36339	2.52756	-0.02220	281.35	0.13871
C	-0.71668	3.31098	-0.00432	294.77	13.63137
C	-0.33457	4.64392	0.00850	309.36	36.96296
C	1.05230	4.65028	0.00501	352.40	22.45105
C	-2.14184	2.88531	-0.00345	357.85	0.05703
C	-2.84595	1.57115	-0.00404	383.67	5.09768
N	-2.32940	0.33961	0.00342	390.35	1.30658
C	-3.33705	-0.54061	0.00576	401.65	9.05663
C	-4.54152	0.14661	-0.00488	423.72	24.14294
C	-4.22662	1.49358	-0.01075	450.67	2.09728
C	-3.26053	-2.04957	0.01557	471.21	6.39548
H	-0.98916	5.50854	0.01883	478.83	11.80509
H	1.68951	5.52756	0.01250	564.68	0.22843
H	3.57902	3.64872	-0.00861	573.09	100.83687
H	-2.82854	3.72221	-0.00195	613.88	0.83938
H	5.59989	1.81251	-0.00263	620.08	51.23609
H	5.66922	-0.89294	0.00210	621.87	0.00710
H	-4.92438	2.32198	-0.01909	644.75	23.33482
H	-5.53808	-0.27534	-0.00884	670.84	2.68395
H	-4.25169	-2.48927	0.02094	679.03	1.05947
H	3.73754	-2.83191	-0.00179	687.49	0.00268
H	1.90221	-4.77233	-0.01234	697.92	0.00343
H	-3.26316	-4.95360	-0.00150	707.85	0.15250
H	-0.92318	-5.99533	-0.09181	712.63	2.13970
H	1.65757	0.37606	-0.09550	723.92	0.01133

725.27	54.46578
733.53	30.22446
740.96	0.94248
742.28	3.10128
760.91	14.30942
766.69	8.10459
780.99	0.01312
789.36	13.17739
798.91	0.19049
805.49	21.21958
813.39	49.56116
819.62	9.10563
823.56	14.31583
830.93	13.20841
854.34	10.83562
882.41	3.75965
901.79	3.82347
917.20	1.21541
920.66	0.33361
921.03	1.16198

1.6.2 Harmonic frequencies

cm⁻¹ Intensity

36.13	0.41820
49.35	0.77722
69.71	1.67602
95.09	1.76643
115.44	1.00699
117.64	0.78802
134.22	0.69032
146.20	0.37694
174.38	1.37025
190.89	0.02923
239.77	0.72780
240.88	5.49915
266.66	0.23999
272.15	4.54716

951.11	343.89209
959.51	465.24295
965.20	58.23731
997.11	2.31249
1008.79	3.20137
1026.50	38.57645
1073.49	97.06857
1080.10	84.22809
1083.60	32.37657
1090.67	51.70354
1115.87	3.90616
1136.74	167.31059
1153.79	124.88696
1166.25	187.72938
1175.05	67.88984
1181.23	96.04515
1203.81	122.75567
1227.52	108.30540
1259.58	56.90729
1271.45	82.19340
1307.89	116.60669
1312.32	147.01713
1334.45	60.11349
1337.19	150.46069
1362.17	10.44070
1379.41	29.59416
1387.53	0.56474
1408.06	65.40469
1411.42	64.31979
1423.57	114.47121
1433.46	196.12755
1449.30	241.31081
1469.79	441.38296
1483.46	388.05567
1518.48	144.31142
1526.98	6.10570
1557.57	728.23840
1565.63	83.50901
1574.97	401.06988
1581.29	431.57571
1608.61	499.99599
1618.99	147.54093
1642.22	232.86178
1659.59	437.79160
3144.91	3349.59340

3150.81	5129.14921
3163.33	4318.42776
3195.69	5585.01013
3203.38	6293.62967
3210.56	1057.19701
3212.10	1155.39788
3228.80	1267.27356
3231.81	12927.67854
3233.36	14253.69469
3247.25	15990.74552
3253.96	9451.31696
3370.63	910.33428
3653.74	15035.56571

2 Nuclear magnetic shieldings of tautomers

Nuclear magnetic resonance shieldings (in ppm)
calculated at the B3LYP/def2-TZVP level.

2.1 1-2

NO.	Atom	ISOTROPIC
1	c	42.43627056
2	c	19.45969193
3	c	31.27634354
4	c	13.83909580
5	n	-69.10244083
6	s	231.30129455
7	c	18.70235566
8	c	51.78305449
9	c	40.98164024
10	c	12.62141608
11	n	-65.68035845
12	c	-2.80339902
13	c	56.13436638
14	c	46.33812632
15	c	71.66191254

16	c	11.17294481
17	n	87.85346177
18	c	16.48985710
19	c	46.07727756
20	c	49.28995160
21	c	78.23944381
22	c	20.52678517
23	n	60.35290816
24	c	29.74374637
25	c	50.67862591
26	c	61.73124866
27	c	38.81347693
28	h	31.49919576
29	h	31.12801162
30	h	34.32526158
31	h	35.65013818
32	h	30.22286914
33	h	29.67504507
34	h	31.62896218
35	h	30.89030891
36	h	32.56897400
37	h	32.84648597
38	h	30.70744033
39	h	27.53767969
40	h	-10.59743703
41	h	-9.85761537

2.2 1-3

NO.	Atom	ISOTROPIC
1	c	40.63770820
2	c	36.57496526
3	c	31.58643944
4	c	7.63142817
5	n	-73.87501920
6	s	221.21746264
7	c	20.08998487
8	c	55.59221872
9	c	63.75888934
10	c	21.30784423
11	n	75.88088091
12	c	6.64429148

13	c	54.96449436
14	c	45.54139036
15	c	78.20115597
16	c	-12.40761379
17	n	-47.20291193
18	c	4.00596980
19	c	41.46589468
20	c	51.43173940
21	c	56.52247062
22	c	18.86773766
23	n	57.07769543
24	c	26.29252162
25	c	52.40355223
26	c	59.30966269
27	c	38.94415533
28	h	30.68949580
29	h	30.81365517
30	h	34.99629424
31	h	35.24458669
32	h	31.33338301
33	h	31.12816694
34	h	31.87409933
35	h	31.47620651
36	h	33.16924064
37	h	34.55048510
38	h	31.28794917
39	h	27.62941527
40	h	-13.39599496
41	h	-13.36063324

2.3 1-4

NO.	Atom	ISOTROPIC
1	c	51.10336753
2	c	23.40918813
3	c	62.72431204
4	c	38.18886199
5	n	121.05594984
6	s	239.06973790
7	c	21.24917947
8	c	67.12796950
9	c	47.78240179

10	c	16.99813850
11	n	-75.05564821
12	c	7.18273153
13	c	47.23330133
14	c	46.60771878
15	c	57.44967125
16	c	6.97992511
17	n	-46.42013013
18	c	-2.01692233
19	c	47.11369841
20	c	37.75171810
21	c	81.53324278
22	c	16.72608509
23	n	94.66462877
24	c	31.69405952
25	c	43.22024749
26	c	52.33733095
27	c	65.62794085
28	h	26.90594315
29	h	26.56496027
30	h	28.32339103
31	h	29.18466917
32	h	26.65865947
33	h	26.32157617
34	h	27.39778519
35	h	27.24439223
36	h	28.54949254
37	h	27.32434699
38	h	27.04606895
39	h	26.28415498
40	h	10.09318294
41	h	25.65064116

2.4 2-3

NO.	Atom	ISOTROPIC
1	c	36.60302655
2	c	23.28207344
3	c	34.74338408
4	c	15.02886371
5	n	-70.25077112
6	s	192.76779182

7	c	13.70568675
8	c	55.58829568
9	c	56.14635582
10	c	21.10761788
11	n	77.72613464
12	c	8.74599037
13	c	51.92510232
14	c	41.31736406
15	c	85.20673762
16	c	5.35836870
17	n	61.69852961
18	c	24.08101821
19	c	43.54137972
20	c	61.06269912
21	c	37.92083340
22	c	11.89144213
23	n	-110.96364583
24	c	1.32271711
25	c	56.55863833
26	c	50.39040377
27	c	24.92916489
28	h	32.37460788
29	h	32.93078042
30	h	36.99588807
31	h	36.02740039
32	h	32.07912427
33	h	31.70951203
34	h	31.41074362
35	h	31.23568788
36	h	33.32253017
37	h	35.52140432
38	h	31.97050820
39	h	27.85648544
40	h	-16.72496146
41	h	-12.19884318

2.5 2-4

NO.	Atom	ISOTROPIC
1	c	50.29513089
2	c	27.31419555
3	c	59.38011632

4	c	38.52191000
5	n	116.65770861
6	s	217.69068265
7	c	20.48858209
8	c	68.37710260
9	c	49.35342653
10	c	18.36022105
11	n	-48.92375717
12	c	6.48265478
13	c	51.40173908
14	c	44.04162883
15	c	77.75825789
16	c	21.14179260
17	n	95.60818806
18	c	25.20052472
19	c	44.91824497
20	c	48.71683314
21	c	73.12754924
22	c	5.98489339
23	n	-67.90228517
24	c	17.49136159
25	c	42.13916733
26	c	49.25579182
27	c	46.03559628
28	h	26.85270361
29	h	26.80926867
30	h	28.34535727
31	h	28.45503243
32	h	26.47944715
33	h	26.06663863
34	h	26.67704124
35	h	26.16649676
36	h	26.90513636
37	h	26.99149139
38	h	26.60777776
39	h	25.67508784
40	h	12.14288850
41	h	25.13418700

2.6 3-4

1	c	49.79545440
2	c	34.25894409
3	c	61.17640310
4	c	38.28227195
5	n	115.62491422
6	s	224.79363541
7	c	19.57045535
8	c	73.14538476
9	c	66.99714123
10	c	33.11089760
11	n	87.17803185
12	c	18.19446151
13	c	54.56296291
14	c	45.81988679
15	c	82.59716994
16	c	-1.68126203
17	n	-37.99784217
18	c	11.79572303
19	c	35.60190135
20	c	48.88144845
21	c	54.74665996
22	c	6.18423877
23	n	-84.87378204
24	c	16.91863885
25	c	44.00270388
26	c	46.52842402
27	c	43.75176970
28	h	26.22123619
29	h	26.47356975
30	h	28.19615611
31	h	27.80878597
32	h	26.70813714
33	h	26.52574875
34	h	26.49063043
35	h	26.08275720
36	h	26.68805574
37	h	27.64391340
38	h	26.77533279
39	h	25.59049893
40	h	25.00653119
41	h	10.19505461

NO. Atom ISOTROPIC

3 Equilibrium geometries of tautomers with substituents

The equilibrium geometries (in Å) of the electronic ground state of the investigated tautomers with substituents optimized at the B3LYP/TZVP level of theory.

3.1 1-2 tautomer

Atom	X	Y	Z
C	-2.32831	-2.95964	0.08935
C	-0.91255	-2.73721	0.05627
C	-2.40407	-4.41684	0.26045
C	-0.29583	-3.98266	0.20812
N	-1.21744	-4.99550	0.33207
S	0.22718	-1.47985	-0.12597
C	1.57174	-2.60971	0.04286
C	1.11370	-3.90782	0.19465
C	2.92224	-2.16674	0.00743
C	3.36905	-0.87620	-0.05020
N	2.52285	0.22308	-0.06974
C	3.30521	1.28929	-0.08406
C	4.73063	0.92217	-0.09104
C	4.76269	-0.43933	-0.06857
C	2.81688	2.63474	-0.07599
C	1.51670	3.05233	-0.04316
N	0.38242	2.25907	-0.04000
C	-0.76166	3.03640	-0.05245
C	-0.30121	4.43015	-0.01944
C	1.05819	4.43549	-0.01735
C	-2.09084	2.70324	-0.10616
C	-2.84717	1.49335	-0.16378
N	-2.40089	0.21678	-0.00658
C	-3.45403	-0.68889	-0.11126
C	-4.61671	0.08107	-0.36447
C	-4.24476	1.42429	-0.40512
C	-3.39553	-2.08568	-0.01535
H	3.56109	3.41818	-0.08845

H	-2.73158	3.57143	-0.14370
H	-4.36162	-2.57236	-0.02822
H	3.66514	-2.95647	0.04686
H	1.78021	-4.75350	0.29355
H	-1.48375	-0.02131	0.33402
H	0.46748	1.25500	-0.11874
C	1.97810	5.61754	0.02380
H	2.82939	5.43622	-0.63808
H	1.46289	6.49018	-0.38321
C	2.49698	5.95250	1.43188
H	1.67457	6.20400	2.10355
H	3.03325	5.10867	1.86815
H	3.17721	6.80595	1.39651
C	-1.21231	5.61961	0.02448
H	-0.67351	6.49178	-0.35179
H	-2.04957	5.47066	-0.66315
C	-1.75813	5.93806	1.42627
H	-2.42334	6.80334	1.39161
H	-2.31705	5.09619	1.83727
H	-0.94638	6.16412	2.11950
C	-5.99006	-0.46085	-0.60770
H	-6.19817	-0.54244	-1.67901
H	-6.12332	-1.45217	-0.17620
H	-6.75115	0.19259	-0.17925
C	-5.15341	2.59235	-0.65685
H	-5.98751	2.26542	-1.28257
H	-4.62860	3.35217	-1.24236
C	-5.71049	3.23237	0.62501
H	-6.28691	2.50939	1.20546
H	-4.90691	3.59865	1.26687
H	-6.36502	4.07388	0.38722
C	5.88106	1.88297	-0.08662
H	6.75657	1.40312	-0.53178
H	5.65167	2.73639	-0.73260
C	6.25224	2.39604	1.31420
H	5.40845	2.90054	1.78895
H	6.54709	1.57009	1.96425
H	7.08431	3.10224	1.26303
C	5.95134	-1.34553	-0.05386
H	6.05556	-1.85596	0.90847
H	5.87607	-2.11993	-0.82164
H	6.87506	-0.79424	-0.23145
C	-3.65779	-5.19567	0.35640
O	-4.77349	-4.71319	0.29272
O	-3.44070	-6.50851	0.52001

C	-4.61052	-7.34369	0.62483	H	1.75154	-4.75568	0.41447
H	-5.21035	-7.22909	-0.28043	H	-1.40483	0.04113	0.06653
H	-5.21637	-7.00119	1.46645	H	1.51767	0.33949	0.03052
C	-4.13641	-8.76769	0.81250	C	1.94647	5.64252	0.12591
H	-4.99714	-9.43467	0.89787	H	2.79682	5.47376	-0.54202
H	-3.53131	-9.09252	-0.03526	H	1.44328	6.53497	-0.25441
H	-3.53552	-8.86246	1.71812	C	2.47071	5.93304	1.54210

3.2 1-3 tautomer

Atom	X	Y	Z				
C	-2.34628	-2.96259	-0.03032	H	1.75154	-4.75568	0.41447
C	-0.92961	-2.77501	-0.11204	H	-1.40483	0.04113	0.06653
C	-2.44014	-4.39520	0.28247	H	1.51767	0.33949	0.03052
C	-0.32249	-3.99638	0.17590	C	1.94647	5.64252	0.12591
N	-1.25880	-4.97667	0.41127	H	2.79682	5.47376	-0.54202
S	0.21545	-1.57557	-0.47926	H	1.44328	6.53497	-0.25441
C	1.55609	-2.66095	-0.10910	C	2.47071	5.93304	1.54210
C	1.09422	-3.93014	0.17977	H	1.65041	6.17773	2.21919
C	2.90045	-2.17017	-0.10478	H	2.99302	5.06993	1.95839
C	3.31845	-0.87302	-0.08615	H	3.16417	6.77703	1.53205
N	2.52424	0.26844	-0.04824	C	-1.25427	5.67493	0.01422
C	3.28467	1.39414	-0.02809	H	-0.71046	6.54495	-0.36231
C	4.67855	0.96944	-0.06484	H	-2.08163	5.52049	-0.68435
C	4.69448	-0.39489	-0.09734	C	-1.82348	6.00977	1.40296
C	2.77542	2.67492	0.02134	H	-2.48579	6.87686	1.35014
C	1.40990	3.05256	0.02799	H	-2.39137	5.17288	1.81257
N	0.34776	2.23592	-0.01788	H	-1.02269	6.23887	2.10802
C	-0.76275	3.06577	-0.04955	C	-5.18126	2.62239	-0.52178
C	-0.34239	4.48533	0.00032	H	-6.03901	2.31856	-1.12688
C	1.00825	4.47682	0.05193	H	-4.69510	3.42270	-1.08541
C	-2.09086	2.73933	-0.14445	C	-5.68527	3.17883	0.81941
C	-2.83881	1.52521	-0.21758	H	-6.22228	2.41453	1.38457
N	-2.37100	0.25057	-0.13461	H	-4.85671	3.52241	1.44153
C	-3.42126	-0.65797	-0.20944	H	-6.36264	4.02085	0.66091
C	-4.60519	0.10882	-0.36770	C	-5.98754	-0.43891	-0.53815
C	-4.24742	1.45532	-0.38033	H	-6.22580	-0.59009	-1.59561
C	-3.38716	-2.06040	-0.11308	H	-6.11527	-1.39929	-0.03930
H	3.49898	3.47585	0.04125	H	-6.73287	0.24556	-0.13250
H	-2.74246	3.60087	-0.18522	C	5.84366	1.91129	-0.03756
H	-4.36629	-2.51815	-0.06749	H	6.69929	1.44500	-0.53120
H	3.67508	-2.92692	-0.07153	H	5.60456	2.79928	-0.62964
				C	6.25223	2.34156	1.38042
				H	5.42505	2.82817	1.89983
				H	6.55550	1.47942	1.97759
				H	7.09004	3.04121	1.34538
				C	5.88118	-1.30071	-0.14563
				H	5.92298	-1.94746	0.73533
				H	5.84972	-1.95198	-1.02303
				H	6.81146	-0.73586	-0.18341
				C	-3.70377	-5.13855	0.47221
				O	-4.81151	-4.64307	0.37836
				O	-3.50613	-6.43360	0.75653
				C	-4.68873	-7.23287	0.95542
				H	-5.29897	-7.19378	0.05073
				H	-5.27660	-6.79990	1.76761

C	-4.23798	-8.64130	1.27298
H	-5.10949	-9.28020	1.43180
H	-3.65064	-9.05744	0.45311
H	-3.62697	-8.66102	2.17656

3.3 1-4 tautomer

Atom	X	Y	Z
C	-2.23294	-2.67984	0.11110
C	-0.81676	-2.55635	0.10663
C	-2.47291	-4.07348	0.17925
C	-0.24433	-3.83358	0.16930
N	-1.25813	-4.74245	0.21344
S	0.37704	-1.32115	0.04552
C	1.65819	-2.53109	0.10375
C	1.16155	-3.82666	0.16709
C	3.03089	-2.15819	0.08132
C	3.47947	-0.86616	0.02820
N	2.59033	0.17866	-0.00638
C	3.30389	1.28611	-0.05464
C	4.75987	0.98195	-0.05295
C	4.85873	-0.37263	-0.00128
C	2.78217	2.61053	-0.11106
C	1.49350	3.09591	-0.12158
N	0.30756	2.39769	-0.08945
C	-0.65834	3.31764	-0.13971
C	-0.11289	4.69644	-0.20062
C	1.23117	4.55731	-0.18924
C	-2.04851	3.07572	-0.15058
C	-2.75004	1.88611	-0.10307
N	-2.24254	0.61994	-0.03323
C	-3.27032	-0.32348	-0.00792
C	-4.51082	0.44444	-0.06499
C	-4.20024	1.76835	-0.12302
C	-3.26504	-1.68840	0.05498
H	3.54436	3.37705	-0.15923
H	-2.67116	3.95634	-0.20867
H	-4.25480	-2.12164	0.06359
H	3.75018	-2.96934	0.10965
H	1.80261	-4.69586	0.20800
H	-1.24318	0.46355	-0.01052
H	-1.18490	-5.74343	0.26241

C	2.26843	5.63895	-0.21723
H	3.10236	5.33896	-0.85855
H	1.84225	6.53078	-0.68414
C	2.81267	6.01852	1.17006
H	2.01285	6.38538	1.81580
H	3.26722	5.16011	1.66692
H	3.56824	6.80334	1.08744
C	-0.92119	5.95700	-0.24963
H	-0.31579	6.75664	-0.68456
H	-1.77000	5.82506	-0.92782
C	-1.44288	6.42049	1.12094
H	-2.06560	5.65656	1.58979
H	-0.61626	6.63120	1.80167
H	-2.03984	7.33008	1.02092
C	-5.14370	2.93248	-0.16869
H	-4.73707	3.70845	-0.82272
H	-6.08130	2.61671	-0.63104
C	-5.44210	3.53562	1.21289
H	-6.12068	4.38689	1.12509
H	-5.90799	2.79673	1.86770
H	-4.52839	3.87891	1.70051
C	5.86820	1.99026	-0.07179
H	6.76743	1.53299	-0.49282
H	5.61016	2.81211	-0.74653
C	6.20248	2.56203	1.31561
H	5.33355	3.04504	1.76578
H	6.52492	1.76963	1.99376
H	7.00468	3.30076	1.24896
C	-5.87125	-0.17327	-0.05514
H	-5.99728	-0.87952	-0.87904
H	-6.04999	-0.72958	0.86852
H	-6.64803	0.58499	-0.14165
C	6.08221	-1.22968	0.02929
H	6.18856	-1.74304	0.98994
H	6.05006	-2.00178	-0.74459
H	6.98733	-0.64255	-0.12858
C	-3.72595	-4.79841	0.21310
O	-4.83906	-4.31171	0.18533
O	-3.51379	-6.14505	0.28248
C	-4.69306	-6.97480	0.32293
H	-5.28896	-6.78373	-0.57130
H	-5.29475	-6.68955	1.18779
C	-4.24137	-8.41615	0.40165
H	-5.11307	-9.07297	0.43368
H	-3.64183	-8.68868	-0.46877

H	-3.64806	-8.59406	1.30034
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3.4 2-3 tautomer

Atom	X	Y	Z
C	-2.31941	-2.68715	0.16073
C	-0.89547	-2.51597	0.12241
C	-2.44938	-4.14949	0.12089
C	-0.32418	-3.79035	0.06654
N	-1.28562	-4.77413	0.06292
S	0.27332	-1.29352	0.18846
C	1.58858	-2.48635	0.09783
C	1.08738	-3.77469	0.04756
C	2.96188	-2.09424	0.12091
C	3.46213	-0.82699	0.06718
N	2.68226	0.31893	-0.10512
C	3.44764	1.45026	-0.01169
C	4.80822	1.01368	0.24700
C	4.81309	-0.35737	0.28391
C	2.96310	2.73675	-0.12477
C	1.62304	3.17791	-0.21794
N	0.47479	2.44122	-0.09706
C	-0.64367	3.26366	-0.20544
C	-0.14972	4.58918	-0.43587
C	1.23071	4.53751	-0.44693
C	-1.97942	2.91784	-0.12025
C	-2.71189	1.72718	0.03951
N	-2.22083	0.45881	0.09984
C	-3.31258	-0.34355	0.18379
C	-4.54345	0.42620	0.20116
C	-4.16764	1.73767	0.10586
C	-3.33445	-1.76094	0.20374
H	3.70174	3.52365	-0.12477
H	-2.61822	3.78683	-0.21311
H	-4.32432	-2.19707	0.24075
H	3.67961	-2.90104	0.21438
H	1.71576	-4.65322	-0.00202
H	0.39754	1.48493	0.21395
H	1.82911	0.29541	-0.63937
C	2.18856	5.67209	-0.66225
H	3.02411	5.33173	-1.28104
H	1.69277	6.45409	-1.24196

C	2.73929	6.28855	0.63428
H	1.93472	6.70018	1.24599
H	3.26165	5.54488	1.23905
H	3.44028	7.09570	0.41103
C	-1.00428	5.80642	-0.62942
H	-0.46031	6.52969	-1.24113
H	-1.89643	5.54440	-1.20353
C	-1.42908	6.48374	0.68413
H	-2.04304	7.36326	0.48000
H	-2.00787	5.80419	1.31146
H	-0.56018	6.80476	1.26083
C	5.95392	1.94718	0.49554
H	6.88948	1.44967	0.23048
H	5.87470	2.80806	-0.17479
C	6.03885	2.44249	1.94803
H	5.12578	2.96307	2.24168
H	6.17966	1.60771	2.63715
H	6.87743	3.13056	2.07364
C	-5.05834	2.94528	0.10588
H	-4.67027	3.70459	-0.58035
H	-6.03662	2.66856	-0.29526
C	-5.25131	3.57287	1.49557
H	-5.69446	2.85370	2.18700
H	-4.29793	3.89077	1.92271
H	-5.90821	4.44478	1.44469
C	5.96490	-1.26320	0.57417
H	5.86995	-1.71857	1.56416
H	6.02026	-2.07809	-0.15131
H	6.91220	-0.72635	0.54731
C	-5.92734	-0.13678	0.29901
H	-6.14084	-0.83836	-0.51162
H	-6.07906	-0.68074	1.23541
H	-6.67831	0.65246	0.25585
C	-3.72895	-4.89299	0.13463
O	-4.82678	-4.37314	0.18755
O	-3.55328	-6.22238	0.08454
C	-4.74917	-7.02580	0.09786
H	-5.37317	-6.74783	-0.75411
H	-5.31513	-6.80485	1.00534
C	-4.32259	-8.47577	0.03665
H	-5.20431	-9.12029	0.04469
H	-3.75608	-8.67759	-0.87373
H	-3.69778	-8.73506	0.89267

3.5 2-4 tautomer

Atom	X	Y	Z
C	-1.94483	-3.28317	-0.36601
C	-0.53563	-3.09703	-0.30122
C	-2.13137	-4.68570	-0.35107
C	0.08234	-4.35594	-0.25050
N	-0.89653	-5.30382	-0.28047
S	0.61742	-1.82745	-0.27325
C	1.93481	-2.99827	-0.19471
C	1.48416	-4.31134	-0.18942
C	3.30085	-2.60447	-0.15074
C	3.78465	-1.32465	-0.15742
N	2.97187	-0.21455	-0.20591
C	3.77789	0.83749	-0.20643
C	5.19839	0.43471	-0.15491
C	5.19518	-0.92407	-0.12389
C	3.31943	2.17852	-0.25964
C	2.01728	2.61566	-0.30745
N	0.87250	1.85252	-0.32047
C	-0.24727	2.65341	-0.38840
C	0.23736	4.03472	-0.40921
C	1.59757	4.00883	-0.36169
C	-1.57729	2.32456	-0.44094
C	-2.32018	1.10363	-0.45154
N	-1.85354	-0.13620	-0.40922
C	-2.97197	-0.96178	-0.45635
C	-4.19831	-0.15814	-0.53374
C	-3.80008	1.13645	-0.53037
C	-3.00343	-2.32829	-0.43758
H	4.07363	2.95230	-0.26573
H	-2.21042	3.19833	-0.49481
H	-3.98661	-2.77648	-0.48375
H	4.01848	-3.41721	-0.11190
H	2.14777	-5.16346	-0.14614
H	0.88623	0.84164	-0.30094
H	-0.78379	-6.30231	-0.25927
C	6.36915	1.36909	-0.11689
H	7.25401	0.86019	-0.50800
H	6.18926	2.21205	-0.79146
C	6.68285	1.90693	1.28868
H	5.82760	2.43873	1.70976
H	6.92912	1.09079	1.97055
H	7.53084	2.59533	1.26190
C	6.35581	-1.86351	-0.06327

H	6.38122	-2.40916	0.88485
H	6.31025	-2.60953	-0.86153
H	7.30397	-1.33425	-0.16079
C	2.54314	5.17158	-0.34873
H	3.41025	4.94201	-0.97437
H	2.05909	6.03318	-0.81384
C	3.02592	5.56733	1.05640
H	2.18793	5.86285	1.68984
H	3.53459	4.73777	1.54965
H	3.72091	6.40797	1.00118
C	-0.64464	5.24579	-0.45797
H	-0.08536	6.07441	-0.89830
H	-1.48511	5.06339	-1.13252
C	-1.18211	5.68230	0.91497
H	-1.82473	6.55961	0.81458
H	-1.76301	4.88799	1.38553
H	-0.36508	5.93747	1.59174
C	-3.35455	-5.46376	-0.39986
O	-4.48266	-5.02066	-0.46661
O	-3.08161	-6.80181	-0.36589
C	-4.21174	-7.70086	-0.39840
H	-4.98432	-7.27060	-1.03468
H	-3.82478	-8.60664	-0.86518
C	-4.74214	-7.98061	0.99484
H	-5.55408	-8.70976	0.93930
H	-3.95951	-8.38979	1.63652
H	-5.13222	-7.07044	1.45050
C	-5.58731	-0.70723	-0.59722
H	-5.70920	-1.39949	-1.43400
H	-5.84201	-1.26104	0.31079
H	-6.32368	0.08786	-0.71422
C	-4.66277	2.36249	-0.56763
H	-5.60997	2.11921	-1.05579
H	-4.19978	3.12978	-1.19553
C	-4.95791	2.95302	0.82039
H	-5.48699	2.22940	1.44344
H	-4.03791	3.22256	1.34240
H	-5.57723	3.84960	0.74014

3.6 3-4 tautomer

Atom	X	Y	Z
------	---	---	---

C	-2.40786	-2.86933	0.05644	H	-2.49572	6.95178	1.06546
C	-1.00547	-2.63633	0.07996	H	-2.29413	5.30746	1.68348
C	-2.54632	-4.27503	0.11120	H	-0.96499	6.45511	1.79581
C	-0.33938	-3.86919	0.14473	C	5.92549	1.96452	0.02529
N	-1.28762	-4.84819	0.16427	H	6.77235	1.43472	-0.41694
S	0.09843	-1.33175	0.04660	H	5.73711	2.82381	-0.62441
C	1.46389	-2.44934	0.11899	C	6.31743	2.46470	1.42486
C	1.06346	-3.77712	0.16740	H	5.49963	3.01844	1.88896
C	2.81148	-1.98898	0.12022	H	6.56571	1.62962	2.08274
C	3.28033	-0.70478	0.08180	H	7.18659	3.12377	1.37036
N	2.53892	0.45805	0.03861	C	-5.06617	2.77811	-0.20573
C	3.35016	1.55079	0.00037	H	-6.02411	2.54061	-0.67553
C	4.72252	1.07141	0.02531	H	-4.60207	3.52729	-0.85376
C	4.67798	-0.29285	0.07452	C	-5.33229	3.39612	1.17610
C	2.87227	2.84274	-0.05763	H	-5.86351	2.69126	1.81858
C	1.50257	3.19804	-0.08107	H	-4.40111	3.66032	1.68042
N	0.48431	2.32856	-0.05833	H	-5.93885	4.30071	1.08912
C	-0.66590	3.08426	-0.11239	C	5.82388	-1.25045	0.11565
C	-0.31653	4.52935	-0.16809	H	5.82914	-1.82603	1.04556
C	1.03493	4.59471	-0.14776	H	5.77411	-1.96801	-0.70782
C	-1.98449	2.69373	-0.13192	H	6.77836	-0.73063	0.04513
C	-2.73781	1.47269	-0.10676	C	-6.05654	-0.26632	-0.15755
N	-2.30943	0.22091	-0.05083	H	-6.20809	-0.97167	-0.97853
C	-3.44851	-0.57387	-0.06083	H	-6.30520	-0.79728	0.76576
C	-4.65548	0.25412	-0.13052	H	-6.77930	0.54081	-0.27634
C	-4.22357	1.53776	-0.15956	C	-3.74504	-5.09049	0.11541
C	-3.48673	-1.93965	-0.01223	O	-4.88815	-4.68545	0.06920
H	3.59993	3.64044	-0.09107	O	-3.43442	-6.41805	0.17921
H	-2.64654	3.54677	-0.18988	C	-4.55031	-7.33284	0.18959
H	-4.46669	-2.39736	-0.02610	H	-5.13753	-7.18141	-0.71791
H	3.56515	-2.76681	0.15507	H	-5.19099	-7.09630	1.04084
H	1.75507	-4.60644	0.21442	C	-3.99600	-8.73752	0.27408
H	-1.13921	-5.84132	0.20757	H	-4.81789	-9.45655	0.28226
H	1.52890	0.60132	0.02328	H	-3.35744	-8.96070	-0.58243
C	1.91933	5.80373	-0.17447	H	-3.41346	-8.87665	1.18649
H	2.76494	5.62419	-0.84609				
H	1.37028	6.64485	-0.60555				
C	2.45718	6.21620	1.20603				
H	1.64006	6.46809	1.88419				
H	3.02835	5.40884	1.66801				
H	3.10959	7.08850	1.12255				
C	-1.27998	5.67712	-0.21678				
H	-0.79524	6.52751	-0.70378				
H	-2.13436	5.42382	-0.85041				
C	-1.79030	6.12339	1.16343				

4 Nuclear magnetic shieldings of tautomers with substituents

Nuclear magnetic resonance shieldings (in ppm)
calculated at the B3LYP/def2-TZVP level.

4.1 1-2

NO.	Atom	ISOTROPIC			
1	c	47.44109303	31	h	30.45349637
2	c	20.33716997	32	h	28.92213394
3	c	36.94220139	33	h	-1.75375438
4	c	18.39266420	34	h	-1.67843561
5	n	-78.80498206	35	c	165.69375802
6	s	244.85294742	36	h	32.30653381
7	c	22.66058916	37	h	31.42058194
8	c	51.88761996	38	c	168.35171850
9	c	48.15249649	39	h	31.90231935
10	c	16.11442759	40	h	31.93203479
11	n	-56.26986678	41	h	31.62772615
12	c	2.42143361	42	c	164.79557018
13	c	40.75145280	43	h	31.42927318
14	c	40.09676315	44	h	32.54374800
15	c	78.44488380	45	c	168.58473342
16	c	17.53509477	46	h	31.71979386
17	n	95.73436190	47	h	32.05688007
18	c	21.47360411	48	h	31.89486137
19	c	35.77374227	49	c	175.64053296
20	c	36.21825621	50	h	31.71819202
21	c	86.12378497	51	h	31.95537950
22	c	26.60952685	52	h	31.97636098
23	n	72.36946878	53	c	165.83003845
24	c	36.05221479	54	h	31.21340363
25	c	36.75160454	55	h	32.21897073
26	c	45.99942559	56	c	170.55673283
27	c	39.26608980	57	h	32.28760702
28	h	31.87235554	58	h	32.70745705
29	h	32.94345821	59	h	31.96516032
30	h	28.10170024	60	c	165.00612621
			61	h	31.08582607
			62	h	32.00506384
			63	c	168.67364651
			64	h	32.22864252
			65	h	32.04459973
			66	h	31.68138559
			67	c	177.39690274
			68	h	31.98950897
			69	h	32.04738964
			70	h	31.42820616
			71	c	13.88076084
			72	o	-60.61795716
			73	o	113.74514528
			74	c	118.94461304
			75	h	28.36925533

76	h	28.31544558
77	c	168.19461784
78	h	31.14181142
79	h	30.86201450
80	h	30.83946134

34	h	-5.02662506
35	c	164.98268042
36	h	32.47470728
37	h	31.41260899
38	c	169.01129237
39	h	32.11702180
40	h	32.22147464
41	h	31.75992985
42	c	164.24027748
43	h	31.42028799
44	h	32.38416009
45	c	166.73953760
46	h	31.76352022
47	h	32.33199326
48	h	32.08188071
49	c	165.61141408
50	h	31.48889346
51	h	32.39699603
52	c	169.96908106
53	h	32.29379761
54	h	32.62455536
55	h	31.98615710
56	c	176.00850707
57	h	32.12671375
58	h	32.23819851
59	h	32.07295917
60	c	166.41098338
61	h	31.44253847
62	h	32.36515702
63	c	169.66388022
64	h	32.27269402
65	h	32.17000676
66	h	31.82079236
67	c	178.71570046
68	h	32.71966444
69	h	32.65363786
70	h	31.71972925
71	c	13.95703331
72	o	-60.53913104
73	o	113.68369277
74	c	118.74051655
75	h	28.42980515
76	h	28.30597069
77	c	168.46434317
78	h	31.13408194

4.2 1-3

NO.	Atom	ISOTROPIC
1	c	46.70328015
2	c	32.37777880
3	c	38.15145550
4	c	12.92471528
5	n	-79.80142427
6	s	229.14355025
7	c	25.06761458
8	c	55.05503649
9	c	67.46814520
10	c	26.34369761
11	n	86.18011089
12	c	11.47118984
13	c	41.45286930
14	c	40.04870421
15	c	86.09986246
16	c	-6.69172659
17	n	-34.63269688
18	c	7.49109862
19	c	30.71843625
20	c	37.44737371
21	c	68.33248526
22	c	23.88889832
23	n	68.97758017
24	c	33.27390688
25	c	37.91731973
26	c	44.17994039
27	c	38.10712701
28	h	32.70850503
29	h	32.61335206
30	h	28.64331010
31	h	32.00885721
32	h	29.53853460
33	h	-4.55076382

79	h	30.90987348
80	h	30.83192128

37	h	29.50291577
38	c	163.20895487
39	h	30.98878718
40	h	30.71304027
41	h	30.61939606
42	c	160.74147324
43	h	29.51671424
44	h	29.65276808
45	c	164.73640509
46	h	30.75857523
47	h	31.02224226
48	h	30.68208819
49	c	161.62830112
50	h	29.57602154
51	h	29.40234723
52	c	166.04701135
53	h	30.73884498
54	h	30.97228240
55	h	30.73199182
56	c	161.48833939
57	h	29.42243685
58	h	29.44483165
59	c	165.01103751
60	h	30.78936159
61	h	31.04996219
62	h	30.68603517
63	c	172.76825656
64	h	29.85387245
65	h	29.91587826
66	h	29.80334764
67	c	175.19068003
68	h	29.92419033
69	h	29.86779103
70	h	29.81103478
71	c	18.45172981
72	o	-49.71081213
73	o	127.55405178
74	c	118.87294307
75	h	27.69344057
76	h	27.68401616
77	c	167.51536553
78	h	30.67842043
79	h	30.51182046
80	h	30.51688496

4.3 1-4

NO.	Atom	ISOTROPIC
1	c	49.84507288
2	c	29.15515468
3	c	59.75424118
4	c	37.23456270
5	n	119.63633070
6	s	251.57551136
7	c	20.74353740
8	c	70.73151277
9	c	58.00788863
10	c	17.23433218
11	n	-59.98312413
12	c	10.94651718
13	c	30.70332906
14	c	39.04218003
15	c	68.67121371
16	c	10.92066009
17	n	-38.43663154
18	c	3.93649398
19	c	32.22763444
20	c	26.11639035
21	c	88.17033330
22	c	22.95600197
23	n	102.25348236
24	c	33.77209224
25	c	35.63383374
26	c	38.38600819
27	c	71.14335789
28	h	25.89901603
29	h	26.54694002
30	h	24.43001953
31	h	25.07609888
32	h	25.36011156
33	h	19.20822994
34	h	23.98514415
35	c	160.60017652
36	h	29.43113031

4.4 2-3

NO.	Atom	ISOTROPIC
1	c	41.93812300
2	c	21.77922551
3	c	41.25304009
4	c	19.35061729
5	n	-77.93300396
6	s	203.39518776
7	c	17.42105871
8	c	54.29603243
9	c	59.47165550
10	c	25.60977761
11	n	85.91154719
12	c	13.14923285
13	c	38.75313820
14	c	35.17011120
15	c	90.64745450
16	c	12.07469655
17	n	72.95155037
18	c	30.66240867
19	c	29.43447151
20	c	47.05535631
21	c	49.49407109
22	c	15.67978013
23	n	-105.58005458
24	c	7.80606836
25	c	45.15640260
26	c	38.87552251
27	c	24.44207128
28	h	34.81923413
29	h	33.41021779
30	h	29.41819005
31	h	33.17953293
32	h	30.30988311
33	h	-9.18083460
34	h	-5.37524106
35	c	168.13613823
36	h	33.34325117
37	h	32.00745887
38	c	170.84375965
39	h	32.68851343
40	h	33.11101061

41	h	32.25481208
42	c	166.64469142
43	h	32.00947674
44	h	33.02143841
45	c	168.84357189
46	h	32.13685449
47	h	32.97467492
48	h	32.61464971
49	c	166.33326848
50	h	32.09312373
51	h	33.36097362
52	c	169.75880118
53	h	31.56651048
54	h	31.62220655
55	h	31.67559719
56	c	165.64847018
57	h	32.95247650
58	h	31.69008172
59	c	167.72906007
60	h	32.21566759
61	h	32.61874925
62	h	31.98990372
63	c	178.68091474
64	h	32.75255254
65	h	33.61518515
66	h	32.26612161
67	c	177.12484473
68	h	32.71787679
69	h	32.63251029
70	h	32.09316678
71	c	14.57432212
72	o	-63.82983967
73	o	114.60632099
74	c	119.41169827
75	h	28.47320059
76	h	28.50007186
77	c	168.05715900
78	h	31.25352572
79	h	30.96318893
80	h	31.00122905

4.5 2-4

NO.	Atom	ISOTROPIC
1	c	48.44240688
2	c	30.97250942
3	c	58.21693763
4	c	38.06491077
5	n	117.07961534
6	s	230.27867998
7	c	18.99031006
8	c	71.27423327
9	c	57.77566182
10	c	18.65049595
11	n	-37.93070905
12	c	9.74282409
13	c	34.63789964
14	c	37.39088136
15	c	85.39302317
16	c	25.97103391
17	n	101.70466325
18	c	30.58626257
19	c	32.56319328
20	c	35.82714171
21	c	79.98356941
22	c	9.68709792
23	n	-58.28326376
24	c	17.23859090
25	c	33.70241850
26	c	34.71308547
27	c	53.72188705
28	h	26.18417633
29	h	26.06510557
30	h	23.64692635
31	h	25.03167603
32	h	25.23871711
33	h	19.58228109
34	h	23.67059713
35	c	162.00612850
36	h	29.39951389
37	h	29.48017574
38	c	165.12347064
39	h	30.82269292
40	h	31.02833063

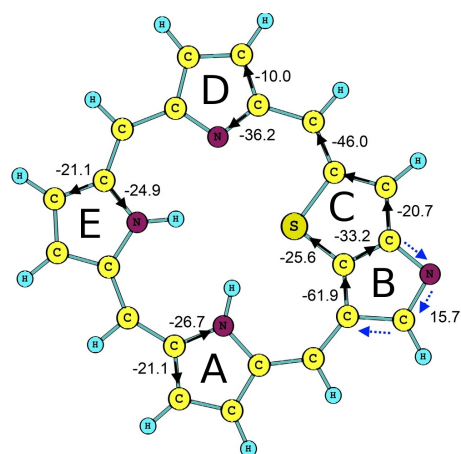
41	h	30.67300871
42	c	174.24043129
43	h	29.89152773
44	h	29.82155196
45	h	29.76862143
46	c	162.24561136
47	h	29.44091068
48	h	29.37003159
49	c	164.77786501
50	h	30.91857738
51	h	30.63990901
52	h	30.59644047
53	c	161.53385974
54	h	29.36660179
55	h	29.43747101
56	c	164.71207063
57	h	30.60730684
58	h	30.62310168
59	h	30.92208548
60	c	19.03962386
61	o	-45.12286177
62	o	127.73698704
63	c	119.66846924
64	h	26.73130535
65	h	28.15952219
66	c	166.71026445
67	h	30.88909177
68	h	30.70235533
69	h	30.27073247
70	c	172.80651035
71	h	29.67602169
72	h	29.74626191
73	h	29.82068606
74	c	161.59752940
75	h	29.35256761
76	h	29.54322092
77	c	165.54816144
78	h	30.99812762
79	h	30.82580686
80	h	30.73892545

4.6 3-4

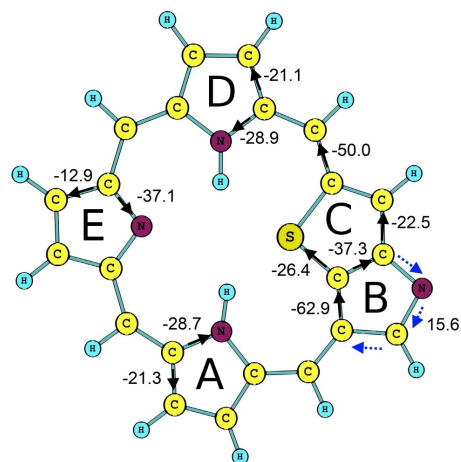
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1	c	48.05645997
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3	c	59.27843234
4	c	37.20016907
5	n	116.13674571
6	s	238.47394502
7	c	18.59938324
8	c	74.64389336
9	c	72.92205065
10	c	35.29630059
11	n	96.35515583
12	c	23.54861208
13	c	38.62584493
14	c	39.99810611
15	c	88.72873664
16	c	3.85181873
17	n	-30.76302156
18	c	15.75644519
19	c	24.51633242
20	c	34.51792392
21	c	63.49995734
22	c	9.34215704
23	n	-73.45493106
24	c	16.11916307
25	c	35.11003501
26	c	32.12113101
27	c	52.66912575
28	h	26.10729397
29	h	25.35572161
30	h	23.45662287
31	h	25.48003096
32	h	25.35079080
33	h	23.58735985
34	h	18.19491035
35	c	162.30404839
36	h	29.46650256
37	h	29.40673693
38	c	164.54434750
39	h	30.94376884
40	h	30.67270478

41	h	30.61580447
42	c	161.05490388
43	h	29.38188360
44	h	29.22944149
45	c	163.07150310
46	h	30.57078273
47	h	30.64615165
48	h	30.94135637
49	c	162.62979577
50	h	29.32999468
51	h	29.37415004
52	c	165.44847508
53	h	30.69536412
54	h	30.96056829
55	h	30.63690206
56	c	161.53841728
57	h	29.29420691
58	h	29.37423423
59	c	165.39239787
60	h	30.96929546
61	h	30.72736832
62	h	30.69120105
63	c	173.65968073
64	h	29.91466357
65	h	29.87692834
66	h	29.61766679
67	c	172.81618513
68	h	29.63742454
69	h	29.69582190
70	h	29.75344615
71	c	18.74095047
72	o	-53.32008339
73	o	126.80363549
74	c	118.69631345
75	h	27.64489713
76	h	27.62204262
77	c	167.76690297
78	h	30.63087421
79	h	30.46720482
80	h	30.46929714

5 Current strengths of the unsubstituted porphyrinoid tautomers

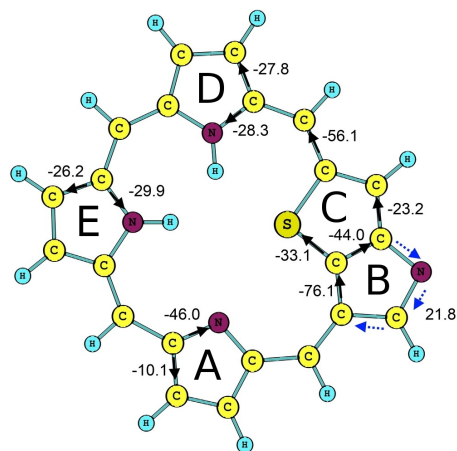


(a) (2.4 kcal/mol)

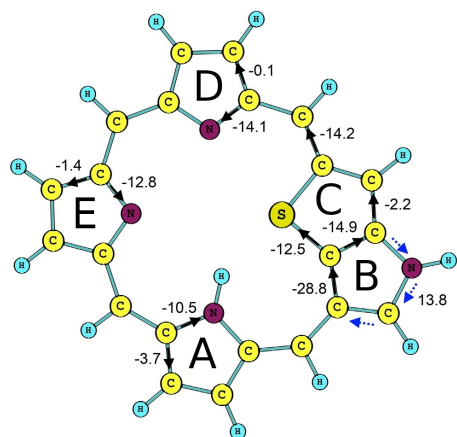


(b) (3.8 kcal/mol)

Figure 1: The molecular structures of the (a) 1-2 and (b) 1-3 tautomers, where position 1 is the lowest inner nitrogen in the picture. The inner nitrogens are numbered clockwise and position 4 is at the outer nitrogen. The current strengths passing chemical bonds and relative energies are also given. The arrows indicate the current pathways.

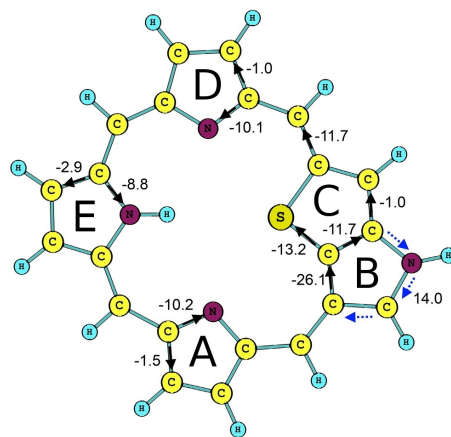


(a) (7.8 kcal/mol)

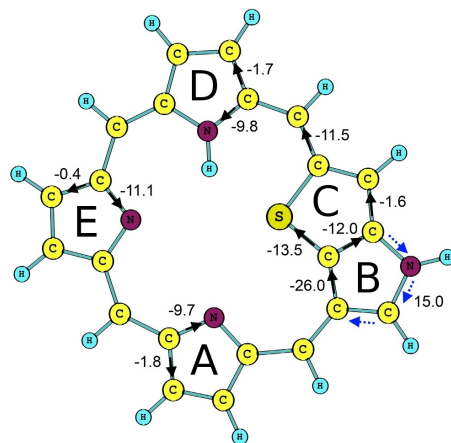


(b) (11.4 kcal/mol)

Figure 2: The molecular structures of the (a) 2-3 and (b) 1-4 tautomers. For the numbering of the inner hydrogens see the caption of Figure 1. The current strengths passing chemical bonds and relative energies are also given. The arrows indicate the current pathways.



(a) (0.0 kcal/mol)



(b) (6.8 kcal/mol)

Figure 3: The molecular structures of the (a) 2-4 and (b) 3-4 tautomers. For the numbering of the inner hydrogens see the caption of Figure 1. The current strengths passing chemical bonds and relative energies are also given. The arrows indicate the current pathways.

6 Porphyrinoid without ethyl formate

The molecular structure and NMR shieldings of the 2-4 substituted porphyrinoid tautomer without the ethyl formate

6.1 Cartesian coordinates

Atom	X	Y	Z
C	-2.12552	-3.39427	-0.36950
C	-0.70618	-3.21227	-0.30967
C	-2.31361	-4.77656	-0.35286
C	-0.09989	-4.46813	-0.26054
N	-1.10277	-5.41383	-0.28706
S	0.45200	-1.95214	-0.28561
C	1.76471	-3.12623	-0.21013
C	1.30347	-4.43573	-0.20430
C	3.13361	-2.73445	-0.16756
C	3.61613	-1.45604	-0.17132
N	2.79579	-0.34661	-0.21710
C	3.59427	0.70789	-0.21301
C	5.01629	0.31353	-0.16123
C	5.02187	-1.04641	-0.13550
C	3.12696	2.05084	-0.26298
C	1.82627	2.48414	-0.31225
N	0.67828	1.72248	-0.32729
C	-0.44193	2.52500	-0.39716
C	0.04730	3.90704	-0.41813
C	1.40579	3.87929	-0.36774
C	-1.77128	2.20210	-0.45010
C	-2.52066	0.97991	-0.45948
N	-2.05762	-0.25852	-0.41634
C	-3.17996	-1.08506	-0.46088
C	-4.40137	-0.28013	-0.53771
C	-3.99966	1.01481	-0.53710
C	-3.19332	-2.44919	-0.43925
H	3.87873	2.82708	-0.26584
H	-2.40171	3.07778	-0.50426

H	-4.17912	-2.90095	-0.48229
H	3.85081	-3.54799	-0.13096
H	1.96134	-5.29268	-0.16322
H	0.68940	0.71193	-0.30872
H	-0.97788	-6.41014	-0.26359
C	6.18122	1.25512	-0.11788
H	7.07108	0.75292	-0.50658
H	5.99820	2.09813	-0.79175
C	6.48654	1.79340	1.28938
H	5.62545	2.31736	1.70844
H	6.73700	0.97797	1.97069
H	7.32908	2.48883	1.26692
C	6.18973	-1.97742	-0.07755
H	6.21706	-2.52916	0.86702
H	6.15235	-2.71860	-0.88084
H	7.13419	-1.44033	-0.16906
C	2.35243	5.04118	-0.35388
H	3.21993	4.81063	-0.97869
H	1.86970	5.90355	-0.81909
C	2.83482	5.43649	1.05156
H	1.99671	5.73390	1.68408
H	3.34126	4.60595	1.54540
H	3.53160	6.27581	0.99691
C	-0.83283	5.11931	-0.46999
H	-0.27147	5.94711	-0.90935
H	-1.67179	4.93714	-1.14662
C	-1.37386	5.55803	0.90085
H	-2.01697	6.43479	0.79770
H	-1.95501	4.76396	1.37149
H	-0.55842	5.81493	1.57892
H	-3.23515	-5.33456	-0.38412
C	-5.79379	-0.82253	-0.59849
H	-5.92240	-1.51295	-1.43669
H	-6.05305	-1.37067	0.31236
H	-6.52679	-0.02444	-0.71661
C	-4.85973	2.24271	-0.57685
H	-5.80966	2.00143	-1.06116
H	-4.39552	3.00546	-1.20934
C	-5.14820	2.84101	0.80924
H	-5.67784	2.12231	1.43773
H	-4.22527	3.10925	1.32653
H	-5.76438	3.73969	0.72716

6.2 Nuclear magnetic resonance shield- ings (in ppm)

NO.	Atom	ISOTROPIC
1	c	51.61927058
2	c	30.27092883
3	c	60.36084095
4	c	39.27519162
5	n	117.69422518
6	s	224.02836421
7	c	21.16928701
8	c	70.04376647
9	c	55.34538116
10	c	18.56381866
11	n	-44.54991979
12	c	7.97256355
13	c	36.96562573
14	c	39.01482837
15	c	84.32609390
16	c	23.64776741
17	n	99.69111367
18	c	27.96351826
19	c	33.75697787
20	c	36.50347974
21	c	80.29281997
22	c	8.57209596
23	n	-63.39355548
24	c	19.11210934
25	c	38.36057931
26	c	36.76347287
27	c	53.47664912
28	h	27.91140724
29	h	27.95226862
30	h	26.59767478
31	h	26.64943522
32	h	26.42637758
33	h	13.52497482
34	h	25.14127358
35	c	162.90497082
36	h	29.89164677
37	h	30.19765158
38	c	166.14996204

39	h	31.19868857
40	h	31.33120255
41	h	30.98002069
42	c	175.26291875
43	h	30.50451139
44	h	30.47566226
45	h	30.24278016
46	c	163.23809498
47	h	30.24323729
48	h	29.94458618
49	c	165.80550197
50	h	31.23715161
51	h	31.02876624
52	h	30.92548991
53	c	162.38755673
54	h	29.94798479
55	h	30.29427856
56	c	165.69808372
57	h	30.94236021
58	h	31.04057814
59	h	31.24173333
60	h	25.61091351
61	c	173.65839930
62	h	30.51927168
63	h	30.52675141
64	h	30.24587849
65	c	162.62050803
66	h	29.89821404
67	h	30.28983747
68	c	166.60337933
69	h	31.35476390
70	h	31.20110749
71	h	31.04533484

7 Current density of the porphyrinoid without ethyl formate

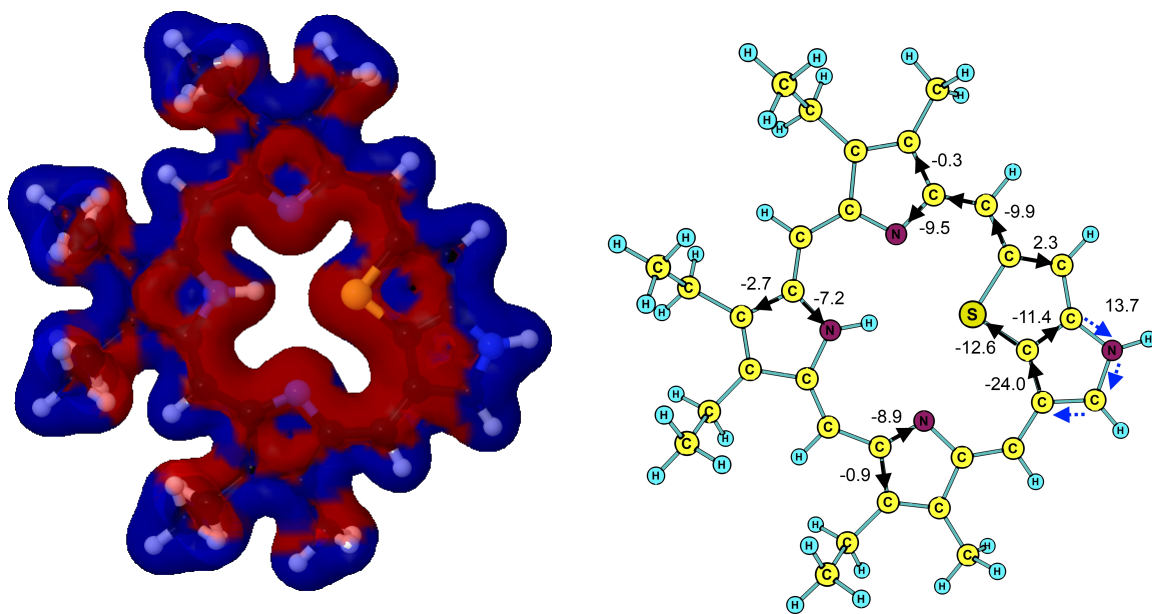


Figure 4: The signed modulus of the magnetically induced current densities and current strengths of the 2-4 substituted porphyrinoid tautomer without the ethyl formate are shown.