

*Electronic Supplementary Information***Predicting the Degree of Aromaticity of Novel Carbaporphyrinoids**Rashid R. Valiev^{*a}, Heike Fliegl,^{*b} Dage Sundholm,^{*c‡}

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1 Molecular structures

The Cartesian coordinates (in Å) of the electronic ground state of the investigated molecules that have been optimized at the B3LYP/def2-TZVP level of theory.

Model 1

Atom	X	Y	Z
H	3.168228383	3.164524455	-0.000642536
O	-0.000000035	-2.116368306	0.000108119
N	2.009308506	0.000000350	-0.000110887
O	-0.000000078	2.116368159	0.000137521
N	-2.009308351	-0.000000102	-0.000042845
C	1.103601565	-2.911576420	0.000602684
C	-1.103601577	-2.911576640	0.000213729
C	1.103601533	2.911576755	0.000080755
C	-1.103601753	2.911576101	0.000799257
C	2.818670456	-1.075537447	-0.000103903
C	2.818670740	1.075537863	-0.000707669
C	-2.818670468	-1.075537623	-0.000611464
C	-2.818670447	1.075537501	-0.000187949
C	0.686086415	-4.261657028	0.001077859
C	-0.686086405	-4.261657029	0.000967691
C	0.686086045	4.261657182	0.000753285
C	-0.686086594	4.261656427	0.001545702
C	4.230546042	-0.674200186	-0.000639361
C	4.230546319	0.674199683	-0.001275246
C	-4.230545980	-0.674199642	-0.001196301
C	-4.230545876	0.674200322	-0.001090750
C	2.394283401	-2.406465402	0.000345185
C	-2.394283543	-2.406465729	-0.000330667
C	-2.394283634	2.406465339	0.000408212
C	2.394283642	2.406465977	-0.000504695
H	1.348676589	-5.111631770	0.001387005
H	-1.348676576	-5.111631717	0.001461978
H	1.348675824	5.111632354	0.000644987
H	-1.348676672	5.111630650	0.002617244
H	5.078726449	-1.342189920	-0.000535409
H	5.078727052	1.342188654	-0.002100129
H	-5.078726523	-1.342189011	-0.001600665

H	-5.078725978	1.342190267	-0.001700062
H	3.168228315	-3.164523620	0.000337927
H	-3.168228326	-3.164524045	-0.000483324
H	-3.168228463	3.164523597	0.000374721

Model 2

Atom	X	Y	Z
H	3.321592119	3.213102594	0.001435122
S	-0.000004451	-1.528231863	0.000047771
N	2.319674834	0.000000122	0.000029679
S	-0.000004688	1.528231814	0.000007491
N	-2.319717848	-0.000000227	-0.000188636
C	1.254389071	-2.730999238	-0.000847845
C	-1.254423213	-2.730941946	0.000361914
C	1.254388983	2.730999380	0.000399973
C	-1.254423284	2.730941676	-0.000939421
C	3.117058757	-1.087553349	-0.000500200
C	3.117058601	1.087553493	0.000923705
C	-3.117019225	-1.087522143	0.000848654
C	-3.117019516	1.087521965	-0.000594427
C	0.686016230	-4.035017046	-0.000961757
C	-0.686118410	-4.034969118	-0.000285778
C	0.686016403	4.035017121	-0.000279021
C	-0.686118282	4.034968953	-0.000981624
C	4.519183904	-0.678091357	0.000080111
C	4.519183766	0.678091339	0.001120413
C	-4.519134857	-0.678065647	0.001128104
C	-4.519135070	0.678065850	0.000207737
C	2.608807574	-2.395176958	-0.001043510
C	-2.608771359	-2.395083275	0.001004267
C	-2.608771618	2.395083021	-0.001136638
C	2.608807367	2.395177126	0.001049769
H	1.295025390	-4.929431512	-0.001373998
H	-1.295145675	-4.929336228	-0.000390463
H	1.295025595	4.929431693	-0.000346538
H	-1.295145360	4.929336122	-0.001406601
H	5.372975552	-1.339139976	-0.000178399

H	5.372975288	1.339139709	0.001902653
H	-5.372899271	-1.339079029	0.001816541
H	-5.372899658	1.339079426	0.000210099
H	3.321592458	-3.213102362	-0.001195369
H	-3.321509908	-3.212961482	0.001412243
H	-3.321510200	3.212961353	-0.001336018

Model 4

Atom	X	Y	Z
H	3.281066160	3.240339370	0.141605722
C	-0.004411824	-2.058331778	-0.196249705
C	2.162239954	-0.011457329	-0.220103000
C	-0.003314648	2.035391288	-0.194573239
C	-2.168383388	-0.011232904	-0.259454368
C	1.193174233	-2.951764567	-0.071221833
C	-1.204027658	-2.951745916	-0.094196698
C	1.194158728	2.929129448	-0.070861121
C	-1.202983051	2.928871123	-0.093043156
C	2.938992745	-1.164858769	-0.019305578
C	2.939421538	1.141752032	-0.019416313
C	-2.949990461	-1.164424918	-0.078347112
C	-2.949573973	1.142106132	-0.077493646
C	0.692649944	-4.263016044	0.036339680
C	-0.705657322	-4.263014057	0.022887534
C	0.693635604	4.240523227	0.035008485
C	-0.704736325	4.240326314	0.022103232
C	4.305169770	-0.688140213	0.273767320
C	4.305457222	0.664550775	0.273565174
C	-4.322717804	-0.687289588	0.181648718
C	-4.322444420	0.665308149	0.182194783
C	2.513525663	-2.506039445	0.000446447
C	-2.525448716	-2.505714405	-0.049782823
C	-2.524525775	2.483128560	-0.048516045
C	2.514541805	2.483117760	0.000081811
H	1.305527902	-5.148441670	0.143530141
H	-1.320373323	-5.148505827	0.118237611
H	1.306421549	5.126334032	0.140119596
H	-1.319523266	5.125983415	0.115881266
H	5.146471832	-1.333208815	0.483298902
H	5.147011630	1.309410888	0.482901085
H	-5.169174089	-1.332160436	0.369665123
H	-5.168656842	1.310303095	0.370851749
H	3.279602025	-3.263414434	0.142994641
H	-3.294533621	-3.262990996	0.075872991
H	-3.293376439	3.240646309	0.077143428
H	-0.011435114	-1.297064837	0.586724155
H	0.004414845	-1.533114008	-1.155530569
H	-0.010110482	1.273503615	0.587707388
H	0.005293708	1.511073191	-1.154400492
H	1.144336204	-0.011619880	-0.524171946
H	-1.143385660	-0.011668229	-0.537909339

Model 3

Atom	X	Y	Z
H	3.207746717	3.251561529	-0.067618617
C	0.005011753	-2.018571272	0.332514019
N	2.245083839	0.016704070	0.019839587
C	-0.016965165	2.002095920	-0.335372173
N	-2.257535950	-0.032467069	-0.021513155
C	1.166305550	-2.803746113	0.165360486
C	-1.138368414	-2.827368554	0.153295205
C	1.126103565	2.810082140	-0.150297637
C	-1.178285734	2.786054242	-0.163504619
C	3.015276132	-1.116171451	0.085505773
C	3.002317933	1.156966922	-0.067156375
C	-3.014154379	-1.173259314	0.063777245
C	-3.028116285	1.099814554	-0.090321941
C	0.705090919	-4.175405189	-0.087179079
C	-0.647055674	-4.189368154	-0.093993270
C	0.634539389	4.170328071	0.105049019
C	-0.717410214	4.156235102	0.097371925
C	4.367034945	-0.658519305	0.032441217
C	4.359389216	0.713247292	-0.051470299
C	-4.371509259	-0.730312909	0.041563507
C	-4.379767700	0.641375199	-0.043487096
C	2.5114446731	-2.418349876	0.137734179
C	-2.490601756	-2.467518293	0.119145149
C	-2.523745483	2.401718496	-0.139061078
C	2.478451198	2.451165826	-0.117952630
H	1.362653835	-5.010681424	-0.281435877
H	-1.285194559	-5.037974592	-0.294982849
H	1.272411913	5.017570310	0.311999447
H	-1.375111092	4.990102014	0.296543895
H	5.230699530	-1.303625967	0.062319399
H	5.215532387	1.366046563	-0.112495455
H	-5.227512371	-1.383723026	0.098582337
H	-5.243735324	1.285712324	-0.078536782
H	3.254897989	-3.205711158	0.085202202
H	-3.220302580	-3.267895895	0.071552085
H	-3.266559628	3.189396654	-0.085642448
H	-1.258473421	-0.030448307	-0.046024993
H	-0.009686742	-1.032812983	0.765913662
H	-0.002018006	1.019216339	-0.775601429
H	1.246487647	0.017386524	0.057937465

Model 5

Atom	X	Y	Z
H	2.982089689	3.304908356	0.095617090
C	-0.305202160	-2.103569643	0.063625302
C	1.774567805	-0.031589760	0.084299735
C	-0.300049682	2.045564973	0.058474196

C	-2.380000995	-0.026437286	0.028857029	C	-1.135125131	3.003014781	0.004312261
C	0.903886014	-3.009546072	0.078068649	C	2.939752493	-1.259207592	-0.167345696
C	-1.516557828	-3.006483856	0.048833219	C	2.968471967	1.150054353	-0.172749150
C	0.911360909	2.948476873	0.070321211	C	-2.932773560	-1.186155160	-0.161561785
C	-1.509160713	2.951495976	0.042424870	C	-2.904257951	1.223109497	-0.148005953
C	2.674501217	-1.235965154	0.099019390	C	0.757839083	-4.271789525	0.395406943
C	2.677513262	1.170542832	0.095561671	C	-0.741153119	-4.327256970	0.423500583
C	-3.282913165	-1.228500462	0.029605594	C	0.779830015	4.287058187	0.440940967
C	-3.279869216	1.178009224	0.027637012	C	-0.719345132	4.232172158	0.419474674
C	0.373167692	-4.357482063	0.072459828	C	4.294494097	-0.747955936	-0.115710132
C	-0.989242207	-4.355765635	0.056032753	C	4.309210215	0.612896626	-0.120403763
C	0.384053460	4.297749976	0.061675430	C	-4.273311589	-0.649322234	-0.101276060
C	-0.978386143	4.299454413	0.045971088	C	-4.258727561	0.711504078	-0.092118233
C	3.957582447	-0.758090017	0.117006925	C	2.542140387	-2.551729960	-0.066497779
C	3.959382812	0.689507900	0.114583657	C	-2.533623965	-2.483264614	-0.068347881
C	-4.564973443	-0.747415554	0.027490393	C	-2.506349944	2.515330932	-0.044410692
C	-4.563102606	0.700192865	0.026493232	C	2.569496215	2.446609597	-0.071809615
C	2.205077552	-2.602922552	0.094031827	H	1.395562507	-5.090475980	0.698196451
C	-2.816786200	-2.596619283	0.034614514	H	-1.142197588	-5.102950948	-0.242223790
C	-2.810360419	2.544885134	0.029813459	H	1.164078371	4.519785480	1.441998934
C	2.211512125	2.538609300	0.087019881	H	-1.355544705	5.048959491	0.730529915
H	0.989877516	-5.246652108	0.080453412	H	5.170948020	-1.379054754	-0.049124654
H	-1.608226985	-5.243387355	0.049585600	H	5.200215568	1.224309175	-0.062322900
H	1.003021042	5.185387697	0.067467304	H	-5.164081265	-1.260949449	-0.041590043
H	-1.595100650	5.188631083	0.037161650	H	-5.135028225	1.342177554	-0.019635868
H	4.853226436	-1.365631038	0.131332226	H	3.314808112	-3.306231639	0.053186388
H	4.856564739	1.294827903	0.126250495	H	-3.304727967	-3.239125208	0.054675907
H	-5.462255488	-1.352739170	0.028067488	H	-3.278596323	3.269239573	0.081608956
H	-5.458839268	1.307780107	0.026413571	H	1.545457289	-0.032038529	-1.255832379
H	2.973762767	-3.371119370	0.104277425	H	-1.514745356	-0.000681414	-1.246820341
H	-3.587408589	-3.362960393	0.028053352	H	1.275625334	-0.012827479	0.482221784
H	-3.579034380	3.313076381	0.021742848	H	-1.236559734	-0.025268177	0.489728178
H	-0.314987550	-1.458204219	0.940766192	H	0.025891903	1.244394949	-0.736545446
H	-0.293765198	-1.455963017	-0.811672170	H	0.006167336	-1.276772969	-0.736961241
H	-0.311056805	1.402084877	0.936983705	H	-1.120471465	-4.567709002	1.424475131
H	-0.290622822	1.396090263	-0.815438525	H	1.178157306	5.066768866	-0.222052276
H	1.138713029	-0.032139617	-0.801071873				
H	-1.730039734	-0.027934287	-0.846446781				
H	1.112921536	-0.029462665	0.950454957				
H	-1.732105329	-0.026559204	0.905148066				

Model 6

Atom	X	Y	Z
H	3.340865634	3.202175468	0.051259163
C	-0.025911236	-2.256971499	-0.313441921
C	2.050100475	-0.039800760	-0.285720940
C	0.060343055	2.221761043	-0.306493841
C	-2.014918520	0.004207733	-0.274333806
C	1.171287927	-3.039856993	-0.013880793
C	-1.164333844	-2.944881016	-0.030114927
C	1.200276166	2.907608571	-0.024184331

Model 7

Atom	X	Y	Z
H	3.229158058	3.319091556	-0.006922455
N	-0.004042436	-2.260817593	0.024458032
C	1.965817146	-0.007717302	-0.033961174
N	0.007917462	2.255701140	0.000584996
C	-1.961396024	0.003001971	-0.034128489
C	1.149495786	-3.036921055	0.040217316
C	-1.161800519	-3.030701331	0.039214248
C	1.165637115	3.026888645	0.007676588
C	-1.145652991	3.033226352	0.007015507
C	2.877619627	-1.214197760	-0.019932153
C	2.883711784	1.194262501	-0.035964912
C	-2.879743160	-1.198643589	-0.022378798

C	-2.872992962	1.209791770	-0.037910186	C	4.285521576	0.563696118	0.016478913
C	0.667266968	-4.404630675	0.111588736	C	-4.315424891	-0.781869736	-0.003776863
C	-0.687070681	-4.400968496	0.111001639	C	-4.400743325	0.567971836	0.007473056
C	0.690876201	4.397480019	0.070786486	C	2.505135485	-2.587050947	-0.015212569
C	-0.663507284	4.401157065	0.070425012	C	-2.346169947	-2.419354540	-0.003137105
C	4.159012391	-0.735916185	-0.027950877	C	-2.593161255	2.368756649	0.031504435
C	4.162496683	0.709405043	-0.037635887	C	2.425968744	2.271165609	0.014550013
C	-4.158427086	-0.713547523	-0.033065383	H	1.292213814	-5.219040205	-0.024322112
C	-4.154210662	0.731723242	-0.042412627	H	-1.389267164	-5.080258694	-0.019728201
C	2.438404485	-2.581084629	0.014520536	H	1.259780055	4.773051761	-0.113003653
C	-2.448128180	-2.567885733	0.011941900	H	-1.216882942	4.996648392	-0.101303977
C	-2.434226191	2.577061399	-0.017667096	H	5.206577869	-1.424445544	0.017288149
C	2.451882964	2.563841225	-0.016001971	H	5.121138318	1.245908893	0.031974099
H	1.315051593	-5.265560337	0.167999735	H	-5.125964257	-1.495677307	-0.024849897
H	-1.339598953	-5.258310687	0.166868536	H	-5.292632621	1.176769869	-0.001186687
H	1.343179933	5.255268964	0.123455097	H	3.242245356	-3.379355894	-0.014681701
H	-1.311242081	5.262371061	0.122755585	H	-3.080841394	-3.217412315	-0.011890625
H	5.051194137	-1.347908215	-0.021025931	H	-3.338853345	3.156107244	0.014370570
H	5.057735024	1.316968642	-0.038245042	H	1.158916853	-0.319598013	-0.047311152
H	-5.053835860	-1.320687831	-0.028170962	H	-0.203239872	0.824161544	0.172443384
H	-5.046144848	1.343978536	-0.044782066				
H	3.211390966	-3.340534185	0.031894059				
H	-3.225245151	-3.323041444	0.027292534				
H	-3.207489441	3.336294952	-0.009665312				
H	1.305966020	0.000572603	0.839597545				
H	-1.342168866	-0.005688351	-0.941051419				
H	1.348698869	-0.013058028	-0.942481829				
H	-1.302748549	0.007238416	0.840350101				
H	0.005312350	1.288470499	-0.240526913				
H	-0.001418833	-1.289372330	-0.197762701				

Model 8

Atom	X	Y	Z
H	3.172037685	3.057164266	0.007581523
N	0.115609252	-2.086681862	-0.012121698
N	2.165821420	-0.183586858	-0.007089590
C	-0.092805079	1.885681104	0.086508700
N	-2.152784206	0.000916224	0.036561548
C	1.144169799	-2.954890337	-0.016445844
C	-1.027987449	-2.843090042	-0.011646152
C	1.060495690	2.642922093	0.026708733
C	-1.217141416	2.746320139	0.035845651
C	2.975897625	-1.285260715	-0.005688327
C	2.904625445	0.980370420	0.006200304
C	-2.881495426	-1.105731400	0.012020546
C	-3.024840898	1.060883076	0.031364130
C	0.667496023	-4.338396752	-0.020646579
C	-0.678322348	-4.267351589	-0.018835738
N	0.642546133	3.981455182	-0.045185663
C	-0.702186440	4.050651427	-0.041648671
C	4.330064856	-0.796362553	0.010245276

Model 9

Atom	X	Y	Z
H	3.295703424	3.234395586	-0.043502819
N	0.061440342	-1.989188829	-0.054821378
N	2.206595877	0.054056871	-0.057380381
C	0.044257831	1.826533220	-0.059751370
N	-2.108158908	0.043531786	-0.057212674
C	1.129170838	-2.791134790	-0.055123397
C	-1.030246581	-2.801720143	-0.055642280
C	1.234319919	2.736881291	-0.052523483
C	-1.139563167	2.763086375	-0.053077609
C	2.971981175	-1.069743067	-0.052428071
C	3.039822674	1.091390073	-0.050658060
C	-2.859652586	-1.059593322	-0.054327761
C	-2.961526601	1.101417789	-0.052453102
C	0.728737594	-4.206790331	-0.056159316
C	-0.620381545	-4.211655551	-0.056414391
N	0.730038613	4.016477722	-0.047094990
C	-0.634342597	4.044499477	-0.046772475
C	4.394631951	-0.703225680	-0.043690024
C	4.439236732	0.647803538	-0.042376540
C	-4.285785026	-0.711195587	-0.048643881
C	-4.347823094	0.641115463	-0.047149533
C	2.479930534	-2.363496149	-0.052848816
C	-2.352820814	-2.378480054	-0.054859502
C	-2.496783080	2.410630216	-0.050940118
C	2.568308125	2.429420071	-0.049345371
H	1.398407996	-5.054343520	-0.056496002
H	-1.285065596	-5.062855360	-0.057105880
H	1.306732356	4.843255959	-0.041694236

H	-1.158914237	4.987887612	-0.041013983
H	5.224837481	-1.394058564	-0.038417278
H	5.312053650	1.283905787	-0.036061184
H	-5.108702930	-1.411031402	-0.045557641
H	-5.228392849	1.266144592	-0.042685224
H	3.221524214	-3.155644779	-0.050166365
H	-3.099122618	-3.166429961	-0.053815039
H	-3.228081040	3.212637170	-0.046135353
H	0.052679240	1.136760914	-0.907239787
H	0.052323011	1.121383268	0.774828794

Model 11

Atom	X	Y	Z
H	3.173450357	3.213294182	-0.000291920
C	0.029505691	-1.860795518	-0.000571224
N	2.205770667	-0.022527081	0.000324110
C	-0.029461100	1.860792892	0.000759132
N	-2.205760727	0.022495094	0.000781943
C	1.135386919	-2.758550260	-0.000979765
C	-1.084260277	-2.697636995	-0.001464808
C	1.084270532	2.697688333	-0.000643886
C	-1.135359355	2.758557177	0.000359367
C	3.001135931	-1.139223829	0.001081798
C	2.964170609	1.108425572	0.000948859
C	-2.964182327	-1.108419320	0.000227479
C	-3.001083363	1.139206017	0.001654767
C	0.659457245	-4.109734486	-0.002338363
N	-0.659076661	-4.091748855	-0.002684035
N	0.659067797	4.091771881	-0.002096426
C	-0.659479962	4.109723490	-0.001465080
C	4.360565314	-0.676564771	0.002497982
C	4.337603704	0.690248565	0.002428869
C	-4.337610983	-0.690209851	0.000969020
C	-4.360530965	0.676574636	0.001956567
C	2.513208845	-2.436727750	0.000104830
C	-2.449440453	-2.405572805	-0.000970255
C	-2.513199848	2.436706906	0.001384484
C	2.449414926	2.405578746	-0.000072348
H	1.206451777	-5.044429699	-0.003022416
H	-1.244890320	-4.914274599	-0.003587674
H	1.244917753	4.914234269	-0.003635332
H	-1.206490384	5.044427694	-0.002502356
H	5.228125413	-1.317680773	0.003376837
H	5.183551968	1.359878608	0.003310414
H	-5.183611831	-1.359787750	0.000735664
H	-5.228107027	1.317686889	0.002652651
H	3.246664550	-3.235510199	0.000311155
H	-3.173470699	-3.213307634	-0.001443523
H	-3.246674145	3.235490766	0.001770890
H	1.169698042	-0.055827856	-0.000433196
H	-1.169727611	0.055748317	0.000565787

Model 10

Atom	X	Y	Z
H	3.193037050	3.242021732	-0.002217364
N	0.010581859	-1.996324508	-0.000020050
N	2.162486176	0.028326343	-0.000788094
C	-0.013319482	1.891762976	-0.000043294
N	-2.160335920	0.049260685	0.000452507
C	1.094004600	-2.816642880	0.000839335
C	-1.073523967	-2.805867873	-0.000545563
C	1.098261348	2.741798212	-0.000813733
C	-1.125073534	2.789097681	0.001161167
C	2.913898096	-1.102296594	0.000399584
C	2.961920761	1.143872406	-0.001467052
C	-2.895686003	-1.089375102	-0.000866741
C	-2.977427808	1.160316533	0.000935203
C	0.677541905	-4.222166761	0.000997358
C	-0.668996847	-4.216114907	-0.000022482
N	0.669344308	4.113884333	-0.000088552
C	-0.656317037	4.132057280	0.001161585
C	4.286413627	-0.686388449	0.000406181
C	4.313418843	0.683176821	-0.000926044
C	-4.280580607	-0.687979810	-0.001269484
C	-4.328118689	0.674125715	-0.000077767
C	2.423960096	-2.414686548	0.001230942
C	-2.406907942	-2.397183029	-0.001285546
C	-2.504606585	2.452327582	0.001665344
C	2.463579522	2.438918971	-0.001724217
H	1.343638107	-5.072095762	0.001734840
H	-1.342462950	-5.060198897	-0.000350766
H	1.257108236	4.933698994	-0.000164972
H	-1.204623622	5.064654822	0.001960371
H	5.128829913	-1.359729651	0.001313599
H	5.182508082	1.322165198	-0.001388894
H	-5.112036986	-1.375047936	-0.002251873
H	-5.205834295	1.301173881	-0.000053238
H	3.173623105	-3.196195909	0.002052088
H	-3.157062605	-3.178015473	-0.001992186
H	-3.243179969	3.246310921	0.002170638
H	1.137504608	0.111059221	-0.000806795
H	-1.135565392	0.156299782	0.000683964

Model 12

Atom	X	Y	Z
H	3.245293640	3.299918641	-0.100527807
C	-0.010952504	-2.113641884	0.496909777
C	2.143270035	0.042996225	0.170664975
C	0.015341901	2.109203249	-0.497637883
C	-2.138926990	-0.046859227	-0.168815111
C	1.161990487	-2.872101445	0.257836769
C	-1.135998995	-2.871330535	0.195681623
C	1.140322684	2.866966823	-0.196476346

C	-1.157631322	2.867649433	-0.258067310	12	C	19.04665484
C	2.944408400	-1.122113483	0.174040295	13	C	19.04670386
C	2.943292709	1.181804920	-0.024651370	14	C	51.77555130
C	-2.938983559	-1.185902016	0.025204964	15	C	51.77557187
C	-2.940366804	1.118047262	-0.172750736	16	C	51.77555674
C	0.700241206	-4.147687773	-0.119803590	17	C	51.77557624
N	-0.645305931	-4.144703126	-0.139826509	18	C	40.50850346
N	0.649737849	4.140377485	0.138896000	19	C	40.50855273
C	-0.695789312	4.143364902	0.119183521	20	C	40.50852846
C	4.333600042	-0.651951099	0.000269201	21	C	40.50855868
C	4.334228968	0.695529054	-0.105606925	22	C	74.87851642
C	-4.329962561	-0.699829346	0.105426329	23	C	74.87851256
C	-4.329485315	0.647730056	0.000183734	24	C	74.87856320
C	2.525356222	-2.442695567	0.219292442	25	C	74.87850936
C	-2.500907161	-2.509542265	0.113939566	26	H	21.58646714
C	-2.521119759	2.438577958	-0.218618352	27	H	21.58646843
C	2.505174329	2.505268973	-0.114265876	28	H	21.58646578
H	1.262861350	-5.022801221	-0.405515979	29	H	21.58646938
H	-1.214574298	-4.905583724	-0.471739561	30	H	22.20480086
H	1.219161376	4.901255542	0.470426858	31	H	22.20480408
H	-1.258412180	5.018513365	0.404817847	32	H	22.20480421
H	5.197351291	-1.300502552	-0.042045840	33	H	22.20480322
H	5.197140322	1.327704931	-0.261082290	34	H	21.12637677
H	-5.192892323	-1.332301526	0.259911964	35	H	21.12637933
H	-5.193400330	1.296141476	0.042080472	36	H	21.12637882
H	3.281352305	-3.217044100	0.133302508			
H	-3.241181292	-3.304153268	0.099566075			
H	-3.276967691	3.213155246	-0.132707275			
H	1.093833566	0.081330100	0.346889334			
H	-1.089079939	-0.084068263	-0.343204132			
H	-0.061417958	-1.143724349	0.941474708			
H	0.066132347	1.139603449	-0.942656070			

Model 2

NO.	Atom	Isotropic
1	H	20.41110384
2	S	169.17695428
3	N	-49.30510016
4	S	169.17691280
5	N	-48.91531759
6	C	24.44498150
7	C	24.51647795
8	C	24.44500651
9	C	24.51647762
10	C	21.29385943
11	C	21.29385719
12	C	21.40830232
13	C	21.40828157
14	C	44.11634364
15	C	44.18898694
16	C	44.11633679
17	C	44.18895485
18	C	43.23291554
19	C	43.23290859
20	C	43.28017074
21	C	43.28016529
22	C	60.89753342
23	C	60.89101503

2 Nuclear magnetic shieldings of tautomers

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

Model 1

NO.	Atom	Isotropic
1	H	21.12638017
2	O	45.73591260
3	N	-64.02240255
4	O	45.73580861
5	N	-64.02234304
6	C	22.71981918
7	C	22.71980321
8	C	22.71980279
9	C	22.71985032
10	C	19.04667884
11	C	19.04666489

24	C	60.89099805
25	C	60.89750223
26	H	21.22888387
27	H	21.23861624
28	H	21.22889343
29	H	21.23861692
30	H	22.17756710
31	H	22.17756382
32	H	22.19535391
33	H	22.19535293
34	H	20.41110012
35	H	20.46622201
36	H	20.46621750

Model 3

NO.	Atom	Isotropic
1	H	21.56397311
2	C	81.71086937
3	N	101.56044308
4	C	81.60355764
5	N	101.55937371
6	C	34.51883548
7	C	34.33469647
8	C	34.14589791
9	C	34.32412650
10	C	41.30558982
11	C	40.99366822
12	C	41.10274827
13	C	41.19596202
14	C	47.15103729
15	C	47.43758878
16	C	47.53417311
17	C	47.17769911
18	C	53.42952444
19	C	53.83197297
20	C	53.80290548
21	C	53.43031484
22	C	72.26092184
23	C	72.57054837
24	C	72.26072242
25	C	72.53240577
26	H	23.27965240
27	H	23.29339811
28	H	23.28140064
29	H	23.26480456
30	H	22.25245308
31	H	22.24483942
32	H	22.25038986
33	H	22.24177629
34	H	21.62208868
35	H	21.62514713

36	H	21.55141155
37	H	39.11587607
38	H	40.97711033
39	H	40.97581265
40	H	39.11518909

Model 4

NO.	Atom	Isotropic
1	H	21.21387440
2	C	143.32175216
3	C	65.12898961
4	C	143.32065641
5	C	65.28987123
6	C	28.10103438
7	C	28.08960693
8	C	28.07792744
9	C	28.09512444
10	C	31.72439711
11	C	31.71578920
12	C	31.82587144
13	C	31.84593443
14	C	38.26983129
15	C	38.33835382
16	C	38.26303165
17	C	38.32906525
18	C	44.86308697
19	C	44.83835970
20	C	44.80260681
21	C	44.84214187
22	C	58.19101022
23	C	58.26638409
24	C	58.27690946
25	C	58.17267135
26	H	21.50749210
27	H	21.51215653
28	H	21.50195763
29	H	21.50890914
30	H	23.54510958
31	H	23.54258208
32	H	23.55532132
33	H	23.55733151
34	H	21.22198761
35	H	21.25853225
36	H	21.26208528
37	H	40.83389238
38	H	39.44237980
39	H	40.83315448
40	H	39.44850703
41	H	39.21893945
42	H	39.21217277

Model 5

NO.	Atom	Isotropic
1	H	32.13746503
2	C	116.75516556
3	C	107.61302620
4	C	116.72326571
5	C	107.92595801
6	C	16.84604088
7	C	16.83475509
8	C	16.84849889
9	C	16.84147957
10	C	12.41181055
11	C	12.43640176
12	C	12.46151181
13	C	12.47421728
14	C	34.34017744
15	C	34.38354970
16	C	34.33046289
17	C	34.35954653
18	C	41.98315418
19	C	41.98055195
20	C	42.06277098
21	C	42.08283972
22	C	58.97875058
23	C	59.05336786
24	C	59.06622534
25	C	58.97824746
26	H	30.21671967
27	H	30.21422560
28	H	30.21461793
29	H	30.21441849
30	H	30.31353075
31	H	30.31444439
32	H	30.30798337
33	H	30.30964870
34	H	32.13475243
35	H	32.13080202
36	H	32.13996828
37	H	9.18526099
38	H	9.17547958
39	H	9.18009803
40	H	9.17496052
41	H	8.95257083
42	H	9.04325127
43	H	8.88340884
44	H	8.85286784

Model 6

NO.	Atom	Isotropic
1	H	25.70033716
2	C	39.59368038

3	C	135.35389973
4	C	39.60293595
5	C	135.33477071
6	C	25.92380459
7	C	27.16148206
8	C	27.13918207
9	C	25.91949802
10	C	27.10831567
11	C	26.06440266
12	C	26.05541383
13	C	27.09650796
14	C	46.11971918
15	C	135.00613386
16	C	134.96619838
17	C	46.10616196
18	C	38.62336529
19	C	38.48864662
20	C	38.47168191
21	C	38.61422012
22	C	62.13758104
23	C	64.64978049
24	C	62.11794418
25	C	64.63644632
26	H	25.57988843
27	H	28.60351298
28	H	28.73110242
29	H	25.57965809
30	H	25.19419371
31	H	25.17350762
32	H	25.17211858
33	H	25.19364354
34	H	25.54871183
35	H	25.69900742
36	H	25.54793821
37	H	27.35324612
38	H	27.35144762
39	H	27.04013587
40	H	27.03892582
41	H	23.39699818
42	H	23.39360560
43	H	28.73462854
44	H	28.59849674

Model 7

NO.	Atom	Isotropic
1	H	53.42202288
2	N	40.32410363
3	C	45.10905307
4	N	39.84640601
5	C	45.13006987
6	C	-14.65355396

7	C	-14.62982192
8	C	-15.04013125
9	C	-14.97914993
10	C	-24.85956391
11	C	-24.75185526
12	C	-24.82554437
13	C	-24.71002825
14	C	49.37500050
15	C	49.45995501
16	C	49.03279178
17	C	49.07497545
18	C	31.32424922
19	C	31.25754314
20	C	31.38007206
21	C	31.33126139
22	C	61.95667960
23	C	62.00594551
24	C	61.95546846
25	C	61.91039706
26	H	43.41737030
27	H	43.42260799
28	H	43.40809261
29	H	43.41534829
30	H	47.01890669
31	H	47.02420432
32	H	47.04680724
33	H	47.05184380
34	H	53.42364360
35	H	53.46303140
36	H	53.46514003
37	H	-52.10963111
38	H	-49.91918231
39	H	-49.87032705
40	H	-52.08264952
41	H	-67.56963422
42	H	-67.78210810

Model 8

NO.	Atom	Isotropic
1	H	23.58745153
2	N	-32.25455968
3	N	98.02315668
4	C	70.11711736
5	N	-77.75949242
6	C	10.24682576
7	C	17.56727753
8	C	48.51520411
9	C	51.44247064
10	C	30.72994346
11	C	39.67937444
12	C	14.69409136

13	C	18.04773789
14	C	46.00626000
15	C	37.02145383
16	N	80.77447369
17	C	44.30178631
18	C	53.03812719
19	C	48.52263071
20	C	44.91767248
21	C	42.51453948
22	C	82.32303498
23	C	62.84053853
24	C	60.97337421
25	C	86.75208332
26	H	23.38350806
27	H	23.08675231
28	H	22.54663865
29	H	22.93385473
30	H	23.38561473
31	H	23.28157764
32	H	23.39990159
33	H	23.25801972
34	H	23.37314889
35	H	22.87228395
36	H	22.87704565
37	H	30.07486465
38	H	31.45107490

Model 9

NO.	Atom	Isotropic
1	H	22.11993462
2	N	-99.78216582
3	N	-65.83190475
4	C	142.13174023
5	N	-93.42602859
6	C	11.17893333
7	C	15.44696193
8	C	30.03635130
9	C	47.18713643
10	C	18.83494081
11	C	12.54692404
12	C	17.35847577
13	C	17.52177625
14	C	41.61102689
15	C	38.10515390
16	N	79.59192357
17	C	47.40407395
18	C	37.22201857
19	C	46.48803621
20	C	41.59639198
21	C	44.38568110
22	C	58.60272329

23	C	55.88060153
24	C	55.90119227
25	C	81.26584813
26	H	22.78361274
27	H	22.61715853
28	H	20.69253303
29	H	21.64316379
30	H	22.63985456
31	H	22.99006313
32	H	22.76027192
33	H	22.76653769
34	H	21.94955846
35	H	21.82269423
36	H	21.30915246
37	H	37.75508216
38	H	37.76134717

33	H	23.33119888
34	H	23.38255402
35	H	23.46986145
36	H	23.16428401
37	H	27.21781982
38	H	26.27852715

Model 10

NO.	Atom	Isotropic
1	H	23.55389130
2	N	-19.20725696
3	N	73.31754267
4	C	-30.79104840
5	N	74.80101874
6	C	15.06605071
7	C	13.56309431
8	C	33.39411634
9	C	36.95462809
10	C	30.53825686
11	C	39.94426958
12	C	30.49972940
13	C	36.27738197
14	C	41.62965173
15	C	42.50449118
16	N	57.79114318
17	C	30.43476446
18	C	54.81823558
19	C	50.68400748
20	C	52.63380226
21	C	48.22366592
22	C	77.79145963
23	C	80.36347521
24	C	65.12523090
25	C	71.49445852
26	H	23.38219014
27	H	23.43098822
28	H	22.40827043
29	H	23.11044721
30	H	23.48722276
31	H	23.34742720
32	H	23.50772669

Model 11

NO.	Atom	Isotropic
1	H	24.46194088
2	C	-26.19797959
3	N	56.13436079
4	C	-26.06108287
5	N	55.69419846
6	C	31.98173923
7	C	27.67826872
8	C	28.04897539
9	C	31.84507716
10	C	32.21336891
11	C	34.21981595
12	C	33.89308494
13	C	31.93698172
14	C	23.92300662
15	N	46.95685376
16	N	47.15762445
17	C	23.85491336
18	C	51.74761156
19	C	53.19324029
20	C	53.05544107
21	C	51.63680828
22	C	67.36149406
23	C	77.69162021
24	C	67.21028341
25	C	77.91768883
26	H	23.24839996
27	H	22.38429910
28	H	22.40031211
29	H	23.24006154
30	H	23.83414223
31	H	23.90424816
32	H	23.85253537
33	H	23.78471021
34	H	23.86817847
35	H	24.28517272
36	H	23.74035957
37	H	23.47799799
38	H	23.53748042

Model 12

NO.	Atom	Isotropic
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1	H	23.69078549
2	C	81.02381131
3	C	59.36952352
4	C	81.06844156
5	C	59.20607308
6	C	48.69827361
7	C	42.15243295
8	C	42.23205650
9	C	48.65377958
10	C	32.20640159
11	C	30.81160179
12	C	30.77644449
13	C	32.09511207
14	C	52.87100831
15	N	91.52091450
16	N	91.59582683
17	C	52.87000334
18	C	44.72722225
19	C	48.17527736
20	C	48.09107816
21	C	44.71181867
22	C	60.92089192
23	C	74.73076754
24	C	60.84922554
25	C	74.86993931
26	H	23.84608819
27	H	23.14016331
28	H	23.14215980
29	H	23.84376434
30	H	24.10304629
31	H	24.20114306
32	H	24.17957772
33	H	24.08497808
34	H	23.33614893
35	H	23.63539002
36	H	23.29208390
37	H	33.33027616
38	H	33.34238422
39	H	33.60144764
40	H	33.60968504