**SYNTHESIS OF NOVEL AROMATIC NITROXIDES AS
POTENTIAL DNA INTERCALATORS. AN EPR
SPECTROSCOPICAL AND DFT COMPUTATIONAL STUDY**

Mario Beyer, Jörg Fritscher, Emiliano Feresin, Olav Schiemann*

*Institut für Physikalische und Theoretische Chemie, Johann Wolfgang Goethe-
Universität, Marie-Curie-Straße 11, D-60439 Frankfurt am Main, Germany*

* Corresponding author. E-mail: o.schiemann@prisner.de

Supporting Information

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Total energies and optimized cartesian coordinates for compounds **1•**, **2•**, **3•**, **4•** and **5•** as obtained from unrestricted PBE0/6-31G(d) computations.

Carbazol-9-oxyl 1•.

Energy = -591.34421 E_h

C	-0.7446454857	0.4955746722	-0.5177236234
C	-1.1251768303	-0.4268788487	0.4750396856
N	0.0309108599	-0.9785814226	1.0465183037
C	1.1516636818	-0.4119652016	0.4217347545
C	0.7130510808	0.5051147857	-0.5518597958
C	2.4887069923	-0.6721232063	0.6778389381
C	3.420099065	0.0264044095	-0.0846207273
C	3.0126359809	0.9449040006	-1.0602142139
C	1.6619868518	1.1919092628	-1.3020737214
C	-1.7365573342	1.1696785087	-1.2224848978
C	-3.0710578871	0.9051035764	-0.9177537373
C	-3.4203668258	-0.0183583439	0.0755512733
C	-2.4452506497	-0.7044219786	0.7933554912
O	0.0580934916	-1.8393736497	1.9667977142
H	2.774520224	-1.3891823874	1.4400949453
H	4.4802118252	-0.1437166147	0.0798349695
H	3.763642723	1.4746738457	-1.6392117269
H	1.3603656092	1.9073011756	-2.0622535445
H	-1.480217111	1.8887153335	-1.9957319874
H	-3.8552055612	1.4248315633	-1.4608020118
H	-4.4693025221	-0.2022732186	0.2894039935
H	-2.6856709794	-1.4249403622	1.5679189672

9,9-Diphenylacridan-10-oxyl 2°.

Energy = -1092.15340 E_h

C	-3.408665148	1.5634318853	0.5782939243
C	-3.9317069008	0.5342291486	1.3596869754
C	-3.13140108	-0.5393541143	1.7162442556
C	-1.8062983304	-0.5851161807	1.2760989436
C	-1.2677511576	0.4185696719	0.4577708125
C	-2.0905264624	1.4984726971	0.1350097872
N	-0.991645095	-1.646352386	1.7155637801
C	0.4080594087	-1.4947807123	1.6881683615
C	0.9905474347	-0.5114886877	0.8752981317
C	0.1297154128	0.2413361664	-0.1380839676
C	1.1805003	-2.3112143996	2.5183065371
C	2.5544852582	-2.1363541617	2.5596061473
C	3.1540981243	-1.14470765	1.7844230893
C	2.37410939	-0.3465749565	0.9523536517
O	-1.5092736515	-2.6288854174	2.3286286999
C	0.7511514936	1.6129039313	-0.4404776001
C	0.006737788	-0.6162393551	-1.4276136416
C	1.0177624186	-1.5037687992	-1.8089431377
C	0.9287538142	-2.2255794912	-2.9967049737
C	-0.1739165624	-2.0762467884	-3.8304008685
C	-1.1874670747	-1.1966709534	-3.4625052091
C	-1.0984009014	-0.4780722251	-2.2743681992
C	0.928397053	2.5166533276	0.616251223
C	1.4847615725	3.7703067398	0.4001068661
C	1.8788663259	4.1496596538	-0.882764898
C	1.7088861813	3.2621952447	-1.937604477
C	1.1486947672	2.0024400137	-1.718805644
H	-4.0263933875	2.4148506858	0.3072675375
H	-4.9610899731	0.5754155256	1.7043893898
H	-3.4925313463	-1.3475727341	2.3413473662
H	-1.6895324346	2.2956288385	-0.4840561497
H	0.6740665033	-3.0565434659	3.1202385732
H	3.1574715349	-2.7661153241	3.2076191944
H	4.2293672408	-0.9949219497	1.8206789013
H	2.8456699591	0.4127672573	0.3357723926
H	1.8843642873	-1.6444814637	-1.1715418075
H	1.7274396187	-2.9125200769	-3.264180543
H	-0.2460684584	-2.6432273826	-4.7546301749
H	-2.0601386141	-1.0717136085	-4.0982917804
H	-1.907247911	0.1919363772	-2.0013625304
H	0.6233332187	2.2276973516	1.618945404
H	1.6111970416	4.4540836621	1.2354289255
H	2.3144567818	5.1303462909	-1.0542972822
H	2.0116710373	3.543830788	-2.9427487658
H	1.0233110258	1.3219092382	-2.5546312476

3,6-Dimethylcarbazol-9-oxyl 3[•].

Energy = -669.88251 E_h

C	-0.5689977627	0.4208544941	-0.3907409632
C	-1.3574320482	-0.098760055	0.6502467957
N	-0.5515850407	-0.8885187848	1.4823447742
C	0.7552853441	-0.8755713289	0.9745499027
C	0.7865720942	-0.0764356104	-0.1841648382
C	1.8751634541	-1.5165692523	1.4755515236
C	3.0661697869	-1.3406818918	0.7771484145
C	3.142642802	-0.5527559582	-0.3826622529
C	1.9887499408	0.0814182919	-0.860653604
C	-1.1658195624	1.2398851111	-1.3437953991
C	-2.529597872	1.5305774589	-1.2513320759
C	-3.281809679	0.9886925681	-0.192211984
C	-2.7125325174	0.1683198446	0.7732067077
C	4.4487564081	-0.3874716195	-1.1104879815
C	-3.1975783663	2.4145639676	-2.2682147413
O	-0.9367216053	-1.5055089051	2.5121895033
H	1.8099299864	-2.1239831521	2.3721306146
H	3.9680470218	-1.828047461	1.1391505662
H	2.0412352669	0.6933672511	-1.7586412761
H	-0.579509201	1.6554100044	-2.1601300831
H	-4.3424274613	1.2213212301	-0.1304411408
H	-3.2859599414	-0.2530546284	1.5922113083
H	4.3816079193	-0.757999384	-2.1404264609
H	5.2553430076	-0.9335826834	-0.6126835372
H	4.7445689502	0.6669787478	-1.1657697383
H	-3.6260216918	3.3086040587	-1.799399746
H	-4.0182305887	1.8917571307	-2.7737950868
H	-2.4911472731	2.7465354984	-3.0347718912

9-Acridanylidenmalonitrile-10-oxyl 4[•].

Energy = -852.92182 E_h

C	-3.5425717827	-0.8260620729	-0.5715645832
C	-3.477292461	-1.7108682654	0.5096186793
C	-2.287176604	-1.888398138	1.1879693478
C	-1.1560086921	-1.1670785788	0.7924281089
C	-1.2119335607	-0.2119867066	-0.2473654944
C	-2.4307761529	-0.088446762	-0.93814478
N	0.0534511306	-1.4297237061	1.4456799349
C	1.2553823289	-0.9841843987	0.8841490491
C	1.2451544426	-0.0256047158	-0.1538794683
C	-0.0240229913	0.5864476794	-0.5383825433
C	2.4491618827	-1.5292059534	1.368012408
C	3.6467252784	-1.1705833245	0.7803879726
C	3.6594153408	-0.2798598733	-0.2978299267
C	2.4800777755	0.2840005916	-0.7514521293
C	-0.1019081344	1.8718877106	-1.0526454545
C	1.0224472647	2.7282047719	-1.2460052544
N	1.8911336057	3.4824223307	-1.4194090534
C	-1.3243895608	2.5499791143	-1.3363992327
N	-2.2810320572	3.1653426318	-1.5807230621
O	0.071784326	-2.1813238565	2.4630730028
H	-4.4657797236	-0.7128831366	-1.1311977879
H	-4.3547007821	-2.2781226328	0.805642654
H	-2.1879771163	-2.5872830819	2.0095813801
H	-2.5022130182	0.5796204469	-1.7866917049
H	2.3946584922	-2.2397810224	2.1837564252
H	4.5746735572	-1.6009568112	1.1450029299
H	4.5946103679	-0.0257540274	-0.7868593816
H	2.5138786186	0.9600158514	-1.5960334655

9-Ethylacridanylideneacyanoacetate-10-oxyl 5[•].

Energy = -1027.68251 E_h

C	1.8850419409	2.3653472342	-1.4803565348
C	1.203037584	3.4337227427	-0.8872510221
C	0.0231001806	3.2100475269	-0.2031084588
C	-0.4697156661	1.9053524044	-0.0932823696
C	0.2422424236	0.8029938444	-0.6045100915
C	1.408717035	1.0731037138	-1.3382712136
N	-1.7166826661	1.7093563012	0.5121696758
C	-2.3977699955	0.4984969566	0.3149471348
C	-1.7198998425	-0.6311851926	-0.1960441677
C	-0.266670822	-0.5507115262	-0.3739403024
C	-3.760945846	0.4569239624	0.62333874
C	-4.4804078333	-0.6964879861	0.3740766528
C	-3.8475856843	-1.8071353842	-0.1907585824
C	-2.4901986121	-1.7738591135	-0.4652253936
O	-2.2915746201	2.6725515605	1.1000935863
C	0.5823929969	-1.6258628272	-0.2759024875
C	2.0852039183	-1.5238470601	-0.2554363178
C	0.1594461085	-2.9715497284	-0.109294421
N	-0.1169030254	-4.092312339	0.0423281346
O	2.8102589265	-2.1147558902	-1.0198248933
O	2.5029622683	-0.7495810851	0.7467601851
C	3.9262644101	-0.5608664948	0.829063002
C	4.1928446689	0.3363219797	2.0127369151
H	2.7827193537	2.5462306377	-2.0639601521
H	1.581099158	4.4467539854	-0.9891978472
H	-0.5545421855	4.015452031	0.2343136506
H	1.9278952411	0.2564877457	-1.830366991
H	-4.2198113265	1.3476984479	1.0350654859
H	-5.5419336766	-0.7278021524	0.6013507624
H	-4.4153512072	-2.7042735944	-0.4175330852
H	-2.0224925494	-2.6439392505	-0.907700998
H	4.2729729792	-0.117728344	-0.1110848184
H	4.4041877265	-1.5402592661	0.9295878206
H	5.2692402742	0.5091075008	2.1117771626
H	3.830790287	-0.120902198	2.9383235143
H	3.6965713778	1.3033197278	1.8870233053