Electronic Supplementary Material (ESI) for Faraday Discussions.

Supporting Information: Donor-Acceptor Preassociation, Excited State Solvation Threshold, and Optical Energy Cost as Challenges in Chemical Applications of Photobases

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Contents

1 Identification of Protonated and Unprotonated forms of 5-Methoxyquinoline from Previous Works

1.1 Steady State

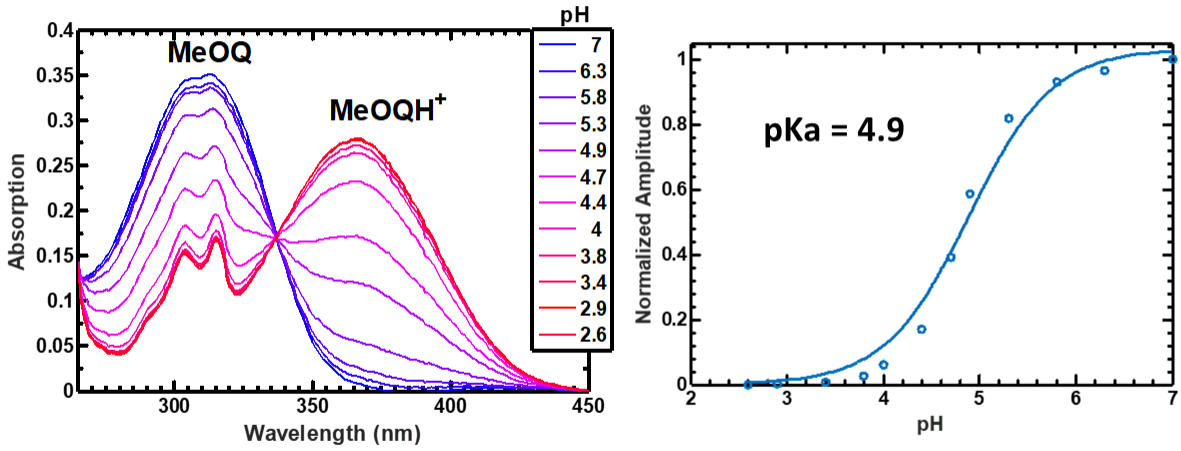

Figure S1: LEFT: Absorption of 5-methoxyquinoline (MeOQ) in water as a function of pH. RIGHT: Titration curve from absorption data. Fit comes from the Henderson-Hasselbach equation. Recreated from our previous work.[S1]

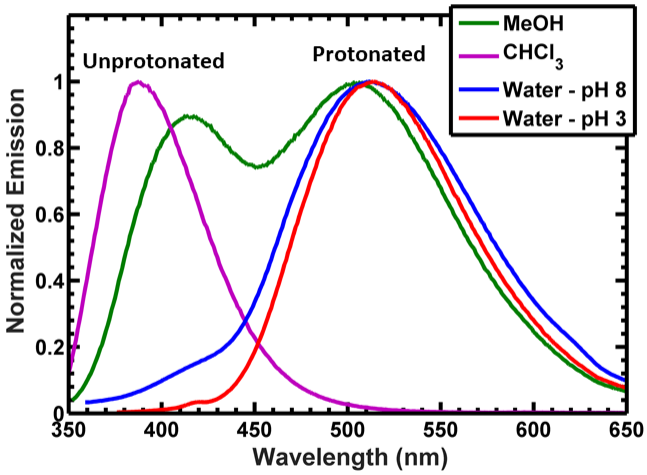

Figure S2: Emission of 5-methoxyquinoline in representative solvents. In CHCl3, there are no acidic protons. Therefore, we know that emission is from the unprotonated form of 5-methoxyquinoline. In acidic water (pH=3) below the ground state pKa of 5-methoxyquinoline (pKa=4.9), we know that 5-methoxyquinoline is mostly protonated in the ground state. Therefore, we know that this emission is from the protonated form. We also see emission from the protonated form in pH 8 water. This is indicative of photobasic behavior. The dual emission in methanol is shown for reference. All spectra obtained from excitation at 340nm. Recreated from our previous work.[S1]

2 Absorption and Emission of 5-methoxyquinoline by Solvent

2.1 2,2,2-trifluoroethanol

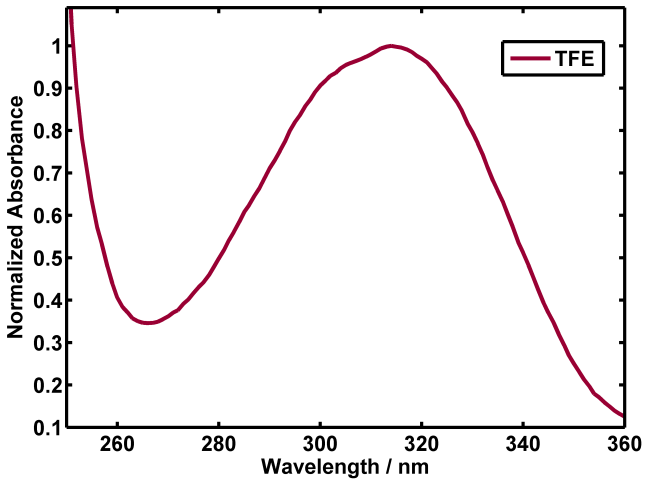

Figure S3: Absorption spectrum for 5-methoxyquinoline in pure 2,2,2-trifluoroethanol.

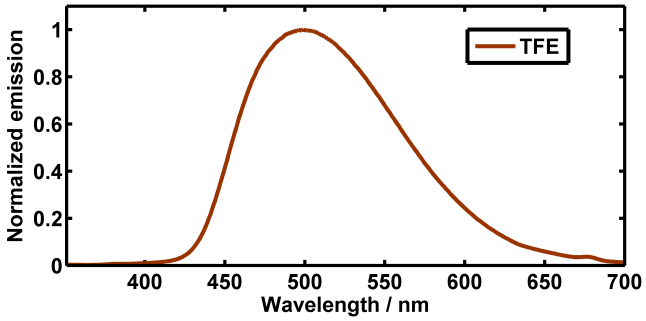

Figure S4: Emission spectrum for 5-methoxyquinoline in pure 2,2,2-trifluoroethanol. Excitation at 310nm.

2.2 DCM

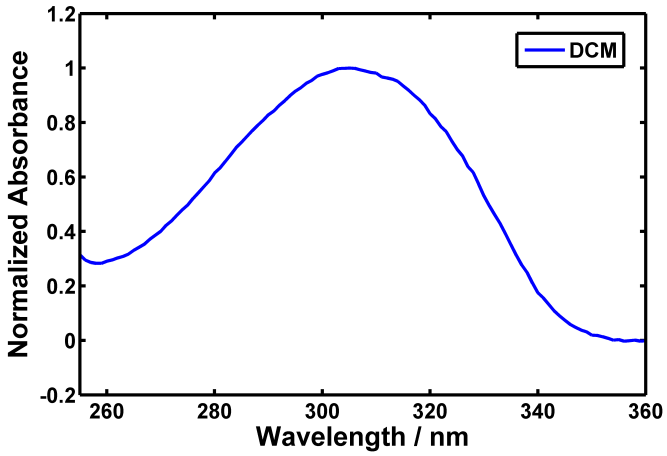

Figure S5: Absorption spectrum for 5-methoxyquinoline in pure DCM.

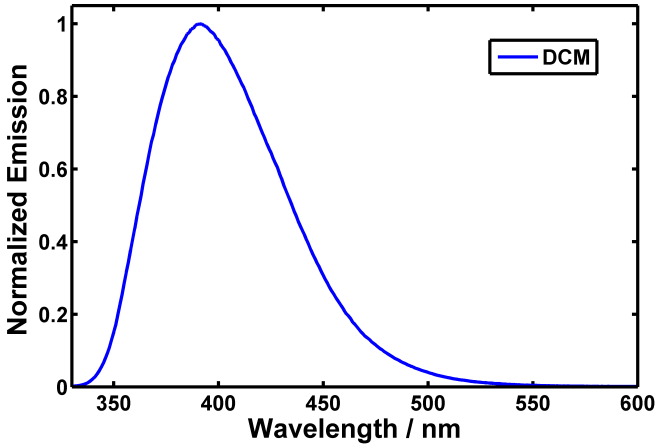

Figure S6: Emission spectrum for 5-methoxyquinoline in pure DCM. Excitation at 310nm.

3 Transition dipole moments, ground state nuclear repulsion energies and cartesian geometries of molecules used in theoretical calculations

The transition dipole moments shown below were used to identify the L_b states, which were used for analysis in the paper. The excited state with the largest transition dipole moment along the short axis of the molecule was assigned as L_b. All geometry optimizations and excited state calculations were performed using QChem.[S2]

3.1 Substituted quinolines

Quinoline

Transition Dipole Moment: -0.0286 X 0.7575 Y 0.0000 Z

Nuclear Repulsion Energy (hartrees): 555.946386

Cartesian Coordinates (angstroms):

1 C -1.2053753152 -1.3970754660 0.0000000000

2 C -2.3938011962 -0.7117605963 0.0000000000

3 C 0.0287126165 -0.6957659721 0.0000000000

4 C -2.4081752013 0.7054932689 0.0000000000

5 C -1.2302111590 1.4084512495 0.0000000000

6 C 0.0148054441 0.7266696463 0.0000000000

7 N 1.1857427009 -1.4183569906 0.0000000000

8 C 2.3201917872 -0.7587036113 0.0000000000

9 C 2.4192967612 0.6550989166 0.0000000000

10 C 1.2654735584 1.3932345854 0.0000000000

11 H -1.1718317146 -2.4821301928 0.0000000000

12 H -3.3362367794 -1.2516625938 0.0000000000

13 H -3.3597641926 1.2286190090 0.0000000000

14 H -1.2340713203 2.4959617205 0.0000000000

15 H 3.2278351025 -1.3602361272 0.0000000000

16 H 3.3977744166 1.1241054931 0.0000000000

17 H 1.2921004207 2.4805025566 0.0000000000

5-Amino Quinoline

Transition Dipole Moment: -0.5496 X 0.9052 Y 0.0000 Z

Nuclear Repulsion Energy (hartrees): 555.9463859572

Cartesian Coordinates (angstroms):

1 C -0.5118801036 -1.9566693904 0.0000000000

2 C -1.8475512585 -1.6436303015 0.0000000000

3 C 0.4455988857 -0.9129596896 0.0000000000

4 C -2.2902683345 -0.3063081068 0.0000000000

5 C -1.3870061364 0.7423236364 0.0000000000

6 C 0.0188516789 0.4487376591 0.0000000000

7 N 1.7650307989 -1.2622737576 0.0000000000

8 C 2.6640640745 -0.3067112378 0.0000000000

9 C 2.3496189350 1.0713920295 0.0000000000

10 C 1.0287060343 1.4407586809 0.0000000000

11 H -0.1514395877 -2.9792898820 0.0000000000

12 H -2.5914255128 -2.4358285578 0.0000000000

13 H -3.3565334750 -0.0941179904 0.0000000000

14 N -1.8351116763 2.0444176771 0.0000000000

15 H 3.7040931773 -0.6285656664 0.0000000000

16 H 3.1411639131 1.8138975622 0.0000000000

17 H 0.7771811528 2.4976511843 0.0000000000

18 H -2.8218755315 2.2381717615 0.0000000000

19 H -1.2175024731 2.8349887810 0.0000000000

5-Bromo Quinoline

Transition Dipole Moment: 0.8586 X -0.5464 Y 0.0000 Z

Nuclear Repulsion Energy (hartrees): 792.1676540774

Cartesian Coordinates (angstroms):

1 C 1.6525554249 -2.0399137029 0.0000000000

2 C 0.4248293201 -2.6469499473 0.0000000000

3 C 1.7488010695 -0.6248109150 0.0000000000

4 C -0.7614002195 -1.8763313700 0.0000000000

5 C -0.6880611435 -0.5069865608 0.0000000000

6 C 0.5646782840 0.1703354555 0.0000000000

7 N 2.9987533645 -0.0798526755 0.0000000000

8 C 3.1007455760 1.2275598545 0.0000000000

9 C 1.9918554232 2.1068224446 0.0000000000

10 C 0.7278666672 1.5790242450 0.0000000000

11 H 2.5782414571 -2.6059835550 0.0000000000

12 H 0.3502758684 -3.7301345424 0.0000000000

13 H -1.7290937725 -2.3652926755 0.0000000000

14 H 4.1111052377 1.6317049078 0.0000000000

15 H 2.1487609775 3.1805522555 0.0000000000

16 H -0.1424531758 2.2272438379 0.0000000000

17 Br -2.3129393956 0.4797457080 0.0000000000

5-Chloro Quinoline

Transition Dipole Moment: 0.6468 X -0.7237 Y 0.0000 Z

Nuclear Repulsion Energy (hartrees): 623.5709186083

Cartesian Coordinates (angstroms):

1 C 0.5133173398 -2.1642711068 0.0000000000

2 C -0.8398579158 -2.3789625956 0.0000000000

3 C 1.0253221086 -0.8412830795 0.0000000000

4 C -1.7467563439 -1.2932727935 0.0000000000

5 C -1.2677154347 -0.0095787729 0.0000000000

6 C 0.1282492410 0.2661140413 0.0000000000

7 N 2.3795642601 -0.6855282754 0.0000000000

8 C 2.8596262353 0.5353498373 0.0000000000

9 C 2.0561487163 1.7007457902 0.0000000000

10 C 0.6929159136 1.5660756846 0.0000000000

11 H 1.2278943381 -2.9808213138 0.0000000000

12 H -1.2346449189 -3.3901702142 0.0000000000

13 H -2.8169474285 -1.4696362309 0.0000000000

14 H 3.9445139052 0.6226974296 0.0000000000

15 H 2.5200978851 2.6813698071 0.0000000000

16 H 0.0467808317 2.4376560209 0.0000000000

17 Cl -2.4136992346 1.3158531603 0.0000000000

5-Cyano Quinoline

Transition Dipole Moment: 0.8311 X -0.9180 Y 0.0000 Z

Nuclear Repulsion Energy (hartrees): 594.1765419265

Cartesian Coordinates (angstroms):

1 C 0.6670064097 -2.0886537775 0.0000000000

2 C -0.6545462945 -2.4573075070 0.0000000000

3 C 1.0393790252 -0.7188646529 0.0000000000

4 C -1.6693752577 -1.4752716162 0.0000000000

5 C -1.3378121320 -0.1370121316 0.0000000000

6 C 0.0290816352 0.2790215713 0.0000000000

7 N 2.3684900412 -0.4164451171 0.0000000000

8 C 2.7085252904 0.8508747391 0.0000000000

9 C 1.7783536240 1.9200299482 0.0000000000

10 C 0.4392080371 1.6348280665 0.0000000000

11 H 1.4626175421 -2.8271708706 0.0000000000

12 H -0.9353550300 -3.5055805188 0.0000000000

13 H -2.7122314212 -1.7750970485 0.0000000000

14 H 3.7756656266 1.0640100320 0.0000000000

15 H 2.1374817807 2.9438125447 0.0000000000

16 H -0.3066887603 2.4252803606 0.0000000000

17 C -2.3738290197 0.8576818789 0.0000000000

18 N -3.1993707729 1.6722248005 0.0000000000

5-Methoxy Quinoline

Transition Dipole Moment: -0.8563 X 0.5102 Y 0.0020 Z

Nuclear Repulsion Energy (hartrees): 650.9191633368

Cartesian Coordinates (angstroms):

1 C 0.5860096533 -2.0986638686 0.1041728437

2 C -0.7701451401 -2.2839225186 0.1008734657

3 C 1.1135418204 -0.7808159605 0.0468964965

4 C -1.6727722191 -1.1914643393 0.0424950785

5 C -1.1837365516 0.0930379236 -0.0145009561

6 C 0.2274148125 0.3267968045 -0.0184706773

7 N 2.4679043610 -0.6261537654 0.0525490438

8 C 2.9482701645 0.5953776273 -0.0062358530

9 C 2.1506034711 1.7606281331 -0.0811279315

10 C 0.7853894068 1.6243640575 -0.0839408715

11 H 1.2851203662 -2.9266687687 0.1533024306

12 H -1.1788454095 -3.2894917735 0.1398547406

13 H -2.7389693216 -1.3866773172 0.0441077221

14 H 4.0336497434 0.6809170876 -0.0006160942

15 H 2.6177367762 2.7388205012 -0.1290039155

16 H 0.1287816249 2.4860711855 -0.1407125343

17 O -1.9449242463 1.2136421721 -0.0729401264

18 C -3.3490846591 1.0724921827 -0.0633440873

19 H -3.6978760516 0.5125928273 -0.9402862461

20 H -3.7504523671 2.0856364682 -0.0964363611

21 H -3.6928298202 0.5775292824 0.8536679602

3.2 Substituted acridines

Acridine

Transition Dipole Moment: 0.0000 X -0.0000 Y -1.0803 Z

Nuclear Repulsion Energy (hartrees): 773.7145851967

Cartesian Coordinates (angstroms): 1 C 2.3801552000 0.0000000000 1.4239999926

2 C 3.5778641000 0.0000000000 0.7705914926

3 C 1.1507144000 0.0000000000 0.6904615926

4 C 3.6329168000 0.0000000000 -0.6563687074

5 C 2.4834611000 0.0000000000 -1.3910122074

6 C 1.2079079000 0.0000000000 -0.7441566074

7 N 0.0000000000 0.0000000000 1.3750144926

8 C -1.1507144000 0.0000000000 0.6904615926

9 C -1.2079079000 0.0000000000 -0.7441566074

10 C -0.0000000000 0.0000000000 -1.4403733074

11 C -2.3801552000 0.0000000000 1.4239999926

12 C -3.5778641000 0.0000000000 0.7705914926

13 C -3.6329168000 0.0000000000 -0.6563687074

14 C -2.4834611000 0.0000000000 -1.3910122074

15 H 2.3167486000 0.0000000000 2.5077116926

16 H 4.5055432000 0.0000000000 1.3357161926

17 H 4.5984920000 0.0000000000 -1.1533155074

18 H 2.5174548000 0.0000000000 -2.4779925074

19 H -0.0000000000 0.0000000000 -2.5292880074

20 H -2.3167486000 0.0000000000 2.5077116926

21 H -4.5055432000 0.0000000000 1.3357161926

22 H -4.5984920000 0.0000000000 -1.1533155074

23 H -2.5174548000 0.0000000000 -2.4779925074

1-Amino Acridine

Transition Dipole Moment: -0.4566 X 1.1387 Y -0.0080 Z

Nuclear Repulsion Energy (hartrees): 884.1615550136

Cartesian Coordinates (angstroms):

1 C 2.7716276235 -1.3158093790 0.0479018096

2 C 3.8782671414 -0.5170496597 0.0237328401

3 C 1.4610728211 -0.7424860081 0.0189384100

4 C 3.7538369012 0.9035666494 -0.0334961344

5 C 2.5199721884 1.4865836622 -0.0608419514

6 C 1.3382434095 0.6836759218 -0.0294705995

7 N 0.4025867414 -1.5629032846 0.0252892644

8 C -0.8273697942 -1.0346130218 0.0054537431

9 C -1.0620447916 0.3859201235 -0.0048382787

10 C 0.0504637083 1.2220671545 -0.0435819727

11 C -1.9439877886 -1.9264441806 -0.0252882844

12 C -3.2106713071 -1.4227301706 -0.0575172412

13 C -3.4556698992 -0.0217553527 -0.0297628733

14 C -2.4201219647 0.8767862702 0.0075797802

15 H 2.8454429441 -2.3981611003 0.0870754254

16 H 4.8688843432 -0.9623421108 0.0450475167

17 H 4.6499744094 1.5167438566 -0.0546049457

18 H 2.4164780084 2.5684292427 -0.1048294779

19 H -0.0643666513 2.3012038121 -0.1123315499

20 H -1.7420193520 -2.9921468923 -0.0273598589

21 H -4.0628596390 -2.0960046750 -0.0868856238

22 H -4.4816858411 0.3383623123 -0.0258246272

23 N -2.6381807263 2.2586864676 -0.0076935776

24 H -2.0453732076 2.7922133114 0.6154301857

25 H -3.6076425963 2.5164938286 0.1266070782

1-Bromo Acridine

Transition Dipole Moment: 0.6620 X -1.0409 Y -0.0000 Z

Nuclear Repulsion Energy (hartrees): 1172.7923068589

Cartesian Coordinates (angstroms):

1 C 3.7762469682 -0.7909732093 0.0000097614

2 C 4.5891630738 0.3049789363 0.0000069274

3 C 2.3533498425 -0.6371967359 0.0000035373

4 C 4.0418501033 1.6241338506 -0.0000025533

5 C 2.6906268550 1.8104714362 -0.0000082249

6 C 1.8052410337 0.6876185250 -0.0000050890

7 N 1.5886106486 -1.7353314699 0.0000057915

8 C 0.2579205664 -1.5956617463 0.0000005949

9 C -0.3940548257 -0.3116935836 -0.0000066804

10 C 0.4183658607 0.8210538225 -0.0000096565

11 C -0.5379120559 -2.7844648948 0.0000022192

12 C -1.8978729419 -2.7052302202 -0.0000023655

13 C -2.5593516171 -1.4422414364 -0.0000083519

14 C -1.8287877966 -0.2916426676 -0.0000101824

15 H 4.1738951040 -1.8008644755 0.0000165636

16 H 5.6683040621 0.1801437620 0.0000117549

17 H 4.7102564493 2.4799172538 -0.0000051252

18 H 2.2637185185 2.8102675227 -0.0000152037

19 H -0.0258362553 1.8119755890 -0.0000155739

20 H -0.0155855809 -3.7353085048 0.0000069456

21 H -2.4998077517 -3.6089575426 -0.0000013715

22 H -3.6436342243 -1.4024521509 -0.0000108886

23 Br -2.7532732959 1.3741562004 -0.0000149025

1-Cyano Acridine

Transition Dipole Moment: -0.4567 X 1.2002 Y 0.0000 Z

Nuclear Repulsion Energy (hartrees): 929.7731082091

Cartesian Coordinates (angstroms):

1 C 3.0222211526 -1.1667444770 0.0000219659

2 C 4.0385496650 -0.2569779291 0.0000157534

3 C 1.6594413075 -0.7301509728 0.0000088897

4 C 3.7674503014 1.1454342405 -0.0000039678

5 C 2.4821516370 1.6011919019 -0.0000171521

6 C 1.3881800023 0.6799167353 -0.0000113328

7 N 0.6926339953 -1.6560764310 0.0000162598

8 C -0.5820268006 -1.2491042837 0.0000043527

9 C -0.9588659076 0.1332097271 -0.0000165715

10 C 0.0558382121 1.0883497481 -0.0000242943

11 C -1.6073068514 -2.2480605808 0.0000137774

12 C -2.9263581777 -1.8983879555 0.0000027082

13 C -3.3125500796 -0.5297006529 -0.0000187339

14 C -2.3613992261 0.4582866295 -0.0000282150

15 H 3.2072017264 -2.2362505713 0.0000369818

16 H 5.0703851508 -0.5963030056 0.0000256721

17 H 4.5962498618 1.8468937799 -0.0000084165

18 H 2.2672711335 2.6667553011 -0.0000325603

19 H -0.1882205247 2.1486879946 -0.0000404422

20 H -1.2901529952 -3.2861391278 0.0000300801

21 H -3.6968905946 -2.6626853129 0.0000109563

22 H -4.3649014639 -0.2640334848 -0.0000279474

23 C -2.7586469189 1.8378089820 -0.0000499500

24 N -3.0583411979 2.9584222357 -0.0000681823

1-Methoxy Acridine

Transition Dipole Moment: -0.4035 X 1.0709 Y -0.1090 Z

Nuclear Repulsion Energy (hartrees): 997.9578097496

Cartesian Coordinates (angstroms):

1 C 3.1237642595 -1.1486305033 0.2095153383

2 C 4.1267623519 -0.2248257911 0.1589893208

3 C 1.7565432947 -0.7460130180 0.0769930556

4 C 3.8378033181 1.1606727470 -0.0293851575

5 C 2.5472960519 1.5839957872 -0.1580607870

6 C 1.4673105080 0.6482726481 -0.1050291724

7 N 0.8064353265 -1.6885498113 0.1241043910

8 C -0.4738992620 -1.3147630364 0.0062493486

9 C -0.8680198853 0.0555836889 -0.1636778782

10 C 0.1301821831 1.0244752215 -0.2261904618

11 C -1.4877286401 -2.3236416757 0.0473610269

12 C -2.8032290945 -1.9833154773 -0.0756711754

13 C -3.2035781163 -0.6240203817 -0.2360489840

14 C -2.2654329997 0.3652023290 -0.2711868157

15 H 3.3235808359 -2.2062228865 0.3506089517

16 H 5.1611720644 -0.5406014544 0.2612349250

17 H 4.6547481802 1.8749108717 -0.0715104637

18 H 2.3184712268 2.6368843501 -0.3045379773

19 H -0.1361059755 2.0667172769 -0.3820028139

20 H -1.1698094459 -3.3533040059 0.1738553507

21 H -3.5680375908 -2.7540925550 -0.0497037980

22 H -4.2536421730 -0.3668347390 -0.3371625036

23 O -2.6249706600 1.6792114811 -0.4377494753

24 C -2.9509232107 2.3453185358 0.7744712053

25 H -3.8254620631 1.8852241473 1.2506722764

26 H -3.1797421264 3.3789277237 0.5093152594

27 H -2.1048103180 2.3218953883 1.4738977060

3.3 Substituted Benzacridines

Benzacridine

Transition Dipole Moment: -0.0254 X -1.2737 Y 0.0000 Z

Nuclear Repulsion Energy (hartrees): 1123.3153144766

Cartesian Coordinates (angstroms):

1 C 3.6348722948 -1.4350804017 -0.0000000000

2 C 4.8226647953 -0.7715234025 -0.0000000000

3 C 2.3881138953 -0.7198227008 -0.0000000000

4 C 2.4245787963 0.7241102992 0.0000000000

5 C 3.7028697968 1.3801881983 0.0000000000

6 C 4.8578478963 0.6610449975 0.0000000000

7 C 1.1667857949 -1.3776951000 -0.0000000000

8 C -0.0495660046 -0.6678024991 -0.0000000000

9 C -0.0115856036 0.7727538008 0.0000000000

10 C 1.2321122968 1.4328421000 0.0000000000

11 N -1.2062307051 -1.3672835983 -0.0000000000

12 C -2.3533483046 -0.6978656975 -0.0000000000

13 C -2.4298603037 0.7446767025 0.0000000000

14 C -1.2413601032 1.4543399017 0.0000000000

15 C -3.5817683052 -1.4444699967 -0.0000000000

16 C -4.7828514047 -0.8048580959 -0.0000000000

17 C -4.8559467037 0.6268552042 0.0000000000

18 C -3.7194723032 1.3748242034 0.0000000000

19 H 3.6059465941 -2.5217755017 -0.0000000000

20 H 5.7572771949 -1.3247862032 -0.0000000000

21 H 3.7267494975 2.4673121983 0.0000000000

22 H 5.8176368966 1.1692861968 0.0000000000

23 H 1.1198045941 -2.4632377999 -0.0000000000

24 H 1.2526944976 2.5212177000 0.0000000000

25 H -1.2546392024 2.5431363017 0.0000000000

26 H -3.5062045059 -2.5273779967 -0.0000000000

27 H -5.7048935051 -1.3792160952 -0.0000000000

28 H -5.8284406034 1.1100321049 0.0000000000

29 H -3.7668357025 2.4612892034 0.0000000000

4-Amino Benzacridine

Transition Dipole Moment: -0.3700 X 1.3527 Y 0.0168 Z

Nuclear Repulsion Energy (hartrees): 1246.3191669501

Cartesian Coordinates (angstroms):

1 C 3.9890587306 -1.3159569585 -0.0433927314

2 C 5.1221695559 -0.5621082420 -0.0249273063

3 C 2.6909297283 -0.7006721378 -0.0180595641

4 C 2.6159848331 0.7400894994 0.0281372534

5 C 3.8383681679 1.4937619200 0.0463524809

6 C 5.0463851200 0.8673741259 0.0207400510

7 C 1.5228768739 -1.4515184878 -0.0345092018

8 C 0.2568895601 -0.8369772340 -0.0103619761

9 C 0.1851093088 0.5984482787 0.0278869039

10 C 1.3711589056 1.3538561901 0.0517969926

11 N -0.8466997604 -1.6185582964 -0.0103535595

12 C -2.0438492761 -1.0436809029 0.0031505856

13 C -2.2269854109 0.3939318237 0.0027417037

14 C -1.0945621328 1.1851366197 0.0380186034

15 C -3.2028923124 -1.8887541508 0.0400637957

16 C -4.4447892755 -1.3343002528 0.0676803737

17 C -4.6373819565 0.0797754102 0.0277014907

18 C -3.5713387752 0.9359316347 -0.0151852455

19 H 4.0457145742 -2.4010232517 -0.0777022151

20 H 6.0962352372 -1.0422638377 -0.0440275233

21 H 3.7773769421 2.5789075768 0.0814744401

22 H 5.9643372115 1.4477480285 0.0344774553

23 H 1.5603348376 -2.5369844776 -0.0641785069

24 H 1.3069737724 2.4400754739 0.0860198270

25 H -1.1684243132 2.2682514275 0.0994804849

26 H -3.0446567993 -2.9617189371 0.0512940427

27 H -5.3236756932 -1.9722773266 0.1008100921

28 H -5.6493210345 0.4772511178 0.0177839577

29 N -3.7313086163 2.3253498391 -0.0107485414

30 H -4.6909063121 2.6224160741 -0.1347626918

31 H -3.1249923575 2.8275364371 -0.6470029132

4-Bromo Benzacridine

Transition Dipole Moment: 0.3893 X -1.2629 Y 0.0000 Z

Nuclear Repulsion Energy (hartrees): 1574.7277614698

Cartesian Coordinates (angstroms):

1 C 4.9099660387 -0.9390406253 0.0000049091

2 C 5.8895480705 0.0051476539 0.0000044774

3 C 3.5223952421 -0.5644847227 0.0000031257

4 C 3.1908675215 0.8415952344 0.0000006610

5 C 4.2599684184 1.8014102853 0.0000001187

6 C 5.5596998310 1.3996622199 0.0000020075

7 C 2.5085365299 -1.5116458053 0.0000037600

8 C 1.1530189076 -1.1311485097 0.0000021568

9 C 0.8238475394 0.2693878948 -0.0000001194

10 C 1.8577285875 1.2249325561 -0.0000009833

11 N 0.2071505397 -2.0955008534 0.0000029453

12 C -1.0718752248 -1.7409542887 0.0000017118

13 C -1.5113243924 -0.3601302098 -0.0000005944

14 C -0.5364999137 0.6222914078 -0.0000016195

15 C -2.0567247741 -2.7865192923 0.0000028609

16 C -3.3819096760 -2.4873538763 0.0000020613

17 C -3.8320790237 -1.1288775376 -0.0000001021

18 C -2.9304535685 -0.1116498020 -0.0000015231

19 H 5.1587621411 -1.9972149559 0.0000066674

20 H 6.9341647097 -0.2926692683 0.0000059254

21 H 4.0062327733 2.8586677015 -0.0000019892

22 H 6.3594857222 2.1343270717 0.0000016141

23 H 2.7387891299 -2.5734432253 0.0000055189

24 H 1.6001880341 2.2823265617 -0.0000030587

25 H -0.8147114631 1.6723762660 -0.0000034683

26 H -1.6946420255 -3.8092645225 0.0000045270

27 H -4.1243049157 -3.2796761295 0.0000032150

28 H -4.8956307577 -0.9179102715 -0.0000005289

29 Br -3.5724896763 1.6777763857 -0.0000040719

4-Chloro Benzacridine

Transition Dipole Moment: -0.2220 X 1.2886 Y -0.0000 Z

Nuclear Repulsion Energy (hartrees): 1342.4496044535

Cartesian Coordinates (angstroms):

1 C 4.3114841164 -1.1944778536 0.0000263012

2 C 5.3915913598 -0.3673050483 0.0000229089

3 C 2.9753066876 -0.6653721158 0.0000189454

4 C 2.8038866444 0.7691871143 0.0000077887

5 C 3.9750113765 1.6019967673 0.0000045458

6 C 5.2209513509 1.0555741079 0.0000118915

7 C 1.8611070324 -1.4919693083 0.0000223823

8 C 0.5569981887 -0.9617439211 0.0000156079

9 C 0.3869925879 0.4675840077 0.0000048539

10 C 1.5225077725 1.3002398051 0.0000009769

11 N -0.4897204730 -1.8156029016 0.0000196751

12 C -1.7210919886 -1.3211961132 0.0000141394

13 C -2.0013170517 0.0996901164 0.0000040015

14 C -0.9254878566 0.9700857032 -0.0000008078

15 C -2.8194684962 -2.2469905352 0.0000188625

16 C -4.1018934336 -1.7975568554 0.0000144554

17 C -4.3953777536 -0.3968948458 0.0000049879

18 C -3.3816064391 0.5078248964 0.0000000855

19 H 4.4386344948 -2.2740354381 0.0000348156

20 H 6.3953241654 -0.7820989879 0.0000283713

21 H 3.8425284265 2.6811958946 -0.0000040814

22 H 6.0991406626 1.6945813628 0.0000093924

23 H 1.9700387728 -2.5730113510 0.0000308658

24 H 1.3859243981 2.3799803626 -0.0000072819

25 H -1.0879505400 2.0442820285 -0.0000087330

26 H -2.5783523111 -3.3049111244 0.0000263472

27 H -4.9303019767 -2.4994276832 0.0000184740

28 H -5.4265021139 -0.0590595980 0.0000018993

29 Cl -3.7615035994 2.2158284410 -0.0000107451

4-Cyano Benzacridine

Transition Dipole Moment: -0.2274 X 1.2919 Y 0.0000 Z

Nuclear Repulsion Energy (hartrees): 1297.6820674338

Cartesian Coordinates (angstroms):

1 C 4.1848175000 -1.2117442098 -0.0001504388

2 C 5.2737830448 -0.3963341009 -0.0001172746

3 C 2.8549752418 -0.6672198872 -0.0000798442

4 C 2.6996871422 0.7690765967 0.0000282070

5 C 3.8797249067 1.5891782666 0.0000603856

6 C 5.1191073326 1.0282942331 -0.0000098730

7 C 1.7317233709 -1.4815609131 -0.0001141666

8 C 0.4337982022 -0.9364560138 -0.0000492301

9 C 0.2801180308 0.4957933375 0.0000565078

10 C 1.4249384839 1.3156564314 0.0000944835

11 N -0.6222061988 -1.7803682597 -0.0000908897

12 C -1.8456899279 -1.2665843238 -0.0000368028

13 C -2.1078789644 0.1514416141 0.0000653546

14 C -1.0260454378 1.0141228765 0.0001132055

15 C -2.9600790685 -2.1745666133 -0.0000855586

16 C -4.2404152679 -1.7132928314 -0.0000385150

17 C -4.5109609249 -0.3115810949 0.0000604114

18 C -3.4839390760 0.5918177380 0.0001105930

19 H 4.3003384818 -2.2924858977 -0.0002327539

20 H 6.2728861255 -0.8220334769 -0.0001710316

21 H 3.7595586202 2.6696480650 0.0001422253

22 H 6.0044843430 1.6572292922 0.0000139599

23 H 1.8286589924 -2.5636140973 -0.0001952714

24 H 1.3005861837 2.3965937656 0.0001759155

25 H -1.1789884916 2.0913743219 0.0001941891

26 H -2.7330952179 -3.2360087112 -0.0001642138

27 H -5.0750765522 -2.4070543308 -0.0000790260

28 H -5.5377561501 0.0398262006 0.0000952770

29 C -3.7646300262 1.9994888847 0.0002056270

30 N -3.9692624908 3.1412938264 0.0002817720

4-Methoxy Benzacridine

Transition Dipole Moment: 0.4497 X -1.2774 Y 0.0000 Z

Nuclear Repulsion Energy (hartrees): 1366.4453236404

Cartesian Coordinates (angstroms):

1 C 4.3955310457 -1.1396779864 -0.0099418972

2 C 5.4675426781 -0.3010997317 -0.0142428361

3 C 3.0542945411 -0.6252296565 -0.0030055168

4 C 2.8680692982 0.8061816121 -0.0009169412

5 C 4.0293192960 1.6514393953 -0.0056392546

6 C 5.2820092769 1.1190662569 -0.0120475652

7 C 1.9478259230 -1.4642928495 0.0017831571

8 C 0.6384877101 -0.9498310515 0.0087962276

9 C 0.4545368277 0.4773074776 0.0106536776

10 C 1.5790978207 1.3222016209 0.0057787711

11 N -0.3990968747 -1.8187859958 0.0136597708

12 C -1.6357150976 -1.3379506659 0.0204056985

13 C -1.9250401948 0.0780761847 0.0225526026

14 C -0.8668140180 0.9642963047 0.0176421809

15 C -2.7337431168 -2.2647522433 0.0260090556

16 C -4.0117571377 -1.8039692712 0.0330359332

17 C -4.3172187011 -0.4039034942 0.0350007542

18 C -3.3046383878 0.5118269864 0.0299098998

19 H 4.5345129756 -2.2178291869 -0.0115804576

20 H 6.4755525227 -0.7056789994 -0.0193249050

21 H 3.8853622412 2.7292823511 -0.0040022106

22 H 6.1530811425 1.7678940795 -0.0155050151

23 H 2.0693236567 -2.5440393717 0.0003982722

24 H 1.4302755943 2.4004493198 0.0073624125

25 H -1.0523208044 2.0345093161 0.0193381141

26 H -2.4995846029 -3.3239385039 0.0245062062

27 H -4.8410406089 -2.5057297681 0.0374912433

28 H -5.3567654085 -0.0973457959 0.0405636236

29 O -3.4632706769 1.8566812630 0.0312229679

30 C -4.7794345479 2.3695315624 0.0397863668

31 H -4.6779112754 3.4550934822 0.0403277401

32 H -5.3199995300 2.0502415658 0.9394239574

33 H -5.3312092176 2.0523317345 -0.8537628136

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lar, D. G.; Warshel, A.; Xu, X.; Aspuru-Guzik, A.; Baer, R.; Bell, A. T.; Besley, N. A.; Chai, J.-D.; Dreuw, A.; Dunietz, B. D.; Furlani, T. R.; Gwaltney, S. R.; Hsu, C.-P.; Jung, Y.; Kong, J.; Lambrecht, D. S.; Liang, W.; Ochsenfeld, C.; Rassolov, V. A.; Slipchenko, L. V.; Subotnik, J. E.; Voorhis, T. V.; Herbert, J. M.; Krylov, A. I.; Gill, P. M.; Head-Gordon, M. Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics* **2015**, *113*, 184–215.