

## SUPPLEMENTARY MATERIAL

### BROMINATION OF ACRIDINE

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### Optimised Geometries of Compounds

#### Acridine

6	0	3.577046	0.766219
6	0	2.38051	1.421988
6	0	1.152532	0.694784
6	0	1.207774	-0.744801
6	0	2.47939	-1.389652
6	0	3.629541	-0.656382
6	0	0	-1.439022
6	0	-1.207774	-0.744801
6	0	-1.152532	0.694784
6	0	-2.38051	1.421988
1	0	-2.321979	2.500941
6	0	-3.577046	0.766219
6	0	-3.629541	-0.656382
6	0	-2.47939	-1.389652

1	0	4.501236	1.327985
1	0	2.321979	2.500941
1	0	2.513358	-2.471529
1	0	4.590529	-1.151856
1	0	0	-2.522575
1	0	-4.501236	1.327985
1	0	-4.590529	-1.151856
1	0	-2.513358	-2.471529
7	0	0	1.377109

### Acridinium Cation

6	0	3.600436	-0.740695
6	0	2.410276	-1.424299
6	0	1.206438	-0.697916
6	0	1.22097	0.731081
6	0	2.478972	1.395719
6	0	3.639617	0.675598
6	0	0	1.408195
6	0	-1.22097	0.731081
6	0	-1.206438	-0.697916
6	0	-2.410276	-1.424299
1	0	-2.391903	-2.505684
6	0	-3.600436	-0.740695
6	0	-3.639617	0.675598
6	0	-2.478972	1.395719
1	0	4.528731	-1.294272
1	0	2.391903	-2.505684
1	0	2.495426	2.476506
1	0	4.594786	1.179519
1	0	0	2.491018
1	0	-4.528731	-1.294272
1	0	-4.594786	1.179519
1	0	-2.495426	2.476506
7	0	0	-1.329673
1	0	0	-2.341344

### 1,1-hydrobromoacridine cation

6	-0.019351	3.588546	-0.795569
6	-0.06918	2.384225	-1.438133
6	-0.038298	1.173919	-0.683733
6	0.044844	1.238172	0.759773
6	0.099454	2.499011	1.381101

6	0.066565	3.64511	0.618542
6	0.060408	0.02259	1.478031
6	-0.00248	-1.166554	0.800592
6	-0.053301	-1.124601	-0.630399
6	-0.030941	-2.326559	-1.367312
1	-0.068177	-2.239905	-2.445612
6	0.062781	-3.585457	-0.755608
6	0.100574	-3.673909	0.608472
6	-0.016771	-2.489334	1.475377
1	-0.043346	4.508843	-1.361035
1	-0.130942	2.307806	-2.513714
1	0.16344	2.56035	2.458639
1	0.106007	4.609985	1.104552
1	0.104885	0.045315	2.55945
1	0.108088	-4.477641	-1.362301
1	0.190478	-4.634177	1.097112
7	-0.078195	0.014264	-1.341209
1	0.624145	-2.540991	2.349973
35	-1.857751	-2.851438	2.29363

## 2,2-hydrobromoacidine cation

6	-0.055896	3.586532	-0.821526
6	-0.051687	2.400391	-1.447587
6	-0.024548	1.153413	-0.708942
6	-0.033788	1.199893	0.750537
6	-0.074034	2.411567	1.392422
6	-0.03753	3.678305	0.650961
6	-0.028471	-0.026054	1.463349
6	-0.009952	-1.218071	0.769499
6	0.007274	-1.152406	-0.677537
6	0.035722	-2.352089	-1.402179
1	0.049747	-2.301781	-2.480726
6	0.043953	-3.560901	-0.735699
6	0.02472	-3.635205	0.679221
6	-0.002199	-2.489359	1.42105
1	-0.069482	4.514009	-1.375164
1	-0.068345	2.326996	-2.525229
1	-0.126043	2.462328	2.472393
1	-0.036078	-0.016607	2.546308
1	0.065051	-4.478872	-1.307044
1	0.031447	-4.601313	1.161966
1	-0.017506	-2.524894	2.501797
7	-0.004789	0.024405	-1.368587
1	-0.713639	4.426315	1.056988

35	1.773357	4.386968	1.269145
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### 3,3-hydrobromoacridine cation

6	-0.056892	3.632943	-0.732709
6	-0.095802	2.324609	-1.387382
6	-0.04388	1.15027	-0.655837
6	-0.030198	1.212921	0.787799
6	-0.064538	2.503777	1.440426
6	-0.07587	3.649061	0.739049
6	0.001706	0.01734	1.472092
6	0.015031	-1.197893	0.762846
6	-0.010214	-1.149057	-0.693727
6	-0.0042	-2.373989	-1.43849
1	-0.023528	-2.305951	-2.516221
6	0.026145	-3.567275	-0.783732
6	0.051451	-3.606002	0.638449
6	0.045907	-2.456142	1.393158
1	-0.162446	2.270367	-2.465052
1	-0.083148	2.526712	2.521469
1	-0.094535	4.611066	1.229202
1	0.013256	0.004503	2.55404
1	0.031544	-4.495216	-1.336854
1	0.075736	-4.566545	1.134434
1	0.065047	-2.510276	2.472676
7	-0.037479	-0.008767	-1.361612
1	-0.678526	4.384858	-1.208707
35	1.81272	4.162651	-1.404114

### 4,4-hydrobromoacridine cation

6	-0.125683	3.633559	-0.715925
6	0.036465	2.391745	-1.491445
6	0.010626	1.116161	-0.715747
6	0.071274	1.187896	0.724499
6	0.010561	2.432999	1.358502
6	-0.110437	3.643202	0.648963
6	0.105677	-0.017856	1.442682
6	0.052499	-1.227567	0.759408
6	-0.053331	-1.180362	-0.676755
6	-0.13502	-2.382941	-1.39237
1	-0.214993	-2.338919	-2.468403

6	-0.106219	-3.587451	-0.718434
6	0.002582	-3.643481	0.689615
6	0.078977	-2.487765	1.419494
1	-0.224198	4.554842	-1.273268
1	-0.571654	2.340774	-2.38824
1	0.033651	2.46369	2.44145
1	-0.188223	4.574414	1.18988
1	0.156798	-0.0012	2.524262
1	-0.166833	-4.510542	-1.278077
1	0.023064	-4.603375	1.184592
1	0.157924	-2.516168	2.497686
7	-0.071686	-0.0015	-1.371522
35	1.905241	2.672596	-2.23551

### 9,9-hydrobromoacridine cation

6	1.565589	-0.055401	3.573354
6	2.079649	-0.411372	2.349214
6	1.323632	-0.175866	1.166403
6	0.010961	0.392476	1.252876
6	-0.475582	0.752418	2.492664
6	0.297121	0.537071	3.63948
6	-0.774213	0.543985	0
6	0.010961	0.392476	-1.252876
6	1.323632	-0.175866	-1.166403
6	2.079649	-0.411372	-2.349214
1	3.059674	-0.852625	-2.240623
6	1.565589	-0.055401	-3.573354
6	0.297121	0.537071	-3.63948
6	-0.475582	0.752418	-2.492664
1	2.132571	-0.219532	4.477596
1	3.059674	-0.852625	2.240623
1	-1.460244	1.189212	2.586343
1	-0.099619	0.834429	4.600595
1	2.132571	-0.219532	-4.477596
1	-0.099619	0.834429	-4.600595
1	-1.460244	1.189212	-2.586343
7	1.917565	-0.46164	0
1	-1.408804	1.423355	0
35	-2.13746	-0.975793	0

### 2,2-hydrobromoacridinium cation

6	-0.077315	3.61912	-0.819903
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6	-0.064936	2.432826	-1.458745
6	-0.035037	1.211846	-0.70645
6	-0.041427	1.216478	0.733986
6	-0.100139	2.442437	1.388762
6	-0.068459	3.702171	0.650945
6	-0.028825	-0.014775	1.42942
6	-0.004828	-1.222842	0.748938
6	0.0122	-1.201127	-0.687522
6	0.042935	-2.380517	-1.414676
1	0.056129	-2.369328	-2.49637
6	0.056036	-3.589397	-0.72545
6	0.038739	-3.643406	0.68264
6	0.008178	-2.48226	1.413336
1	-0.090792	4.547366	-1.374684
1	-0.073513	2.388174	-2.539839
1	-0.192783	2.48357	2.466259
1	-0.037887	-0.008345	2.5127
1	0.079818	-4.512061	-1.289685
1	0.049282	-4.602558	1.179716
1	-0.005554	-2.50566	2.494325
7	-0.005849	0.031156	-1.324513
1	-0.664933	4.504925	1.074347
35	1.826964	4.142049	1.272799
1	-0.00072	0.023726	-2.340273

#### 4,4-hydrobromoacridinium cation

6	-0.093205	3.670997	-0.701224
6	0.002137	2.432311	-1.496048
6	-0.01076	1.16689	-0.712943
6	0.030727	1.197417	0.70527
6	0.015691	2.454106	1.356786
6	-0.052765	3.67005	0.668174
6	0.055309	-0.021275	1.411946
6	0.026114	-1.240849	0.743635
6	-0.037206	-1.233817	-0.69035
6	-0.079406	-2.419921	-1.412565
1	-0.128433	-2.413955	-2.493339
6	-0.055614	-3.620416	-0.716516
6	0.008824	-3.659493	0.691983
6	0.048272	-2.493369	1.415272
1	-0.170744	4.596998	-1.256472
1	-0.673956	2.424791	-2.348653

1	0.046303	2.466596	2.440203
1	-0.081855	4.600086	1.217312
1	0.091506	-0.004823	2.494464
1	-0.086926	-4.548795	-1.270542
1	0.025831	-4.61458	1.196942
1	0.095338	-2.510677	2.495355
7	-0.056272	-0.00614	-1.331396
35	1.834103	2.641169	-2.319521
1	-0.075948	-0.02055	-2.34779

### 9,9-hydrobromoacridinium cation

6	1.570252	-0.041087	3.593613
6	2.091701	-0.41636	2.386615
6	1.328665	-0.172466	1.20811
6	0.014815	0.407801	1.259899
6	-0.469091	0.791698	2.492719
6	0.300486	0.580454	3.644731
6	-0.761891	0.519942	0
6	0.014815	0.407801	-1.259899
6	1.328665	-0.172466	-1.20811
6	2.091701	-0.41636	-2.386615
1	3.069912	-0.874569	-2.313781
6	1.570252	-0.041087	-3.593613
6	0.300486	0.580454	-3.644731
6	-0.469091	0.791698	-2.492719
1	2.125438	-0.203672	4.506144
1	3.069912	-0.874569	2.313781
1	-1.445122	1.249281	2.578004
1	-0.088898	0.90198	4.602014
1	2.125438	-0.203672	-4.506144
1	-0.088898	0.90198	-4.602014
1	-1.445122	1.249281	-2.578004
7	1.869397	-0.433579	0
1	-1.488496	1.323919	0
35	-1.90767	-1.180659	0
1	2.807034	-0.836686	0