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**Electronic Supporting Information**

# Butadiene dyes based on 3-(dicyanomethylidene)indan-1-one and 1,3-bis(dicyanomethylidene)indane: Synthesis, characterization and solvatochromic behaviour

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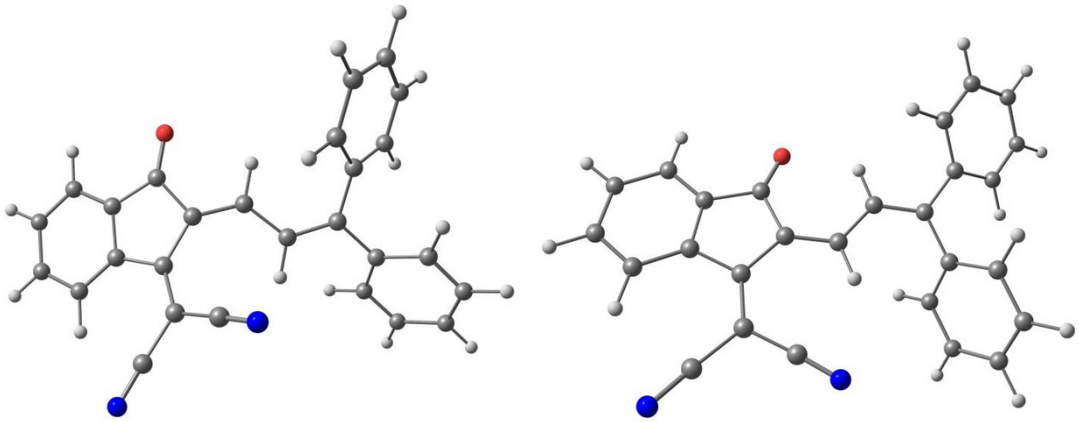
**Contents:**

**Fig. S1** Optimized structures, cartesian coordinates and total electronic energies (Hartree) for the computed species (*E*)-**4a** and (*Z*)-**4a**.



**(*E*)-4a: E(gas) = -1223.22193600**

C -4.911387 1.862439 -1.035037
C -6.072768 1.100551 -1.194317
C -6.069639 -0.265152 -0.877560
C -4.923609 -0.900268 -0.384644
C -3.757407 -0.142740 -0.222576
C -3.769977 1.227403 -0.559770
C -2.416632 1.800777 -0.345661
C -2.413047 -0.492332 0.308649
C -1.543276 0.652260 0.057064
C -0.180146 0.789976 -0.047987
C 0.814407 -0.229403 -0.133875
C 2.171529 -0.004708 -0.173314
C 2.755392 1.316826 0.157549
C 2.342162 2.026343 1.301366
C 2.888582 3.275845 1.600701
C 3.850120 3.840701 0.759589
C 4.274621 3.143608 -0.377532
C 3.743416 1.888702 -0.669111
C 3.091045 -1.110414 -0.523847
C 4.358209 -1.212417 0.084548
C 5.211072 -2.274388 -0.214247
C 4.824942 -3.248413 -1.139621
C 3.577046 -3.153170 -1.764227
C 2.719414 -2.097773 -1.459051
O -2.073296 2.961723 -0.514287
H 3.274798 -3.897798 -2.495957
H 1.764127 -2.019650 -1.970446
H 4.661647 -0.467942 0.814208
H 6.176703 -2.343446 0.279708
H -4.884349 2.921672 -1.274642
H -6.981577 1.564790 -1.567546
H -6.976371 -0.848323 -1.013851
H -4.958300 -1.956429 -0.149182
H 0.144963 1.817407 -0.209004
H 0.475887 -1.254641 -0.237290
H 4.077152 1.351466 -1.552530
H 5.021528 3.578790 -1.036411

H 2.564143 3.804198 2.493175
H 1.615327 1.577280 1.971995
C -2.115475 -1.614291 1.062247
C -0.928746 -1.731646 1.851156
C -3.027580 -2.702332 1.233761
N 0.000671 -1.841666 2.545205
N -3.741847 -3.611886 1.376263
H 4.271928 4.815452 0.990216
H 5.492231 -4.073112 -1.375813

**(*Z*)-4a: E(gas) = -1223.22763125**

C 4.187663 -2.825131 -0.452759
C 5.566173 -2.607365 -0.387193
C 6.062437 -1.330079 -0.090750
C 5.207674 -0.247764 0.146312
C 3.823549 -0.458784 0.082061
C 3.342254 -1.747271 -0.217435
C 1.860969 -1.734551 -0.234027
C 2.667178 0.455318 0.279961
C 1.444688 -0.332338 0.074577
C 0.134852 0.095005 0.141996
C -1.011301 -0.744831 -0.000860
C -2.315409 -0.298314 0.009794
C -2.668654 1.141588 -0.062836
C -2.124984 1.973571 -1.058560
C -2.460960 3.326806 -1.118584
C -3.337973 3.873508 -0.179571
C -3.890218 3.056909 0.812999
C -3.570338 1.701356 0.863448
C -3.421080 -1.281011 0.066218
C -4.655339 -1.012555 -0.561112
C -5.685379 -1.952215 -0.546254
C -5.513422 -3.174549 0.109662
C -4.300992 -3.450825 0.750374
C -3.266977 -2.517301 0.728304
O 1.143818 -2.703429 -0.460644
H -4.163487 -4.392117 1.275835
H -2.339467 -2.735766 1.248779
H -4.796696 -0.070161 -1.080929
H -6.622783 -1.730066 -1.049389
H 3.770831 -3.802080 -0.680121
H 6.257294 -3.426605 -0.565729
H 7.136202 -1.170655 -0.042440
H 5.633037 0.720906 0.371605
H -0.056769 1.141718 0.350280
H -0.828730 -1.807807 -0.097337
H -4.002491 1.071085 1.635858
H -4.569627 3.477717 1.549535
H -2.032823 3.953757 -1.895877
H -1.455164 1.548310 -1.800829
C 2.771336 1.795004 0.608664
C 1.655251 2.664715 0.813303
C 4.019712 2.469069 0.789552
N 0.788294 3.422832 0.991885
N 5.008605 3.064488 0.949404
H -6.318905 -3.904005 0.126634
H -3.590589 4.929619 -0.219681

**Fig. S2** Plot of $\lambda_{max}$ ($CH_2Cl_2$ solution) *vs* Hammett coefficients for compounds **5a-f**.

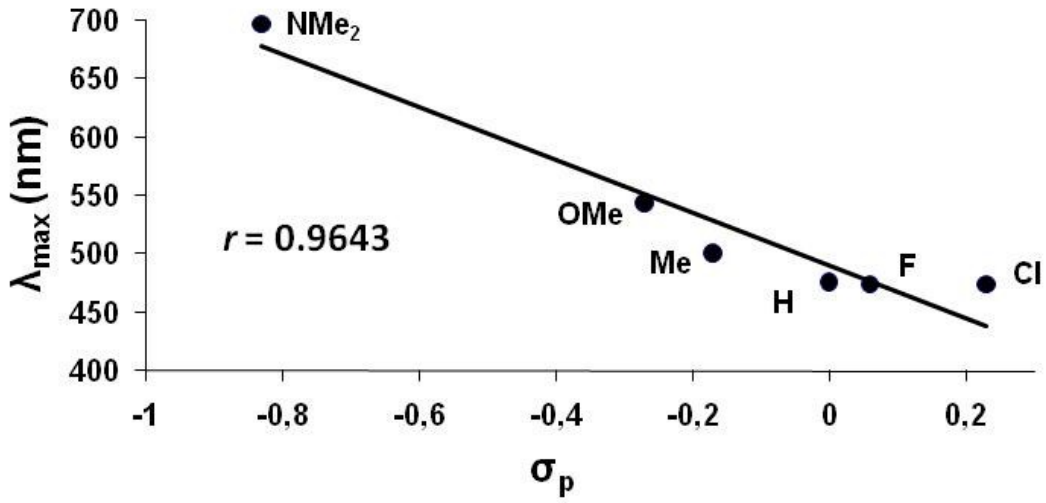
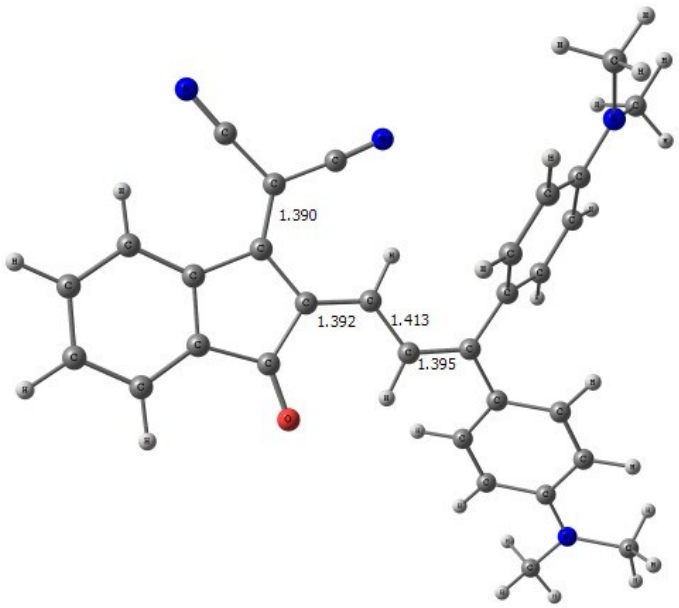


**Fig. S3** Optimized structure, cartesian coordinates and total electronic energy (Hartree) for the computed species **4f**.

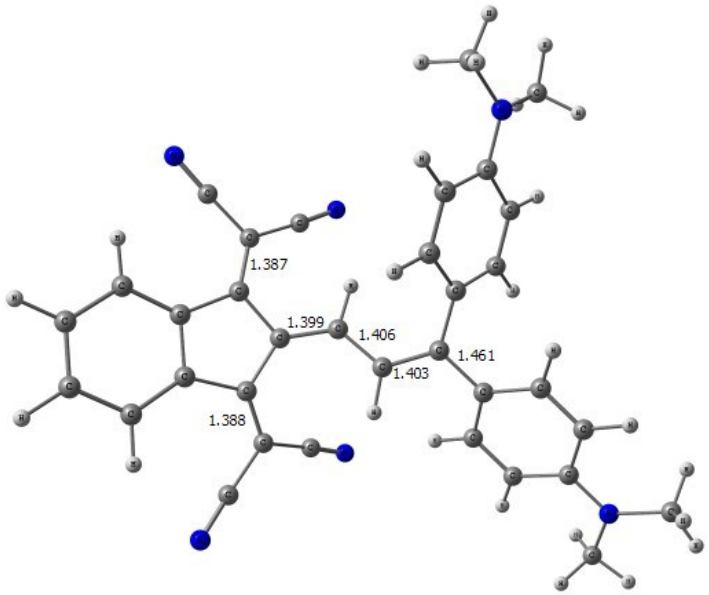



**E(gas) = -1491.18635506**

C -4.604886 -3.827598 0.641068
C -6.000538 -3.861456 0.549625
C -6.708226 -2.706369 0.192755
C -6.052130 -1.498650 -0.080403
C -4.655143 -1.458818 0.009872
C -3.959758 -2.627797 0.370136
C -2.501837 -2.344755 0.402639
C -3.667166 -0.363607 -0.211760
C -2.340324 -0.912594 0.039471
C -1.115022 -0.256553 -0.034548
C 0.149553 -0.857912 0.154586
C 1.365026 -0.173631 0.116692
C 1.436340 1.292900 0.199852
C 0.659956 2.024247 1.123313
C 0.693820 3.408877 1.179427
C 1.502750 4.157379 0.287077
C 2.298008 3.425671 -0.634242
C 2.272706 2.039437 -0.657934
C 0.542985 6.251316 1.129704
C 2.614118 -0.934988 0.010553
C 3.829086 -0.448724 0.543462
C 5.007019 -1.178253 0.482754
C 5.046212 -2.453884 -0.138290
C 3.830815 -2.944276 -0.686779
C 2.661202 -2.206695 -0.606065
C 7.443165 -2.653803 0.355273
O -1.628263 -3.164920 0.678252
H 8.249297 -3.369256 0.190479
H 7.729715 -1.705528 -0.118759
H 7.356270 -2.483569 1.437163
H 3.803607 -3.903773 -1.188161
H 1.762276 -2.613871 -1.057672

H 3.839623 0.513059 1.045700
H 5.899398 -0.759095 0.930900
H -4.025366 -4.703993 0.915035
H -6.538933 -4.782158 0.755011
H -7.791666 -2.741488 0.124425
H -6.636361 -0.630584 -0.352944
H -1.118498 0.795794 -0.294829
H 0.664113 6.019937 2.194755
H 0.695246 7.324006 1.005307
H -0.488977 6.011199 0.837709
H 0.165677 -1.930445 0.301237
H 2.881446 1.518404 -1.390884
H 2.924412 3.943022 -1.350260
H 0.077536 3.910690 1.914443
H 0.035716 1.488127 1.831535
C -4.007548 0.927980 -0.594718
C -5.352707 1.358796 -0.811716
C -3.067037 1.979633 -0.818996
N -6.430968 1.761638 -0.999453
N -2.353835 2.881280 -1.016474
N 6.210443 -3.184334 -0.208487
N 1.521526 5.535265 0.320060
C 6.213434 -4.501946 -0.828431
H 5.529262 -5.192605 -0.317648
H 5.924954 -4.453636 -1.887073
H 7.218514 -4.920981 -0.773166
C 2.269636 6.275848 -0.685817
H 3.329562 5.996856 -0.673386
H 1.881320 6.111905 -1.702373
H 2.206740 7.341760 -0.463434

**Fig. S4** Optimized structure, cartesian coordinates and total electronic energy (Hartree) for the computed species **5f**.




**E(gas) = -1639.72799120**

C 4.771383 -2.989799 -1.100220
C 6.065375 -2.641719 -1.503819
C 6.563201 -1.355291 -1.278786
C 5.777042 -0.382411 -0.651209
C 4.474847 -0.712140 -0.265262
C 3.973813 -2.021075 -0.485812
C 2.603750 -2.092821 0.060857
C 3.420095 0.091195 0.385329
C 2.201664 -0.725284 0.377469
C 0.927101 -0.148070 0.363344
C -0.324304 -0.704571 0.046968
C -1.502045 0.047646 -0.073412
C -1.476790 1.512155 -0.201174
C -0.576773 2.171691 -1.065493
C -0.532475 3.554013 -1.165016
C -1.382891 4.371421 -0.375460
C -2.298240 3.711075 0.487040
C -2.349486 2.327701 0.551486
C -2.793222 -0.634763 -0.089342
C -3.908036 -0.094021 -0.773103
C -5.128143 -0.747274 -0.825039
C -5.318427 -1.993895 -0.169472
C -4.206386 -2.534870 0.532023
C -2.989300 -1.877219 0.562839
H -4.299768 -3.468186 1.073056
H -2.182924 -2.316503 1.141539
H -3.799451 0.845966 -1.304230
H -5.935461 -0.293635 -1.386501
H 4.407248 -3.992406 -1.279942

H 6.686165 -3.384294 -1.996001
H 7.570989 -1.101788 -1.593530
H 6.184557 0.605282 -0.483765
H 0.907898 0.915883 0.565276
H -0.416515 -1.772157 -0.090705
H -3.050032 1.861243 1.237356
H -2.960683 4.283369 1.124166
H 0.168616 4.000680 -1.858660
H 0.080547 1.581214 -1.696704
C 3.585241 1.359013 0.922731
C 4.800232 2.103817 0.817439
C 2.586323 2.039684 1.687097
N 5.767615 2.750872 0.746484
N 1.817238 2.637172 2.328121
C -6.686562 -3.935488 0.454619
H -5.984424 -4.680925 0.060205
H -6.532575 -3.857614 1.539055
H -7.698865 -4.301619 0.282506
C -2.136073 6.555124 0.452694
H -3.205203 6.349840 0.321016
H -1.877730 6.382712 1.507403
H -1.970881 7.609473 0.229125
C 1.922498 -3.265772 0.357435
C 0.795963 -3.322822 1.231280
C 2.365601 -4.557156 -0.066584
N -0.104048 -3.425060 1.965429
N 2.683830 -5.625299 -0.408584
N -6.526141 -2.646437 -0.207132
N -1.328944 5.744630 -0.449646
C -7.659678 -2.053802 -0.903865
H -7.917863 -1.069940 -0.490699
H -7.460341 -1.934443 -1.977366
H -8.527636 -2.703866 -0.792595
C -0.284486 6.390839 -1.234125
H 0.721602 6.137080 -0.871415
H -0.350815 6.110629 -2.292423
H -0.408188 7.472189 -1.169608

**Table S1** Melting points of compounds **4-5a-f**[a]

| Compound | M.p. (ºC) | Compound | M.p. (ºC) |
|---|---|---|---|
| **4a** | 266 (dec.) | **5a** | 284 (dec.) |
| **4b** | 261 (dec.) | **5b** | 289 (dec.) |
| **4c** | 270 (dec.) | **5c** | 295 (dec.) |
| **4d** | 273 (dec.) | **5d** | 307 (dec.) |
| **4e** | 265 (dec.) | **5e** | 290 (dec.) |
| **4f** | 277 (dec.) | **5f** | 301 (dec.) |

[a] Measured with a Büchi B-545 melting point apparatus