Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: COSMO-RI-ADC(2) Excitation Energies And Excited State Gradients†

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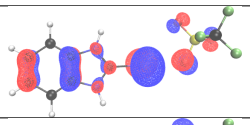
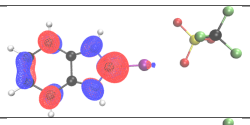
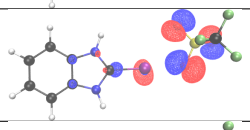
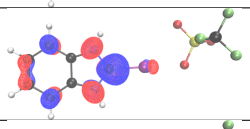
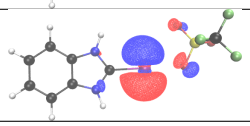
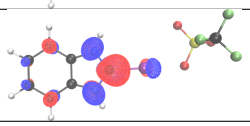
1 Natural Transition Orbitals

Table 1: Vertical excitation energies (VEE), transition moments (OS), dipole moments (μ) and NTOs of 2-Iodobenzimidazolium.otf complex calculated in vacuum at ADC(2)/def2-TZVPP level of theory (The isosurface chosen to visualize is 0.05).

EEL	VEE	OS	μ	OCC	VIR	Contrib.
1	4.55	0.41	12.59			91.54%
2	4.67	0.08	1.08			96.89%
3	5.15	0.00	10.23			99.76%

2 Cartesian coordinates of the studied molecules

- **DMABN** MP2/def2-TZVPP optimized geometry of the ground state in vacuum:
  C -0.8614494 -1.9266209 0.7585447
  C 0.0756059 -2.5988760 -0.0317852
  C 0.9323351 -1.8547817 -0.8484680
  C 0.8502980 -0.4711480 -0.8779105
  C -0.1011966 0.2231015 -0.1029742
  C -0.9432094 -0.5429704 0.7288794
  H -1.5215945 -2.4905026 1.4031153
  H 1.6691444 -2.3627162 -1.4553781
  H 1.5342083 0.0677134 -1.5146653
  H -1.6737161 -0.0607953 1.3592987
  N -0.2121943 1.5966106 -0.1655166
  C 0.1627977 -4.0239660 0.0018321
  N 0.2342548 -5.1945397 0.0292641
  C -0.9636589 2.2692168 0.8748552
  H -0.5504525 2.0921931 1.8741168
  H -0.9511072 3.3368334 0.6766942
  H -2.0027079 1.9455420 0.8690906
  C 0.8728198 2.3427348 -0.7700960
  H 0.9942642 2.0657372 -1.8155376
  H 0.6274084 3.4000412 -0.7368242
  H 1.8281503 2.1871926 -0.2565355

- **DMABN** COSMO-MP2/def2-TZVPP optimized geometry of the ground state in acetonitrile solution:
  C -0.6707951 -0.8134369 0.7798387
  C 0.2661211 -1.4824523 -0.0170481
  C 1.1295705 -0.7413339 -0.8329054
  C 1.0539517 0.6422266 -0.8538808
  C 0.1020854 1.3382622 -0.0740591
  C -0.7448580 0.5701873 0.7574283
  H -1.3344092 -1.3756681 1.4232028
  H 1.8655386 -1.2475170 -1.4432617
  H 1.7407564 1.1815051 -1.4876921
  H -1.4728464 1.0527896 1.3909534

N -0.0014627 2.7028673 -0.1286447
C 0.3466662 -2.9055808 0.0092139
N 0.4127013 -4.0764341 0.0305139
C -0.7766460 3.3842812 0.8939528
H -0.3706925 3.2207313 1.8970631
H -0.7660672 4.4483983 0.6806468
H -1.8118949 3.0496393 0.8795863
C 1.0679927 3.4581649 -0.7585265
H 1.1808318 3.1696771 -1.8015872
H 0.8078754 4.5114692 -0.7290566
H 2.0274068 3.3166378 -0.2513178

- **DMABN** COSMO-ADC(2)/def2-TZVPP optimized geometry of the ICT state in non-equilibrium solution limit (acetonitrile):
  C -0.1898504 -0.8001372 1.1529399
  C 0.1436617 -1.4585007 -0.0851161
  C 0.6267677 -0.6712921 -1.1734917
  C 0.8434708 0.6791602 -1.0265310
  C 0.6229528 1.3125293 0.2537931
  C -0.0028468 0.5480552 1.2961759
  H -0.5927830 -1.3847658 1.9707602
  H 0.8563837 -1.1525640 -2.1169409
  H 1.1985544 1.2707657 -1.8622357
  H -0.2750925 1.0417840 2.2224480
  N 0.2808921 2.6886716 0.1406608
  C -0.0473507 -2.8373214 -0.2333872
  N -0.2067448 -4.0062563 -0.3546624
  C -1.1050865 3.1424278 0.1347440
  H -1.1899714 4.0003519 0.7975361
  H -1.3578425 3.4441128 -0.8830255
  H -1.7387172 2.3219865 0.4561855
  C 1.3438523 3.6551116 -0.0541287
  H 2.0096594 3.2816935 -0.8306384
  H 0.9291396 4.6207680 -0.3215367
  H 1.9027773 3.7078333 0.8808708

- **DMABN** COSMO-ADC(2)/def2-TZVPP optimized geometry of the ICT state in equilibrium solution limit (acetonitrile):
  C -0.2533603 -0.8080496 1.1187412
  C 0.1436584 -1.4573983 -0.1093495
  C 0.7027775 -0.6690960 -1.1574789
  C 0.9270848 0.6771855 -0.9835970
  C 0.6128657 1.3102230 0.2803138
  C -0.0675760 0.5369787 1.2811454
  H -0.6975656 -1.4003686 1.9085980
  H 0.9875049 -1.1471790 -2.0870716
  H 1.3421947 1.2663942 -1.7918993
  H -0.3801353 1.0195615 2.2002274
  N 0.2738454 2.6821757 0.1397024
  C -0.0535476 -2.8313484 -0.2825931
  N -0.2195436 -3.9976850 -0.4244692
  C -1.0932336 3.1647158 0.2639118
  H -1.0945859 4.0571393 0.8855575
  H -1.4570955 3.4190266 -0.7337029
  H -1.7061971 2.3788871 0.6937174
  C 1.3223647 3.6342528 -0.1680536
  H 2.0581003 3.1577962 -0.8107927
  H 0.8996664 4.5172161 -0.6355860
  H 1.8046039 3.8939864 0.7770989

- **2-Iodobenzimidazolium · OTF** MP2/def2-TZVPP optimized geometry of the ground state in vacuum:
  S 4.9201145 1.1182332 0.1209306
  O 6.1465768 1.6225221 0.6695918
  O 4.5123334 -0.2290496 0.4525769
  O 3.7910406 2.0877204 0.1847409
  C 5.2149435 1.0480287 -1.6925832
  F 4.1010525 0.6553112 -2.3345727
  F 5.5636269 2.2403289 -2.1783619
  F 6.1825274 0.1784169 -1.9861722
  N -0.6671093 -0.9118184 0.4185568
  N -1.5228679 1.0644022 0.3192845
  C -2.0376874 -1.0941013 0.4473133

C -2.5954836 0.1923779 0.3827111
C -2.8332124 -2.2355639 0.5219549
C -3.9738116 0.3956716 0.3898848
C -4.2056839 -2.0319474 0.5290365
C -0.3555174 0.3948395 0.3409758
C -4.7649979 -0.7418393 0.4642565
H 0.0424144 -1.6299892 0.4488826
H -2.4048248 -3.2261810 0.5716012
H -4.4046154 1.3852594 0.3401027
I 1.5604660 1.1686525 0.2685158
H -4.8640891 -2.8867536 0.5857357
H -5.8401731 -0.6352754 0.4726743
H -1.5650220 2.0707547 0.2623632

- **2-Iodobenzimidazolium** · **OTF** COSMO-MP2/def2-TZVPP optimized geometry of the ground state in aqueous solution:

S 5.0878680 1.6044945 0.0472828
O 6.2448479 2.4456389 0.2821679
O 4.8947847 0.5174363 0.9872068
O 3.8687100 2.3312745 -0.2999819
C 5.4984233 0.7404988 -1.5202462
F 4.5047981 -0.0755555 -1.8884640
F 5.7021756 1.6144132 -2.5110511
F 6.6067386 0.0053679 -1.3841091
N -0.8270236 -0.9475282 0.0002959
N -1.6036133 1.0089523 0.5215236
C -2.1807936 -1.1159243 0.2048593
C -2.6837758 0.1512721 0.5424311
C -3.0032411 -2.2396974 0.1276206
C -4.0347232 0.3592206 0.8197318
C -4.3462210 -2.0319877 0.4034017
C -0.4945335 0.3346512 0.1938775
C -4.8516349 -0.7585727 0.7425557
H -0.1658203 -1.6684237 -0.2578275
H -2.6126658 -3.2128660 -0.1320416
H -4.4177909 1.3355805 1.0785509

I 1.3709904 1.1235692 0.0166583
H -5.0276927 -2.8697657 0.3578141
H -5.9075625 -0.6528995 0.9480235
H -1.6222443 2.0008509 0.7197199

- **2-Iodobenzimidazolium** · **OTF** COSMO-ADC(2)/def2-TZVPP optimized geometry of the first excited state in aqueous solution:

S 2.7575975 1.5520718 0.4125927
O 3.0323106 1.7874511 1.8099013
O 1.4519414 2.1537239 0.0039281
O 3.8231717 1.7558164 -0.5365386
C 2.4022949 -0.2500063 0.3235939
F 2.0687415 -0.6020079 -0.9200078
F 3.4814032 -0.9480823 0.6813310
F 1.4004512 -0.5745863 1.1381920
N -0.7138502 -0.0210757 -2.0006968
N -1.3597924 1.5499567 -0.6520714
C -1.1164795 -0.6548884 -0.8437565
C -1.5269130 0.3679268 0.0360415
C -1.1625071 -1.9987595 -0.4788100
C -1.9911765 0.0883842 1.3200131
C -1.6140334 -2.2733878 0.8060676
C -0.8865104 1.3170770 -1.8986515
C -2.0174873 -1.2510299 1.6881584
H -0.3482365 -0.4728629 -2.8275412
H -0.8528264 -2.7833851 -1.1547257
H -2.3040997 0.8728904 1.9947169
I 1.0145825 2.7259226 -2.4359985
H -1.6564455 -3.3010706 1.1401670
H -2.3596309 -1.5176754 2.6787913
H -1.5225056 2.4775972 -0.2846968