

**Role of Solvent and Effect of Substituent on Azobenzene Isomerization
by Using Room Temperature Ionic Liquids as Reaction Media**

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II. Hammett plots in BM₂IM Tf₂N (**a**) and BMIM PF₆ (**b**).

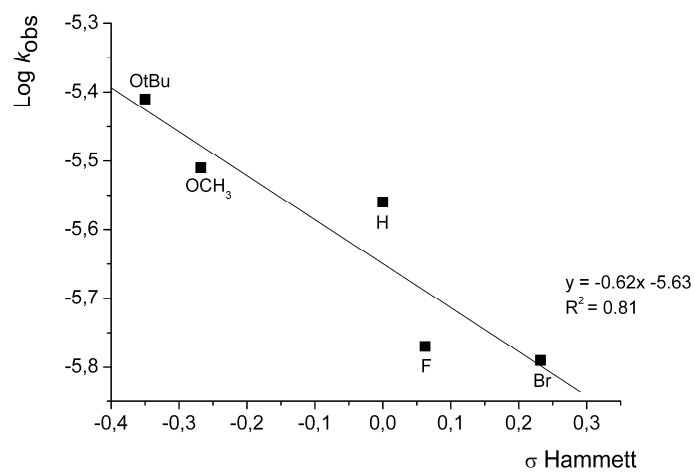
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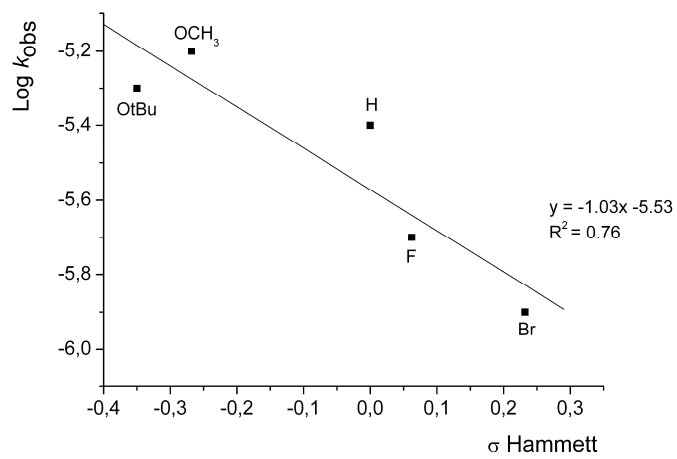
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II. Hammett plots in BM₂IM Tf₂N (a) and BMIM PF₆ (b).

(a)

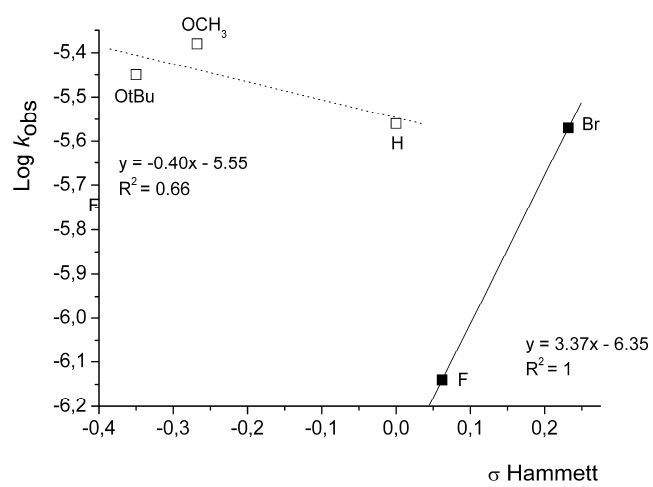


(b)

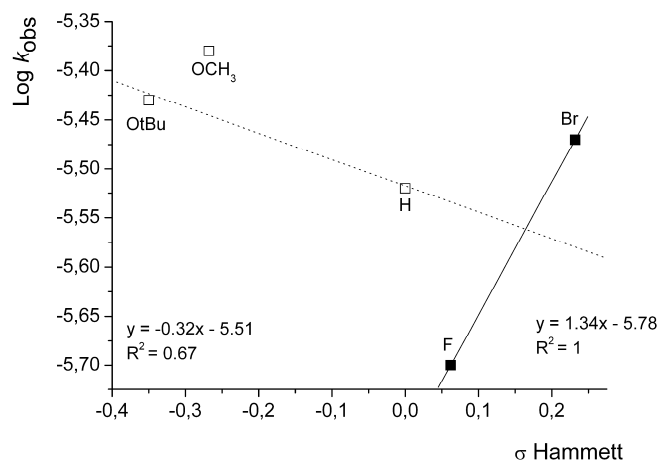


III. Hammett plots in HMIM Tf₂N (c) and BMIM Tf₂N (d).

(c)



(d)



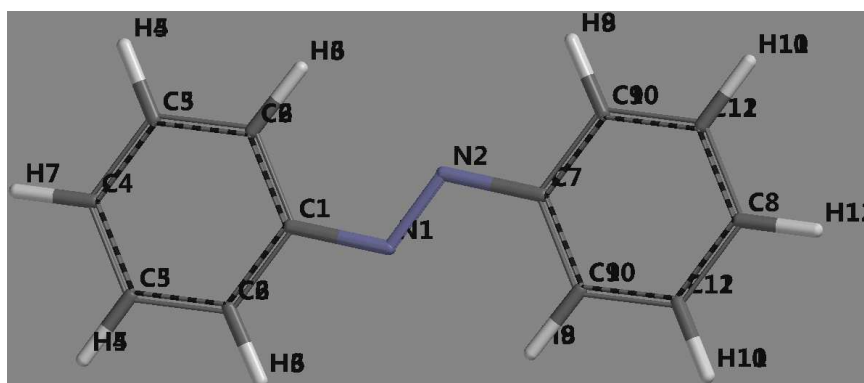
IV. Computational Data.

The calculations were performed by using DFT at the B3LYP/6-31G** level (Wavefunction Spartan 14v1.1.8 software) for the geometry optimization and computing the HOMO energy.

HOMO and LUMO energies in eV of the *trans* isomers

<i>p</i> -Substituent	HOMO <i>trans</i>	LUMO <i>trans</i>
H	-6.13	-2.18
OCH ₃	-5.71	-1.99
OtBu	-5.94	-2.09
Br	-6.26	-2.41
F	-6.17	-2.24

TRANS-AZOBENZENE: -572.777853 au

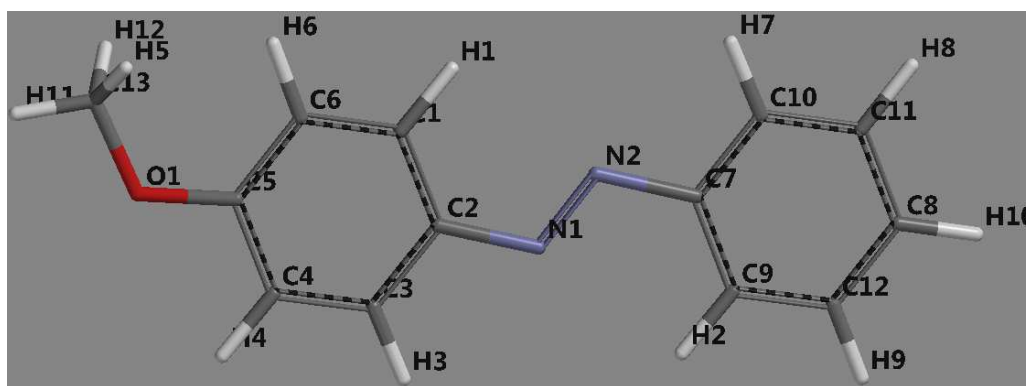


Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 N N1	-0.3844584	-0.4994573	-0.0000018
2 N N2	0.3844584	0.4994573	-0.0000018
3 C C1	-1.7680053	-0.1853008	-0.0000018
4 C C4	-4.5342861	0.2012076	-0.0000018
5 C C2	-2.2931227	1.1183296	0.0077934
6 C C6	-2.6337223	-1.2867011	-0.0084906
7 C C5	-4.0139713	-1.0936363	-0.0080729
8 C C3	-3.6702023	1.3036792	0.0086669
9 H H3	-1.6067020	1.9569677	0.0139120
10 H H6	-2.1991787	-2.2812041	-0.0147562

11 H H5	-4.6813579	-1.9501788	-0.0142675
12 H H4	-4.0783695	2.3103520	0.0157667
13 H H7	-5.6094320	0.3550771	-0.0000018
14 C C7	1.7680053	0.1853008	-0.0000018
15 C C8	4.5342861	-0.2012076	-0.0000018
16 C C9	2.6337223	1.2867011	-0.0084906
17 C C10	2.2931227	-1.1183296	0.0077934
18 C C11	3.6702023	-1.3036792	0.0086669
19 C C12	4.0139713	1.0936363	-0.0080729
20 H H8	2.1991787	2.2812041	-0.0147562
21 H H9	1.6067020	-1.9569677	0.0139120
22 H H10	4.0783695	-2.3103520	0.0157667
23 H H11	4.6813579	1.9501788	-0.0142675
24 H H12	5.6094320	-0.3550771	-0.0000018

TRANS-4-OCH₃-AZOBENZENE: -687.304524 au

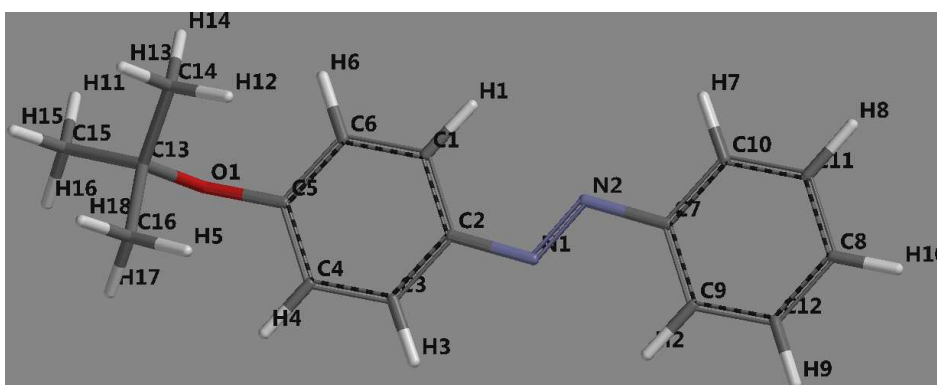


Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 H H1	-0.8454873	-1.7495777	-0.0049203
2 C C1	-1.4652735	-0.8601763	-0.0020039
3 C C4	-3.0157237	1.4672305	0.0054560
4 C C2	-0.8390525	0.3961155	0.0007237
5 C C6	-2.8512045	-0.9591886	-0.0010705
6 C C5	-3.6354299	0.2075376	0.0033428
7 C C3	-1.6332560	1.5550015	0.0038493
8 H H6	-3.3147968	-1.9383510	-0.0038163
9 H H3	-1.1344607	2.5188600	0.0053052
10 H H4	-3.6416637	2.3529821	0.0083433
11 N N1	0.5565054	0.6071648	0.0003373
12 N N2	1.2567353	-0.4433277	0.0016021
13 C C7	2.6575089	-0.2214890	0.0011742
14 C C8	5.4457380	-0.0213644	0.0016144
15 C C9	3.2702415	1.0437924	-0.0033460
16 C C10	3.4488829	-1.3777599	0.0056473
17 C C11	4.8388310	-1.2781306	0.0059593
18 C C12	4.6568639	1.1360289	-0.0031260

19 H H2	2.6420481	1.9270610	-0.0070222
20 H H7	2.9486518	-2.3409467	0.0089647
21 H H8	5.4469361	-2.1778971	0.0096565
22 H H9	5.1313607	2.1133390	-0.0066826
23 H H10	6.5287917	0.0603085	0.0018217
24 O O1	-4.9958138	0.2202149	0.0060401
25 C C13	-5.6890282	-1.0199822	0.0050240
26 H H5	-5.4655064	-1.6080711	-0.8940110
27 H H11	-6.7503684	-0.7687469	0.0146694
28 H H12	-5.4517085	-1.6176276	0.8942160

TRANS-4-OtBu-AZOBENZENE: -805.259217 au

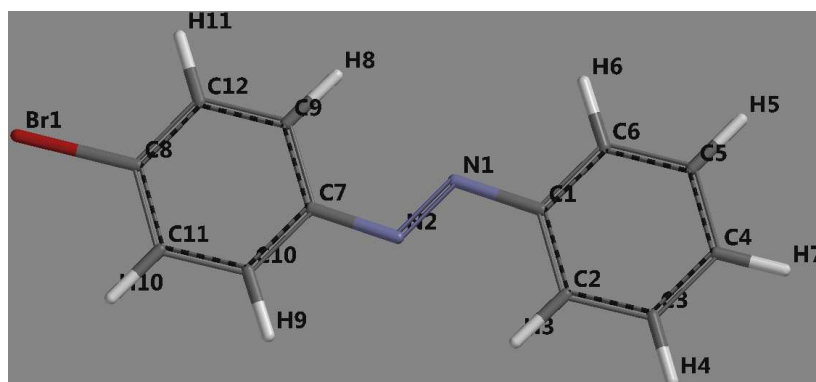


Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 H H1	0.3344269	-1.7830487	0.5261108
2 C C1	-0.3066199	-0.9096352	0.4990805
3 C C4	-1.9123139	1.3860858	0.4477521
4 C C2	0.2810782	0.3563219	0.3234528
5 C C6	-1.6817556	-1.0208269	0.6401034
6 C C5	-2.4989167	0.1232586	0.5991964
7 C C3	-0.5322068	1.4970663	0.3088989
8 H H6	-2.1471082	-1.9884143	0.7957839
9 H H3	-0.0558461	2.4647535	0.1898958
10 H H4	-2.5444864	2.2673778	0.4556483
11 N N1	1.6671582	0.5904607	0.1650356
12 O O1	-3.8497733	0.0058389	0.8122731
13 C C13	-4.7697126	-0.1621535	-0.3188705
14 C C14	-4.4097146	-1.4129117	-1.1282198
15 H H12	-3.4269757	-1.3190241	-1.5989205
16 H H13	-5.1486092	-1.5703807	-1.9200463
17 H H14	-4.4034695	-2.2986882	-0.4860811
18 C C15	-6.1261398	-0.3296453	0.3664509
19 H H11	-6.1185912	-1.2078569	1.0183881
20 H H15	-6.9182850	-0.4538422	-0.3775488
21 H H16	-6.3536932	0.5488248	0.9768298
22 C C16	-4.7576896	1.0892197	-1.2043148

23 H H5	-3.7775909	1.2474901	-1.6634685
24 H H17	-5.0146244	1.9770614	-0.6186283
25 H H18	-5.4915861	0.9876989	-2.0107273
26 N N2	2.3827005	-0.4486601	0.1529135
27 C C7	3.7715303	-0.2108340	-0.0090081
28 C C8	6.5373520	0.0210653	-0.3301209
29 C C9	4.3581812	1.0602767	-0.1372450
30 C C10	4.5769056	-1.3566245	-0.0398649
31 C C11	5.9562220	-1.2413671	-0.2018162
32 C C12	5.7343567	1.1682581	-0.2960696
33 H H2	3.7188216	1.9351337	-0.1105709
34 H H7	4.0958646	-2.3238550	0.0633389
35 H H8	6.5755793	-2.1328488	-0.2295922
36 H H9	6.1900543	2.1494905	-0.3944747
37 H H10	7.6119552	0.1154888	-0.4561961

TRANS-4-BROMOAZOBENZENE: -3146.05719 au

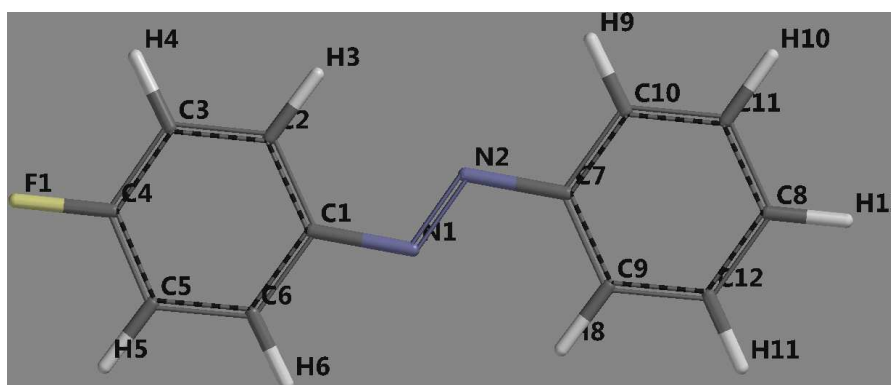


Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 N N1	2.0594298	-0.4599697	0.0000000
2 N N2	1.3321528	0.5699784	0.0000000
3 C C1	3.4536662	-0.2031397	0.0000000
4 C C4	6.2323593	0.0697546	0.0000000
5 C C2	4.0313569	1.0786714	0.0000000
6 C C6	4.2731558	-1.3396238	0.0000000
7 C C5	5.6598636	-1.2030799	0.0000000
8 C C3	5.4145321	1.2072218	0.0000000
9 H H3	3.3803429	1.9450776	0.0000000
10 H H6	3.7984733	-2.3155360	0.0000000
11 H H5	6.2919181	-2.0858787	0.0000000
12 H H4	5.8636951	2.1962068	0.0000000
13 H H7	7.3128319	0.1797470	0.0000000
14 C C7	-0.0610165	0.3120869	0.0000000
15 C C8	-2.8264594	0.0426606	0.0000000
16 C C9	-0.6427553	-0.9675713	0.0000000
17 C C10	-0.8818555	1.4466212	0.0000000

18 C	C11	-2.2684542	1.3199641	0.0000000
19 C	C12	-2.0247892	-1.1044702	0.0000000
20 H	H8	0.0045364	-1.8368478	0.0000000
21 H	H9	-0.4115754	2.4244626	0.0000000
22 H	H10	-2.9043655	2.1972061	0.0000000
23 H	H11	-2.4814459	-2.0880690	0.0000000
24 Br	Br1	-4.7313929	-0.1454327	0.0000000

TRANS-4-FLUOROAZOBENZENE: -672.009951 au

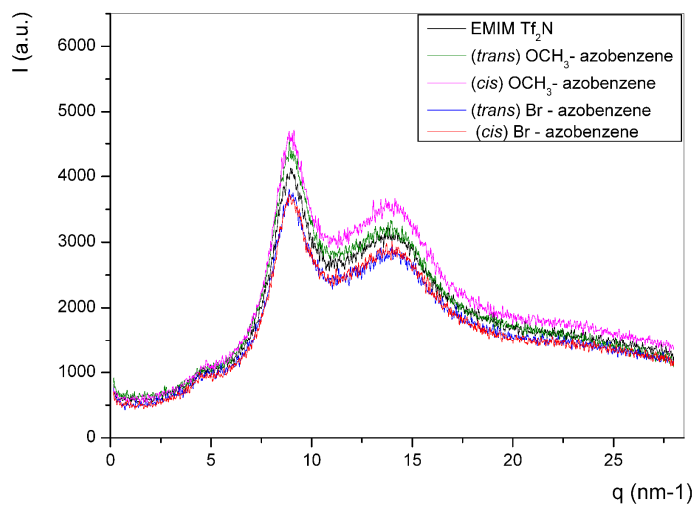


Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 N N1	-0.0784484	-0.5311304	0.0000000
2 N N2	-0.8316965	0.4802355	0.0000000
3 C C1	1.3071562	-0.2397240	0.0000000
4 C C4	4.0525715	0.1026188	0.0000000
5 C C2	1.8540893	1.0565814	0.0000000
6 C C6	2.1583905	-1.3535171	0.0000000
7 C C5	3.5405857	-1.1899615	0.0000000
8 C C3	3.2306031	1.2303152	0.0000000
9 H H3	1.1814417	1.9060785	0.0000000
10 H H6	1.7121678	-2.3424161	0.0000000
11 H H5	4.2180193	-2.0364876	0.0000000
12 H H4	3.6812610	2.2169441	0.0000000
13 C C7	-2.2197010	0.1893137	0.0000000
14 C C8	-4.9921429	-0.1499617	0.0000000
15 C C9	-2.7669921	-1.1053739	0.0000000
16 C C10	-3.0666250	1.3054428	0.0000000
17 C C11	-4.4497988	1.1359101	0.0000000
18 C C12	-4.1469691	-1.2670896	0.0000000
19 H H8	-2.0954189	-1.9559580	0.0000000
20 H H9	-2.6155002	2.2925313	0.0000000
21 H H10	-5.1024498	2.0037085	0.0000000
22 H H11	-4.5721555	-2.2666870	0.0000000
23 H H12	-6.0697199	-0.2855221	0.0000000
24 F F1	5.3889286	0.2756465	0.0000000

V. Additional SWAXS spectra.

Azobenzene derivatives at 3×10^{-2} M in EMIM Tf₂N before and after UV irradiation.



Azobenzene derivatives at 3×10^{-2} M in BMIM BF₄ before and after UV irradiation.

