Supplementary Material

Ring-closure reaction of 2-benzoylbenzenediazonium salts in 1-butyl-3-methylimidazolium ionic liquids

Takao Okazaki,* Hiroyuki Yamamoto, and Toshikazu Kitagawa*

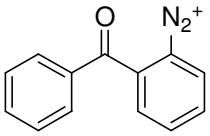
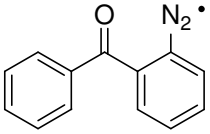
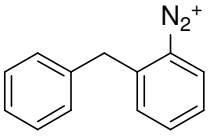
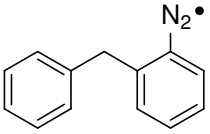
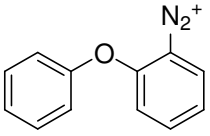
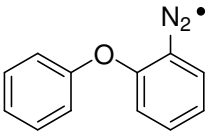
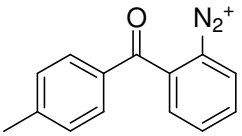
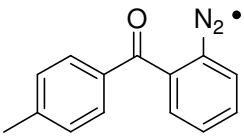
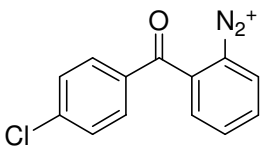
Department of Chemistry for Materials, Graduate School of Engineering, Mie University, Tsu, Mie 514-8507, Japan
Email: okazaki@chem.mie-u.ac.jp

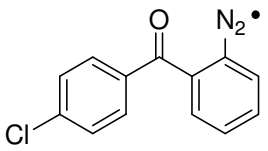
Table of Contents

Table S1. Energy (E), Zero Point Energy (ZPE), and Gibbs Free Energy (G) of the Optimized Structures by the DFT Calculations

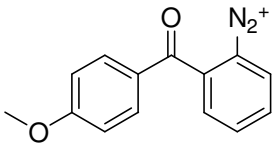
Compound	Method E, hartree	ZPE, hartree	G, hartree
N_2	B3LYP/6-31G(d)		
	-109.5241291	0.005599	-109.536980
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)		
	-109.5634692	0.005271	-109.576648
$CF_3SO_3^-$ (Anion)	B3LYP/6-31G(d)		
	-961.497981	0.027271	-961.503223
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)		
	-961.8622215	0.025944	-961.868260
$CF_3SO_3^{\bullet}$ (Radical)	B3LYP/6-31G(d)		
	-961.3301452	0.024465	-961.340550
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)		
	-961.58935	0.023233	-961.600631
Tf_2N^- (Anion)	B3LYP/6-31G(d)		
	-1827.2053211	0.053381	-1827.196091
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)		
	-1827.7675014	0.051280	-1827.758252
$Tf_2N^{\bullet}$ (Radical)	B3LYP/6-31G(d)		
	-1827.0244237	0.051762	-1827.018835
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)		
	-1827.5017241	0.049930	-1827.495495

Table S2. Energy (E), Zero Point Energy (ZPE), and Gibbs Free Energy (G) of the Optimized Structures by the DFT Calculations

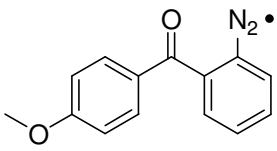
Compound	Method E, hartree	ZPE, hartree	G, hartree
	B3LYP/6-31G(d) -685.2375795	0.190379	-685.086946
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) -685.504027	0.186944	-685.356066
	B3LYP/6-31G(d) -685.4652558	0.188163	-685.318572
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) -685.6764469	0.185149	-685.531627
	B3LYP/6-31G(d) -611.2232641	0.208599	-611.055404
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) -611.4687816	0.205292	-611.302082
	B3LYP/6-31G(d) -611.4545038	0.207078	-611.290108
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) -611.6368586	0.203915	-611.472895
	B3LYP/6-31G(d) -647.1248178	0.184220	-646.980855
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) -647.3808024	0.180785	-647.238459
	B3LYP/6-31G(d) -647.3478744	0.182181	-647.206996
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) -647.5464763	0.179305	-647.406675
	B3LYP/6-31G(d) -724.5590248	0.217868	-724.383791
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) -724.8332791	0.214399	-724.659678
	B3LYP/6-31G(d) -724.7841835	0.215705	-724.612690
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) -725.0055894	0.212561	-724.835229
	B3LYP/6-31G(d) -1144.8297024	0.180627	-1144.690958
	PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d) -1145.1276564	0.177440	-1144.991292



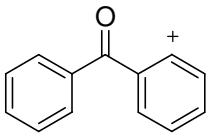
B3LYP/6-31G(d)
-1145.0609312 0.178463 -1144.926101
PCM(EtOH)-B3LYP/6-31G(d)//B3LYP/6-31G(d)
-1145.3009738 0.175596 -1145.167785



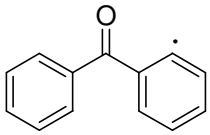
B3LYP/6-31G(d)
-799.7685318 0.223284 -799.588247
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
-800.0673942 0.219457 -799.890024



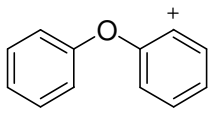
B3LYP/6-31G(d)
-799.9904877 0.221044 -799.814298
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
-800.2400788 0.217665 -800.065955



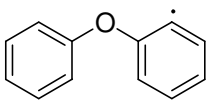
B3LYP/6-31G(d)
-575.6543704 0.176540 -575.516950
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
-575.8931358 0.172719 -575.758314



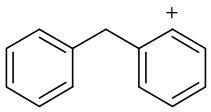
B3LYP/6-31G(d)
-575.9474497 0.178762 -575.807271
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
-576.1231091 0.175621 -575.985589



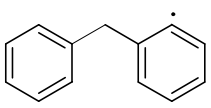
B3LYP/6-31G(d)
-537.5282793 0.170180 -537.395509
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
-537.7528857 0.166580 -537.622822



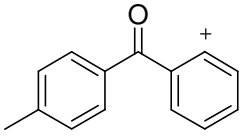
B3LYP/6-31G(d)
-537.8245442 0.172606 -537.689694
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
-537.9886035 0.169562 -537.856022



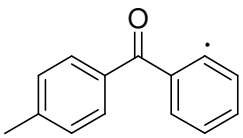
B3LYP/6-31G(d)
-501.6500972 0.195285 -501.493261
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
-501.860728 0.191606 -501.705938



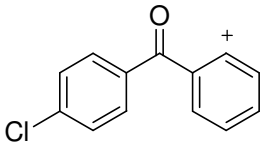
B3LYP/6-31G(d)
-501.9283453 0.197283 -501.770667
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
-502.0779658 0.194152 -501.921461



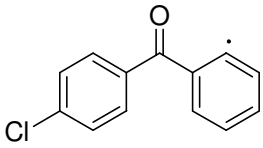
B3LYP/6-31G(d)
-614.9763326 0.203897 -614.815210
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
-615.2230574 0.200110 -615.062771



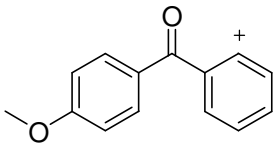
B3LYP/6-31G(d)
-615.2665097 0.206317 -615.101781
PCM(EtOH)-B3LYP/6-31+G(2d,p)//B3LYP/6-31G(d)
-615.4523694 0.203070 -615.289299



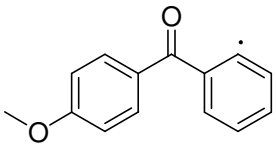
B3LYP/6-31G(d)
-1035.2461306 0.166777 -1035.120468
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
-1035.5163327 0.163211 -1035.393038



B3LYP/6-31G(d)
-1035.5431482 0.169038 -1035.414951
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
-1035.7472779 0.166033 -1035.621525



B3LYP/6-31G(d)
A fluorenonium ion was obtained as the optimized structure
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
A fluorenonium ion was obtained as the optimized structure



B3LYP/6-31G(d)
-690.4728525 0.211586 -690.303248
PCM(EtOH)-B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d)
-690.6867002 0.208076 -690.519981
