SUPPORTING INFORMATION

First Observation of Ultrafast Intramolecular Proton Transfer Rate between Electronic Ground States in Solution

Yuichi Masuda,* Tomoko Nakano, and Midori Sugiyama

Department of Chemistry, Faculty of Science, Ochanomizu University, Bunkyo-ku, Tokyo 112-8610, Japan

Table S1 Reaction conditions for synthesis of ^{17}O-enriched compounds.

	BA	Fluvene	DBM
	reaction mixture content		
substance (^{17}O un-enriched)	100 mg	132 mg	101 mg
^{17}O labeled water (^{17}O abundance)	60 mg (46.3%)	158 mg (42.0%)	105 mg (46.3%)
hydroichloric acid(37 w/w %)	6 μl	12 μl	10μl
dioxane	0.6 g	1.2 g	0.5g
	reaction condition		
temperature	60 ºC	80 ºC	80 ºC
reaction time	2 hr	3 days	46 hr
	^{17}O abundance of product		
	32.8	30.5 %	29.5 %

Table S2 Atomic coordinate of Fulvene with MO calculations (MP2: 6-311++G(d,p)).

atom	x	y	z
C(1)	-1.511	0.883	0.063
C(2)	-0.116	0.834	0.140
C(3)	0.734	1.996	0.161
H(3)	0.386	3.022	0.126
C(4)	2.050	1.575	0.319
H(4)	2.916	2.222	0.406
C(5)	2.073	0.156	0.380
H(5)	2.953	-0.458	0.533
C(6)	0.754	-0.330	0.283
C(7)	0.372	-1.716	0.387
C(8)	-2.224	2.141	-0.230
C(9)	1.427	-2.761	0.294
C(o)	-3.359	2.476	0.530
H(o)	-3.678	1.813	1.329
C(o)	-1.813	2.976	-1.284
H(o)	-0.968	2.683	-1.900
C(m)	-4.050	3.661	0.264
H(m)	-4.916	3.927	0.863
C(m)	-2.524	4.149	-1.558
H(m)	-2.214	4.786	-2.383
C(p)	-3.634	4.499	-0.780
H(p)	-4.180	5.415	-0.992
C(o')	1.390	-3.838	1.196
H(o')	0.610	-3.866	1.952
C(o')	2.411	-2.721	-0.709
H(o')	2.410	-1.908	-1.430
C(m')	2.351	-4.848	1.117
H(m')	2.331	-5.671	1.827
C(m')	3.354	-3.750	-0.800
H(m')	4.104	-3.728	-1.587
C(p')	3.335	-4.807	0.119
H(p')	4.075	-5.600	0.052
O(OH)	-2.304	-0.139	0.263
H(OH)	-1.736	-0.976	0.467
O(O···H)	-0.810	-2.096	0.584