Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Supplementary Data

Synthesis, Structures, Redox and Photophysical Properties of Benzodifuran-functionalised Pyrene and Anthracene Fluorophores

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Calculated and experimental structural parameters of **1**.

	X-ray	B3LYP/TZVP		X-ray	B3LYP/TZVP
bond length [Å]			**bond angle [deg]**		
C1-N1	1.324	1.345	C17-C16-C36	117.8	120.3
C1-O1	1.342	1.352	C14-C16-C36	135	134.0
C1-C14	1.412	1.380	C18-C17-O1	124.8	123.8
C14-C15	1.403	1.406	C18-C17-C16	126.2	126.4
C14-C16	1.415	1.449	O1-C17-C16	109	109.8
C15-N2	1.147	1.157	C17-C18-C19	117.2	113.3
C16-C17	1.409	1.398	C18-C19-C20	116	120.3
C16-C36	1.429	1.414	C36-C20-C19	128.3	126.4
C17-C18	1.353	1.396	C20-C36-C16	114.4	113.3
C17-O1	1.387	1.387	C20-C36-C37	125.1	123.4
C18-C19	1.405	1.414	C16-C36-C37	120.6	123.3
C19-C20	1.416	1.398	C38-C37-C36	176.5	178.5
C20-C36	1.356	1.396	C37-C38-C39	177.4	177.8
C36-C37	1.459	1.408	C44-C39-C40	123.7	119.7
C37-C38	1.184	1.211	C44-C39-C38	119.4	118.9
C38-C39	1.470	1.416	C40-C39-C38	116.9	121.4
C39-C44	1.373	1.407	C51-C40-C39	123.3	122.4
C39-C40	1.434	1.419	C51-C40-C41	121.8	118.6
C40-C51	1.383	1.432	C39-C40-C41	114.9	119.0
C40-C41	1.440	1.424	C42-C41-C48	119.8	119.7
C41-C42	1.410	1.425	C42-C41-C40	122.3	120.3
C41-C48	1.435	1.425	C48-C41-C40	117.8	120.0
C42-C43	1.404	1.403	C43-C42-C41	118.2	118.9
C42-C45	1.453	1.432	C43-C42-C45	121.2	122.2
C43-C44	1.393	1.381	C41-C42-C45	120.5	118.9
C45-C46	1.366	1.358	C44-C43-C42	121.8	121.2
C46-C47	1.414	1.433	C39-C44-C43	119	120.9
C47-C54	1.398	1.401	C46-C45-C42	118.7	121.4
C47-C48	1.432	1.425	C45-C46-C47	122.3	121.3
C48-C49	1.339	1.424	C54-C47-C46	123.2	122.3
C49-C52	1.430	1.401	C54-C47-C48	116.7	119.1
C49-C50	1.479	1.432	C46-C47-C48	120.1	118.6
C50-C51	1.380	1.358	C49-C48-C47	120.3	119.7
C52-C53	1.376	1.389	C49-C48-C41	121.2	120.2
C53-C54	1.336	1.390	C47-C48-C41	118.5	120.1
bond angle [deg]			C48-C49-C52	121.1	119.2
N1-C1-O1	114	116.4	C48-C49-C50	119.5	118.4
N1-C1-C14	134.1	131.8	C52-C49-C50	119.4	122.5
O1-C1-C14	111.7	111.8	C51-C50-C49	120.6	121.5
C15-C14-C1	126.6	123.9	C50-C51-C40	119.1	121.4
C15-C14-C16	128.3	130.4	C53-C52-C49	118.2	120.8
C1-C14-C16	105	105.7	C54-C53-C52	120.7	120.5
N2-C15-C14	177.5	177.2	C53-C54-C47	122.9	120.8
C17-C16-C14	107.2	105.7	C1-O1-C17	107.1	106.9

Calculated and experimental structural parameters of **2**.

	X-ray	B3LYP/TZVP		X-ray	B3LYP/TZVP
bond length [Å]			**bond angle [deg]**		
O1-C1	1.372	1.351	C34-C22-C23	117.8	118.2
O1-C17	1.387	1.388	N1-C1-O1	114.9	116.5
N1-C1	1.342	1.344	N1-C1-C14	134.6	131.7
N2-C15	1.154	1.158	O1-C1-C14	110.4	111.8
C17-C18	1.391	1.398	C17-C18-C16	113.3	113.0
C17-C16	1.396	1.400	C17-C18-C19	121.4	121.2
C22-C21	1.417	1.420	C16-C18-C19	125.4	125.7
C22-C34	1.423	1.422	C27-C26-C21	122.3	122.6
C22-C23	1.435	1.439	C27-C26-C25	118.2	118.1
C1-C14	1.388	1.380	C21-C26-C25	119.6	119.3
C18-C16	1.422	1.414	C24-C25-C30	122.2	121.4
C18-C19	1.454	1.411	C24-C25-C26	119.1	119.6
C26-C27	1.417	1.424	C30-C25-C26	118.7	119.0
C26-C21	1.422	1.422	C22-C21-C26	119.8	120.3
C26-C25	1.439	1.438	C22-C21-C20	120.4	120.5
C25-C24	1.383	1.396	C26-C21-C20	119.7	119.2
C25-C30	1.424	1.427	C28-C27-C26	121.3	121.1
C21-C20	1.462	1.417	C24-C23-C31	121.8	121.5
C27-C28	1.359	1.368	C24-C23-C22	119.1	119.6
C23-C24	1.392	1.395	C31-C23-C22	119.1	118.9
C23-C31	1.434	1.427	C19-C20-C21	178.1	177.5
C20-C19	1.156	1.213	C25-C24-C23	112.6	121.8
C16-C14	1.444	1.450	C17-C16-C18	119.1	119.8
C14-C15	1.410	1.405	C17-C16-C14	106.0	105.5
C31-C32	1.362	1.365	C18-C16-C14	134.9	134.7
C32-C33	1.423	1.419	C20-C19-C18	174.0	174.7
C33-C34	1.355	1.367	C1-C14-C15	126.2	122.7
C28-C29	1.414	1.419	C1-C14-C16	106.4	105.8
C29-C30	1.368	1.364	C15-C14-C16	127.3	131.5
bond angle [deg]			C32-C31-C23	120.7	121.0
C1-O1-C17	107.3	107.0	C31-C32-C33	120.0	120.1
O1-C17-C18	122.4	123.0	C34-C33-C32	120.6	120.7
O1-C17-C16	109.9	109.9	C27-C28-C29	121.1	120.7
C18-C17-C16	127.7	127.1	N2-C15-C14	179.3	175.6
C21-C22-C34	122.5	122.4	C30-C29-C28	119.6	119.9
C21-C22-C23	119.7	119.4	C29-C30-C25	121.2	121.1

Cartesian coordinates of the optimized ground-state geometry of **1** (B3LYP/TZVP):

C	2.113109	2.516940	0.000000
C	2.541060	1.205089	0.000000
C	1.336369	0.399509	0.000000
C	0.273556	1.307761	0.000000
O	0.763659	2.605411	0.000000
C	-1.086450	0.992040	0.000000
C	-1.336369	-0.399509	0.000000
C	-0.273556	-1.307761	0.000000
C	1.086450	-0.992040	0.000000
C	-2.541060	-1.205089	0.000000
C	-2.113109	-2.516940	0.000000
O	-0.763659	-2.605411	0.000000
N	-2.787605	-3.680179	0.000000
C	2.108141	-1.961386	0.000000
C	3.008872	-2.770988	0.000000
C	-3.893856	-0.821137	0.000000
N	-5.021470	-0.560220	0.000000
C	-2.108141	1.961386	0.000000
C	-3.008872	2.770988	0.000000
C	3.893856	0.821137	0.000000
N	5.021470	0.560220	0.000000
N	2.787605	3.680179	0.000000
H	-2.290828	-4.553509	0.000000
H	-3.792724	-3.681584	0.000000
H	2.290828	4.553509	0.000000
H	3.792724	3.681584	0.000000
C	-4.097602	3.675706	0.000000
C	-3.891559	5.079961	0.000000
C	-5.023428	5.943725	0.000000
C	-6.340916	5.401673	0.000000
C	-6.500378	4.008143	0.000000
C	-5.407838	3.163165	0.000000
C	-2.584796	5.664488	0.000000
C	-2.412821	7.011416	0.000000
C	-3.528780	7.909078	0.000000
C	-4.841073	7.357173	0.000000
C	-7.457170	6.298102	0.000000
C	-7.282747	7.644442	0.000000
C	-5.972094	8.224544	0.000000
C	-5.766857	9.610330	0.000000
C	-4.482038	10.139514	0.000000
C	-3.374046	9.301731	0.000000
C	4.097602	-3.675706	0.000000
C	5.407838	-3.163165	0.000000
C	6.500378	-4.008143	0.000000
C	6.340916	-5.401673	0.000000
C	5.023428	-5.943725	0.000000

C	3.891559	-5.079961	0.000000
C	2.584796	-5.664488	0.000000
C	2.412821	-7.011416	0.000000
C	3.528780	-7.909078	0.000000
C	4.841073	-7.357173	0.000000
C	7.457170	-6.298102	0.000000
C	7.282747	-7.644442	0.000000
C	5.972094	-8.224544	0.000000
C	5.766857	-9.610330	0.000000
C	4.482038	-10.139514	0.000000
C	3.374046	-9.301731	0.000000
H	5.548667	-2.089619	0.000000
H	7.500266	-3.589412	0.000000
H	8.455363	-5.875155	0.000000
H	8.140275	-8.307779	0.000000
H	6.626130	-10.271244	0.000000
H	4.343484	-11.214079	0.000000
H	2.374833	-9.722714	0.000000
H	1.414016	-7.433773	0.000000
H	1.727919	-5.002692	0.000000
H	-5.548667	2.089619	0.000000
H	-7.500266	3.589412	0.000000
H	-1.727919	5.002692	0.000000
H	-1.414016	7.433773	0.000000
H	-2.374833	9.722714	0.000000
H	-4.343484	11.214079	0.000000
H	-6.626130	10.271244	0.000000
H	-8.140275	8.307779	0.000000
H	-8.455363	5.875155	0.000000

Cartesian coordinates of the optimized ground-state geometry of **2** (B3LYP/TZVP):

C	1.653129	2.839691	0.000000
C	2.302815	1.622308	0.000000
C	1.258305	0.616258	0.000000
C	0.053194	1.328047	0.000000
O	0.310478	2.691543	0.000000
C	-1.240205	0.797685	0.000000
C	-1.258305	-0.616258	0.000000
C	-0.053194	-1.328047	0.000000
C	1.240205	-0.797685	0.000000
C	-2.302815	-1.622308	0.000000
C	-1.653129	-2.839691	0.000000
O	-0.310478	-2.691543	0.000000
N	-2.117794	-4.100934	0.000000
C	2.374648	-1.636394	0.000000
C	3.279143	-2.444516	0.000000
C	-3.703071	-1.509625	0.000000
N	-4.860584	-1.506244	0.000000

C	-2.374648	1.636394	0.000000
C	-3.279143	2.444516	0.000000
C	3.703071	1.509625	0.000000
N	4.860584	1.506244	0.000000
N	2.117794	4.100934	0.000000
H	-1.479191	-4.876363	0.000000
H	-3.108067	-4.274339	0.000000
H	1.479191	4.876363	0.000000
H	3.108067	4.274339	0.000000
C	4.292940	-3.433885	0.000000
C	5.663849	-3.062689	0.000000
C	6.672841	-4.087991	0.000000
C	6.291046	-5.429863	0.000000
C	4.949107	-5.813415	0.000000
C	3.922442	-4.806639	0.000000
C	4.569012	-7.188880	0.000000
C	3.255191	-7.557264	0.000000
C	2.242342	-6.563138	0.000000
C	2.564104	-5.233958	0.000000
C	8.047218	-3.703607	0.000000
C	8.408219	-2.387355	0.000000
C	7.411751	-1.376496	0.000000
C	6.084639	-1.704354	0.000000
C	-4.292940	3.433885	0.000000
C	-3.922442	4.806639	0.000000
C	-4.949107	5.813415	0.000000
C	-6.291046	5.429863	0.000000
C	-6.672841	4.087991	0.000000
C	-5.663849	3.062689	0.000000
C	-6.084639	1.704354	0.000000
C	-7.411751	1.376496	0.000000
C	-8.408219	2.387355	0.000000
C	-8.047218	3.703607	0.000000
C	-2.564104	5.233958	0.000000
C	-2.242342	6.563138	0.000000
C	-3.255191	7.557264	0.000000
C	-4.569012	7.188880	0.000000
H	5.342305	-0.919916	0.000000
H	7.700110	-0.332698	0.000000
H	9.455067	-2.108381	0.000000
H	8.800250	-4.483672	0.000000
H	7.058426	-6.196967	0.000000
H	5.351885	-7.938945	0.000000
H	2.980061	-8.604944	0.000000
H	1.202540	-6.868912	0.000000
H	1.786319	-4.482126	0.000000
H	-5.342305	0.919916	0.000000
H	-7.700110	0.332698	0.000000
H	-9.455067	2.108381	0.000000
H	-8.800250	4.483672	0.000000

H	-7.058426	6.196967	0.000000
H	-5.351885	7.938945	0.000000
H	-2.980061	8.604944	0.000000
H	-1.202540	6.868912	0.000000
H	-1.786319	4.482126	0.000000