crystals

Supplementary Materials: Molecular Structure, Spectroscopic and DFT Computational Studies of Arylidene-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione

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Table S1. The calculated bond distances and bond angles compared to the experimental data of **1.**

Parameter	Calculated	Experimental	Parameter	Calculated	Experimental
R(1-8)	1.228	1.213	A(1-8-6)	117.8	118.6
R(2-13)	1.221	1.209	A(1-8-19)	125.5	125.2
R(3-18)	1.225	1.214	A(2-13-6)	121.9	121.2
R(4-25)	1.361	1.359	A(2-13-7)	122.0	121.5
R(5-26)	1.364	1.358	A(3-18-7)	119.0	119.9
R(5-31)	1.425	1.431	A(3-18-19)	123.8	123.3
R(6-8)	1.401	1.395	A(4-25-23)	120.4	118.2
R(6-9)	1.469	1.465	A(4-25-26)	120.3	121.8
R(6-13)	1.397	1.375	A(26-5-31)	118.7	118.0
R(7-13)	1.395	1.365	A(5-26-25)	113.7	115.4
R(7-14)	1.468	1.477	A(5-26-27)	126.2	124.6
R(7-18)	1.395	1.389	A(8-6-9)	116.2	117.5
R(8-19)	1.471	1.475	A(8-6-13)	126.0	125.7
R(18-19)	1.491	1.485	A(6-8-19)	116.6	116.2
R(19-20)	1.373	1.357	A(9-6-13)	117.7	116.8
R(20-22)	1.448	1.455	A(6-13-7)	116.1	117.3
R(22-23)	1.421	1.413	A(13-7-14)	118.1	116.9
R(22-29)	1.411	1.384	A(13-7-18)	125.3	125.4
R(23-25)	1.382	1.368	A(14-7-18)	116.6	117.7
R(25-26)	1.413	1.383	A(7-18-19)	117.2	116.8
R(26-27)	1.395	1.384	A(8-19-18)	118.7	118.4
R(27-29)	1.392	1.411	A(8-19-20)	127.7	127.4
			A(18-19-20)	113.6	114.2
			A(19-20-22)	138.6	137.8
			A(20-22-23)	114.8	114.2
			A(20-22-29)	127.2	127.9
			A(23-22-29)	118.1	117.8
			A(22-23-25)	121.5	121.7
			A(22-29-27)	120.6	120.6
			A(23-25-26)	119.3	120.0
			A(25-26-27)	120.1	120.1
			A(26-27-29)	120.4	119.8

Table S2. The calculated bond distances and bond angles compared to the experimental data of **2.**

Parameter	Calculated	Experimental	Parameter	Calculated	Experimental
R(1-8)	1.226	1.218	A(1-8-6)	120.1	119.4
R(2-13)	1.22	1.224	A(1-8-19)	123.3	123.7
R(3-18)	1.229	1.213	A(2-13-6)	121.5	120.5
R(4-25)	1.359	1.363	A(2-13-7)	121.3	121.4
R(4-31)	1.423	1.433	A(3-18-7)	118.9	118.0
R(5-26)	1.354	1.346	A(3-18-19)	124.9	124.9
R(6-8)	1.397	1.381	A(25-4-31)	117.6	117.4
R(6-9)	1.468	1.471	A(4-25-23)	125.0	125.2
R(6-13)	1.391	1.367	A(4-25-26)	115.2	114.3
R(7-13)	1.394	1.373	A(5-26-25)	117.1	117.4
R(7-14)	1.468	1.465	A(5-26-27)	123.3	123.3
R(7-18)	1.403	1.399	A(8-6-9)	119.3	118.1
R(8-19)	1.493	1.482	A(8-6-13)	124.9	124.7
R(18-19)	1.472	1.455	A(6-8-19)	116.7	116.9
R(19-20)	1.376	1.367	A(9-6-13)	115.9	117.2
R(20-22)	1.445	1.439	A(6-13-7)	117.2	118.2
R(22-23)	1.419	1.405	A(13-7-14)	115.3	117.6
R(22-29)	1.413	1.403	A(13-7-18)	125.6	124.3
R(23-25)	1.386	1.37	A(14-7-18)	119.1	118.1
R(25-26)	1.419	1.403	A(7-18-19)	116.2	117.1
R(26-27)	1.396	1.38	A(8-19-18)	119.6	118.6
R(27-29)	1.388	1.372	A(8-19-20)	113.2	114.0
			A(18-19-20)	127.2	127.4
			A(19-20-22)	139.0	138.2
			A(20-22-23)	127.2	127.4
			A(20-22-29)	114.9	114.8
			A(23-22-29)	117.9	117.8
			A(22-23-25)	121.2	120.7
			A(22-29-27)	121.2	121.4
			A(23-25-26)	119.8	120.6
			A(25-26-27)	119.6	119.3
			A(26-27-29)	120.4	120.3