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UV-absorbing benzamide-based dendrimer precursors: synthesis, theoretical calculation, and spectroscopic characterization

Chidera C. Nnadiekwe[a], Ahmed Nada[a], Ismail Abdulazeez[b], Mohammad R. Imam[c], Muhammad Ramzan Saeed Ashraf Janjua[a], Abdulaziz A. Al-Saadi[* a,d]

[a]*Chemistry Department, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia.*
[b]*Interdisciplinary Research Center for Membranes & Water Security, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia.*
[b]*Medical Sciences Department, American University of Iraq, Sulaimani, Kurdistan Region, Iraq 46001.*
[d]*Interdisciplinary Research Center for Refining & Advanced Chemicals, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia.*
** Corresponding author: A.A. Al-Saadi (asaadi@kfupm.edu.sa)*

Supplementary Information

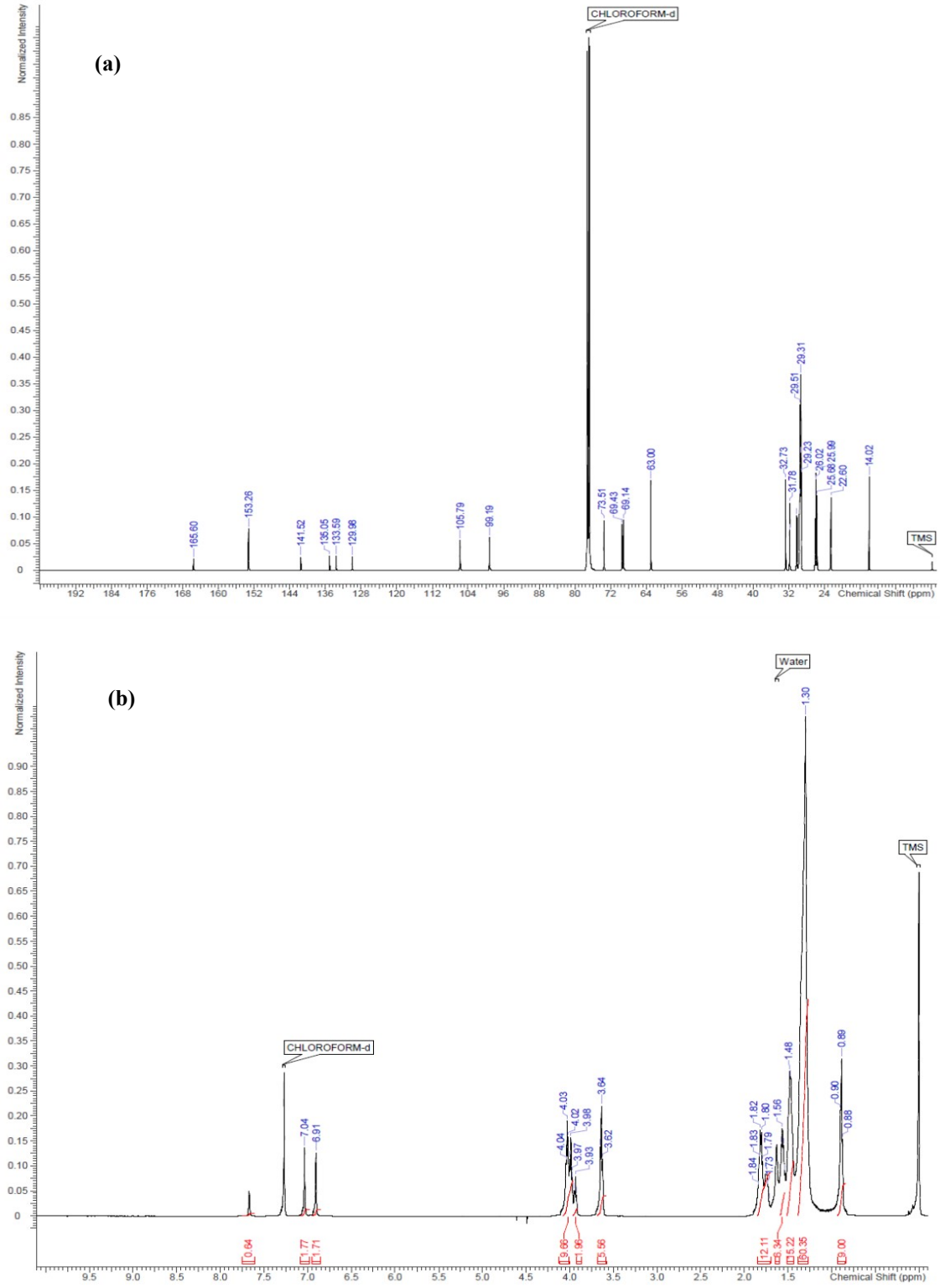

Figure S1: (a) ^{13}C-NMR and (b) ^{1}H-NMR spectra of the Janus (***J*1**) benzamide structure.

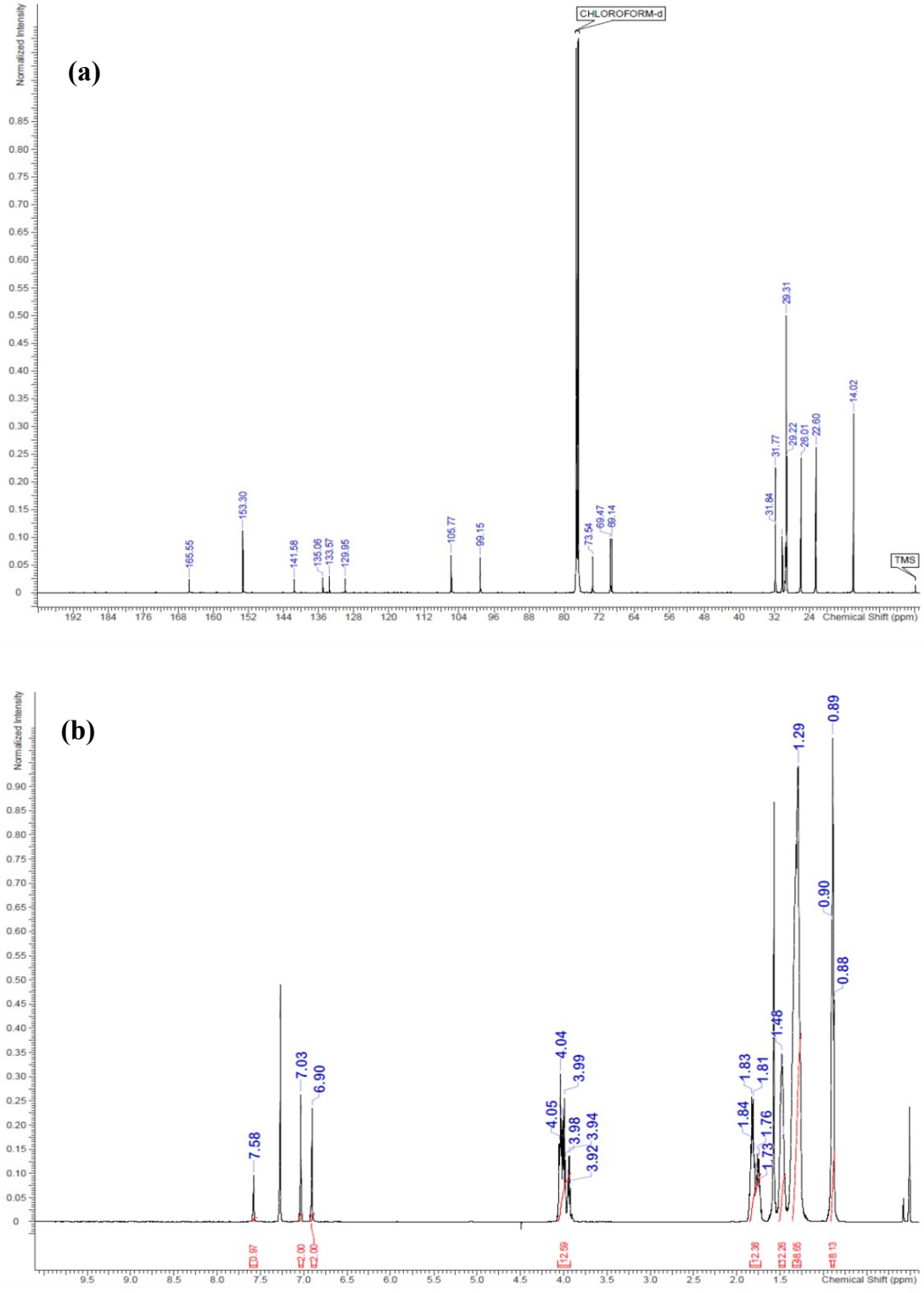

Figure S2: (a) ^{13}C-NMR and (b) ^{1}H-NMR spectra of the Twin (***T*1)** benzamide structure.

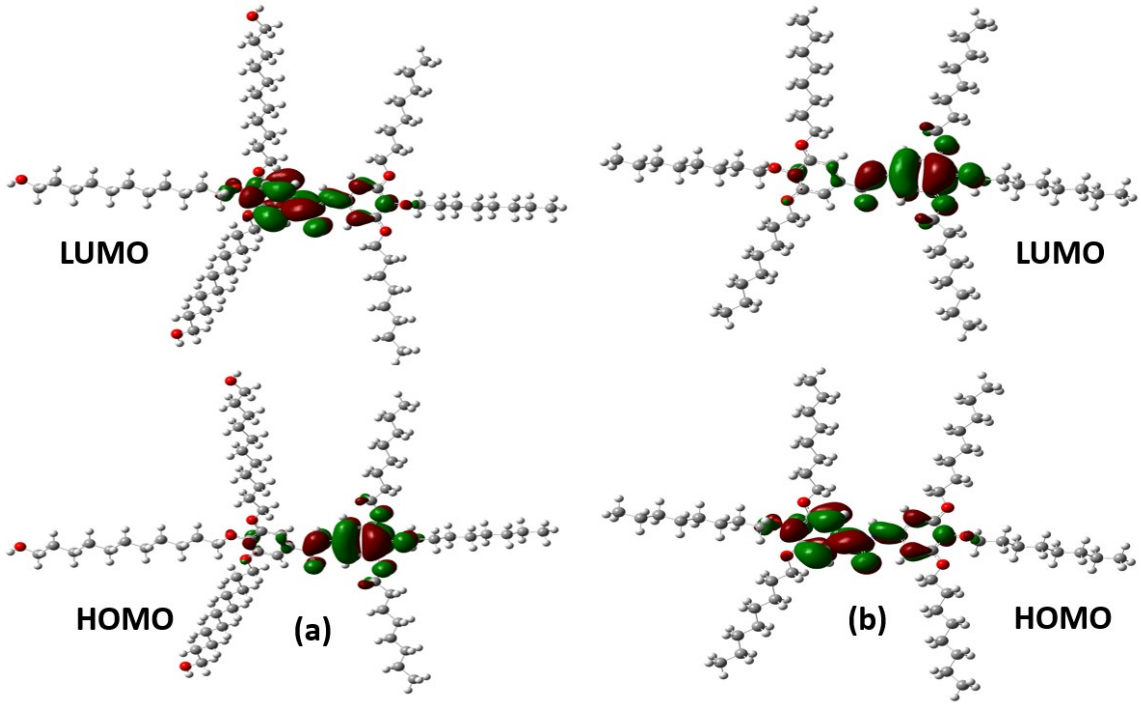

Figure S3: Frontier orbitals of (a) Janus **(*J*1)** and (b) Twin **(*T*1)** benzamide structures.

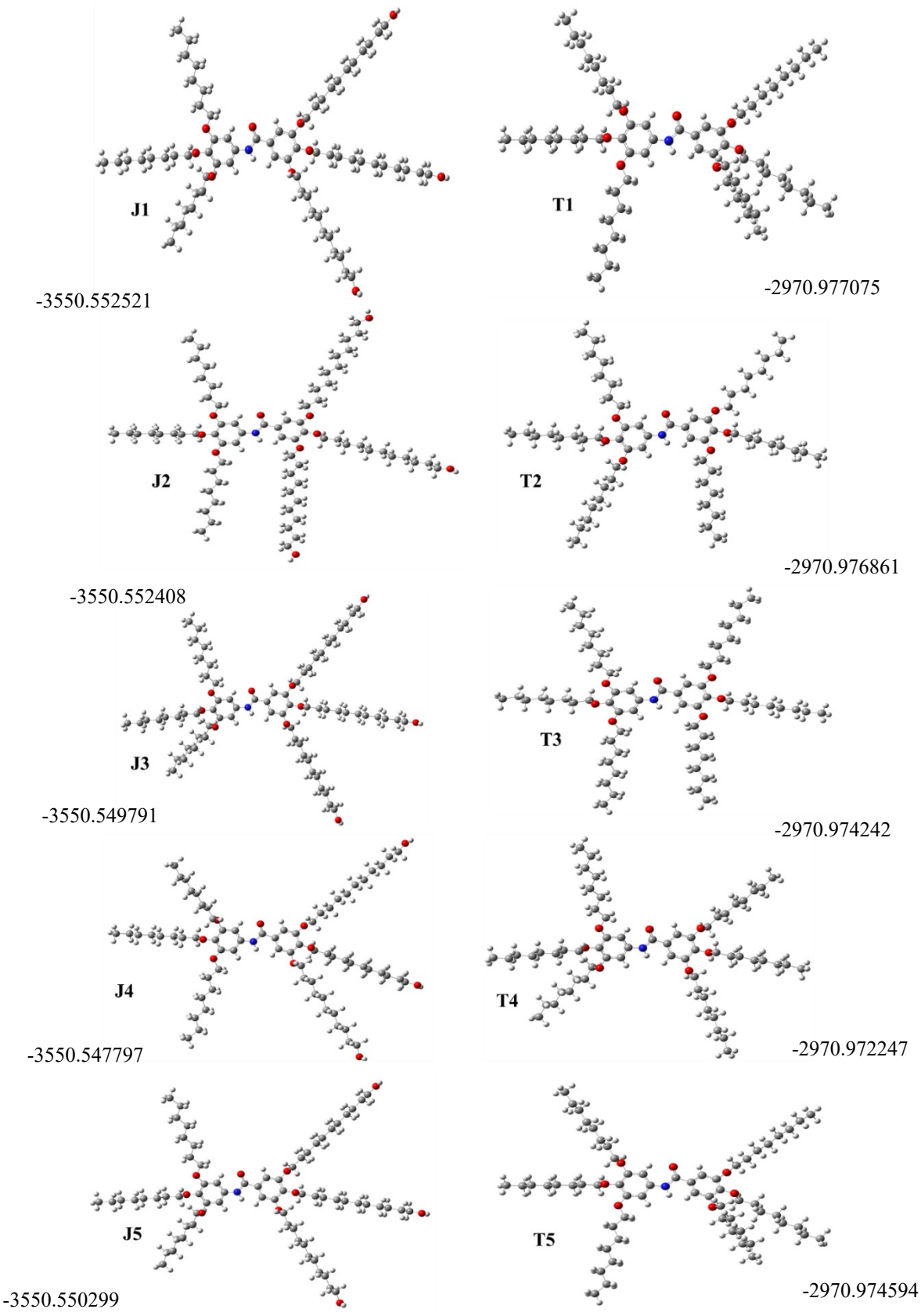

Figure S4: Optimized structures with their computed total energies (Hartree) of the different configurations of the Janus, denoted with the "***J***" series, and the Twin, denoted with the "***T***" series (Refer to **Table 1** for structural and stability details).

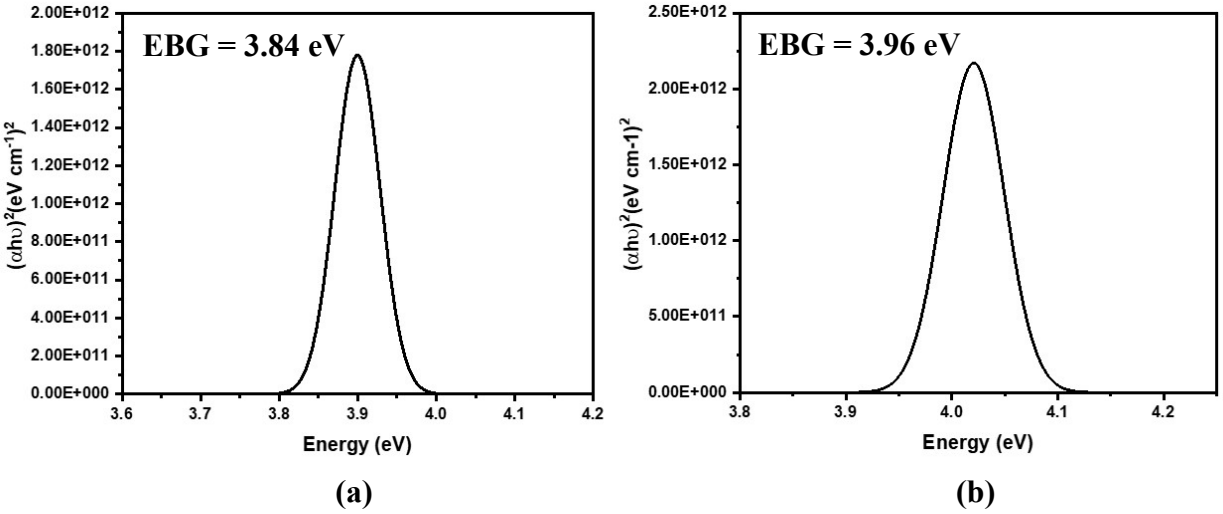

Figure S5: Theoretical UV-Vis energy gaps for (a) Janus **(*J*1)**, and (b) Twin **(*T*1)** benzamides-computed at the B3LYP level using the Tauc plot extrapolation.

Table S1: Selected bond distances calculated at the B3LYP/6-311G(d) level for the Janus and the Twin benzamides in their two most stable configurations.

	Janus Benzamide		**Twin Benzamide**	
Bond Distances	***J1***	***J2***	***T1***	***T2***
O(2)-C(1)	1.221	1.221	1.221	1.220
C(1)-C(5)	1.504	1.504	1.504	1.503
C(1)-N(3)	1.376	1.377	1.377	1.378
N(3)-C(13)	1.411	1.411	1.411	1.410
C(8)-O(23)	1.360	1.360	1.360	1.364
O(23)-C(75)	1.426	1.426	1.426	1.428
C(12)-O(22)	1.365	1.364	1.364	1.370
O(22)-C(51)	1.439	1.438	1.438	1.442
C(10)-O(21)	1.359	1.359	1.359	1.362
O(21)-C(27)	1.430	1.430	1.430	1.437
C(18)-O(24)	1.362	1.362	1.362	1.373
O(24)-C(147)	1.424	1.424	1.424	1.440

C(20)-O(25)	1.369	1.369	1.369	1.373
O(25)-C(123)	1.435	1.435	1.435	1.439
C(16)-O(26)	1.360	1.360	1.360	1.360
O(26)-C(99)	1.429	1.429	1.429	1.430

Table S2: Selected bond angles calculated at the B3LYP/6-311G(d) level for the Janus and the Twin benzamides in their two most stable configurations.

	Janus Benzamide		**Twin Benzamide**	
Bond Angles	***J1***	***J2***	***T1***	***T2***
O(2)-C(1)-N(3)	123.858	123.844	123.931	123.890
O(2)-C(1)-C(5)	121.415	121.464	121.744	121.457
C(1)-N(3)-C(13)	129.236	129.234	129.224	129.240
C(5)-C(1)-N(3)	114.722	114.686	114.320	114.646
C(8)-O(23)-C(75)	119.100	118.930	119.192	118.997
C(12)-O(22)-C(51)	115.013	115.815	117.346	115.602
C(10)-O(21)-C(27)	118.808	118.698	121.473	118.700
C(16)-O(26)-C(99)	118.755	118.810	118.956	118.799
C(18)-O(24)-C(147)	119.196	119.020	116.005	118.992
C(20)-O(25)-C(123)	115.236	115.150	115.002	115.232
C(195)-C(198)-O(205)	107.891	107.899	-	-
C(186)-C(189)-O(201)	107.915	107.918	-	-
C(177)-C(180)-O(203)	107.919	107.901	-	-

Table S3: The dihedral angles of the different configurations of the Janus and Twin benzamide systems.

	Janus Benzamide		**Janus Benzamide**	
Dihedral Angles	***J1***	***J2***	***T1***	***T2***
C(15)-C(18)-O(24)-C(147)	2.955	3.302	111.212	2.433
C(20)-C(18)-O(24)-C(147)	-176.834	-176.433	-71.049	-177.386
C(18)-C(20)-O(25)-C(123)	-92.321	-94.357	-100.577	-94.385
C(16)-C(20)-O(25)-C(123)	89.840	87.803	80.867	87.661
C(14)-C(16)-O(26)-C(99)	-2.134	-3.900	-2.122	-1.719
C(20)-C(16)-O(26)-C(99)	177.778	176.081	178.545	178.258
O(2)-C(1)-N(3)-C(13)	-3.800	-3.341	-2.852	-3.389
C(13)-N(3)-C(1)-C(5)	176.929	177.508	177.825	177.462
O(2)-C(1)-N(3)-C(5)	179.269	179.150	179.321	179.147
C(6)-C(8)-O(23)-C(75)	5.357	-1.240	4.536	4.012
C(12)-C(8)-O(23)-C(75)	-175.357	178.023	-174.674	-176.550
C(8)-C(12)-O(22)-C(51)	-95.561	97.128	-68.573	-96.474
C(10)-C(12)-O(22)-C(51)	85.515	-86.082	116.471	85.043
C(12)-C(10)-O(21)-C(27)	177.048	-177.168	-40.759	178.258
C(7)-C(10)-O(21)-C(27)	-2.952	2.586	142.952	-1.696