Electronic Supplementary Information

Unprecedented selectivity in molecular recognition of carbohydrates by a metal-organic framework

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Experimental

1. Synthesis and characterization of NU-1000

The NU-1000 MOF was synthesized by following the reported method.[S1] Powder X-ray diffraction (PXRD) data were collected on a Rigaku model ATX-G diffractometer equipped with a Cu rotating anode X-ray source. N_2 sorption isotherm measurements were performed on a Micromeritics Tristar II 3020 (Micromeritics, Norcross, GA) at 77 K. Between 30 and 50 mg of material was used for each measurement. Scanning electron microscopy (SEM) images and energy dispersive spectroscopy (EDX) profiles were collected on a Hitachi SU8030. Samples were activated and coated with OsO_4 to ~8 nm thickness in a Denton Desk III TSC Sputter Coater (Moorestown, NJ) before SEM imaging.

2. Adsorption of carbohydrates on NU-1000

In this adsorption study, four carbohydrates were tested: glucose; cellobiose; maltose; and lactose (Sigma). An aqueous stock solution with high concentration of carbohydrate was initially prepared in a volumetric flask and was used as prepared or after dilution in Milli-Q water (18 MΩ cm). For glucose and cellobiose, 10 mg of NU-1000 was dispersed in 10 mL of the stock solution, and in the case of maltose and lactose, 5 mg of the material was used in 1.5 mL of the stock solution. The suspension was ultrasonicated for 1 min to disperse NU-1000 well, vortexed for at least 90 min at 297 K, and then filtered with a syringeless filter device Mini-UniPrep equipped with a polytetrafluoroethylene membrane (0.2 μm mesh, Whatman). The filtrate was diluted 3–5 times in distilled water. The amount of residual carbohydrate in the filtrate was quantified by high-performance liquid chromatography (HPLC, Shimadzu, Prominence HPLC System, refractive index detector) equipped with an Aminex HPX-87H column (Bio-Rad, ø7.8 × 300 mm, mobile phase: 5 mM H_2SO_4 0.6 mL min^{-1}, column temperature: 323 K). The subtraction of mass of carbohydrate quantified by HPLC from that of carbohydrate charged provided a value of sugar uptake. After the filtration, the solid phase was dried and analyzed by N_2 sorption measurement at 77 K, PXRD measurement, and SEM (*vide supra*) after washing with distilled water three times, washed with acetone three times, and dried in air.

Adsorption isotherms for carbohydrates (Fig. 1) were quantitatively analyzed by the reported method for adsorption process in an aqueous solution.[S2,S3] Type II adsorption follows the BET equation, but the equation can be approximated to be eqn (S1) at low c/c_{sat}.

$$\theta_A \equiv \frac{N_A}{N_C} = CX \qquad \text{(S1)}$$

where N_A and N_C are the adsorption uptake of carbohydrate and the number of pyrene unit in NU-1000, respectively. X is equal to c/c_{sat}. C is given by

$$C = \exp\left(-\frac{\Delta\Delta G_1}{RT}\right) \qquad \text{(S2)}$$

where R is the gas constant and T is the adsorption temperature. $\Delta\Delta G_1$ is defined by eqn (S3).

$$\Delta\Delta G_1 = \left(\Delta G_{\text{desolvation-pyrene}} + \Delta G_{\text{adsorption-sugar-pyrene}}\right) - \left(\Delta G_{\text{desolvation-particle}} + \Delta G_{\text{adsorption-sugar-particle}}\right) \qquad \text{(S3)}$$

In eqn (S3), we reference two different processes: (i) desolvation of water molecules from pyrene unit and sugar molecule in aqueous solution ($\Delta G_{\text{desolvation-pyrene}}$), followed by sugar molecule adsorption on the pyrene unit ($\Delta G_{\text{adsorption-sugar-pyrene}}$) and (ii) desolvation of water molecules from sugar particle and sugar molecule in aqueous solution ($\Delta G_{\text{desolvation-particle}}$), in addition to sugar molecule adsorption on the particle ($\Delta G_{\text{adsorption-sugar-particle}}$). Assuming $\Delta G_{\text{desolvation}}$ is the same for the pyrene unit and particle, it follows that the value of ($\Delta G_{\text{desolvation-pyrene}} - \Delta G_{\text{desolvation-particle}}$) is approximately zero. Accordingly,

$$\Delta\Delta G_1 = \Delta G_{\text{adsorption-sugar-pyrene}} - \Delta G_{\text{adsorption-sugar-particle}} \qquad \text{(S4)}$$

Hence, $\Delta\Delta G_1$ is equal to the Gibbs free energy change in sugar adsorption on the pyrene unit, based on sugar adsorption on the particle as a reference state. Then, from the inset in Fig. 1, the values of $\Delta\Delta G_1$ for cellobiose and lactose have been calculated to be –9.5 and –7.8 kJ mol^{-1}, respectively, indicating that lactose adsorption on NU-1000 is thermodynamically similar to cellobiose adsorption.

3. Density Functional Theory calculations

As a model representing the interaction between each adsorbate and NU-1000, a cluster formed by the adsorbate and the 1,3,6,8-tetrakis(*p*-benzoate)pyrene unit (Fig. S7a) of NU-1000 was considered. The adsorbate molecules are β-glucose (Fig. S7b) and cellobiose (β-anomer, Fig. S7c). Initially, we optimized the structure of the individual adsorbates and pyrene unit separately and then the structure of the supersystems (adsorbate plus pyrene unit, Fig. S8). Four hydrogen atoms were added to the unit to keep an electro-neutrality of the system and only the carbon atoms of carboxylate groups were kept fixed during the geometry optimization of the systems to maintain a rigidity of the MOF structure.

For β-glucose and cellobiose substrate, full geometry optimizations were performed at the PBE-D3,[S4,S5] M06-2X,[S6] and M06-L[S7] levels of theory as implemented in the Gaussian 09 software.[S8] The pyrene unit was obtained from a previously optimized structure using periodic DFT.[S9] The def2-TZVP[S10] basis set functions were used for all the atoms (C, H, and O atoms). Frequency calculations were performed to verify the nature of the stationary points. Gibbs free energies (ΔG) and enthalpies (ΔH) at 298.15 K were computed by adding zero-point vibrational energies, and thermal vibrational-rotational entropy using the quasi-harmonic approximation. Solvation effects were included for all systems using the SMD implicit solvation model with water as a solvent by performing single-point calculations or geometry optimization in the cases this is specified.[S11]

Additionally, single-point calculations with different functionals were performed on the PBE-D3/def2-TZVP gas-phase optimized geometries. The functionals under consideration were the B3LYP-D3,[S5,S12] M06-HF,[S6] PBE0-D3,[S12,S13] PBE-D3, M06-L, and M06-2X, with a basis set including an additional polarization function (def2-TZVPP). The extra polarization functions are important for the accurate description of non-covalent interactions. Solvation effects were applied in all higher-level single-point calculations.

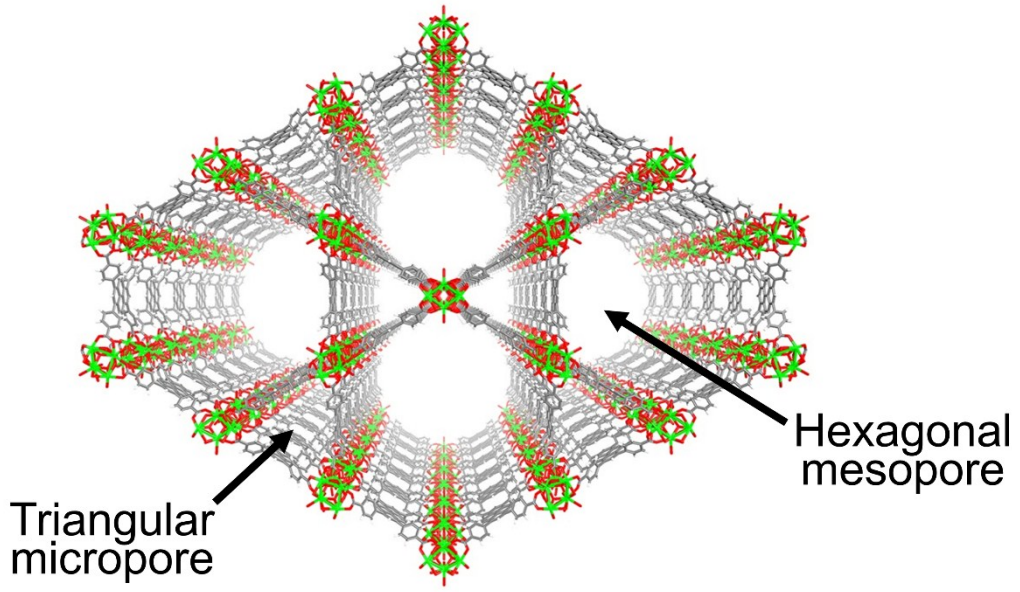

Fig. S1 Pore structure of NU-1000. The pore size distribution is shown in Fig. S3.

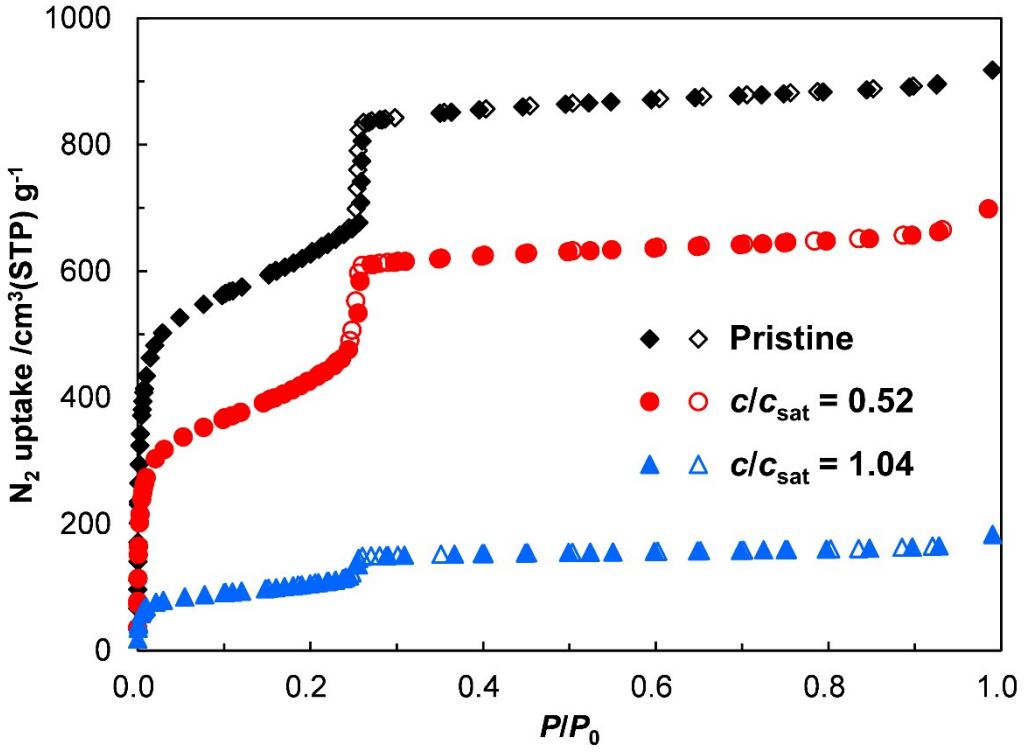

Fig. S2 N_2 physisorption isotherms of NU-1000 before and after cellobiose adsorption, recorded at 77 K. Closed dots = adsorption branch; open dots = desorption branch.

The pore-volume degreases at c/c_{sat} = 0.52 and 1.04 are determined to be 0.36 and 1.13 $cm^3\ g_{NU\text{-}1000}^{-1}$, respectively. These values are close to the volumes that the adsorbed cellobiose possesses if it has a crystalline state density (0.53 $cm^3\ g_{NU\text{-}1000}^{-1}$ at c/c_{sat} = 0.52 and 1.32 $cm^3\ g_{NU\text{-}1000}^{-1}$ at c/c_{sat} = 1.04).[S14]

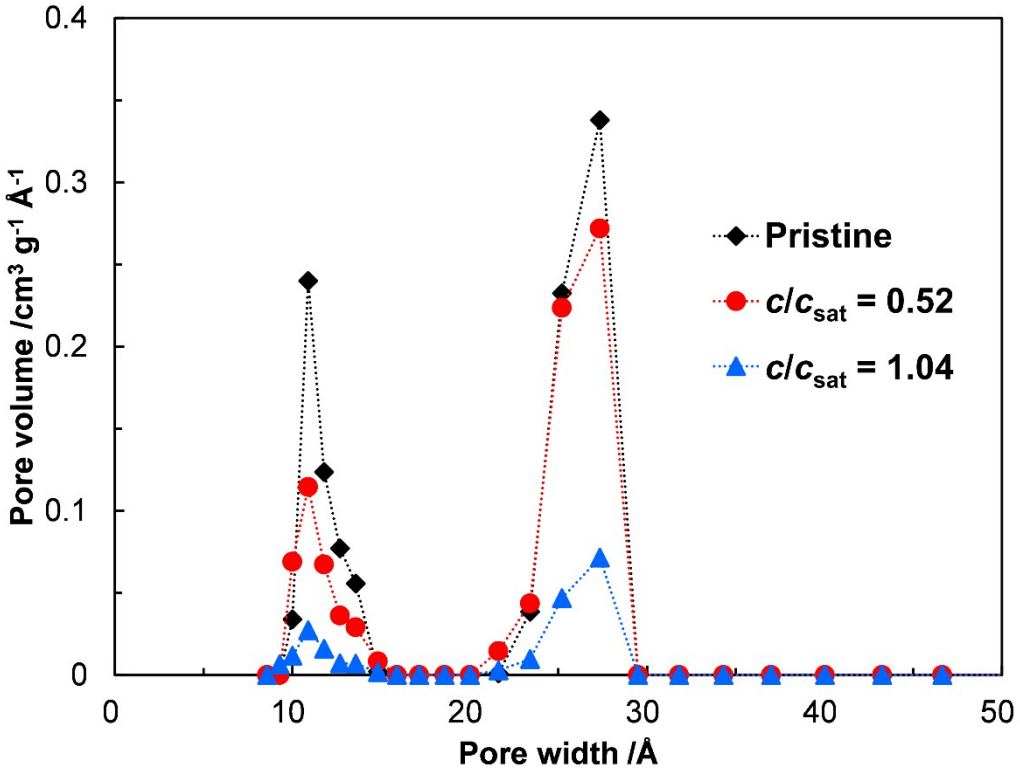

Fig. S3 Pore size distribution of NU-1000 before and after cellobiose adsorption.

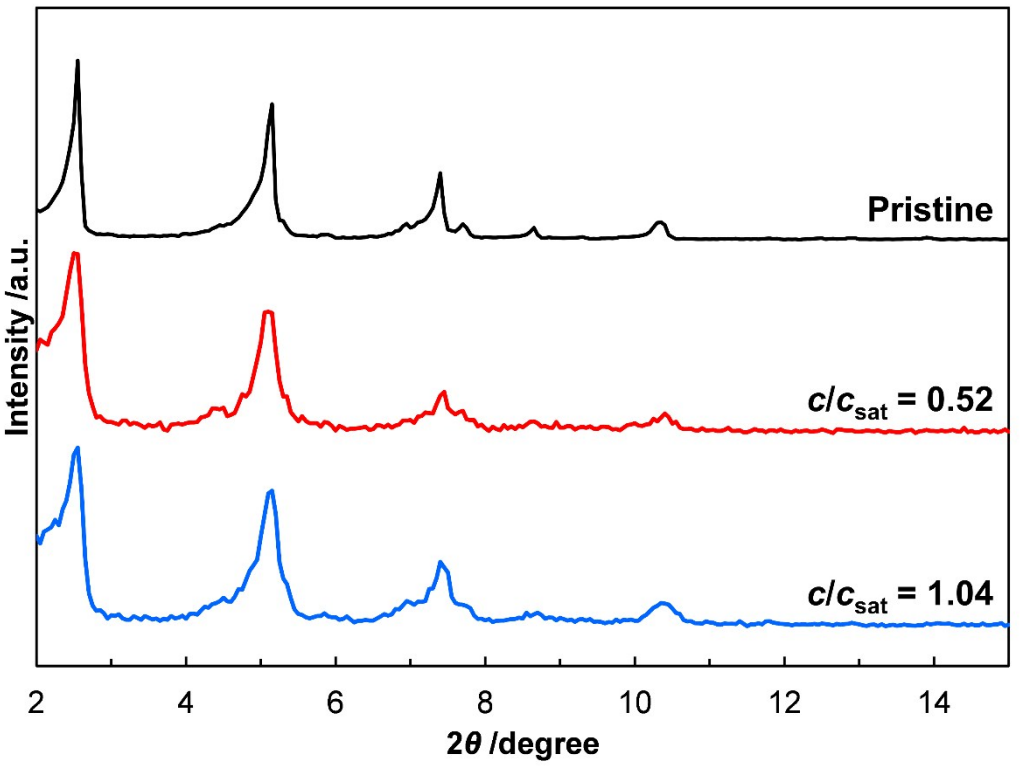

Fig. S4 PXRD patterns of NU-1000 before and after cellobiose adsorption.

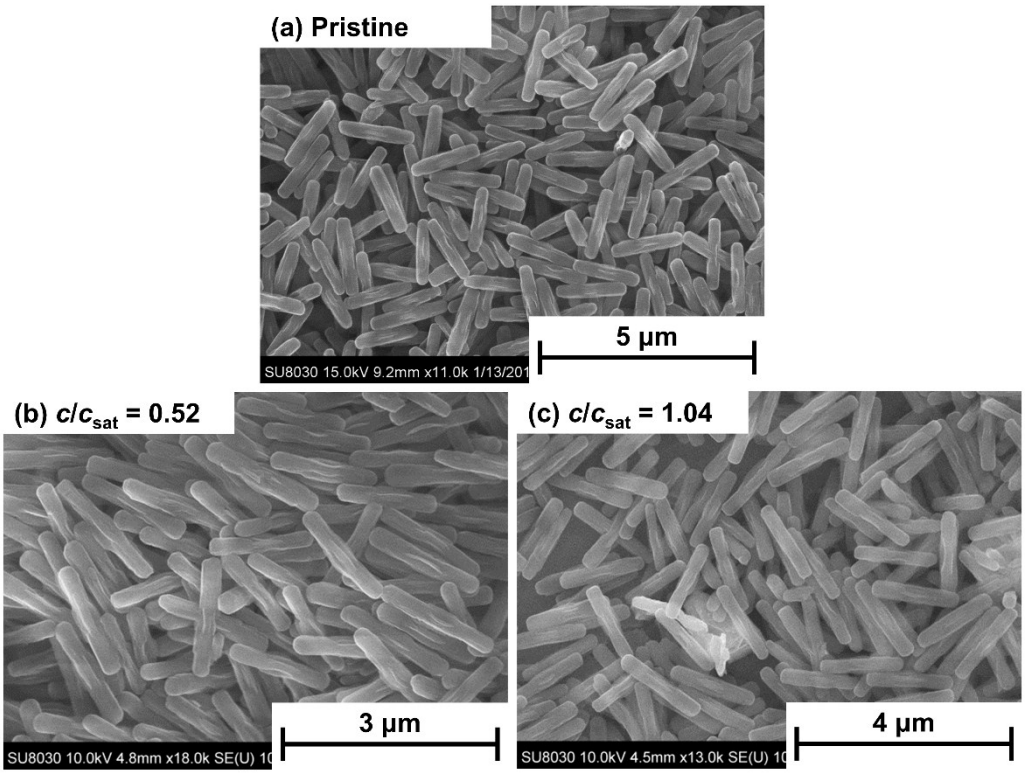

Fig. S5 SEM images of NU-1000 before and after cellobiose adsorption.

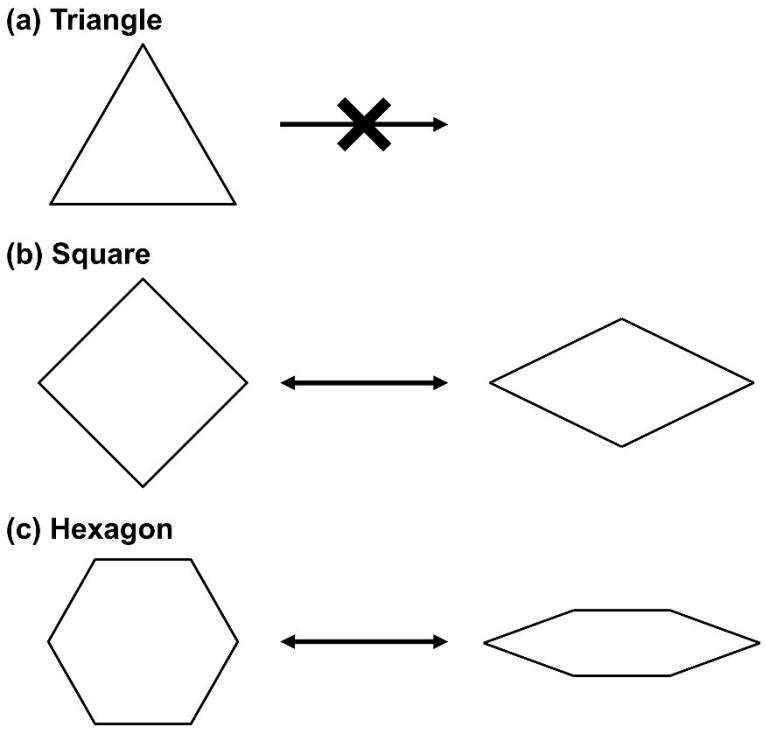

Fig. S6 Geometric deformation of polygons with preserving side-length. In contrast to square and hexagon, triangle cannot be converted to other shape without change of side-length.[S15,S16]

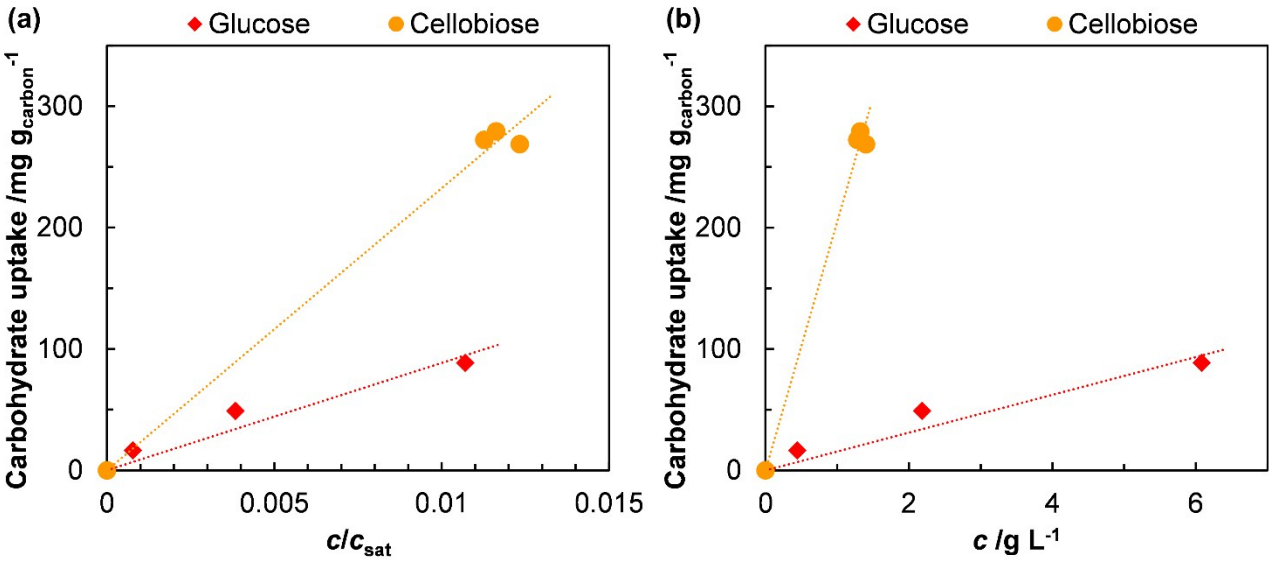

Fig. S7 Adsorption isotherms of glucose and cellobiose on mesoporous carbon nanoparticles at low concentration, based on (a) concentration relative to saturation concentration (c/c_{sat}) and (b) concentration (c, unit: g L^{-1}). Data were taken from previously reported adsorption isotherms.[S17]

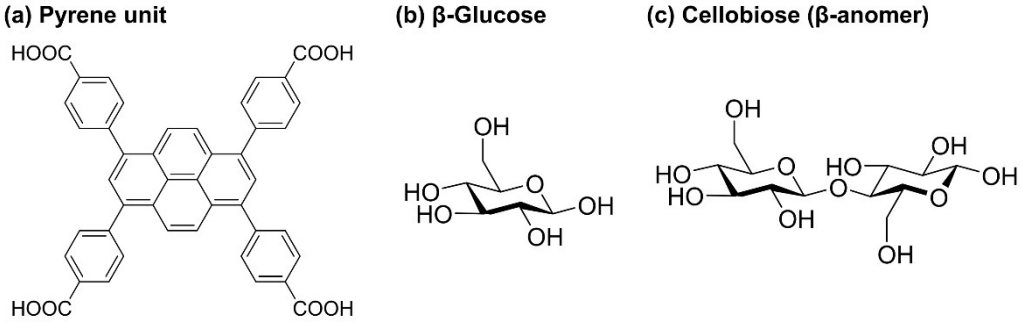

Fig. S8 Subsystem models for DFT calculations.

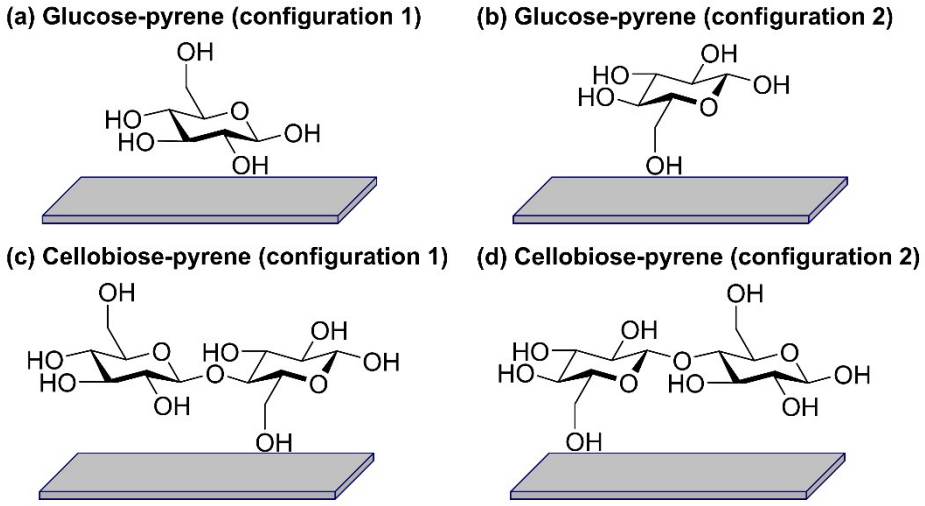

Fig. S9 Supersystem models formed by carbohydrate and pyrene unit for DFT calculations. The grey plates represent the pyrene unit.

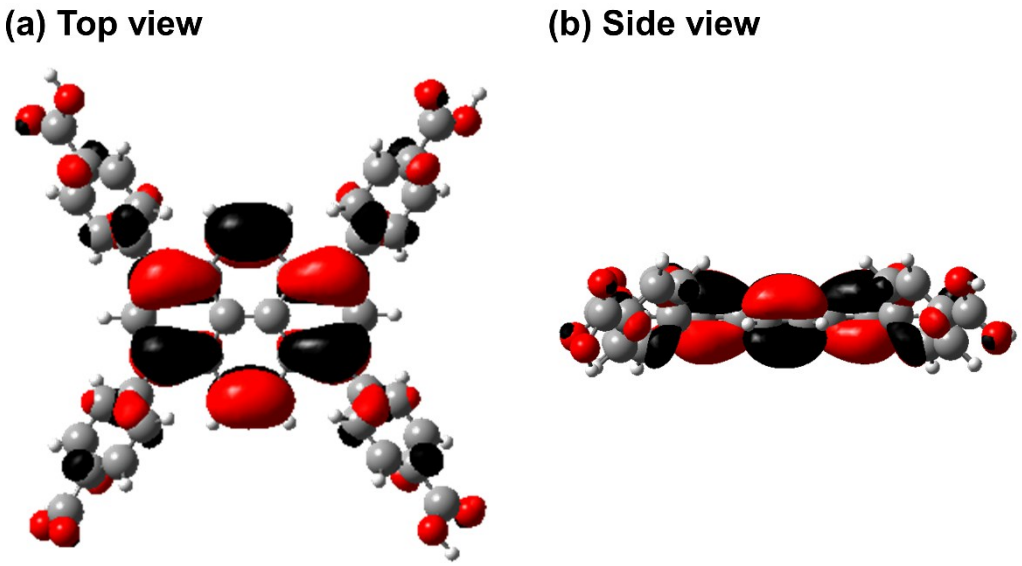

Fig. S10 Highest occupied molecular orbital (HOMO) of pyrene unit, calculated at the PBE-D3 level of theory.

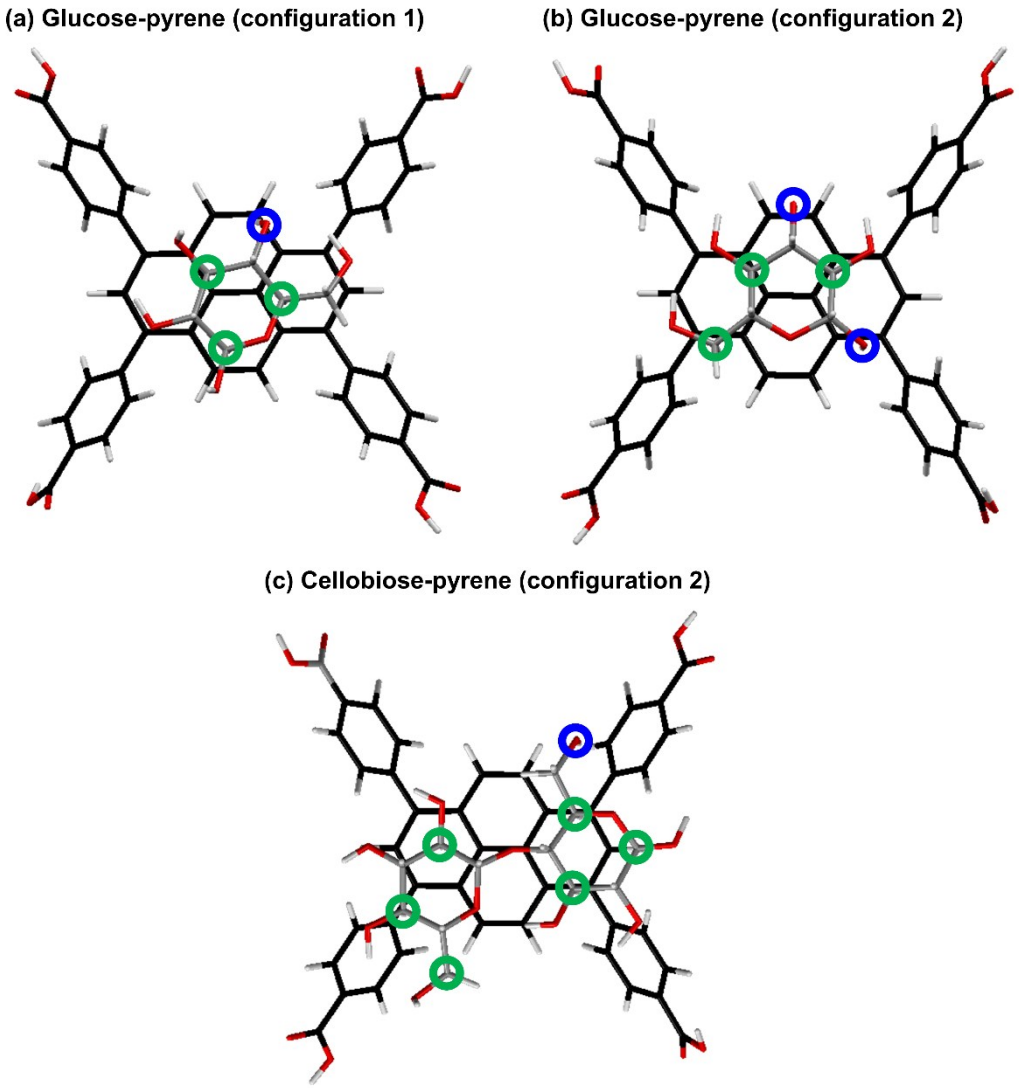

Fig. S11 Optimized geometries of the supersystem models, calculated using the PBE-D3 functional, including solvent effects. The structure of cellobiose-pyrene (configuration 1) is shown in Fig. 3. The green circles represent CH groups facing pyrene unit, and the blue circles highlight OH groups interacting with the unit. Legends: black = carbon atoms of pyrene unit; grey = carbon atoms of carbohydrate; red = oxygen atoms; and white = hydrogen atoms.

Table S1 Calculated binding energies including solvent effects with the def2-TZVP basis set and different density functionals[a]

Functional	Adsorbate	ΔH	ΔG	$\Delta\Delta H^b$	$\Delta\Delta G^b$
PBE-D3	β-Glucose	–14.4	–0.5	–3.3	–2.3
	Cellobiose	–17.7	–2.8		
M06-L	β-Glucose	–12.4	1.7	–5.2	–3.4
	Cellobiose	–17.6	–1.7		
M06-2X	β-Glucose	–14.6	–2.3	–5.9	–3.7
	Cellobiose	–20.5	–6.0		

[a] Both ΔH and ΔG values (unit: kcal mol^{-1}) shown here are the averaged energy of configuration 1 and configuration 2 (see Fig. S9). [b] Difference between cellobiose and β-glucose.

Table S2 Single-point binding energy calculations with different density functionals, using the def2-TZVPP basis set and solvent effects[a]

Functional	Adsorbate	ΔH	ΔG	$\Delta\Delta H^b$	$\Delta\Delta G^b$
PBE-D3	β-Glucose	–14.3	–0.4	–6.5	–4.8
(0% HF)	Cellobiose	–20.8	–5.1		
M06-L	β-Glucose	–9.9	4.0	–6.9	–5.2
(0% HF)	Cellobiose	–16.8	–1.1		
B3LYP-D3	β-Glucose	–15.5	–1.6	–6.4	–4.7
(20% HF)	Cellobiose	–22.0	–6.3		
PBE0-D3	β-Glucose	–13.5	0.4	–6.5	–4.7
(25% HF)	Cellobiose	–20.0	–4.3		
M06-2X	β-Glucose	–9.3	4.7	–4.2	–2.4
(54% HF)	Cellobiose	–13.4	2.2		
M06-HF	β-Glucose	–8.7	5.2	–2.5	–0.7
(100% HF)	Cellobiose	–11.2	4.4		

[a] Both ΔH and ΔG values (unit: kcal mol^{-1}) shown here are the averaged energy of configuration 1 and configuration 2 (see Fig. S9). [b] Difference between cellobiose and β-glucose.

To investigate the DFT functional sensitivity of the interaction between carbohydrates and the pyrene unit, we performed single point calculations at the PBE-D3/def2-TZVP gas phase optimized geometries. Six different functionals, namely B3LYP-D3, M06-2X, M06-HF, M06-L, PBE0-D3, and PBE-D3, with the def2-TZVPP basis set for all atoms were tested including solvent effects. The calculated energies are shown in Table S2. The three functionals with the empirical D3 correction (PBE-D3, PBE0-D3, and B3LYP-D3) predict ΔG from 0.4 to −1.6 kcal mol^{-1} for β-glucose, and from –4.3 to –6.3 kcal mol^{-1} for cellobiose. These functionals containing dispersion correction have shown to describe correctly dispersive effects for similar systems.[S18,S19] The corresponding values from the M06-L, M06-2X, and M06-HF functionals are significantly higher. Overall, the relative energy differences ($\Delta\Delta G$, Table S2) between cellobiose and glucose for functionals with 0 to 25% Hartee-Fock (HF) exchange is on average ~4.9 kcal/mol. On the other hand, larger HF percentage underestimates $\Delta\Delta G$ (–2.4 kcal mol^{-1} for M06-2X and –0.7 kcal mol^{-1} for M06-HF). Thus, functionals with a higher contribution of HF exchange underestimate the binding energies of cellobiose, resulting in small differences in the monomer and dimer binding energies.

Computational results (shown in unit of Ångström)

1. Glucose (PBE-D3)

Number of atoms = 24

SCF(SCRF) = -686.73857373

C	-1.67744500	0.12813700	0.19977500	H	-0.63444600	1.24663900	-1.30229300
C	-0.64800300	1.19452800	-0.19652100	O	-1.07830800	2.49770800	0.21374900
C	0.74067200	0.80628700	0.29714400	H	-0.86807500	2.59944900	1.16010700
C	1.07695800	-0.60920200	-0.21995200	H	0.74236100	0.76293900	1.40224800
O	0.07767800	-1.52655900	0.22839100	O	1.74257100	1.77735100	-0.03951800
C	2.42597300	-1.12196700	0.29052400	H	1.54952400	2.11665100	-0.93205800
C	-1.22796200	-1.25128500	-0.30296600	H	1.11382400	-0.58626000	-1.33084000
O	-2.07948900	-2.28455700	0.06027000	H	-2.27107800	-2.20247400	1.01260600
H	-1.19370000	-1.25572400	-1.40999200	H	2.51672800	-2.18389700	0.02060900
H	-1.71288200	0.07310500	1.31283800	H	2.43943100	-1.05534700	1.39741400
O	-2.95196200	0.43808600	-0.33449400	O	3.52463700	-0.44064300	-0.29822100
H	-3.06065700	1.40188800	-0.21790400	H	3.35678000	0.51295800	-0.16217400

2. Cellobiose (PBE-D3)

Number of atoms = 45

SCF(SCRF) = -1297.09422060

C	-1.80878500	-1.24765200	0.35231800	O	-3.27554300	3.49496100	-0.00045900
C	-3.17635000	-1.70905200	-0.15175300	H	-2.98731000	3.76025500	0.88898400
C	-4.22151600	-0.63684300	0.14316600	O	-0.87205200	-2.24381100	-0.05711300
C	-2.60557100	1.12727300	0.13228700	H	0.01724200	-1.93841800	0.23027300
C	-1.44936500	0.15271800	-0.14423200	O	-0.28988600	0.65400100	0.55856400
H	-3.13547400	-1.82827400	-1.25278200	C	0.93765300	0.50542700	-0.05390900
H	-1.85550400	-1.19905600	1.46018600	C	1.87710300	1.61559700	0.41235400
H	-2.71146600	1.22869000	1.23481200	C	3.26883400	1.37422100	-0.16146300
H	-1.24007800	0.12151200	-1.22972000	C	3.78856200	-0.01775200	0.17314100
H	-4.32829300	-0.50377000	1.24413700	C	2.75488300	-1.06921900	-0.26316300
O	-3.54894900	-2.92491700	0.48405800	H	0.84223100	0.52189900	-1.16084700
H	-2.76453600	-3.50150500	0.42588800	H	3.20482900	1.45201000	-1.26716000
O	-5.42299000	-1.00377700	-0.45571200	H	3.92240600	-0.09476800	1.27158800
H	-6.07840200	-0.31730000	-0.23809600	H	2.66737700	-1.04177800	-1.37057000
O	-3.80334800	0.60581100	-0.43646300	H	1.92176700	1.57857500	1.51821500
C	-2.35886800	2.50689800	-0.47097800	O	1.35041800	2.85790400	-0.03931800
H	-1.31120700	2.79875000	-0.28642000	H	2.07141500	3.50717100	0.05995600
H	-2.51595700	2.43737100	-1.55854600	O	4.11519800	2.40386700	0.35011900

H	5.00968400	2.22540600	0.00699700	H	3.19403400	-2.50053300	1.28859000
O	5.03526600	-0.15832100	-0.50527000	O	4.39799200	-2.90565800	-0.30394300
H	5.30870900	-1.09128700	-0.38582600	H	4.29581600	-3.13947900	-1.24292200
C	3.11778000	-2.48507200	0.19140400	O	1.48972900	-0.77842800	0.34456500
H	2.31987400	-3.18779300	-0.10399700				

3. Pyrene unit (PBE-D3)

Number of atoms = 78

SCF(SCRF) = -2292.50627135

C	2.82737400	-1.24851700	-0.07084900	C	-3.69145800	-2.44871500	-0.03202400
C	-2.88371100	-1.20408000	-0.07156500	C	3.66184900	2.44850000	-0.04903800
C	2.84676800	1.20897900	-0.08429800	C	-3.65238600	2.50965700	-0.00704500
C	-2.86462100	1.25320700	-0.06336800	C	4.64915300	-2.73678200	-0.94461400
C	1.40598500	-1.25044600	-0.08622100	C	-4.71451600	-2.66474100	-0.97127200
C	-1.46221500	-1.22885200	-0.08633100	C	4.68823000	2.64946000	-0.98989100
C	1.42537400	1.23324200	-0.09401500	C	-4.67564800	2.75504400	-0.94177900
C	-1.44297600	1.25480700	-0.08421400	C	0.64549500	-2.45769200	-0.18319100
C	5.40641400	-3.90255100	-0.89501000	C	-0.71969700	-2.44739500	-0.18458400
C	-5.47210900	-3.83482500	-0.95110100	C	0.68279300	2.45149800	-0.19255200
C	5.47270100	3.79999100	-0.96482800	C	-0.68243300	2.46191500	-0.18662200
C	-5.41788500	3.93108700	-0.89897800	C	3.50618000	-0.02524300	-0.09126100
C	5.16280300	-4.86555300	0.09553800	C	-3.54411600	0.02981700	-0.07858300
C	-5.24104300	-4.82267700	0.01894300	C	0.69927400	-0.00315700	-0.07938800
C	5.25476800	4.78193900	0.01366900	C	-0.73607700	0.00755600	-0.07698100
C	-5.16521400	4.89490000	0.08860100	H	6.19316300	-4.09379100	-1.62609300
C	5.99271800	-6.10135700	0.09589100	H	-6.27012400	-3.94718300	-1.69075900
C	-6.01194600	-6.10953500	0.09980400	H	6.25364100	3.94621400	-1.71079900
C	6.05198700	6.03741200	0.08457400	H	-6.19830600	4.13049000	-1.63467400
C	-5.97429200	6.14506600	0.07797700	H	3.96877500	-5.36732500	1.82575700
C	4.15286300	-4.63269200	1.04209400	H	-4.10019600	-5.34438900	1.76139600
C	-4.25119000	-4.59161100	0.98648600	H	4.09596300	5.34418600	1.73520700
C	4.24599300	4.58273900	0.96856800	H	-3.97295500	5.38500100	1.82346900
C	-4.16374900	4.65046700	1.04131400	H	2.62206000	-3.28766500	1.73542500
C	3.39401700	-3.46712600	0.98519700	H	-2.72206100	-3.26771000	1.71863100
C	-3.48560300	-3.43133400	0.95626100	H	2.69270300	3.28283500	1.69553200
C	3.46233600	3.43461100	0.93688400	H	-2.65243100	3.28850800	1.74413400
C	-3.41995800	3.47490800	0.99105900	H	4.83460700	-2.00181200	-1.73029300
C	3.62013100	-2.50119500	-0.01356100	H	-4.90217200	-1.91151900	-1.73877000

H	4.85275500	1.89905500	-1.76560000	O	7.00445700	6.11486300	-0.89151100
H	-4.86667000	2.02090100	-1.72695000	O	-6.84883700	6.40332400	-0.72944800
H	-1.21094800	3.40881100	-0.29385500	O	5.66176400	-6.96024000	1.10519600
H	1.22482000	3.39017100	-0.30514100	O	-6.07035500	-6.79288000	1.09766000
H	-1.26085200	-3.38699700	-0.29311400	O	5.89458600	6.91829100	0.91090800
H	1.17400600	-3.40471600	-0.28993700	O	-5.63523600	7.00265900	1.08553200
H	4.59745100	-0.03365300	-0.04959500	H	7.45605800	6.97118100	-0.74494000
H	-4.63532400	0.03899300	-0.03229200	H	-6.22574500	7.77610200	0.97683100
O	6.87708100	-6.34839300	-0.70438300	H	-6.42988000	-5.90949200	-1.77002400
O	-6.66830400	-6.50346400	-1.03340200	H	6.26623100	-7.72382800	1.00386000

4. Glucose-pyrene (configuration 1) (PBE-D3)

Number of atoms = 102

SCF(SCRF) = -2979.26939278

C	2.69034000	-1.34289200	-0.95724400	C	3.10271200	-3.59363300	0.10851500
C	-3.00384600	-0.96501000	-0.94027900	C	-3.70688200	-3.12876400	0.14670200
C	2.85817600	1.11028100	-0.89439400	C	3.61316800	3.27057800	0.19285600
C	-2.84513800	1.48646600	-0.85284300	C	-3.31028100	3.65389900	0.35345700
C	1.27231500	-1.25910300	-1.02446300	C	3.40421400	-2.64424700	-0.88683700
C	-1.58890800	-1.06844700	-1.01451400	C	-3.87504400	-2.16674000	-0.86875800
C	1.44124700	1.21899400	-0.92666200	C	3.74903300	2.29666500	-0.81525500
C	-1.42746200	1.40780600	-0.90767700	C	-3.55590200	2.78687300	-0.72830400
C	5.12338500	-4.14871100	-1.73355600	C	4.43546100	-2.94071600	-1.79753100
C	-5.74362500	-3.47136300	-1.72702600	C	-4.91938700	-2.34817400	-1.79087500
C	5.64328400	3.55550600	-1.69837800	C	4.78863700	2.45633400	-1.74958700
C	-5.17944800	4.38727500	-1.58602500	C	-4.51356500	3.16879900	-1.68577100
C	4.80785900	-5.09561300	-0.74750900	C	0.44219800	-2.41617100	-1.16121300
C	-5.55820400	-4.44019700	-0.72792400	C	-0.92075700	-2.32558800	-1.15580400
C	5.48529600	4.52805700	-0.69917400	C	0.76736100	2.48355400	-0.93977300
C	-4.91452300	5.25685300	-0.51731500	C	-0.59716700	2.57288900	-0.92618900
C	5.57030500	-6.37873900	-0.73295600	C	3.44048800	-0.16252800	-0.91982000
C	-6.41256500	-5.67032400	-0.59456100	C	-3.59305400	0.30369800	-0.89053300
C	6.35558600	5.73390900	-0.60022100	C	0.64129600	0.02847800	-0.98681400
C	-5.64204000	6.55935500	-0.47071000	C	-0.79220200	0.12335000	-0.98260900
C	3.79452400	-4.80138100	0.17935500	H	5.91197900	-4.38404500	-2.44967200
C	-4.54149000	-4.23966700	0.21866500	H	-6.55846200	-3.55803100	-2.45163600
C	4.46548900	4.36760000	0.25063400	H	6.43337900	3.66807100	-2.44056400
C	-3.98013700	4.87181500	0.45804200	H	-5.90840600	4.69180200	-2.33836000

H	3.55217300	-5.52126200	0.96091600	H	-5.83252400	8.13386200	0.53742000
H	-4.42309800	-4.97401400	1.01653000	H	-6.81082700	-5.52101100	-2.47251800
H	4.36096700	5.11684200	1.03654700	H	5.73777700	-8.01127800	0.18289100
H	-3.78184200	5.53096900	1.30317800	C	-1.40678700	-0.74680600	3.08793200
H	2.32992500	-3.37185000	0.84792000	C	-0.86731200	0.60350200	2.60763800
H	-2.93953900	-2.97766200	0.90726100	C	0.57896100	0.81061300	3.04498100
H	2.84081000	3.15655200	0.95409200	C	1.42588300	-0.41654100	2.63622100
H	-2.60285300	3.35247800	1.12945500	O	0.83406300	-1.61935900	3.14036900
H	4.68038800	-2.21784100	-2.57817700	C	2.85508200	-0.36497200	3.18006000
H	-5.07565400	-1.60576700	-2.57601100	C	-0.47254800	-1.86190400	2.60140000
H	4.90967500	1.71443600	-2.54132000	O	-0.88116800	-3.14008900	2.96635100
H	-4.71461600	2.50781400	-2.53121600	H	-0.42970200	-1.86327700	1.49642200
H	-1.07067700	3.55415600	-0.95195900	H	-1.39806300	-0.76835000	4.20169400
H	1.36265100	3.39528900	-0.98741200	O	-2.71564500	-0.97242900	2.58894800
H	-1.52005900	-3.22894700	-1.26673300	H	-3.16731300	-0.10652900	2.60807400
H	0.91587200	-3.39045300	-1.27934100	H	-0.90122500	0.59085400	1.50480500
H	4.52582300	-0.23775900	-0.83220800	O	-1.75183500	1.67224700	2.97204800
H	-4.68025500	0.37166900	-0.81031300	H	-1.58879700	1.89614700	3.90657700
O	6.45143300	-6.67479400	-1.51956100	H	0.62625100	0.90828100	4.14583800
O	-7.09204400	-6.06681500	-1.71399000	O	1.12313400	2.03513600	2.52997500
O	7.31703300	5.77177900	-1.56941600	H	0.82056800	2.13147800	1.60423400
O	-6.45511400	6.93367600	-1.29613300	H	1.47586500	-0.45118300	1.53011300
O	5.17604000	-7.21423100	0.27209200	H	-1.09422600	-3.13583800	3.91782200
O	-6.51827300	-6.30555400	0.43050600	H	3.33666200	-1.33176300	2.97198800
O	6.24406100	6.60731700	0.24102200	H	2.81726200	-0.23904600	4.28117700
O	-5.30043100	7.31540800	0.61390800	O	3.64615700	0.63876000	2.55925700
H	7.81852800	6.59651000	-1.40491100	H	3.11814600	1.46075900	2.58028600

5. Glucose-pyrene (configuration 2) (PBE-D3)

Number of atoms = 102

SCF(SCRF) = -2979.27055985

C	-2.84474200	-1.13528400	-0.90051000	C	1.54893600	1.14621000	-1.01225900
C	2.85615300	-1.37807200	-0.82786000	C	-5.40616100	-3.68523000	0.24643300
C	-2.73805400	1.31948100	-0.91933600	C	5.18152600	-4.12432000	0.38175400
C	2.96259200	1.07686400	-0.88712400	C	-5.05632200	4.05917500	0.30160600
C	-1.42707100	-1.21025900	-0.98202500	C	5.43925100	3.66781200	0.34690800
C	1.43731300	-1.33502900	-0.93725600	C	-5.36081800	-4.63170800	-0.78824400
C	-1.32244900	1.27078900	-1.02717100	C	5.02122100	-5.11101400	-0.60307500

C	-4.95501000	5.01116900	-0.72472300	H	-2.98799800	-3.14592500	-2.73877500
C	5.44335100	4.59861100	-0.70320700	H	2.80258300	-3.45850300	-2.60383600
C	-6.25372100	-5.82338400	-0.69838200	H	-2.76649900	3.35717900	-2.75539600
C	5.73463700	-6.43623600	-0.58312800	H	3.20976000	3.05108100	-2.76822200
C	-5.70140400	6.30280600	-0.70411700	H	-4.61551900	-1.84535800	1.04191400
C	6.31427300	5.80456700	-0.57830000	H	4.62444400	-2.16557300	1.08407500
C	-4.48094200	-4.42753600	-1.86307200	H	-4.40482800	2.13888900	1.03866200
C	4.16827100	-4.84416900	-1.68531300	H	4.62048700	1.82255400	1.11380500
C	-4.12149700	4.74611400	-1.82199100	H	1.42611700	3.32035900	-0.96390700
C	4.63233800	4.36503600	-1.82504000	H	-1.01137500	3.42581500	-0.96383400
C	-3.66074500	-3.30244800	-1.89336600	H	1.12176100	-3.48001700	-0.73917500
C	3.46281800	-3.64778200	-1.75556200	H	-1.31052000	-3.37248400	-0.78831200
C	-3.39687400	3.56018900	-1.88763900	H	-4.54438500	0.16752800	-0.76100400
C	3.82675100	3.22989900	-1.88548600	H	4.66090800	-0.22035400	-0.68730900
C	-3.70061700	-2.34996800	-0.85850000	O	-7.03463100	-6.04292600	0.20926700
C	3.60172200	-2.66302100	-0.75813100	O	6.21117500	-6.85689300	0.62595500
C	-3.48590300	2.60188800	-0.86032500	O	-6.47992000	6.44304600	0.40784600
C	3.81102400	2.29658600	-0.83310900	O	7.02946400	6.05058900	0.37543500
C	-4.59166700	-2.55601500	0.21157600	O	-6.11013000	-6.67122300	-1.75979000
C	4.49078600	-2.91500600	0.30096200	O	5.89407800	-7.12180100	-1.56803100
C	-4.33320100	2.86973600	0.23028000	O	-5.63985500	7.15549700	-1.57093800
C	4.63791300	2.53042000	0.28186800	O	6.23062300	6.62919400	-1.66307700
C	-0.73099100	-2.45559100	-0.89220800	H	-6.91576800	7.31484300	0.31343900
C	0.63185000	-2.51515200	-0.86596500	H	6.83643800	7.37414700	-1.47085500
C	-0.51768900	2.45487200	-1.00980900	H	5.90275300	-6.25250200	1.32750600
C	0.84926900	2.39614100	-1.00692800	H	-6.73736600	-7.40419400	-1.59208500
C	-3.45614600	0.12095500	-0.83548600	C	1.45303500	0.57487500	2.56679900
C	3.57350700	-0.17659800	-0.77506700	C	0.23958300	1.42676800	2.92995300
C	-0.65796900	-0.00132500	-1.03851600	C	-1.05276200	0.69790900	2.58936300
C	0.77711200	-0.06359100	-1.02341700	C	-1.06955800	-0.67869600	3.26666300
H	-6.08525200	-3.85629200	1.08285300	O	0.09274500	-1.40742000	2.85954400
H	5.87225900	-4.26797100	1.21731200	C	-2.26144000	-1.53522600	2.83143500
H	-5.70083000	4.25585600	1.15822000	C	1.34778800	-0.81293100	3.21697300
H	6.07077600	3.85863000	1.21585500	O	2.35351700	-1.68277200	2.80193200
H	-4.44540500	-5.15187500	-2.67654700	H	1.44253900	-0.72812600	4.31645600
H	4.07376800	-5.59828200	-2.46783500	H	1.44919800	0.40950800	1.47001900
H	-4.06094900	5.48598400	-2.62137800	O	2.66445700	1.20291700	2.96962800
H	4.63868400	5.07477100	-2.65206700	H	2.53779400	2.15700700	2.80381500

H	0.25661700	1.63858200	4.01301600	H	-1.08708000	-0.53998400	4.36714200
O	0.29557200	2.72211700	2.30689400	H	2.29720200	-1.74306100	1.82800700
H	0.30215200	2.58626200	1.33451200	H	-2.18945800	-2.51827000	3.31932500
H	-1.09561800	0.53175500	1.49601300	H	-2.17317900	-1.69742700	1.74015100
O	-2.19291200	1.45946900	3.01109100	O	-3.52488100	-0.97693300	3.17813500
H	-2.03080900	2.38067000	2.73058400	H	-3.45341100	-0.00777700	3.06117000

6. Cellobiose-pyrene (configuration 1) (PBE-D3)

Number of atoms = 123

SCF(SCRF) = -3589.63670523

C	-1.86042600	1.27198800	-1.59874400	C	-2.65801900	2.52299300	-1.55572700
C	3.81461100	1.20286200	-0.95580200	C	4.60362600	2.44731700	-0.76286200
C	-1.88336600	-1.19323400	-1.65951600	C	-2.70641000	-2.42972800	-1.67662500
C	3.78464600	-1.25386200	-0.95901200	C	4.54333600	-2.51719300	-0.76961700
C	-0.43989400	1.26923600	-1.49659700	C	-3.71010100	2.73866200	-2.46935100
C	2.41177900	1.23121900	-1.17610100	C	5.72790100	2.70863400	-1.56458200
C	-0.46370700	-1.21900100	-1.54880800	C	-3.73501900	-2.59670100	-2.62391200
C	2.38281200	-1.24801300	-1.19087200	C	5.67418100	-2.79454100	-1.56088300
C	-4.47404300	3.90234000	-2.43044100	C	0.33558500	2.47111800	-1.50995400
C	6.47581400	3.87333800	-1.39382800	C	1.69269000	2.45326000	-1.35814800
C	-4.53695700	-3.73631000	-2.62721400	C	0.28765700	-2.43542800	-1.59396800
C	6.39169200	-3.97554300	-1.39667300	C	1.64218900	-2.44947400	-1.41496100
C	-4.21437800	4.89607000	-1.47078100	C	-2.53453200	0.04689100	-1.69993200
C	6.13172700	4.80767100	-0.40362400	C	4.46435000	-0.03356700	-0.87406000
C	-4.33714400	-4.74688000	-1.67257100	C	0.25909500	0.01701900	-1.44089200
C	6.00575400	-4.91242200	-0.42558900	C	1.68537700	-0.00002000	-1.27265700
C	-5.03970000	6.14217600	-1.49522300	H	-5.27363900	4.07228300	-3.15302900
C	6.89060400	6.08326500	-0.16255200	H	7.35565100	4.02023600	-2.02719700
C	-5.15261000	-5.99544000	-1.63000800	H	-5.31781800	-3.85142900	-3.37877700
C	6.79980200	-6.17021300	-0.30649200	H	7.25645700	-4.19894800	-2.02310900
C	-3.18389500	4.68045800	-0.53820200	H	-2.98521000	5.43205700	0.22613300
C	5.03559300	4.52683900	0.42685000	H	4.79381500	5.23193800	1.22331800
C	-3.32737400	-4.58122000	-0.71293300	H	-3.18713900	-5.35927600	0.03897200
C	4.89431700	-4.63197100	0.38649500	H	4.59323500	-5.34243300	1.15627700
C	-2.42389700	3.51264500	-0.57762800	H	-1.65456200	3.34115800	0.17833100
C	4.27752000	3.37372800	0.24768300	H	3.44823600	3.16843100	0.92646500
C	-2.52709100	-3.44396400	-0.71479000	H	-1.77865700	-3.31934100	0.06711200
C	4.17226700	-3.45130100	0.21744000	H	3.32531900	-3.24213400	0.87521800

H	-3.90987700	1.99020000	-3.23836700	O	3.62122200	0.86977600	2.35030800
H	6.00786800	1.99488100	-2.34192300	H	4.23882900	0.18599600	2.66493200
H	-3.88999100	-1.82787300	-3.38346100	O	1.97596400	-0.71467600	2.32598100
H	5.97215900	-2.08175600	-2.33251400	C	0.47618000	-2.56735900	2.23945200
H	2.17936300	-3.39681300	-1.45905000	H	-0.54573900	-2.88849800	2.50377800
H	-0.23579300	-3.37088900	-1.78814500	H	0.54923300	-2.50642100	1.14336600
H	2.24880400	3.39022400	-1.38626000	O	1.45998700	-3.52333300	2.63730300
H	-0.16912000	3.42315000	-1.66902700	H	1.31752300	-3.72821900	3.57685900
H	-3.62657700	0.05380000	-1.74228000	O	-0.92479800	2.20990400	2.26269500
H	5.53605900	-0.04663300	-0.66394300	H	-1.84673700	1.90206400	2.43287400
O	-5.93562900	6.36442700	-2.28824200	O	-1.62858900	-0.62024100	2.96734800
O	7.67329300	6.53246000	-1.19159500	C	-2.74846500	-0.50115900	2.16358400
O	-6.09444300	-6.04420400	-2.61781500	C	-3.79192800	-1.55570600	2.51990600
O	7.76447900	-6.45491800	-0.99354000	C	-4.96653000	-1.37332500	1.56166800
O	-4.68201300	7.02492500	-0.51959100	C	-5.53381400	0.03970700	1.63448800
O	6.83649500	6.71256200	0.87028500	C	-4.41384700	1.08251500	1.47498500
O	-5.01619100	-6.88946600	-0.81458200	H	-2.47391100	-0.58417400	1.09162100
O	6.33149300	-6.99976500	0.67228000	H	-4.59676000	-1.54099500	0.52926000
H	-6.55906900	-6.89685200	-2.49152000	H	-6.00336300	0.17404300	2.63081900
H	6.92289600	-7.77991400	0.65411200	H	-4.04227600	1.04354400	0.43228100
H	7.51932400	5.97721800	-1.97920900	H	-4.12269400	-1.38018700	3.56185700
H	-5.28112800	7.79228600	-0.62588500	O	-3.21393700	-2.84795700	2.38234300
C	-0.04051500	1.23226700	2.81182600	H	-3.96251300	-3.46194100	2.25576600
C	1.36566000	1.61479200	2.35914300	O	-5.93747400	-2.36636700	1.89348400
C	2.35771700	0.56337700	2.84863700	H	-6.67013100	-2.26727700	1.25927000
C	0.71622100	-1.17439400	2.81212900	O	-6.50459800	0.14939400	0.59476600
C	-0.38441200	-0.19195200	2.37647800	H	-6.73435300	1.10082400	0.53085100
H	1.39558500	1.59845500	1.25363700	C	-4.89798000	2.50027600	1.78234700
H	-0.07755000	1.26795500	3.92023400	H	-4.04133200	3.19389900	1.78147700
H	0.72672700	-1.22346600	3.92324200	H	-5.35698000	2.52367400	2.78227400
H	-0.47028000	-0.21942100	1.27470800	O	-5.90846700	2.91972400	0.85640600
H	2.35249000	0.51710600	3.96132700	H	-5.46340400	3.22942800	0.04450400
O	1.73200100	2.89817500	2.85536400	O	-3.33601900	0.80840500	2.38563200
H	0.94694600	3.46296000	2.72630900				

7. Cellobiose-pyrene (configuration 2) (PBE-D3)

Number of atoms = 123

SCF(SCRF) = -3589.63540577

C	-3.11486000	-0.35166400	-1.36985500	C	-0.26710100	2.82797700	-1.04831800
C	2.49228900	-1.44737400	-1.48632900	C	1.07155600	2.56809000	-1.10135400
C	-2.63464700	2.05253900	-1.18039000	C	-3.52865000	0.98084900	-1.25436100
C	2.96481500	0.95973700	-1.35931100	C	3.38727800	-0.37302400	-1.43078200
C	-1.72043600	-0.64092300	-1.37137900	C	-0.77707800	0.43913500	-1.32524100
C	1.09586100	-1.18783700	-1.42974000	C	0.63060200	0.16509800	-1.35978800
C	-1.23818900	1.79188500	-1.21105700	H	-7.07808800	-2.40011400	0.01010900
C	1.57266500	1.24373100	-1.30279000	H	5.23617700	-4.93050700	-0.11503200
C	-6.23213300	-2.39440500	-0.67861400	H	-5.34613200	5.23137600	0.87802800
C	4.48954900	-4.60639400	-0.84618400	H	6.77373800	3.02659900	0.39415200
C	-4.64426700	5.00700400	0.07485800	H	-4.98003500	-4.19337700	-3.28719500
C	5.98291000	3.02798500	-0.35683700	H	2.85198100	-5.58506700	-3.65311600
C	-6.13095500	-3.42118400	-1.62899300	H	-3.11687600	6.50416700	-2.57089700
C	4.07511300	-5.44219100	-1.89420800	H	4.87848200	4.91053800	-2.97352000
C	-4.28363800	6.01491500	-0.83263500	H	-3.25553400	-2.42144200	-3.16541000
C	5.93488800	4.08154300	-1.27987300	H	1.91084000	-3.28645100	-3.41922000
C	-7.18151000	-4.47525300	-1.64165100	H	-2.14432700	4.21633500	-2.78965300
C	4.57865000	-6.84272900	-2.09826100	H	3.17033900	3.11324300	-3.02922600
C	-4.82542600	7.39977000	-0.75430300	H	-5.34924000	-0.61435000	0.14187500
C	6.97917800	5.14045100	-1.19288400	H	4.30061900	-2.70384700	0.12700300
C	-5.05184400	-3.41627200	-2.52648400	H	-4.37920100	2.94768700	0.66952200
C	3.14874700	-4.94248300	-2.82315400	H	5.06064500	1.21705600	0.34760100
C	-3.37817500	5.71694700	-1.86236600	H	1.77782000	3.38665100	-0.96121800
C	4.91380300	4.10242600	-2.24324100	H	-0.60896200	3.84394300	-0.85363700
C	-4.07889900	-2.42366400	-2.44962000	H	0.47609900	-3.26955100	-1.30174100
C	2.62825200	-3.66061900	-2.68656600	H	-1.91395100	-2.80567100	-1.25036000
C	-2.83515000	4.44180200	-1.97535400	H	-4.59800100	1.19857800	-1.26221900
C	3.95339700	3.09531100	-2.26934500	H	4.45729100	-0.58006000	-1.50027300
C	-4.15133800	-1.40646300	-1.47813200	O	-8.12828400	-4.52503300	-0.87693400
C	3.02982900	-2.82402600	-1.62678600	O	5.20841100	-7.43186200	-1.03838700
C	-3.18435300	3.42611500	-1.06531400	O	-5.69461600	7.56933900	0.28569400
C	3.98510700	2.03780400	-1.33994300	O	7.89440300	5.15128300	-0.39038700
C	-5.26404200	-1.39881600	-0.61230400	O	-6.97992000	-5.41064300	-2.61597300
C	3.98152100	-3.31472200	-0.71815200	O	4.44769600	-7.45535300	-3.13513300
C	-4.10456500	3.72786600	-0.04445300	O	-4.54260600	8.30396100	-1.51959600
C	5.02564500	2.01868400	-0.39166600	O	6.81008900	6.12490100	-2.12375800
C	-1.21113500	-1.97708400	-1.33254200	H	-5.97854000	8.50509400	0.23567800
C	0.12834400	-2.23827800	-1.36090800	H	7.54427400	6.75483100	-1.97210100

H	5.15458700	-6.84653700	-0.25931700	O	0.36122000	0.11521800	2.13114400
H	-7.72278000	-6.04234500	-2.52727300	C	-0.82649000	-0.21699900	2.75268300
C	2.11299400	-1.55393800	2.52953400	C	-1.93221800	0.71773800	2.26187600
C	3.52107000	-1.77195900	3.08331000	C	-3.27118600	0.25402300	2.82329300
C	4.43366500	-0.63701500	2.63146700	C	-3.53835500	-1.20116400	2.46905400
C	2.61695600	0.88810900	2.38286100	C	-2.37408900	-2.07705600	2.94888100
C	1.58496900	-0.15201300	2.84685500	H	-0.73404600	-0.16107700	3.85827000
H	3.48614700	-1.74297100	4.18981000	H	-3.24440800	0.34807100	3.92829300
H	2.15874100	-1.63560600	1.42389300	H	-3.58655700	-1.29140300	1.36706500
H	2.72146600	0.78294800	1.28249300	H	-2.32683600	-2.05137900	4.05838500
H	1.40924400	-0.04850000	3.93367900	H	-1.95854600	0.65478000	1.15963100
H	4.53018600	-0.65831800	1.51946800	O	-1.60931900	2.03395200	2.69311600
O	4.03984900	-3.01755900	2.62392400	H	-2.38432500	2.59019000	2.49352600
H	3.30617100	-3.65301100	2.72900800	O	-4.28727200	1.11418900	2.29417900
O	5.66773100	-0.76845000	3.26184300	H	-5.13468400	0.77309600	2.63512300
H	6.20683800	0.00338900	3.01108400	O	-4.78753900	-1.54520600	3.06327800
O	3.86711200	0.61618900	3.01948300	H	-4.90727800	-2.50672000	2.91652200
C	2.21287000	2.32231500	2.69929500	C	-2.49317100	-3.52345700	2.45916800
H	1.17548000	2.47692300	2.35521100	H	-1.60966700	-4.10267000	2.77859000
H	2.24175700	2.47040700	3.78973600	H	-2.51797300	-3.52102700	1.35932200
O	3.10983500	3.28628800	2.15255500	O	-3.71277500	-4.14664500	2.88518000
H	3.13211400	3.16660100	1.18647600	H	-3.62101900	-4.38373600	3.82440400
O	1.31231100	-2.60555700	3.06491700	O	-1.15339700	-1.58383400	2.38020800
H	0.40079000	-2.47324700	2.71461000				

8. Glucose (M06-L)

Number of atoms = 24

SCF(SCRF) = -687.37512170

C	-1.66224500	0.12489400	0.19901300	O	-2.92850800	0.43151300	-0.31881400
C	-0.64528600	1.18311900	-0.19848200	H	-3.04328300	1.38331500	-0.19902900
C	0.73258700	0.80120500	0.29285800	H	-0.62882100	1.23149100	-1.29640500
C	1.07026400	-0.60267500	-0.21778100	O	-1.07386600	2.47221600	0.20903800
O	0.07729100	-1.50952500	0.22545100	H	-0.84729800	2.58388600	1.13964400
C	2.40829600	-1.11073500	0.28771100	H	0.72879800	0.76137600	1.39039100
C	-1.21569600	-1.24105900	-0.30281900	O	1.72208500	1.76392100	-0.04376300
O	-2.05777600	-2.26739400	0.05346100	H	1.52543900	2.10772000	-0.92247500
H	-1.17656600	-1.23943900	-1.40237200	H	1.09986700	-0.57670700	-1.32110900
H	-1.68810800	0.06925800	1.30443700	H	-2.23947400	-2.19649200	0.99780500

H	2.50238400	-2.16473200	0.02530200	O	3.49593700	-0.43394900	-0.28982400
H	2.41851900	-1.05158200	1.38626800	H	3.33972500	0.50915700	-0.14985500

9. Cellobiose (M06-L)

Number of atoms = 45

SCF(SCRF) = -1298.30257038

C	-1.87467100	-1.19486100	0.54980100	C	0.93859100	0.52372300	0.00745100
C	-3.21641900	-1.64290200	0.00244000	C	1.89954700	1.52678200	0.61192400
C	-4.21253000	-0.50742400	0.11415000	C	3.26779100	1.32668500	-0.00265300
C	-2.51991700	1.14965500	0.00360600	C	3.74961600	-0.09783500	0.15299000
C	-1.41277200	0.10363200	-0.08024800	C	2.69782200	-1.04705700	-0.41524400
H	-3.10608200	-1.87108100	-1.06867100	H	0.84359000	0.69818000	-1.08064200
H	-1.99708800	-1.00337700	1.62896500	H	3.19119100	1.53372800	-1.08330800
H	-2.68489800	1.37777900	1.07166300	H	3.87107200	-0.31915600	1.22529000
H	-1.14218000	-0.06749800	-1.13100600	H	2.61860700	-0.86633500	-1.50117400
H	-4.36111500	-0.24322800	1.17919700	H	1.95394200	1.33052700	1.69289000
O	-3.68642800	-2.76043500	0.71552700	O	1.41583900	2.82252300	0.35260900
H	-2.94228200	-3.37156000	0.77264200	H	2.14886200	3.42495800	0.52849900
O	-5.38989300	-0.87750300	-0.49790600	O	4.13598200	2.25891600	0.60625700
H	-6.00229000	-0.13845900	-0.42371800	H	5.01605300	2.10190200	0.24553500
O	-3.70093800	0.62772800	-0.56918000	O	4.98610400	-0.17360500	-0.52417300
C	-2.16204200	2.42403900	-0.72995600	H	5.25351100	-1.10309200	-0.52167400
H	-1.13323900	2.70260900	-0.47771200	C	3.01005100	-2.50926000	-0.15730800
H	-2.20220700	2.22475300	-1.80313500	H	2.19723800	-3.13674100	-0.53661200
O	-3.06826500	3.47799900	-0.48853700	H	3.07218400	-2.67533900	0.91975600
H	-2.88596700	3.82556600	0.38904300	O	4.26722800	-2.89058800	-0.69446700
O	-0.98189400	-2.26838200	0.34321400	H	4.16667300	-3.00422400	-1.64463900
H	-0.08645300	-1.95162300	0.53453100	O	1.45057000	-0.79859700	0.21550100
O	-0.27574700	0.60702300	0.63397400				

10. Pyrene unit (M06-L)

Number of atoms = 78

SCF(SCRF) = -2294.87265492

C	-2.82314400	-1.24884000	0.03654100	C	1.45787300	-1.22222100	0.04463700
C	2.87465000	-1.20210000	0.03909200	C	-1.42652100	1.22537300	0.04747600
C	-2.84309900	1.20564700	0.04522400	C	1.43808800	1.24831700	0.04143700
C	2.85516800	1.25260700	0.03133700	C	-5.45243100	-3.85071600	0.83757400
C	-1.40645500	-1.24500400	0.04363100	C	5.52180200	-3.77319600	0.88607900

C	-5.52025500	3.74200000	0.89645100	H	-6.27394100	-3.99321000	1.52811200
C	5.46014700	3.88126200	0.83727600	H	6.34300800	-3.83687300	1.59366900
C	-5.16343300	-4.86902500	-0.07032500	H	-6.33513400	3.84069800	1.60080800
C	5.25170500	-4.81515600	-0.00163500	H	6.27617100	4.03383700	1.53219000
C	-5.26011300	4.77679900	-0.00226600	H	-3.87761900	-5.44962600	-1.68666800
C	5.16261200	4.89675400	-0.07120700	H	4.00668700	-5.42372700	-1.61942600
C	-5.99098300	-6.10485900	-0.04821400	H	-4.01364100	5.41496200	-1.61324200
C	6.01360300	-6.10878700	-0.05752800	H	3.87762200	5.45949900	-1.69467600
C	-6.05455300	6.03376700	-0.04379600	H	-2.54552100	-3.39102800	-1.63864400
C	5.97161100	6.14568500	-0.04267500	H	2.64164700	-3.37007100	-1.62069300
C	-4.10550400	-4.68109400	-0.96057200	H	-2.62199600	3.37785900	-1.61040000
C	4.20469500	-4.63383100	-0.90630100	H	2.57035000	3.38559500	-1.65094000
C	-4.20508800	4.62199100	-0.90149700	H	-4.93182600	-1.92058500	1.59079500
C	4.11206100	4.69425900	-0.96717200	H	4.99003500	-1.83110300	1.60265000
C	-3.35080500	-3.52095000	-0.92629200	H	-4.94745500	1.81498100	1.61997700
C	3.44031100	-3.48164200	-0.89784600	H	4.95933100	1.94554100	1.58993100
C	-3.42367500	3.48093700	-0.88965000	H	1.19270500	3.38317100	0.27421600
C	3.37159000	3.52485500	-0.93579400	H	-1.21524200	3.36357400	0.28095300
C	-3.61810000	-2.50027600	-0.00517200	H	1.24525400	-3.36108500	0.27943800
C	3.68590800	-2.44414500	0.01217700	H	-1.16170300	-3.37964600	0.27608900
C	-3.66130800	2.44271400	0.02138000	H	-4.57626100	-0.03587700	0.02951500
C	3.64508200	2.50806500	-0.01190600	H	4.60889200	0.03988900	0.01965500
C	-4.69940600	-2.69029500	0.86454200	O	-6.90999800	-6.30533200	0.70545400
C	4.76167100	-2.61389900	0.88955300	O	6.89888100	-6.33944500	0.93775000
C	-4.73844500	2.59861400	0.90154200	O	-7.04442100	6.04900700	0.87672300
C	4.72111600	2.71126900	0.86128200	O	6.88288100	6.35892400	0.71679100
C	-0.64253800	-2.43969600	0.15184000	O	-5.60039000	-7.00420800	-0.97871000
C	0.71274300	-2.42894200	0.15331600	O	5.86497900	-6.92005400	-0.92797500
C	-0.68153800	2.43206700	0.15450600	O	-5.85668200	6.94953800	-0.80206200
C	0.67379200	2.44305000	0.15088900	O	5.57269400	7.04002900	-0.97429700
C	-3.49240200	-0.02716200	0.05951200	H	-7.49360600	6.89909900	0.76730000
C	3.52496600	0.03063900	0.05267500	H	6.15572900	7.80557400	-0.87213100
C	-0.70101900	-0.00407000	0.03106000	H	6.86114600	-5.62671600	1.58649600
C	0.73248600	0.00733600	0.02985200	H	-6.19538900	-7.76100900	-0.88055300

11. Glucose-pyrene (configuration 1) (M06-L)

Number of atoms = 102

SCF(SCRF) = -2982.26835903

C	2.60929800	-1.38229200	-0.92062400	C	0.69158400	2.42698900	-0.87141000
C	-3.07037800	-0.99863500	-0.83120000	C	-0.66277400	2.51684800	-0.84733600
C	2.78120700	1.06800500	-0.85533600	C	3.35188200	-0.20366900	-0.89163400
C	-2.90976900	1.45054900	-0.75344400	C	-3.64866400	0.26834600	-0.78568000
C	1.19527500	-1.29194300	-0.96643400	C	0.56685100	-0.01070000	-0.90378900
C	-1.66004900	-1.09939500	-0.91363500	C	-0.86469300	0.08512500	-0.88248500
C	1.36805800	1.17312000	-0.85526800	H	5.92968600	-4.31005300	-2.36085700
C	-1.49725300	1.36479000	-0.80779300	H	-6.76868200	-3.43310200	-2.17153600
C	5.09909500	-4.12806400	-1.69079700	H	6.38697700	3.49927600	-2.47080000
C	-5.90339800	-3.41446100	-1.51579600	H	-6.13055900	4.49890500	-2.17124400
C	5.58792100	3.44489500	-1.74390500	H	3.36842400	-5.65637700	0.77516400
C	-5.33610200	4.26771800	-1.47303200	H	-4.34655400	-5.13369000	0.91889500
C	4.72939200	-5.13646600	-0.80113100	H	4.25971600	5.17947600	0.82286200
C	-5.64514000	-4.46305300	-0.63206300	H	-3.69397000	5.64087400	1.13895900
C	5.41648000	4.48592700	-0.83157400	H	2.15719300	-3.52647000	0.71878300
C	-4.98675700	5.22668700	-0.52248000	H	-2.86457100	-3.15902500	0.82676600
C	5.49133000	-6.41671500	-0.81577900	H	2.75527300	3.23435900	0.84890300
C	-6.48822400	-5.70211600	-0.51610000	H	-2.52369400	3.48572400	1.03431000
C	6.28182300	5.69631600	-0.80573000	H	4.71214800	-2.16283300	-2.43370800
C	-5.71257700	6.52786700	-0.51580700	H	-5.30019700	-1.51137200	-2.27927400
C	3.65950200	-4.89636600	0.06282400	H	4.87975000	1.56203000	-2.46447100
C	-4.53737500	-4.33958200	0.20850500	H	-4.94989300	2.33279700	-2.29388100
C	4.38200700	4.38467700	0.09810200	H	-1.12494900	3.49276400	-0.89572900
C	-3.96567000	4.92096200	0.37872500	H	1.27669700	3.33298300	-0.94784900
C	2.97130600	-3.69437800	0.02238100	H	-1.58469400	-3.23654400	-1.23088700
C	-3.70410900	-3.23653600	0.14617000	H	0.82316800	-3.39755700	-1.28309600
C	3.53448000	3.29225700	0.09969700	H	4.43177400	-0.27881300	-0.83391900
C	-3.29946500	3.70795000	0.31162400	H	-4.72828400	0.33720400	-0.70846100
C	3.32432600	-2.68258800	-0.88007900	O	6.41637700	-6.65903400	-1.54930100
C	-3.94578800	-2.19420700	-0.75978800	O	-7.42019200	-5.89654600	-1.47676000
C	3.67837300	2.25095300	-0.82627400	O	7.24830600	5.65967700	-1.74993900
C	-3.62398800	2.74995200	-0.65754600	O	-6.59430600	6.82832300	-1.28030000
C	4.41491800	-2.92576800	-1.72412300	O	5.03026000	-7.30094600	0.09605900
C	-5.07691000	-2.30304900	-1.57421900	O	-6.36528800	-6.50013200	0.37026000
C	4.73803400	2.35044600	-1.73494900	O	6.15339900	6.61849000	-0.04047700
C	-4.67305200	3.05391000	-1.53397400	O	-5.27184400	7.35864400	0.45483500
C	0.36047500	-2.43382900	-1.12281200	H	7.74789400	6.48219400	-1.64848900
C	-0.99225200	-2.34286200	-1.09345700	H	-5.80041700	8.16507100	0.37260200

H	-7.35050900	-5.20741900	-2.14805600	H	-2.86492000	-0.11810300	2.56686000
H	5.58612500	-8.08791300	0.00597700	H	-0.61596500	0.72333900	1.54483200
C	-1.09897000	-0.69703200	3.03902800	O	-1.53848700	1.68672600	3.03150400
C	-0.61096300	0.68560400	2.64146100	H	-1.40613500	1.87531000	3.96800600
C	0.80859900	0.93202600	3.10079900	H	0.84930600	0.97033000	4.19767700
C	1.69619600	-0.22306500	2.62509900	O	1.28795000	2.19367800	2.65258600
O	1.16080500	-1.45522900	3.08088800	H	0.93339800	2.34063000	1.76266900
C	3.12705500	-0.12867800	3.11923500	H	1.71309600	-0.20538400	1.52310700
C	-0.11480500	-1.73493400	2.52263800	H	-0.63841200	-3.10104900	3.75906100
O	-0.45687900	-3.03723900	2.81389600	H	3.63942000	-1.06191200	2.88012800
H	-0.06385900	-1.66977700	1.42575400	H	3.12872900	-0.03345800	4.21510900
H	-1.11680300	-0.77097300	4.14240100	O	3.84265200	0.91126600	2.49845900
O	-2.37181900	-0.94673300	2.49731500	H	3.30871900	1.71177900	2.58840000

12. Glucose-pyrene (configuration 2) (M06-L)

Number of atoms = 102

SCF(SCRF) = -2982.27057448

C	-2.92299900	-1.34933700	-0.76780500	C	4.25401500	-4.57865600	-1.76401900
C	2.77050700	-1.19807200	-0.86775900	C	-4.49540000	4.46682800	-1.64990500
C	-2.98867200	1.10398900	-0.74301100	C	3.92834600	4.72042000	-1.86784800
C	2.70906000	1.25553200	-0.89722400	C	-3.50263500	-3.62934000	-1.68213200
C	-1.50851100	-1.32151600	-0.83990000	C	3.46620700	-3.44278800	-1.79954500
C	1.35333900	-1.24523000	-0.89019200	C	-3.69378800	3.33998600	-1.67571000
C	-1.57560600	1.14924000	-0.82374000	C	3.20947700	3.53725500	-1.85669800
C	1.28997900	1.22632500	-0.90356100	C	-3.69447100	-2.61599300	-0.73572900
C	-5.40295600	-3.99970800	0.29165400	C	3.60162700	-2.43064700	-0.84033600
C	5.35019300	-3.75737600	0.19140800	C	-3.82578000	2.32992300	-0.71371300
C	-5.60983800	3.62925100	0.29869100	C	3.47627800	2.52714300	-0.92342200
C	5.23802700	3.93677600	-0.02197600	C	-4.67246900	-2.82478200	0.24449900
C	-5.19383700	-5.00934100	-0.64747100	C	4.57344400	-2.60810000	0.14902800
C	5.20286200	-4.76832400	-0.75810100	C	-4.80948300	2.49753500	0.26718500
C	-5.46218300	4.63370500	-0.65840000	C	4.52169700	2.75170800	-0.01818900
C	4.94753900	4.94424200	-0.94123600	C	-0.72200100	-2.50383100	-0.77355800
C	-5.99507600	-6.26041600	-0.54764400	C	0.63261000	-2.46884100	-0.79860300
C	6.00516400	-6.04098900	-0.77902500	C	-0.85252600	2.37262000	-0.76327300
C	-6.28689700	5.87405700	-0.67094100	C	0.50276700	2.41039600	-0.80479100
C	5.73287700	6.20981000	-0.89354500	C	-3.61292600	-0.14060800	-0.69587800
C	-4.23724600	-4.80238600	-1.64202500	C	3.40016700	0.04478000	-0.85232400

C	-0.82720200	-0.06685700	-0.87235800	O	-6.17980200	6.76275400	-1.47785700
C	0.60513200	-0.02836300	-0.90431100	O	5.34189800	7.09310600	-1.83770700
H	-6.14401000	-4.15922300	1.06454800	H	-7.66509200	6.73991400	0.23986700
H	6.08852800	-3.83500800	0.98336300	H	5.90668300	7.87077300	-1.72433200
H	-6.35285900	3.73998500	1.07686400	H	6.56653600	-5.65899400	1.00735300
H	6.03095500	4.10554300	0.69545400	H	-6.25355300	-7.91744000	-1.36301900
H	-4.07243800	-5.56625400	-2.38971500	C	2.09995800	0.01603900	2.55863100
H	4.15104400	-5.34793100	-2.51853300	C	1.31827700	1.22423600	3.02603700
H	-4.39044700	5.23769400	-2.40278300	C	-0.13605800	1.07902200	2.64552400
H	3.70179000	5.47977600	-2.60390200	C	-0.68756900	-0.22916200	3.19478900
H	-2.77556600	-3.48437300	-2.47181900	O	0.09869100	-1.29259800	2.67917500
H	2.73900400	-3.32378100	-2.59363100	C	-2.11430300	-0.49276600	2.74856400
H	-2.96227600	3.22478100	-2.46633700	C	1.46279300	-1.26780100	3.07582100
H	2.43342700	3.38137800	-2.59583700	O	2.06965200	-2.40448300	2.58588900
H	-4.83785100	-2.06011900	0.99534800	H	1.54404200	-1.31821000	4.17139500
H	4.69839200	-1.84903400	0.91321500	H	2.02596900	-0.02495100	1.45808700
H	-4.92778700	1.73708300	1.03038300	O	3.44992000	0.08250100	2.95664400
H	4.75751100	1.98615700	0.71265000	H	3.68997600	1.01805300	2.93842400
H	1.00362000	3.36593000	-0.72404100	H	1.40293100	1.32203300	4.11393500
H	-1.40267500	3.29566600	-0.64299600	O	1.87875600	2.42993700	2.50887900
H	1.18490100	-3.39455800	-0.70777300	H	1.86444000	2.35975600	1.54170800
H	-1.22194800	-3.45479600	-0.65603400	H	-0.19858700	1.02066400	1.54690300
H	-4.69534300	-0.17008800	-0.64471800	O	-0.90919800	2.16632300	3.12002500
H	4.48396100	0.07103700	-0.84846300	H	-0.41812100	2.97207900	2.91518300
O	-6.82990600	-6.47747700	0.29354500	H	-0.64123600	-0.20829800	4.29518300
O	6.73652800	-6.31698000	0.32249800	H	2.05476900	-2.34830700	1.61950700
O	-7.18665600	5.90424500	0.33611800	H	-2.39625000	-1.50403500	3.04659600
O	6.61825700	6.43909300	-0.10957700	H	-2.13382400	-0.46323300	1.65026600
O	-5.68483700	-7.14972400	-1.51687600	O	-3.05177300	0.39114200	3.31238800
O	6.01393200	-6.79302000	-1.71268600	H	-2.69377900	1.28428600	3.21843400

13. Cellobiose-pyrene (configuration 1) (M06-L)

Number of atoms = 123

SCF(SCRF) = -3593.20512582

C	-1.84395200	1.32855200	-1.47898600	C	-0.43044200	1.30497700	-1.35306600
C	3.82581200	1.18516500	-0.90346100	C	2.42224300	1.23003500	-1.07640200
C	-1.89169500	-1.12917000	-1.58450100	C	-0.47967200	-1.16865200	-1.45636100
C	3.76619600	-1.26626100	-0.93409700	C	2.36340400	-1.23619300	-1.12563000

C	-4.40520400	3.97763400	-2.37783200	H	-5.39528100	-3.64967000	-3.31433300
C	6.55018900	3.77462200	-1.35162000	H	7.26848300	-4.15588300	-1.97634100
C	-4.60065600	-3.58551400	-2.58334300	H	-2.94665500	5.52168400	0.24885400
C	6.38074500	-3.96926800	-1.38535100	H	4.84875200	5.25454300	1.14297900
C	-4.14829300	4.98825900	-1.44804600	H	-3.21495700	-5.33646000	-0.05609600
C	6.21517700	4.75229700	-0.41384500	H	4.47114300	-5.45236000	0.97580600
C	-4.39557100	-4.64395800	-1.69605300	H	-1.65433800	3.43290500	0.26098500
C	5.95357500	-4.95740700	-0.49787500	H	3.47952500	3.21752200	0.89690700
C	-4.94608200	6.24815400	-1.51247300	H	-1.78306600	-3.33775400	0.02697600
C	6.98512900	6.02634900	-0.20569500	H	3.23339300	-3.35078800	0.74558700
C	-5.21846400	-5.88606900	-1.70659700	H	-3.87525100	2.04782100	-3.12373200
C	6.73331300	-6.22397300	-0.40957800	H	6.06592300	1.89367100	-2.24550500
C	-3.14579600	4.76653900	-0.50008900	H	-3.95747800	-1.66374900	-3.25738100
C	5.09669600	4.51880800	0.38866800	H	6.02140900	-2.03812000	-2.22663400
C	-3.36539300	-4.52922700	-0.76241800	H	2.12450100	-3.35926700	-1.44446900
C	4.81028700	-4.71083300	0.26497400	H	-0.26820600	-3.30039500	-1.74624200
C	-2.40769500	3.59204800	-0.50216500	H	2.26737300	3.37908200	-1.24824100
C	4.32387100	3.38065900	0.23671000	H	-0.12851400	3.44346600	-1.47720700
C	-2.55171000	-3.41032300	-0.73222800	H	-3.60361500	0.13579100	-1.69208100
C	4.10511400	-3.52569500	0.12568600	H	5.52559600	-0.08519900	-0.69337200
C	-2.63214500	2.58641400	-1.45491100	O	-5.81283700	6.46830300	-2.31918500
C	4.64051800	2.41318000	-0.72689600	O	7.94575800	6.31302000	-1.11418900
C	-2.73121600	-2.35171100	-1.63384400	O	-6.17405700	-5.86294900	-2.66228300
C	4.51433800	-2.53868200	-0.78081800	O	7.72046200	-6.47228100	-1.05532700
C	-3.66949500	2.80327700	-2.37498000	O	-4.58622800	7.13038500	-0.55696500
C	5.78451000	2.62852300	-1.50079400	O	6.78179100	6.77689500	0.70708100
C	-3.78777800	-2.46393300	-2.54688500	O	-5.06699800	-6.81844200	-0.95835900
C	5.67963900	-2.78327600	-1.51801600	O	6.21102100	-7.09005800	0.48703100
C	0.35968500	2.48881600	-1.34294000	H	-6.64336100	-6.70594800	-2.58726300
C	1.70986200	2.45301500	-1.21929300	H	6.78429400	-7.86934600	0.46514500
C	0.25895600	-2.38227200	-1.52875900	H	7.94697600	5.64833500	-1.81301900
C	1.60475100	-2.41451100	-1.36326700	H	-5.15445100	7.90428900	-0.67897100
C	-2.51992300	0.11564700	-1.61906400	C	-0.06991200	1.16903000	2.82308500
C	4.45445800	-0.05739700	-0.86152000	C	1.32253300	1.53104200	2.35207000
C	0.25500600	0.05084600	-1.32438900	C	2.31070900	0.49361300	2.84070100
C	1.68036000	0.01490600	-1.17216900	C	0.66496700	-1.21957700	2.84905800
H	-5.18326000	4.13961200	-3.11323900	C	-0.41964500	-0.24459900	2.40135600
H	7.42818800	3.87729600	-1.98238800	H	1.33225500	1.48419500	1.25358600

H	-0.09623200	1.21267500	3.92394600	C	-5.50054500	0.01762400	1.53270400
H	0.68512300	-1.24153000	3.95253000	C	-4.37934100	1.05146100	1.43963200
H	-0.49277000	-0.28085100	1.30409800	H	-2.46905100	-0.61408800	1.09490400
H	2.32079100	0.46424700	3.94676800	H	-4.50827700	-1.52394100	0.45357600
O	1.69418900	2.81225900	2.80307300	H	-6.00951600	0.13933900	2.50243100
H	0.91902500	3.37259100	2.67142000	H	-3.96806700	1.02100600	0.41802200
O	3.55503800	0.78373900	2.32032300	H	-4.19142200	-1.40793100	3.48575800
H	4.16974700	0.10799200	2.62569400	O	-3.24767900	-2.86372400	2.34977400
O	1.91628000	-0.77947200	2.35099400	H	-3.98444300	-3.47103100	2.20131200
C	0.41851500	-2.61244200	2.31153800	O	-5.90457000	-2.37733100	1.71621400
H	-0.61741200	-2.89833500	2.52246100	H	-6.60081400	-2.27146000	1.05854900
H	0.54059100	-2.58078900	1.22503600	O	-6.41528500	0.13668800	0.46259600
O	1.34571100	-3.56764600	2.78343000	H	-6.66890400	1.06966500	0.40808000
H	1.11414200	-3.78566500	3.69058700	C	-4.85723900	2.45905800	1.73737400
O	-0.93528500	2.14487700	2.27668100	H	-4.00012000	3.13800000	1.79937400
H	-1.84957200	1.87030500	2.46440600	H	-5.36429600	2.48151400	2.70408700
O	-1.66395000	-0.66128900	2.97044500	O	-5.79996500	2.89357700	0.77216200
C	-2.76290300	-0.53764800	2.15830700	H	-5.31552000	3.13824500	-0.02825800
C	-3.81478600	-1.58174100	2.46722900	O	-3.35000900	0.75447700	2.37653600
C	-4.93325000	-1.38413000	1.46293800				

14. Cellobiose-pyrene (configuration 2) (M06-L)

Number of atoms = 123

SCF(SCRF) = -3593.20517120

C	3.15150500	0.38396800	-1.28395600	C	4.41070600	-5.96879900	-0.76385800
C	-2.45449700	1.39079000	-1.53433600	C	-5.83467000	-4.17118600	-1.23080700
C	2.70598700	-2.02377200	-1.09583500	C	7.16897800	4.56066900	-1.52770700
C	-2.89387100	-1.01977900	-1.39795800	C	-4.62081200	6.77784100	-1.97253400
C	1.75731800	0.64471000	-1.33967300	C	4.96666700	-7.34703700	-0.68618600
C	-1.06052900	1.14753500	-1.46725900	C	-6.86616000	-5.23864600	-1.11340000
C	1.31236600	-1.78088300	-1.17018400	C	5.05412400	3.47653900	-2.40398800
C	-1.50205000	-1.27756100	-1.32230100	C	-3.11893000	4.94200800	-2.71112500
C	6.23367900	2.46774400	-0.57995100	C	3.45100100	-5.68970300	-1.73704900
C	-4.54685100	4.46752300	-0.85830000	C	-4.75548700	-4.25431300	-2.11202000
C	4.80535900	-4.93934300	0.09129300	C	4.09834700	2.47708600	-2.33469700
C	-5.94754500	-3.03737700	-0.42812800	C	-2.58345400	3.66987300	-2.62514600
C	6.12994800	3.49663700	-1.51585900	C	2.89410500	-4.42829200	-1.84274200
C	-4.11052300	5.37166800	-1.82695400	C	-3.81203600	-3.24305800	-2.17251500

C	4.17304400	1.45539800	-1.37901200	O	8.10819700	4.61400100	-0.77419400
C	-3.01427500	2.76074400	-1.64949400	O	-5.68779200	7.12047300	-1.21817000
C	3.27424900	-3.38963100	-0.98240800	O	5.88281700	-7.47915000	0.29898200
C	-3.90299900	-2.10668200	-1.35729500	O	-7.82270000	-5.19215600	-0.38270500
C	5.28309400	1.46444300	-0.52159000	O	6.94960400	5.48453700	-2.48916500
C	-4.01854800	3.18803900	-0.77735600	O	-4.12597000	7.58127000	-2.71321400
C	4.25131900	-3.67361900	-0.02079800	O	4.65124500	-8.25881700	-1.40840800
C	-5.00535400	-2.02520700	-0.49551500	O	-6.61622700	-6.28710800	-1.92799700
C	1.22329100	1.96336600	-1.32978700	H	6.17658500	-8.40052800	0.26422600
C	-0.10984200	2.20222700	-1.38828400	H	-7.33464100	-6.91752500	-1.77648800
C	0.35274300	-2.81685000	-1.00760300	H	-5.99782700	6.35730400	-0.71584200
C	-0.97925900	-2.57936900	-1.08463300	H	7.67235000	6.12345100	-2.41264700
C	3.57523300	-0.93630100	-1.13707200	C	-2.22465700	1.55755500	2.37335300
C	-3.32515600	0.30421100	-1.47736400	C	-3.61988600	1.74578800	2.93987300
C	0.83176200	-0.44333800	-1.30915600	C	-4.49817500	0.60506800	2.47269500
C	-0.57688100	-0.19173500	-1.37784600	C	-2.66885500	-0.87771200	2.26032000
H	7.07249000	2.47383400	0.10481000	C	-1.66953000	0.18353800	2.71224100
H	-5.29009600	4.74299400	-0.11566700	H	-3.57347000	1.69537000	4.03781300
H	5.54789900	-5.13597500	0.85293700	H	-2.29336300	1.61172500	1.27196500
H	-6.78116900	-2.97291500	0.25935700	H	-2.77088200	-0.78459800	1.16450600
H	4.97035100	4.24931300	-3.15607700	H	-1.50091300	0.10154600	3.79469000
H	-2.77975000	5.63500100	-3.47032700	H	-4.55428000	0.62398900	1.36081500
H	3.15550900	-6.48281200	-2.41208500	O	-4.15953000	2.97536900	2.51374000
H	-4.65988100	-5.11755100	-2.75646100	H	-3.44560100	3.61895700	2.61003600
H	3.28385000	2.47484800	-3.04800400	O	-5.74140800	0.70742100	3.05661300
H	-1.82419200	3.36347700	-3.33450800	H	-6.23264100	-0.09090400	2.83307900
H	2.16345900	-4.23201900	-2.61779700	O	-3.92097700	-0.62296200	2.87236500
H	-2.99183700	-3.32343100	-2.87498000	C	-2.24721500	-2.29130800	2.58877400
H	5.38002400	0.68231000	0.22289000	H	-1.21198200	-2.43283500	2.25917000
H	-4.36181400	2.52961800	0.01151700	H	-2.27318300	-2.43283200	3.67113400
H	4.55612500	-2.88875100	0.66233900	O	-3.11922200	-3.25895200	2.04701400
H	-5.10023500	-1.16400000	0.15648700	H	-3.13347400	-3.14565600	1.08893100
H	-1.66468600	-3.40113800	-0.92771500	O	-1.45274000	2.62996800	2.86694100
H	0.69803200	-3.81603500	-0.78200900	H	-0.55308100	2.52578300	2.51656900
H	-0.46659800	3.22211900	-1.34083800	O	-0.44152000	-0.06582600	2.02124100
H	1.90215400	2.79961200	-1.23919200	C	0.72596800	0.27389000	2.65737900
H	4.64055000	-1.13303500	-1.10205500	C	1.83845900	-0.65557400	2.21070200
H	-4.39069300	0.49548400	-1.54477300	C	3.14640600	-0.19029600	2.80814600

C	3.42197000	1.24514300	2.43207800	H	4.99810900	-0.70730300	2.67860200
C	2.25362500	2.12574400	2.85583800	O	4.64698800	1.59164700	3.03946400
H	0.60735400	0.23678000	3.75503100	H	4.79351600	2.53311200	2.86942700
H	3.08188500	-0.25845200	3.90611500	C	2.38507900	3.54879500	2.34129400
H	3.49089000	1.30496100	1.33451900	H	1.49825400	4.13203900	2.61055200
H	2.17703700	2.12223200	3.95647800	H	2.43793400	3.52168900	1.25050000
H	1.90712500	-0.58148100	1.11719400	O	3.57949800	4.17188200	2.78346500
O	1.51422700	-1.96369200	2.61436400	H	3.46252800	4.43797400	3.70081500
H	2.30408600	-2.50036300	2.47574400	O	1.05974900	1.61774900	2.27305500
O	4.16557100	-1.05345200	2.33453300				

15. Glucose (M06-2X)

Number of atoms = 24

SCF(SCRF) = -687.24159941

C	-1.67745800	0.12487200	0.18137100	H	-0.62692700	1.26878200	-1.28948900
C	-0.65437300	1.18221200	-0.19880200	O	-1.04017300	2.47077900	0.26132100
C	0.72676500	0.80342900	0.29489300	H	-1.10980500	2.44594400	1.22370400
C	1.07690700	-0.59419400	-0.20936700	H	0.71795500	0.76870200	1.39586100
O	0.08536800	-1.49429500	0.24374500	O	1.69877200	1.72299700	-0.15668000
C	2.42110700	-1.08728700	0.30602300	H	1.33927900	2.61325500	-0.06399300
C	-1.19910000	-1.24712100	-0.29346900	H	1.11086300	-0.57614400	-1.30822600
O	-2.03991700	-2.27079700	0.08136500	H	-2.14128100	-2.25717200	1.04001000
H	-1.16113300	-1.26084000	-1.38944000	H	2.50266000	-2.15066800	0.08245900
H	-1.74915200	0.08060200	1.28269400	H	2.45076000	-0.96895400	1.39702300
O	-2.92766300	0.39847000	-0.39105300	O	3.50113500	-0.44156700	-0.32092400
H	-3.07673900	1.34970600	-0.33689800	H	3.36024700	0.51063000	-0.25979800

16. Cellobiose (M06-2X)

Number of atoms = 45

SCF(SCRF) = -1298.04932119

C	-1.90304100	-1.19134000	0.59081100	H	-1.14933600	-0.12291100	-1.11663300
C	-3.24952900	-1.62871300	0.03810400	H	-4.40874700	-0.19028600	1.15079800
C	-4.22722300	-0.46933900	0.09986700	O	-3.75603800	-2.70129800	0.79086900
C	-2.50227800	1.15220800	-0.01557000	H	-3.05075500	-3.35501800	0.86020000
C	-1.41111600	0.08372800	-0.07140700	O	-5.39389700	-0.83725800	-0.53939400
H	-3.13552100	-1.90126200	-1.01913700	H	-5.98778800	-0.07914400	-0.54048400
H	-2.02809800	-0.97708600	1.66214600	O	-3.68511300	0.64122800	-0.58644200
H	-2.66748500	1.41288400	1.04202100	C	-2.10702000	2.40023800	-0.78169100

H	-1.07175500	2.65724500	-0.53840400	H	2.64203300	-0.83614900	-1.53673500
H	-2.17612300	2.17783500	-1.84840500	H	1.93212500	1.29361000	1.71416900
O	-2.97799500	3.48408600	-0.54050400	O	1.40468900	2.79788100	0.38734400
H	-2.75943700	3.86835100	0.31269800	H	2.10976400	3.41785200	0.60929000
O	-1.02090600	-2.27743600	0.41219200	O	4.13535900	2.22567900	0.69038900
H	-0.12157900	-1.97938600	0.60688100	H	5.02697000	2.07610500	0.35478300
O	-0.27466500	0.57298000	0.63473000	O	4.99140900	-0.16699600	-0.51264500
C	0.94078700	0.50903900	0.00014700	H	5.27929000	-1.08889000	-0.53006100
C	1.89347100	1.50381200	0.63813200	C	3.01106200	-2.51138800	-0.22200400
C	3.27300000	1.32379000	0.03464500	H	2.20388500	-3.12379200	-0.63223900
C	3.75112700	-0.10905500	0.15499400	H	3.06004200	-2.69241500	0.85280300
C	2.70310900	-1.03984500	-0.45643000	O	4.27205500	-2.88017000	-0.75542100
H	0.84100500	0.72607100	-1.07542200	H	4.18691400	-3.02277500	-1.70277500
H	3.21620500	1.56927400	-1.03622700	O	1.45027800	-0.80984900	0.16062800
H	3.86290700	-0.35969800	1.21918400				

17. Pyrene unit (M06-2X)

Number of atoms = 78

SCF(SCRF) = -2294.30700360

C	-2.82314400	-1.24884000	0.03654100	C	5.97161100	6.14568500	-0.04267500
C	2.87465000	-1.20210000	0.03909200	C	-4.10550400	-4.68109400	-0.96057200
C	-2.84309900	1.20564700	0.04522400	C	4.20469500	-4.63383100	-0.90630100
C	2.85516800	1.25260700	0.03133700	C	-4.20508800	4.62199100	-0.90149700
C	-1.40645500	-1.24500400	0.04363100	C	4.11206100	4.69425900	-0.96717200
C	1.45787300	-1.22222100	0.04463700	C	-3.35080500	-3.52095000	-0.92629200
C	-1.42652100	1.22537300	0.04747600	C	3.44031100	-3.48164200	-0.89784600
C	1.43808800	1.24831700	0.04143700	C	-3.42367500	3.48093700	-0.88965000
C	-5.45243100	-3.85071600	0.83757400	C	3.37159000	3.52485500	-0.93579400
C	5.52180200	-3.77319600	0.88607900	C	-3.61810000	-2.50027600	-0.00517200
C	-5.52025500	3.74200000	0.89645100	C	3.68590800	-2.44414500	0.01217700
C	5.46014700	3.88126200	0.83727600	C	-3.66130800	2.44271400	0.02138000
C	-5.16343300	-4.86902500	-0.07032500	C	3.64508200	2.50806500	-0.01190600
C	5.25170500	-4.81515600	-0.00163500	C	-4.69940600	-2.69029500	0.86454200
C	-5.26011300	4.77679900	-0.00226600	C	4.76167100	-2.61389900	0.88955300
C	5.16261200	4.89675400	-0.07120700	C	-4.73844500	2.59861400	0.90154200
C	-5.99098300	-6.10485900	-0.04821400	C	4.72111600	2.71126900	0.86128200
C	6.01360300	-6.10878700	-0.05752800	C	-0.64253800	-2.43969600	0.15184000
C	-6.05455300	6.03376700	-0.04379600	C	0.71274300	-2.42894200	0.15331600

C	-0.68153800	2.43206700	0.15450600	H	-4.94745500	1.81498100	1.61997700
C	0.67379200	2.44305000	0.15088900	H	4.95933100	1.94554100	1.58993100
C	-3.49240200	-0.02716200	0.05951200	H	1.19270500	3.38317100	0.27421600
C	3.52496600	0.03063900	0.05267500	H	-1.21524200	3.36357400	0.28095300
C	-0.70101900	-0.00407000	0.03106000	H	1.24525400	-3.36108500	0.27943800
C	0.73248600	0.00733600	0.02985200	H	-1.16170300	-3.37964600	0.27608900
H	-6.27394100	-3.99321000	1.52811200	H	-4.57626100	-0.03587700	0.02951500
H	6.34300800	-3.83687300	1.59366900	H	4.60889200	0.03988900	0.01965500
H	-6.33513400	3.84069800	1.60080800	O	-6.90999800	-6.30533200	0.70545400
H	6.27617100	4.03383700	1.53219000	O	6.89888100	-6.33944500	0.93775000
H	-3.87761900	-5.44962600	-1.68666800	O	-7.04442100	6.04900700	0.87672300
H	4.00668700	-5.42372700	-1.61942600	O	6.88288100	6.35892400	0.71679100
H	-4.01364100	5.41496200	-1.61324200	O	-5.60039000	-7.00420800	-0.97871000
H	3.87762200	5.45949900	-1.69467600	O	5.86497900	-6.92005400	-0.92797500
H	-2.54552100	-3.39102800	-1.63864400	O	-5.85668200	6.94953800	-0.80206200
H	2.64164700	-3.37007100	-1.62069300	O	5.57269400	7.04002900	-0.97429700
H	-2.62199600	3.37785900	-1.61040000	H	-7.49360600	6.89909900	0.76730000
H	2.57035000	3.38559500	-1.65094000	H	6.15572900	7.80557400	-0.87213100
H	-4.93182600	-1.92058500	1.59079500	H	6.86114600	-5.62671600	1.58649600
H	4.99003500	-1.83110300	1.60265000	H	-6.19538900	-7.76100900	-0.88055300

18. Glucose-pyrene (configuration 1) (M06-2X)

Number of atoms = 102

SCF(SCRF) = -2981.56662885

C	2.61760700	-1.37693100	-0.89787800	C	5.39929900	4.49428500	-0.82380400
C	-3.05172800	-1.01364800	-0.84930200	C	-4.98243200	5.19694900	-0.53301400
C	2.77898900	1.06739500	-0.83753800	C	5.52344200	-6.40737800	-0.78286900
C	-2.89979700	1.42877600	-0.77324600	C	-6.45823100	-5.72694300	-0.48842900
C	1.20901100	-1.29278800	-0.95703800	C	6.27881900	5.70789100	-0.79565300
C	-1.64698800	-1.10917900	-0.92964600	C	-5.71803600	6.50521500	-0.51119600
C	1.37207000	1.16708000	-0.85323000	C	3.74815500	-4.85138800	0.15374300
C	-1.49330500	1.34878200	-0.82713500	C	-4.57109200	-4.29654100	0.30113700
C	5.05132000	-4.16132400	-1.73984200	C	4.43265200	4.34921400	0.16851600
C	-5.79440000	-3.52304600	-1.60619900	C	-4.05057600	4.84393700	0.44194400
C	5.51103200	3.51096000	-1.80296300	C	3.05330300	-3.64959600	0.11135000
C	-5.24130700	4.30548900	-1.57071400	C	-3.74218200	-3.18700000	0.22495100
C	4.75079000	-5.12067600	-0.77658900	C	3.58687500	3.25123300	0.17218400
C	-5.59684100	-4.49065100	-0.62327800	C	-3.37919500	3.63020900	0.36846300

C	3.34050500	-2.68473300	-0.85902000	H	-4.72038600	0.31271800	-0.72203400
C	-3.92389700	-2.22386100	-0.77441700	O	6.38924100	-6.67700700	-1.56803600
C	3.67576400	2.26405900	-0.81451700	O	-7.13281200	-6.10963800	-1.59039700
C	-3.61923800	2.73716000	-0.68029700	O	7.17638000	5.72334200	-1.79644100
C	4.35825800	-2.96032400	-1.77654700	O	-6.52291100	6.84669700	-1.33213300
C	-4.97331800	-2.40390200	-1.67552400	O	5.14314900	-7.24647100	0.19576900
C	4.66144000	2.41200900	-1.79311200	O	-6.55147700	-6.34794700	0.52602000
C	-4.57175000	3.09187800	-1.63954600	O	6.20493300	6.58297900	0.02143600
C	0.37550100	-2.45370600	-1.09522600	O	-5.37968500	7.27422900	0.53824300
C	-0.97200900	-2.36720700	-1.07801800	H	7.69383700	6.53506500	-1.69760200
C	0.69004800	2.43262400	-0.85605900	H	-5.89761200	8.08877400	0.46880200
C	-0.65896300	2.51783300	-0.83972900	H	-6.84997800	-5.59897600	-2.35647800
C	3.36081100	-0.19963900	-0.85685700	H	5.68983800	-8.04078400	0.11418100
C	-3.64061700	0.24732500	-0.79757400	C	-1.18125700	-0.59353000	2.97347600
C	0.57871600	-0.01655200	-0.91140800	C	-0.62446700	0.76348100	2.56956100
C	-0.85900500	0.07490300	-0.90294000	C	0.79358900	0.95263800	3.07211200
H	5.83054500	-4.37307300	-2.46040300	C	1.64662400	-0.24100500	2.62324200
H	-6.61035200	-3.60409800	-2.31591400	O	1.05066700	-1.44000000	3.08482200
H	6.25878100	3.60916100	-2.57795800	C	3.06767800	-0.19960000	3.16416500
H	-5.96658000	4.58102800	-2.32530700	C	-0.21882200	-1.68331800	2.51311700
H	3.51395700	-5.58236600	0.91547400	O	-0.62980800	-2.95581300	2.85375600
H	-4.43698100	-5.03054400	1.08499400	H	-0.15009900	-1.66583400	1.41970600
H	4.35828700	5.10649800	0.93811200	H	-1.25324600	-0.64556400	4.07291800
H	-3.85213500	5.52139700	1.26127300	O	-2.43313700	-0.81492400	2.37812600
H	2.28529500	-3.45032600	0.85094500	H	-2.91485900	0.02201600	2.37499000
H	-2.95729500	-3.04472900	0.95963100	H	-0.60173500	0.79198700	1.47616000
H	2.85307100	3.15210000	0.96133500	O	-1.50593100	1.81014800	2.93712800
H	-2.66618900	3.36092100	1.13991800	H	-1.40883900	1.99296500	3.87901700
H	4.59623300	-2.22827800	-2.53848200	H	0.80115700	0.98322100	4.16950800
H	-5.14302500	-1.66456700	-2.44867800	O	1.33541900	2.18383400	2.62519200
H	4.75106100	1.66230500	-2.56961300	H	0.88901800	2.43872000	1.80593300
H	-4.77275700	2.41509900	-2.46098200	H	1.70164200	-0.24047200	1.52603200
H	-1.12957900	3.49076500	-0.86662500	H	-0.76175600	-2.99851000	3.80822300
H	1.27806700	3.33899600	-0.90506100	H	3.53499200	-1.16334400	2.96068200
H	-1.56481600	-3.26407100	-1.19124600	H	3.03978000	-0.06135000	4.25264300
H	0.84681700	-3.41790900	-1.22444700	O	3.85108100	0.78515600	2.53337900
H	4.44008100	-0.27040100	-0.78838800	H	3.37782400	1.62358900	2.58819600

19. Glucose-pyrene (configuration 2) (M06-2X)

Number of atoms = 102

SCF(SCRF) = -2981.56716481

C	2.86390600	-1.07634500	0.85850400	C	-4.64568600	2.64541600	-0.25806400
C	-2.81396000	-1.23991700	0.84202500	C	0.73781700	-2.36372900	0.91258500
C	2.79549200	1.36923000	0.80632500	C	-0.61086800	-2.40469300	0.90188900
C	-2.88740300	1.20748400	0.81936000	C	0.59595300	2.53363300	0.82890300
C	1.45652700	-1.12314000	0.95005100	C	-0.75556500	2.49588400	0.84092100
C	-1.40455100	-1.20878900	0.93415400	C	3.49225200	0.16259000	0.76301300
C	1.38892700	1.33921500	0.90186400	C	-3.51276000	-0.03643100	0.76388300
C	-1.47947300	1.25606600	0.91005500	C	0.70976700	0.08815900	0.96661100
C	5.36299000	-3.71182500	-0.22883800	C	-0.72908900	0.04586900	0.96206100
C	-5.18370400	-3.99501100	-0.25224600	H	6.01936500	-3.91978500	-1.06385000
C	5.20012700	4.06059200	-0.35932300	H	-5.87367200	-4.15296400	-1.07354100
C	-5.43250500	3.78890900	-0.30197000	H	5.88156900	4.22977400	-1.18178500
C	5.33042200	-4.60545900	0.83838800	H	-6.13419400	3.94590300	-1.11094300
C	-5.03706300	-4.94222300	0.75780900	H	4.44959100	-5.03239800	2.74805600
C	5.06426600	5.02749300	0.63354900	H	-4.08456400	-5.37537300	2.61808200
C	-5.32763700	4.75912600	0.69154200	H	4.09080800	5.54369000	2.46341500
C	6.21528000	-5.81605000	0.79228200	H	-4.34804500	5.29782600	2.52265900
C	-5.78104000	-6.26088000	0.78708600	H	3.02280300	-3.02304500	2.75312200
C	5.83310700	6.31540900	0.61558700	H	-2.78702600	-3.27048800	2.66986100
C	-6.18901300	5.98539200	0.59829000	H	2.77451800	3.44970300	2.57395600
C	4.47860000	-4.34825600	1.91117100	H	-2.95335000	3.27093200	2.59995100
C	-4.17582400	-4.65450100	1.81612100	H	4.58185800	-1.90364600	-1.07678700
C	4.18317000	4.79494500	1.68740900	H	-4.59549000	-2.08304100	-1.02317900
C	-4.42802200	4.55924700	1.73686200	H	4.56820700	2.14439000	-1.08311600
C	3.67510500	-3.21709400	1.91018400	H	-4.73178500	1.90041100	-1.04093500
C	-3.45406900	-3.47245600	1.84061400	H	-1.31166900	3.41927500	0.75214900
C	3.44559500	3.62270200	1.74141500	H	1.09768500	3.48629400	0.72854300
C	-3.64047900	3.41738500	1.77546100	H	-1.11000300	-3.36048400	0.82305200
C	3.70361300	-2.31325200	0.84481300	H	1.29899500	-3.28510800	0.84053700
C	-3.58118400	-2.52425400	0.81865100	H	4.57355100	0.18941800	0.69302500
C	3.56643700	2.64759600	0.74564800	H	-4.59411800	-0.06929800	0.69830100
C	-3.72666900	2.44388800	0.77593700	O	6.96609100	-6.07651600	-0.10567200
C	4.56210500	-2.57707400	-0.22633700	O	-6.25722100	-6.70668900	-0.38969900
C	-4.47329500	-2.79924300	-0.21870200	O	6.65007700	6.41762400	-0.44616600
C	4.46154200	2.88520800	-0.29962000	O	-6.97374500	6.19802400	-0.28291300

O	6.08328400	-6.59838000	1.87809800	H	-1.53657400	-1.27682800	-4.19682500
O	-5.94618300	-6.88780700	1.78861500	H	-1.62454500	0.05781900	-1.46420600
O	5.74078500	7.17256100	1.44930000	O	-2.88960100	0.62099100	-2.99671800
O	-5.98982800	6.83824200	1.61760500	H	-2.85823200	1.58302200	-2.92249100
H	7.10139400	7.27078400	-0.37494200	H	-0.55972400	1.13881000	-4.10743600
H	-6.58143900	7.59089500	1.47547900	O	-0.65601100	2.34979400	-2.51061100
H	-5.92866800	-6.17000300	-1.11924400	H	-0.60951400	2.31937900	-1.54319400
H	6.68622800	-7.34606600	1.76016600	H	0.90100200	0.37173600	-1.54941800
C	-1.64518000	0.13079300	-2.56039700	O	1.88754500	1.23454600	-3.14938000
C	-0.51208100	1.03254300	-3.01839500	H	1.66594800	2.15970100	-2.98541300
C	0.83105200	0.43913100	-2.64388600	H	0.92923800	-0.92752400	-4.30200700
C	0.93868700	-0.97726600	-3.20368300	H	-2.22390000	-2.25990500	-1.66430300
O	-0.15284000	-1.73816900	-2.72315500	H	2.16829000	-2.72351900	-3.11807000
C	2.18839800	-1.70548400	-2.72855800	H	2.14055000	-1.76523700	-1.63436100
C	-1.43403400	-1.27944700	-3.10479900	O	3.38706900	-1.10497400	-3.16281700
O	-2.36263800	-2.17998000	-2.61822600	H	3.28073300	-0.14572400	-3.12761600

20. Cellobiose-pyrene (configuration 1) (M06-2X)

Number of atoms = 123

SCF(SCRF) = -3592.38193467

C	-1.87875400	1.25102800	-1.49395200	C	-5.19225600	-5.99082000	-1.66202900
C	3.77654800	1.16563200	-0.89786800	C	6.76174600	-6.20993600	-0.36010500
C	-1.90414900	-1.20101900	-1.57650200	C	-3.24439900	4.67379400	-0.53414900
C	3.73952700	-1.28117700	-0.91041800	C	5.06621600	4.49889300	0.39357100
C	-0.47045400	1.24186800	-1.37567100	C	-3.39138400	-4.57957500	-0.68238600
C	2.38112800	1.19495700	-1.08776100	C	4.86733000	-4.67816400	0.35814200
C	-0.49659000	-1.22716400	-1.45915400	C	-2.49560200	3.50254600	-0.51905600
C	2.34479400	-1.26646100	-1.11968100	C	4.30193800	3.34913100	0.25995800
C	-4.41826900	3.89745600	-2.47828400	C	-2.58865600	-3.44912400	-0.66062400
C	6.42383800	3.82239400	-1.45810900	C	4.14650900	-3.49900700	0.21465100
C	-4.52545100	-3.74003400	-2.62339700	C	-2.67825700	2.51342700	-1.49380000
C	6.33232000	-4.00254500	-1.41987200	C	4.58242600	2.41442400	-0.74342300
C	-4.20808400	4.88832200	-1.52026000	C	-2.73305700	-2.44262500	-1.62230500
C	6.12458500	4.76312400	-0.47470300	C	4.50292000	-2.55595500	-0.75492800
C	-4.36291500	-4.74086800	-1.66811800	C	-3.66750800	2.72963200	-2.46113900
C	5.96258400	-4.94440200	-0.46285000	C	5.66692600	2.66377400	-1.58521100
C	-5.02687200	6.14667500	-1.59321000	C	-3.72284400	-2.60691700	-2.59523100
C	6.90553900	6.04356800	-0.28273000	C	5.61416000	-2.82405400	-1.55963200

C	0.31161700	2.44658400	-1.36865000	H	-6.56906100	-6.86144100	-2.58243800
C	1.65538700	2.42333000	-1.24065900	H	6.88072900	-7.81621000	0.59043800
C	0.25509200	-2.44862600	-1.52021800	H	7.42307100	5.94512200	-2.12159400
C	1.59471300	-2.46694400	-1.35135300	H	-5.29416200	7.78924500	-0.73573400
C	-2.55062500	0.03344200	-1.60906700	C	-0.01099700	1.30699300	2.85168800
C	4.41911600	-0.06847500	-0.82505600	C	1.37579700	1.69035100	2.36958700
C	0.22380600	-0.00287600	-1.33886800	C	2.37685700	0.64112300	2.81620900
C	1.65451800	-0.02482300	-1.18043000	C	0.74731200	-1.07809400	2.80532200
H	-5.16736200	4.06255900	-3.24192000	C	-0.35465600	-0.10076200	2.39492300
H	7.26996100	3.95549800	-2.12334400	H	1.37261500	1.68832400	1.27265500
H	-5.27555700	-3.85223800	-3.39416500	H	-0.02544500	1.32737000	3.95064800
H	7.18308400	-4.21166200	-2.05530800	H	0.77585000	-1.13902500	3.90489500
H	-3.08438500	5.42533400	0.22760900	H	-0.43493400	-0.10513500	1.29957800
H	4.85493200	5.20889600	1.18250000	H	2.41262900	0.59484600	3.91684300
H	-3.27509300	-5.35263200	0.06662600	O	1.75496900	2.94841700	2.87129200
H	4.57676600	-5.39467700	1.11432200	H	0.99893200	3.53644100	2.75536800
H	-1.76353100	3.34187500	0.26558400	O	3.61278800	0.95303900	2.28233900
H	3.49916200	3.15715500	0.96252900	H	4.21874500	0.22781200	2.47147700
H	-1.85936400	-3.32997100	0.13128500	O	1.98668300	-0.61776600	2.30985600
H	3.30669900	-3.30286100	0.87379400	C	0.49423000	-2.45129700	2.21566400
H	-3.82998100	1.98192700	-3.22748500	H	-0.52008900	-2.76995900	2.47238000
H	5.91474800	1.94673200	-2.35832500	H	0.57071000	-2.36586400	1.12965800
H	-3.85264200	-1.84411400	-3.35314900	O	1.46220500	-3.40451700	2.60553600
H	5.90402400	-2.10696300	-2.31798900	H	1.29865300	-3.66311600	3.51669900
H	2.12586800	-3.40675500	-1.41280400	O	-0.89823900	2.27900700	2.33683800
H	-0.26852500	-3.37234400	-1.72155500	H	-1.80740400	1.98938000	2.51566800
H	2.20783700	3.35247800	-1.26542400	O	-1.57856100	-0.53846400	2.97137400
H	-0.18863500	3.39433100	-1.50503300	C	-2.69330600	-0.46304200	2.16991700
H	-3.63432600	0.04168800	-1.67814000	C	-3.70935300	-1.52620400	2.54246300
H	5.48836900	-0.08518200	-0.64495400	C	-4.87897500	-1.38083500	1.58392000
O	-5.85933800	6.36287000	-2.42792100	C	-5.46758300	0.01554200	1.64436100
O	7.62464600	6.47058300	-1.34008300	C	-4.36746700	1.06252100	1.45650700
O	-6.08702200	-6.02632400	-2.66471000	H	-2.41517200	-0.57713400	1.11045400
O	7.70584400	-6.47791100	-1.05041600	H	-4.50656600	-1.55127000	0.56159100
O	-4.72504400	7.01549000	-0.61583700	H	-5.92295900	0.15673600	2.63482800
O	6.90082100	6.66456600	0.73613100	H	-4.00634300	1.00892200	0.42042300
O	-5.08406100	-6.87454500	-0.85837400	H	-4.04169300	-1.34750100	3.57237800
O	6.30928600	-7.03538900	0.60004400	O	-3.11247400	-2.79299800	2.41643400

H	-3.82915600	-3.43632800	2.34128700	H	-4.01321900	3.15965800	1.76396500
O	-5.82415900	-2.37062200	1.92204200	H	-5.35827000	2.50274100	2.70696600
H	-6.57238800	-2.28516100	1.32017800	O	-5.81842100	2.87070300	0.76943600
O	-6.44118700	0.08678600	0.62638600	H	-5.35560300	3.13430900	-0.03676900
H	-6.71803900	1.00886200	0.53495000	O	-3.29644800	0.81596500	2.35247200
C	-4.86298000	2.47265600	1.73495100				

21. Cellobiose-pyrene (configuration 2) (M06-2X)

Number of atoms = 123

SCF(SCRF) = -3592.38140779

C	3.01180600	0.33763100	-1.43176900	C	4.03520900	1.41465200	-1.57889600
C	-2.58697300	1.34411400	-1.49298900	C	-3.14823000	2.72091400	-1.63642400
C	2.57356900	-2.05956600	-1.17747500	C	3.14920700	-3.43317600	-1.04912300
C	-3.01970800	-1.05685000	-1.31261600	C	-4.02785300	-2.15690700	-1.21197900
C	1.62328600	0.59906900	-1.42021600	C	5.14790300	1.45395200	-0.73041300
C	-1.19759500	1.10333100	-1.44600600	C	-4.09574200	3.19758300	-0.73220500
C	1.18286400	-1.81781600	-1.19755800	C	4.09918300	-3.70697200	-0.06127700
C	-1.63366900	-1.31349600	-1.28288900	C	-4.91151800	-2.20860700	-0.13099000
C	6.10494400	2.45095300	-0.84748500	C	1.09026900	1.93253500	-1.39848600
C	-4.62228700	4.47821100	-0.85257400	C	-0.23818400	2.17046500	-1.40764500
C	4.65506400	-4.97467000	0.06694900	C	0.22057100	-2.86995800	-1.03057400
C	-5.85673600	-3.22030100	-0.02891300	C	-1.10746300	-2.63487200	-1.08947200
C	5.98689300	3.43103100	-1.82974200	C	3.44573800	-0.97987300	-1.29116300
C	-4.22876200	5.31670700	-1.89204300	C	-3.46115800	0.26082100	-1.40651600
C	4.28278300	-5.99761700	-0.80030600	C	0.70236600	-0.48480300	-1.33267600
C	-5.94805800	-4.20056500	-1.01165000	C	-0.71335600	-0.23103600	-1.35804600
C	7.03586100	4.49774400	-1.91029600	H	6.95282500	2.48493400	-0.17549800
C	-4.76048600	6.71811600	-2.09056900	H	-5.36278800	4.78319000	-0.12112500
C	4.85014000	-7.38180700	-0.70369000	H	5.37957400	-5.17050000	0.84558100
C	-6.98881400	-5.26967600	-0.86239400	H	-6.52652200	-3.26803000	0.81955300
C	4.90220600	3.38426600	-2.70289400	H	4.81172500	4.12669700	-3.48393200
C	-3.30535100	4.83322000	-2.81886400	H	-3.01962200	5.47335900	-3.64320100
C	3.35097800	-5.72920500	-1.80122700	H	3.07656500	-6.52369100	-2.48301100
C	-5.07169000	-4.15950300	-2.09515100	H	-5.13672200	-4.91620300	-2.86487200
C	3.94284000	2.38963800	-2.57715200	H	3.11341000	2.35998700	-3.27254500
C	-2.76857400	3.56293000	-2.68839200	H	-2.05104300	3.20820200	-3.41827100
C	2.79271500	-4.46686400	-1.92240900	H	2.07949500	-4.27086100	-2.71347800
C	-4.12277900	-3.15168700	-2.18945700	H	-3.44906900	-3.12592600	-3.03735200

H	5.24678400	0.70169700	0.04362600	O	-5.49866600	0.81951800	3.14175000
H	-4.41039500	2.58379000	0.10097100	H	-5.99116800	0.01091200	2.96249000
H	4.40038300	-2.91558700	0.61689100	O	-3.66581900	-0.48504100	2.90259100
H	-4.83111200	-1.47203600	0.66046900	C	-1.94456500	-2.10885000	2.67237400
H	-1.79773900	-3.46134400	-0.97690400	H	-0.90352000	-2.23018700	2.35860400
H	0.57336200	-3.87395000	-0.84198200	H	-2.00081800	-2.21017700	3.75814200
H	-0.59648500	3.18940500	-1.35678600	O	-2.77454900	-3.11605200	2.13647900
H	1.77652300	2.76550600	-1.33869700	H	-2.65710100	-3.13568200	1.18076800
H	4.51093400	-1.17805000	-1.29905100	O	-1.24723500	2.80890500	2.86945700
H	-4.52840300	0.44900600	-1.44751700	H	-0.32620300	2.68112900	2.59896100
O	7.98092400	4.57887700	-1.17587100	O	-0.21552600	0.14799300	2.00454000
O	-5.36735400	7.28925500	-1.03398700	C	0.96916900	0.31249800	2.68133500
O	5.73713600	-7.51197400	0.29795100	C	2.04302100	-0.53559300	2.01654100
O	-7.77646900	-5.33056800	0.03950400	C	3.39355900	-0.20556100	2.62360300
O	6.81112600	5.37485400	-2.90380000	C	3.67204700	1.28208700	2.54725900
O	-4.65571400	7.31043800	-3.12175100	C	2.54091200	2.03736100	3.23836200
O	4.55696800	-8.28883700	-1.43167500	H	0.86629700	0.02362600	3.73903700
O	-6.95435000	-6.17117000	-1.85930500	H	3.38702900	-0.50356800	3.68165300
H	6.04552000	-8.42914400	0.28339400	H	3.67856500	1.58807700	1.49147300
H	-7.65512700	-6.81433500	-1.68105900	H	2.51944800	1.76294900	4.30437100
H	-5.28005100	6.73971600	-0.24786700	H	2.05378600	-0.28240400	0.95317300
H	7.53244700	6.01953900	-2.87918400	O	1.69951700	-1.88372900	2.21997600
C	-2.00847900	1.73078500	2.37476300	H	2.34704600	-2.43299700	1.76134400
C	-3.40408800	1.89149500	2.95591700	O	4.38188200	-0.94044700	1.92834500
C	-4.27193300	0.72774800	2.51486500	H	5.23582000	-0.68544600	2.29974000
C	-2.41245400	-0.71887600	2.29100700	O	4.93403400	1.47969800	3.14173500
C	-1.42690400	0.36756900	2.71817100	H	5.08845000	2.43078700	3.21741800
H	-3.34817200	1.85872200	4.05139000	C	2.66341200	3.54709300	3.08961200
H	-2.07975800	1.78748100	1.27706400	H	1.79415200	4.03250000	3.54172000
H	-2.51060300	-0.66109900	1.19619300	H	2.67504500	3.79316000	2.02636000
H	-1.24664600	0.30203300	3.79852300	O	3.87672100	4.03595900	3.63462900
H	-4.37399800	0.73646700	1.41449100	H	3.79455700	4.10089800	4.59076300
O	-3.97693800	3.09988900	2.51640500	O	1.32090800	1.69108800	2.60987300
H	-3.30006100	3.77934400	2.62452400				

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