1	SUPPORTING INFORMATION FOR:			
2	Efficient structural and energetic screening of fullerene encapsulation in a large			
3	supramolecular double decker macrocycle			
4	Fabian Bohle and Stefan Grimme*			
5				

6 <u>GFN2-xTB:</u>

7 Version 6.1 of GFN2-xTB¹ was used, as implemented in the *xtb* code. All GFN2-xTB calculations were 8 carried out with the GBSA implicit solvation model and CHCl₃ as solvent. For all calculations (optimizations and hessian calculations) the 'very tight' settings were used (verytight: E_{conv} (energy 9 convergence) = $1 \cdot 10^{-7}$ E_h; G_{conv}(gradient convergence) = $2 \cdot 10^{-4}$ E_h· α^{-1} ; accuracy(for integral cutoffs and 10 SCF criteria) = 0.05). Vibrational frequencies were calculated for thermostatistical correction to free 11 12 energy and to verify that the optimized geometries are indeed minimum structures on the electronic potential hypersurface (check for no imaginary modes). The thermostatistical contributions to free 13 energy are calculated in the rigid-rotor-harmonic-oscillator approach (RRHO)² and include zero point 14 15 vibrational energies at 298.15 K. To reduce the error of the harmonic approximation for low-lying 16 vibrational frequencies as well as numerical noise in the calculations, the RRHO-scheme (an interpolation between the rigid-rotor (RR)- to the harmonic oscillator (HO) is applied at low-lying 17 frequencies (every vibrational mode below 50 cm⁻¹). 18

19

20 <u>xTB-IFF:</u>

21 The intermolecular forcefield xTB-IFF³ is implemented in a standalone code called *xtbiff* and is generated from 'low cost' quantum mechanical (OM) input data (atomic partial charges, localized 22 molecular orbitals and frontier orbital energies and densities have to be provided), here generated by 23 24 GFN2-xTB(GBSA(CHCl₃)). The QM data from each fragment is used to dock the intermolecular 25 fragments and generate the best docking position. The docking itself is run in gas phase, but the provided QM input data is generated within the GBSA implicit solvation model. xTB-IFF returns the 26 27 intermolecular interaction energy and several docking geometries sorted by their interaction energies. Since only rigid fragments are docked, the best xTB-IFF geometry has to be optimized once more by 28 29 GFN2-xTB(GBSA).

30

31 <u>B97-3c/COSMO reference calculations:</u>

32 B97-3c/COSMO(ε =4.8)⁴ reference single-point calculations were performed with the TURBOMOLE.7.2.1 program package⁵. The resolution-of-identity (RI) approximation for Coulomb 33 integrals was generally applied⁶ using the matching default auxiliary basis sets⁷. The integration of the 34 exchange-correlation contribution was performed on the numerical quadrature grids m4. The default 35 convergence criteria for single-points [10⁻⁷ E_h] was applied. To be able to compare to the GFN2-36 37 xTB(GBSA) calculations the implicit solvent model COSMO was applied.

38

39 <u>Reaction path calculation:</u>

40 The reaction path is calculated to get a good guess on the transition state structure. To start from 41 reasonable geometries reactants and products are optimized with GFN2-xTB(GBSA(CHCl₃)). The 42 reaction path is then calculated with the growing string method GSM⁸ using GFN2-

- xTB(GBSA(CHCl₃)) as the underlying electronic structure method. The reaction path was calculated
 with 20 nodes on the reaction string. Geometries close to the estimated transition state were picked and
 hessians were calculated to find the imaginary mode of the transition state. On the examined reaction
 path no transition state could be obtained (no single imaginary mode was obtainable).
- 47
- 48 TABLE I: Lowest lying fullerene isomers determined by GFN2-xTB(GBSA(CHCl₃) free energy:

 (https://dx.doi.org/10.1063/1.5012601) 5. TURBOMOLE V7.2.1 2017, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989–2007, TURBOMOLE GmbH, since 2007; available from http://www. turbomole.com. 6. K. Eichkorn, O. Treutler, H. Öhm, M. Häser, R. Ahlrichs, <i>Chem. Phys. Lett.</i> 242 (1995) 652 (https://dx.doi.org/10.1016/0009-2614(95)00838-U) 7. F. Weigend, <i>Phys. Chem. Chem. Phys.</i> 8 (2006) 1057 (https://dx.doi.org/10.1039/b515623h) 		Full	erene isomer name within the manuscript:	Fullerene name from <i>Tomaneks</i> ' ⁹ ESI:		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			C ₆₀	C ₆₀		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$						
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$						
$ \begin{array}{ccccc} C_{78} & C_{78-C2v-3} \\ C_{80} & C_{80,D5h-6} \\ C_{84} & C_{84+D2-22} \\ C_{90} & C_{90-C2-45} \\ C_{96-D2-183} \\ C_{100-D2-449} \end{array} $						
Cs0 Cs0 Cs0-D5h-6 Cs4 Cs4-D2-22 Cs0-C2-45 Cs0 Cs0-C2-45 Cs0-D2-245 Cs0 Cs0-D2-249 Cs0-D2-249 Image: Cs0 Cs0-D2-249 Cs0-D2-249 Cs0 Cs0-D2-249 Cs0-D2-249 Cs0 Cs0-D2-249 Cs0-D2-249 Cs0 REFERENCES: Cs0-D2-249 Cs0 Cs0-D2-249 Cs0-D2-249 Cs0 Cs1-Ds1-Ds1-Ds1-Ds1-Ds1-Ds1-Ds1-Ds1-Ds1-D						
C84 C84D2-22 C90 C96C245 C96 C96C245 C96 C96C245 C96 C96C245 C96 C100-D22449 60 REFERENCES: 51 1. C. Bannwarth, S. Ehlert, S. Grimme, J. Chem. Theory Comput. 15 (2019) 1652 (https://dx.doi.org/10.1021/acs.jctc.8b01176) 2. 53 2. S. Grimme, Chem. Eur. J. 18 (2012) 9955 (https://dx.doi.org/10.1002/chem.201200497) 54 3. S. Grimme, C. Bannwarth, E. Caldeweyher, J. Pisarek, A. Hansen, J. Chem. Phys. 147 (2017) 55 161708 (https://dx.doi.org/10.1063/1.4991798) 56 4. J. G. Brandenburg, C. Bannwarth, A. Hansen, S. Grimme, J. Chem. Phys. 148 (2018) 064104 (https://dx.doi.org/10.1063/1.5012601) 58 5. TURBOMOLE V7.2.1 2017, a development of University of Karlsruhe and 59 Forschungszentrum Karlsruhe GmbH, 1989–2007, TURBOMOLE GmbH, since 2007; 50 available from http://www. turbomole.com. 51 6. K. Eichkorn, O. Treutler, H. Öhm, M. Häser, R. Ahlrichs, Chem. Phys. Lett. 242 (1995) 652 52 (https://dx.doi.org/10.1016/0009-2614(95)00838-U) 53 7. F. Weigend, Phys. Chem. Chem. Phys. 8 (2006) 1057 (https://dx.doi.org/10.103						
$\begin{array}{c} \begin{array}{c} C_{90} \\ C_{96} \\ C_{96} \\ C_{96} \\ C_{96} \\ C_{96} \\ C_{96} \\ C_{100-D2-449} \end{array} \\ \end{array}$						
C_{100} $C_{100-D2.449}$ 19 REFERENCES: 11 C. Bannwarth, S. Ehlert, S. Grimme, J. Chem. Theory Comput. 15 (2019) 1652 (https://dx.doi.org/10.1021/acs.jctc.8b01176) 12 S. Grimme, Chem. Eur. J. 18 (2012) 9955 (https://dx.doi.org/10.1002/chem.201200497) 13 S. Grimme, C. Bannwarth, E. Caldeweyher, J. Pisarek, A. Hansen, J. Chem. Phys. 147 (2017) 161708 (https://dx.doi.org/10.1063/1.4991798) 14 J. G. Brandenburg, C. Bannwarth, A. Hansen, S. Grimme, J. Chem. Phys. 148 (2018) 064104 (https://dx.doi.org/10.1063/1.5012601) 15 TURBOMOLE V7.2.1 2017, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989–2007, TURBOMOLE GmbH, since 2007; available from http://www. turbomole.com. 16 K. Eichkorn, O. Treutler, H. Öhm, M. Häser, R. Ahlrichs, Chem. Phys. Lett. 242 (1995) 652 (https://dx.doi.org/10.1016/0009-2614(95)00838-U) 17 F. Weigend, Phys. Chem. Chem. Phys. 8 (2006) 1057 (https://dx.doi.org/10.1039/b515623h) 18 P. M. Zimmerman, J. Chem. Phys. 138 (2013) 184102 (https://dx.doi.org/10.1063/1.4804162) 19 David Tománek, Guide Through the Nanocarbon Jungle, Morgan & Claypool Publishers, San Rafael, USA, 2014 (http://dx.doi.org/10.1088/978-1-627-05273-3)						
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