Supplementary material

Supramolecular self assembled chlorophyll derivative fullerene donor - acceptor system for photoinduced charge separation; Zn *pyro*-pheophorbide *a* – fulleronicotine dyad

Jari Kavakka, Sami Heikkinen, Ilkka Kilpeläinen, Nikolai V. Tkachenko and Juho Helaja

1. Characterization of *pyro*-pheophorbide *a* (1) and fulleronicotine (2)

Characterizations: **1**: ^{1}H NMR (500MHz, DMSO, 27 ^{o}C): δ = 9.64 (s, 1 H, 10-H), 9.33 (s, 1 H, 5-H), 8.59 (s, 1H, 20-H), 8.19 (dd, $^3J_{cis}$ = 11.5 Hz, $^3J_{trans}$ = 18.0 Hz, 1 H, 3^1-H), 6.26 (dd, $^2J_{gem}$ = 1.5 Hz, $^3J_{trans}$ = 18.0 Hz, 1 H, 3^2_{trans}-H), 6.08 (dd, $^2J_{gem}$ = 1.5 Hz, $^3J_{cis}$ = 11.5 Hz, 1 H, 3^2_{cis}-H), 5.14 (d, $^2J_{gem}$ = 19.5 Hz, 1 H, 13^2-H), 5.08 (d, $^2J_{gem}$ = 19.5 Hz, 1 H, $13^{2'}$-H), 4.57 (m, 1 H, 18-H), 4.30 (m, 1 H, 17-H), 3.81 (m, 2 H, 8^1-H), 3.62, 3.376, 3.286 (each s, 3 H, 12^1-, 2^1-, 7^1-H), 2.61-1.27 (m, 4 H, 17^1-, 17^2-H), 1.80 (d, $^3J_{181\text{-}18}$ = 7.0 Hz, 3 H, 18^1-H), 1.70 (t, $^3J_{82\text{-}81}$ = 7.5 Hz, 3 H, 8^2-H). HRMS (ESI + H^+): calcd. for $C_{33}H_{32}N_4O_3Zn$ 596.1760; found 596.1746.; **2**: ^{1}H NMR: (300 MHz, 1:1 CS_2:$CDCl_3$, 27 °C): δ = 9.01 (s, 1 H, 2-H), 8.59 (dd, J = 4.6Hz, J = 1.5Hz, 1 H, 6-H), 8.16 (d, J = 7.3Hz, 1 H, 4-H), 7.37 (dd, J = 8.9Hz, J = 4.9Hz, 1 H, 5-H), 5.00 (d, J = 9.46 Hz, 1 H, 9_a-H), 4.97 (s, 1 H, 7-H), 4.29 (d, J = 9.5 Hz, 1 H, 9_b-H), 2.80 (s, NMe). HRMS (ESI + H^+): calcd. For $C_{68}H_{11}N_2$ 855.0917; found 855.0922. The characterization data is equivalent with earlier reports **1** [J. S. Kavakka, S. Heikkinen, J. Helaja *Eur. J. Org. Chem.* 2008, 4932–4937] and **2** [T. Da Ros, M. Prato, F. Novello, M. Maggini, E. Banfi *J. Org. Chem.* 1996, **61**, 9070-9072].

2. UV/Vis titration of Zn *pyro*-pheophorbide *a* (1) – fulleronicotine (2) dyad in $CHCl_3$

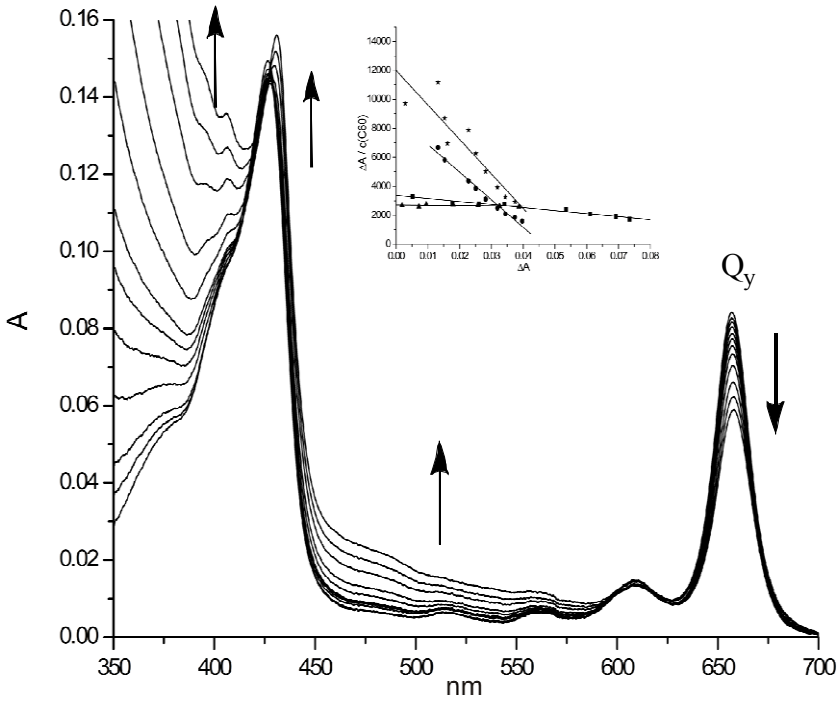


Fig. S1 UV/Vis titration of Zn-*pyro*-pheophorbide *a* (**1**) (3,85 μM) adding amounts fulleronicotine (**2**) (0 – 32.0 μM) in $CHCl_3$. The arrows show the directions of spectral changes. The inset chart illustrates very approximate Scatchard binding analysis (analyzed from Q_y band intensity) for **1** and **2** in $CHCl_3$ (K_a= 190 000 M^{-1}), in toluene (Ka =290 000 M^{-1}) methyl ester of **1** and **2** (Ka = 1700 M^{-1}) in toluene and in $CHCl_3$ (K_a= 21 000 M^{-1}). Overlapping of C_{60} signals with chlorin signals hinders reliable quantitative peak top intensity analysis; therefore abovementioned K_a values are very approximate in nature.

3. Stern-Volmer plots of fluorescence emission titrations

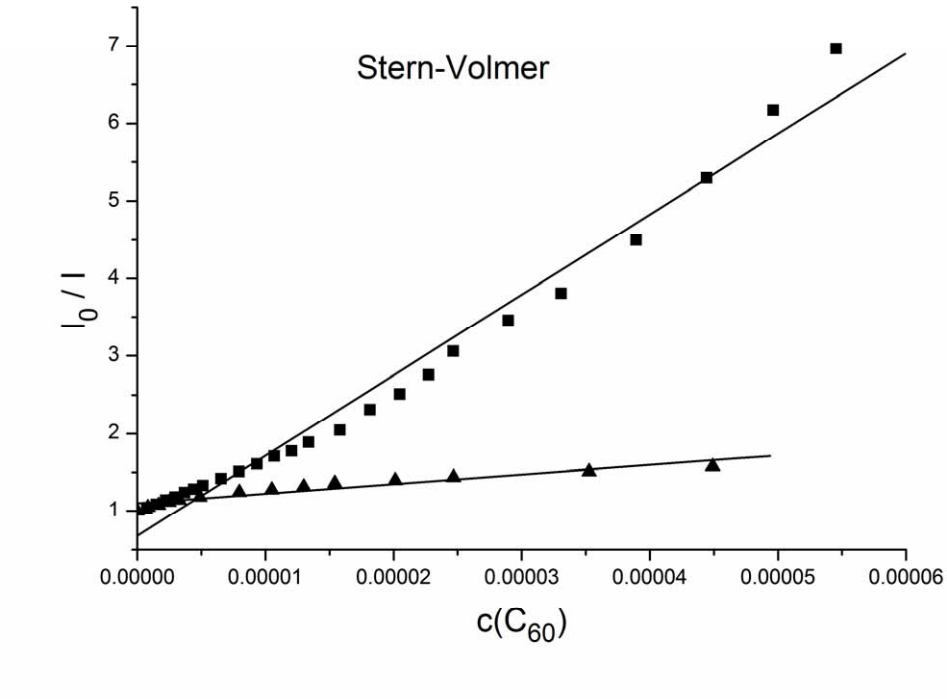


Fig. S2 The straight line fitted to squares shows quenching of **1** adding **2** (slope =103767), whereas the line fitted to triangles analysis quenching of methyl ester of **1** adding **2** (slope =12383).

4. Time resolved transient absorption and emission measurement of Zn *pyro*-pheophorbide *a* (1) – fulleronicotine (2)

The femtosecond pump-probe and up-conversion instruments were used to for time resolved measurements of absorption and emission, respectively. The instruments used were described elsewhere [N. V. Tkachenko, L. Rantala, A. Y. Tauber, J. Helaja, P. H. Hynninen, H. Lemmetyinen, *J. Am. Chem. Soc.* (1999), **121**, 9378-9387.]. In brief, Ti:sapphire laser pumped by CW Nd laser was used to generate 50 fs at 820 nm. The second harmonic at 410 nm was used to excite samples in up-conversion experiments. The sample emission was mixed with the laser fundamental harmonic and the signal at sum frequency was passed through a color filter and monochromator and detected by a photomultiplier working in single photon counting mode. In pump-probe experiments the pulses from the same laser were reduced in repetition rate from 90 MHz to 10 Hz by a pulse picker and amplified by Ti:sapphire multi-pass amplifier. The resulting 1 mJ pulses were split in to two beams. One was used as the pump after a second harmonic generator and another was passed to a white continuum generator and was used as probe. The time resolution of both instruments was 150-200 fs (FWHM).

The transient absorption measurements in the visible part of the spectrum had to be fitted by four exponential at least to obtain a reasonable fit quality. The resulting decay component spectra and their lifetime are presented in **Fig. S3**. The strongest signal in the range is near 660 nm is due to the bleaching of the ground state of the chlorin chromophore. A more complex fit model as compared to that used to fit data in the near IR (**Fig. 4**) is needed to account for the photochemistry of the chlorin-fullerene complexes and non-bound chlorins. Also the actual number of intermediate states is likely greater than four, but they could not be resolved for this experimental data, which resulted in discrepancies in lifetimes obtained from the data fits in the visible and near IR regions. However, the results in the near IR are believed to be more reliable for the monitoring of the charge separated state since in this part of the spectrum the signal is mainly due to the fullerene chromophore, and in particular the band at 1020 nm is typical for the fullerene anion.

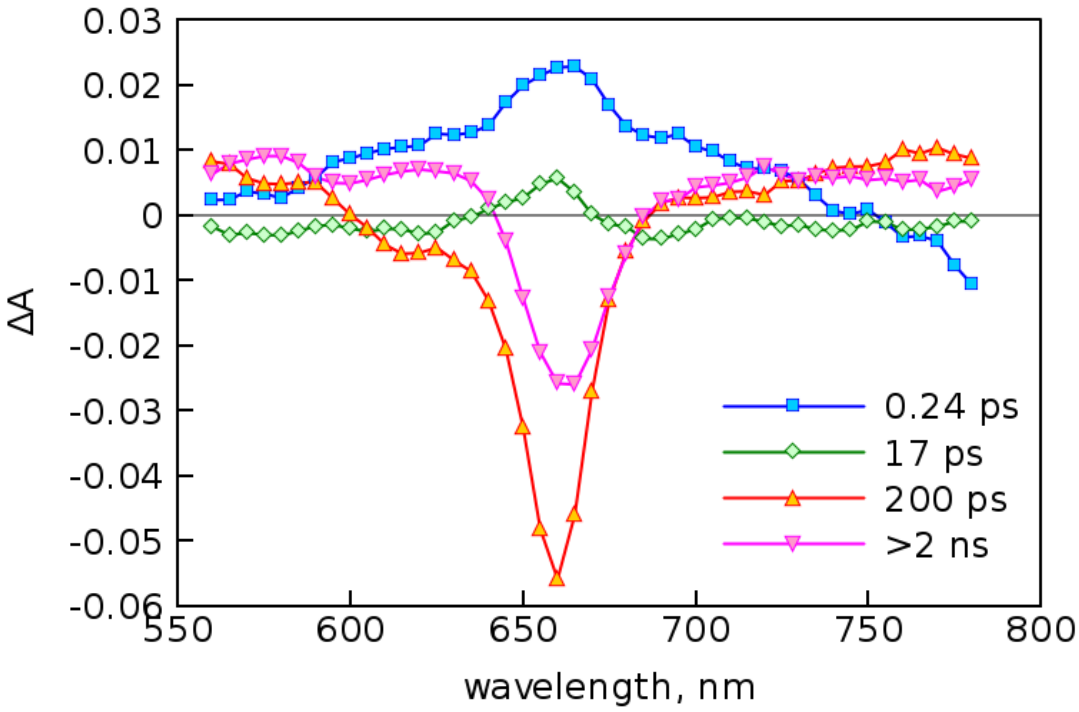


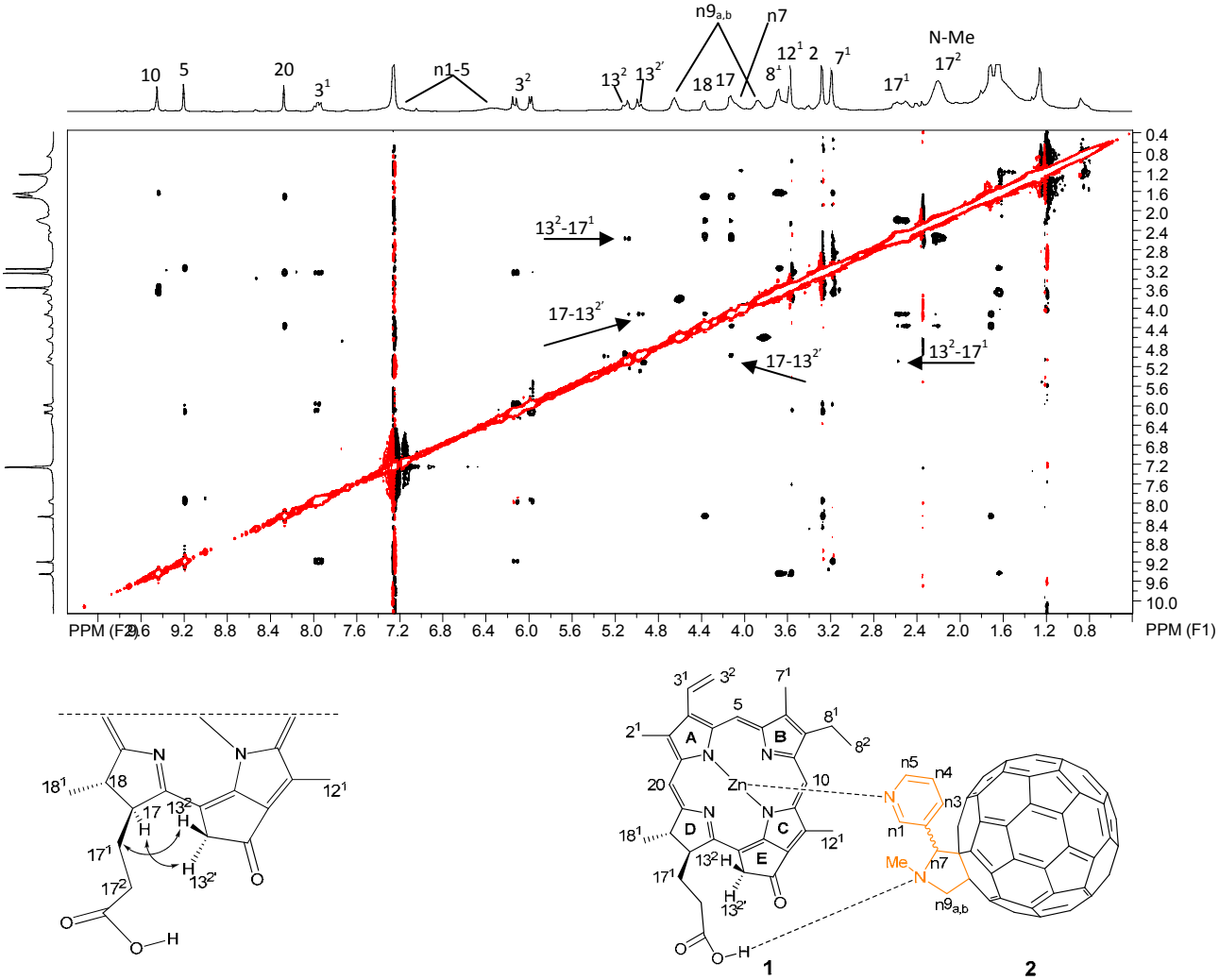
Fig. S3 Transient absorption decay component spectra of 1:1 complex of **1** and **2** in toluene obtained for 4-exponential fits of pump-probe measurements carried out in the visible part of the spectrum. The component lifetimes are indicated on the plots. Excitation wavelength was 410 nm.

5. ROESY spectrum of Zn *pyro*-pheophorbide *a* (1) – fulleronicotine (2) dyad in $CDCl_3$

All NMR experiments were performed at 27 °C using Varian Unity INOVA 500 NMR-spectrometer (500 MHz ^{1}H-frequency) equipped with 5 mm triple-resonance (^{1}H, ^{13}C, ^{15}N) probehead incorporating z-gradient coil.

Phase-sensitive ROESY-experiment was acquired with 16 transients and 200 increments using spectral width of 6153 Hz in both dimensions and relaxation delay of 2 s. Mixing was accomplished using 400 ms spinlock with RF-power of 1.9 kHz. The acquired data matrix 1231 x 200 (complex points) was apodized using squared cosine weighting function in both dimensions and zero-filled up to 2048 x 2048 (complex points) prior to Fourier transform.

ROESY spectrum of Zn *pyro*-pheophorbide *a* (**1**) and fulleronicotine (**2**) complex including partial assignation:



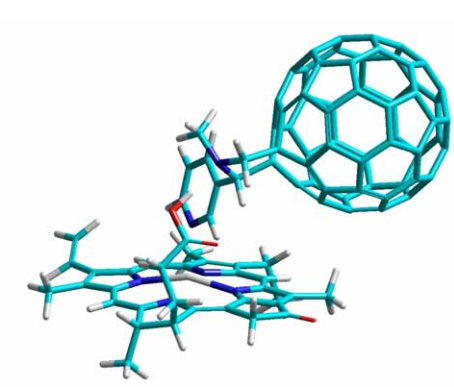
ROESY correlation:
1) Assignation of 13^2-CH_2 protons based on the correlation observed in between H-17– H -$13^{2'}$.
2) Indication spatial proximity of 17^1 CH_2 to 13^2 (both protons are above the macrocyclic plane).
These correlations combined with the absence of the correlation in between (CH_2) 17^2-(CH_2)13^2 protons agrees well with the global minima structures depicted *wide infra*.

6. Molecular modeling of Zn *pyro*-pheophorbide *a* (1) – fulleronicotine (2) dyad

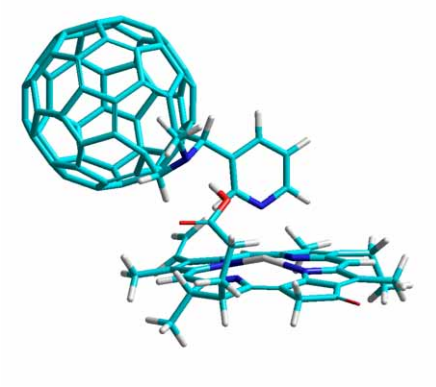
Geometry optimizations for Zn *pyro*-pheophorbide *a* (**1**) - fulleronicotine (**2**) complexes were performed with DFT B3LYP method on 6-31G(d) level using GAUSSIAN03 program. The optimizations were run as 4 processor paraller job in HP CP4000 BL ProLiant supercluster in the National Centre for Scientific Computing (CSC) in Espoo. Molecules and MO's were visualized with Gaussian view 3.09.

Prior to the DFT calculations conformational search was performed for the propionic acid side chain and for the pyrrolidine moiety of fulleronicotine with semiempirical RM1 method [G. B. Rocha, R. O. Freire, A. M. Simas, J. J. P. Steward *J. Comp. Chem.* **2006**, *27*, 1101–1111.] (via HyperChem interface). In the search all the propionic side chain rotamers and fulleronicotine pyrrolidine orientations were systematically studied. Structures showing (pyridine-Zn, COOH- *N*-pyrrolidine) 'two point' coordination were chosen for further optimizations on the DFT level [similarly as in J. S. Kavakka, S. Heikkinen, J. Helaja *Eur. J. Org. Chem.* 2008, 4932-4937.]. Due to rather extensive size of the DFT calculations, geometry optimizations were terminated after 20-25 optimization steps if the energy level of the complex structure still persisted >5 kcal/mol above so far found global minimum (After 20-25 steps only minor energy changes could observed, although due to flat potential surfaces complete refined optimization was achieved typically after 50-100 steps). As a result of this method only one local minimum could be found (in addition to the found global minima) for each β-ligated (above the chlorin plane) *R*- and *S*-fulleronicotine, respectively. In the case the chlorin α-ligation (**2** below the plane) there is less such rotamers for the propionic acid side chain, in which **1** could achieve 'two point' coordination with fulleronicotine **2**. For *R* and *S*-fulleronicotines the α-ligated minimum energy complexes are lying above 9 and 11 kcal/mol higher energy level than the corresponding β-ligated global energy minima. The reason for higher energy arises obviously from structural distortions in chlorin D-ring. This can be measured as a large H_{17}-H_{18} dihedral angle (165° and 170° for *R*- and *S*-**2**, respectively). Experimentally this wide torsion angle would result 9-10 Hz coupling in between there protons in the ^{1}H NMR spectra [J. Helaja, A. Y. Tauber, I. Kilpeläinen, P. Hynninen, *Magn. Reson. Chem.* 1997, **35**, 619-628]. However, this large coupling ($J_{17\text{-}18}$) was not observed in the ^{1}H NMR spectra of **1** + **2** adduct.

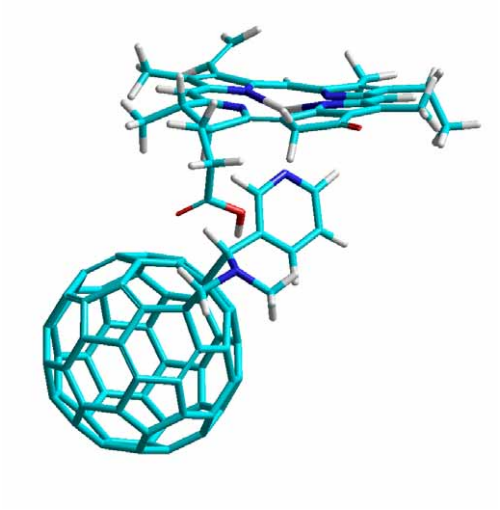
R-Fulleronicotine complexes



A *R* 0 kcal/mol

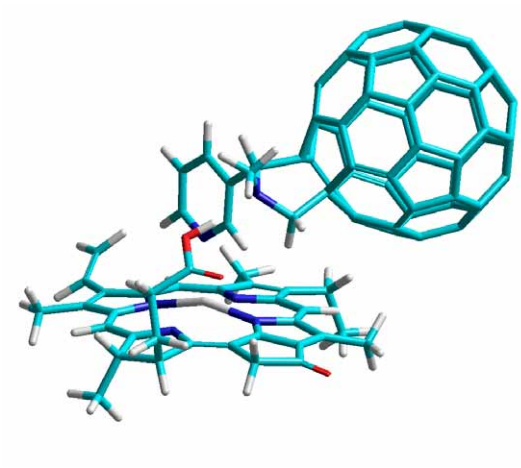


B R 3.313 kcal/mol

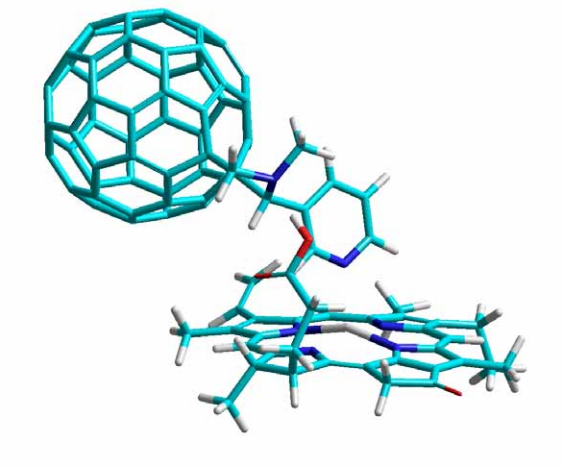


R 9.05 kcal/mol

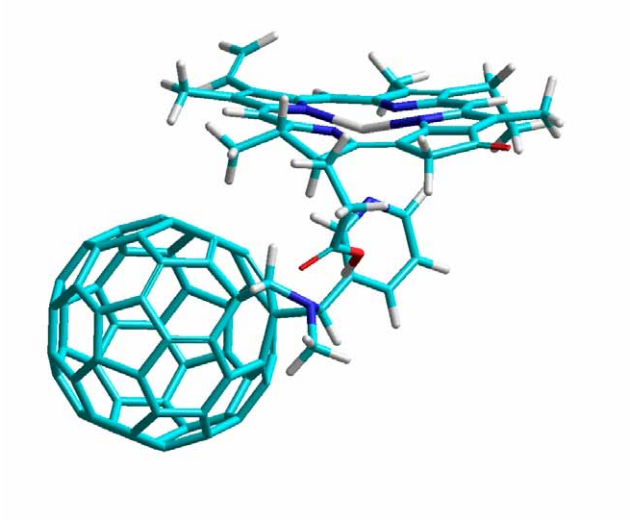
S-Fulleronicotine complexes



A *S* 0 kcal/mol



B *S* 1.78 kcal/mol



S 11.13 kcal/mol

XYZ coordinates of B3LYP 6-31G(d) optimized *R*- and *S*-fulleronicotine (2) - Zn *pyro*-pheophorbide *a* (1)

R-Fulleronicotine complexes

A

153
0.000000
Zn 5.1127 0.3878 0.2991
C 6.6135 -2.4294 0.3567
C 6.7372 -3.8231 0.9713
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B

153
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S-Fulleronicotine and **1** complexes

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