Supporting Information

Area-Selective Passivation of sp^2 Carbon Surfaces by Supramolecular Self-Assembly

Zhi Li,[a] Hans Van Gorp,[a] Peter Walke,[a] Thanh Hai Phan,[a,b] Yasuhiko Fujita,[a] John Greenwood,*[,c] Oleksandr Ivasenko,*[,a] Kazukuni Tahara,[d,e] Yoshito Tobe,[e] Hiroshi Uji-i[a,f] and Stijn F. L. Mertens,*[,a,g] Steven De Feyter*[,a]

S1. Removal of nPC adlayers

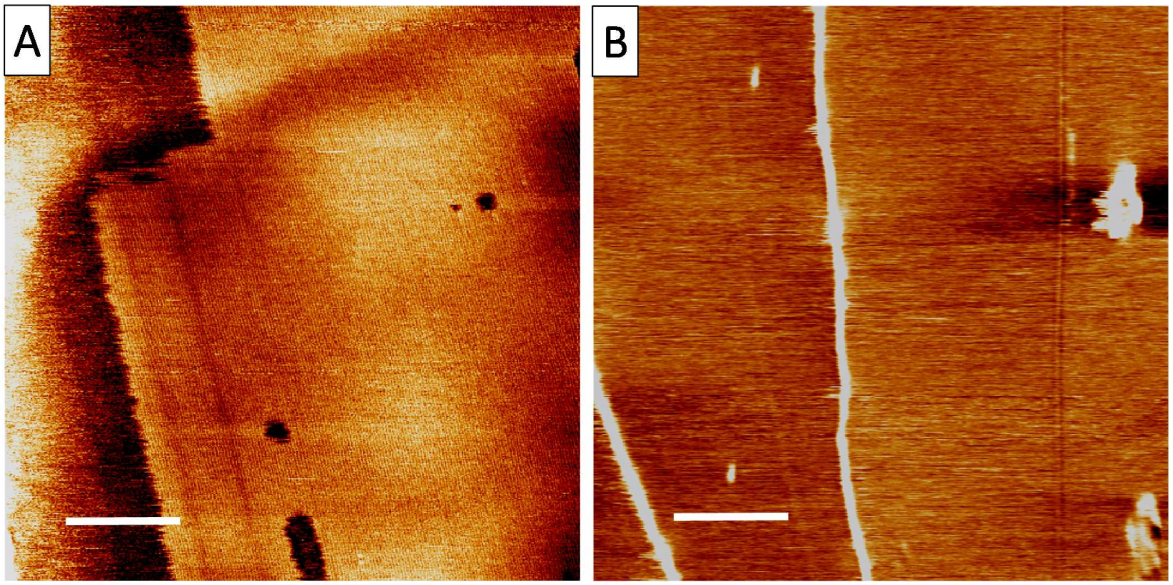


Fig. S1. AFM of a self-assembled monolayer of *n*-PC on HOPG. A: before washing; B: after washing by hot toluene (80 °C). Scale bar for both images: 200 nm. The AFM images show that the *n*-PC layer can be easily removed from the HOPG surface by washing with 10 mL hot toluene (80 °C), leaving the HOPG surface uncovered. This proves that the protection of HOPG surface by this method is reversible.

S2. Electrochemical stability of nPC adlayers

Electrochemical STM allows in situ real space imaging of the substrate–electrolyte interface surface with submolecular resolution under electrochemical potential control. As shown in Fig. S2, imaging of the partially nPC-covered HOPG in 0.1M $HClO_4$ started at the open circuit potential (–0.1 V *vs*. Pt quasi-reference). The lamellar structure of the nPC adlayer can be clearly recognised. A stepwise change of the substrate potential down to –0.5 V (Fig. S2B–E) reveals no dynamics (including adsorption, desorption, or phase rearrangement) of the nPC adlayer, although some image drift is apparent. The same stable behavior is observed for stepwise substrate potential changes up to 0.4V above the open circuit potential. This proves that the physisorbed nPC layer on HOPG surface is stable in an electrochemical environment over a wide potential range, which is an important requirement for a passivating layer. This property stands in marked contrast with the behavior of n-alkanes on gold, where extensive restructuring is observed under electrochemical conditions.[1]

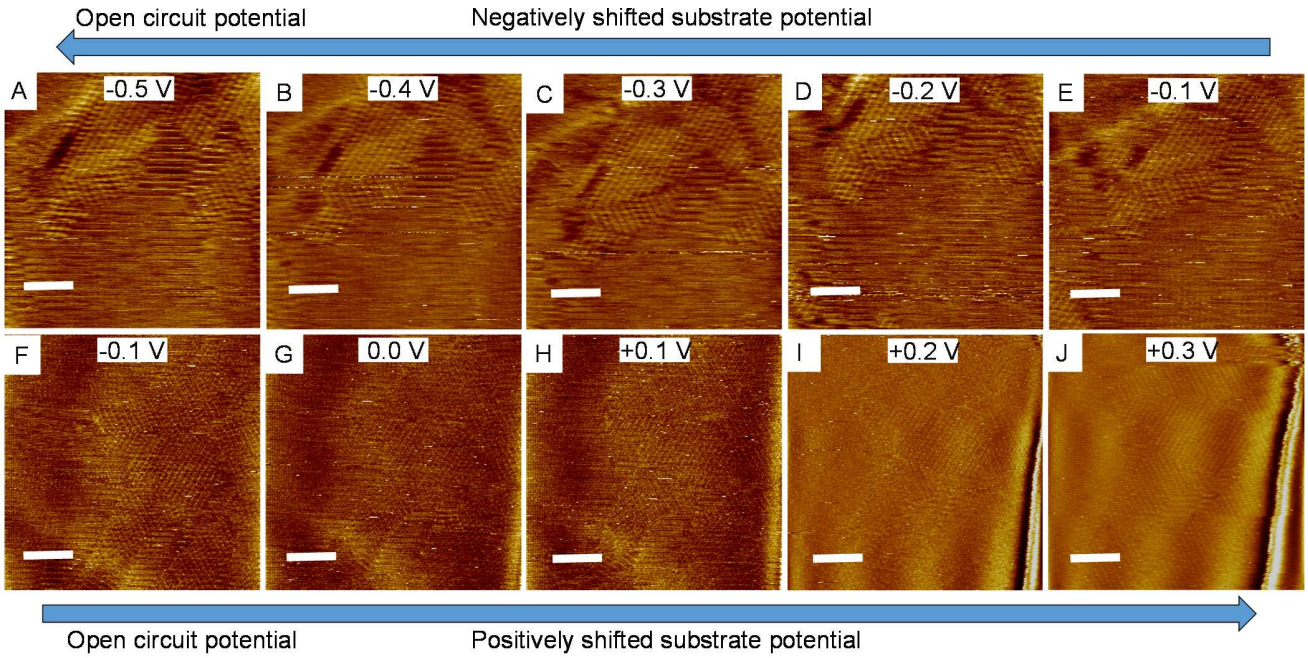


Fig. S2. *In-situ* electrochemical STM (EC-STM) images of *n*-PC on HOPG in 0.1M $HClO_4$. Reference electrode: Pt wire; counter electrode: Pt wire. The Open circuit potential = 0.1V vs Pt wire. A) E_s = -0.5 V, E_b = 0.41 V, I_t = 0.36 nA; B) E_s = -0.4 V, E_b = 0.51 V, I_t = 0.36 nA; C) E_s = -0.3 V, E_b = 0.61 V, I_t = 0.36 nA; D) E_s = -0.2 V, E_b = 0.71 V, I_t = 0.36 nA; E) E_s = -0.1 V, E_b = 0.77 V, I_t = 0.36 nA; F) E_s = -0.1 V, E_b = 0.70 V, I_t = 0.15 nA; G) E_s = 0 V, E_b = 0.80 V, I_t = 0.15 nA; H) E_s = +0.1 V, E_b = 0.90 V, I_t = 0.15 nA; I) E_s = +0.2 V, E_b = 0.86 V, I_t = 0.15 nA; I) E_s = +0.3 V, E_b = 1.10 V, I_t = 0.15 nA. Scale bar for all the images is 50 nm.

S3. Effect of thermal annealing on the quality of nPC films

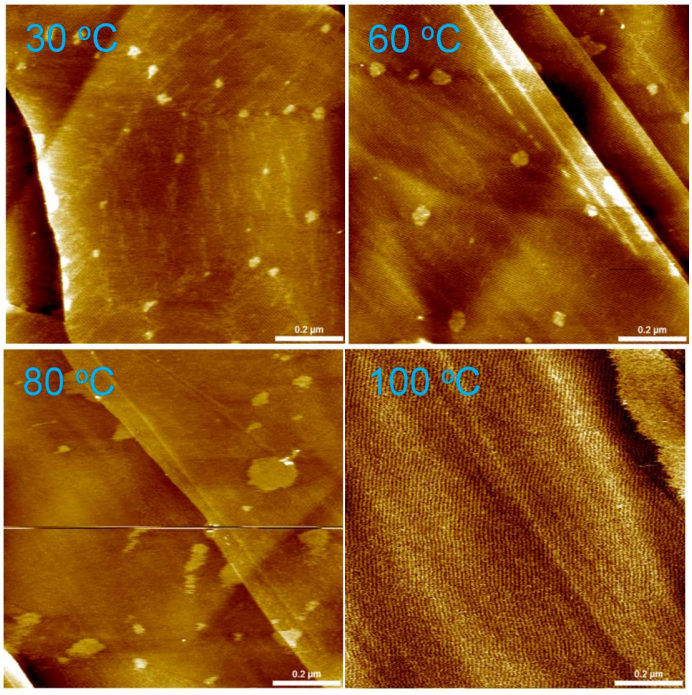


Fig. S3. AFM images of nPC recorded at the given temperatures.

S4. Molecular modelling

All density functional theory calculations at B97D/6-31G(d) level were done using Gaussian G09 software.[2] B97D functional (Grimme's functional including dispersion)- one of the most accurate general purpose GGAs.[3] To cut down calculation expenses the estimation was performed using n-pentane, 3-pentyl radical and ovalene ($C_{32}H_{14}$) as small models of nPC, secondary $C_{50}H_{101}$ radicals and graphene sheet, respectively. Ovalene is sufficiently large to accommodate fully extended C5 alkyl chain. Reaction enthalpies were estimated as the difference of calculated heats of formation of starting materials and products, e.g. hydrogen abstraction from physisorbed n-pentane on ovalene by TBP radicals:

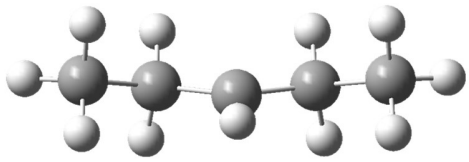
$C_5H_{12}/C_{32}H_{14} + TBP\cdot = \cdot C_5H_{11}/C_{32}H_{14} + TBP\text{-}H \qquad \Delta H_{reaction}$

$\Delta H_{reaction} = \Delta H_{\cdot C5H11/C32H14} + \Delta H_{TBP\text{-}H} - \Delta H_{C5H12/C32H14} - \Delta H_{TBP\cdot}$ = (-1424.0329429) + (-546.3611831) – (-1424.6998372) – (-545.6765516) = -0.0177372 hartrees (~11.1 kcal/mol)

Physisorbed and chemisorbed 3-pentyl radicals on ovalene are isomers and their stability (heat of formation) can be compared directly: -1424.0329429 hartrees vs. -1424.0168702 hartrees (-0.016 hartrees (-10.0 kcal/mol)), corroborating that physisorbed secondary alkyl radicals are more stable than covalently grafted.

Heat of formation, charge, spin multiplicity and xyz coordinates of DFT optimized models are listed below.

C_5H_{11} physisorbed on $C_{34}H_{12}$



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 C                  1.23060500    3.09298200   -0.12263800
 C                 -1.23376300    1.66831200   -0.33672600
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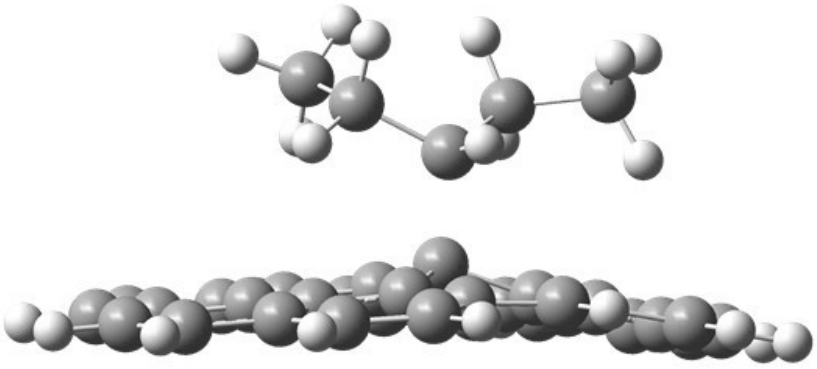
C_5H_{11} covalently grafted to $C_{34}H_{12}$



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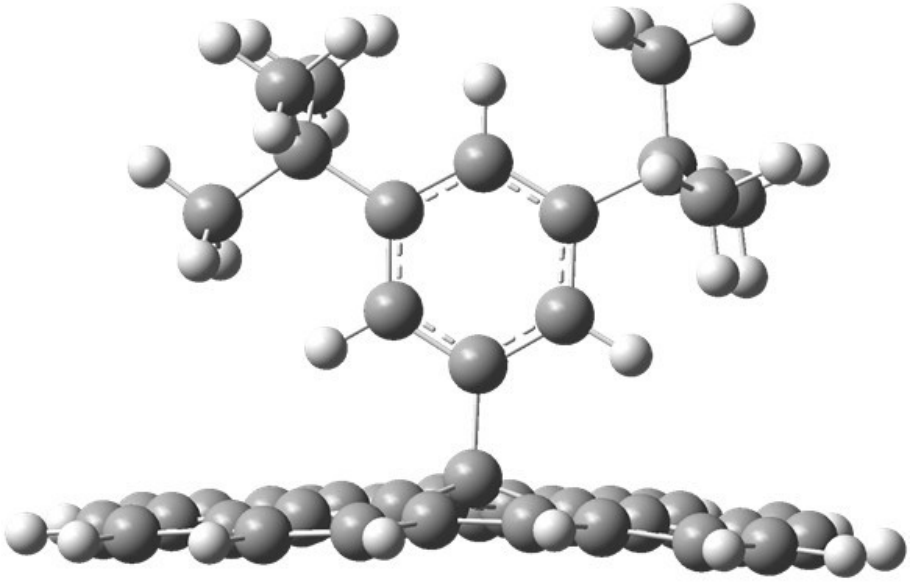
TBP covalently grafted to $C_{32}H_{14}$



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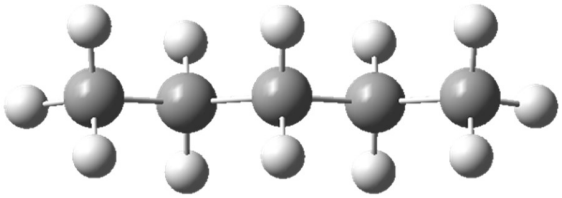
C_5H_{12} physisorbed on $C_{32}H_{14}$



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C	-0.96872700	-0.46816900	0.00000000
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C	-3.09552300	-0.13277600	-1.23058500
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C	-0.96363300	-0.45390900	2.47219700
C	-1.66725500	-0.32774100	3.71294100

C	-3.08634800	-0.10963300	3.68271900
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C	0.45285100	-0.66275600	-2.47200100
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C	3.26933700	-1.03665800	2.49337200
C	2.58418000	-0.94219600	3.68240300
C	1.16214900	-0.74804600	3.71238600
C	0.43721200	-0.62285900	4.92788700
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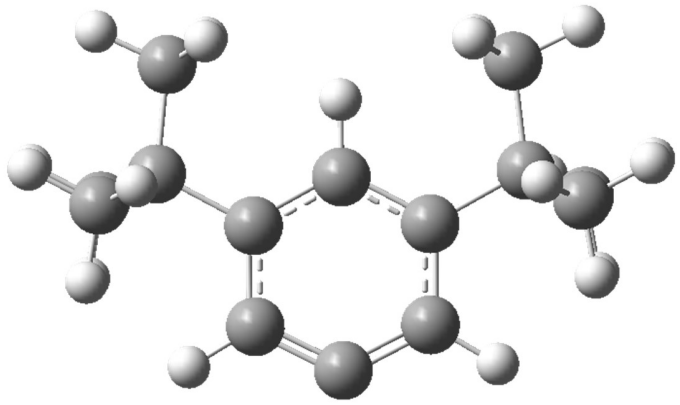
H	4.35259300	-1.17726400	2.48865600
H	3.11868600	-1.00536100	4.63310900
H	0.98278300	-0.68627000	5.87226800
H	-1.47592200	-0.31949500	5.87319000
H	-3.61616700	-0.01495400	-4.63352200
H	-4.85123100	0.15254300	-2.48963700
H	-3.61616700	-0.01495400	4.63352200
H	-4.85123100	0.15254300	2.48963700
H	-4.85199400	0.14347800	0.00000000
C	1.55988800	2.62854200	0.00000000
C	0.71278300	2.68149800	1.28140100
C	1.56548400	2.61221300	2.55818400
C	0.71278300	2.68149800	-1.28140100
C	1.56548400	2.61221300	-2.55818400
H	2.28090600	3.46769500	0.00000000
H	0.11157700	3.60883000	1.28166400
H	-0.00400400	1.84598900	1.27092500
H	0.93652300	2.59190300	3.46288200
H	2.18731600	1.70377700	2.56069500
H	2.23960100	3.48347200	2.62582200
H	-0.00400400	1.84598900	-1.27092500
H	0.11157700	3.60883000	-1.28166400
H	0.93652300	2.59190300	-3.46288200
H	2.23960100	3.48347200	-2.62582200
H	2.18731600	1.70377700	-2.56069500
H	2.16002000	1.70211300	0.00000000

TBP radical



HF=-545.6765516 hartrees

0 2

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C	0.00000000	-1.22979200	1.75923400
C	0.00000000	-1.23967200	0.34048200
C	0.00000000	0.00000000	-0.33101200
C	0.00000000	-2.59192500	-0.39963700
C	0.00000000	2.59192500	-0.39963700
C	0.00000000	2.42807700	-1.93454700
C	-1.26343400	3.39574700	0.00106500
C	1.26343400	3.39574700	0.00106500
C	0.00000000	-2.42807700	-1.93454700
C	1.26343400	-3.39574700	0.00106500
C	-1.26343400	-3.39574700	0.00106500
H	0.00000000	2.16812900	2.31806000
H	0.00000000	-2.16812900	2.31806000
H	0.00000000	0.00000000	-1.41728100
H	0.00000000	3.42262500	-2.40781100
H	0.89368200	1.88355700	-2.27883500
H	-0.89368200	1.88355700	-2.27883500
H	-1.26500400	4.37266300	-0.51071800
H	-2.17672100	2.84933700	-0.28354000
H	-1.29570700	3.57607900	1.08637800
H	1.26500400	4.37266300	-0.51071800
H	1.29570700	3.57607900	1.08637800
H	2.17672100	2.84933700	-0.28354000
H	0.00000000	-3.42262500	-2.40781100
H	-0.89368200	-1.88355700	-2.27883500
H	0.89368200	-1.88355700	-2.27883500
H	1.26500400	-4.37266300	-0.51071800
H	2.17672100	-2.84933700	-0.28354000
H	1.29570700	-3.57607900	1.08637800
H	-1.26500400	-4.37266300	-0.51071800
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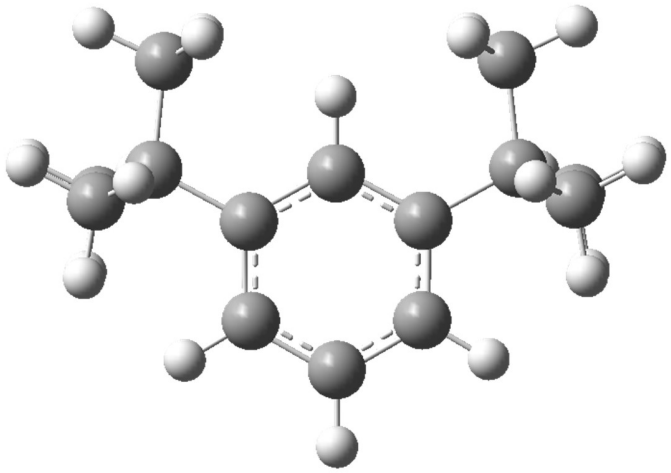
TBP-H



HF=-546.3611831 hartrees

0 1

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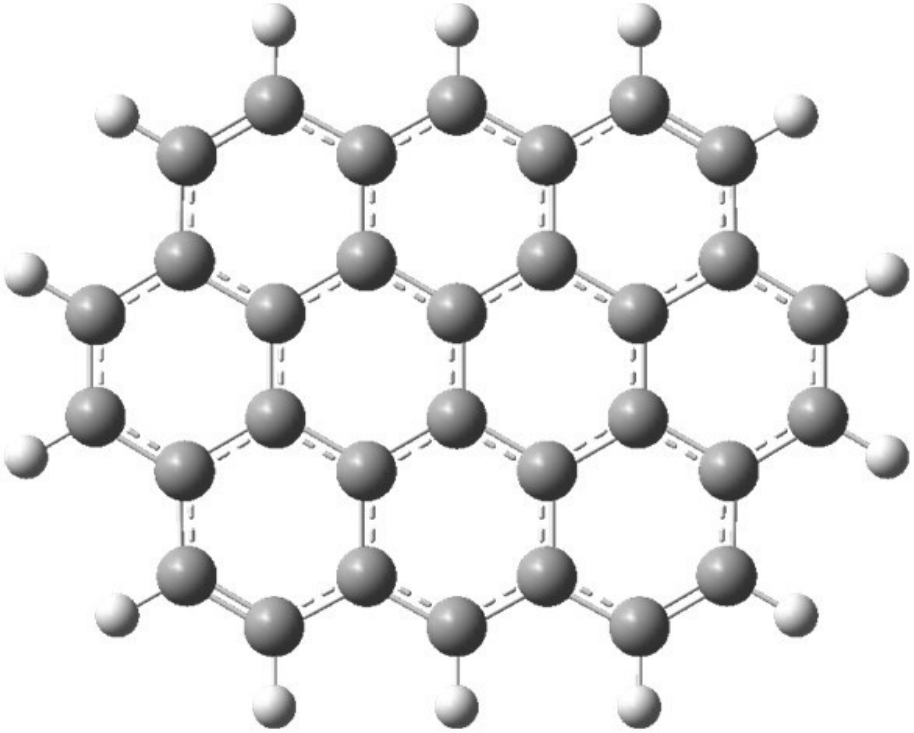
C	0.00000000	1.21460900	1.71295800
C	0.00000000	0.00000000	2.41032000
C	0.00000000	-1.21460900	1.71295800
C	0.00000000	-1.23519700	0.30433800
C	0.00000000	0.00000000	-0.37326300
C	0.00000000	-2.58712600	-0.43453300
C	0.00000000	2.58712600	-0.43453300
C	0.00000000	2.42942300	-1.96957900
C	-1.26302400	3.39135000	-0.03268300
C	1.26302400	3.39135000	-0.03268300
C	0.00000000	-2.42942300	-1.96957900
C	1.26302400	-3.39135000	-0.03268300
C	-1.26302400	-3.39135000	-0.03268300
H	0.00000000	2.15447800	2.26831500
H	0.00000000	0.00000000	3.50290700
H	0.00000000	-2.15447800	2.26831500
H	0.00000000	0.00000000	-1.46006000
H	0.00000000	3.42518500	-2.44039000
H	0.89340500	1.88575000	-2.31627500
H	-0.89340500	1.88575000	-2.31627500
H	-1.26381000	4.37061000	-0.54024900
H	-2.17659100	2.84688500	-0.32060900
H	-1.29662700	3.56677900	1.05342000
H	1.26381000	4.37061000	-0.54024900
H	1.29662700	3.56677900	1.05342000
H	2.17659100	2.84688500	-0.32060900
H	0.00000000	-3.42518500	-2.44039000
H	-0.89340500	-1.88575000	-2.31627500
H	0.89340500	-1.88575000	-2.31627500
H	1.26381000	-4.37061000	-0.54024900
H	2.17659100	-2.84688500	-0.32060900
H	1.29662700	-3.56677900	1.05342000
H	-1.26381000	-4.37061000	-0.54024900

H	-1.29662700	-3.56677900	1.05342000
H	-2.17659100	-2.84688500	-0.32060900

$C_{32}H_{14}$



HF=-1227.0537226 hartrees

0 1

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C	0.00000000	-1.23407200	-1.43172600
C	0.00000000	-2.47289400	-0.71627400
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C	0.00000000	-3.68355700	-2.86669300
C	0.00000000	-2.49452600	-3.55855800
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C	0.00000000	2.47289400	-0.71627400
C	0.00000000	3.71415900	-1.43095000
C	0.00000000	3.68355700	-2.86669300
C	0.00000000	2.49452600	-3.55855800
C	0.00000000	1.23078900	-2.87260400
C	0.00000000	0.00000000	-3.55750100
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C	0.00000000	-2.47289400	0.71627400
C	0.00000000	-3.71415900	1.43095000
C	0.00000000	-4.92977200	0.69434000

C	0.00000000	-4.92977200	-0.69434000
C	0.00000000	-3.68355700	2.86669300
C	0.00000000	-2.49452600	3.55855800
C	0.00000000	2.49452600	3.55855800
C	0.00000000	3.68355700	2.86669300
C	0.00000000	3.71415900	1.43095000
C	0.00000000	4.92977200	0.69434000
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H	0.00000000	0.00000000	4.65073200
H	0.00000000	-5.87471100	1.24281600
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H	0.00000000	5.87471100	-1.24281600
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H	0.00000000	0.00000000	-4.65073200

References

1. Y. He, T. Ye and E. Borguet, *J. Phys. Chem. B*, 2002, **106**, 11264-11271.
2. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09 Revision A.02*, Gaussian, Inc., Wallingford, CT, USA, 2009.
3. S. Grimme, *J. Comput. Chem.*, 2006, **27**, 1787-1799.