

SUPPORTING INFORMATION

All-carbon supramolecular complexation of a bilayer molecular nanographene with [60] and [70]fullerenes

Manuel Buendía,^a Anton J. Stasyuk,^{b,c} Salvatore Filippone,^a Miquel Solà^{*b} and Nazario Martín^{*a,d}

^a Departamento de Química Orgánica I, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, Ciudad Universitaria s/n, 28040 Madrid, Spain. E-mail: nazmar@ucm.es

^b Institut de Química Computacional i Catàlisi (IQCC) and Departament de Química, Universitat de Girona, M. Aurèlia Capmany, 69, 17003 Girona, Spain. E-mail: miquel.sola@udg.edu

^c Departament de Farmàcia i Tecnologia Farmacèutica, i Físicoquímica, Facultat de Farmàcia i Ciències de l'Alimentació & Institut de Química Teòrica i Computacional (IQTCUB), Av. Joan XXIII 27-31, Universitat de Barcelona (UB), Barcelona, Spain.

^d IMDEA-Nanociencia, C/ Faraday, 9, Campus de Cantoblanco, 28049 Madrid, Spain.

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1. General

Unless otherwise noted, all materials were obtained from commercial suppliers and used without further purification. C₆₀ 99.5 % and C₇₀ 99 % were purchased from Solenne, chlorobenzene-d⁵ (PhCl-d⁵) 99 % atom % D was purchased from Aldrich, and **CNG-1** was prepared according to the procedure reported in the literature.¹ ¹H NMR spectra of the titration were recorded at 300 MHz (Bruker AVIII) at 298 K, and all NMR experiments for the assignment of **CNG-1** proton signals at 700MHz (Bruker AVIII) (¹H NMR: 700 MHz; ¹³C NMR: 176 MHz) at 300 K. Chemical shifts for ¹H NMR are expressed in parts per million (ppm) relative to the solvent. Data are reported as follows: chemical shift, multiplicity (s = singlet, bs = broad singlet, d = doublet), coupling constant (Hz), and integration.

¹ **1.** Buendía, M.; Fernández-García, J. M.; Perles, J.; Filippone, S.; Martín, N. Enantioselective synthesis of a two-fold inherently chiral molecular nanographene. *Nat. Synth.* **2024**, *3* (4), 545-553. DOI: 10.1038/s44160-024-00484-x.

2. Assignment of CNG-1 proton signals

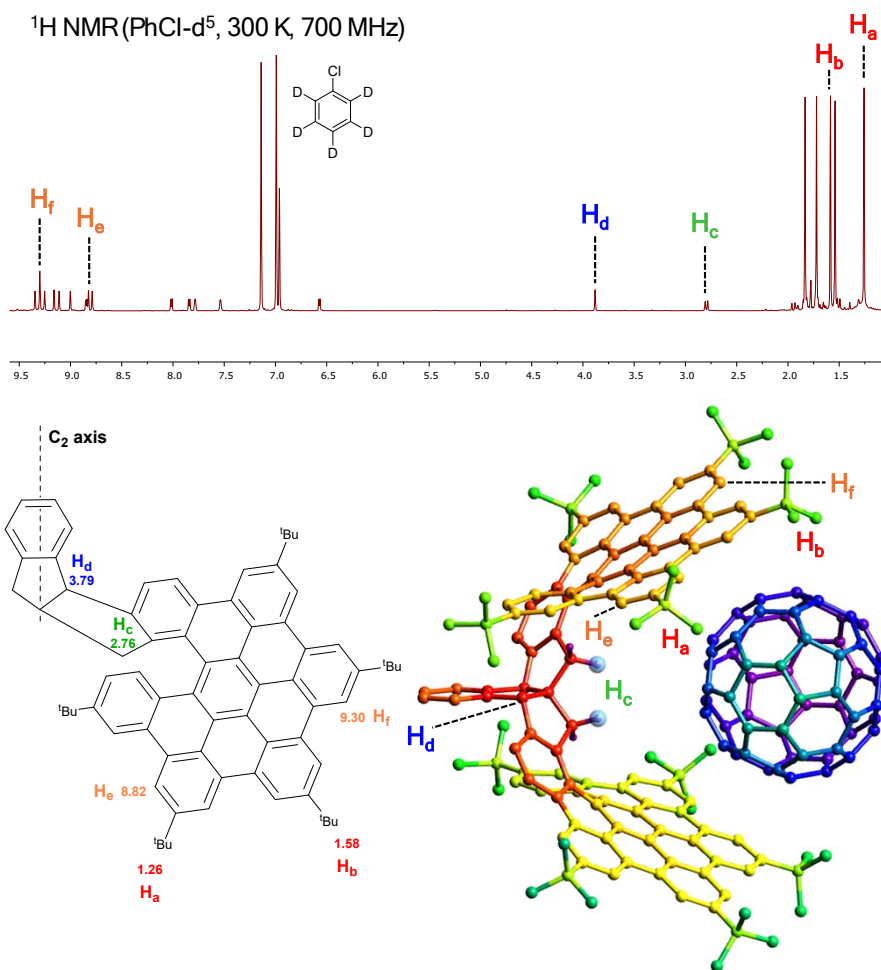


Figure S1. Assignment of CNG-1 proton signals H_a - H_f in $^1\text{H NMR}$ spectra (top; PhCl- d^5 , 300 K, 700 MHz); in half of the molecule (bottom left; chemical shifts in ppm); and in the CNG-1- C_{60} complex representation (bottom right).

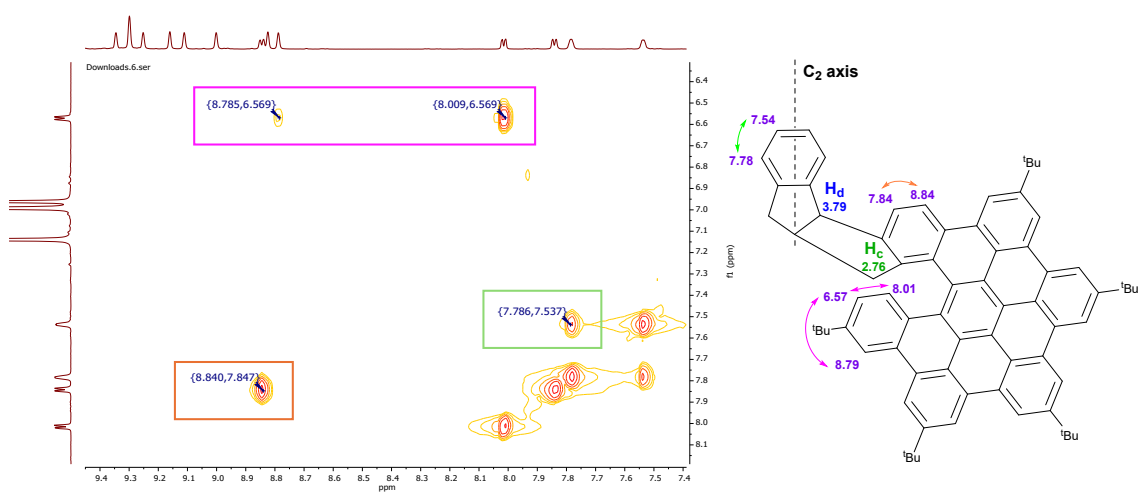


Figure S2. Expansion of COSY experiment of CNG-1 showing proton-proton correlations between aromatic proton signals (PhCl- d^5 , 300 K, 700 MHz).

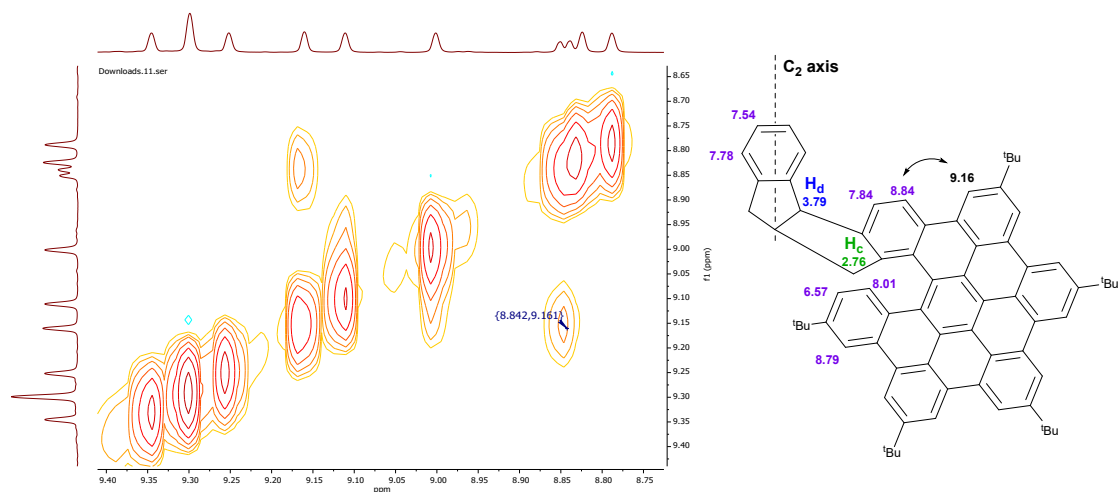


Figure S3. Expansion of 2D NOESY experiment of **CNG-1** showing a short distance proton-proton dipolar interaction between protons at the edge of the nanographene layer (PhCl-d⁵, 300 K, 700 MHz).

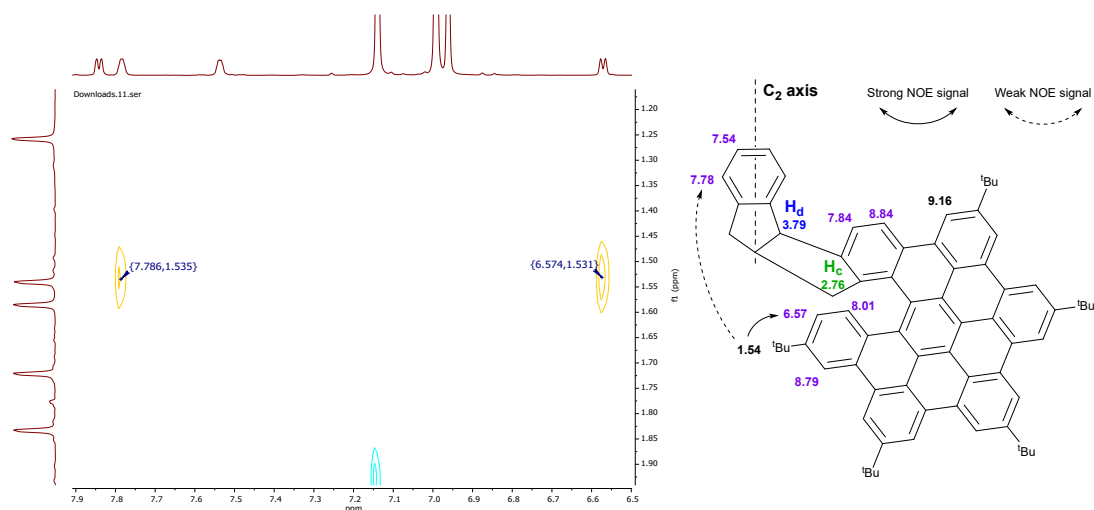


Figure S4. Expansion of 2D NOESY experiment of **CNG-1** showing proton-proton short distance and long distance dipolar interactions between *tert*-butyl proton at 1.54 ppm and its neighboring protons (PhCl-d⁵, 300 K, 700 MHz).

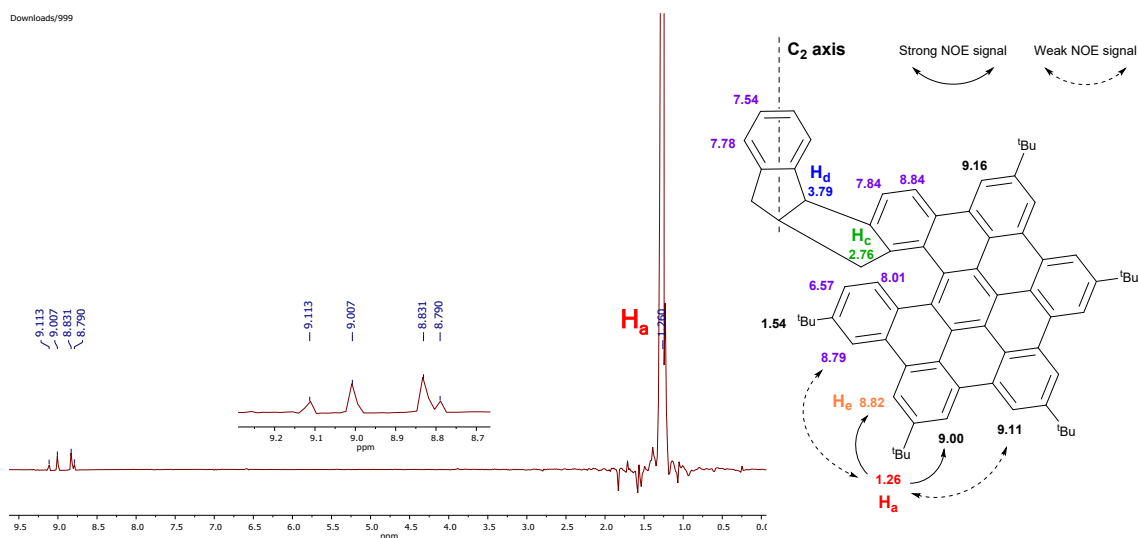


Figure S5. 1D NOESY experiment of **CNG-1** and its expansion, showing proton-proton short distance and long distance dipolar interactions between *tert*-butyl proton at 1.26 ppm and its neighboring protons at the edge of the nanographene (PhCl-d⁵, 300 K, 700 MHz).

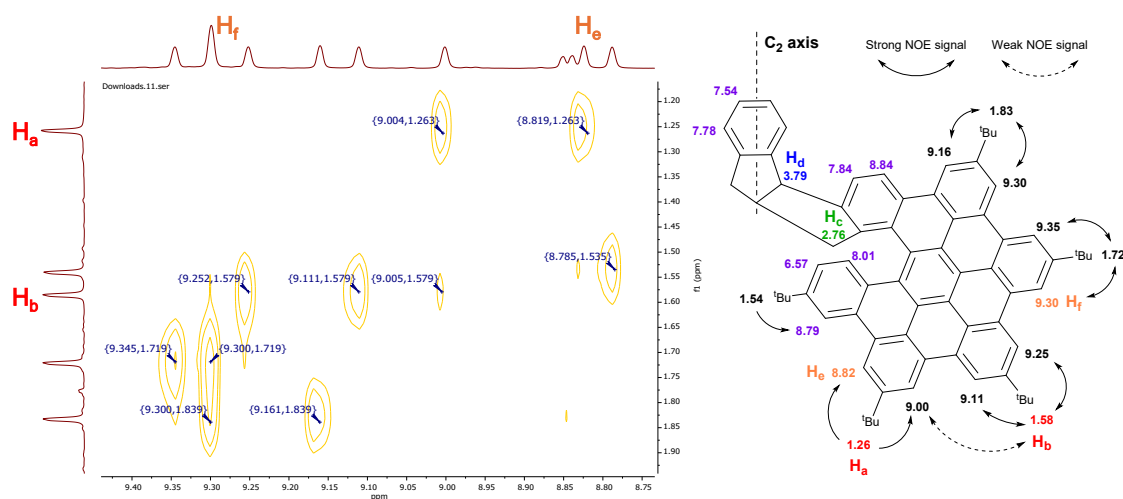


Figure S6. Expansion of 2D NOESY experiment of **CNG-1** showing proton-proton short distance and long distance dipolar interactions between all five anisochronous *tert*-butyl protons and their neighboring protons at the edge of the nanographene (PhCl-d⁵, 300 K, 700 MHz).

3. Titrations monitored by ^1H NMR

3.1. CNG-1 and C_{60} in PhCl-d^5

Table S1. Experimental data of the ^1H NMR titration between host CNG-1 and guest C_{60} .

Stock solutions in PhCl-d^5						Initial CNG-1 n (mol)		Initial Volume (mL)	
Composition	Volume (mL)	Mw ($\text{g}\cdot\text{mol}^{-1}$)	Mass (mg)	Molarity (M)	n (mol)	CNG-1 Molarity (M)	5,00E-07	5,00E-04	0,5
CNG-1	2,5	1748,49	2,19	5,00E-04	1,25E-06				
C_{60} +CNG-1 (5,00E-04 M)	2	720,64	13,69	9,50E-03	1,90E-05				
						C_{60} Solution Molarity (M)		9,50E-03	

	Aliquot (mL)	Volume of C_{60} +CNG-1 added (mL)	Total CNG-1			Total C_{60}			Total volume (mL)	δ_c (ppm)
			Equivalents related to Initial CNG-1	n (mol)	CNG-1 Molarity [H_0] (M)	Equivalents related to Total CNG-1	n (mol)	C_{60} Molarity [G_0] (M)		
CNG-1 stock solution	0,000	0,000	1,00	2,50E-07	5,00E-04	0,00	0,00E+00	0,00E+00	0,500	2,761
Addition 1	0,010	0,010	1,02	2,55E-07	5,00E-04	0,37	9,50E-08	1,86E-04	0,510	2,765
Addition 2	0,010	0,020	1,04	2,60E-07	5,00E-04	0,73	1,90E-07	3,65E-04	0,520	2,765
Addition 3	0,010	0,030	1,06	2,65E-07	5,00E-04	1,08	2,85E-07	5,38E-04	0,530	2,768
Addition 4	0,015	0,045	1,09	2,73E-07	5,00E-04	1,57	4,28E-07	7,84E-04	0,545	2,771
Addition 5	0,015	0,060	1,12	2,80E-07	5,00E-04	2,04	5,70E-07	1,02E-03	0,560	2,774
Addition 6	0,020	0,080	1,16	2,90E-07	5,00E-04	2,62	7,60E-07	1,31E-03	0,580	2,779
Addition 7	0,020	0,100	1,20	3,00E-07	5,00E-04	3,17	9,50E-07	1,58E-03	0,600	2,782
Addition 8	0,025	0,125	1,25	3,13E-07	5,00E-04	3,80	1,19E-06	1,90E-03	0,625	2,785
Addition 9	0,030	0,155	1,31	3,28E-07	5,00E-04	4,50	1,47E-06	2,25E-03	0,655	2,789
Addition 10	0,035	0,190	1,38	3,45E-07	5,00E-04	5,23	1,81E-06	2,62E-03	0,690	2,792
Addition 11	0,035	0,225	1,45	3,63E-07	5,00E-04	5,90	2,14E-06	2,95E-03	0,725	2,796
Addition 12	0,045	0,270	1,54	3,85E-07	5,00E-04	6,66	2,57E-06	3,33E-03	0,770	2,800
Addition 13	0,050	0,320	1,64	4,10E-07	5,00E-04	7,41	3,04E-06	3,71E-03	0,820	2,804
Addition 14	0,060	0,380	1,76	4,40E-07	5,00E-04	8,20	3,61E-06	4,10E-03	0,880	2,809
Addition 15	0,070	0,450	1,90	4,75E-07	5,00E-04	9,00	4,28E-06	4,50E-03	0,950	2,813
Addition 16	0,075	0,525	2,05	5,13E-07	5,00E-04	9,73	4,99E-06	4,87E-03	1,025	2,816
Addition 17	0,090	0,615	2,23	5,58E-07	5,00E-04	10,48	5,84E-06	5,24E-03	1,115	2,819
Addition 18	0,105	0,720	2,44	6,10E-07	5,00E-04	11,21	6,84E-06	5,61E-03	1,220	2,823
Addition 19	0,120	0,840	2,68	6,70E-07	5,00E-04	11,91	7,98E-06	5,96E-03	1,340	2,824
Addition 20	0,140	0,980	2,96	7,40E-07	5,00E-04	12,58	9,31E-06	6,29E-03	1,480	2,826
Addition 21	0,160	1,140	3,28	8,20E-07	5,00E-04	13,21	1,08E-05	6,60E-03	1,640	2,829
Addition 22	0,160	1,300	3,60	9,00E-07	5,00E-04	13,72	1,24E-05	6,86E-03	1,800	2,830
Addition 23	0,200	1,500	4,00	1,00E-06	5,00E-04	14,25	1,43E-05	7,13E-03	2,000	2,833
C_{60} +CNG-1 stock solution	-	-	4,00	1,00E-06	5,00E-04	19,00	4,75E-06	9,50E-03	0,500	2,848

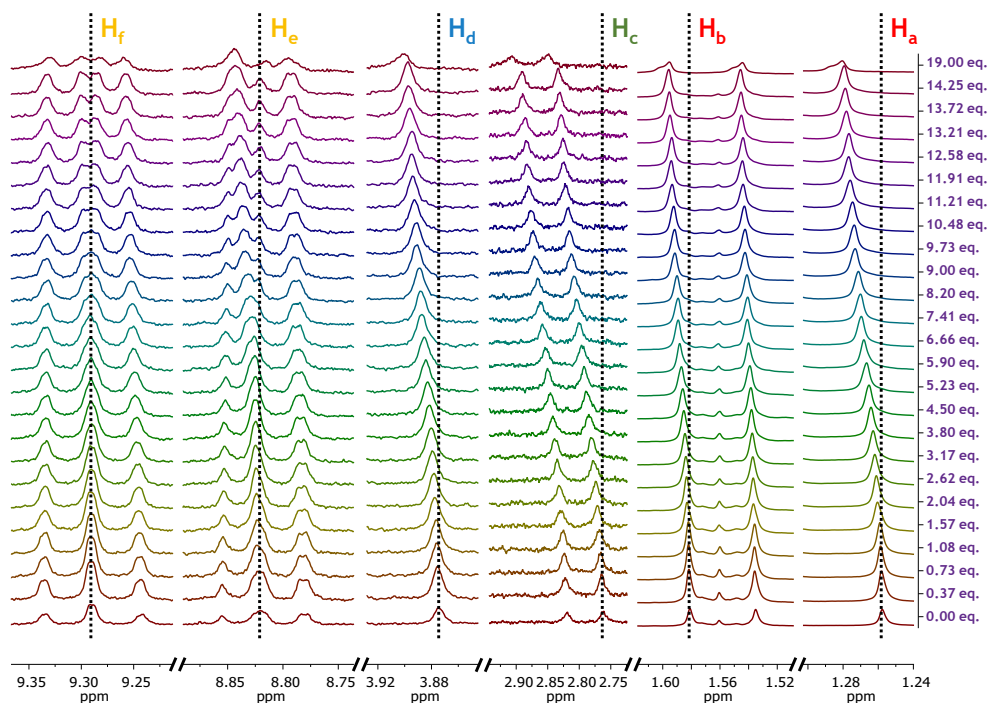


Figure S7. Partial ^1H NMR spectra of the titration between host CNG-1 and guest C_{60} , showcasing six signals (H_a to H_f , see manuscript for the definition) with the greatest chemical shifts (PhCl-d^5 , 298 K, 300 MHz).

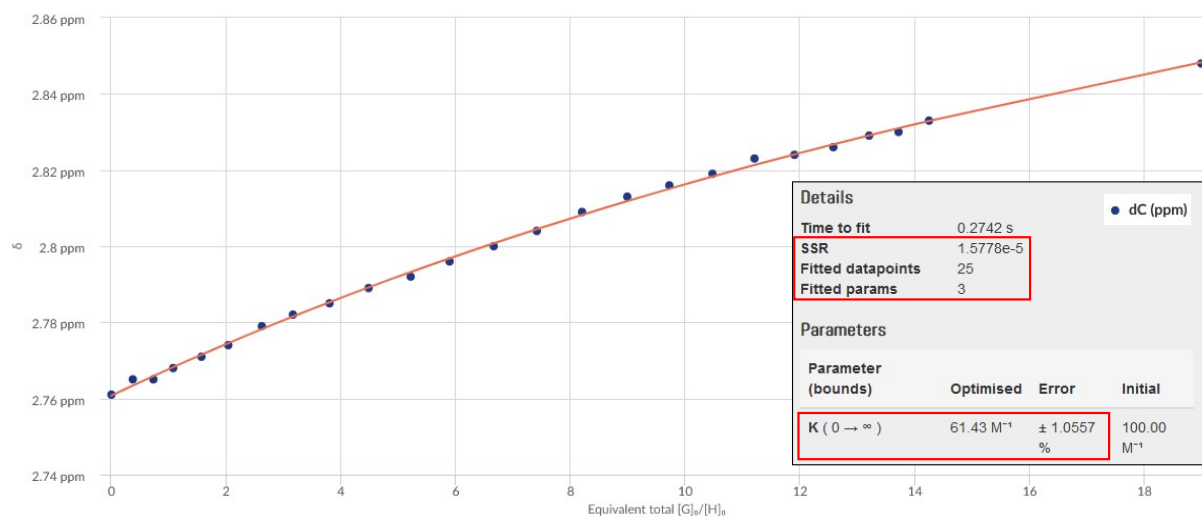


Figure S8. Dataset points of the titration between host **CNG-1** and guest **C₆₀**, representing chemical shifts of signal H_c (δ_c) vs equivalents of guest ($[G]_0/[H]_0$), and non-linear fitting model adjusted for a 1:1 stoichiometry.

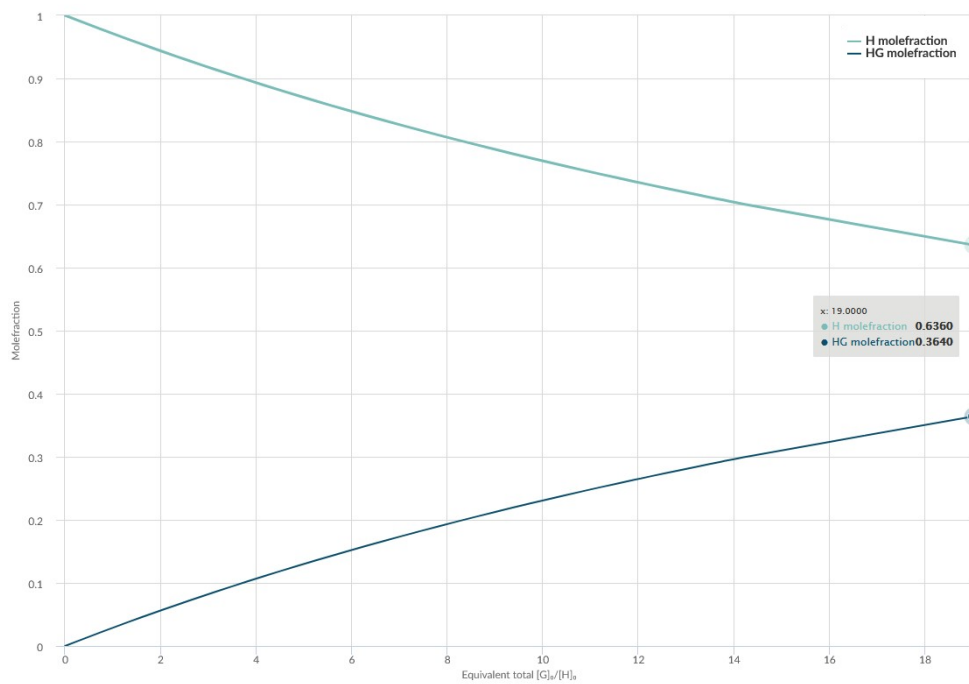


Figure S9. Molar fractions of free **CNG-1** host (H) and supramolecular complex **CNG-1⊃C₆₀** (HG) at each point of the titration.

3.2. CNG-1 and C₇₀ in PhCl-d⁵

Table S2. Experimental data of the ¹H NMR titration between host CNG-1 and guest C₇₀.

Stock solutions in PhCl-d ⁵						Initial CNG-1 n (mol)	
Composition	Volume (mL)	Mw (g·mol ⁻¹)	Mass (mg)	Molarity (M)	n (mol)	CNG-1 Molarity (M)	2,50E-07
CNG-1	2,5	1748,49	2,19	5,00E-04	1,25E-06	CNG-1 Molarity (M)	5,00E-04
C ₇₀ +CNG-1 (5,00E-04 M)	2	840,75	6,73	4,00E-03	8,00E-06	Initial Volume (mL)	0,5
						C ₇₀ Solution Molarity (M)	4,00E-03

	Aliquot (mL)	Volume of C ₇₀ +CNG-1 added (mL)	Total CNG-1			Total C ₇₀			Total volume (mL)	H _c δ _c (ppm)
			Equivalents related to Initial CNG-1	n (mol)	CNG-1 Molarity [H] ₀ (M)	Equivalents related to Total CNG-1	n (mol)	C ₇₀ Molarity [G] ₀ (M)		
CNG-1 stock solution	0,000	0,000	1,00	2,50E-07	5,00E-04	0,00	0,00E+00	0,00E+00	0,500	2,763
Addition 1	0,010	0,010	1,02	2,55E-07	5,00E-04	0,16	4,00E-08	7,84E-05	0,510	2,764
Addition 2	0,010	0,020	1,04	2,60E-07	5,00E-04	0,31	8,00E-08	1,54E-04	0,520	2,767
Addition 3	0,010	0,030	1,06	2,65E-07	5,00E-04	0,45	1,20E-07	2,26E-04	0,530	2,769
Addition 4	0,015	0,045	1,09	2,73E-07	5,00E-04	0,66	1,80E-07	3,30E-04	0,545	2,771
Addition 5	0,015	0,060	1,12	2,80E-07	5,00E-04	0,86	2,40E-07	4,29E-04	0,560	2,772
Addition 6	0,020	0,080	1,16	2,90E-07	5,00E-04	1,10	3,20E-07	5,52E-04	0,580	2,777
Addition 7	0,020	0,100	1,20	3,00E-07	5,00E-04	1,33	4,00E-07	6,67E-04	0,600	2,778
Addition 8	0,025	0,125	1,25	3,13E-07	5,00E-04	1,60	5,00E-07	8,00E-04	0,625	2,782
Addition 9	0,030	0,155	1,31	3,28E-07	5,00E-04	1,89	6,20E-07	9,47E-04	0,655	2,784
Addition 10	0,035	0,190	1,38	3,45E-07	5,00E-04	2,20	7,60E-07	1,10E-03	0,690	2,786
Addition 11	0,035	0,225	1,45	3,63E-07	5,00E-04	2,48	9,00E-07	1,24E-03	0,725	2,790
Addition 12	0,045	0,270	1,54	3,85E-07	5,00E-04	2,81	1,08E-06	1,40E-03	0,770	2,793
Addition 13	0,050	0,320	1,64	4,10E-07	5,00E-04	3,12	1,28E-06	1,56E-03	0,820	2,794
Addition 14	0,060	0,380	1,76	4,40E-07	5,00E-04	3,45	1,52E-06	1,73E-03	0,880	2,799
Addition 15	0,070	0,450	1,90	4,75E-07	5,00E-04	3,79	1,80E-06	1,89E-03	0,950	2,801
Addition 16	0,075	0,525	2,05	5,13E-07	5,00E-04	4,10	2,10E-06	2,05E-03	1,025	2,802
Addition 17	0,090	0,615	2,23	5,58E-07	5,00E-04	4,41	2,46E-06	2,21E-03	1,115	2,805
Addition 18	0,105	0,720	2,44	6,10E-07	5,00E-04	4,72	2,88E-06	2,36E-03	1,220	2,805
Addition 19	0,120	0,840	2,68	6,70E-07	5,00E-04	5,01	3,36E-06	2,51E-03	1,340	2,809
Addition 20	0,140	0,980	2,96	7,40E-07	5,00E-04	5,30	3,92E-06	2,65E-03	1,480	2,809
Addition 21	0,160	1,140	3,28	8,20E-07	5,00E-04	5,56	4,56E-06	2,78E-03	1,640	2,808
Addition 22	0,160	1,300	3,60	9,00E-07	5,00E-04	5,78	5,20E-06	2,89E-03	1,800	2,809
Addition 23	0,200	1,500	4,00	1,00E-06	5,00E-04	6,00	6,00E-06	3,00E-03	2,000	2,810
C ₇₀ +CNG-1 stock solution	-	-	4,00	1,00E-06	5,00E-04	8,00	2,00E-06	4,00E-03	0,500	2,812

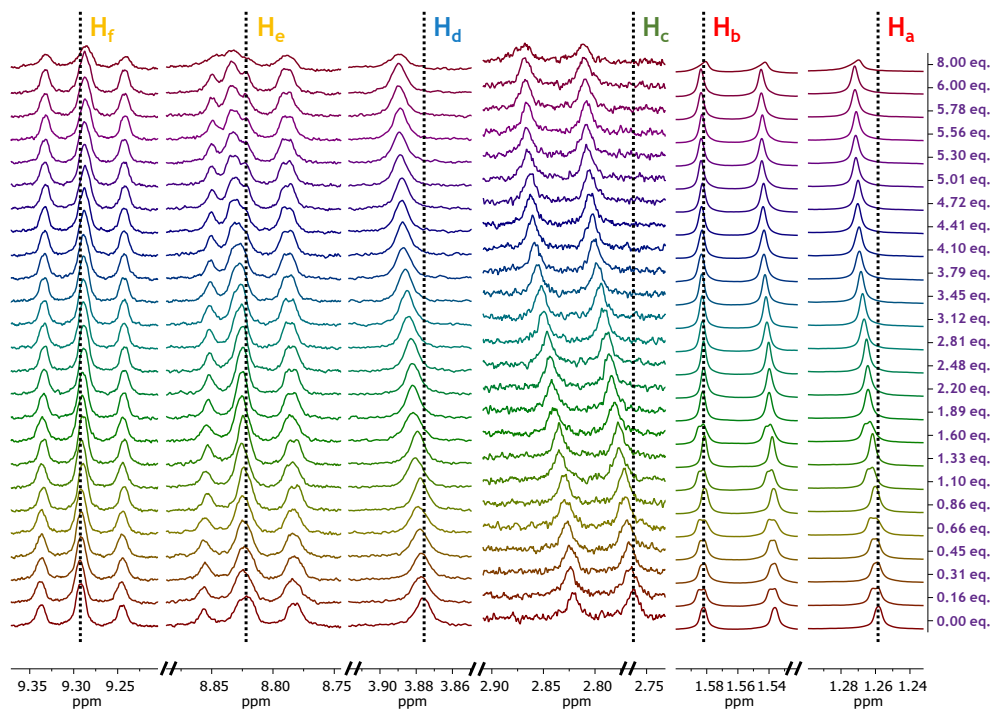


Figure S10. Partial ¹H NMR spectra of the titration between host CNG-1 and guest C₇₀, showcasing six signals (H_a to H_f, see manuscript for the definition) with the greatest chemical shifts (PhCl-d⁵, 298 K, 300 MHz).

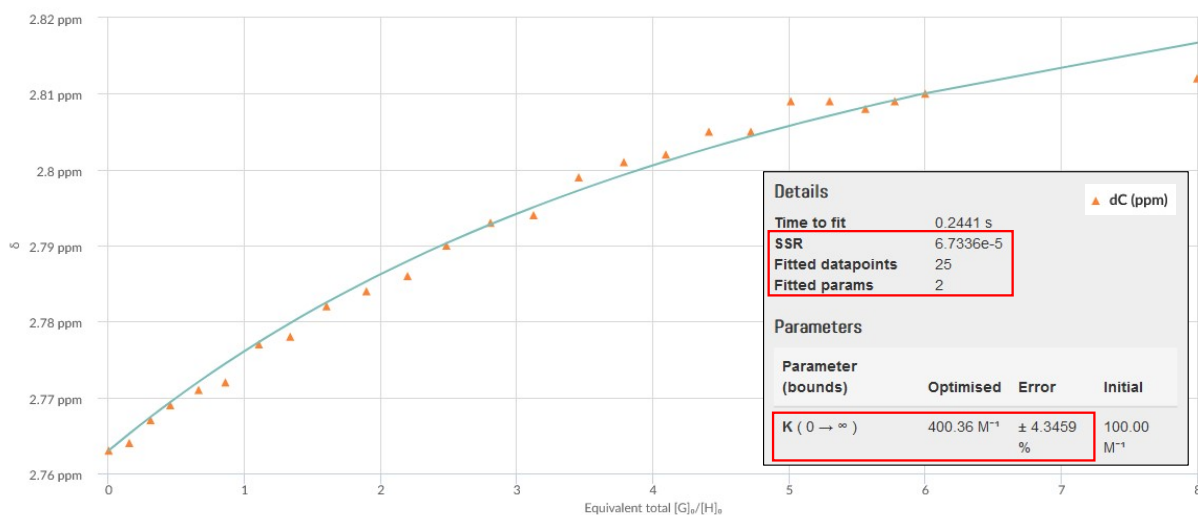


Figure S11. Dataset points of the titration between host **CNG-1** and guest C_{70} , representing chemical shifts of signal H_c (δ_c) vs equivalents of guest ($[G]_0/[H]_0$), and non-linear fitting model adjusted for a 1:1 stoichiometry.

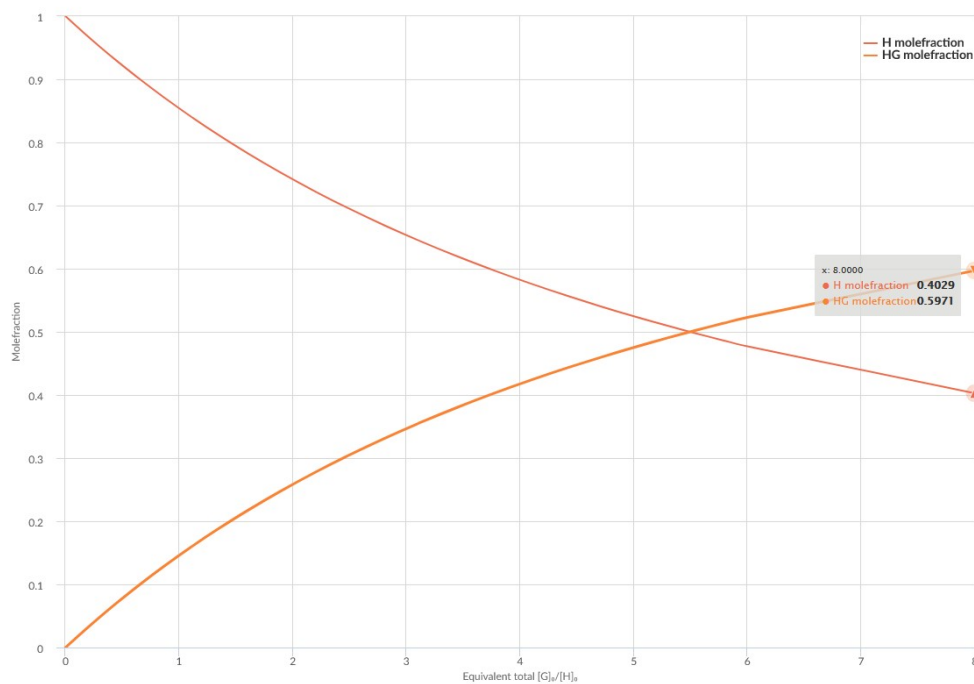


Figure S12. Molar fractions of free **CNG-1** host (H) and supramolecular complex **CNG-1**→ C_{70} (HG) at each point of the titration.

4. Theoretical calculations

Quantum-chemical calculations

Geometry optimization of the complexes was performed employing the DFT BLYP^{1,2} exchange–correlation functional with Ahlrichs' def2-SVP basis set.^{3,4} The empirical dispersion D3 correction was computed with the Becke–Johnson damping function.^{5,6} Interaction energy was computed using the BLYP functional coupled with TZVP basis⁷ for the BLYP-D3(BJ)/def2-SVP optimized geometries. Its decomposition analysis (EDA)^{8,9} was performed using the Amsterdam Density Functional (ADF) program.¹⁰ Molecular structures and frontier molecular orbitals were visualized by Chemcraft 1.8. program.¹¹

Energy decomposition analysis

The interaction energy between the **CNG-1** and the fullerene in the gas phase was examined in the framework of the Kohn-Sham MO model using a quantitative energy decomposition into electrostatic interactions, Pauli repulsive orbital interactions and attractive orbital interactions, to which a term ΔE_{disp} was added to account for the dispersion correction:¹²⁻¹⁴

$$\Delta E_{\text{int}} = \Delta E_{\text{elstat}} + \Delta E_{\text{Pauli}} + \Delta E_{\text{oi}} + \Delta E_{\text{disp}} \quad (1)$$

The term ΔV_{elstat} corresponds to the classical electrostatic interactions between the unperturbed charge distributions of the prepared (i.e. deformed) fragments and is usually attractive. The Pauli repulsion, ΔE_{Pauli} , comprises the destabilizing interactions between occupied orbitals and is responsible for any steric repulsion. The orbital interactions, ΔE_{oi} , account for electron-pair bonding, charge transfer (i.e., donor–acceptor interactions between occupied orbitals on one moiety and unoccupied orbitals on the other, including HOMO-LUMO interactions) and polarization (empty-occupied orbital mixing on one fragment due to the presence of another fragment). The term ΔE_{disp} accounts for the dispersion corrections.^{15,16}

Non-covalent interaction (NCI) index

The NCI method¹⁷⁻¹⁹ relies on two scalar fields to map local bonding properties: the electron density (ρ) and the reduced-density gradient (RDG, s) defined as:

$$s = \frac{1}{2(3\pi)^{1/3}} \frac{|\nabla\rho|}{\rho^{4/3}} \quad (2)$$

The combination of s and ρ allows a rough partition of real space into bonding regions: high- s low- ρ corresponds to non-interacting density tails, low- s high- ρ to covalent bonds, and low- s low- ρ to non-covalent interactions. The NCI analysis was carried out at the BLYP-D3(BJ)/def2-SVP level using Multiwfn program.²⁰

Complexation, interaction and deformation energies

The interaction energies were calculated directly from the electronic energy of complex and electronic energies of its subsystems. For **Host**⊃**C_{xxx}**, the interaction energy can be expressed as follows:

$$E_{\text{int}} = E_{\text{Host} \supset C_{xxx}} - (E_{\text{Host}} + E_{C_{xxx}}) \quad (3)$$

Deformation (or strain) energy for each of studied complexes has been determined using following equation:

$$E_{Strain} = (E_{Host}^{Complex\ geom.} - E_{Host}^{Eq.\ geom.}) + (E_{C_{XXX}}^{Complex\ geom.} - E_{C_{XXX}}^{Eq.\ geom.}) \quad (4)$$

At the same time, complexation energy comprises both interaction ($\Delta E_{int.}$) and deformation ($E_{def.}$) energies. Thus $\Delta E_{Complex.}$ can be represented as following:

$$E_{Complex} = E_{int} + E_{def} \quad (5)$$

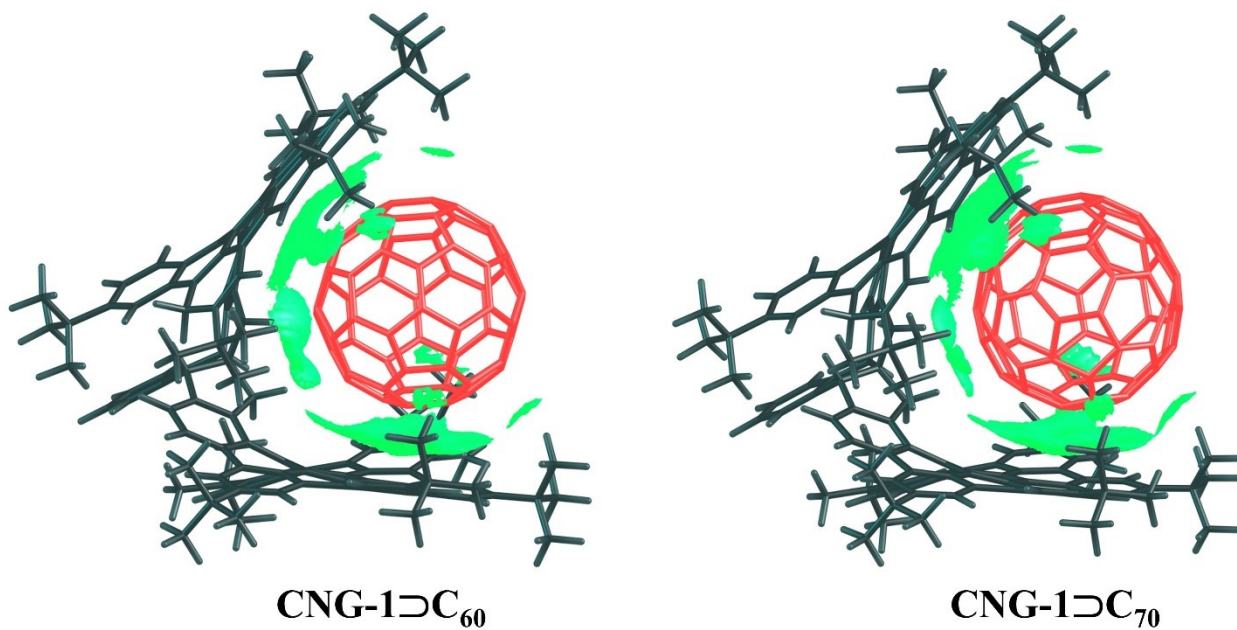


Figure S13. NCI isosurfaces for **CNG-1⊃C₆₀** and **CNG-1⊃C₇₀** complexes.

Cartesian coordinates

CNG-1 nanographene tweezers

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	-0.849728000	2.528368000	2.078255000
6	-0.156166000	3.208995000	3.098329000
6	-0.129842000	2.637325000	0.741091000
6	1.145490000	3.538045000	1.019404000
6	1.103297000	3.881043000	2.568017000
6	2.496331000	2.788639000	0.794226000
6	0.982713000	4.787925000	0.096843000
6	3.108393000	2.581580000	2.169727000
6	-0.361715000	4.643728000	-0.596878000
6	4.340024000	1.941402000	2.510492000
6	4.921902000	2.236036000	3.791076000
6	4.159315000	2.964470000	4.746048000
6	2.890456000	3.460912000	4.442047000
6	2.388638000	3.302775000	3.133430000
6	-0.916838000	3.385753000	-0.319445000
6	-2.052837000	2.925219000	-1.016679000
6	-2.575009000	3.703356000	-2.050681000
6	-2.032058000	4.979484000	-2.368974000
6	-0.968954000	5.510766000	-1.558667000
6	-0.641755000	3.191827000	4.417360000
6	-1.844601000	2.517927000	4.706312000
6	-2.557265000	1.868535000	3.678873000
6	-2.059441000	1.870746000	2.361104000
1	0.146883000	1.622608000	0.384706000
1	1.049468000	4.975104000	2.750911000
1	3.199068000	3.405338000	0.193434000
1	2.337818000	1.869115000	0.211212000
1	1.101278000	5.714033000	0.678731000
1	1.777344000	4.820042000	-0.679016000
1	4.590005000	3.186049000	5.729992000
1	2.326304000	4.028392000	5.194796000
1	-2.479187000	1.936214000	-0.801518000
1	-3.389659000	3.293275000	-2.659483000
1	-0.091506000	3.698275000	5.220823000
1	-2.230981000	2.505822000	5.735789000
1	-3.500977000	1.351821000	3.906286000
1	-2.617388000	1.362821000	1.563882000
6	6.509395000	1.073626000	1.680433000
6	5.084536000	1.095847000	1.567645000
6	4.471802000	0.311322000	0.533308000
6	5.251926000	-0.035421000	-0.614627000
6	6.673593000	0.146125000	-0.601644000
6	7.309593000	0.599936000	0.590926000
6	8.750908000	0.624019000	0.685880000
6	7.462691000	-0.176299000	-1.768034000
6	4.600193000	-0.523960000	-1.812998000
6	7.139067000	1.467809000	2.923683000
6	3.108992000	-0.228224000	0.625949000
6	8.556716000	1.346568000	3.084764000
6	9.119262000	1.564452000	4.364608000
6	8.338015000	1.910489000	5.481024000
6	6.950594000	2.078195000	5.288468000
6	6.334043000	1.896593000	4.033675000

CNG-1C₆₀

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	-1.212005000	2.084866000	1.277890000
6	-0.568320000	2.712931000	2.370255000
6	-0.499083000	2.387227000	-0.036544000
6	0.807088000	3.153245000	0.405192000
6	0.558543000	3.615153000	1.887159000
6	2.072981000	2.253379000	0.507085000
6	0.936302000	4.364926000	-0.542906000
6	2.797174000	2.715893000	1.764374000
6	-0.446278000	4.533204000	-1.148865000
6	4.159513000	2.536171000	2.162255000
6	4.648800000	3.340877000	3.254513000
6	3.733823000	4.118977000	4.012167000
6	2.378095000	4.184298000	3.680680000
6	1.923969000	3.507925000	2.534185000
6	-1.196190000	3.360184000	-0.983795000
6	-2.373220000	3.160555000	-1.740865000
6	-2.705084000	4.079406000	-2.743953000
6	-1.951988000	5.274268000	-2.938942000
6	-0.902612000	5.571940000	-2.009320000
6	-1.039319000	2.521677000	3.678569000
6	-2.179899000	1.720087000	3.892116000
6	-2.842952000	1.122897000	2.801421000
6	-2.357390000	1.299879000	1.489384000
1	-0.268947000	1.439442000	-0.570967000
1	0.193804000	4.657979000	1.932245000
1	2.716041000	2.297686000	-0.392386000
1	1.747211000	1.204511000	0.603922000
1	1.367038000	5.242206000	-0.036156000
1	1.615156000	4.123126000	-1.380512000
1	4.103026000	4.731893000	4.843422000
1	1.696982000	4.815837000	4.259425000
1	-2.978745000	2.252939000	-1.604273000
1	-3.544689000	3.851641000	-3.412595000
1	-0.522439000	2.991186000	4.527285000
1	-2.554842000	1.562663000	4.913911000
1	-3.734663000	0.503525000	2.975322000
1	-2.870798000	0.821043000	0.643306000
6	6.496611000	2.039523000	1.460658000
6	5.113026000	1.669154000	1.447318000
6	4.734024000	0.505214000	0.703370000
6	5.598867000	0.034551000	-0.334439000
6	6.949538000	0.494371000	-0.412457000
6	7.419929000	1.444662000	0.538572000
6	8.782432000	1.922315000	0.466886000
6	7.814796000	0.028840000	-1.472804000
6	5.058418000	-0.801737000	-1.383799000
6	6.984301000	2.969206000	2.456930000
6	3.525487000	-0.277594000	0.969518000
6	8.367312000	3.330234000	2.494765000
6	8.862716000	4.043289000	3.611012000
6	8.032772000	4.423145000	4.681288000
6	6.653138000	4.145429000	4.575443000
6	6.099864000	3.465413000	3.470882000

6	9.554607000	0.282865000	-0.451655000	6	9.656108000	1.474514000	-0.577170000
6	10.963661000	0.314046000	-0.325527000	6	10.903720000	2.119044000	-0.743487000
6	11.604664000	0.673190000	0.872107000	6	11.318311000	3.182449000	0.075183000
6	10.795857000	1.007770000	1.977885000	6	10.484855000	3.546448000	1.153624000
6	9.387638000	0.991210000	1.920701000	6	9.238387000	2.931340000	1.379798000
6	6.821791000	-0.580621000	-2.985710000	6	7.280514000	-0.768269000	-2.538426000
6	7.619854000	-0.855531000	-4.119465000	6	8.129880000	-1.156329000	-3.597040000
6	9.021864000	-0.750881000	-4.096676000	6	9.484643000	-0.782730000	-3.648680000
6	9.633879000	-0.369809000	-2.886224000	6	9.985293000	0.019549000	-2.605228000
6	8.896721000	-0.087099000	-1.716749000	6	9.180154000	0.466663000	-1.537377000
6	3.185703000	-0.753698000	-1.825346000	6	3.685549000	-1.208958000	-1.345159000
6	2.547285000	-1.063948000	-3.047389000	6	3.090360000	-1.731573000	-2.514257000
6	3.260920000	-1.196727000	-4.251474000	6	3.819565000	-1.903772000	-3.707008000
6	4.660902000	-1.037819000	-4.205984000	6	5.200701000	-1.623607000	-3.680787000
6	5.354826000	-0.717854000	-3.019413000	6	5.847083000	-1.096337000	-2.542663000
6	2.423652000	-0.353158000	1.864874000	6	2.900690000	-0.295562000	2.242708000
6	1.126218000	-0.860414000	1.943211000	6	1.704725000	-0.982303000	2.457467000
6	0.442489000	-1.303747000	0.781428000	6	1.082791000	-1.715266000	1.413031000
6	1.136053000	-1.231371000	-0.436559000	6	1.749011000	-1.769570000	0.176694000
6	2.455163000	-0.722262000	-0.550073000	6	2.964612000	-1.085960000	-0.071112000
6	2.570690000	-1.510520000	-5.598822000	6	3.157012000	-2.325843000	-5.037672000
6	13.144099000	0.714905000	1.014301000	6	12.604152000	3.991722000	-0.205484000
6	9.899046000	-1.041071000	-5.336845000	6	10.415586000	-1.191771000	-4.812652000
6	8.944815000	2.120845000	6.887817000	6	8.577194000	5.128839000	5.945076000
6	-0.973713000	-1.922028000	0.823814000	6	-0.240394000	-2.487872000	1.610208000
6	-1.594865000	-1.857318000	2.239515000	6	-0.914526000	-2.144840000	2.960413000
6	-0.885508000	-3.414288000	0.394760000	6	0.058048000	-4.013215000	1.572028000
6	-1.903807000	-1.160088000	-0.160060000	6	-1.227399000	-2.124304000	0.466542000
6	1.039297000	-1.672005000	-5.448260000	6	1.653606000	-2.647169000	-4.866822000
6	3.145279000	-2.834459000	-6.176782000	6	3.864778000	-3.586180000	-5.607102000
6	2.843125000	-0.348130000	-6.594933000	6	3.295478000	-1.148059000	-6.045672000
6	9.056552000	-1.447570000	-6.569167000	6	9.668131000	-1.997163000	-5.901960000
6	10.880980000	-2.201520000	-5.011024000	6	11.572014000	-2.067460000	-4.254906000
6	10.708257000	0.236242000	-5.699235000	6	11.001728000	0.086607000	-5.475765000
6	13.865618000	0.333938000	-0.299975000	6	13.392575000	3.437456000	-1.415861000
6	13.581244000	-0.286713000	2.120129000	6	13.528395000	3.956990000	1.042828000
6	13.582660000	2.151997000	1.413627000	6	12.203728000	5.461863000	-0.520507000
6	10.479965000	1.928791000	6.900171000	6	10.114875000	5.295585000	5.907110000
6	8.315775000	1.096534000	7.873491000	6	8.210125000	4.285090000	7.198084000
6	8.632706000	3.565251000	7.371182000	6	7.938428000	6.540183000	6.065635000
1	10.197125000	1.437285000	4.490421000	1	9.933619000	4.260138000	3.654065000
1	6.330088000	2.366075000	6.144335000	1	5.986109000	4.472604000	5.380771000
1	11.573835000	0.047415000	-1.191429000	1	11.538633000	1.820884000	-1.580124000
1	11.283156000	1.304316000	2.912858000	1	10.787547000	4.372812000	1.807209000
1	7.128381000	-1.169788000	-5.043127000	1	7.715011000	-1.766004000	-4.402872000
1	10.725525000	-0.290906000	-2.855961000	1	11.031994000	0.336639000	-2.647275000
1	1.462125000	-1.194036000	-3.051383000	1	2.023296000	-1.971514000	-2.492484000
1	5.228739000	-1.153087000	-5.135054000	1	5.782955000	-1.766212000	-4.596972000
1	2.928084000	-0.056410000	2.789376000	1	3.356968000	0.257999000	3.070988000
1	0.650191000	-0.924820000	2.928047000	1	1.252069000	-0.946813000	3.454701000
1	0.652891000	-1.625208000	-1.337602000	1	1.331346000	-2.391924000	-0.623483000
1	-2.621733000	-2.273371000	2.217066000	1	-1.885700000	-2.672964000	3.037875000
1	-1.657526000	-0.818714000	2.614813000	1	-1.111140000	-1.060269000	3.055312000
1	-1.011732000	-2.453124000	2.968847000	1	-0.296704000	-2.464722000	3.822402000
1	-0.496482000	-3.522871000	-0.636417000	1	0.511535000	-4.313230000	0.606994000
1	-1.887932000	-3.888241000	0.431210000	1	-0.875832000	-4.596709000	1.707870000
1	-0.212121000	-3.977548000	1.070881000	1	0.763350000	-4.296234000	2.378608000
1	-1.534841000	-1.211512000	-1.202450000	1	-0.840036000	-2.422973000	-0.526581000
1	-1.973731000	-0.091700000	0.117338000	1	-1.413212000	-1.034208000	0.449036000
1	-2.926023000	-1.589714000	-0.141304000	1	-2.197833000	-2.639879000	0.615461000

1	0.588316000	-1.902378000	-6.433591000	1	1.221917000	-2.951391000	-5.840722000
1	0.562747000	-0.745890000	-5.070929000	1	1.083273000	-1.766862000	-4.510997000
1	0.779344000	-2.500064000	-4.759691000	1	1.489328000	-3.477779000	-4.152014000
1	2.659756000	-3.076489000	-7.144216000	1	3.400641000	-3.887593000	-6.568052000
1	2.968680000	-3.678330000	-5.480372000	1	3.783968000	-4.437096000	-4.901589000
1	4.235872000	-2.767152000	-6.355890000	1	4.940322000	-3.406106000	-5.798090000
1	2.357946000	-0.552799000	-7.571243000	1	2.819449000	-1.406275000	-7.013817000
1	3.926401000	-0.210324000	-6.778707000	1	4.355483000	-0.898865000	-6.244085000
1	2.442931000	0.608019000	-6.203081000	1	2.808746000	-0.233512000	-5.653287000
1	9.723710000	-1.641906000	-7.431981000	1	10.367949000	-2.262449000	-6.718644000
1	8.350777000	-0.646992000	-6.866051000	1	8.841065000	-1.409878000	-6.347138000
1	8.473296000	-2.370970000	-6.383220000	1	9.247770000	-2.941069000	-5.502519000
1	11.522597000	-2.425353000	-5.887765000	1	12.260538000	-2.366726000	-5.071454000
1	10.327169000	-3.123218000	-4.742831000	1	11.176016000	-2.987503000	-3.780654000
1	11.546217000	-1.949134000	-4.162728000	1	12.166317000	-1.525152000	-3.493666000
1	11.340976000	0.054080000	-6.591877000	1	11.676276000	-0.188431000	-6.311824000
1	11.374292000	0.548769000	-4.871755000	1	11.585744000	0.695010000	-4.759009000
1	10.028622000	1.082346000	-5.923331000	1	10.195424000	0.728221000	-5.879725000
1	13.610826000	1.028092000	-1.124957000	1	12.794055000	3.478252000	-2.347098000
1	13.613757000	-0.694991000	-0.624466000	1	13.712642000	2.389146000	-1.253821000
1	14.962778000	0.378326000	-0.152664000	1	14.304619000	4.044731000	-1.578899000
1	13.278162000	-1.319826000	1.857537000	1	13.821878000	2.916536000	1.287299000
1	13.126037000	-0.040884000	3.099169000	1	13.032856000	4.386648000	1.935024000
1	14.683192000	-0.270066000	2.246045000	1	14.451666000	4.542626000	0.857073000
1	13.273960000	2.886396000	0.643250000	1	11.553884000	5.509687000	-1.415693000
1	14.685325000	2.205510000	1.521542000	1	13.106860000	6.076126000	-0.713609000
1	13.134596000	2.464814000	2.376383000	1	11.650108000	5.925628000	0.318637000
1	10.989170000	2.646999000	6.227650000	1	10.441533000	5.919066000	5.051564000
1	10.770057000	0.904121000	6.595025000	1	10.632019000	4.318380000	5.839551000
1	10.869671000	2.095426000	7.923769000	1	10.460269000	5.795415000	6.833551000
1	8.525955000	0.057854000	7.549249000	1	8.645644000	3.268470000	7.129296000
1	7.216672000	1.212928000	7.940227000	1	7.114675000	4.175478000	7.314967000
1	8.732574000	1.231940000	8.892554000	1	8.600042000	4.767647000	8.117520000
1	9.063151000	4.314415000	6.677158000	1	8.215146000	7.170863000	5.198170000
1	9.063295000	3.738482000	8.378676000	1	8.289866000	7.048392000	6.986614000
1	7.543239000	3.751469000	7.434648000	1	6.833563000	6.491143000	6.105055000
6	-0.638190000	7.373944000	-3.161986000	6	-0.254468000	7.597713000	-3.273335000
6	-0.478150000	6.868413000	-1.833518000	6	-0.271143000	6.889445000	-2.037092000
6	0.166813000	7.707845000	-0.862996000	6	0.337491000	7.483144000	-0.888267000
6	1.046757000	8.737454000	-1.323759000	6	1.318889000	8.498005000	-1.089293000
6	1.061280000	9.106663000	-2.708446000	6	1.470000000	9.113727000	-2.371463000
6	0.135746000	8.495432000	-3.603987000	6	0.620344000	8.717786000	-3.445524000
6	0.010466000	8.973449000	-4.961523000	6	0.754371000	9.331144000	-4.744051000
6	1.968914000	10.125169000	-3.184511000	6	2.506287000	10.096872000	-2.582363000
6	1.962320000	9.376651000	-0.399353000	6	2.275280000	8.767619000	-0.037631000
6	-1.635937000	6.795853000	-4.036987000	6	-1.145244000	7.191509000	-4.337615000
6	-0.093731000	7.621955000	0.580041000	6	-0.034531000	7.166178000	0.498113000
6	-1.886100000	7.371639000	-5.327412000	6	-1.123555000	7.891069000	-5.588550000
6	-2.994292000	6.911319000	-6.069490000	6	-2.115480000	7.593897000	-6.546369000
6	-3.851327000	5.893678000	-5.602137000	6	-3.110034000	6.616916000	-6.327502000
6	-3.549674000	5.296894000	-4.364684000	6	-3.075008000	5.896327000	-5.118492000
6	-2.444404000	5.703206000	-3.581932000	6	-2.100922000	6.139703000	-4.123270000
6	0.889891000	10.000201000	-5.448473000	6	1.776882000	10.314516000	-4.972570000
6	0.740223000	10.442162000	-6.780297000	6	1.980534000	10.777082000	-6.289178000
6	-0.233477000	9.915146000	-7.651612000	6	1.229350000	10.307341000	-7.384349000
6	-1.083577000	8.910210000	-7.156263000	6	0.199257000	9.382618000	-7.130780000
6	-0.989772000	8.426776000	-5.831574000	6	-0.065561000	8.888648000	-5.834045000
6	2.935908000	10.705358000	-2.293862000	6	3.471007000	10.359199000	-1.548656000
6	3.828704000	11.671659000	-2.800452000	6	4.489867000	11.299992000	-1.792333000
6	3.811109000	12.091128000	-4.146440000	6	4.621381000	11.967808000	-3.027498000

6	2.846559000	11.526050000	-4.997434000	6	3.700231000	11.659185000	-4.042994000
6	1.915596000	10.558953000	-4.550957000	6	2.652150000	10.726318000	-3.860871000
6	1.927420000	9.047408000	0.997675000	6	2.168125000	8.086905000	1.220701000
6	2.933773000	9.552350000	1.844887000	6	3.287271000	8.043784000	2.071360000
6	3.955073000	10.405572000	1.379463000	6	4.497854000	8.694712000	1.739315000
6	3.933168000	10.773021000	0.023003000	6	4.518591000	9.502609000	0.587069000
6	2.955448000	10.291432000	-0.879701000	6	3.420993000	9.577056000	-0.303512000
6	-1.253431000	6.990693000	1.105754000	6	-1.317955000	6.671844000	0.846046000
6	-1.478893000	6.888534000	2.478974000	6	-1.695776000	6.495235000	2.178765000
6	-0.567899000	7.446045000	3.413266000	6	-0.813204000	6.805538000	3.246199000
6	0.543423000	8.129349000	2.895410000	6	0.466200000	7.281354000	2.904007000
6	0.802109000	8.248747000	1.506495000	6	0.872848000	7.478774000	1.559672000
6	-5.069920000	5.472365000	-6.456399000	6	-4.183712000	6.369223000	-7.412875000
6	-0.784152000	7.381398000	4.942178000	6	-1.275914000	6.760318000	4.722200000
6	5.036623000	10.908122000	2.363567000	6	5.756156000	8.440478000	2.596346000
6	4.826235000	13.154105000	-4.627142000	6	5.775806000	12.976054000	-3.229114000
6	-0.328537000	10.448159000	-9.100076000	6	1.605298000	10.764821000	-8.812283000
6	-2.028451000	6.542372000	5.317857000	6	-2.595101000	5.967017000	4.892517000
6	-0.980369000	8.823202000	5.491000000	6	-1.507319000	8.226449000	5.191621000
6	0.466027000	6.744161000	5.611108000	6	-0.207056000	6.102794000	5.633153000
6	4.354376000	11.717555000	3.502521000	6	5.473731000	8.826299000	4.074245000
6	6.077617000	11.822655000	1.675786000	6	6.977815000	9.250496000	2.102724000
6	5.783357000	9.687050000	2.970155000	6	6.101826000	6.926745000	2.502496000
6	4.587742000	14.475679000	-3.843329000	6	7.132373000	12.248168000	-3.013145000
6	4.689771000	13.454389000	-6.138780000	6	5.629498000	14.128222000	-2.196664000
6	6.270700000	12.646129000	-4.359656000	6	5.777829000	13.588309000	-4.649753000
6	-0.608985000	11.976839000	-9.065842000	6	3.045707000	10.265108000	-9.123758000
6	-1.460598000	9.765356000	-9.903709000	6	1.558150000	12.315451000	-8.895531000
6	1.017495000	10.183937000	-9.832188000	6	0.647460000	10.190643000	-9.882683000
6	-4.577025000	4.974455000	-7.844212000	6	-3.487242000	5.976791000	-8.746289000
6	-6.007359000	6.697826000	-6.646801000	6	-5.005796000	7.672345000	-7.619862000
6	-5.884008000	4.335733000	-5.794290000	6	-5.159961000	5.234035000	-7.024267000
1	-3.212837000	7.377477000	-7.036248000	1	-2.127364000	8.159255000	-7.485069000
1	-4.186529000	4.491726000	-3.989732000	1	-3.814405000	5.110170000	-4.943425000
1	1.404180000	11.228340000	-7.154539000	1	2.787993000	11.490862000	-6.480175000
1	-1.835105000	8.475607000	-7.819885000	1	-0.390012000	8.996452000	-7.966568000
1	4.561297000	12.123223000	-2.123421000	1	5.209114000	11.514709000	-0.994001000
1	2.813121000	11.843795000	-6.042024000	1	3.809305000	12.140888000	-5.016925000
1	2.927927000	9.263636000	2.901569000	1	3.230237000	7.431327000	2.979877000
1	4.708757000	11.443996000	-0.353578000	1	5.436623000	10.035514000	0.326982000
1	-1.996499000	6.575547000	0.418151000	1	-2.046458000	6.460123000	0.056346000
1	-2.385601000	6.378518000	2.823062000	1	-2.708354000	6.132696000	2.386867000
1	1.224936000	8.624386000	3.596032000	1	1.162632000	7.577635000	3.698179000
1	-2.958988000	6.994099000	4.921551000	1	-3.443261000	6.456459000	4.376210000
1	-2.127998000	6.491562000	6.420472000	1	-2.858146000	5.904749000	5.967162000
1	-1.958214000	5.506986000	4.935573000	1	-2.502024000	4.934556000	4.502151000
1	-1.865040000	9.302779000	5.026946000	1	-2.264458000	8.727417000	4.556607000
1	-0.101214000	9.463749000	5.283495000	1	-0.572598000	8.817875000	5.132092000
1	-1.134331000	8.802134000	6.589397000	1	-1.864476000	8.248688000	6.241904000
1	0.654419000	5.732632000	5.205665000	1	-0.054892000	5.041010000	5.361813000
1	0.320665000	6.658131000	6.707167000	1	-0.535752000	6.136358000	6.691118000
1	1.378470000	7.346895000	5.438615000	1	0.770850000	6.617506000	5.575186000
1	3.624042000	11.102673000	4.063349000	1	4.649335000	8.225883000	4.505447000
1	3.813589000	12.593588000	3.092370000	1	5.195095000	9.895930000	4.158161000
1	5.111769000	12.084953000	4.224829000	1	6.372588000	8.652442000	4.696812000
1	6.617963000	11.295184000	0.865073000	1	7.256877000	8.981369000	1.064993000
1	6.830546000	12.156691000	2.416681000	1	7.852794000	9.035179000	2.747479000
1	5.609191000	12.729682000	1.245201000	1	6.793933000	10.342807000	2.140780000
1	6.276222000	9.091513000	2.176211000	1	6.271254000	6.624230000	1.451492000
1	5.094318000	9.014353000	3.516440000	1	5.285801000	6.295216000	2.898718000

1	6.561931000	10.024517000	3.684464000	1	7.017279000	6.689710000	3.077295000
1	5.304243000	15.256434000	-4.171221000	1	7.976312000	12.956070000	-3.141797000
1	4.717179000	14.334959000	-2.752639000	1	7.254925000	11.423435000	-3.741316000
1	3.560493000	14.854176000	-4.014917000	1	7.209445000	11.810014000	-1.999583000
1	4.856141000	12.548462000	-6.754429000	1	4.665519000	14.658105000	-2.331844000
1	5.443339000	14.208253000	-6.440658000	1	6.449751000	14.865080000	-2.317565000
1	3.691176000	13.863565000	-6.389192000	1	5.664853000	13.752561000	-1.155664000
1	6.463911000	11.699489000	-4.902614000	1	4.841723000	14.141514000	-4.861960000
1	6.447580000	12.458526000	-3.283022000	1	5.907608000	12.813298000	-5.430708000
1	7.014158000	13.396931000	-4.697006000	1	6.618339000	14.303161000	-4.747989000
1	-0.680394000	12.381090000	-10.096297000	1	3.350414000	10.566212000	-10.147065000
1	0.193947000	12.530877000	-8.542110000	1	3.103509000	9.160835000	-9.054328000
1	-1.562716000	12.191201000	-8.543640000	1	3.786544000	10.679253000	-8.412798000
1	-1.494009000	10.180232000	-10.930484000	1	1.829421000	12.657094000	-9.915147000
1	-2.452954000	9.935581000	-9.441589000	1	2.263230000	12.789369000	-8.185528000
1	-1.303003000	8.672244000	-9.990858000	1	0.541593000	12.691407000	-8.664020000
1	0.974018000	10.563851000	-10.873419000	1	0.944773000	10.554166000	-10.886028000
1	1.239227000	9.098775000	-9.868754000	1	-0.400222000	10.506374000	-9.707969000
1	1.865555000	10.683943000	-9.325402000	1	0.675455000	9.083622000	-9.908815000
1	-3.897539000	4.106249000	-7.731685000	1	-2.882748000	5.056889000	-8.618122000
1	-4.027699000	5.763429000	-8.393539000	1	-2.812827000	6.776258000	-9.109065000
1	-5.436298000	4.662639000	-8.472621000	1	-4.241811000	5.788402000	-9.537107000
1	-6.889819000	6.420885000	-7.259343000	1	-5.785181000	7.521379000	-8.394712000
1	-5.491471000	7.534109000	-7.157293000	1	-4.364958000	8.514622000	-7.945380000
1	-6.369306000	7.072185000	-5.668590000	1	-5.507726000	7.974469000	-6.679171000
1	-5.274562000	3.420908000	-5.656203000	1	-4.633242000	4.269953000	-6.881049000
1	-6.747326000	4.068098000	-6.435182000	1	-5.907758000	5.089625000	-7.828985000
1	-6.282516000	4.637484000	-4.805696000	1	-5.713959000	5.465936000	-6.093286000
				6	2.925755000	6.316743000	-5.764404000
				6	3.320064000	7.404701000	-4.962485000
				6	2.636673000	5.020115000	-5.143994000
				6	3.438922000	7.239960000	-3.512394000
				6	2.750493000	4.866951000	-3.745248000
				6	3.149352000	6.002691000	-2.909045000
				6	3.605267000	6.070777000	-7.041064000
				6	4.397105000	8.295205000	-5.404839000
				6	3.140646000	3.971820000	-6.035705000
				6	3.738080000	4.620623000	-7.208348000
				6	4.587175000	8.027325000	-3.059829000
				6	4.642234000	6.927934000	-7.467225000
				6	5.043490000	8.066594000	-6.633927000
				6	5.177422000	8.682217000	-4.226796000
				6	3.363296000	3.659783000	-3.186213000
				6	4.007216000	5.501955000	-1.829481000
				6	3.727756000	2.806501000	-5.498145000
				6	3.839943000	2.646332000	-4.044536000
				6	4.141192000	4.053271000	-2.004001000
				6	5.403452000	7.554695000	-2.016769000
				6	4.902327000	4.081709000	-7.795112000
				6	5.111908000	6.262684000	-1.391886000
				6	5.852232000	6.367876000	-8.074289000
				6	6.500358000	8.210865000	-6.728439000
				6	6.573982000	8.831697000	-4.315697000
				6	5.979335000	4.972582000	-8.235940000
				6	4.939707000	2.247900000	-6.109354000
				6	7.250185000	8.585653000	-5.592412000
				6	6.999412000	7.160185000	-7.618697000
				6	5.514265000	2.871750000	-7.237389000
				6	6.858960000	7.704976000	-2.108539000
				6	5.369060000	3.422291000	-1.728726000

6	5.119418000	1.991343000	-3.759665000
6	7.432929000	8.329801000	-3.237668000
6	6.391190000	5.606795000	-1.102032000
6	5.798253000	1.741328000	-5.035330000
6	5.866857000	2.385372000	-2.633915000
6	6.516912000	4.212915000	-1.268456000
6	7.257264000	4.315850000	-7.950003000
6	7.472049000	6.498053000	-1.544979000
6	6.969976000	3.017196000	-7.333707000
6	8.229474000	6.527046000	-7.343020000
6	8.527327000	7.927492000	-5.304590000
6	8.639777000	7.769299000	-3.850100000
6	8.360884000	5.077588000	-7.513198000
6	9.007278000	6.917081000	-6.163214000
6	7.199233000	1.884381000	-5.129500000
6	7.316797000	2.540294000	-2.739569000
6	7.722975000	3.661656000	-1.892540000
6	7.797304000	2.531509000	-6.300382000
6	8.636300000	5.959676000	-2.135866000
6	9.230491000	6.607349000	-3.309670000
6	7.973287000	2.288540000	-3.955183000
6	8.767294000	4.509995000	-2.307932000
6	9.221980000	4.573156000	-6.438773000
6	9.621242000	5.710044000	-5.603897000
6	8.945208000	3.325578000	-5.843846000
6	9.730053000	5.557444000	-4.204711000
6	9.055798000	3.169236000	-4.390804000
6	9.445387000	4.260788000	-3.584476000

CNG-1D_{C₇₀}

Gas-phase. BLYP-D3(BJ)/def2-SVP

Atom	X	Y	Z
6	-1.220899000	2.195356000	1.357289000
6	-0.556944000	2.766883000	2.468355000
6	-0.489004000	2.496919000	0.052370000
6	0.820602000	3.246889000	0.510019000
6	0.597008000	3.648346000	2.013499000
6	2.091674000	2.346248000	0.543776000
6	0.938588000	4.500992000	-0.383190000
6	2.826040000	2.732203000	1.819290000
6	-0.416003000	4.649178000	-1.050199000
6	4.190976000	2.518906000	2.191823000
6	4.700223000	3.266995000	3.313995000
6	3.800367000	4.013056000	4.121084000
6	2.440689000	4.100567000	3.814225000
6	1.967041000	3.487279000	2.639825000
6	-1.161442000	3.469446000	-0.911006000
6	-2.307456000	3.255646000	-1.710341000
6	-2.613217000	4.169313000	-2.725190000
6	-1.863687000	5.369564000	-2.898724000
6	-0.846494000	5.680003000	-1.937404000
6	-1.041603000	2.560698000	3.769725000
6	-2.215648000	1.802494000	3.958091000
6	-2.898932000	1.264432000	2.849286000
6	-2.399766000	1.454791000	1.544446000
1	-0.260368000	1.545120000	-0.475707000
1	0.264221000	4.699948000	2.108255000
1	2.728336000	2.455620000	-0.354781000
1	1.774861000	1.290383000	0.567756000

1	1.306856000	5.367974000	0.184065000
1	1.677991000	4.341663000	-1.188921000
1	4.183134000	4.581223000	4.977340000
1	1.771915000	4.705625000	4.435102000
1	-2.905224000	2.339761000	-1.597147000
1	-3.427195000	3.931824000	-3.421302000
1	-0.509585000	2.985085000	4.632950000
1	-2.601886000	1.634311000	4.973932000
1	-3.817515000	0.679979000	3.003035000
1	-2.930482000	1.021823000	0.684588000
6	6.515607000	1.994067000	1.464508000
6	5.123154000	1.659083000	1.439072000
6	4.719477000	0.515125000	0.674657000
6	5.580762000	0.028828000	-0.360293000
6	6.942716000	0.458607000	-0.425681000
6	7.428147000	1.390644000	0.536504000
6	8.809004000	1.815403000	0.496523000
6	7.813130000	-0.037201000	-1.468365000
6	5.045920000	-0.835488000	-1.391072000
6	7.026322000	2.878765000	2.491452000
6	3.497273000	-0.248370000	0.939791000
6	8.419912000	3.195737000	2.547622000
6	8.928328000	3.871961000	3.680733000
6	8.105055000	4.252091000	4.755266000
6	6.721058000	4.003764000	4.642951000
6	6.154047000	3.363215000	3.521825000
6	9.684435000	1.347368000	-0.536736000
6	10.970296000	1.926186000	-0.655672000
6	11.423777000	2.940589000	0.202639000
6	10.577371000	3.331324000	1.261286000
6	9.292557000	2.782454000	1.439507000
6	7.284130000	-0.854963000	-2.521497000
6	8.138616000	-1.255378000	-3.572293000
6	9.492488000	-0.882412000	-3.625338000
6	9.995364000	-0.085452000	-2.579875000
6	9.188594000	0.371606000	-1.517717000
6	3.673324000	-1.245887000	-1.348785000
6	3.106546000	-1.870858000	-2.481403000
6	3.862008000	-2.153362000	-3.635019000
6	5.234124000	-1.834724000	-3.615960000
6	5.853489000	-1.197954000	-2.519174000
6	2.869612000	-0.253796000	2.212702000
6	1.656997000	-0.909928000	2.426066000
6	1.019001000	-1.626216000	1.379974000
6	1.693624000	-1.708176000	0.150522000
6	2.929721000	-1.059769000	-0.094837000
6	3.244481000	-2.784706000	-4.903698000
6	12.770414000	3.668443000	-0.009476000
6	10.421201000	-1.282133000	-4.794337000
6	8.660834000	4.931741000	6.027951000
6	-0.331514000	-2.352631000	1.566689000
6	-0.991475000	-2.006475000	2.922785000
6	-0.093757000	-3.887784000	1.503210000
6	-1.302942000	-1.932324000	0.428800000
6	1.744615000	-3.116364000	-4.721836000
6	3.997482000	-4.100016000	-5.247420000
6	3.383912000	-1.781426000	-6.082875000
6	9.663183000	-2.050322000	-5.903002000
6	11.561472000	-2.186945000	-4.250044000
6	11.031607000	0.000179000	-5.428373000

6	13.554179000	3.107282000	-1.219704000
6	13.650779000	3.517984000	1.261529000
6	12.482695000	5.173907000	-0.274617000
6	10.201748000	5.066433000	5.996235000
6	8.271964000	4.085944000	7.272752000
6	8.051306000	6.355255000	6.156523000
1	10.004189000	4.058340000	3.734794000
1	6.061411000	4.325337000	5.456210000
1	11.612211000	1.607419000	-1.479191000
1	10.908749000	4.122176000	1.943857000
1	7.726506000	-1.866413000	-4.378014000
1	11.045382000	0.219730000	-2.616257000
1	2.044424000	-2.129312000	-2.457787000
1	5.834530000	-2.057496000	-4.503772000
1	3.336978000	0.286208000	3.042975000
1	1.203959000	-0.863020000	3.422640000
1	1.263118000	-2.326313000	-0.645525000
1	-1.979282000	-2.503491000	2.995788000
1	-1.153195000	-0.917872000	3.033878000
1	-0.381896000	-2.358125000	3.778288000
1	0.351014000	-4.190045000	0.534872000
1	-1.051185000	-4.434874000	1.625153000
1	0.595800000	-4.213181000	2.307447000
1	-0.923663000	-2.225697000	-0.569081000
1	-1.450658000	-0.836325000	0.431417000
1	-2.291702000	-2.415279000	0.566562000
1	1.346520000	-3.572154000	-5.649808000
1	1.145458000	-2.208016000	-4.514141000
1	1.578675000	-3.837007000	-3.896707000
1	3.564433000	-4.566944000	-6.155406000
1	3.922925000	-4.827654000	-4.414698000
1	5.072098000	-3.920436000	-5.444172000
1	2.969689000	-2.216438000	-7.015289000
1	4.441113000	-1.513934000	-6.272829000
1	2.840509000	-0.841764000	-5.866888000
1	10.358372000	-2.302934000	-6.727519000
1	8.842443000	-1.441055000	-6.329891000
1	9.232073000	-2.999299000	-5.527748000
1	12.250638000	-2.479121000	-5.068618000
1	11.150052000	-3.110617000	-3.796386000
1	12.157920000	-1.667394000	-3.474679000
1	11.697202000	-0.268894000	-6.273401000
1	11.631862000	0.578961000	-4.700694000
1	10.237985000	0.667604000	-5.813981000
1	12.988793000	3.227284000	-2.164779000
1	13.795179000	2.033243000	-1.093120000
1	14.511074000	3.653875000	-1.332301000
1	13.867716000	2.450711000	1.467307000
1	13.155923000	3.940618000	2.157428000
1	14.615962000	4.048061000	1.129209000
1	11.843752000	5.296979000	-1.170672000
1	13.429441000	5.726969000	-0.442294000
1	11.958839000	5.648702000	0.577570000
1	10.544248000	5.691283000	5.147944000
1	10.699078000	4.079458000	5.921089000
1	10.554252000	5.550296000	6.928437000
1	8.685356000	3.060634000	7.196671000
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5. References

- 1 A. D. Becke, Phys. Rev. A 1988, **38**, 3098-3100.
- 2 C. Lee, W. Yang and R. G. Parr, Phys. Rev. B 1988, **37**, 785-789.
- 3 F. Weigend and R. Ahlrichs, Phys. Chem. Chem. Phys. 2005, **7**, 3297-3305.
- 4 F. Weigend, Phys. Chem. Chem. Phys. 2006, **8**, 1057-1065.
- 5 S. Grimme, J. Antony, S. Ehrlich and H. Krieg, J. Chem. Phys. 2010, **132**, 154104.
- 6 S. Grimme, S. Ehrlich and L. Goerigk, J. Comput. Chem. 2011, **32**, 1456-1465.
K. Eichkorn, F. Weigend, O. Treutler, R. Ahlrichs; Theor. Chem. Acc. 1997, **97**, 119.
- 7 K. Eichkorn, F. Weigend, O. Treutler, R. Ahlrichs; Theor. Chem. Acc. 1997, **97**, 119.
- 8 K. Morokuma, J. Chem. Phys. 1971, **55**, 1236-1244.
- 9 F. M. Bickelhaupt, E. J. Baerends, in *Reviews in Computational Chemistry*, vol. 15 (Eds.: K.B. Lipkowitz, D.B. Boyd), John Wiley & Sons, Inc., 2000, pp. 1-86.
- 10 ADF 2018, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, E.J. Baerends, T. Ziegler, A.J. Atkins, J. Autschbach, O. Baseggio, D. Bashford, A. Bérces, F.M. Bickelhaupt, C. Bo, P.M. Boerrigter, L. Cavallo, C. Daul, D.P. Chong, D.V. Chulhai, L. Deng, R.M. Dickson, J.M. Dieterich, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, A. Förster, C. Fonseca Guerra, M. Franchini, A. Ghysels, A. Giammona, S.J.A. van Gisbergen, A. Goetz, A.W. Götz, J.A. Groeneveld, O.V. Gritsenko, M. Grüning, S. Gusarov, F.E. Harris, P. van den Hoek, Z. Hu, C.R. Jacob, H. Jacobsen, L. Jensen, L. Joubert, J.W. Kaminski, G. van Kessel, C. König, F. Kootstra, A. Kovalenko, M.V. Krykunov, E. van Lenthe, D.A. McCormack, A. Michalak, M. Mitoraj, S.M. Morton, J. Neugebauer, V.P. Nicu, L. Noodleman, V.P. Osinga, S. Patchkovskii, M. Pavanello, C.A. Peeples, P.H.T. Philipsen, D. Post, C.C. Pye, H. Ramanantoanina, P. Ramos, W. Ravenek, J.I. Rodríguez, P. Ros, R. Rüger, P.R.T. Schipper, D. Schlüns, H. van Schoot, G. Schreckenbach, J.S. Seldenthuis, M. Seth, J.G. Snijders, M. Solà, M. Stener, M. Swart, D. Swerhone, V. Tognetti, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E.M. van Wezenbeek, G. Wiesenekker, S.K. Wolff, T.K. Woo, A.L. Yakovlev
- 11 G. A. Zhurko, Chemcraft 1.80 (build 523b) - graphical program for visualization of quantum chemistry computations. (<https://chemcraftprog.com>).
- 12 T. Ziegler and A. Rauk, Theor. Chim. Acta 1977, **46**, 1-10.
- 13 T. Ziegler and A. Rauk, Inorg. Chem. 1979, **18**, 1558-1565.
- 14 T. Ziegler and A. Rauk, Inorg. Chem. 1979, **18**, 1755-1759.
- 15 S. Grimme, J. Comput. Chem. 2004, **25**, 1463-1473.
- 16 S. Grimme, J. Comput. Chem. 2006, **27**, 1787-1799.
- 17 E. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. Cohen and W. Yang, J. Am. Chem. Soc. 2010, **132**, 6498-6506.
- 18 J. Contreras-García, E. Johnson, S. Keinan, R. Chaudret, J. Piquemal, D. Beratan and W. Yang, J. Chem. Theory Comput. 2011, **7**, 625-632.
- 19 J. Contreras-García, W. Yang and E. Johnson, J. Phys. Chem. A, 2011, **115**, 12983-12990.
- 20 T. Lu and F. Chen, J. Comput. Chem. 2012, **33**, 580-592.