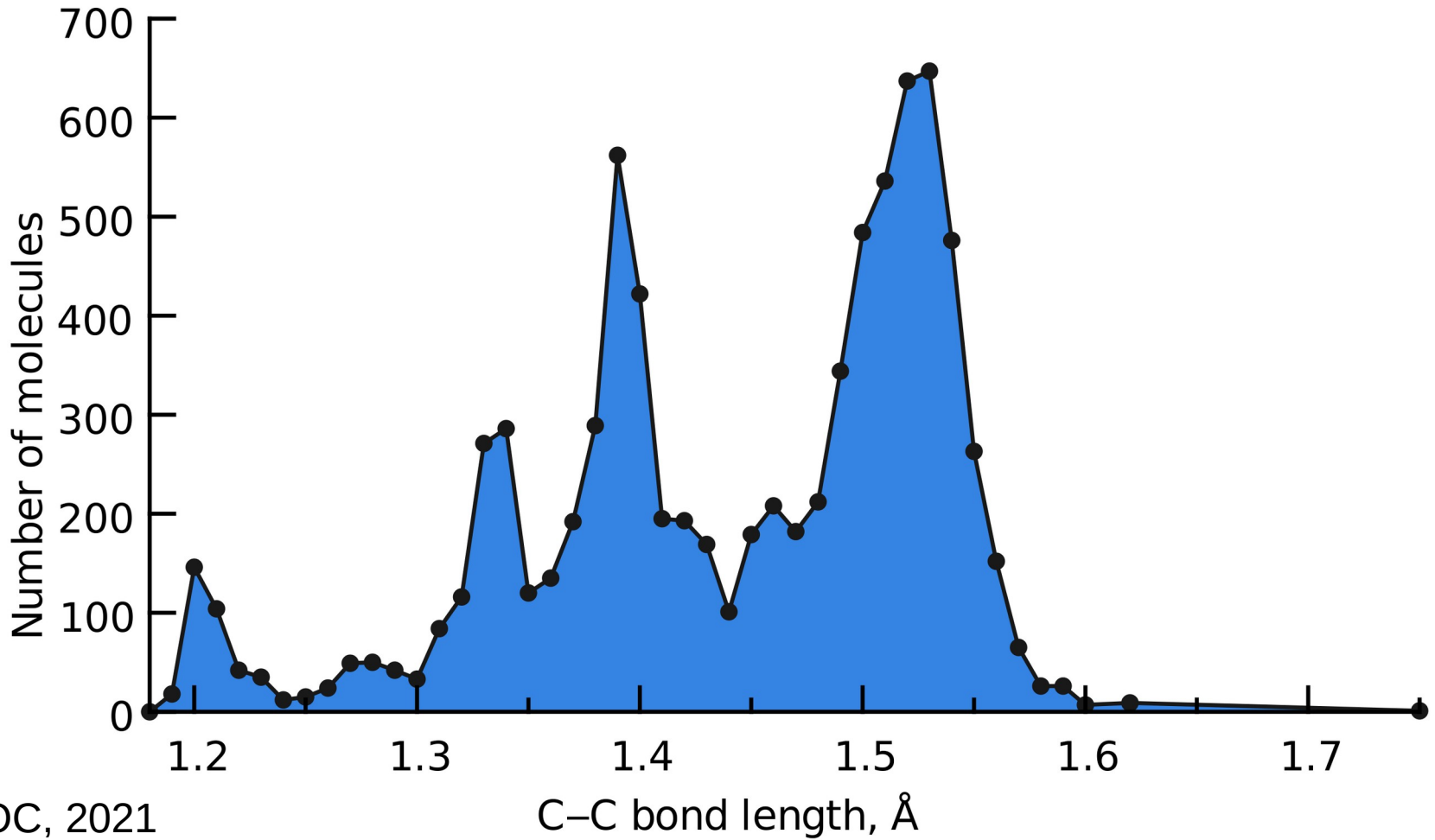
Was ist die längste C—C Bindung?

Yury V. Vishnevskiy

Uni-Bielefeld

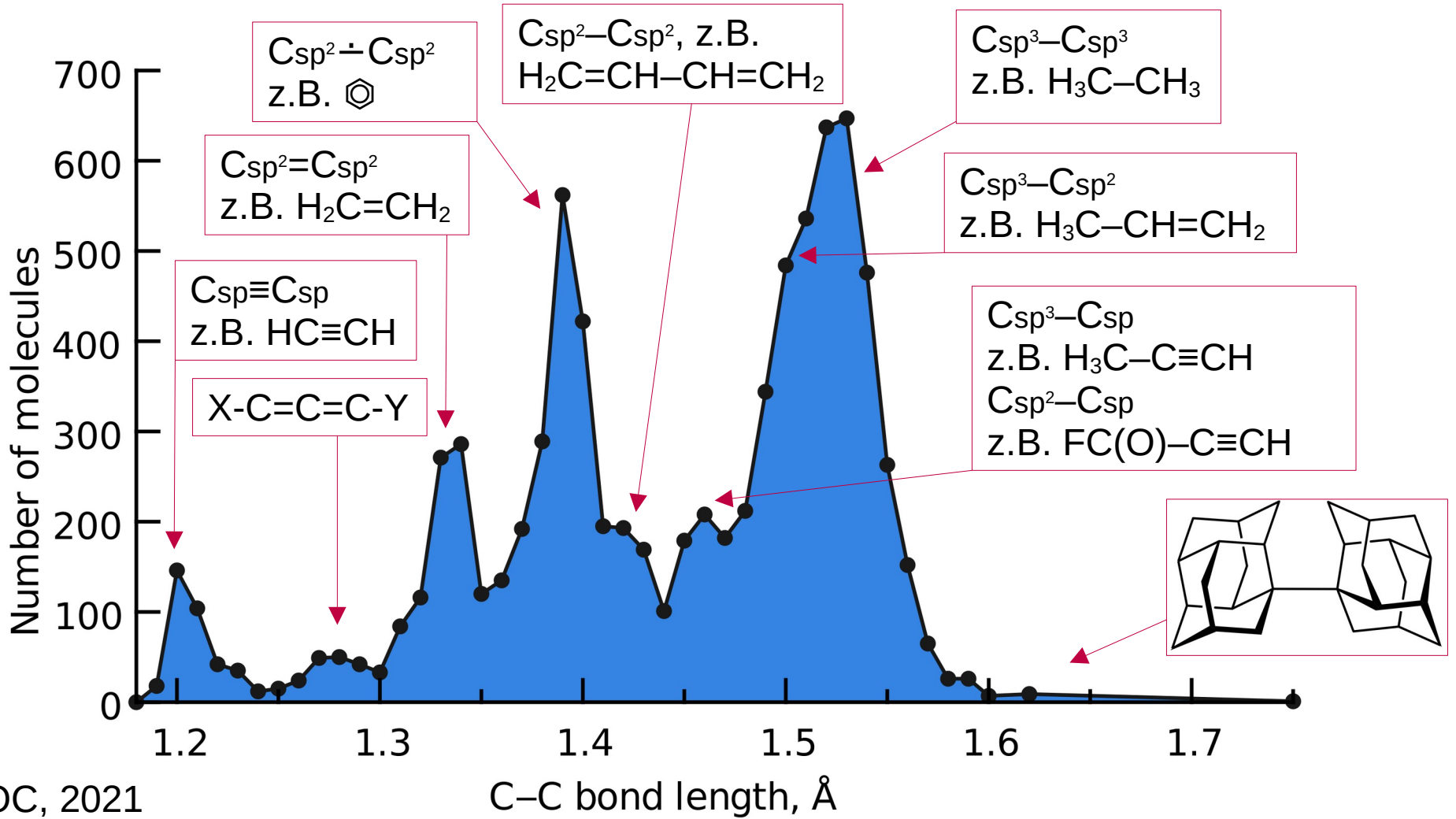
Oktober 2022

r(C–C): Experiment



MOGADOC, 2021

r(C–C): Experiment



MOGADOC, 2021

Overcoming lability of extremely long alkane carbon–carbon bonds through dispersion forces

Peter R. Schreiner[1], Lesya V. Chernish[2], Pavel A. Gunchenko[2], Evgeniya Yu. Tikhonchuk[2], Heike Hausmann[1], Michael Serafin[3], Sabine Schlecht[3], Jeremy E. P. Dahl[4], Robert M. K. Carlson[4] & Andrey A. Fokin[1,2]

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Stable Alkanes Containing Very Long Carbon–Carbon Bonds

Andrey A. Fokin,*[,⊥,‡] Lesya V. Chernish,[⊥] Pavel A. Gunchenko,[⊥] Evgeniya Yu. Tikhonchuk,[⊥] Heike Hausmann,[‡] Michael Serafin,[§] Jeremy E. P. Dahl,[∥] Robert M. K. Carlson,[∥] and Peter R. Schreiner*[,‡]

Chem

Article

Longest C–C Single Bond among Neutral Hydrocarbons with a Bond Length beyond 1.8 Å

Yusuke Ishigaki,[1,*] Takuya Shimajiri,[1] Takashi Takeda,[1,2] Ryo Katoono,[1] and Takanori Suzuki[1,3,*]

Long Carbon–Carbon Bonding beyond 2 Å in Tris(9-fluorenylidene)methane

Takashi Kubo,* Yuki Suga, Daisuke Hashizume,* Hiroki Suzuki, Tatsuya Miyamoto, Hiroshi Okamoto, Ryohei Kishi, and Masayoshi Nakano

Cite This: *J. Am. Chem. Soc.* 2021, 143, 14360–14366

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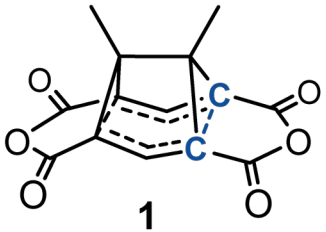

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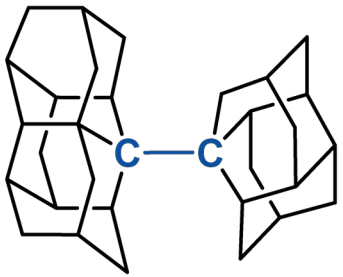

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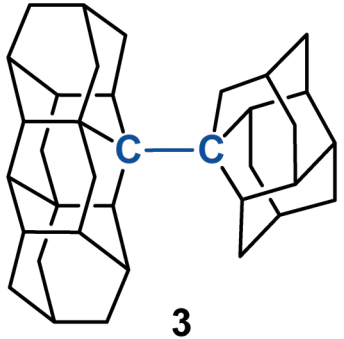

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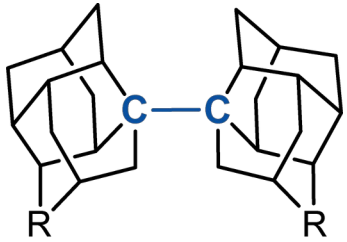
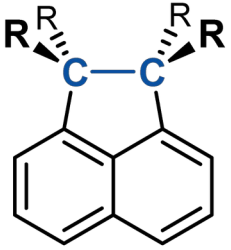
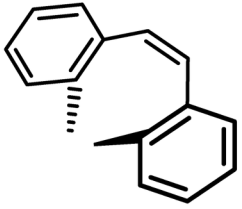
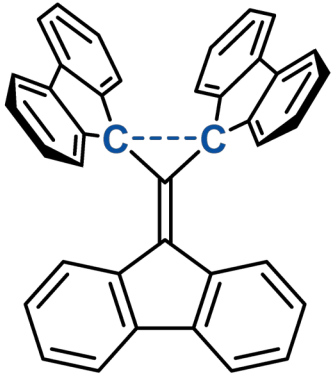


R = CH_2 (**4a**)
R = O (**4b**)



R = H (**5a**) – *this work*
R = 4-*t*-Bu-C_6H_4 (**5b**)
R = C_6H_5 (**5c**)

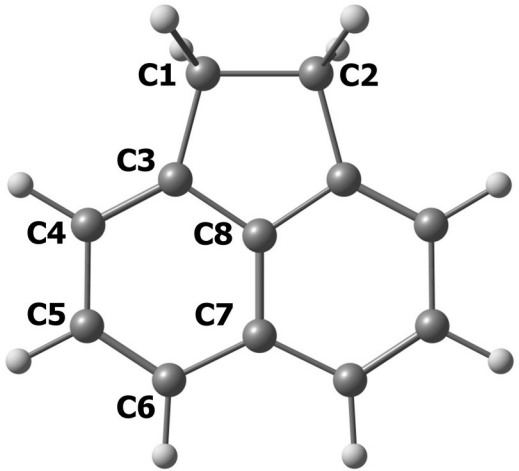
R,R =  (**5d**)



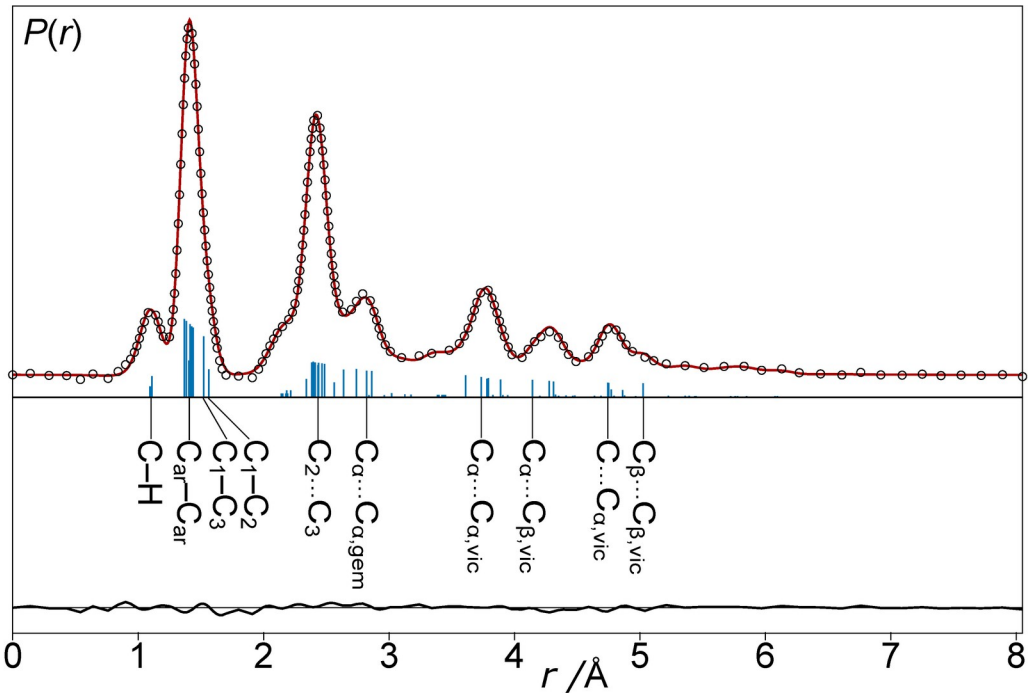
6

	d(C–C) (s) [Å]	*d*(C–C) (g) [Å]
1	1.670(1)	1.737(44)
2	1.704(4)	n.a.
3	1.71	n.a.
4a	1.647(4)	1.630(5)
4b	1.642(2)	1.632(5)
5a		
5b	1.708(4)	n.a.
5c	1.701(3)	n.a.
5d	1.746(3)	n.a.
6	2.0415(5)	n.a.

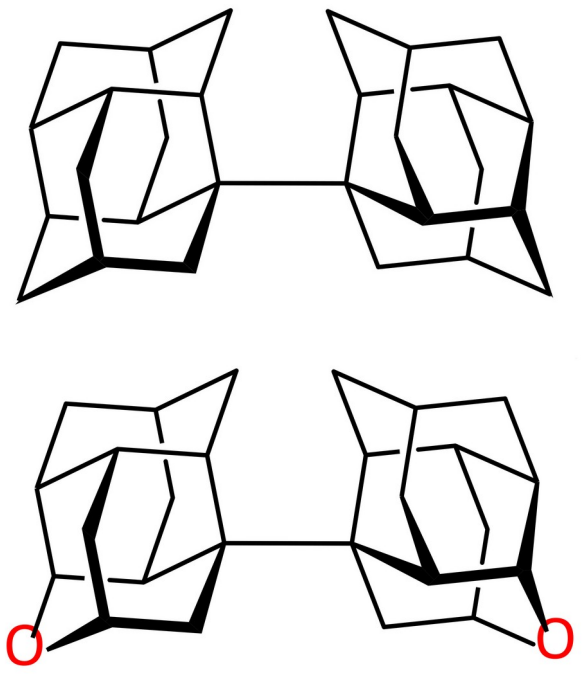
r(C–C) in Acenaphthen



Methode	r_e(C1—C2), Å
GED+MW	1.560(4)
XRD	1.5640(4)
CCSD(T)	1.562
r^{2}SCAN-3c	1.564
PBEh-3c	1.556

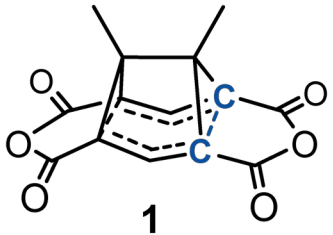


Benchmark C—C



Fokin, A. A.; Zhuk, T. S.; Blomeyer, S.; Pérez, C.; Chernish, L. V.; Pashenko, A. E.; Antony, J.; Vishnevskiy, Y. V.; Berger, R. J. F.; Grimme, S.; Logemann, C.; Schnell, M.; Mitzel, N. W.; Schreiner, P. R. *Intramolecular London Dispersion Interaction Effects on Gas-Phase and Solid-State Structures of Diamondoid Dimers.* J. Am. Chem. Soc. 2017, 139 (46), 16696–16707. DOI: 10.1021/jacs.7b07884.

Method	Oxa-dimer	Dimer
XRD	1.643(1)	1.647(4)
GED	1.632(9)	**1.630(5)**
GED+MW	**1.632(5)**	-
B3LYP/cc-pVTZ	1.662	1.674
TPSS/cc-pVTZ	1.658	1.668
HF/cc-pVTZ	1.652	1.664
B97-D3/cc-pVTZ	1.651	1.662
r^{2}SCAN-3c	**1.645**	**1.655**
TPSS-D3/cc-pVTZ	1.642	1.652
B3LYP-D3/cc-pVTZ	1.642	1.653
ωB97XD/cc-pVTZ	1.638	1.648
PBE0/cc-pVTZ	1.637	1.648
M06-2X/cc-pVTZ	1.636	1.647
PBEh-3c	**1.632**	**1.642**
SCS(1.2;2/3)-MP2/def2-QZVP	1.629	1.640
PBE0-D3/cc-pVTZ	1.628	1.638
B3PW91-D3/cc-pVTZ	1.627	1.636
PW6B95-D3/def2-QZVP	1.626	1.636
ae-MP2/cc-pwCVTZ	1.622	1.633



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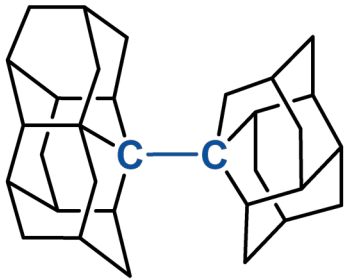

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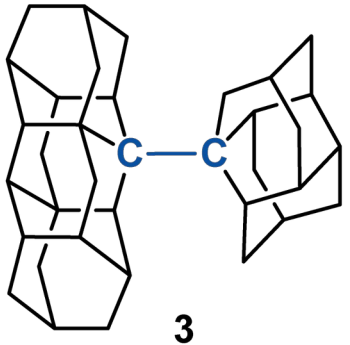

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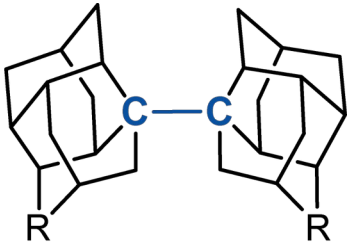
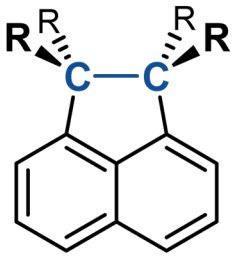


R = CH_2 (**4a**)

R = O (**4b**)



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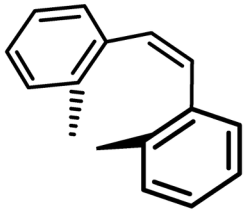
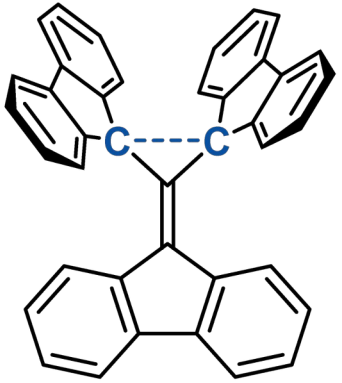
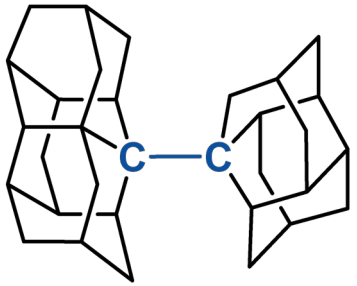
R,R =  (**5d**)



6

	d(C–C) (s) [Å]	*d*(C–C) (g) [Å]	
1	1.670(1)	1.737(44)	[1.633]
2	1.704(4)	[1.686]	
3	1.71	[1.694]	
4a	1.647(4)	1.630(5)	
4b	1.642(2)	1.632(5)	[PBEh-3c]
5a	1.5640(4)	1.560(4)	
5b	1.708(4)	[1.680]	
5c	1.701(3)	[1.678]	
5d	1.746(3)	[1.704]	
6	2.0415(5)	[1.653]	



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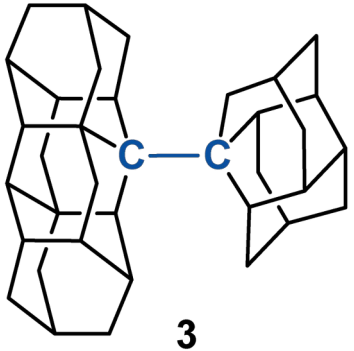

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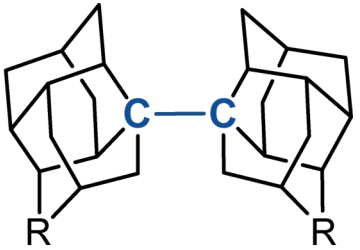
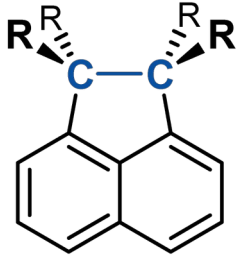


R = CH_2 (**4a**)

R = O (**4b**)



R = H (**5a**) – *this work*

R = 4-*t*-Bu-C_6H_4 (**5b**)

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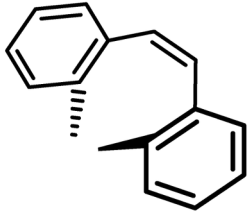
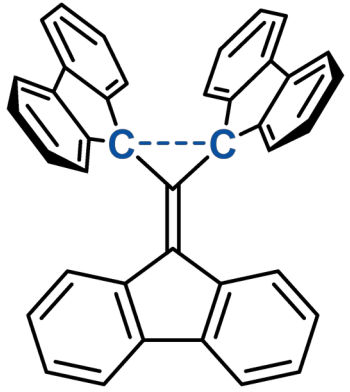


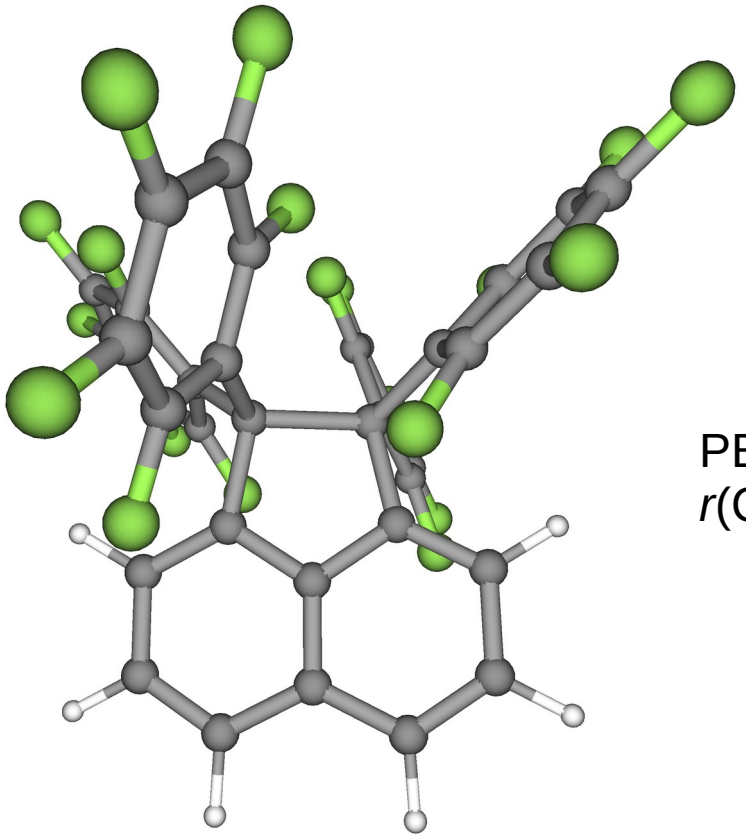
R,R = (**5d**)



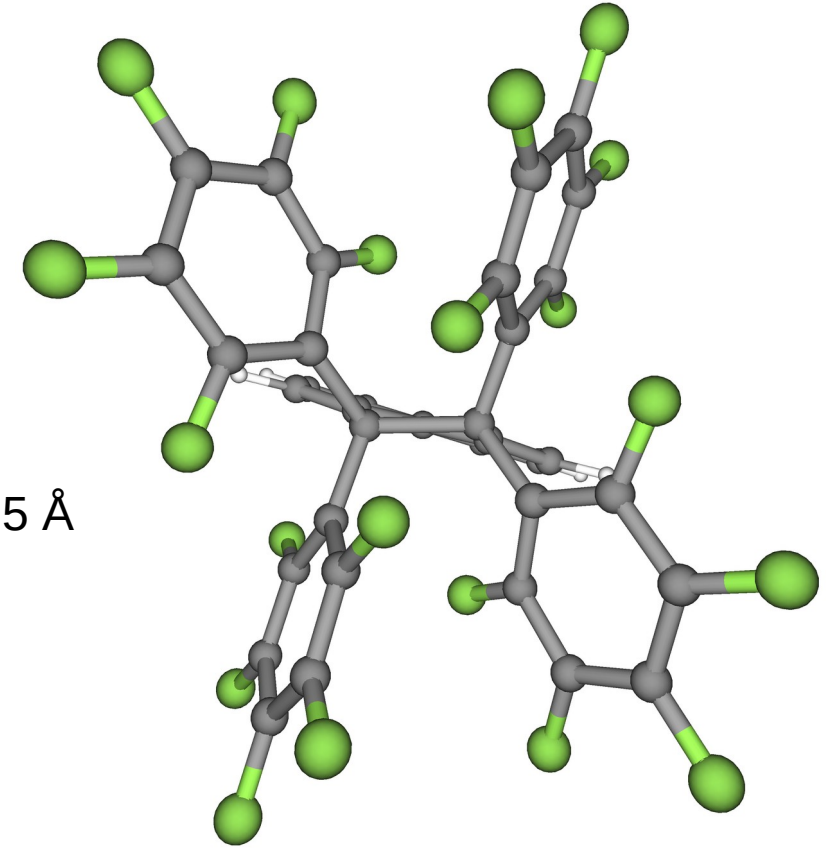
6

	d(C–C) (s) [Å]	*d*(C–C) (g) [Å]	*d*(C-C) (g) [Å] im F-Derivat
2	1.704(4)	[1.686]	[3.918]**
3	1.71	[1.694]	[3.936]**
4a	1.647(4)	1.630(5)	[2.417]*
4b	1.642(2)	1.632(5)	[2.168]*
5a	1.5640(4)	1.560(4)	[1.584]
5b	1.708(4)	[1.680]	[1.700]
5c	1.701(3)	[1.678]	[1.725]
5d	1.746(3)	[1.704]	[1.691]
6	2.0415(5)	[1.653]	[1.691]

5c mit R=C_6F_5



PBEh-3c:
r(C—C) = 1.725 Å



Noch länger C—C ?

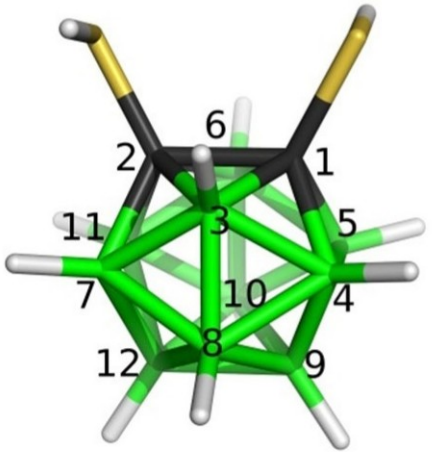
ChemPubSoc Europe
DOI: 10.1002/chem.201805145
CHEMISTRY A European Journal Full Paper

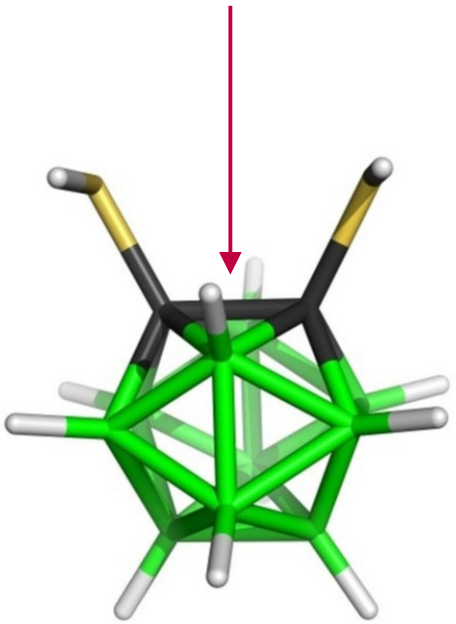
Carboranes

Icosahedral Carbaboranes with Peripheral Hydrogen–Chalcogenide Groups: Structures from Gas Electron Diffraction and Chemical Shielding in Solution

Tomáš Baše,[a] Josef Holub,[a] Jindřich Fanfrlík,[b] Drahomír Hnyk,*[a] Paul D. Lane,[c, d] Derek A. Wann,[c] Yury V. Vishnevskiy,*[e] Denis Tikhonov,[e, f, g] Christian G. Reuter,[e] and Norbert W. Mitzel*[e]

r_e = 1.750(28) Å



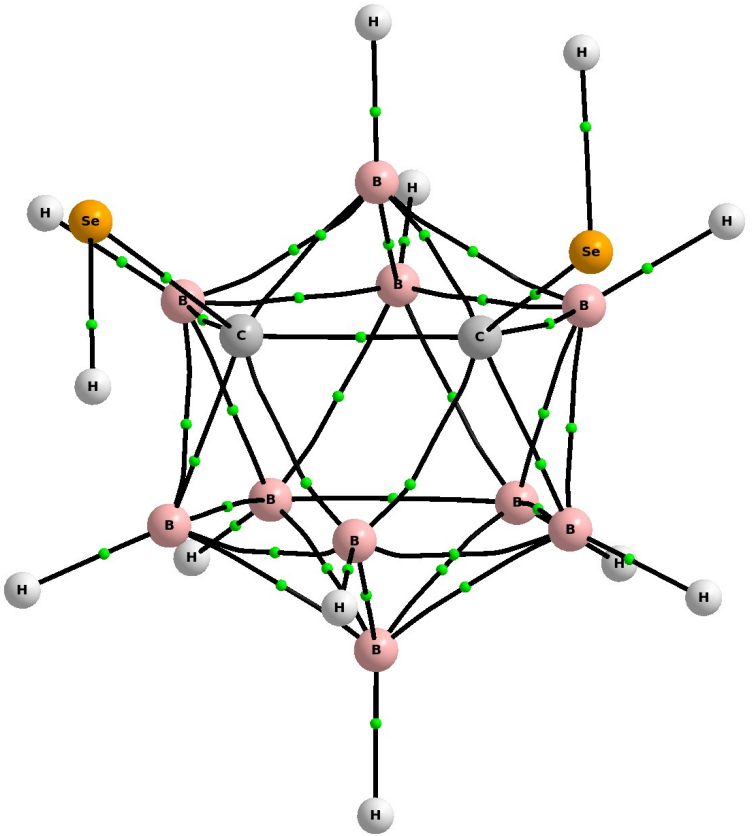


1,2-$(EH)_2$-closo-1,2-$C_2B_{10}H_{10}$

E = S, Se

QTAIM

1,2-$(SeH)_2$-closo-1,2-$C_2B_{10}H_{10}$



ρ = 0.16 a.u.
$\Delta\rho$ = -0.08 a.u.