Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic supplementary information

Locating the hydrogen atoms in endohedral clusterfullerenes by density functional theory

Bo Li, Lei Lou and Peng Jin*

School of Materials Science and Engineering, Hebei University of Technology, Tianjin 300130, China.

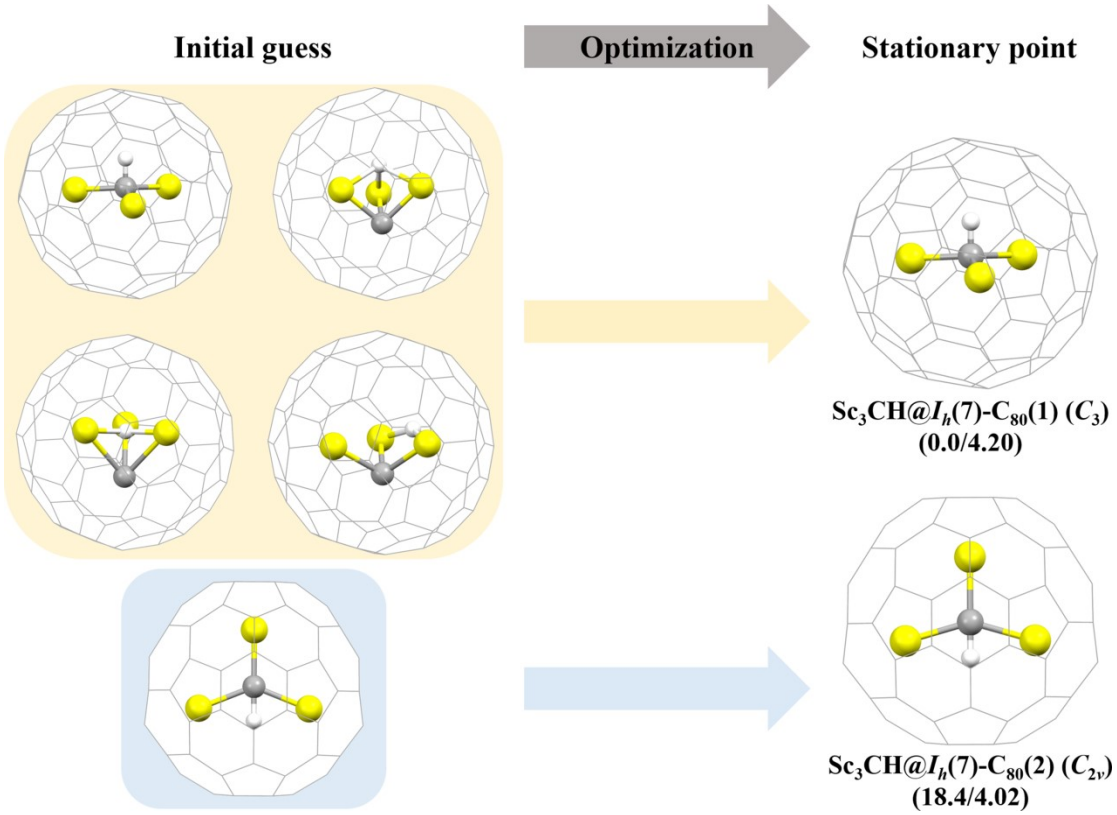

Fig. S1 Initial guessed isomer structures and respective optimized results of $Sc_3CH@I_h(7)$-C_{80}. The point-group symmetries and relative energies (kcal/mol)/HOMO-LUMO gap energies (eV) are given in parentheses.

Table S1 Relative energies (kcal/mol)/SOMO-LUMO gaps (eV) of two $Sc_4C_2H@I_h(7)$-C_{80} isomers obtained using different functionals and basis sets (C/H).

isomer	basis sets	M06-2X	B3LYP	ωB97X-D
$Sc_4C_2H@I_h(7)$-$C_{80}(1)$	6-31G*	0.0/3.57	0.0/1.82	0.0/5.12
	6-311+G**	0.0/3.53	0.0/1.83	0.0/5.10
$Sc_4C_2H@I_h(7)$-$C_{80}(2)$	6-31G*	12.6/2.36	1.6/0.87	5.0/3.84
	6-	11.7/2.43	0.1/1.10	3.1/3.87

311+G**

Table S2 Natural population analysis (NPA) charges and natural electron configuration populations of HCFs at the B3LYP/6-31G*~SDD level of theory. Please see Fig. 2 in main text for the atom numbering.

compound	atom	charge	population
$Sc_3CH@I_h(7)$-C_{80}	Sc1	+1.56	$4s^{0.10}3d^{0.57}4p^{0.08}4d^{0.41}5p^{0.30}$
	Sc2	+1.56	$4s^{0.10}3d^{0.57}4p^{0.08}4d^{0.41}5p^{0.30}$
	Sc3	+1.56	$4s^{0.10}3d^{0.57}4p^{0.08}4d^{0.41}5p^{0.30}$
	C	-1.89	$2s^{1.40}2p^{4.48}3p^{0.01}$
	H	+0.29	$1s^{0.71}$
$Sc_4CNH@I_h(7)$-C_{80}	Sc1	+1.47	$4s^{0.13}3d^{0.68}4d^{0.36}5p^{0.41}$
	Sc2	+1.37	$4s^{0.15}3d^{0.66}4d^{0.42}5p^{0.46}$
	Sc3	+1.35	$4s^{0.15}3d^{0.67}4d^{0.43}5p^{0.47}$
	Sc4	+1.20	$4s^{0.16}3d^{0.91}4d^{0.27}5p^{0.54}$
	C	-1.21	$2s^{1.22}2p^{3.90}3p^{0.02}$
	N	-1.14	$2s^{1.48}2p^{4.70}3p^{0.01}$
	H	-0.36	$1s^{1.36}$
$Sc_4C_2H@I_h(7)$-C_{80}(1)	Sc1	+1.20	$4s^{0.17}3d^{0.69}4p^{0.57}4d^{0.41}$
	Sc2	+1.21	$4s^{0.18}3d^{0.74}4p^{0.55}4d^{0.40}$
	Sc3	+1.09	$4s^{0.17}3d^{0.88}4p^{0.59}4d^{0.33}$
	Sc4	+1.18	$4s^{0.18}3d^{0.74}4p^{0.55}4d^{0.42}$
	C1	-0.86	$2s^{1.18}2p^{3.65}3p^{0.03}$
	C2	-0.89	$2s^{1.18}2p^{3.67}3p^{0.02}$
	H	-0.35	$1s^{1.35}$
$Sc_4C_2H@I_h(7)$-C_{80}(2)	Sc1	+1.43	$4s^{0.13}3d^{0.65}4p^{0.42}4d^{0.41}$
	Sc2	+1.37	$4s^{0.13}3d^{0.69}4p^{0.44}4d^{0.43}$
	Sc3	+1.45	$4s^{0.12}3d^{0.66}4p^{0.40}4d^{0.41}$
	Sc4	+1.34	$4s^{0.14}3d^{0.74}4p^{0.50}4d^{0.35}$
	C1	-1.23	$2s^{1.12}2p^{4.08}3p^{0.03}$
	C2	-1.45	$2s^{1.21}2p^{4.23}3p^{0.01}$
	H	+0.28	$1s^{0.72}$

Table S3 Vertical ionization potential (VIP), vertical electron affinity (VEA), adiabatic ionization potential (AIP) and adiabatic electron affinity (AEA) of $Sc_3CH@I_h(7)$-C_{80}, $Sc_4CNH@I_h(7)$-C_{80} and two $Sc_4C_2H@I_h(7)$-C_{80} isomers obtained using different functionals (unit: eV).

compound	functionals	VIP	VEA	AIP	AEA
$Sc_3CH@I_h(7)$-C_{80}	M06-2X	7.1	1.8	7.0	2.3
	B3LYP	7.0	1.8	6.6	1.9
$Sc_4CNH@I_h(7)$-C_{80}	M06-2X	6.3	1.7	5.9	1.9
	B3LYP	5.1	1.9	4.9	2.0

$Sc_4C_2H@I_h(7)$-$C_{80}(1)$	M06-2X	6.6	1.9	6.6	2.0
	B3LYP	6.6	1.9	6.4	1.9
$Sc_4C_2H@I_h(7)$-$C_{80}(2)$	M06-2X	5.8	1.9	5.3	2.1
	B3LYP	5.0	2.0	4.9	2.1

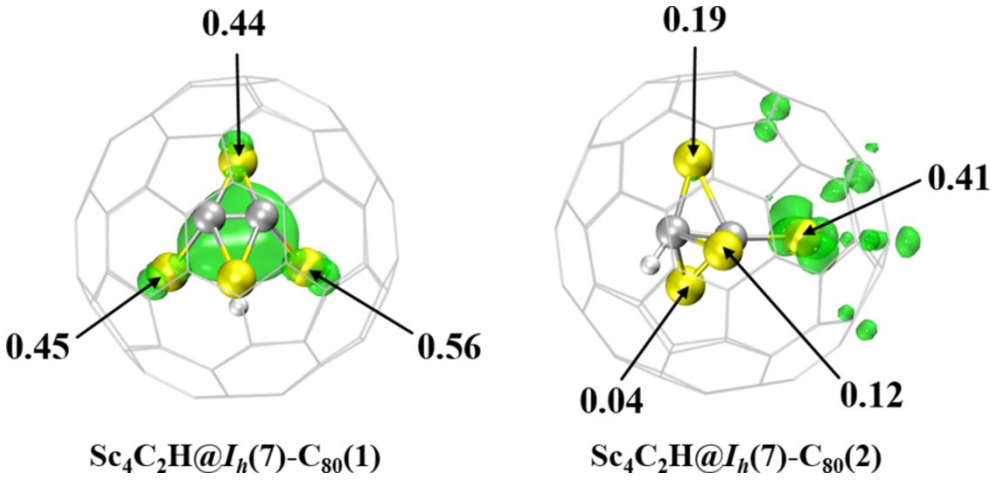

Fig. S2 Spin density distribution (with spin population values for selected atoms) of two $Sc_4C_2H@I_h$-C_{80} isomers (isovalue: ±0.006 au).

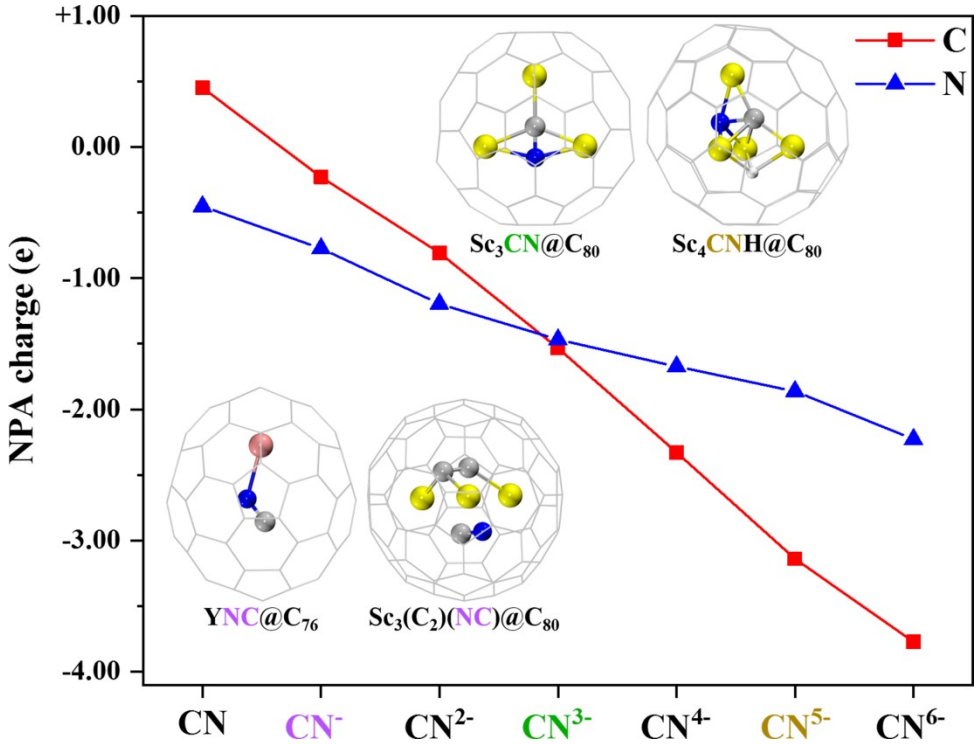

Fig. S3 NPA charges of the atoms in CN^{q-} (q = 0-6) at the M06-2X/6-31++G* level of theory and the corresponding representative clusterfullerenes.

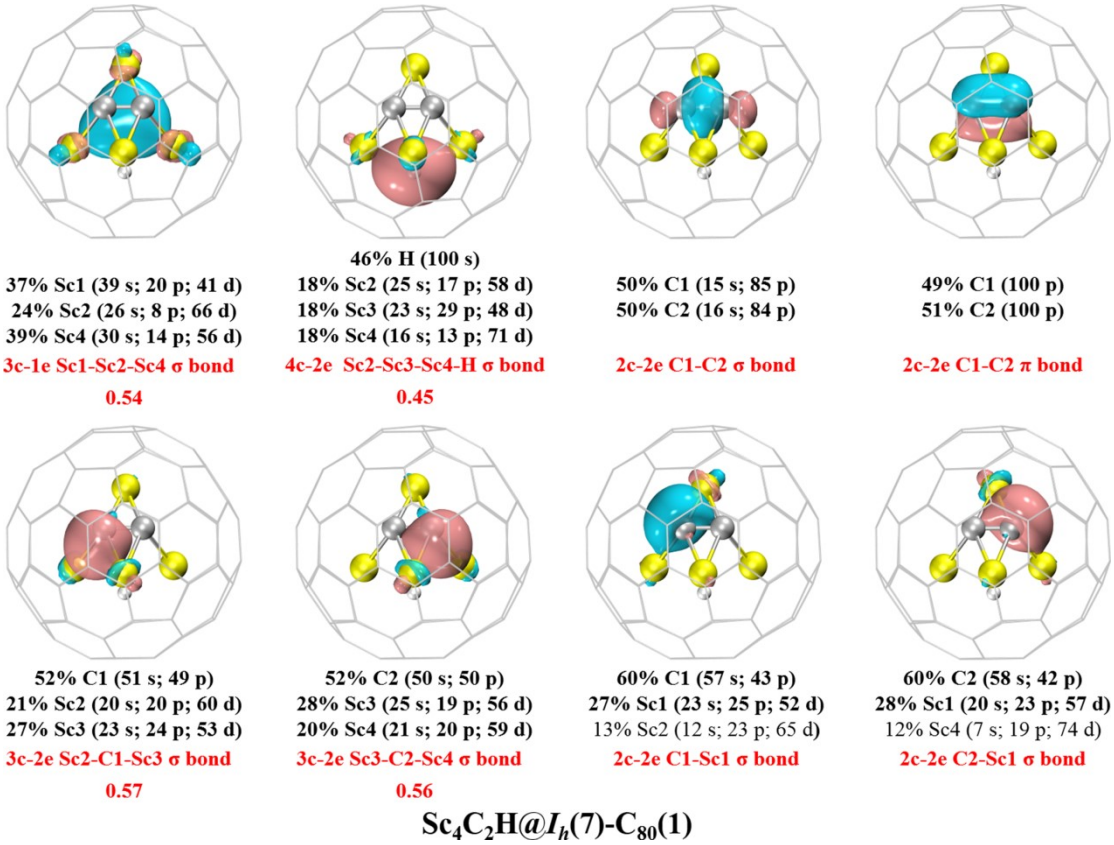

Fig. S4 LMOs (isovalue: ±0.06 au) of $Sc_4C_2H@I_h$-C_{80}(1) with atomic orbital compositions (%) at the B3LYP/6-31G*~SDD level of theory. The atoms mainly contributing to the orbital are highlighted in bold. The normalized multicenter bond order values are given in red.

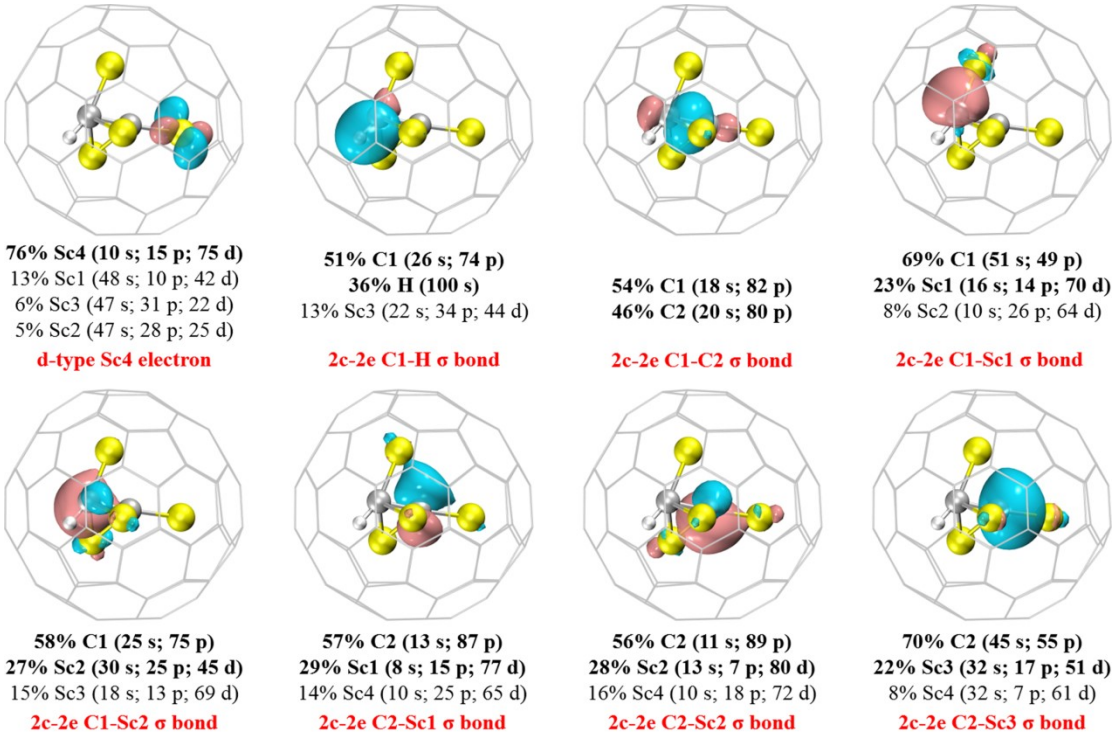

Fig. S5 LMOs (isovalue: ±0.06 au) of $Sc_4C_2H@I_h$-C_{80}(2) with atomic orbital compositions (%) at the B3LYP/6-31G*~SDD level of theory.

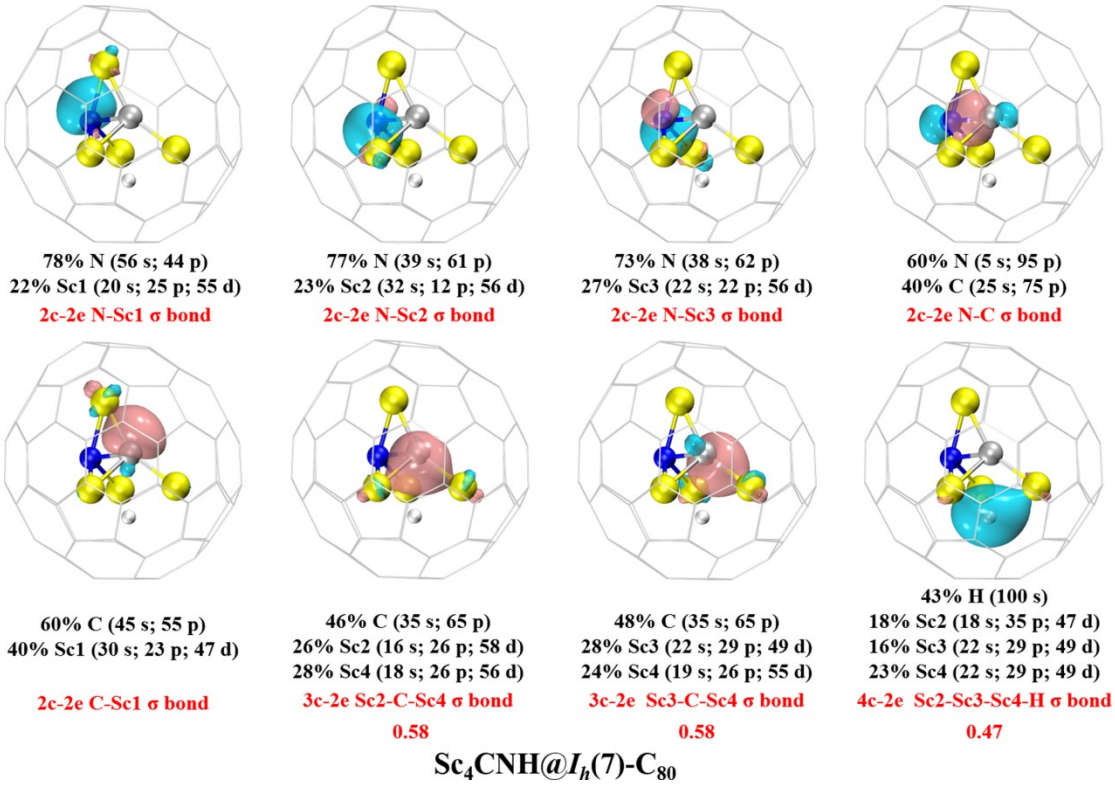

Fig. S6 LMOs (isovalue: ±0.06 au) of $Sc_4CNH@I_h$-C_{80} with atomic orbital compositions (%).

Table S4 Interatomic distances (*d*, Å), Wiberg bond orders (WBOs) and density descriptors (unit: au) at the intracluster (purple) and cluster-cage (green) BCPs of two $Sc_4C_2H@I_h(7)$-C_{80} isomers. Please see Fig. 8 in the main text for the atom numbering.

compound	A-B	*d*	WBO	ρ	$\nabla^2\rho$	*H*	H/ρ	$\|V\|/G$	G/ρ	δ(A,B)
$Sc_4C_2H@I_h(7)$-C_{80}(1)	Sc1-C1	2.12	0.76	0.08	0.30	-0.02	-0.20	1.18	1.12	0.83
	Sc1-C2	2.10	0.78	0.09	0.27	-0.02	-0.24	1.23	1.04	0.84
	Sc2-C1	2.12	0.81	0.08	0.24	-0.02	-0.22	1.22	1.01	0.81
	Sc2-H	2.03	0.30	0.04	0.10	-0.01	-0.17	1.22	0.73	0.32
	Sc3-C1	2.14	0.74	0.08	0.28	-0.02	-0.20	1.19	1.09	0.77
	Sc3-C2	2.12	0.77	0.08	0.26	-0.02	-0.24	1.24	1.01	0.81
	Sc3-H	2.09	0.27	0.04	0.11	-0.01	-0.13	1.16	0.80	0.27
	Sc4-C2	2.13	0.77	0.07	0.23	-0.02	-0.21	1.21	1.00	0.77
	Sc4-H	2.03	0.30	0.04	0.10	-0.01	-0.17	1.23	0.73	0.32
	C1-C2	1.34	1.42	0.33	-0.82	-0.38	-1.14	3.19	0.52	0.91
	C1-H	2.48	0.00	0.03	0.06	0.00	-0.09	1.16	0.58	0.00
	C2-H	2.48	0.00	0.03	0.06	0.00	-0.08	1.13	0.59	0.00
	Sc1-C3	2.20	0.52	0.07	0.24	-0.01	-0.18	1.17	1.08	0.72
	Sc2-C8	2.24	0.51	0.06	0.21	-0.01	-0.18	1.18	1.01	0.71
	Sc3-C9	2.21	0.51	0.06	0.24	-0.01	-0.17	1.16	1.08	0.71
	Sc3-C13	2.25	0.47	0.06	0.24	-0.01	-0.13	1.12	1.11	0.68
	Sc4-C16	2.24	0.50	0.06	0.21	-0.01	-0.17	1.17	1.02	0.70
	C1-C4	3.08	0.01	0.01	0.03	0.00	0.08	0.87	0.65	0.01
	C1-C5	3.05	0.01	0.01	0.04	0.00	0.12	0.84	0.70	0.02
	C1-C6	3.09	0.01	0.01	0.03	0.00	0.09	0.87	0.68	0.01
	C1-C7	3.17	0.00	0.01	0.03	0.00	0.09	0.86	0.66	0.01
	C2-C17	3.14	0.01	0.01	0.04	0.00	0.11	0.85	0.75	0.01
	C2-C18	3.16	0.01	0.01	0.03	0.00	0.09	0.86	0.68	0.01
	C2-C19	3.06	0.01	0.01	0.04	0.00	0.10	0.86	0.69	0.01
	C2-C20	3.10	0.01	0.01	0.03	0.00	0.08	0.88	0.67	0.02
	C2-C21	3.03	0.01	0.01	0.04	0.00	0.11	0.84	0.73	0.01
	H-C10	2.56	0.00	0.02	0.05	0.00	0.08	0.88	0.73	0.01
	H-C11	2.63	0.00	0.01	0.04	0.00	0.06	0.91	0.66	0.00
	H-C12	2.52	0.00	0.02	0.05	0.00	0.10	0.87	0.77	0.01
	H-C14	2.56	0.00	0.01	0.05	0.00	0.09	0.88	0.75	0.01
	H-C15	2.62	0.01	0.02	0.05	0.00	0.08	0.88	0.72	0.01
$Sc_4C_2H@I_h(7)$-C_{80}(2)	Sc1-C1	2.04	0.99	0.10	0.23	-0.03	-0.32	1.35	0.92	1.01
	Sc1-C2	2.21	0.65	0.06	0.21	-0.01	-0.17	1.17	1.01	0.60
	Sc2-C1	2.17	0.75	0.07	0.22	-0.02	-0.23	1.24	0.98	0.76
	Sc2-C2	2.11	0.77	0.08	0.24	-0.02	-0.26	1.26	1.00	0.71
	Sc3-C1	2.19	0.73	0.07	0.23	-0.01	-0.20	1.19	1.02	0.76

Sc3-C2	2.10	0.77	0.08	0.25	-0.02	-0.24	1.23	1.05	0.77
Sc4-C2	1.97	1.07	0.10	0.34	-0.03	-0.31	1.27	1.13	0.96
C1-C2	1.49	0.79	0.24	-0.42	-0.21	-0.85	3.01	0.42	0.48
C1-H	1.09	0.57	0.26	-0.78	-0.25	-0.97	5.39	0.22	0.52
Sc1-C3	2.25	0.50	0.06	0.21	-0.01	-0.17	1.17	1.02	0.70
Sc2-C7	2.26	0.47	0.06	0.22	-0.01	-0.15	1.15	1.05	0.68
Sc2-C8	2.23	0.50	0.06	0.23	-0.01	-0.17	1.16	1.07	0.70
Sc3-C9	2.23	0.51	0.06	0.22	-0.01	-0.18	1.18	1.04	0.71
Sc4-C10	2.20	0.53	0.07	0.23	-0.01	-0.21	1.20	1.04	0.73
C1-C4	3.16	0.01	0.01	0.04	0.00	0.06	0.91	0.68	0.01
C1-C5	2.95	0.01	0.01	0.05	0.00	0.11	0.85	0.76	0.02
H-C6	2.10	0.02	0.03	0.09	0.00	0.01	1.01	0.83	0.03

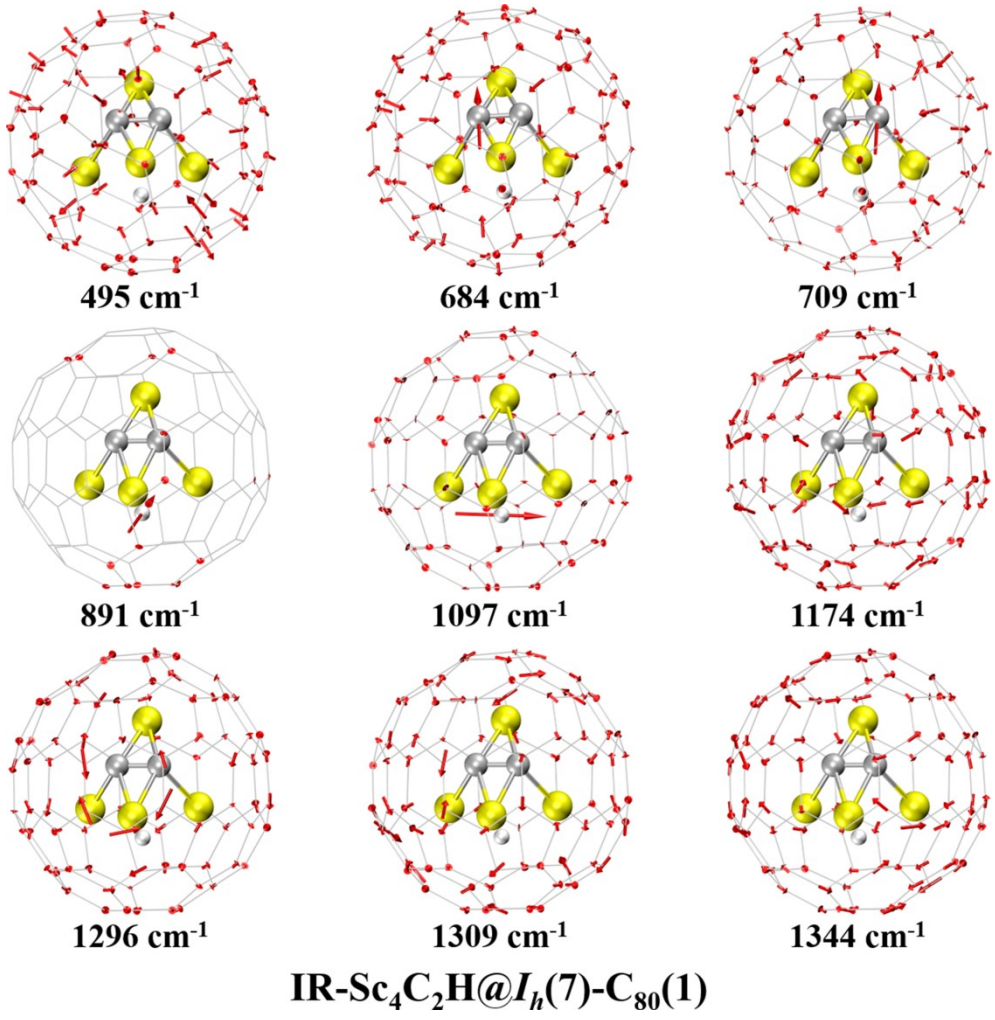

Fig. S7 Main IR vibrational modes of $Sc_4C_2H@I_h(7)$-$C_{80}(1)$.

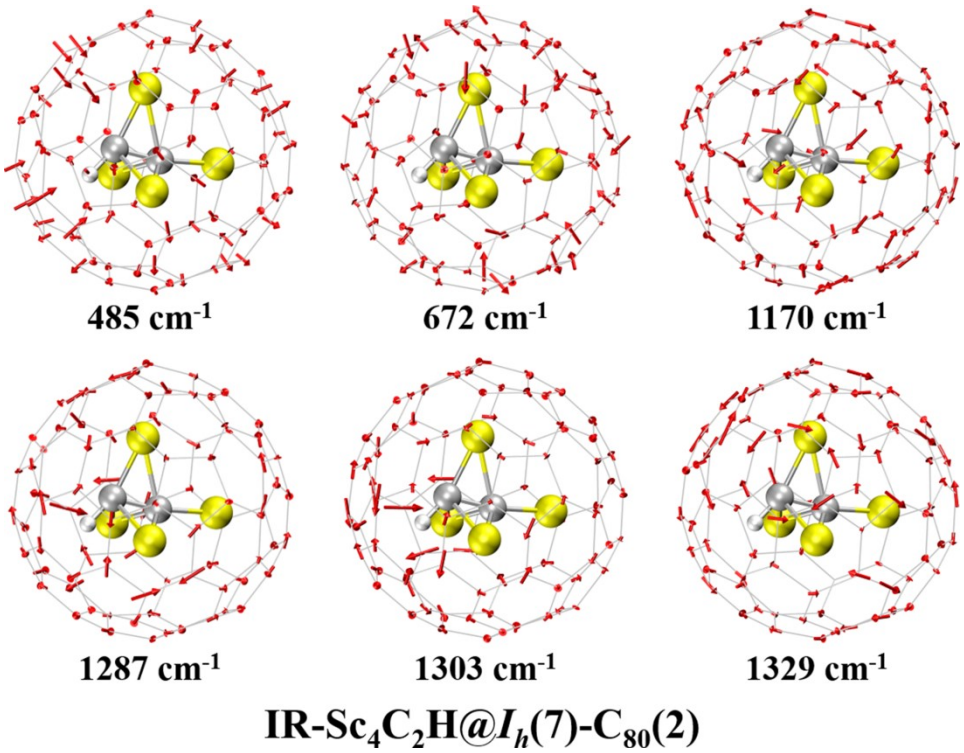

Fig. S8 Main IR vibrational modes of $Sc_4C_2H@I_h(7)$-$C_{80}(2)$.

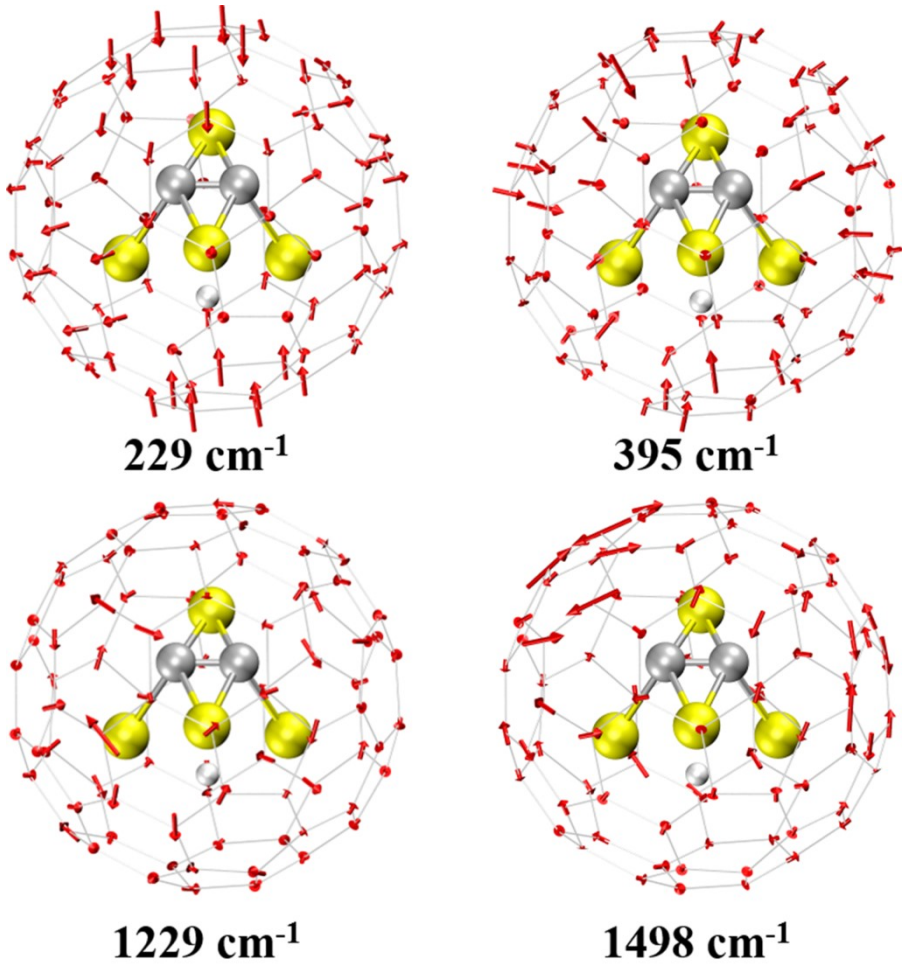

Fig. S9 Main Raman vibrational modes of $Sc_4C_2H@I_h(7)$-$C_{80}(1)$.

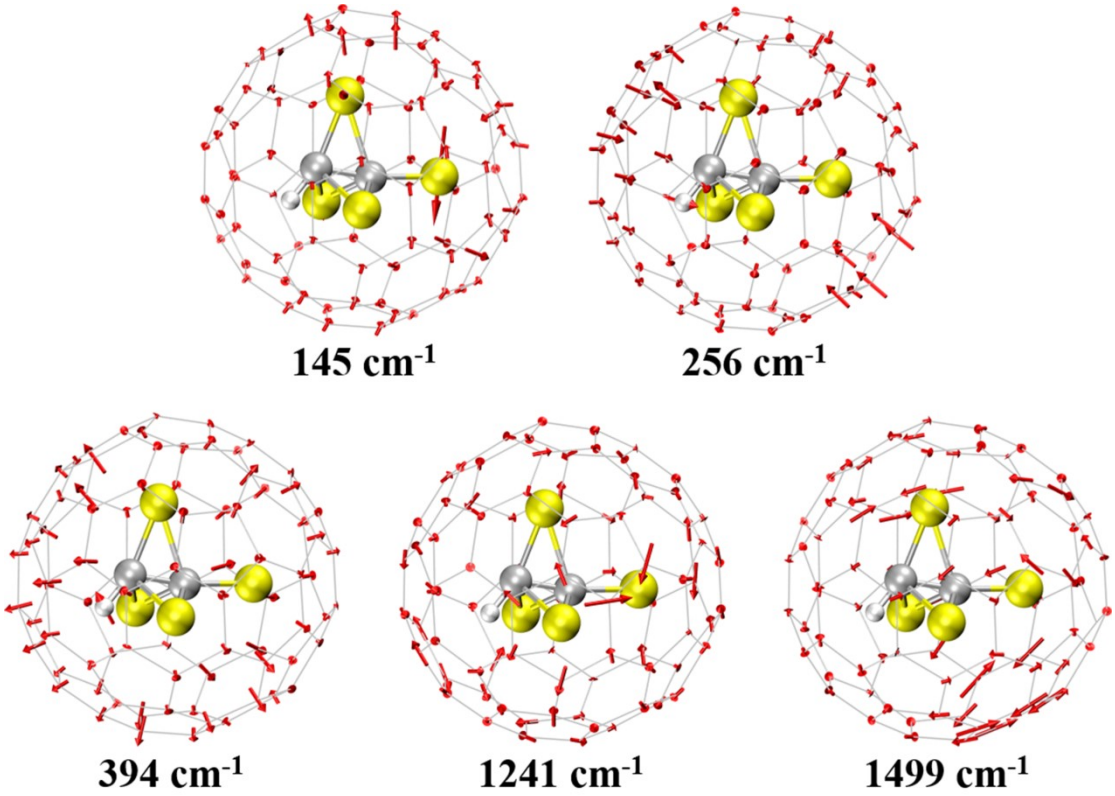

Fig. S10 Main Raman vibrational modes of $Sc_4C_2H@I_h(7)$-$C_{80}(2)$.

Optimized Cartesian Coordinates (M06-2X/6-31G*~SDD)

$Sc_3CH@I_h(7)$-C_{80}

C	1.63188500	1.72464900	3.32961800
C	1.46477700	2.88129600	2.49673200
C	0.07343500	3.24005600	2.50268600
C	0.34707400	1.36487700	3.85266700
C	-0.61261600	2.29412700	3.34390800
C	0.00000000	0.00000000	4.06740000
C	1.00848100	-0.98301300	3.85266700
C	2.59903900	0.73080100	3.03198300
C	2.29308000	-0.61652200	3.34390800
C	3.47147700	0.95782300	1.90490100
C	2.26018000	3.07887300	1.34678400
C	3.28236000	2.10379000	1.07368700
C	1.67494600	3.72831500	0.23103700
C	-0.55060600	3.84313900	1.36991500
C	0.28384900	4.08550200	0.23610300
C	-1.95493800	3.57141400	1.11652000
C	-1.93241200	1.88543300	3.03198300
C	-2.56523800	2.52747600	1.90490100
C	-1.35555500	-0.38186400	3.85266700

C	-2.30953200	0.55092900	3.32961800
C	-1.68046400	-1.67760500	3.34390800
C	0.67764700	-2.27557800	3.32961800
C	-0.66662700	-2.61623400	3.03198300
C	2.76925300	-1.68362400	2.50268600
C	1.76288700	-2.70918200	2.49673200
C	4.07040400	-0.09268100	1.11652000
C	3.60355900	-1.44473100	1.36991500
C	3.72202700	1.77711200	-0.25181400
C	4.25370000	0.42069600	-0.25242800
C	2.04038300	3.37238700	-1.10545300
C	3.01714700	2.36684600	-1.36691300
C	-0.21845300	3.95414000	-1.11535600
C	0.87742400	3.49437300	-1.93111300
C	-2.49118300	3.47346400	-0.25242800
C	-1.58695500	3.61563800	-1.39292000
C	-3.46311600	1.79071200	1.07368700
C	-3.40003800	2.33481400	-0.25181400
C	-3.22766400	-0.17211400	2.49673200
C	-2.84268800	-1.55643200	2.50268600
C	-3.79647200	0.41793700	1.34678400
C	-3.05295300	-2.39840800	1.36991500
C	-0.90623900	-3.48529900	1.90490100
C	-2.11546600	-3.47873300	1.11652000
C	1.53629200	-3.49681000	1.34678400
C	0.18075600	-3.89450200	1.07368700
C	3.39622400	-2.28857100	0.23610300
C	2.39134300	-3.31470300	0.23103700
C	3.92471200	-0.43347600	-1.39292000
C	3.53361200	-1.78788400	-1.11535600
C	2.83336400	1.55469200	-2.51108200
C	3.23836500	0.16596900	-2.49595200
C	0.66607800	2.62664000	-3.03674500
C	1.68587400	1.68393400	-3.35146500
C	-1.76291600	2.72152200	-2.49595200
C	-0.67746200	2.27343500	-3.32866000
C	-3.55832200	1.42950300	-1.36691300
C	-2.76308500	1.67641900	-2.51108200
C	-4.06628800	-0.41361200	0.23103700
C	-3.68007300	-1.79693100	0.23610300
C	-3.94076400	0.08083000	-1.10545300
C	-3.31515900	-2.16625600	-1.11535600
C	-3.46492800	-0.98731500	-1.93111300
C	-1.76251700	-3.89416000	-0.25242800

C	-0.32198900	-4.11192600	-0.25181400
C	-2.33775700	-3.18216200	-1.39292000
C	1.90038100	-3.45321700	-1.10545300
C	2.58750400	-2.50705800	-1.93111300
C	0.54117500	-3.79634900	-1.36691300
C	2.30758400	-0.55001800	-3.32866000
C	1.35462200	0.38245700	-3.84533100
C	1.94169800	-1.89016000	-3.03674500
C	-1.00852800	0.98190800	-3.84533100
C	-2.30126700	0.61804300	-3.35146500
C	-2.60777600	-0.73648000	-3.03674500
C	0.00000000	0.00000000	-4.06437400
C	-1.47544900	-2.88749100	-2.49595200
C	-0.07027900	-3.23111100	-2.51108200
C	0.61539300	-2.30197700	-3.35146500
C	-1.63012100	-1.72341700	-3.32866000
C	-0.34609300	-1.36436500	-3.84533100
C	0.00000000	0.00000000	0.25052700
Sc	2.08917300	0.00000000	-0.00359800
Sc	-1.04458600	1.80927700	-0.00359800
Sc	-1.04458600	-1.80927700	-0.00359800
H	0.00000000	0.00000000	1.38176000

$Sc_4CNH@I_h(7)$-C_{80}

C	-1.05503300	-2.83880900	2.73608200
C	-3.12228600	-2.71398600	-0.34984300
C	-4.04296500	-0.81882300	0.67126300
C	0.70097500	-1.64494600	3.68604300
C	-2.78884800	0.37774900	2.90628700
C	-3.86457900	-1.49487600	-0.58735500
C	1.28809800	-3.32789800	1.92281100
C	0.69828200	-3.95135600	0.79342800
C	-0.99469200	-3.86144400	-0.79564500
C	-0.54375000	0.48140200	4.01609400
C	-2.17425700	-3.22527000	-1.30043700
C	-1.63666000	-1.71923100	3.43526100
C	-1.70814200	1.12859500	3.48903400
C	-3.39909700	1.19423600	1.89391100
C	-4.01924600	0.61883700	0.74431800
C	1.93864700	-0.94550700	3.42487300
C	1.32517400	-3.84905000	-0.48752600
C	0.28245100	-3.79555800	-1.47835400
C	2.55639100	-2.68711200	1.76972500
C	-3.61062200	-0.73795000	-1.76146200

C	-1.64532400	2.40210600	2.83474100
C	0.69308300	1.16627900	3.81462400
C	-1.63865300	-3.37909200	1.53803900
C	-2.69783600	2.46034600	1.85433600
C	-2.05229900	-2.56742200	-2.58091700
C	2.87182300	-1.50388500	2.51005800
C	-3.96948700	1.41908100	-0.46799700
C	1.91834900	0.46462900	3.53652300
C	-2.71743800	-1.29365800	-2.74192800
C	-3.67152700	0.70645900	-1.68600900
C	0.43378200	-3.07791900	-2.70254600
C	-0.76749600	-2.49772300	-3.28280700
C	0.76804600	2.44682000	3.17454100
C	-2.85253200	-2.79858600	1.05628400
C	-0.39781000	3.06288600	2.64010500
C	3.71847900	-0.66205700	1.69484000
C	2.75511700	1.30530900	2.72604900
C	-1.86950700	-0.44896500	-3.53412600
C	3.92499300	-1.34000100	0.43241600
C	-2.82539600	1.53805400	-2.49933200
C	2.02781300	2.52792900	2.50253900
C	2.72198000	-2.41753700	-1.87302200
C	-0.67424400	-1.17027100	-3.85181700
C	1.67656200	-2.37655900	-2.85659800
C	-3.41541700	-1.63119600	1.68906800
C	3.69972300	0.77096800	1.78639300
C	-2.57529200	2.77488400	-1.80560300
C	-0.25303500	3.82604000	1.45712800
C	-1.30873300	3.87449500	0.47294700
C	-1.88464200	0.97744100	-3.42817200
C	4.11469100	-0.59660900	-0.78646800
C	3.44763000	-1.17133900	-1.92398400
C	1.74681600	-1.09984000	-3.51388100
C	2.16620100	3.22478400	1.27647700
C	0.56915300	-0.45322700	-3.97648600
C	-2.77070200	-1.04891900	2.82676100
C	1.01089600	3.89968300	0.78309000
C	-0.66735500	3.97587700	-0.81679200
C	-1.25805900	3.37421000	-1.96135000
C	4.00583100	1.55954500	0.58871000
C	2.82759200	-0.35992900	-2.94385900
C	-0.68383700	1.67326100	-3.68506000
C	4.22062900	0.87715100	-0.71261200
C	3.14935600	2.71735600	0.33931100

C	0.75300000	3.99009600	-0.62024000
C	0.53705800	0.96166600	-3.93601900
C	0.37677700	-2.79650600	2.89846100
C	-0.36107900	2.85770800	-2.94124500
C	2.77058600	1.05480100	-2.82557200
C	3.47000400	1.65075600	-1.70375600
C	2.84878100	2.77901900	-1.06126700
C	1.63542500	3.38986600	-1.55608500
C	1.62017300	1.70499400	-3.35561500
C	1.06137500	2.87277700	-2.74146100
C	-3.29716300	2.74161100	-0.53192600
C	3.19038200	-2.58886400	0.49026400
C	-2.59051700	3.24472900	0.65119000
C	-0.53304000	-0.96471700	4.03729200
C	2.55234500	-3.13401200	-0.65927200
C	0.13530000	0.42962900	-0.12406500
C	-0.73099900	-3.95759800	0.60723200
Sc	2.16135000	0.49777600	-0.06007700
Sc	-0.51938300	-1.29360300	-1.35104800
Sc	-1.67524500	1.28034800	-0.22500900
Sc	-0.45123000	-0.60304200	1.77878100
N	0.72392300	-0.87916600	0.18189000
H	-1.73384700	-0.69183700	0.17095400

$Sc_4C_2H@I_h(7)$-C_{80}(1)

C	0.26158000	-1.72695000	-3.69084700
C	-1.97588200	-1.12825600	-3.41623300
C	1.45721700	-2.21523700	-3.09192400
C	-3.12819200	-1.00478000	-2.57399700
C	-3.23219400	-2.01122000	-1.54768000
C	0.12380800	-0.34835600	-4.06219000
C	-1.24928900	0.02253200	-3.90309900
C	-1.02898000	-2.21329300	-3.30101900
C	-1.14867800	-3.19322800	-2.28237800
C	0.05198000	-3.73070000	-1.73040900
C	-2.27989900	-3.08297200	-1.42023200
C	1.34120900	-3.26153200	-2.13977400
C	2.55202700	-1.29073900	-2.92598500
C	-3.63134400	0.33710400	-2.26117500
C	-3.71048000	-1.68071500	-0.22384000
C	1.16941600	0.58530900	-3.83454400
C	-1.61458300	1.33388400	-3.50366500
C	0.13454800	-4.07496200	-0.33598700
C	-2.17876600	-3.43176800	-0.03203400

C	4.24512400	0.37658000	-0.16851800
C	4.03730500	-0.62952500	0.84775300
C	3.58473200	-1.97030700	0.51723800
C	3.09674800	0.98550600	2.52563200
C	3.51637500	-0.32760400	2.16842800
C	2.83388200	-2.48005200	1.63262000
C	1.64705500	-1.32404800	3.47665900
C	2.79878900	-1.47136900	2.64968800
C	-1.17202400	-0.57300800	3.85256000
C	-2.41170200	-0.07974300	3.35002900
C	-3.20517700	-0.87121700	2.44614000
C	-3.85078100	0.01803800	1.51007600
C	-2.55900700	1.29705000	2.98084300
C	-3.45016400	1.35829400	1.85114200
C	-1.45906500	2.20604100	3.11628700
C	3.77225000	1.68979600	0.21143700
C	4.02971500	-0.02474100	-1.56771600
C	3.24827700	1.98974000	1.52426800
C	3.10613900	2.57902100	-0.72034400
C	3.26625100	0.86965500	-2.44979300
C	3.52882900	-1.38003100	-1.86425300
C	2.79993200	2.17959600	-2.05414200
C	2.40479200	0.08337800	-3.28687400
C	1.61590400	2.70868800	-2.64673400
C	3.28488400	-2.35844800	-0.82513800
C	2.23190200	-3.31159100	-1.01262000
C	0.81054000	1.92146100	-3.53899600
C	2.30051800	3.06431200	1.40428800
C	2.21737900	3.42482500	0.00966900
C	1.00238900	3.90373500	-0.56102500
C	0.72829200	3.56717200	-1.91068600
C	1.48454400	-3.81049500	0.10288800
C	1.99510200	1.12396800	3.42240900
C	1.74785100	-3.38614400	1.43368800
C	0.58421500	-2.28118700	3.32083800
C	1.27683500	-0.02045900	3.89819400
C	-1.42912800	3.77347200	-0.11251400
C	-0.61882200	3.31274400	-2.35899300
C	-1.70322500	3.36351300	-1.45636300
C	-0.10902500	4.09524100	0.34137300
C	-0.56856400	2.29416500	-3.36802600
C	-2.17621400	3.25787700	0.99779500
C	-2.80039900	2.45078900	-1.63590200
C	-0.02763200	3.82319500	1.77130500

C	1.19311100	3.23333900	2.30477700
C	0.64063700	-3.35305700	2.36255400
C	-0.79461400	-1.91914300	3.50985800
C	-0.72238800	-3.67426200	1.95279000
C	-1.60790200	-2.75943700	2.67360200
C	-2.77530000	-2.17134400	2.05212200
C	-0.10630000	0.34161400	4.07088200
C	-0.24974700	1.71382700	3.69064700
C	-3.04842600	-2.55445600	0.70738900
C	-4.13044300	-0.36049300	0.15076400
C	-0.98093100	-3.96679700	0.54998900
C	1.05322300	2.20683800	3.29092000
C	-3.23907600	2.30596900	0.81784000
C	-1.32949100	3.28211800	2.16309300
C	-3.58776000	1.95165400	-0.53663200
C	-4.12833500	0.65296200	-0.89887400
C	-2.80355000	1.46521400	-2.67790700
Sc	-0.03242100	1.73772500	0.94617300
C	0.11235800	0.64718500	-0.87914800
Sc	2.05895900	-0.08938100	-0.58299000
Sc	-1.93862100	0.12985300	-0.84996100
C	0.03806900	-0.68718600	-0.82897500
Sc	-0.34326700	-1.68602900	0.99799600
H	-1.25117000	0.12515400	1.12469500

$Sc_4C_2H@I_h(7)$-C_{80}(2)

C	-2.76533800	3.18732700	0.41559500
C	-1.75195600	2.12725300	-2.99399900
C	0.22390500	3.24161600	-2.47623500
C	-2.05425900	2.44543700	2.49834700
C	0.87768400	4.02487400	0.13127800
C	-0.36736100	2.26968700	-3.34047600
C	-3.77420100	1.02935800	1.35312200
C	-4.13507200	0.65045700	0.03040700
C	-3.47159000	0.59169500	-2.19411900
C	0.28871100	3.26046900	2.41163500
C	-2.43975800	0.88999300	-3.12343900
C	-1.53605800	3.93597600	0.75781000
C	1.27738600	3.63386100	1.46179200
C	1.92002500	3.57258600	-0.76326700
C	1.58917700	3.12955000	-2.07512600
C	-1.70726400	1.38242500	3.39603300
C	-4.08849600	-0.72772000	-0.38321900
C	-3.68426400	-0.76364300	-1.76424800

C	-3.46133100	-0.01127000	2.28906300
C	0.38638400	1.17321500	-3.83089700
C	2.54865400	2.97983200	1.38746400
C	0.62396900	2.23954700	3.34141700
C	-3.01562100	2.69602000	-0.92255500
C	2.94482100	2.91663700	0.00236900
C	-1.70553300	-0.20680800	-3.70291200
C	-2.43779800	0.17108000	3.28684200
C	2.36438900	2.07219800	-2.62390700
C	-0.35841700	1.31949600	3.82798500
C	-0.31129000	-0.06141500	-4.02929700
C	1.76377700	1.10723900	-3.49061600
C	-2.89923600	-1.84128500	-2.28950000
C	-1.96200500	-1.58507200	-3.37456600
C	1.88224100	1.55623800	3.25351500
C	-2.03020500	3.02354700	-1.90898400
C	2.83287800	1.87334400	2.24080000
C	-1.79426700	-1.09625600	3.53049600
C	0.27994600	0.05379400	4.05883200
C	0.32830500	-1.33784900	-3.89239800
C	-2.40314100	-2.06198200	2.64161300
C	2.40257900	-0.15274000	-3.27084100
C	1.67039400	0.21340200	3.69526800
C	-2.96075300	-2.86145000	0.00192900
C	-0.68811200	-2.31089100	-3.49776800
C	-2.55865500	-2.88773100	-1.37679400
C	-0.80396300	3.73761200	-1.58920400
C	-0.41718700	-1.19263300	3.94907900
C	3.43975600	0.03183600	-2.28011800
C	3.66121700	0.80706200	1.72677400
C	4.23190400	0.78389400	0.38391800
C	1.69080800	-1.37949800	-3.41591100
C	-1.63870900	-3.15527800	2.11553700
C	-1.94688900	-3.52964600	0.76806100
C	-1.29512600	-3.58595200	-1.47273900
C	2.38136200	-0.86172700	3.12623000
C	-0.31764600	-3.29301400	-2.48847900
C	-0.50187700	4.18179200	-0.25474200
C	3.37868200	-0.54094300	2.13712200
C	4.24932500	-0.63917300	-0.04335300
C	3.79964300	-1.04179300	-1.37765500
C	0.34734100	-2.35952500	3.52330500
C	-0.92178600	-3.97030500	-0.14276100
C	2.08044400	-2.46083200	-2.56873300

C	-0.26555100	-3.32518800	2.59294200
C	1.71401300	-2.13285900	3.05619300
C	3.70447100	-1.42093300	1.05542300
C	1.05239700	-3.34744900	-2.06816600
C	-3.07069600	2.28784000	1.50362400
C	3.07175200	-2.27948300	-1.54978700
C	0.44237000	-4.00019400	0.24668200
C	0.74373300	-3.66653600	1.61494100
C	1.95341900	-2.94850500	1.90300600
C	2.92235500	-2.62046300	0.88654200
C	1.43006100	-3.73294000	-0.73772400
C	2.67462100	-3.08779300	-0.42618900
C	3.41558200	1.41817700	-1.87203400
C	-3.43372200	-1.39150600	1.88369700
C	3.75462600	1.84171100	-0.52829500
C	-1.10015100	3.41492300	2.04009600
C	-3.69925300	-1.75802800	0.52736200
C	-1.22234700	-0.22751300	0.10212800
C	0.22543500	0.11518000	0.06848900
C	-3.74057500	1.46854000	-1.09027000
Sc	-0.08166400	-1.30109100	1.60446200
Sc	-0.55249000	-1.08158900	-1.62075300
Sc	2.18522700	0.16812200	-0.12388700
Sc	-0.84383700	1.92507300	0.09740100
H	-1.85043800	0.07377700	0.93766600