

Supplementary Materials

Photoreactions of $\text{Sc}_3\text{N}@\text{C}_{80}$ with Disilirane, Silirane, and Digermirane: A Photochemical Method to Separate I_h and D_{5h} Isomers

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Materials and General Methods: All chemicals were reagent grade, purchased from Wako Pure Chemical Industries Ltd. $\text{Sc}_3\text{N@C}_{80}$ was purchased from Luna Innovations Inc. 1,2-dichlorobenzene (ODCB) was distilled from P_2O_5 under vacuum before use. Toluene was distilled from benzophenone sodium ketyl under dry N_2 prior to use. Reagents were used as purchased unless otherwise specified. High-performance liquid chromatography (HPLC) was performed on an LC-908 apparatus (Japan Analytical Industry Co. Ltd.) monitored using a UV3702 detector. Analytical HPLC was performed on a PU-1586 pump with a UV-1575 detector (JASCO Corp.). Buckyprep-M (i.d. 10 mm \times 250 mm, 4.6 mm \times 250 mm), 5PBB (i.d. 4.6 mm \times 250 mm), and 5PYE (i.d. 4.6 mm \times 250 mm) columns (Nacalai Tesque Inc.) were used for HPLC separation. Toluene was used as the eluent for HPLC. The ^1H and ^{13}C NMR measurements were conducted on a JEOL ECA-500 spectrometer (JEOL Ltd.). MALDI-TOF mass experiments were performed (Autoflex III smartbeam, Bruker Daltonics) with 1,1,4,4-tetraphenyl-1,3-butadiene (TPB) as the matrix in both positive and negative ion modes. Absorption spectra were measured using a UV spectrophotometer (UV-3150, Shimadzu Corp.). Cyclic voltammograms and differential pulse voltammograms were recorded on an electrochemical analyzer (BAS CV50W, BAS Inc.). The reference electrode was a saturated calomel reference electrode (SCE). The glassy carbon electrode was used as the working electrode, and a platinum wire was used as the counter electrode. All potentials are referenced to the ferrocene/ferrocenium couple (Fc/Fc^+) as the standard. $(n\text{-Bu})_4\text{NPF}_6$ (0.1 M) in ODCB was used as the supporting electrolyte solution. The cyclic voltammograms were recorded using a scan rate of 20 mV/s. The differential pulse voltammograms were obtained using a pulse amplitude of 50 mV, a pulse width of 50 ms, a pulse period of 200 ms, and a scan rate of 50 mV/s.

Complete list of authors for Ref 51.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Rev. C.01. Gaussian Inc.: Wallingford, CT, 2013.

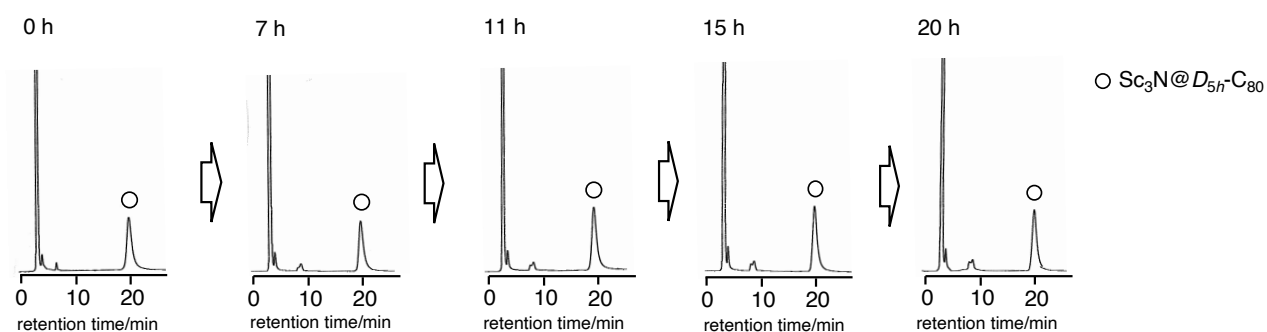


Figure S1. HPLC profiles of the photoreaction of $\text{Sc}_3\text{N}@D_{5h}\text{-C}_{80}$ with **1**. HPLC conditions: Buckyprep-M column (ϕ 4.6 x 250 mm), Eluent: toluene, Flow rate: 1.0 ml/min, Detection wavelength: 330 nm.

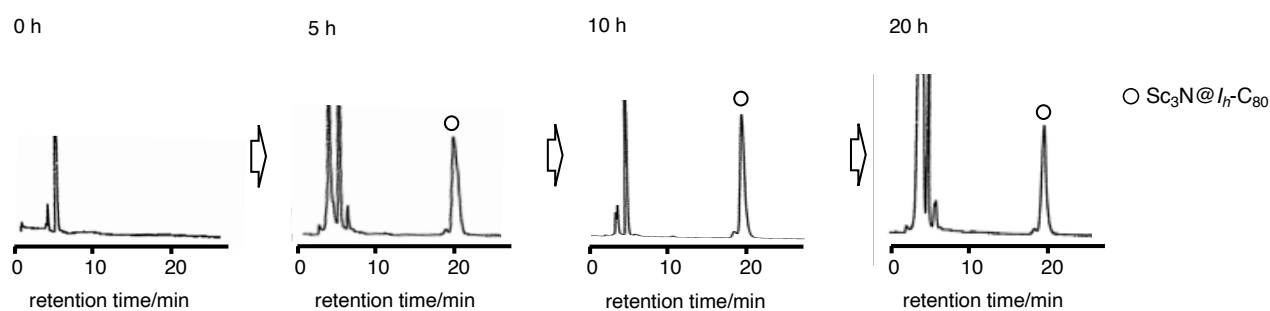


Figure S2. HPLC profiles of the thermolysis of the mixture of **2** and **3**. HPLC conditions: 5PYE column (ϕ 4.6 x 250 mm), Eluent: toluene, Flow rate: 1.0 ml/min, Detection wavelength: 330 nm.

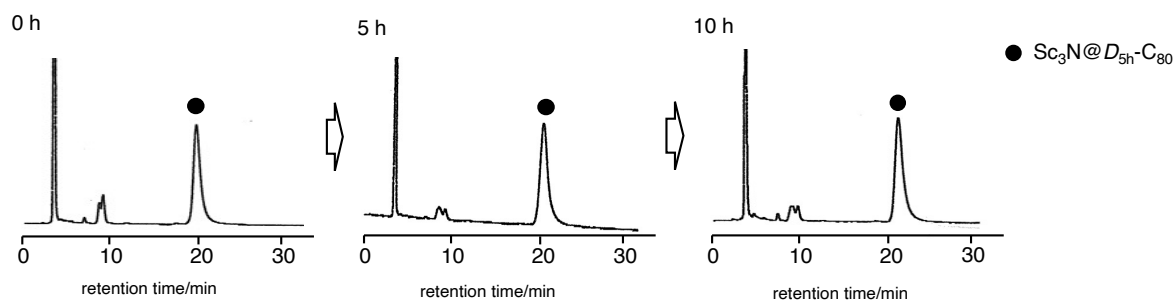


Figure S3. HPLC profiles of the photoreaction of $\text{Sc}_3\text{N}@D_{5h}\text{-C}_{80}$ with **4**. HPLC conditions: Buckyprep-M column (ϕ 4.6 x 250 mm), Eluent: toluene, Flow rate: 1.0 ml/min, Detection wavelength: 330 nm.

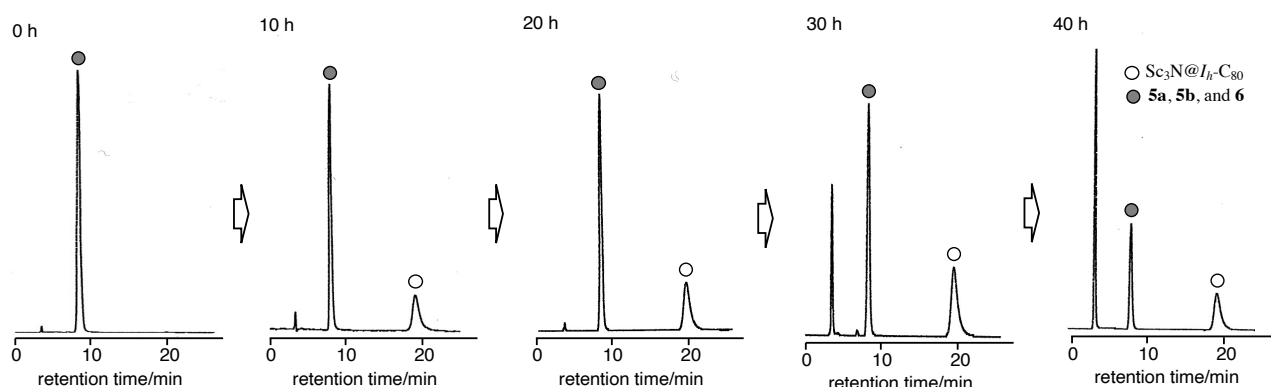


Figure S4. HPLC profiles of the thermolysis of the mixture of **5a**, **5b**, and **6**. HPLC conditions: 5PYE column (ϕ 4.6 x 250 mm), Eluent: toluene, Flow rate: 1.0 ml/min, Detection wavelength: 330 nm.

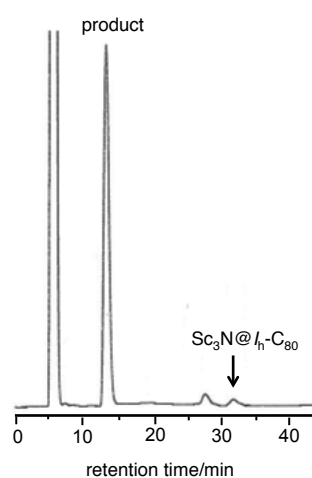


Figure S5. HPLC profile of the reaction mixture of $\text{Sc}_3\text{N}@I_h\text{-C}_{80}$ and **7**. Conditions: Buckyrep-M (ϕ 10 × 250 mm); Eluent, toluene; Flow rate, 3.0 mL/min; Detection wavelength, 330 nm.

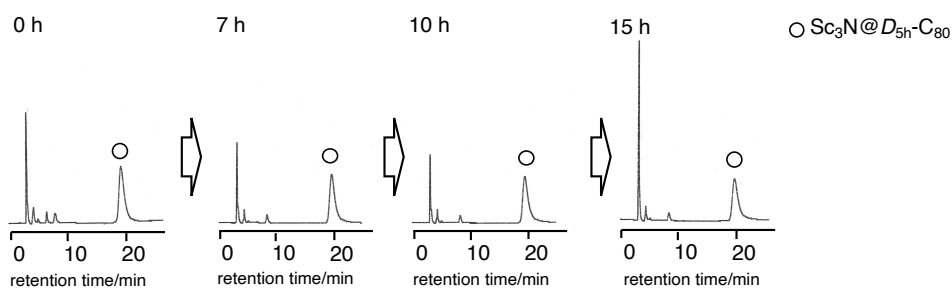


Figure S6. HPLC profiles of the photolysis of $\text{Sc}_3\text{N}@D_{5h}\text{-C}_{80}$ with **7**. HPLC conditions: Buckyprep-M column ($\phi 4.6 \times 250$ mm), Eluent: toluene, Flow rate: 1.0 ml/min, Detection wavelength: 330 nm.

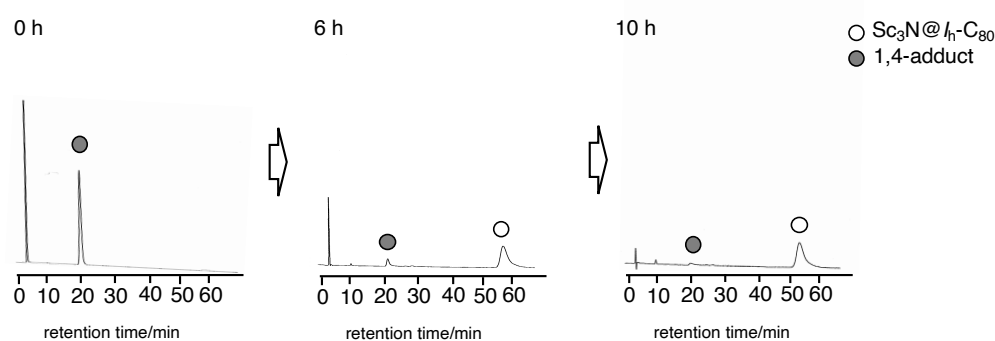


Figure S7. HPLC profiles of the thermolysis of **9**. HPLC conditions: 5PBB column ($\phi 4.6 \times 250$ mm), Eluent: toluene, Flow rate: 1.0 ml/min, Detection wavelength: 330 nm.

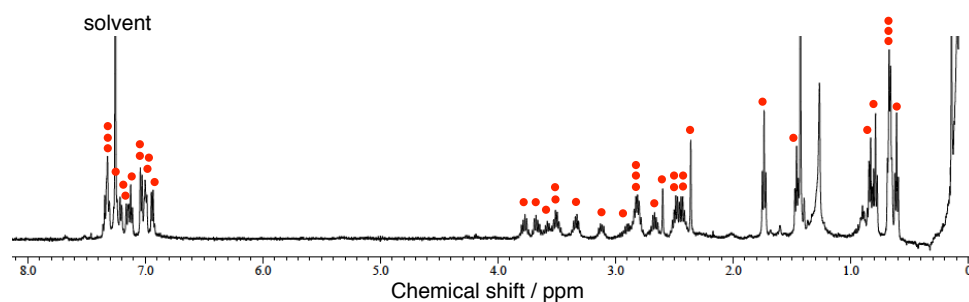


Figure S8. 500 MHz ^1H NMR spectrum of **9** recorded at 293 K in $\text{CS}_2/\text{CDCl}_3$ (1:3).

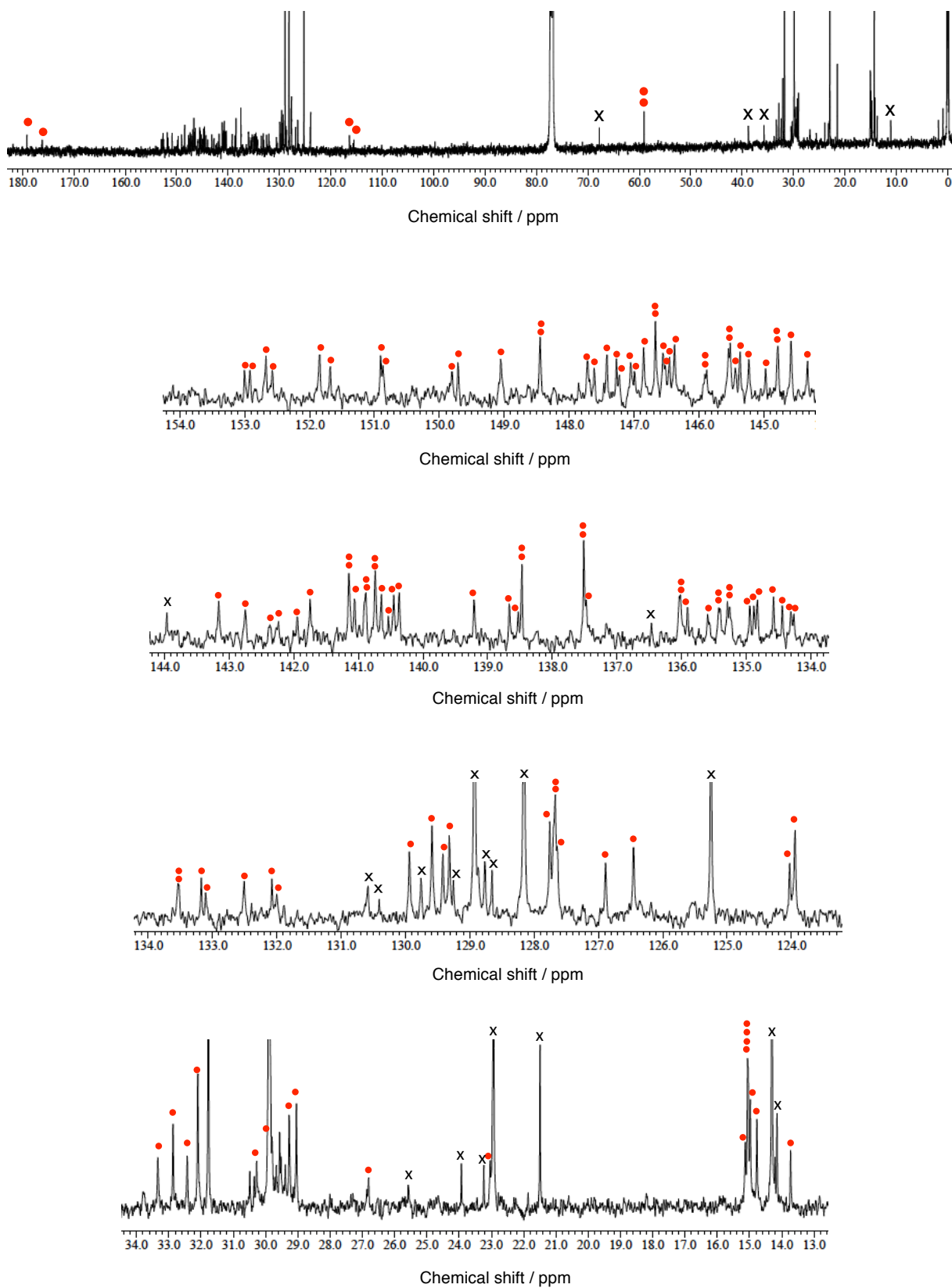


Figure S9. 125 MHz ^{13}C NMR spectra of **9** recorded at 293 K in $\text{CS}_2/\text{CDCl}_3$ (1:3).

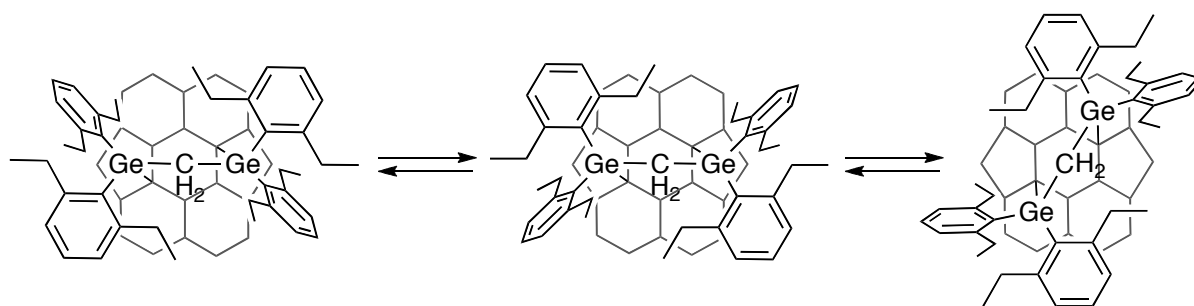
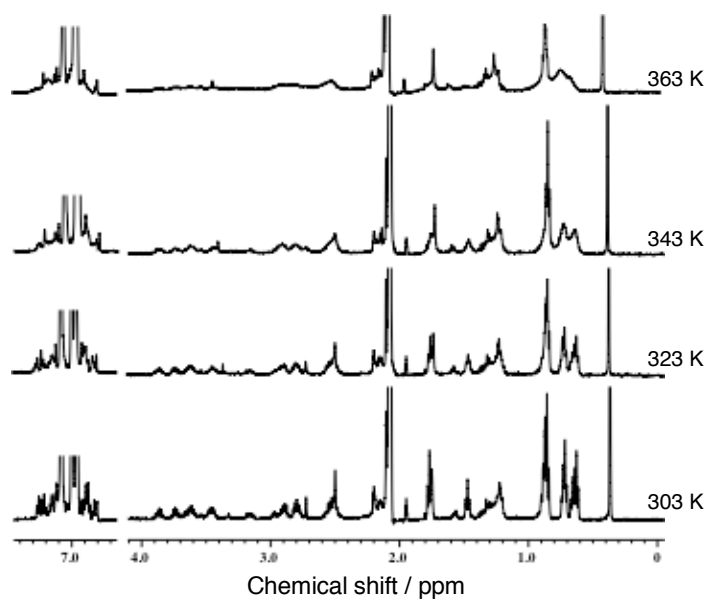


Figure S10. 500 MHz VT ^1H NMR spectra of **9** recorded in toluene- d_8 (above). Possible isomerization between conformers (below).

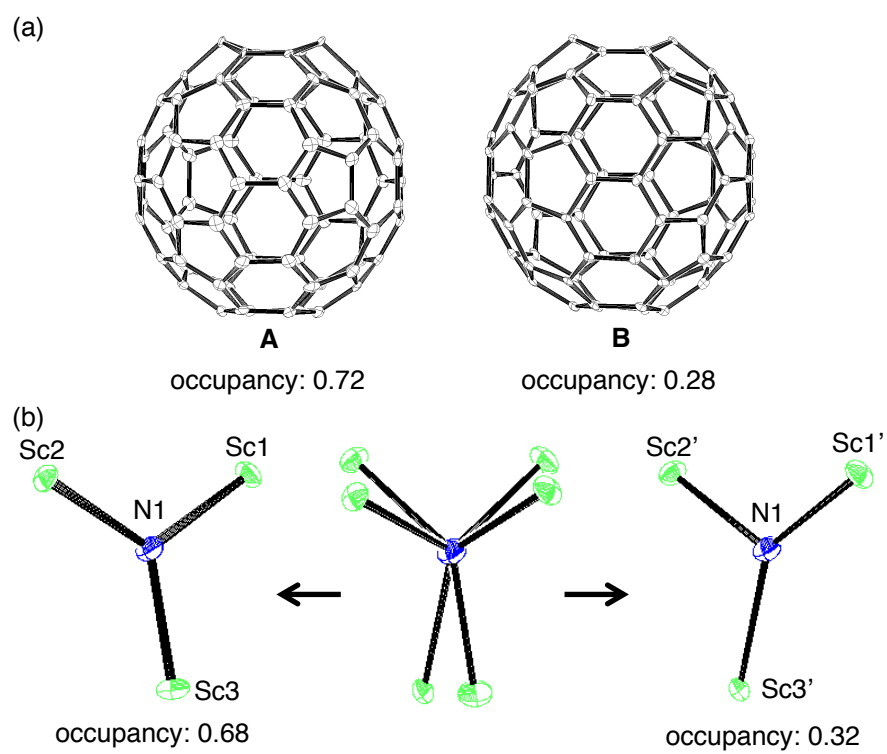


Figure S11. Disorder of (a) C_{80} cage and (b) Sc_3N cluster with occupancies in the crystal of **9**.

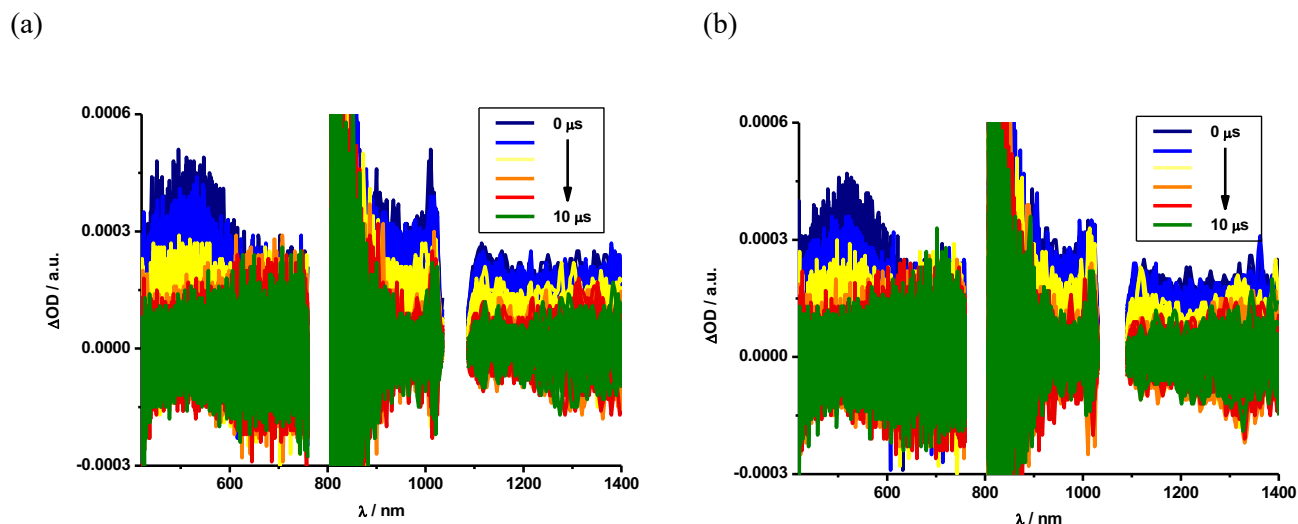


Figure S12. Raw data of all the transient absorption measurements of $\text{Sc}_3\text{N}@I_h\text{-C}_{80}$ ($\lambda_{\text{ex}} = 387 \text{ nm}$, $E = 400 \text{ nJ}$) in the absence (a) and the presence (b) of **7**.

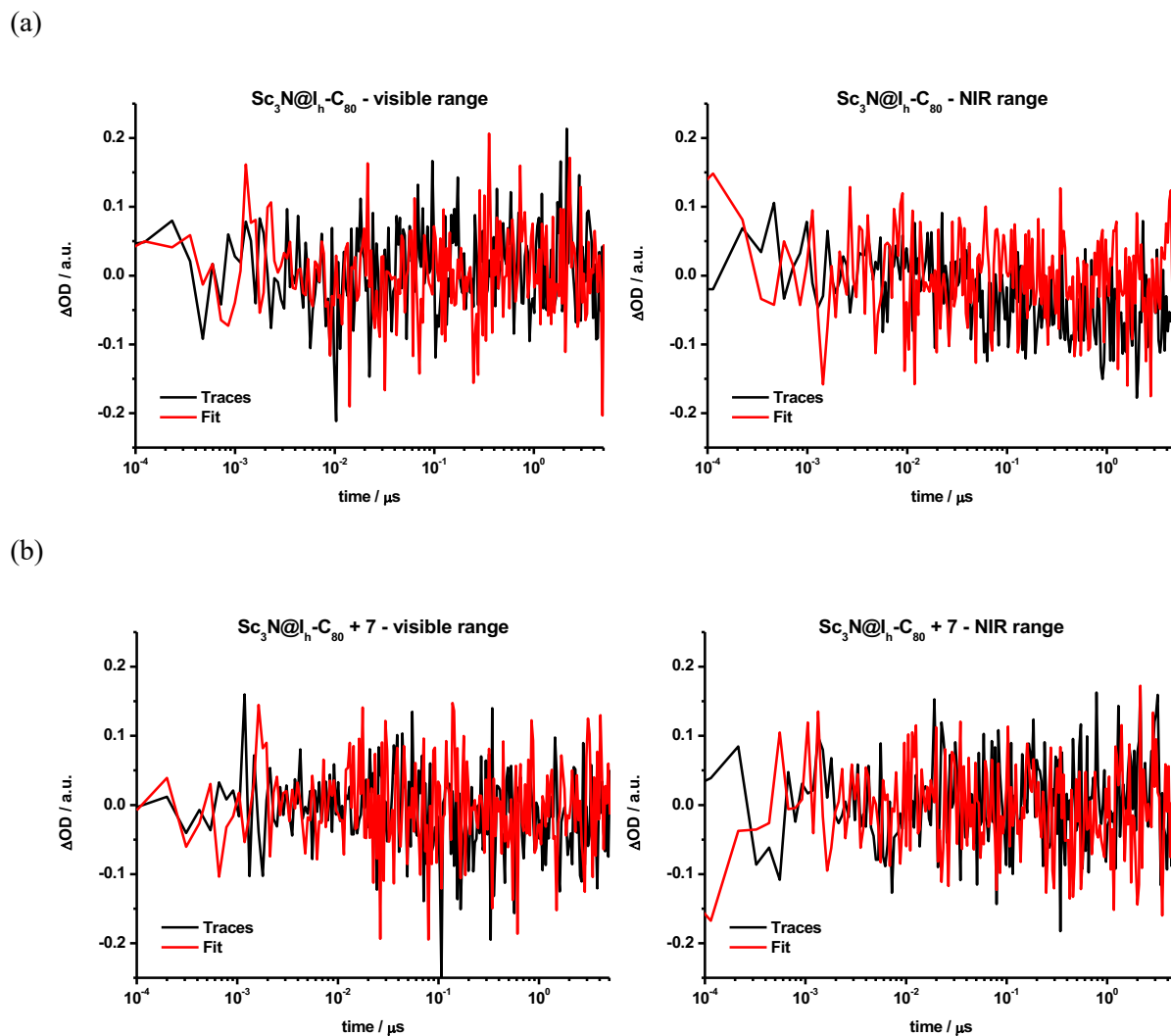


Figure S13. Residuals of the decay profiles from the transient absorption measurements (Figures 8 and S12) using $\text{Sc}_3\text{N}@I_h\text{-C}_{80}$ in the absence (a) and the presence (b) of 200 times equimolar amounts of **7** at the visible and NIR regions.

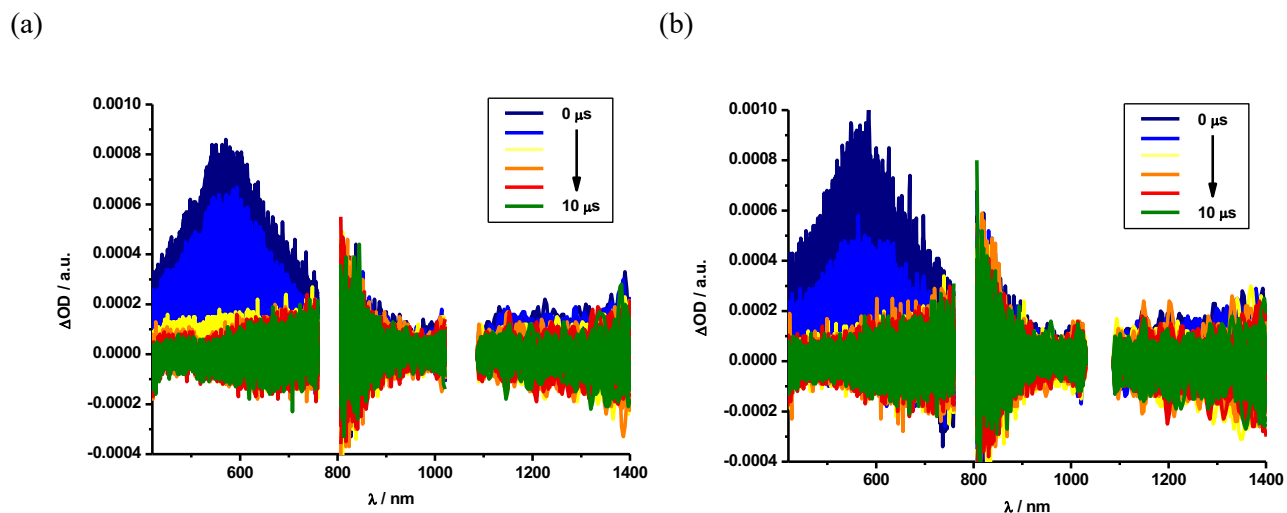


Figure S14. Raw data of all the transient absorption measurements of $\text{Sc}_3\text{N}@D_{5h}\text{-C}_{80}$ ($\lambda_{\text{ex}} = 387 \text{ nm}$, $E = 400 \text{ nJ}$) in the absence (a) and the presence (b) of **7**.

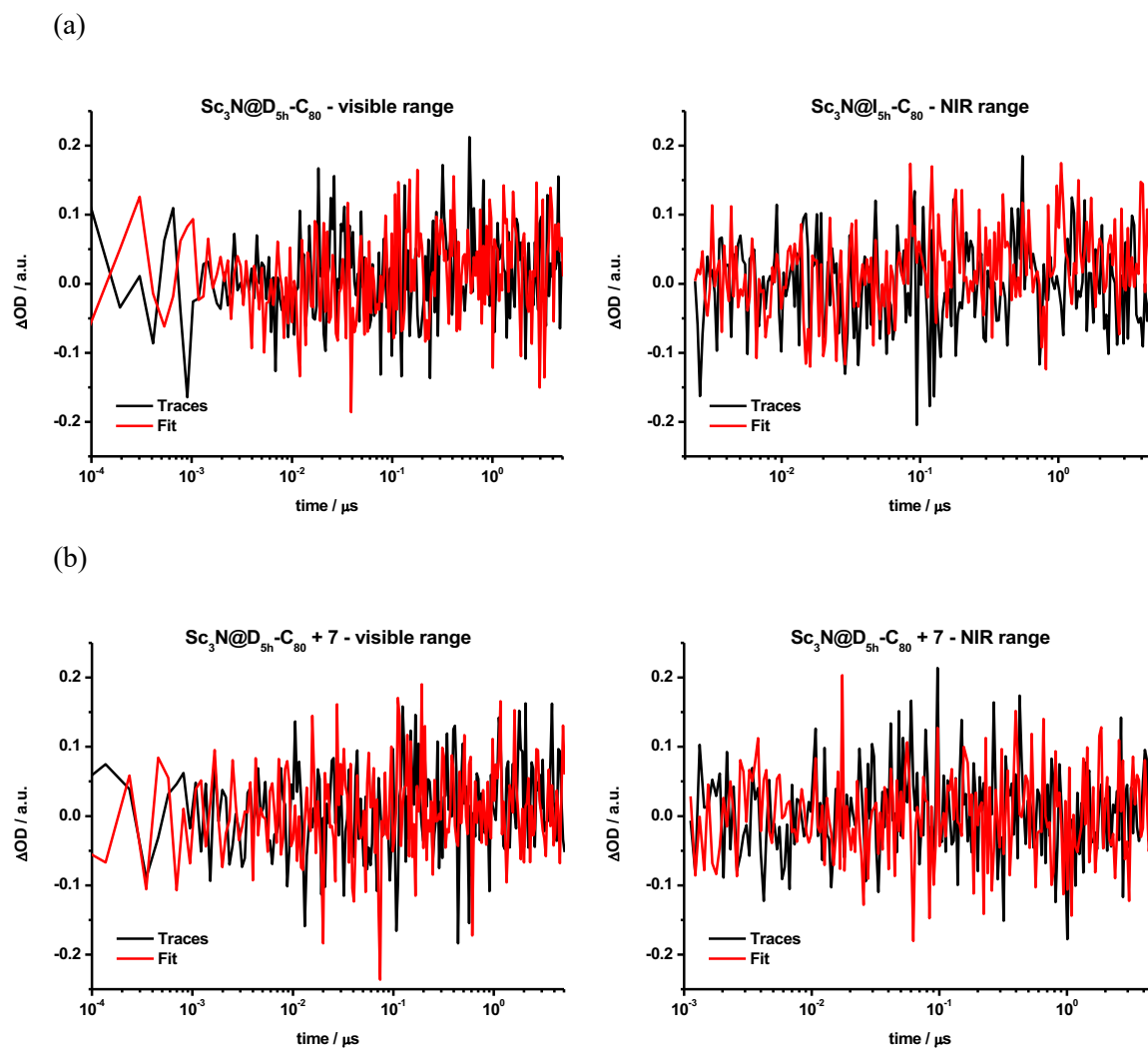


Figure S15. Residuals of the decay profiles from the transient absorption measurements (Figures 10 and S14) using $\text{Sc}_3\text{N}@D_{5h}\text{-C}_{80}$ in the absence (a) and the presence (b) of 200 times equimolar amounts of **7** at the visible and NIR regions.

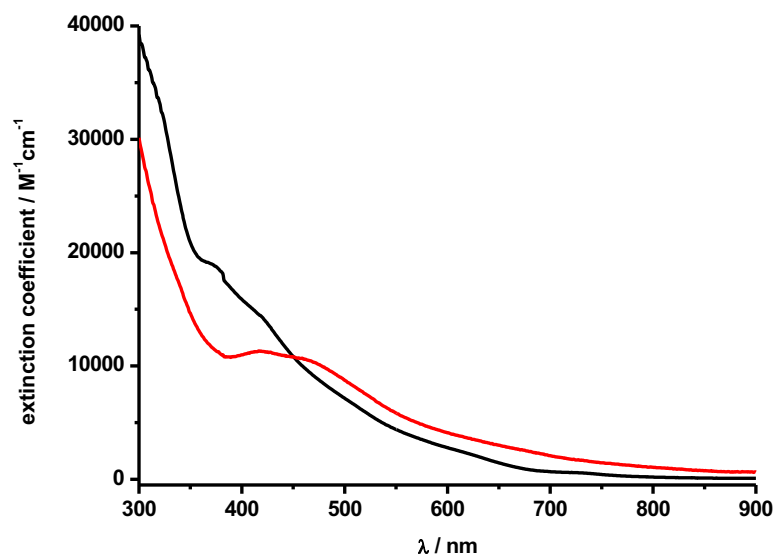


Figure S16. UV-Visible spectra of $\text{Sc}_3\text{N}@I_h\text{-C}_{80}$ (black) and $\text{Sc}_3\text{N}@D_{5h}\text{-C}_{80}$ (red) in toluene.

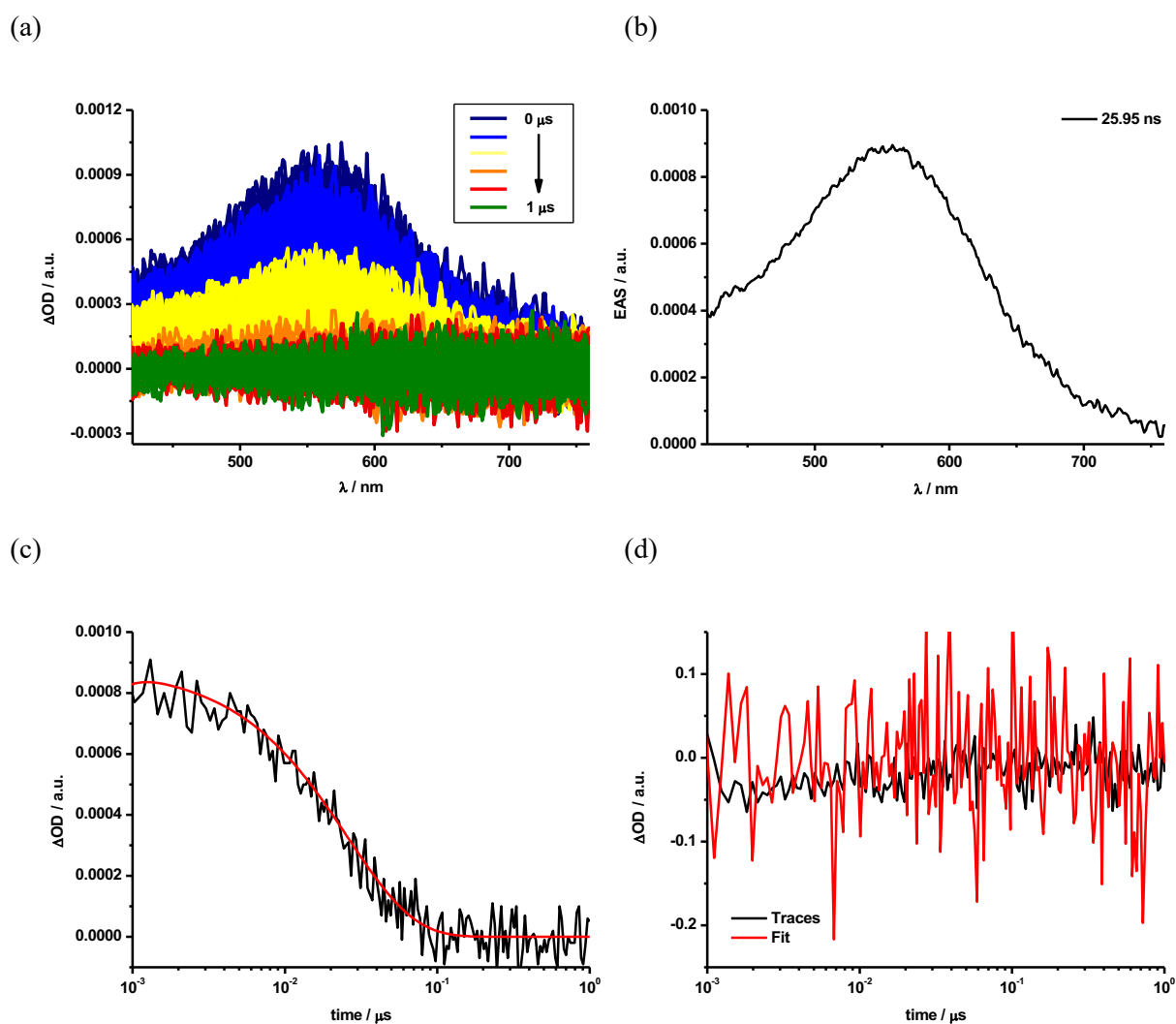


Figure S17. (a) Raw data of the transient absorption measurements of pure toluene ($\lambda_{\text{ex}} = 387 \text{ nm}$, $E = 400 \text{ nJ}$). (b) Respective evolution associated spectra (EAS) of the triplet excited state of pure toluene at the respective relative delay time. (c) Respective decay profiles of the transient absorption measurements at 555 nm. (d) Respective residuals of the decay profile from the transient absorption measurement.

Table S1. Ten lowest excited states of $\text{Sc}_3\text{N}@I_h\text{-C}_{80}$ calculated by TD-B3LYP/6-31G*~SDD.

Excited State	Excitation Energy (eV)	Wavelength (nm)	Contribution
T ₁	1.8208	680.93	HOMO -> LUMO
T ₂	1.9152	647.38	HOMO-1 -> LUMO
T ₃	1.9158	647.18	HOMO-2 -> LUMO
S ₁	1.9539	634.54	HOMO -> LUMO
T ₄	2.0441	606.54	HOMO -> LUMO+1
T ₅	2.0449	606.29	HOMO -> LUMO+2
S ₂	2.0483	605.30	HOMO-1 -> LUMO HOMO -> LUMO+1
S ₃	2.0493	605.02	HOMO-2 -> LUMO HOMO -> LUMO+2
T ₆	2.0713	598.59	HOMO-1 -> LUMO+1 HOMO-2 -> LUMO+2
T ₇	2.0905	593.09	HOMO-3 -> LUMO HOMO-1 -> LUMO+1

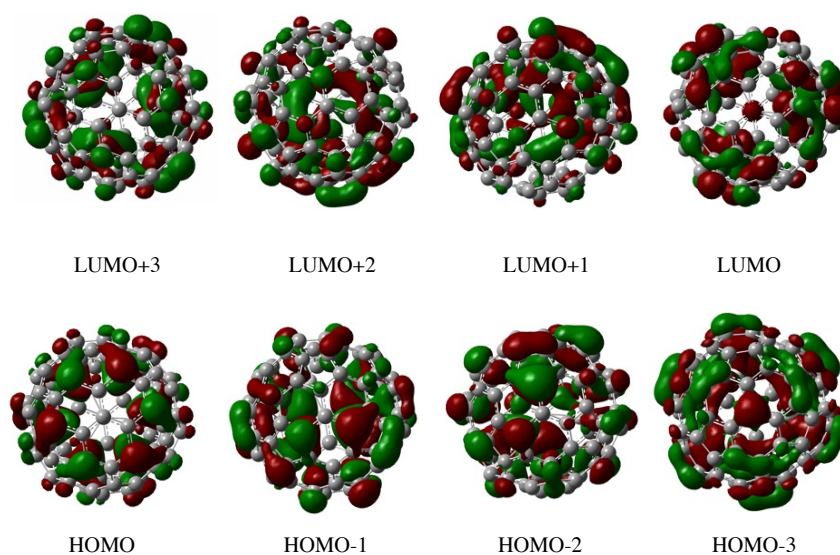
**Figure S18.** Selected molecular orbitals of $\text{Sc}_3\text{N}@I_h\text{-C}_{80}$.

Table S2. Ten lowest excited states of $\text{Sc}_3\text{N}@D_{5h}\text{-C}_{80}$ calculated by TD-B3LYP/6-31G*~SDD.

Excited State	Excitation Energy (eV)	Wavelength (nm)	Contribution
T ₁	1.4945	829.62	HOMO -> LUMO HOMO-1 -> LUMO
S ₁	1.6184	766.08	HOMO -> LUMO HOMO-1 -> LUMO
T ₂	1.6513	750.84	HOMO-1 -> LUMO+1 HOMO -> LUMO+1
T ₃	1.7092	725.41	HOMO-1 -> LUMO HOMO -> LUMO+3
T ₄	1.7392	712.90	HOMO-2 -> LUMO HOMO -> LUMO+1
T ₅	1.7418	711.83	HOMO-2 -> LUMO HOMO -> LUMO+1
T ₆	1.7905	692.46	HOMO -> LUMO+3 HOMO-1 -> LUMO+2
S ₂	1.7965	690.12	HOMO-1 -> LUMO HOMO -> LUMO+1
S ₃	1.8146	683.25	HOMO -> LUMO+1 HOMO-1 -> LUMO
T ₇	1.8213	680.73	HOMO -> LUMO+2 HOMO -> LUMO+3

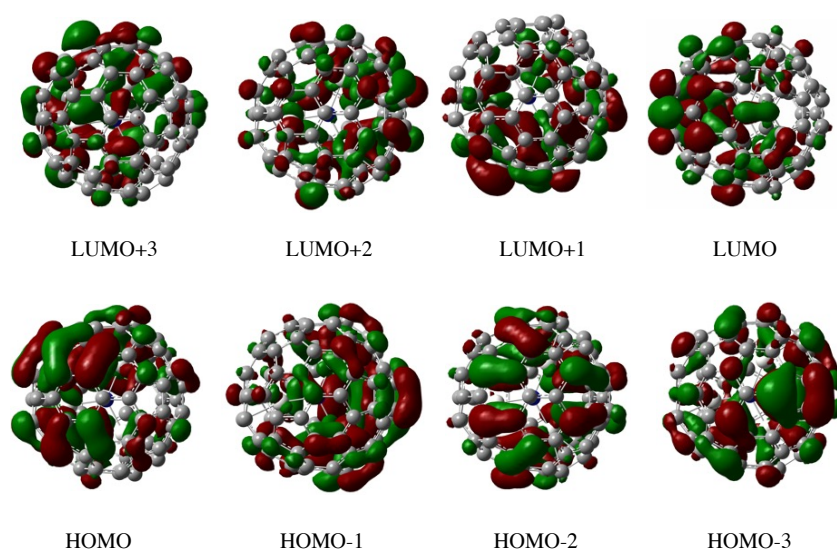
**Figure S19.** Selected molecular orbitals of $\text{Sc}_3\text{N}@D_{5h}\text{-C}_{80}$.

Table S3. Cartesian coordinates of optimized structures.Sc₃N@I_h-C₈₀

Sc	-0.20297500	2.02489500	0.00000000
Sc	-0.20993400	-1.02212200	1.74685900
Sc	-0.20993400	-1.02212200	-1.74685900
N	-0.10854300	0.00314900	0.00000000
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C	1.40199600	3.03598300	2.37066800
C	1.12246100	3.78216900	1.16288000
C	2.55644500	2.20968300	2.38861800
C	0.27500600	1.41110700	3.87196500
C	1.11591700	-0.88437900	3.85516000
C	1.39871400	0.53384500	3.81613200
C	2.55566400	0.96048600	3.11154800
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C	1.28167000	-2.25754800	3.15608900
C	-0.11680800	-2.34168000	3.39519200
C	-0.84835200	-1.20031900	3.86515700
C	-0.18936300	0.04223000	4.10402100
C	-0.92500200	1.23476300	3.84431000
C	-0.26493600	2.41109000	3.36282400
C	-1.17046900	3.10193800	2.46253200
C	-0.71205500	3.77134900	1.29125400
C	0.72400400	3.92137700	1.13396900
C	1.37786500	4.05047000	-0.15761500
C	2.59221600	3.25898800	-0.11892400
C	3.02503000	2.41971700	-1.22689600
C	3.81915100	1.28290000	-0.90332400
C	3.77442900	0.10759100	-1.72227100
C	3.87985300	-1.04963600	-0.88171700
C	3.19451500	-2.26346800	-1.19259200
C	2.84544200	-3.12903300	-0.06361300
C	1.62887400	-3.93169100	-0.09008100
C	0.96606600	-3.80846600	1.19276800
C	-0.47701200	-3.75562800	1.34999400

C	-0.98045900	-3.09735600	2.50861300
C	-2.25001300	-2.43106600	2.49389600
C	-2.16631600	-1.24112100	3.27827500
C	-2.85794500	-0.04918800	2.87595300
C	-2.24701600	1.18719900	3.25247100
C	-2.39727600	2.35988800	2.44813300
C	-3.18112700	2.32245000	1.28850000
C	-3.85480000	1.11352800	0.90825200
C	-3.73287200	-0.08838200	1.67953300
C	-3.88569600	-1.33262600	0.94128900
C	-3.03848800	-2.43356400	1.32509900
C	-2.55487700	-3.09738300	0.15633300
C	-1.28409400	-3.76533700	0.13699900
C	-0.63809100	-3.84915800	-1.13529700
C	0.79555100	-3.87814900	-1.24732700
C	1.16235300	-3.09439100	-2.39740500
C	2.34193900	-2.26961800	-2.40182300
C	2.29195800	-1.11772400	-3.24176700
C	2.99889700	0.07415700	-2.88455800
C	2.21841100	1.21345000	-3.26490300
C	2.18886800	2.37084100	-2.43640000
C	0.97006400	3.13993300	-2.44382400
C	0.55548700	3.95138300	-1.32458500
C	-0.87273400	3.81164400	-1.19877500
C	-1.53373100	3.72378500	0.07726700
C	-2.77682100	3.02286100	0.10882500
C	-3.24890000	2.27743200	-1.03521100
C	-3.93039400	1.10149200	-0.55619400
C	-3.95132900	-0.12228700	-1.30728400
C	-3.97760000	-1.35932800	-0.54486500
C	-3.11540500	-2.43834900	-0.99592600
C	-2.37296700	-2.42220100	-2.23256500
C	-1.16484100	-3.17472200	-2.30121400
C	-0.05233400	-2.70034600	-3.07435500
C	-0.12282400	-1.47735800	-3.80563400
C	1.07164400	-0.71234300	-3.91265600
C	1.02664200	0.72130800	-3.92611600
C	-0.21212600	1.41418200	-3.82442400
C	-0.21687300	2.64900700	-3.10661600
C	-1.35420500	3.07200100	-2.34611700
C	-2.52497900	2.26385500	-2.26279000
C	-2.55237100	1.06687800	-3.03663500

C	-3.22202600	-0.10888700	-2.54539800
C	-2.47904100	-1.25418300	-3.03193100
C	-1.37657700	-0.78308600	-3.81547500
C	-1.42097100	0.64982400	-3.81601400

Compound 2

N	2.55629900	0.04256600	-0.02513200
C	-4.38130300	0.01923500	-0.06288600
C	6.41795300	-0.31388200	-1.43237100
C	5.64654800	-0.53887700	-2.61996900
C	4.94601800	0.52466000	-3.31468400
C	4.91395100	-1.76112100	-2.83282800
C	3.79415200	-0.04110700	-3.94649100
C	3.76768100	-1.45525200	-3.64262800
C	2.57874800	0.69784400	-4.02612700
C	2.54207400	-2.18005700	-3.48854100
C	1.35442400	-0.05623300	-3.89801500
C	1.29341800	-1.49065100	-3.72812000
C	0.21793600	0.51647300	-3.24010600
C	0.08122500	-1.80296900	-2.96323400
C	-0.53803000	-0.53605300	-2.62532700
C	-1.29325100	-0.27414900	-1.42529900
C	6.39500500	-1.37129400	-0.45693300
C	5.65863300	-2.59396800	-0.66576500
C	6.38736800	-1.09639500	0.96923700
C	4.88199700	-2.79295100	-1.84700900
C	5.20758400	-3.07188700	0.61261500
C	5.64913100	-2.15357500	1.61889800
C	3.68512500	-3.55700500	-1.72496500
C	3.96365700	-3.76722300	0.74696700
C	4.87008800	-1.90749300	2.79464900
C	3.23237600	-4.03832600	-0.45164600
C	2.52548900	-3.23555700	-2.51952700
C	3.22804600	-3.58273800	1.95181600
C	3.67630900	-2.66869200	2.96738300
C	1.79775000	-4.01116400	-0.45468400
C	1.34679100	-3.52392800	-1.73251900
C	1.78685500	-3.56997600	1.94326100
C	2.51368700	-2.08283600	3.58195000
C	1.05796800	-3.72877600	0.72886700
C	1.34729400	-2.64407500	2.94314200
C	0.10340200	-2.80997300	-1.89597300

C	-0.16740600	-3.00773900	0.56163800
C	-0.65141500	-2.56925500	-0.71648100
C	0.18061700	-1.86430500	2.72658800
C	-0.60690700	-2.08890500	1.56416000
C	-1.67114700	-1.43103700	-0.51295100
C	-1.33790000	-1.03461900	0.93413100
C	-6.75647000	-3.30885400	-3.66650600
C	-7.09985600	-3.11383500	-2.32980300
C	-5.43475600	-3.05243800	-4.02489500
C	-6.17676500	-2.68873600	-1.36474900
C	-4.47975200	-2.62044600	-3.09664000
C	-6.72232400	-2.57345200	0.04818500
C	-4.82317500	-2.42396100	-1.73521500
C	-3.08747400	-2.38154100	-3.62232700
C	-4.37412000	-1.32955500	2.94878600
C	-3.75354400	-3.03313300	1.09829500
C	-4.04158200	-2.72225300	2.45643200
C	-3.21647400	-4.90765800	-0.61998700
C	-3.49451000	-4.39794400	0.78283400
C	-4.05651900	-3.73244000	3.42558300
C	-3.51611500	-5.37311000	1.78846200
C	-3.79206700	-5.06737700	3.11954500
H	-5.00068100	0.12801300	-0.95619700
H	-8.12520000	-3.30191700	-2.01665100
H	-5.12888600	-3.18901300	-5.06040500
H	-7.81623200	-2.60049200	0.02979000
H	-6.43479900	-1.64546400	0.54785200
H	-2.33583600	-2.93949500	-3.05846100
H	-2.81082500	-1.32369900	-3.58156100
H	-4.31625300	-1.28675600	4.04077000
H	-3.69295700	-0.57300900	2.55571800
H	-2.71098800	-5.87774500	-0.57441000
H	-2.57471800	-4.24236200	-1.20203400
H	-4.28068200	-3.46198900	4.45571200
H	-3.30743200	-6.40590100	1.51574100
C	6.40105200	0.24628300	1.47590200
C	5.62501400	0.47307100	2.65992400
C	4.90897400	-0.58579000	3.33224000
C	4.89911300	1.70306400	2.87736900
C	3.75466400	-0.00990900	3.95776400
C	3.74137600	1.40613000	3.67368100
C	2.53191800	-0.73581200	4.03553400

C	2.52335800	2.14163700	3.50170700
C	1.31299600	0.03192200	3.90285400
C	1.26439500	1.46716400	3.73427200
C	0.17538200	-0.53013500	3.23555700
C	0.05898700	1.79172700	2.95812400
C	-0.57024800	0.53068500	2.61718200
C	-1.30545900	0.27619800	1.40059200
C	6.51416400	1.32763300	0.50624200
C	5.68065200	2.49804800	0.70721700
C	6.52590400	1.05096100	-0.94062800
C	4.88161100	2.72306800	1.88818300
C	5.20926800	2.95877000	-0.56815200
C	5.69355000	2.06132000	-1.57436700
C	3.70031300	3.50351900	1.74649700
C	3.98929400	3.70557100	-0.71934200
C	4.91155200	1.83904800	-2.77011500
C	3.26252600	3.99866600	0.47145500
C	2.52776800	3.19150800	2.52833200
C	3.27787400	3.54138300	-1.93546900
C	3.73073800	2.61778100	-2.94506400
C	1.82719300	3.98317000	0.45988800
C	1.36115700	3.49199400	1.73027900
C	1.83568500	3.54272300	-1.94117900
C	2.56642100	2.04564400	-3.57144000
C	1.09871200	3.70695200	-0.73148900
C	1.40016100	2.61904900	-2.94420000
C	0.11002300	2.79042900	1.88293000
C	-0.13750500	2.99672900	-0.57544400
C	-0.64044900	2.56487800	0.69583400
C	0.22245500	1.85126400	-2.73773000
C	-0.57576900	2.08354800	-1.58419400
C	-1.66858200	1.43571100	0.48332000
C	-1.32634500	1.03732300	-0.96201500
C	-6.80258400	3.19787700	3.62967100
C	-7.13013500	3.02033400	2.28624100
C	-5.47598600	2.97719400	3.99241400
C	-6.18802700	2.64014800	1.32132800
C	-4.50143100	2.58965200	3.06405700
C	-6.71474000	2.54468900	-0.10019200
C	-4.83068500	2.40205900	1.69813800
C	-3.10719800	2.38556800	3.59954800
C	-4.28030800	1.45898600	-3.03737200

C	-3.72688000	3.10092100	-1.10475600
C	-3.98967200	2.83723300	-2.47930700
C	-3.21664600	4.91777400	0.68311800
C	-3.48713600	4.45645200	-0.73759600
C	-4.00908200	3.88323100	-3.40904900
C	-3.51238100	5.46883600	-1.70650100
C	-3.77792600	5.21121900	-3.04897900
H	-5.10487100	-0.08261300	0.75019500
H	-8.15745900	3.18780400	1.96790200
H	-5.18094400	3.10724600	5.03192300
H	-7.80882800	2.56812900	-0.09669300
H	-6.41662100	1.62513600	-0.60915200
H	-2.35662900	2.90414400	2.99959000
H	-2.83133500	1.32670400	3.62772400
H	-4.20587200	1.46832800	-4.12911500
H	-3.58454500	0.70266900	-2.66949400
H	-2.73582000	5.90131000	0.67344300
H	-2.55470500	4.24673200	1.23543700
H	-4.20777100	3.64721100	-4.45279500
H	-3.31367800	6.49223500	-1.39418400
Sc	1.54038100	0.90256600	1.51981300
Sc	1.57733600	-0.98021500	-1.48961800
Sc	4.53850000	0.34472800	-0.07515700
C	-3.77297000	-6.13084600	4.19127600
H	-2.77656500	-6.21566400	4.64538800
H	-4.47799500	-5.90132200	4.99765200
H	-4.02888700	-7.11489200	3.78417100
C	-7.76655100	-3.80100700	-4.67534500
H	-7.52930900	-3.44885600	-5.68497400
H	-7.78869600	-4.89859600	-4.71092300
H	-8.77897300	-3.46487500	-4.42651100
C	-7.83490300	3.63857600	4.63983700
H	-7.58504500	3.28868700	5.64714900
H	-7.90457800	4.73385400	4.68380900
H	-8.83144000	3.26121600	4.38579100
C	-3.82757300	6.32081400	-4.07182500
H	-3.38146900	6.00964000	-5.02303700
H	-4.86338500	6.61885500	-4.28315100
H	-3.29568000	7.21167300	-3.72235700
H	-4.14248300	-5.04232800	-1.19017400
H	-5.39332600	-1.02859800	2.67449800
H	-6.36674600	3.37968600	-0.71711900

H	-3.01954900	2.76549200	4.62243700
H	-4.14262800	5.00635100	1.26170100
H	-5.29598300	1.12189700	-2.79369500
H	-3.00217100	-2.69456200	-4.66771800
H	-6.38061000	-3.39764900	0.68283800
Si	-3.65580900	-1.75378900	-0.33568700
Si	-3.64673600	1.77576900	0.29096200

Compound **9**

N	0.00000000	0.00000000	2.88276300
C	0.00000000	0.00000000	-4.24316500
C	-1.48854900	0.00364100	6.74088000
C	-2.68578200	0.00394100	5.95218100
C	-3.16273000	-1.16690100	5.24336000
C	-3.13098700	1.16911700	5.22366900
C	-3.88741800	-0.72352000	4.09133200
C	-3.86318300	0.72206600	4.07251700
C	-3.82610400	-1.45763100	2.87102400
C	-3.83241700	1.46781900	2.84916400
C	-3.84272700	-0.68717100	1.64788100
C	-3.94088800	0.75426700	1.59541600
C	-3.09170400	-1.12246900	0.50612900
C	-3.24682400	1.21177900	0.38472800
C	-2.68678400	0.03177900	-0.24844500
C	-1.44294000	0.00639700	-0.97918100
C	-0.72616500	1.23550900	6.77605100
C	-1.14883000	2.36663500	5.97842900
C	0.73768200	1.23220900	6.77647600
C	-2.35111300	2.36020200	5.19621500
C	0.01577200	3.06782100	5.51842000
C	1.17182400	2.36101900	5.97843000
C	-2.36615700	3.14597500	4.00890900
C	0.02160300	3.80799500	4.29077000
C	2.38238300	2.35748400	5.20309400
C	-1.20470400	3.86309000	3.56269300
C	-3.07687400	2.68335800	2.84339600
C	1.24407500	3.86246000	3.56703700
C	2.40966900	3.14857200	4.01787900
C	-1.19601900	3.84428900	2.12746200
C	-2.35396400	3.12109400	1.67114800
C	1.24465600	3.85809700	2.12623800
C	3.12808000	2.69571400	2.85531600

C	0.02348000	3.79518300	1.39247400
C	2.40223300	3.13661800	1.68794700
C	-2.37697500	2.39371000	0.42707700
C	0.00000000	3.06058500	0.16385700
C	-1.16937200	2.38686200	-0.32277200
C	2.34242700	2.33860100	0.51520500
C	1.16039900	2.34835800	-0.27669000
C	-0.74859400	1.30712200	-1.32136400
C	0.73806000	1.19523800	-1.00633400
C	-4.35660900	2.24045400	-6.54088000
C	-3.02863900	2.32666500	-6.94045100
C	-4.64586300	2.10739100	-5.18858200
C	-1.97783400	2.25951600	-6.01352500
C	-3.62531200	2.04315800	-4.22707900
C	-0.58004100	2.39598500	-6.60473000
C	-2.27020800	2.09073300	-4.63189400
C	-4.05213900	1.91967500	-2.77826700
C	2.75798300	1.99615100	-3.90589500
C	0.57021100	3.36261500	-3.48080700
C	1.96939600	3.28294700	-3.70962700
C	-1.47249600	4.88229800	-2.89928900
C	-0.00966600	4.63916900	-3.24900100
C	2.73325100	4.45882700	-3.74775400
C	0.79552500	5.78741500	-3.29212300
C	2.15798700	5.70764000	-3.55009800
C	-0.27700900	3.80312800	-7.14956100
C	-5.01756300	3.01724600	-2.29972600
C	3.23370700	1.77171300	-5.35308000
C	-2.25914700	5.64426400	-3.97948800
H	-0.82587100	-0.26086000	-4.90875100
H	-5.15715900	2.27862900	-7.27506700
H	-2.78964600	2.44230200	-7.99536900
H	-5.68189400	2.04748300	-4.86525800
H	-0.47441100	1.66789500	-7.42078700
H	0.18991300	2.14371300	-5.87683100
H	-3.16993400	1.93691600	-2.14179500
H	-4.52140100	0.93932000	-2.61454100
H	3.64380000	2.04213400	-3.25821500
H	2.19297200	1.12918700	-3.56395100
H	-1.50385200	5.46131900	-1.96643100
H	-1.98878300	3.94634800	-2.67819800
H	3.80498700	4.38068800	-3.91818300

H	0.34053600	6.75585200	-3.09676100
H	2.76900400	6.60625700	-3.57176100
H	0.71752700	3.82776300	-7.60961100
H	-1.00734200	4.10582800	-7.90794800
H	-0.29443100	4.54581000	-6.34622300
H	-5.96297200	3.00005800	-2.85154300
H	-5.25117100	2.87797000	-1.23855900
H	-4.57824500	4.01290000	-2.42493000
H	2.39126100	1.68905900	-6.04842800
H	3.85626800	2.60645500	-5.69413300
H	3.82262200	0.85159900	-5.42923100
H	-3.28269900	5.84330300	-3.64150200
H	-1.78978400	6.60780500	-4.20661000
H	-2.31680100	5.06788600	-4.90736300
C	1.48854900	-0.00364100	6.74088000
C	2.68578200	-0.00394100	5.95218100
C	3.16273000	1.16690100	5.24336000
C	3.13098700	-1.16911700	5.22366900
C	3.88741800	0.72352000	4.09133200
C	3.86318300	-0.72206600	4.07251700
C	3.82610400	1.45763100	2.87102400
C	3.83241700	-1.46781900	2.84916400
C	3.84272700	0.68717100	1.64788100
C	3.94088800	-0.75426700	1.59541600
C	3.09170400	1.12246900	0.50612900
C	3.24682400	-1.21177900	0.38472800
C	2.68678400	-0.03177900	-0.24844500
C	1.44294000	-0.00639700	-0.97918100
C	0.72616500	-1.23550900	6.77605100
C	1.14883000	-2.36663500	5.97842900
C	-0.73768200	-1.23220900	6.77647600
C	2.35111300	-2.36020200	5.19621500
C	-0.01577200	-3.06782100	5.51842000
C	-1.17182400	-2.36101900	5.97843000
C	2.36615700	-3.14597500	4.00890900
C	-0.02160300	-3.80799500	4.29077000
C	-2.38238300	-2.35748400	5.20309400
C	1.20470400	-3.86309000	3.56269300
C	3.07687400	-2.68335800	2.84339600
C	-1.24407500	-3.86246000	3.56703700
C	-2.40966900	-3.14857200	4.01787900
C	1.19601900	-3.84428900	2.12746200

C	2.35396400	-3.12109400	1.67114800
C	-1.24465600	-3.85809700	2.12623800
C	-3.12808000	-2.69571400	2.85531600
C	-0.02348000	-3.79518300	1.39247400
C	-2.40223300	-3.13661800	1.68794700
C	2.37697500	-2.39371000	0.42707700
C	0.00000000	-3.06058500	0.16385700
C	1.16937200	-2.38686200	-0.32277200
C	-2.34242700	-2.33860100	0.51520500
C	-1.16039900	-2.34835800	-0.27669000
C	0.74859400	-1.30712200	-1.32136400
C	-0.73806000	-1.19523800	-1.00633400
C	4.35660900	-2.24045400	-6.54088000
C	3.02863900	-2.32666500	-6.94045100
C	4.64586300	-2.10739100	-5.18858200
C	1.97783400	-2.25951600	-6.01352500
C	3.62531200	-2.04315800	-4.22707900
C	0.58004100	-2.39598500	-6.60473000
C	2.27020800	-2.09073300	-4.63189400
C	4.05213900	-1.91967500	-2.77826700
C	-2.75798300	-1.99615100	-3.90589500
C	-0.57021100	-3.36261500	-3.48080700
C	-1.96939600	-3.28294700	-3.70962700
C	1.47249600	-4.88229800	-2.89928900
C	0.00966600	-4.63916900	-3.24900100
C	-2.73325100	-4.45882700	-3.74775400
C	-0.79552500	-5.78741500	-3.29212300
C	-2.15798700	-5.70764000	-3.55009800
C	0.27700900	-3.80312800	-7.14956100
C	5.01756300	-3.01724600	-2.29972600
C	-3.23370700	-1.77171300	-5.35308000
C	2.25914700	-5.64426400	-3.97948800
H	0.82587100	0.26086000	-4.90875100
H	5.15715900	-2.27862900	-7.27506700
H	2.78964600	-2.44230200	-7.99536900
H	5.68189400	-2.04748300	-4.86525800
H	0.47441100	-1.66789500	-7.42078700
H	-0.18991300	-2.14371300	-5.87683100
H	3.16993400	-1.93691600	-2.14179500
H	4.52140100	-0.93932000	-2.61454100
H	-3.64380000	-2.04213400	-3.25821500
H	-2.19297200	-1.12918700	-3.56395100

H	1.50385200	-5.46131900	-1.96643100
H	1.98878300	-3.94634800	-2.67819800
H	-3.80498700	-4.38068800	-3.91818300
H	-0.34053600	-6.75585200	-3.09676100
H	-2.76900400	-6.60625700	-3.57176100
H	-0.71752700	-3.82776300	-7.60961100
H	1.00734200	-4.10582800	-7.90794800
H	0.29443100	-4.54581000	-6.34622300
H	5.96297200	-3.00005800	-2.85154300
H	5.25117100	-2.87797000	-1.23855900
H	4.57824500	-4.01290000	-2.42493000
H	-2.39126100	-1.68905900	-6.04842800
H	-3.85626800	-2.60645500	-5.69413300
H	-3.82262200	-0.85159900	-5.42923100
H	3.28269900	-5.84330300	-3.64150200
H	1.78978400	-6.60780500	-4.20661000
H	2.31680100	-5.06788600	-4.90736300
Ge	-0.65657400	1.74068200	-3.41110300
Ge	0.65657400	-1.74068200	-3.41110300
Sc	1.65179000	-0.60880600	1.85428100
Sc	-1.65179000	0.60880600	1.85428100
Sc	0.00000000	0.00000000	4.88726300