Electronic Supplementary Material (ESI) for ChemComm.

SUPPORTING INFORMATION of SYNTHESES, STRUCTURES, AND COMPUTATIONS

Carbene-mediated synthesis of a germanium tris(dithiolene) dianion

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SUPPORTING INFORMATIONS of SYNTHESES

Materials and Methods

General.

The syntheses of air-sensitive compounds were performed under purified argon using Schlenk techniques and an inert atmosphere drybox (M-Braun LabMaster SP). Chemicals were purchased from Aldrich and Strem and used as received. THF was dried and distilled under argon from Na/benzophenone prior to use. 1,2-difluorobenzene, C_6D_5F, CD_3CN were dried and distilled from CaH_2, which were then stored over 3A molecular sieves over one week before the use. ^1H NMR and $^{13}C\{^1H\}$ NMR spectra were recorded on a Bruker Avance III HD 400 MHz spectrometer or on a Varian Unity Inova 500 MHz spectrometer. X-ray intensity data for **4** and **5** were measured at 135K on a Bruker D8 Quest PHOTON 100 CMOS X-ray diffractometer system with Incoatec Microfocus Source (IμS) monochromated Mo Kα radiation (λ = 0.71073 Å, sealed tube) using phi and omega-scan technique.

Compound **4**: To a Schlenk tube charged with **3** (0.350 g, 0.236 mmol) in THF (5 mL) was added dropwise 3 mL of THF solution of [:C{N(Pr^i)CMe}$_2$] (0.043g, 0.238 mmol). The reaction mixture was stirred under ambient temperature overnight. After filtration, the volatiles were removed from the filtrate in vacuo, giving raw compound **4** as red solid (0.251 g, 87.5% yield). X-ray quality red crystals of **4** were achieved by recrystallization in 1,2-difluorobenzene. Mp: gradually decomposed (> 152^{o}C) and melt (> 297^{o}C). ^1H NMR (499.80 MHz, C_6D_5F): δ 1.23 [d, 12H, CH(CH_3)$_2$, dithiolene], 1.35 [d, 12H, CH(CH_3)$_2$, dithiolene], 1.48 [d, 12H, CH(CH_3)$_2$, dithiolene], 1.52 [d, 12H, CH(CH_3)$_2$, dithiolene], 1.60 [d, 12H, CH(CH_3)$_2$, NHC], 1.84 [s, 6H, CH_3CCCH_3], 3.01 [m, 4H, CH(CH$_3$)$_2$, dithiolene], 3.31 [m, 4H, CH(CH$_3$)$_2$, dithiolene], 6.26 [m, 2H, CH(CH$_3$)$_2$, NHC], 7.19 [d, 4H, Ar-*H*], 7.28 [d, 4H, Ar-*H*], 7.32 [t, 4H, Ar-*H*]. Crystal data for **4·(1,2-difluorobenzene)**: $C_{71}H_{92}F_2GeN_6S_6$, fw = 1332.45, monoclinic, $P2_1/n$, a = 13.8170(10) Å, b = 27.779(2) Å, c = 19.3544(13) Å, β = 107.003(2)^o, V = 7103.9(9) Å^3, Z = 4, R1 = 0.0400 for 17647 data (I>2σ(I)), wR_2 = 0.0886 (all data).

Compound **5**: ***Method 1*** (without addition of water). To a 250 mL Schlenk flask charged with **3** (0.400 g, 0.269 mmol) in THF (150 mL) was added dropwise 5 mL THF solution of [:C{N(Pr^i)CMe}$_2$] (0.096g, 0.532 mmol). The reaction mixture was stirred under ambient temperature for 24h, giving a dark blue solution with a small amount of white precipitate. After filtration, the filtrate was concentrated under vacuo to approximately 30 mL. The resulting blue microcrystalline powder (i.e., raw compound **5)** was subsequently isolated and drying in vacuo (0.212 g, 75.7% yield, calculated by supposing that two equivalents of **3** gives one equivalent of **5**). ***Method 2*** (with addition of water). To a 250 mL Schlenk flask charged with **3** (0.400g, 0.269 mmol) in THF (140 mL) was added dropwise 10 mL THF solution of [:C{N(Pr^i)CMe}$_2$] (0.098g, 0.544 mmol). After 30 min, 9.85 mL of H_2O/THF mixture (0.1% v/v) was added dropwise to the reaction mixture, which was then stirred for another 16h. During this course compound **5** was observed as a blue microcrystalline powder, which was isolated by filtration. The filtrate was concentrated in vacuo to approximately 10 mL, giving the second crop of **5**. Yield: 0.203 g (71.7%). X-ray quality dark blue crystals of **5** were achieved by recrystallization in 1,2-

diflurobenzene. Mp: gradually decomposed (> 163°C) and melt (> 266°C). ^{1}H NMR (400.14 MHz, CD_3CN): δ 0.81 [bs, 12H, CH(CH_3)$_2$, dithiolene], 1.15 [bd, 60H, CH(CH_3)$_2$, dithiolene], 1.47 [d, 36H, CH(CH_3)$_2$, imidazolium], 2.19 [s, 18H, CH_3CCCH_3, imidazolium], 3.0 [bd, 12H, CH(CH$_3$)$_2$, dithiolene], 4.45 [m, 6H, CH(CH$_3$)$_2$, imidazolium], 7.12-7.32 [1,2-difluorobenzene and 18H, Ar-H (dithiolene)] 8.75 [s, 3H, NC(H)N]. ^{13}C{^{1}H} NMR (100.62 MHz, CD_3CN): δ 9.05 (CH$_3$CCCH$_3$), 23.23, 24.76, 24.98 [CH(CH$_3$)$_2$], 29.83 [CH(CH$_3$)$_2$, dithiolene], 51.59 [CH(CH$_3$)$_2$, imidazolium], 124.41[S(N)CC(N)S], 126.48, 126.53, 126.59 (1,2-difluorobenzene), 126.22, 127.80, 137.22, 148.99 [Ar-C], 129.67 [CH$_3$$CCCH_3$], 131.37 [N$C$(H)N], 150.31, 150.46, 152.77, 152.90 (1,2-diflurobenzene), 161.56 [NC(=S)N]. Crystal data for **(5)$_2$·(1,2-difluorobenzene)$_8$**: $C_{276}H_{362}Cl_2F_{16}Ge_2N_{24}S_{18}$, fw= 5113.03, triclinic, P-1, a = 18.9013(12) Å, b = 22.8865(15) Å, c = 32.511(2) Å, α = 82.466(2)°, β = 86.258(2)°, γ = 88.632(2)°, V = 13911.0(15) Å^3, Z = 2, R1 = 0.0692 for 32495 data (I>2σ(I)), wR_2 = 0.1717(all data).

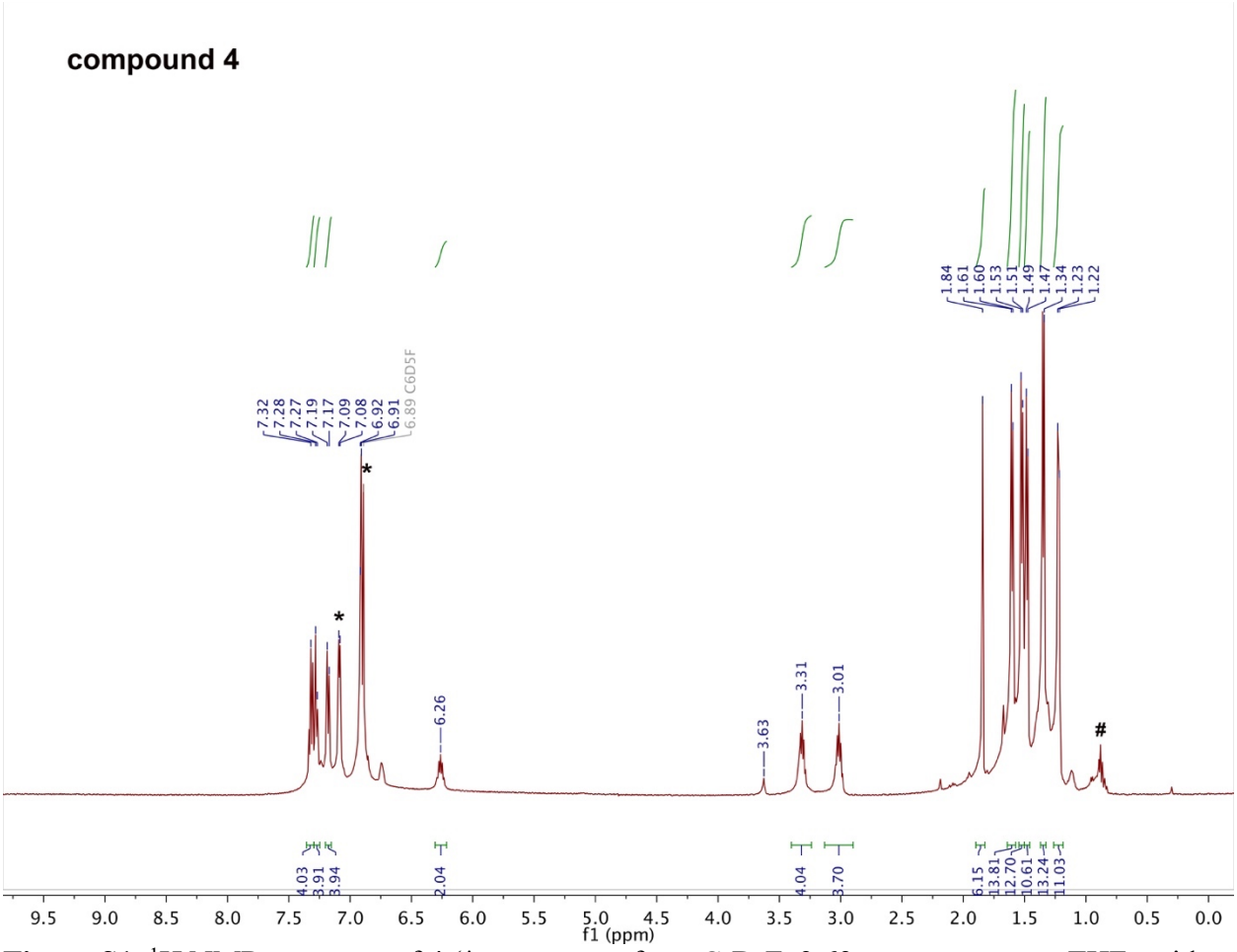

Figure S1. ^{1}H NMR spectrum of **4** (* resonances from C_6D_5F, 3.63 ppm resonance, THF residue, # resonances of hexane solvent that was used to rinse the crystals of **4**).

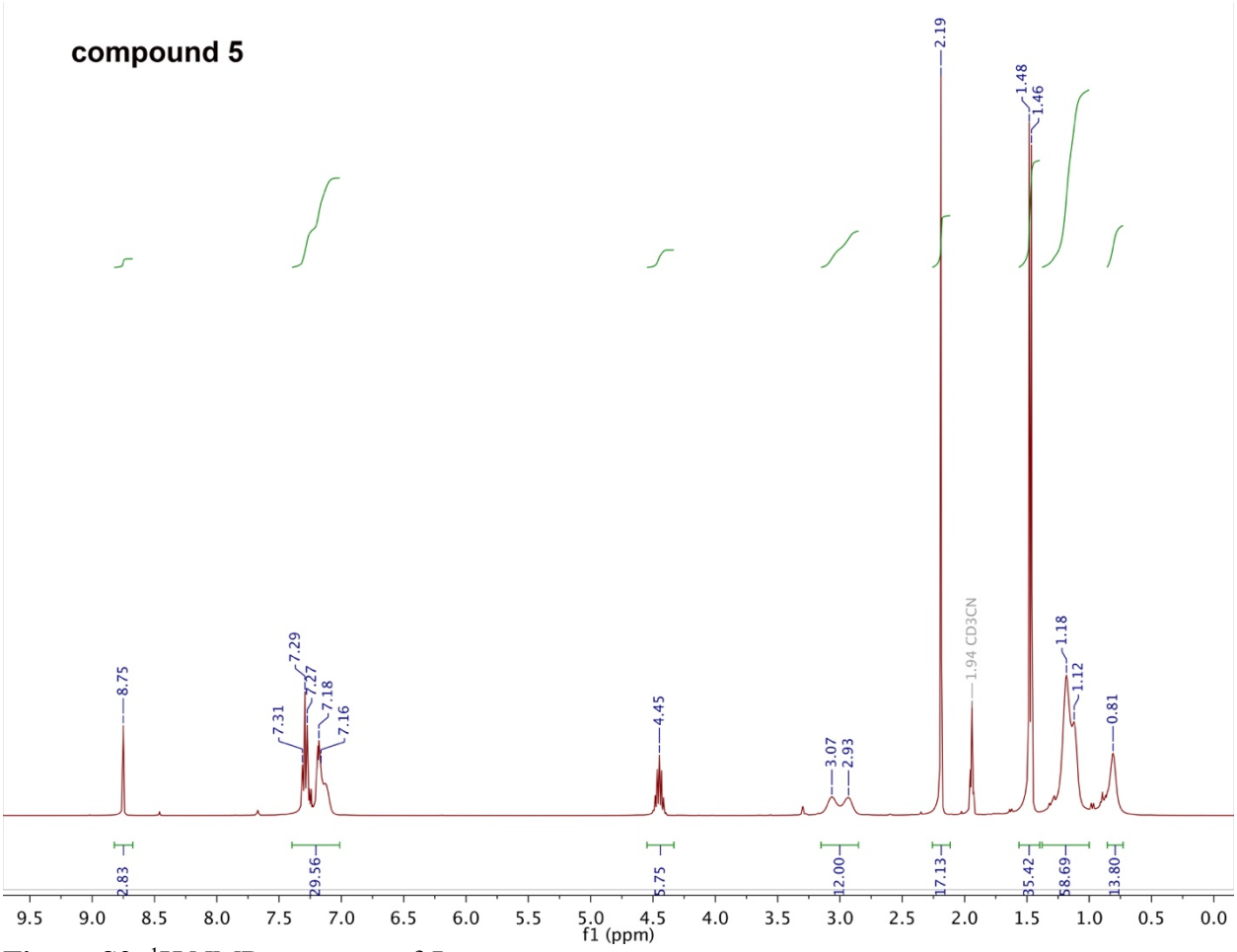

Figure S2. ^{1}H NMR spectrum of **5**.

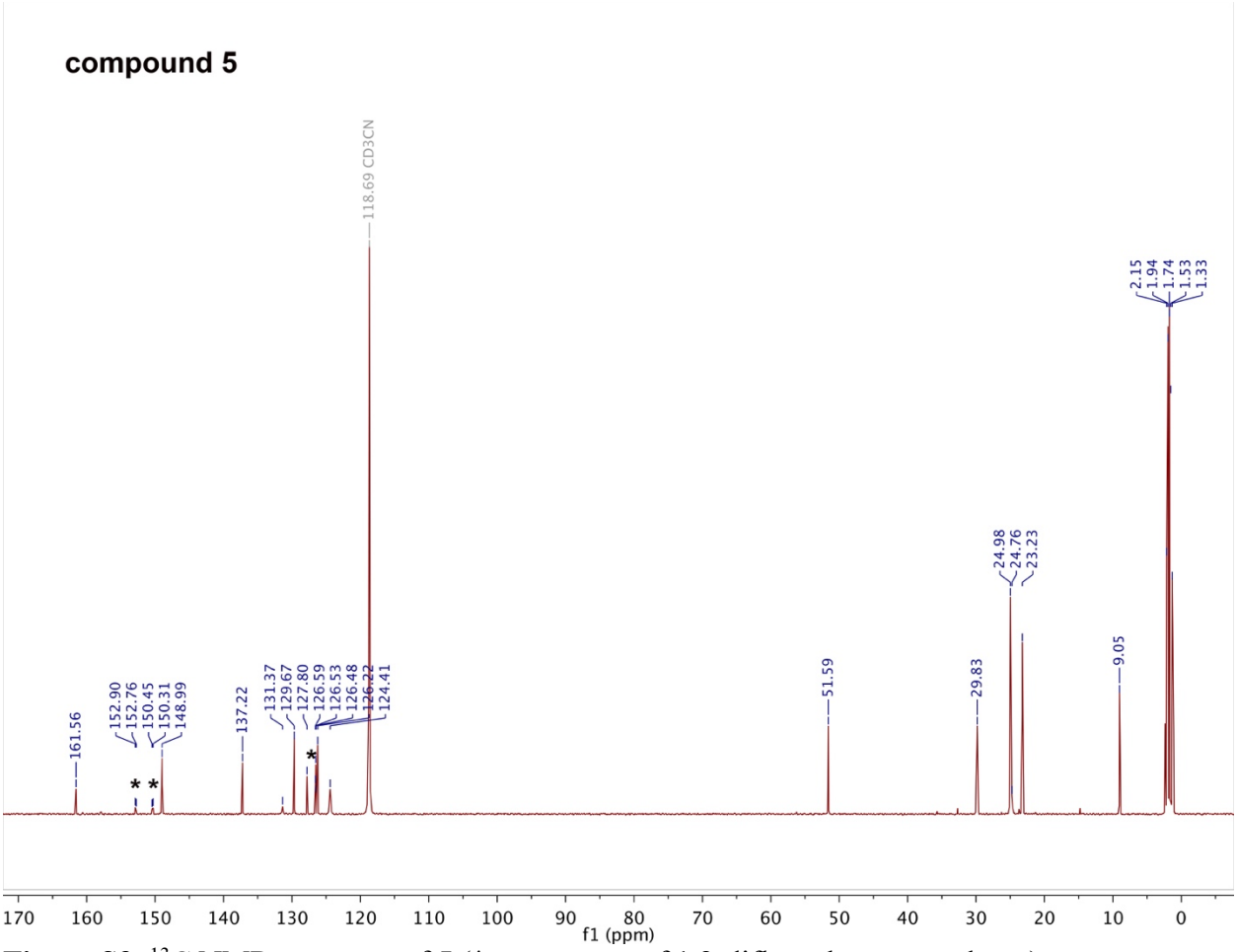

Figure S3. ^{13}C NMR spectrum of **5** (* resonances of 1,2-difluorobenzene solvent).

SUPPORTING INFORMATIONS of COMPUTATIONS

All computations employed the Gaussian09 programs:

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

Table S1. Coordinates of the B3LYP/6-311G** optimized geometry of **4-Me**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	-0.367511	0.000532	0.003942
2	16	0	4.336562	4.712802	-0.569561
3	16	0	0.907304	1.008408	1.698638
4	16	0	-0.535191	2.153050	-1.141934
5	16	0	4.354028	-4.703774	0.551929
6	16	0	0.921495	-0.994548	-1.688864
7	16	0	-0.527638	-2.151317	1.145131
8	7	0	2.789161	2.882515	0.791204
9	7	0	1.885513	3.604207	-1.068911
10	7	0	2.809542	-2.868977	-0.770258
11	7	0	1.882354	-3.603461	1.073028
12	7	0	-3.254009	-0.711774	-0.831051
13	7	0	-3.262586	0.701347	0.821002
14	6	0	3.007468	3.719412	-0.281412
15	6	0	1.522868	2.311929	0.695285
16	6	0	0.958328	2.757025	-0.466070
17	6	0	3.014224	-3.715492	0.294536
18	6	0	1.539633	-2.299659	-0.689191
19	6	0	0.966832	-2.749535	0.466019
20	6	0	-2.455338	-0.003386	-0.002399
21	6	0	-4.591538	-0.449834	-0.530874
22	6	0	-4.596935	0.433253	0.512204
23	6	0	-5.778768	1.034094	1.203249
24	6	0	-5.766114	-1.056018	-1.229585
25	1	0	-6.681355	0.491152	0.924770
26	1	0	-5.923513	2.081888	0.928509
27	1	0	-5.693102	0.980708	2.288800
28	1	0	-5.673508	-1.002458	-2.314556
29	1	0	-6.672911	-0.517018	-0.957192
30	1	0	-5.908053	-2.104390	-0.955580
31	6	0	-2.748617	1.579817	1.912781

32	1	0	-1.675128	1.616456	1.740438
33	6	0	-2.728980	-1.588082	-1.919299
34	1	0	-1.656498	-1.620004	-1.739982
35	6	0	-3.259956	3.016599	1.797893
36	1	0	-3.125256	3.394699	0.783049
37	1	0	-4.305941	3.122054	2.088118
38	1	0	-2.668023	3.645027	2.466990
39	6	0	-2.964863	0.946640	3.289909
40	1	0	-4.017359	0.908417	3.577417
41	1	0	-2.557199	-0.065810	3.322807
42	1	0	-2.437894	1.543299	4.037764
43	6	0	-2.938894	-0.956071	-3.297928
44	1	0	-2.535253	0.058059	-3.328294
45	1	0	-2.404489	-1.550587	-4.042198
46	1	0	-3.989649	-0.922361	-3.592289
47	6	0	-3.234700	-3.027106	-1.807548
48	1	0	-3.105053	-3.404440	-0.791756
49	1	0	-4.278271	-3.137223	-2.104638
50	1	0	-2.635607	-3.652982	-2.472650
51	6	0	3.757843	-2.703030	-1.860092
52	1	0	4.765198	-2.680946	-1.447860
53	1	0	3.689296	-3.536348	-2.564548
54	1	0	3.542291	-1.765631	-2.371099
55	6	0	1.663281	-4.317355	2.318862
56	1	0	2.580022	-4.855786	2.550900
57	1	0	1.429856	-3.609987	3.116469
58	1	0	0.839250	-5.027435	2.212938
59	6	0	1.697820	4.342854	-2.306421
60	1	0	0.832118	3.931740	-2.822961
61	1	0	1.543003	5.404618	-2.099618
62	1	0	2.588176	4.239750	-2.925999
63	6	0	3.726987	2.675168	1.881788
64	1	0	3.983758	1.617032	1.960780
65	1	0	4.618402	3.258095	1.658404
66	1	0	3.294766	3.015105	2.826163

Table S2. Coordinates of the B3LYP/6-311G** optimized geometry of **Δ-[5-Me]$^{2-}$**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	0.000057	-0.000111	0.509333
2	16	0	-5.127810	-4.376737	-0.876809
3	16	0	-1.386221	-1.457838	1.992204
4	16	0	-2.066322	0.252601	-0.920859
5	16	0	6.354565	-2.251553	-0.876739
6	16	0	1.955497	-0.471956	1.992399
7	16	0	0.814642	-1.915958	-0.920826
8	16	0	-1.227182	6.628821	-0.876609
9	16	0	-0.569209	1.929179	1.992397
10	16	0	1.252155	1.663312	-0.920591
11	7	0	-3.293524	-3.080327	0.736341
12	7	0	-3.709136	-2.012866	-1.112154
13	7	0	4.314491	-1.311813	0.736483
14	7	0	3.598055	-2.205405	-1.112129
15	7	0	-1.021196	4.392122	0.736536
16	7	0	0.111122	4.218538	-1.111943
17	6	0	-4.019156	-3.151252	-0.420064
18	6	0	-2.579141	-1.874769	0.797913
19	6	0	-2.839922	-1.203029	-0.366850
20	6	0	4.738863	-1.904547	-0.419985
21	6	0	2.913249	-1.296250	0.798059
22	6	0	2.462027	-1.857911	-0.366788
23	6	0	-0.719919	5.056052	-0.419868
24	6	0	-0.334065	3.170825	0.798147
25	6	0	0.378106	3.060935	-0.366613
26	6	0	0.675917	4.498726	-2.415901
27	1	0	1.759780	4.629030	-2.343559
28	1	0	0.469124	3.664681	-3.089052
29	1	0	0.218858	5.414934	-2.785103
30	6	0	-1.902672	4.887927	1.772913
31	1	0	-2.409794	5.769314	1.384832

32	1	0	-2.621462	4.109985	2.035908
33	1	0	-1.332762	5.157811	2.667599
34	6	0	-4.234125	-1.663736	-2.416108
35	1	0	-4.888692	-0.790077	-2.343773
36	1	0	-3.408381	-1.426014	-3.089282
37	1	0	-4.799264	-2.517540	-2.785281
38	6	0	-3.282328	-4.091600	1.772729
39	1	0	-3.792672	-4.971208	1.384832
40	1	0	-2.249252	-4.325682	2.035379
41	1	0	-3.800496	-3.732678	2.667586
42	6	0	3.558348	-2.834489	-2.416154
43	1	0	3.129512	-3.838409	-2.343898
44	1	0	2.939237	-2.238444	-3.089172
45	1	0	4.580319	-2.896488	-2.785452
46	6	0	5.184574	-0.796447	1.772942
47	1	0	6.201446	-0.797874	1.384877
48	1	0	4.870210	0.214968	2.036067
49	1	0	5.133354	-1.425067	2.667544

SUPPORTING INFORMATIONS of X-RAY

Compound **4**

Table S3. Sample and crystal data for **4**.

Identification code	**4**	
Chemical formula	$C_{71}H_{92}F_2GeN_6S_6$	
Formula weight	1332.45 g/mol	
Temperature	135(2) K	
Wavelength	0.71073 Å	
Crystal size	0.130 x 0.250 x 0.290 mm	
Crystal system	monoclinic	
Space group	$P2_1/n$ (No. 14)	
Unit cell dimensions	a = 13.8170(10) Å	α = 90°
	b = 27.779(2) Å	β = 107.003(2)°
	c = 19.3544(13) Å	γ = 90°
Volume	7103.9(9) $Å^3$	
Z	4	
Density (calculated)	1.246 g/cm^3	
Absorption coefficient	0.657 mm^{-1}	
F(000)	2824	

Table S4. Data collection and structure refinement for **4**.

Theta range for data collection	1.77 to 31.00°
Index ranges	-20<=h<=20, -40<=k<=40, -28<=l<=28
Reflections collected	289193
Independent reflections	22607 [R(int) = 0.0768]
Max. and min. transmission	0.7463 and 0.6874
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	22607 / 0 / 765
Goodness-of-fit on F^2	1.043
Δ/σ_{max}	0.002
Final R indices	17647 data; I>2σ(I) R1 = 0.0400, wR2 = 0.0812
	all data R1 = 0.0622, wR2 = 0.0886
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0323P)^2+4.8862P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.526 and -0.452 eÅ^{-3}
R.M.S. deviation from mean	0.069 eÅ^{-3}

Table S5. Bond lengths (Å) for **4**.

Ge1-C55	2.0101(14)	Ge1-S5	2.2610(4)
Ge1-S3	2.2667(4)	Ge1-S2	2.4052(4)
Ge1-S6	2.4136(4)	S1-C1	1.6684(16)
S2-C2	1.7269(15)	S3-C3	1.7459(15)
S4-C28	1.6771(15)	S5-C29	1.7430(15)
S6-C30	1.7263(14)	N1-C1	1.3706(19)
N1-C2	1.3955(19)	N1-C16	1.4405(19)
N2-C1	1.371(2)	N2-C3	1.3951(19)
N2-C4	1.4416(19)	N3-C28	1.3668(19)
N3-C29	1.3975(18)	N3-C43	1.4388(19)
N4-C28	1.3698(18)	N4-C30	1.4000(18)
N4-C31	1.4355(19)	C2-C3	1.350(2)
C4-C9	1.398(2)	C4-C5	1.397(2)
C5-C6	1.397(2)	C5-C13	1.515(2)
C6-C7	1.376(3)	C7-C8	1.381(3)
C8-C9	1.393(2)	C9-C10	1.517(2)
C10-C12	1.519(3)	C10-C11	1.526(3)
C13-C15	1.529(3)	C13-C14	1.526(3)
C16-C17	1.394(2)	C16-C21	1.403(2)
C17-C18	1.395(2)	C17-C25	1.515(2)
C18-C19	1.376(3)	C19-C20	1.384(3)
C20-C21	1.394(2)	C21-C22	1.519(2)
C22-C23	1.530(2)	C22-C24	1.527(2)
C25-C27	1.529(3)	C25-C26	1.529(3)
C29-C30	1.349(2)	C31-C32	1.396(2)

C31-C36	1.396(2)	C32-C33	1.398(2)
C32-C40	1.516(2)	C33-C34	1.381(3)
C34-C35	1.376(3)	C35-C36	1.394(2)
C36-C37	1.514(2)	C37-C39	1.517(3)
C37-C38	1.517(3)	C40-C42	1.523(2)
C40-C41	1.524(2)	C43-C48	1.402(2)
C43-C44	1.396(2)	C44-C45	1.400(2)
C44-C52	1.517(2)	C45-C46	1.377(3)
C46-C47	1.378(3)	C47-C48	1.394(2)
C48-C49	1.519(2)	C49-C51	1.527(2)
C49-C50	1.532(2)	C52-C53	1.524(3)
C52-C54	1.524(3)	N5-C55	1.3456(18)
N5-C56	1.3900(19)	N5-C63	1.4836(19)
N6-C55	1.3464(19)	N6-C57	1.3910(18)
N6-C58	1.4894(19)	C56-C57	1.358(2)
C56-C62	1.493(2)	C57-C61	1.490(2)
C58-C60	1.518(2)	C58-C59	1.522(2)
C63-C65	1.516(2)	C63-C64	1.523(2)
F1-C66	1.3192(18)	F2-C67	1.3217(17)
C66-C67	1.39	C66-C71	1.39
C67-C68	1.39	C68-C69	1.39
C69-C70	1.39	C70-C71	1.39

Table S6. Bond angles (°) for **4**.

C55-Ge1-S5	121.80(4)	C55-Ge1-S3	122.13(4)
S5-Ge1-S3	116.070(16)	C55-Ge1-S2	87.52(4)
S5-Ge1-S2	88.212(15)	S3-Ge1-S2	94.586(14)
C55-Ge1-S6	87.52(4)	S5-Ge1-S6	94.173(14)
S3-Ge1-S6	88.291(15)	S2-Ge1-S6	175.027(14)
C2-S2-Ge1	93.64(5)	C3-S3-Ge1	96.74(5)
C29-S5-Ge1	96.63(5)	C30-S6-Ge1	93.36(5)
C1-N1-C2	110.21(12)	C1-N1-C16	126.87(12)
C2-N1-C16	122.87(12)	C1-N2-C3	110.25(12)
C1-N2-C4	124.29(13)	C3-N2-C4	124.61(13)
C28-N3-C29	109.83(12)	C28-N3-C43	125.28(12)
C29-N3-C43	124.72(12)	C28-N4-C30	110.05(12)
C28-N4-C31	126.63(12)	C30-N4-C31	123.30(12)
N2-C1-N1	105.09(12)	N2-C1-S1	126.99(11)
N1-C1-S1	127.91(12)	C3-C2-N1	107.24(13)
C3-C2-S2	127.36(12)	N1-C2-S2	125.36(11)
C2-C3-N2	107.19(13)	C2-C3-S3	126.37(12)
N2-C3-S3	126.11(11)	C9-C4-C5	123.23(14)
C9-C4-N2	117.76(14)	C5-C4-N2	119.00(14)
C6-C5-C4	117.09(16)	C6-C5-C13	120.51(15)
C4-C5-C13	122.39(15)	C7-C6-C5	121.05(16)
C6-C7-C8	120.43(16)	C7-C8-C9	121.25(17)
C4-C9-C8	116.95(15)	C4-C9-C10	123.04(14)
C8-C9-C10	120.01(15)	C9-C10-C12	111.34(16)
C9-C10-C11	110.90(16)	C12-C10-C11	110.94(17)

C5-C13-C15	110.56(16)	C5-C13-C14	110.77(17)
C15-C13-C14	111.54(19)	C17-C16-C21	123.40(14)
C17-C16-N1	118.18(14)	C21-C16-N1	118.28(14)
C16-C17-C18	116.95(16)	C16-C17-C25	123.11(15)
C18-C17-C25	119.95(16)	C19-C18-C17	121.21(17)
C20-C19-C18	120.59(16)	C19-C20-C21	120.90(17)
C20-C21-C16	116.92(16)	C20-C21-C22	121.25(15)
C16-C21-C22	121.82(14)	C21-C22-C23	110.60(14)
C21-C22-C24	113.53(14)	C23-C22-C24	109.44(14)
C17-C25-C27	111.00(17)	C17-C25-C26	111.09(16)
C27-C25-C26	110.62(18)	N3-C28-N4	105.58(12)
N3-C28-S4	127.41(11)	N4-C28-S4	126.98(11)
C30-C29-N3	107.62(12)	C30-C29-S5	126.55(11)
N3-C29-S5	125.62(11)	C29-C30-N4	106.91(12)
C29-C30-S6	126.94(11)	N4-C30-S6	126.09(11)
C32-C31-C36	123.36(14)	C32-C31-N4	117.94(13)
C36-C31-N4	118.60(14)	C31-C32-C33	116.88(16)
C31-C32-C40	121.72(14)	C33-C32-C40	121.36(15)
C34-C33-C32	121.05(17)	C33-C34-C35	120.52(17)
C36-C35-C34	121.04(17)	C35-C36-C31	117.14(16)
C35-C36-C37	120.96(15)	C31-C36-C37	121.81(14)
C39-C37-C36	113.35(16)	C39-C37-C38	110.38(17)
C36-C37-C38	109.91(16)	C32-C40-C42	109.76(15)
C32-C40-C41	113.82(15)	C42-C40-C41	111.70(16)
C48-C43-C44	123.36(14)	C48-C43-N3	117.99(14)
C44-C43-N3	118.64(14)	C45-C44-C43	117.05(15)
C45-C44-C52	120.48(15)	C43-C44-C52	122.39(14)

C46-C45-C44	120.84(16)	C47-C46-C45	120.65(16)
C46-C47-C48	121.33(16)	C43-C48-C47	116.71(15)
C43-C48-C49	121.29(14)	C47-C48-C49	121.98(15)
C48-C49-C51	112.63(15)	C48-C49-C50	112.29(14)
C51-C49-C50	108.95(15)	C44-C52-C53	110.27(14)
C44-C52-C54	111.93(16)	C53-C52-C54	111.58(18)
C55-N5-C56	109.50(12)	C55-N5-C63	123.33(12)
C56-N5-C63	126.75(12)	C55-N6-C57	109.44(12)
C55-N6-C58	123.47(12)	C57-N6-C58	126.94(12)
N5-C55-N6	107.22(12)	N5-C55-Ge1	125.20(11)
N6-C55-Ge1	127.59(11)	C57-C56-N5	106.93(13)
C57-C56-C62	128.45(14)	N5-C56-C62	124.61(14)
C56-C57-N6	106.91(13)	C56-C57-C61	127.96(14)
N6-C57-C61	125.07(14)	N6-C58-C60	110.53(13)
N6-C58-C59	111.88(13)	C60-C58-C59	113.71(14)
N5-C63-C65	109.68(13)	N5-C63-C64	112.37(13)
C65-C63-C64	115.09(14)	F1-C66-C67	118.88(12)
F1-C66-C71	121.12(12)	C67-C66-C71	120.0
F2-C67-C68	121.10(12)	F2-C67-C66	118.89(12)
C68-C67-C66	120.0	C67-C68-C69	120.0
C68-C69-C70	120.0	C71-C70-C69	120.0
C70-C71-C66	120.0		

Compound **5**

Table S7. Sample and crystal data for **5**.

Identification code	**5**	
Chemical formula	$C_{276}H_{362}Cl_2F_{16}Ge_2N_{24}S_{18}$	
Formula weight	5113.03 g/mol	
Temperature	135(2) K	
Wavelength	0.71073 Å	
Crystal size	0.130 x 0.200 x 0.290 mm	
Crystal system	triclinic	
Space group	P-1(No. 2)	
Unit cell dimensions	a = 18.9013(12) Å	α = 82.466(2)°
	b = 22.8865(15) Å	β = 86.258(2)°
	c = 32.511(2) Å	γ = 88.632(2)°
Volume	13911.0(15) $Å^3$	
Z	2	
Density (calculated)	1.221 g/cm^3	
Absorption coefficient	0.437 mm^{-1}	
F(000)	5432	

Table S8. Data collection and structure refinement for **5**.

Theta range for data collection	1.75 to 26.02°
Index ranges	-23<=h<=23, -28<=k<=28, -40<=l<=40
Reflections collected	357769
Independent reflections	54763 [R(int) = 0.1404]
Coverage of independent reflections	99.9%
Absorption correction	Multi-Scan
Max. and min. transmission	0.7454 and 0.6971
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	54763 / 956 / 3152
Goodness-of-fit on F^2	1.004
Δ/σ_{max}	0.005
Final R indices	32495 data; I>2σ(I) R1 = 0.0692, wR2 = 0.1415
	all data R1 = 0.1413, wR2 = 0.1717
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0658P)^2+26.1833P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.818 and -1.136 eÅ^{-3}
R.M.S. deviation from mean	0.081 eÅ^{-3}

Table S9. Bond lengths (Å) for **5**.

Ge1-S6	2.4156(11)	Ge1-S2	2.4161(11)
Ge1-S9	2.4174(11)	Ge1-S5	2.4263(11)
Ge1-S3	2.4286(11)	Ge1-S8	2.4310(11)
Ge2-S15	2.3887(10)	Ge2-S12	2.4102(10)
Ge2-S17	2.4306(11)	Ge2-S18	2.4331(11)
Ge2-S11	2.4375(11)	Ge2-S14	2.4381(11)
S1-C1	1.681(4)	S2-C2	1.719(4)
S3-C3	1.721(4)	S4-C28	1.686(4)
S5-C29	1.723(4)	S6-C30	1.716(4)
S7-C55	1.686(4)	S8-C56	1.731(4)
S9-C57	1.714(4)	S13-C204	1.680(4)
S15-C206	1.712(4)	S14-C205	1.726(4)
S16-C207	1.682(4)	S18-C209	1.714(4)
S17-C208	1.723(4)	S10-C201	1.684(4)
S12-C203	1.724(4)	S11-C202	1.718(4)
N1-C1	1.360(5)	N1-C2	1.409(5)
N1-C16	1.441(5)	N2-C1	1.368(5)
N2-C3	1.404(5)	N2-C4	1.447(5)
N3-C28	1.366(5)	N3-C29	1.403(5)
N3-C43	1.439(5)	N4-C28	1.360(5)
N4-C30	1.403(5)	N4-C31	1.431(5)
N5-C55	1.350(5)	N5-C56	1.408(5)
N5-C70	1.438(5)	N6-C55	1.368(5)
N6-C57	1.401(5)	N6-C58	1.431(5)
N16-C204	1.365(5)	N16-C206	1.394(5)
N16-C16A	1.434(5)	N15-C204	1.368(5)

N15-C205	1.405(5)	N15-C4A	1.436(5)
N18-C207	1.363(5)	N18-C209	1.406(5)
N18-C43A	1.440(5)	N17-C207	1.367(5)
N17-C31A	1.431(5)	N17-C208	1.410(5)
N14-C201	1.362(5)	N14-C203	1.400(5)
N14-C70A	1.441(5)	N13-C201	1.358(5)
N13-C202	1.406(5)	N13-C58A	1.440(5)
C2-C3	1.352(5)	C4-C5	1.388(6)
C4-C9	1.402(6)	C5-C6	1.405(6)
C5-C13	1.507(6)	C6-C7	1.365(7)
C7-C8	1.378(7)	C8-C9	1.403(6)
C9-C10	1.509(6)	C10-C12	1.529(7)
C10-C11	1.513(6)	C13-C14	1.533(6)
C13-C15	1.528(7)	C16-C17	1.386(6)
C16-C21	1.401(6)	C17-C18	1.393(6)
C17-C25	1.514(6)	C18-C19	1.375(6)
C19-C20	1.371(6)	C20-C21	1.391(6)
C21-C22	1.511(6)	C22-C23	1.509(6)
C22-C24	1.514(7)	C25-C26	1.520(6)
C25-C27	1.519(7)	C29-C30	1.353(5)
C31-C36	1.392(6)	C31-C32	1.405(6)
C32-C33	1.387(6)	C32-C40	1.513(6)
C33-C34	1.373(7)	C34-C35	1.371(7)
C35-C36	1.394(6)	C36-C37	1.521(6)
C37-C39	1.518(6)	C37-C38	1.520(6)
C40-C41	1.520(6)	C40-C42	1.524(6)
C43-C44	1.396(6)	C43-C48	1.391(6)

C44-C45	1.393(6)	C44-C52	1.519(6)
C45-C46	1.371(6)	C46-C47	1.373(6)
C47-C48	1.392(6)	C48-C49	1.518(6)
C49-C50	1.518(6)	C49-C51	1.521(7)
C52-C53	1.527(7)	C52-C54	1.530(6)
C56-C57	1.349(5)	C58-C63	1.398(6)
C58-C59	1.402(6)	C59-C60	1.402(6)
C59-C67	1.500(6)	C60-C61	1.371(7)
C61-C62	1.383(8)	C62-C63	1.397(7)
C63-C64	1.511(7)	C64-C66	1.520(7)
C64-C65	1.533(7)	C67-C69	1.513(7)
C67-C68	1.517(7)	C70-C75	1.394(6)
C70-C71	1.389(5)	C71-C72	1.395(6)
C71-C79	1.523(6)	C72-C73	1.379(6)
C73-C74	1.372(6)	C74-C75	1.387(6)
C75-C76	1.526(6)	C76-C78	1.520(7)
C76-C77	1.515(8)	C79-C81	1.536(6)
C79-C80	1.517(6)	C206-C205	1.353(5)
C4A-C5A	1.392(6)	C4A-C9A	1.392(6)
C5A-C6A	1.394(6)	C5A-C13A	1.516(6)
C6A-C7A	1.368(7)	C7A-C8A	1.371(7)
C8A-C9A	1.384(6)	C9A-C10A	1.520(7)
C10A-C11A	1.518(7)	C10A-C12A	1.517(7)
C13A-C15A	1.498(7)	C13A-C14A	1.522(7)
C16A-C21A	1.396(6)	C16A-C17A	1.397(6)
C17A-C18A	1.389(6)	C17A-C25A	1.516(6)
C18A-C19A	1.383(6)	C19A-C20A	1.375(7)

C20A-C21A	1.395(6)	C21A-C22A	1.509(6)
C22A-C23A	1.514(7)	C22A-C24A	1.524(8)
C25A-C27A	1.523(7)	C25A-C26A	1.521(6)
C209-C208	1.350(5)	C31A-C36A	1.394(6)
C31A-C32A	1.391(6)	C32A-C33A	1.400(6)
C32A-C40A	1.515(6)	C33A-C34A	1.375(7)
C34A-C35A	1.367(7)	C35A-C36A	1.402(6)
C36A-C37A	1.512(6)	C37A-C39A	1.521(7)
C37A-C38A	1.513(7)	C40A-C41A	1.517(6)
C40A-C42A	1.541(6)	C43A-C48A	1.392(6)
C43A-C44A	1.397(6)	C44A-C45A	1.404(6)
C44A-C52A	1.507(7)	C45A-C46A	1.373(7)
C46A-C47A	1.367(7)	C47A-C48A	1.403(6)
C48A-C49A	1.514(6)	C49A-C50A	1.515(6)
C49A-C51A	1.516(7)	C52A-C53A	1.508(7)
C52A-C54A	1.537(7)	C203-C202	1.345(5)
C58A-C63A	1.395(6)	C58A-C59A	1.390(6)
C59A-C60A	1.384(6)	C59A-C67A	1.523(6)
C60A-C61A	1.383(6)	C61A-C62A	1.377(6)
C62A-C63A	1.393(6)	C63A-C64A	1.514(6)
C64A-C65A	1.523(6)	C64A-C66A	1.524(7)
C67A-C68A	1.530(6)	C67A-C69A	1.516(7)
C70A-C75A	1.393(6)	C70A-C71A	1.394(6)
C71A-C72A	1.396(6)	C71A-C79A	1.519(7)
C72A-C73A	1.377(7)	C73A-C74A	1.358(8)
C74A-C75A	1.400(7)	C75A-C76A	1.505(7)
C76A-C77A	1.522(7)	C76A-C78A	1.513(7)

C79A-C81A	1.511(7)	C79A-C80A	1.536(6)
N7-C82	1.329(5)	N7-C83	1.385(5)
N7-C90	1.489(5)	N8-C82	1.327(5)
N8-C84	1.384(5)	N8-C85	1.492(5)
C82-H82	0.958(18)	C83-C84	1.354(6)
C83-C89	1.491(6)	C84-C88	1.485(6)
C85-C87	1.512(6)	C85-C86	1.511(6)
C90-C91	1.495(7)	C90-C92	1.506(7)
N9-C93	1.330(6)	N9-C94	1.379(5)
N9-C01	1.494(6)	N10-C93	1.327(6)
N10-C95	1.382(5)	N10-C96	1.484(5)
C93-H93	0.950(19)	C94-C95	1.352(6)
C94-C00	1.482(6)	C95-C99	1.474(6)
C96-C97	1.509(6)	C96-C98	1.505(6)
C01-C03	1.481(8)	C01-C02	1.508(8)
N11-C04	1.322(6)	N11-C05	1.381(6)
N11-C012	1.480(7)	N12-C04	1.326(6)
N12-C06	1.371(6)	N12-C07	1.491(6)
C04-H04	0.955(19)	C05-C06	1.361(7)
C05-C011	1.479(7)	C06-C010	1.496(7)
C07-C08	1.500(7)	C07-C09	1.499(7)
C012-C013	1.489(11)	C012-C014	1.536(11)
N19-C210	1.324(5)	N19-C83A	1.383(5)
N19-C90A	1.489(5)	N20-C210	1.331(5)
N20-C84A	1.384(5)	N20-C85A	1.488(5)
C210-H210	0.967(18)	C83A-C84A	1.355(6)
C83A-C89A	1.496(6)	C84A-C88A	1.484(6)

C85A-C87A	1.506(6)	C85A-C86A	1.519(7)
C90A-C92A	1.489(7)	C90A-C91A	1.509(7)
N21-C211	1.331(6)	N21-C94A	1.394(5)
N21-C01A	1.475(5)	N22-C211	1.333(6)
N22-C95A	1.371(6)	N22-C96A	1.495(6)
C211-H211	0.973(19)	C94A-C95A	1.352(6)
C94A-C0A	1.478(6)	C95A-C99A	1.490(6)
C96A-C98A	1.482(8)	C96A-C97A	1.479(8)
C01A-C03A	1.512(6)	C01A-C02A	1.511(6)
N23-C212	1.330(6)	N23-C05A	1.388(6)
N23-C01D	1.490(6)	N24-C212	1.328(6)
N24-C06A	1.390(6)	N24-C07A	1.475(6)
C212-H212	0.966(19)	C05A-C06A	1.344(7)
C05A-C01C	1.494(7)	C06A-C01B	1.494(7)
C07A-C08A	1.501(7)	C07A-C09A	1.521(7)
C01D-C01F	1.509(7)	C01D-C01E	1.497(7)
F1-C02B	1.358(6)	F2-C02G	1.334(6)
C02B-C02C	1.357(9)	C02B-C02G	1.350(8)
C02C-C02D	1.402(9)	C02D-C02E	1.360(8)
C02E-C02F	1.342(8)	C02F-C02G	1.345(7)
F3-C03B	1.348(6)	F4-C03G	1.347(5)
C03B-C03G	1.359(8)	C03B-C03C	1.355(7)
C03C-C03D	1.373(7)	C03D-C03E	1.349(8)
C03E-C03F	1.379(8)	C03F-C03G	1.372(8)
F5-C04B	1.334(14)	F6-C04G	1.322(13)
C04B-C04C	1.39	C04B-C04G	1.39
C04C-C04D	1.39	C04D-C04E	1.39

C04E-C04F	1.39	C04F-C04G	1.39
F7-C05B	1.331(10)	F8-C05G	1.336(11)
C05B-C05C	1.370(15)	C05B-C05G	1.380(14)
C05C-C05D	1.377(14)	C05D-C05E	1.370(13)
C05E-C05F	1.382(13)	C05F-C05G	1.317(15)
F7'-C05H	1.318(17)	F8'-C05M	1.335(18)
C05H-C05I	1.37(2)	C05H-C05M	1.38(2)
C05I-C05J	1.39(2)	C05J-C05K	1.37(2)
C05K-C05L	1.38(2)	C05L-C05M	1.31(2)
F9-C06B	1.337(12)	F10-C06G	1.316(14)
C06B-C06C	1.401(16)	C06B-C06G	1.331(17)
C06C-C06D	1.388(14)	C06D-C06E	1.356(13)
C06E-C06F	1.293(16)	C06F-C06G	1.47(2)
F9'-C06H	1.332(13)	F10'-C06M	1.311(15)
C06H-C06M	1.324(19)	C06H-C06I	1.373(19)
C06I-C06J	1.397(18)	C06J-C06K	1.369(17)
C06K-C06L	1.316(17)	C06L-C06M	1.46(2)
F11-C07B	1.413(14)	F12-C07G	1.330(12)
C07B-C07C	1.39	C07B-C07G	1.39
C07C-C07D	1.39	C07D-C07E	1.39
C07E-C07F	1.39	C07F-C07G	1.39
F11'-C07H	1.406(10)	F11'-C07M	2.602(15)
F12'-C07M	1.389(10)	C07H-C07I	1.39
C07H-C07M	1.39	C07I-C07J	1.39
C07J-C07K	1.39	C07K-C07L	1.39
C07L-C07M	1.39	F13-C08B	1.568(14)
F14-C08G	1.455(13)	C08B-C08C	1.39

C08B-C08G	1.39	C08C-C08D	1.39
C08D-C08E	1.39	C08E-C08F	1.39
C08F-C08G	1.39	F15-C09B	1.380(13)
F16-C09G	1.482(14)	C09B-C09C	1.39
C09B-C09G	1.39	C09C-C09D	1.39
C09D-C09E	1.39	C09E-C09F	1.39
C09F-C09G	1.39		

Table S10. Bond angles (°) for **5**.

S6-Ge1-S2	88.30(4)	S6-Ge1-S9	87.37(4)
S2-Ge1-S9	87.20(4)	S6-Ge1-S5	88.51(4)
S2-Ge1-S5	94.63(4)	S9-Ge1-S5	175.44(4)
S6-Ge1-S3	176.49(4)	S2-Ge1-S3	89.07(4)
S9-Ge1-S3	94.83(4)	S5-Ge1-S3	89.39(4)
S6-Ge1-S8	95.57(4)	S2-Ge1-S8	173.99(4)
S9-Ge1-S8	88.39(4)	S5-Ge1-S8	90.06(4)
S3-Ge1-S8	87.23(4)	S15-Ge2-S12	175.26(4)
S15-Ge2-S17	96.94(4)	S12-Ge2-S17	87.54(4)
S15-Ge2-S18	86.91(4)	S12-Ge2-S18	94.90(4)
S17-Ge2-S18	87.21(4)	S15-Ge2-S11	87.67(4)
S12-Ge2-S11	88.03(3)	S17-Ge2-S11	172.82(4)
S18-Ge2-S11	87.55(4)	S15-Ge2-S14	88.86(4)
S12-Ge2-S14	89.62(4)	S17-Ge2-S14	89.49(4)
S18-Ge2-S14	174.28(4)	S11-Ge2-S14	96.12(4)
C2-S2-Ge1	94.07(13)	C3-S3-Ge1	93.74(13)
C29-S5-Ge1	93.70(13)	C30-S6-Ge1	94.44(13)
C56-S8-Ge1	92.46(13)	C57-S9-Ge1	93.45(14)
C206-S15-Ge2	94.95(13)	C205-S14-Ge2	93.74(13)
C209-S18-Ge2	92.91(13)	C208-S17-Ge2	92.44(13)
C203-S12-Ge2	93.87(13)	C202-S11-Ge2	94.55(13)
C1-N1-C2	110.7(3)	C1-N1-C16	125.8(3)
C2-N1-C16	123.4(3)	C1-N2-C3	110.2(3)
C1-N2-C4	123.7(3)	C3-N2-C4	126.0(3)
C28-N3-C29	110.1(3)	C28-N3-C43	123.4(3)

C29-N3-C43	126.3(3)	C28-N4-C30	110.4(3)
C28-N4-C31	124.3(3)	C30-N4-C31	125.0(3)
C55-N5-C56	110.4(3)	C55-N5-C70	124.3(3)
C56-N5-C70	125.2(3)	C55-N6-C57	110.2(3)
C55-N6-C58	126.5(3)	C57-N6-C58	122.8(3)
C204-N16-C206	110.6(3)	C204-N16-C16A	127.4(3)
C206-N16-C16A	121.9(3)	C204-N15-C205	110.5(3)
C204-N15-C4A	124.0(3)	C205-N15-C4A	125.5(3)
C207-N18-C209	110.0(3)	C207-N18-C43A	124.5(3)
C209-N18-C43A	123.3(3)	C207-N17-C31A	125.3(3)
C207-N17-C208	109.6(3)	C31A-N17-C208	124.6(3)
C201-N14-C203	110.1(3)	C201-N14-C70A	124.6(3)
C203-N14-C70A	125.2(3)	C201-N13-C202	110.5(3)
C201-N13-C58A	125.1(3)	C202-N13-C58A	124.3(3)
N2-C1-N1	105.3(3)	N2-C1-S1	128.4(3)
N1-C1-S1	126.4(3)	C3-C2-N1	106.5(3)
C3-C2-S2	127.2(3)	N1-C2-S2	125.3(3)
C2-C3-N2	107.3(3)	C2-C3-S3	125.7(3)
N2-C3-S3	126.7(3)	C5-C4-C9	123.5(4)
C5-C4-N2	118.5(4)	C9-C4-N2	118.0(4)
C4-C5-C6	116.6(4)	C4-C5-C13	123.9(4)
C6-C5-C13	119.4(4)	C7-C6-C5	121.5(4)
C6-C7-C8	120.7(4)	C7-C8-C9	120.8(4)
C4-C9-C8	116.9(4)	C4-C9-C10	122.4(4)
C8-C9-C10	120.7(4)	C9-C10-C12	113.8(4)
C9-C10-C11	111.1(4)	C12-C10-C11	109.4(4)
C5-C13-C14	110.6(4)	C5-C13-C15	111.9(4)

C14-C13-C15	110.6(4)	C17-C16-C21	123.9(4)
C17-C16-N1	118.3(4)	C21-C16-N1	117.8(4)
C16-C17-C18	116.7(4)	C16-C17-C25	122.0(4)
C18-C17-C25	121.3(4)	C19-C18-C17	121.2(4)
C20-C19-C18	120.4(4)	C19-C20-C21	121.5(4)
C16-C21-C20	116.3(4)	C16-C21-C22	122.4(4)
C20-C21-C22	121.3(4)	C21-C22-C23	113.0(4)
C21-C22-C24	110.8(4)	C23-C22-C24	110.8(4)
C26-C25-C17	112.6(4)	C26-C25-C27	112.4(4)
C17-C25-C27	109.9(4)	N4-C28-N3	105.6(3)
N4-C28-S4	126.6(3)	N3-C28-S4	127.8(3)
C30-C29-N3	107.0(3)	C30-C29-S5	126.0(3)
N3-C29-S5	126.4(3)	C29-C30-N4	106.9(3)
C29-C30-S6	126.1(3)	N4-C30-S6	125.8(3)
C36-C31-C32	122.8(4)	C36-C31-N4	119.0(4)
C32-C31-N4	118.2(4)	C33-C32-C31	117.1(4)
C33-C32-C40	122.2(4)	C31-C32-C40	120.7(4)
C34-C33-C32	121.0(4)	C33-C34-C35	121.0(4)
C34-C35-C36	120.7(4)	C31-C36-C35	117.3(4)
C31-C36-C37	121.6(4)	C35-C36-C37	121.0(4)
C36-C37-C39	112.7(4)	C36-C37-C38	109.2(4)
C39-C37-C38	111.7(4)	C32-C40-C41	113.1(4)
C32-C40-C42	111.3(4)	C41-C40-C42	110.2(4)
C44-C43-C48	123.2(4)	C44-C43-N3	118.5(4)
C48-C43-N3	118.3(4)	C43-C44-C45	117.2(4)
C43-C44-C52	121.8(4)	C45-C44-C52	121.0(4)
C46-C45-C44	121.1(4)	C45-C46-C47	120.1(4)

C46-C47-C48	121.8(4)	C43-C48-C47	116.5(4)
C43-C48-C49	122.9(4)	C47-C48-C49	120.5(4)
C48-C49-C50	112.4(4)	C48-C49-C51	110.9(4)
C50-C49-C51	111.2(4)	C44-C52-C53	111.9(4)
C44-C52-C54	111.4(4)	C53-C52-C54	110.2(4)
N5-C55-N6	105.6(3)	N5-C55-S7	128.5(3)
N6-C55-S7	125.9(3)	C57-C56-N5	106.9(3)
C57-C56-S8	125.7(3)	N5-C56-S8	126.9(3)
C56-C57-N6	106.9(3)	C56-C57-S9	126.5(3)
N6-C57-S9	125.7(3)	C63-C58-C59	123.7(4)
C63-C58-N6	118.0(4)	C59-C58-N6	118.2(4)
C60-C59-C58	116.6(4)	C60-C59-C67	121.2(4)
C58-C59-C67	122.1(4)	C61-C60-C59	121.3(5)
C60-C61-C62	120.5(5)	C61-C62-C63	121.3(5)
C58-C63-C62	116.6(5)	C58-C63-C64	121.4(4)
C62-C63-C64	122.1(4)	C63-C64-C66	113.6(5)
C63-C64-C65	111.4(4)	C66-C64-C65	110.2(4)
C59-C67-C69	108.8(4)	C59-C67-C68	114.2(4)
C69-C67-C68	111.4(5)	C75-C70-C71	122.5(4)
C75-C70-N5	118.8(4)	C71-C70-N5	118.6(3)
C70-C71-C72	117.3(4)	C70-C71-C79	122.9(3)
C72-C71-C79	119.8(4)	C73-C72-C71	121.2(4)
C72-C73-C74	120.1(4)	C73-C74-C75	121.1(4)
C70-C75-C74	117.8(4)	C70-C75-C76	121.1(4)
C74-C75-C76	121.0(4)	C78-C76-C75	111.7(5)
C78-C76-C77	111.3(5)	C75-C76-C77	111.1(4)
C71-C79-C81	110.4(3)	C71-C79-C80	111.7(4)

C81-C79-C80	111.6(4)	N16-C204-N15	105.0(3)
N16-C204-S13	126.8(3)	N15-C204-S13	128.2(3)
C205-C206-N16	107.4(3)	C205-C206-S15	126.9(3)
N16-C206-S15	125.0(3)	C206-C205-N15	106.5(3)
C206-C205-S14	125.3(3)	N15-C205-S14	127.7(3)
C5A-C4A-C9A	123.2(4)	C5A-C4A-N15	118.3(4)
C9A-C4A-N15	118.6(4)	C4A-C5A-C6A	116.8(4)
C4A-C5A-C13A	122.0(4)	C6A-C5A-C13A	121.2(4)
C7A-C6A-C5A	120.8(5)	C6A-C7A-C8A	121.1(4)
C9A-C8A-C7A	120.7(5)	C4A-C9A-C8A	117.3(4)
C4A-C9A-C10A	122.0(4)	C8A-C9A-C10A	120.8(4)
C9A-C10A-C11A	111.9(4)	C9A-C10A-C12A	111.8(5)
C11A-C10A-C12A	110.8(5)	C15A-C13A-C5A	112.7(4)
C15A-C13A-C14A	110.6(4)	C5A-C13A-C14A	112.9(4)
C21A-C16A-C17A	123.0(4)	C21A-C16A-N16	118.2(4)
C17A-C16A-N16	118.3(4)	C16A-C17A-C18A	117.0(4)
C16A-C17A-C25A	122.5(4)	C18A-C17A-C25A	120.5(4)
C19A-C18A-C17A	121.3(4)	C20A-C19A-C18A	120.4(4)
C19A-C20A-C21A	120.8(4)	C16A-C21A-C20A	117.4(4)
C16A-C21A-C22A	121.6(4)	C20A-C21A-C22A	120.9(4)
C21A-C22A-C23A	112.6(4)	C21A-C22A-C24A	110.5(4)
C23A-C22A-C24A	110.5(5)	C17A-C25A-C27A	110.2(4)
C17A-C25A-C26A	112.2(4)	C27A-C25A-C26A	111.5(4)
N18-C207-N17	106.0(3)	N18-C207-S16	127.0(3)
N17-C207-S16	127.0(3)	C208-C209-N18	107.1(3)
C208-C209-S18	126.1(3)	N18-C209-S18	125.5(3)
C209-C208-N17	107.2(3)	C209-C208-S17	125.2(3)

N17-C208-S17	126.9(3)	C36A-C31A-C32A	122.4(4)
C36A-C31A-N17	118.0(4)	C32A-C31A-N17	119.6(4)
C31A-C32A-C33A	117.6(4)	C31A-C32A-C40A	122.5(4)
C33A-C32A-C40A	120.0(4)	C34A-C33A-C32A	120.9(4)
C33A-C34A-C35A	120.6(4)	C34A-C35A-C36A	120.9(4)
C31A-C36A-C35A	117.6(4)	C31A-C36A-C37A	122.8(4)
C35A-C36A-C37A	119.6(4)	C36A-C37A-C39A	110.5(4)
C36A-C37A-C38A	112.6(4)	C39A-C37A-C38A	111.5(4)
C32A-C40A-C41A	112.1(4)	C32A-C40A-C42A	110.9(4)
C41A-C40A-C42A	110.3(4)	C48A-C43A-C44A	123.6(4)
C48A-C43A-N18	116.7(4)	C44A-C43A-N18	119.7(4)
C43A-C44A-C45A	116.3(4)	C43A-C44A-C52A	122.7(4)
C45A-C44A-C52A	120.9(4)	C46A-C45A-C44A	121.5(5)
C47A-C46A-C45A	120.5(5)	C46A-C47A-C48A	121.3(5)
C43A-C48A-C47A	116.8(4)	C43A-C48A-C49A	123.0(4)
C47A-C48A-C49A	120.2(4)	C48A-C49A-C50A	111.2(4)
C48A-C49A-C51A	112.3(4)	C50A-C49A-C51A	111.4(4)
C44A-C52A-C53A	111.4(4)	C44A-C52A-C54A	110.9(4)
C53A-C52A-C54A	110.4(4)	N14-C201-N13	105.4(3)
N14-C201-S10	127.7(3)	N13-C201-S10	126.8(3)
C202-C203-N14	107.3(3)	C202-C203-S12	126.3(3)
N14-C203-S12	126.0(3)	C203-C202-N13	106.6(3)
C203-C202-S11	125.6(3)	N13-C202-S11	126.7(3)
C63A-C58A-C59A	123.2(4)	C63A-C58A-N13	118.2(4)
C59A-C58A-N13	118.6(4)	C58A-C59A-C60A	117.1(4)
C58A-C59A-C67A	122.5(4)	C60A-C59A-C67A	120.4(4)
C61A-C60A-C59A	121.7(4)	C60A-C61A-C62A	119.7(4)

C63A-C62A-C61A	121.2(4)	C58A-C63A-C62A	117.1(4)
C58A-C63A-C64A	121.9(4)	C62A-C63A-C64A	120.9(4)
C63A-C64A-C65A	112.4(4)	C63A-C64A-C66A	110.6(4)
C65A-C64A-C66A	111.1(4)	C59A-C67A-C68A	111.7(4)
C59A-C67A-C69A	111.1(4)	C68A-C67A-C69A	111.4(4)
C75A-C70A-C71A	123.2(4)	C75A-C70A-N14	118.5(4)
C71A-C70A-N14	118.2(4)	C70A-C71A-C72A	117.0(4)
C70A-C71A-C79A	122.3(4)	C72A-C71A-C79A	120.7(4)
C73A-C72A-C71A	120.8(5)	C72A-C73A-C74A	120.8(4)
C73A-C74A-C75A	121.4(5)	C70A-C75A-C74A	116.8(5)
C70A-C75A-C76A	122.3(4)	C74A-C75A-C76A	120.9(5)
C75A-C76A-C77A	112.6(4)	C75A-C76A-C78A	111.7(5)
C77A-C76A-C78A	110.4(5)	C71A-C79A-C81A	112.4(4)
C71A-C79A-C80A	113.0(4)	C81A-C79A-C80A	110.0(4)
C82-N7-C83	108.7(3)	C82-N7-C90	125.0(4)
C83-N7-C90	126.0(4)	C82-N8-C84	108.7(3)
C82-N8-C85	126.3(3)	C84-N8-C85	124.9(3)
H82-C82-N8	125(2)	H82-C82-N7	126(2)
N8-C82-N7	108.8(4)	C84-C83-N7	106.8(4)
C84-C83-C89	130.5(4)	N7-C83-C89	122.7(4)
C83-C84-N8	107.0(4)	C83-C84-C88	130.2(4)
N8-C84-C88	122.8(4)	N8-C85-C87	109.7(3)
N8-C85-C86	110.9(3)	C87-C85-C86	112.6(4)
N7-C90-C91	109.8(4)	N7-C90-C92	110.4(4)
C91-C90-C92	112.9(5)	C93-N9-C94	108.8(4)
C93-N9-C01	125.1(4)	C94-N9-C01	125.8(4)
C93-N10-C95	109.2(4)	C93-N10-C96	124.7(4)

C95-N10-C96	125.9(4)	H93-C93-N10	127(3)
H93-C93-N9	125(3)	N10-C93-N9	108.3(4)
C95-C94-N9	107.2(4)	C95-C94-C00	130.2(4)
N9-C94-C00	122.6(4)	C94-C95-N10	106.6(4)
C94-C95-C99	130.3(4)	N10-C95-C99	123.2(4)
N10-C96-C97	110.8(4)	N10-C96-C98	110.1(4)
C97-C96-C98	112.5(4)	N9-C01-C03	109.2(5)
N9-C01-C02	110.3(4)	C03-C01-C02	113.7(5)
C04-N11-C05	108.7(4)	C04-N11-C012	124.6(5)
C05-N11-C012	126.6(5)	C04-N12-C06	108.4(4)
C04-N12-C07	124.4(4)	C06-N12-C07	126.4(4)
H04-C04-N11	126(3)	H04-C04-N12	125(3)
N11-C04-N12	109.2(4)	N11-C05-C06	106.3(4)
N11-C05-C011	123.1(5)	C06-C05-C011	130.6(5)
N12-C06-C05	107.4(4)	N12-C06-C010	122.3(4)
C05-C06-C010	130.3(5)	N12-C07-C08	110.8(4)
N12-C07-C09	108.9(4)	C08-C07-C09	112.9(5)
C013-C012-N11	110.0(6)	C013-C012-C014	108.8(6)
N11-C012-C014	109.5(6)	C210-N19-C83A	108.8(4)
C210-N19-C90A	125.4(4)	C83A-N19-C90A	125.9(4)
C210-N20-C84A	108.4(4)	C210-N20-C85A	125.7(4)
C84A-N20-C85A	125.8(4)	H210-C210-N20	125(2)
H210-C210-N19	125(2)	N20-C210-N19	109.0(4)
C84A-C83A-N19	106.8(4)	C84A-C83A-C89A	130.2(4)
N19-C83A-C89A	123.0(4)	C83A-C84A-N20	107.0(4)
C83A-C84A-C88A	130.4(4)	N20-C84A-C88A	122.6(4)
N20-C85A-C87A	111.3(4)	N20-C85A-C86A	109.2(4)

C87A-C85A-C86A	112.6(4)	N19-C90A-C92A	111.2(4)
N19-C90A-C91A	109.2(4)	C92A-C90A-C91A	113.3(5)
C211-N21-C94A	108.5(4)	C211-N21-C01A	125.5(4)
C94A-N21-C01A	126.0(4)	C211-N22-C95A	108.8(4)
C211-N22-C96A	126.0(4)	C95A-N22-C96A	125.2(4)
H211-C211-N21	123(3)	H211-C211-N22	129(3)
N21-C211-N22	108.5(4)	C95A-C94A-N21	106.4(4)
C95A-C94A-C0A	129.8(4)	N21-C94A-C0A	123.7(4)
C94A-C95A-N22	107.7(4)	C94A-C95A-C99A	130.4(5)
N22-C95A-C99A	122.0(4)	C98A-C96A-N22	109.2(5)
C98A-C96A-C97A	114.0(5)	N22-C96A-C97A	111.1(5)
N21-C01A-C03A	110.0(4)	N21-C01A-C02A	110.3(4)
C03A-C01A-C02A	111.9(4)	C212-N23-C05A	108.7(4)
C212-N23-C01D	124.8(4)	C05A-N23-C01D	126.5(4)
C212-N24-C06A	108.6(4)	C212-N24-C07A	124.9(4)
C06A-N24-C07A	126.1(4)	H212-C212-N24	126(3)
H212-C212-N23	125(3)	N24-C212-N23	108.6(4)
C06A-C05A-N23	107.0(4)	C06A-C05A-C01C	130.1(4)
N23-C05A-C01C	122.8(4)	C05A-C06A-N24	107.1(4)
C05A-C06A-C01B	130.0(5)	N24-C06A-C01B	122.9(5)
N24-C07A-C08A	111.6(4)	N24-C07A-C09A	109.3(4)
C08A-C07A-C09A	112.2(5)	C01F-C01D-N23	110.0(4)
C01F-C01D-C01E	111.9(4)	N23-C01D-C01E	110.2(4)
C02C-C02B-C02G	120.3(5)	C02C-C02B-F1	121.2(6)
C02G-C02B-F1	118.5(6)	C02B-C02C-C02D	117.5(5)
C02E-C02D-C02C	120.7(6)	C02D-C02E-C02F	119.8(6)
C02G-C02F-C02E	119.8(6)	F2-C02G-C02F	120.4(5)

F2-C02G-C02B	117.6(5)	C02F-C02G-C02B	121.9(6)
C03G-C03B-F3	118.4(5)	C03G-C03B-C03C	120.8(5)
F3-C03B-C03C	120.7(5)	C03D-C03C-C03B	118.7(5)
C03E-C03D-C03C	121.1(5)	C03D-C03E-C03F	120.3(5)
C03G-C03F-C03E	118.4(6)	C03B-C03G-F4	119.1(6)
C03B-C03G-C03F	120.6(5)	F4-C03G-C03F	120.2(6)
C04C-C04B-C04G	120.0	C04C-C04B-F5	132.3(14)
C04G-C04B-F5	107.6(14)	C04D-C04C-C04B	120.0
C04C-C04D-C04E	120.0	C04D-C04E-C04F	120.0
C04E-C04F-C04G	120.0	F6-C04G-C04F	124.9(15)
F6-C04G-C04B	114.9(15)	C04F-C04G-C04B	120.0
C05C-C05B-F7	124.2(13)	C05C-C05B-C05G	120.3(10)
F7-C05B-C05G	115.5(13)	C05B-C05C-C05D	119.1(10)
C05C-C05D-C05E	119.5(10)	C05F-C05E-C05D	120.2(10)
C05G-C05F-C05E	120.3(10)	C05F-C05G-F8	117.3(11)
C05F-C05G-C05B	120.7(10)	F8-C05G-C05B	121.9(12)
C05I-C05H-C05M	119.1(19)	C05I-C05H-F7'	128(3)
C05M-C05H-F7'	112(3)	C05H-C05I-C05J	120(2)
C05I-C05J-C05K	120(2)	C05L-C05K-C05J	118(2)
C05M-C05L-C05K	122(2)	C05L-C05M-C05H	120(2)
C05L-C05M-F8'	115(3)	C05H-C05M-F8'	125(3)
C06C-C06B-C06G	121.4(12)	C06C-C06B-F9	118.0(13)
C06G-C06B-F9	120.4(14)	C06B-C06C-C06D	117.7(11)
C06E-C06D-C06C	117.9(12)	C06F-C06E-C06D	126.3(14)
C06E-C06F-C06G	114.5(14)	F10-C06G-C06B	118.0(15)
F10-C06G-C06F	122.3(15)	C06B-C06G-C06F	117.9(13)
C06M-C06H-F9'	117.5(17)	C06M-C06H-C06I	122.0(15)

F9'-C06H-C06I	120.4(18)	C06J-C06I-C06H	114.3(16)
C06K-C06J-C06I	121.3(18)	C06L-C06K-C06J	122.6(18)
C06M-C06L-C06K	110.2(19)	C06L-C06M-C06H	119.5(16)
C06L-C06M-F10'	117.6(17)	C06H-C06M-F10'	117.5(18)
C07C-C07B-C07G	120.0	C07C-C07B-F11	90.1(13)
C07G-C07B-F11	148.3(13)	C07D-C07C-C07B	120.0
C07E-C07D-C07C	120.0	C07D-C07E-C07F	120.0
C07E-C07F-C07G	120.0	C07F-C07G-C07B	120.0
C07F-C07G-F12	158.7(8)	C07B-C07G-F12	80.9(8)
C07H-F11'-C07M	21.3(5)	F11'-C07H-C07I	102.9(10)
F11'-C07H-C07M	137.1(10)	C07I-C07H-C07M	120.0
C07H-C07I-C07J	120.0	C07K-C07J-C07I	120.0
C07J-C07K-C07L	120.0	C07M-C07L-C07K	120.0
F11'-C07M-C07L	141.6(5)	F11'-C07M-C07H	21.6(5)
C07L-C07M-C07H	120.0	F11'-C07M-F12'	83.0(9)
C07L-C07M-F12'	135.4(10)	C07H-C07M-F12'	104.6(10)
F13-C08B-C08C	102.0(19)	F13-C08B-C08G	133.1(19)
C08C-C08B-C08G	120.0	C08D-C08C-C08B	120.0
C08E-C08D-C08C	120.0	C08F-C08E-C08D	120.0
C08E-C08F-C08G	120.0	F14-C08G-C08F	142.1(19)
F14-C08G-C08B	96.7(19)	C08F-C08G-C08B	120.0
F15-C09B-C09C	97.1(19)	F15-C09B-C09G	139.6(18)
C09C-C09B-C09G	120.0	C09B-C09C-C09D	120.0
C09E-C09D-C09C	120.0	C09D-C09E-C09F	120.0
C09G-C09F-C09E	120.0	F16-C09G-C09F	155.2(16)
F16-C09G-C09B	83.5(16)	C09F-C09G-C09B	120.0