Supporting Information

REACTION OF AN OVEROWDED 1,2-DIARYL-1,2-DIBROMODISILENE WITH 1-VINYLCYCLOHEPTA-1,3,5-TRIENE: ISOLATION OF A 2-VINYLSILACYCLOPROPANE DERIVATIVE AND ITS THERMAL CONVERSION TO A SILACYCLOPENTA-3-ENE DERIVATIVE

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1. Spectroscopic Data

Figure S1. ^{1}H NMR spectrum of **5** (400 MHz, C_6D_6, 298 K).

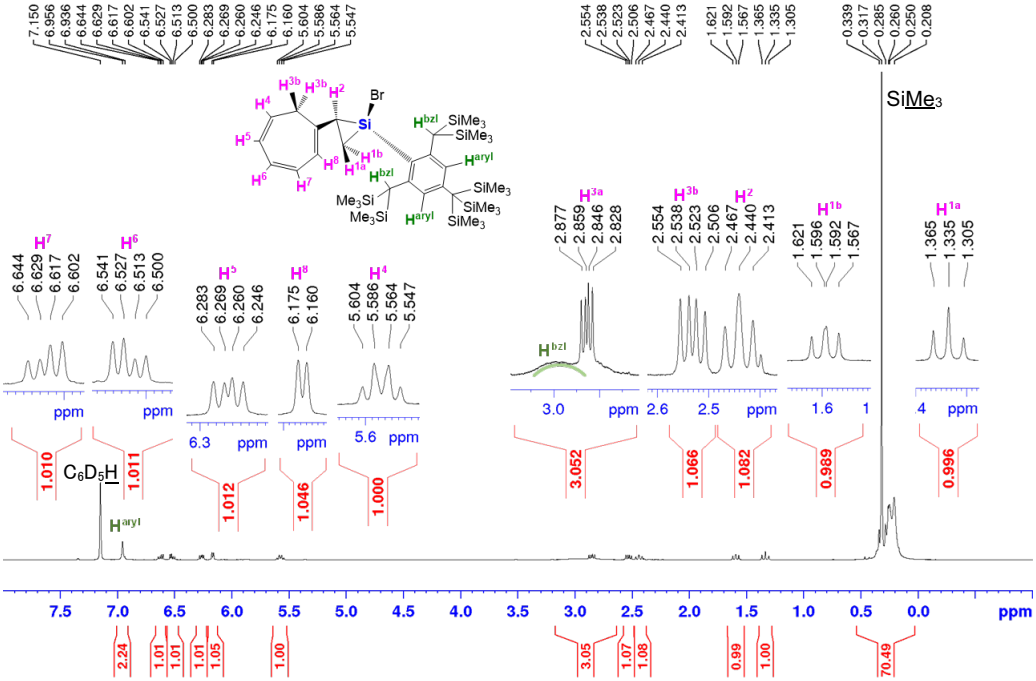


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **5** (100 MHz, C_6D_6, 298 K). As seen in other systems with a Bbt group, some of aromatic ring carbons (C_A, C_B) and *o*-benzyl carbons (C_E) of Bbt group were severely broadened and could not be observed. Normally, these can be observed by increasing the temperature, but in this system, it was not possible because the reaction to **6** proceeded at elevated temperature. We tried to detect them by using long-range correlations at room temperature but could not observe any significant correlation. Regarding the assignment of C_D, it is considered to be appropriate from the comparison of the signal position and shape with the related compound, but a clear correlation could not be confirmed in the HMBC measurement under various conditions. There is a room to be C_B.

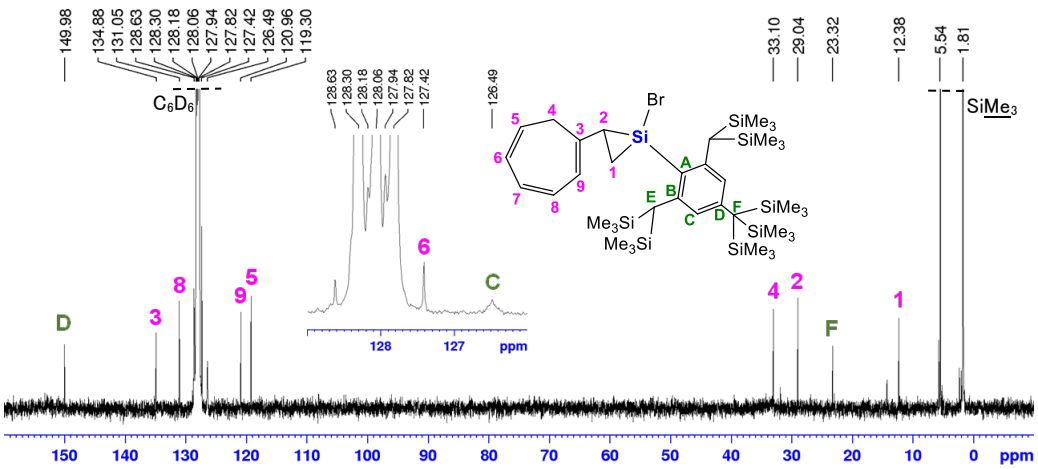


Figure S3. $^{13}C\{^{1}H\}$ DEPT135 NMR spectrum of **5** (100 MHz, C_6D_6, 298 K). (x: C_6D_5H)

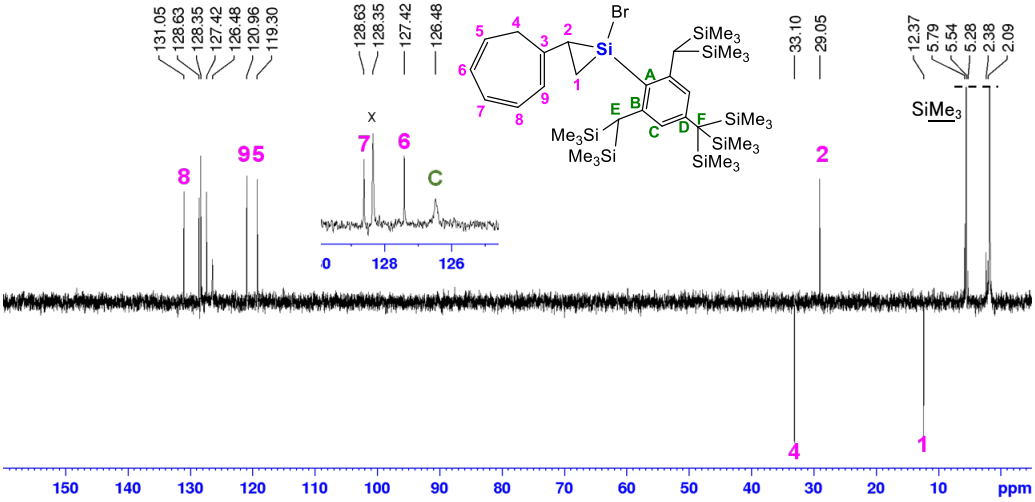


Figure S4. $^{29}Si\{^{1}H\}$ NMR spectrum of **5** (79.5 MHz, C_6D_6, 298 K).

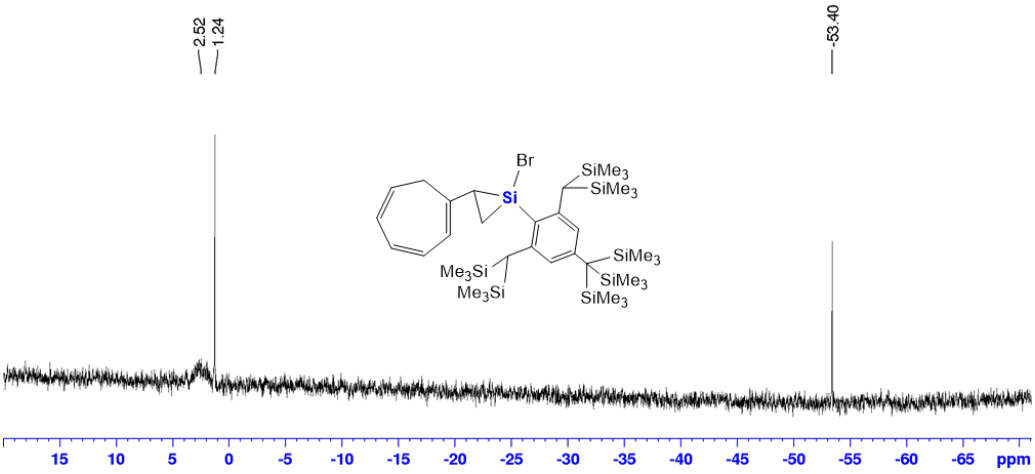


Figure S5. HRMS (DART-TOF) spectrum of **5**.

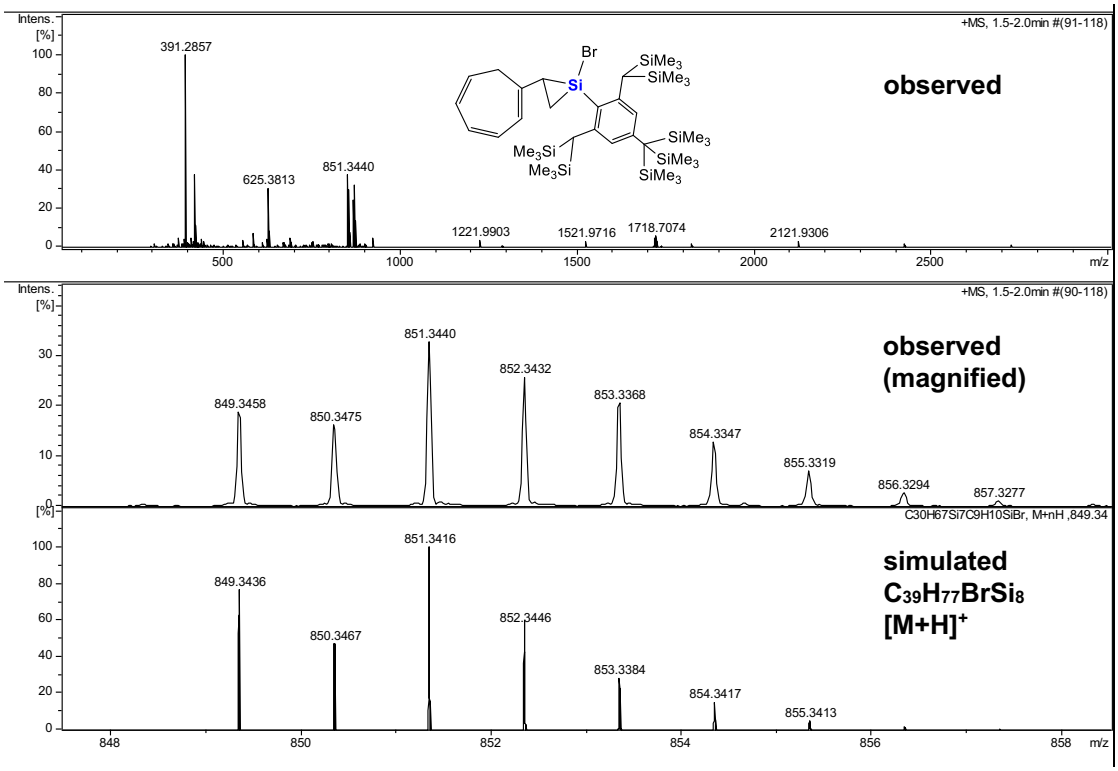


Figure S6. ^{1}H NMR spectrum of **6** (400 MHz, C_6D_6, 298 K). (x: impurity)

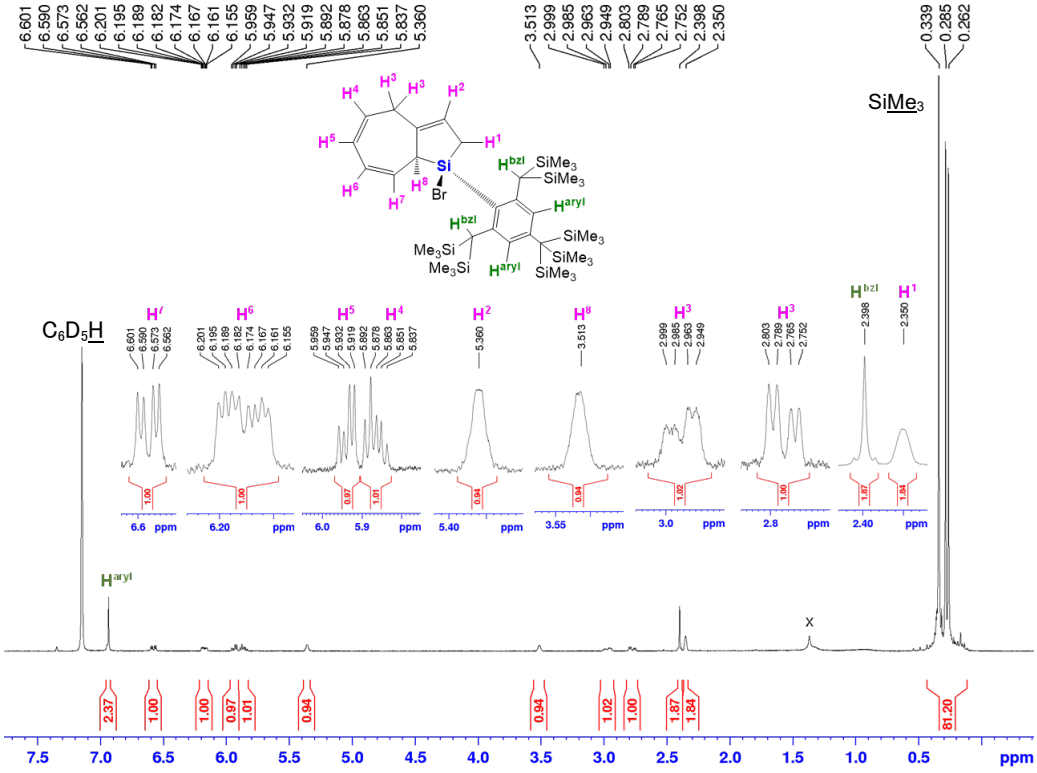


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of **6** (100 MHz, C_6D_6, 298 K). (x: hexane)

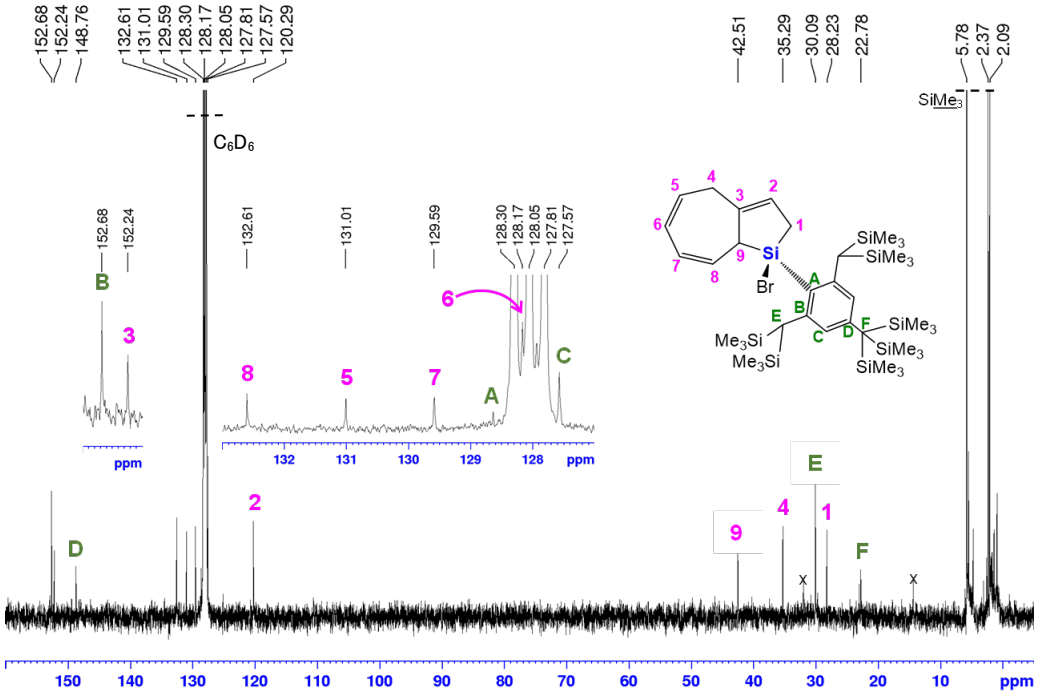


Figure S8. $^{13}C\{^{1}H\}$ DEPT 135 NMR spectrum of **6** (100 MHz, C_6D_6, 298 K). (x: C_6D_5H)

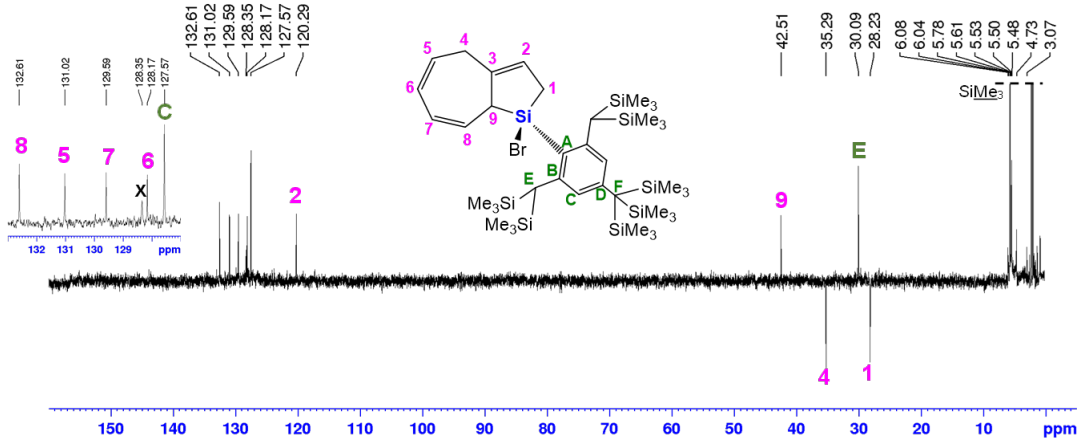


Figure S9. $^{29}Si\{^{1}H\}$ NMR spectrum of **6** (79.5 MHz, C_6D_6, 298 K).

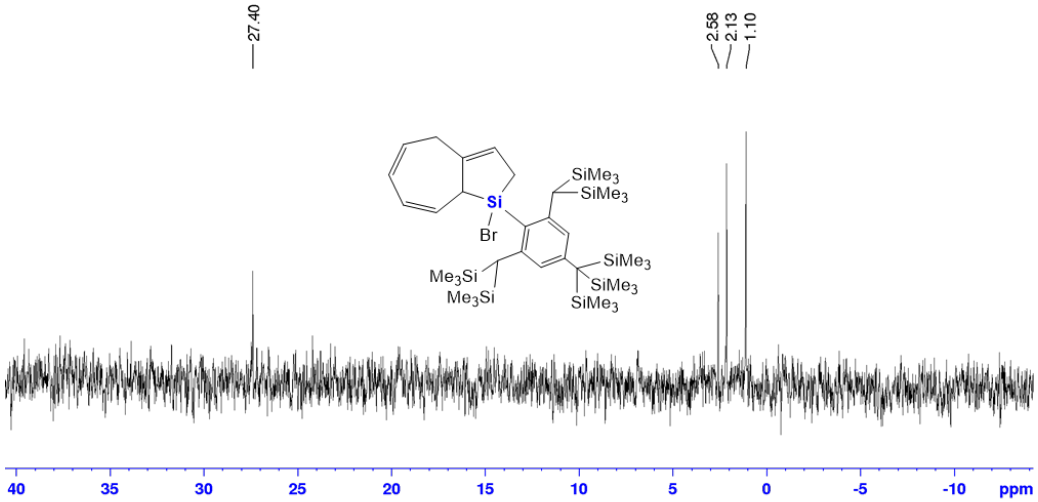
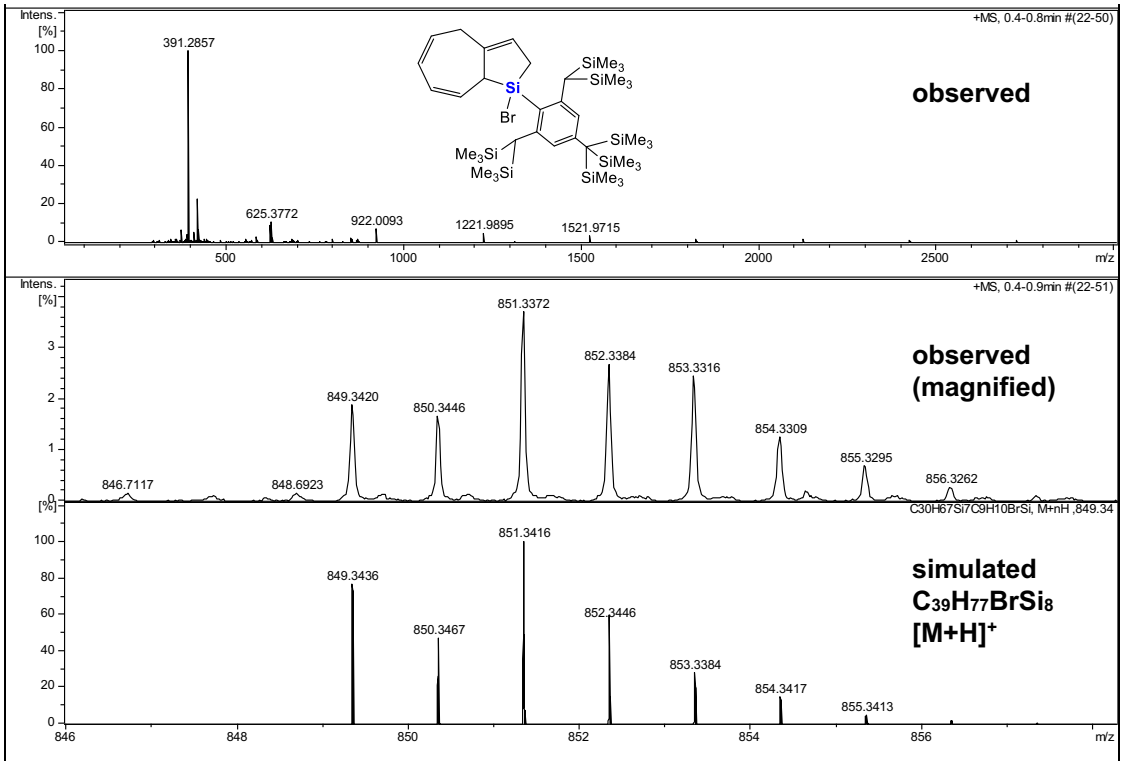


Figure S10. HRMS (DART-TOF) spectrum of **6**.



2. X-Ray Diffraction Studies

Figure S11. Disorder of the 2-cyclohepta-1,3,5-trien-1-ylsilacyclopropane moiety of **5** [major (83%): Si1, Br1, and C1-C9; minor (17%): Si1 (shared), Br2, and C10-C18) with thermal ellipsoid plots (50% probability).

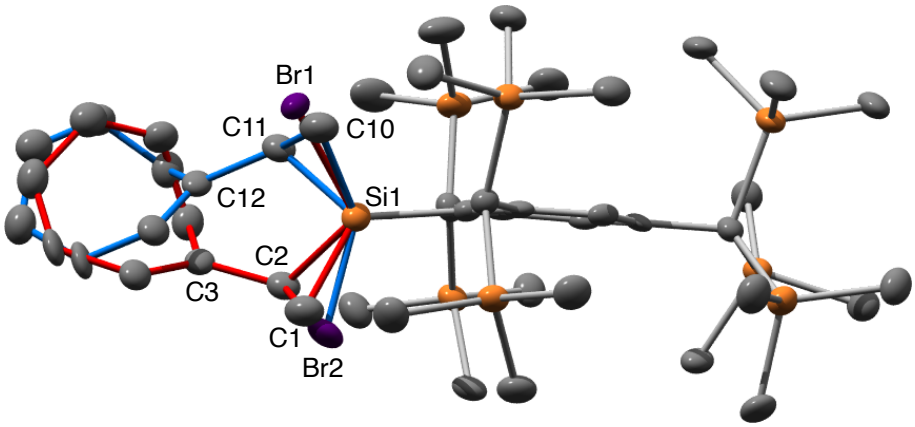


Table 1. Crystallographic data for **5** and **6**.

	5	**6**
Empirical formula	$C_{39}H_{77}BrSi_8$	$C_{39}H_{77}BrSi_8$
Formula weight	850.63	850.63
Temperature (K)	103(2)	90(2)
Crystal system	Triclinic	Orthorhombic
Crystal size (mm)	0.20×0.15×0.03	0.10×0.05×0.04
Space group	*P*–1 (#2)	$Pna2_1$ (#33)
a (Å)	12.9420(6)	15.4322(10)
b (Å)	13.1605(8)	23.6128(15)
c (Å)	15.0753(8)	13.0485(10)
α (°)	94.500(5)	90
β (°)	91.762(4)	90
γ (°)	110.513(5)	90
V (Å^3)	2392.8(2)	4754.8(6)
Z	2	4
$D_{calcd.}$ (g•cm^{-3})	1.181	1.188
μ (mm^{-1})	1.085	1.092
F(000)	916	1832
θ range (°)	1.683 to 27.500	2.172 to 27.497
Reflections collected	32445	69482
Independent reflections	10865 [R_{int} = 0.0892]	10728 [R_{int} = 0.1620]
Completeness to θ_{max}	99.4%	99.9%
Data/restraints/parameters	10865/6/491	6456/0/373
Goodness of fit	1.093	1.013
R_1 [I>2σ(I)]	0.0683	0.0628
wR_2 [I>2σ(I)]	0.1203	0.0913
R_1 (all data)	0.1198	0.1296
wR_2 (all data)	0.1354	0.1101
Largest diff. peak (e•Å)	0.564	0.514
Largest diff. hole (e•Å)	–0.362	–0.588