

Table S1. Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$).
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Sn(1)	0.817032(6)	0.457938(13)	0.635876(5)	31(1)
F(1)	0.55539(7)	1.01325(16)	0.54705(6)	60(1)
F(2)	0.52572(8)	1.19578(18)	0.55887(8)	88(1)
F(3)	0.53960(11)	1.28568(18)	0.62930(10)	110(1)
F(4)	0.58654(9)	1.18363(19)	0.68850(8)	94(1)
F(5)	0.61616(7)	0.99801(17)	0.67785(6)	64(1)
F(6)	0.65606(7)	0.99148(15)	0.55188(5)	54(1)
F(7)	0.74296(8)	1.05059(16)	0.55647(7)	69(1)
F(8)	0.80063(7)	1.0050(2)	0.61979(8)	82(1)
F(9)	0.76856(7)	0.89681(17)	0.67862(6)	70(1)
F(10)	0.68295(6)	0.83840(14)	0.67530(5)	52(1)
F(11)	0.53247(6)	0.89181(14)	0.66329(5)	53(1)
F(12)	0.50804(7)	0.74399(18)	0.70770(6)	68(1)
F(13)	0.55436(8)	0.56718(19)	0.71177(7)	80(1)
F(14)	0.62693(8)	0.54228(15)	0.66907(7)	68(1)
F(15)	0.65179(6)	0.68851(14)	0.62254(5)	49(1)
F(16)	0.51527(6)	0.84362(15)	0.58241(5)	51(1)
F(17)	0.48127(6)	0.73398(17)	0.52245(6)	65(1)
F(18)	0.53794(7)	0.65084(16)	0.47293(6)	63(1)
F(19)	0.62999(6)	0.68195(14)	0.48531(5)	52(1)
F(20)	0.66473(5)	0.78468(14)	0.54549(5)	46(1)
C(1)	0.74921(10)	0.4635(2)	0.60989(8)	33(1)
C(2)	0.71720(11)	0.3958(2)	0.62140(9)	42(1)
C(3)	0.67393(11)	0.3956(3)	0.60127(10)	53(1)
C(4)	0.66299(12)	0.4619(3)	0.57089(10)	55(1)
C(5)	0.69540(11)	0.5292(3)	0.56079(9)	49(1)
C(6)	0.73878(10)	0.5315(2)	0.57949(8)	37(1)
C(7)	0.72840(12)	0.3221(2)	0.65458(10)	46(1)
C(8)	0.69921(13)	0.3405(3)	0.68843(11)	61(1)
C(9)	0.72652(16)	0.2139(3)	0.64149(13)	80(1)
C(10)	0.61581(14)	0.4619(4)	0.54863(13)	84(2)
C(11A)	0.57896(19)	0.4969(5)	0.57091(18)	75(1)
C(11B)	0.5773(7)	0.4289(19)	0.5710(6)	75(1)
C(12A)	0.6068(3)	0.3662(7)	0.5299(3)	75(1)
C(12B)	0.6136(3)	0.4350(7)	0.5089(3)	75(1)
C(14)	0.77387(11)	0.6062(2)	0.56802(9)	41(1)
C(15)	0.77557(16)	0.6147(3)	0.52429(10)	73(1)
C(16)	0.76825(12)	0.7096(3)	0.58716(12)	59(1)
C(17)	0.85490(10)	0.3245(2)	0.63150(8)	34(1)
C(18)	0.87194(10)	0.2751(2)	0.66525(8)	37(1)
C(19)	0.89783(11)	0.1890(2)	0.66151(9)	44(1)
C(20)	0.90663(12)	0.1518(2)	0.62588(9)	46(1)
C(21)	0.88875(11)	0.2028(2)	0.59266(9)	45(1)
C(22)	0.86319(10)	0.2895(2)	0.59469(8)	37(1)
C(23)	0.86355(11)	0.3150(2)	0.70537(8)	40(1)

C(24)	0.90620(13)	0.3587(3)	0.72623(10)	62(1)
C(25)	0.84174(14)	0.2363(3)	0.72973(10)	63(1)
C(26)	0.93624(15)	0.0585(3)	0.62321(11)	65(1)
C(27)	0.91177(17)	-0.0247(3)	0.60250(19)	102(2)
C(28)	0.98011(16)	0.0797(4)	0.60627(19)	115(2)
C(29)	0.84473(11)	0.3451(2)	0.55838(9)	44(1)
C(30)	0.88204(13)	0.3721(3)	0.53218(10)	59(1)
C(31)	0.80460(13)	0.2890(3)	0.53691(11)	67(1)
C(32)	0.84714(10)	0.5841(2)	0.66478(8)	34(1)
C(33)	0.82797(10)	0.6215(2)	0.69754(8)	39(1)
C(34)	0.84796(12)	0.7062(3)	0.71528(10)	53(1)
C(35)	0.88581(13)	0.7525(3)	0.70175(11)	57(1)
C(36)	0.90377(11)	0.7126(3)	0.66945(10)	51(1)
C(37)	0.88511(10)	0.6277(2)	0.65047(9)	40(1)
C(38)	0.78651(11)	0.5721(2)	0.71279(9)	41(1)
C(39)	0.79515(15)	0.5413(3)	0.75511(10)	64(1)
C(40)	0.74406(12)	0.6385(3)	0.70562(11)	59(1)
C(41)	0.90661(16)	0.8446(3)	0.72313(15)	83(1)
C(42)	0.87328(15)	0.9306(3)	0.72054(13)	78(1)
C(43A)	0.9320(5)	0.8345(12)	0.7541(5)	75(1)
C(43B)	0.9525(2)	0.8674(5)	0.71426(19)	75(1)
C(44)	0.90673(11)	0.5839(3)	0.61584(10)	42(1)
C(45)	0.91457(14)	0.6601(3)	0.58465(11)	66(1)
C(46)	0.95017(12)	0.5261(3)	0.62848(12)	58(1)
C(47)	0.58632(11)	0.9932(3)	0.61234(10)	44(1)
C(48)	0.56405(12)	1.0503(3)	0.58328(11)	50(1)
C(49)	0.54875(13)	1.1482(3)	0.58884(13)	64(1)
C(50)	0.55615(15)	1.1915(3)	0.62394(15)	72(1)
C(51)	0.57920(14)	1.1403(3)	0.65336(13)	68(1)
C(52)	0.59352(12)	1.0446(3)	0.64730(11)	52(1)
C(53)	0.66453(10)	0.9077(2)	0.61217(9)	39(1)
C(54)	0.68301(11)	0.9638(2)	0.58371(9)	42(1)
C(55)	0.72792(12)	0.9961(3)	0.58534(11)	49(1)
C(56)	0.75696(11)	0.9725(3)	0.61744(12)	53(1)
C(57)	0.74072(11)	0.9197(3)	0.64673(10)	50(1)
C(58)	0.69570(11)	0.8886(2)	0.64403(9)	43(1)
C(59)	0.59474(10)	0.7989(2)	0.64071(8)	39(1)
C(60)	0.55799(10)	0.8072(3)	0.66341(8)	44(1)
C(61)	0.54427(11)	0.7316(3)	0.68702(9)	50(1)
C(62)	0.56733(12)	0.6423(3)	0.68892(10)	55(1)
C(63)	0.60387(12)	0.6302(3)	0.66728(10)	51(1)
C(64)	0.61612(10)	0.7069(2)	0.64383(9)	42(1)
C(65)	0.59163(10)	0.8230(2)	0.56746(8)	38(1)
C(66)	0.54545(10)	0.8045(2)	0.55896(9)	42(1)
C(67)	0.52685(10)	0.7496(3)	0.52818(10)	48(1)
C(68)	0.55494(11)	0.7081(2)	0.50282(9)	47(1)
C(69)	0.60138(11)	0.7236(2)	0.50936(9)	42(1)
C(70)	0.61850(10)	0.7784(2)	0.54122(8)	38(1)
B(1)	0.60939(11)	0.8812(3)	0.60824(10)	39(1)

Calculation of Structure and Bonding for Sn complex.

Geometry calculations:

The starting geometry was the x-ray structure. Geometry optimization was done using DFT/B3LYP [Becke, 1988 #1] [Lee, 1988 #2], with the effective core potential basis set LACVP**[Hay, 1985 #111] for the Sn, and the 6-31G basis set for all other atoms, as implemented in the *Jaguar* program [Jaguar, 1991-2000 #3]. Although the x-ray structure has a C_3 symmetry, no symmetry constraints were imposed during the optimization.

There are very minor changes in the geometry before and after optimizations, the main changes are deviation from strict C_3 symmetry (x-ray structure) to an almost symmetrical structure (calculated structure) and a small enlargement of the geometry (x-ray structure is smaller than calculated structure), as is expected when moving from bulk to gas phases. Table 1 display some distances and dihedral angles for the calculated, minimized structure.

Figure A. Numbering scheme for the Sn complex.

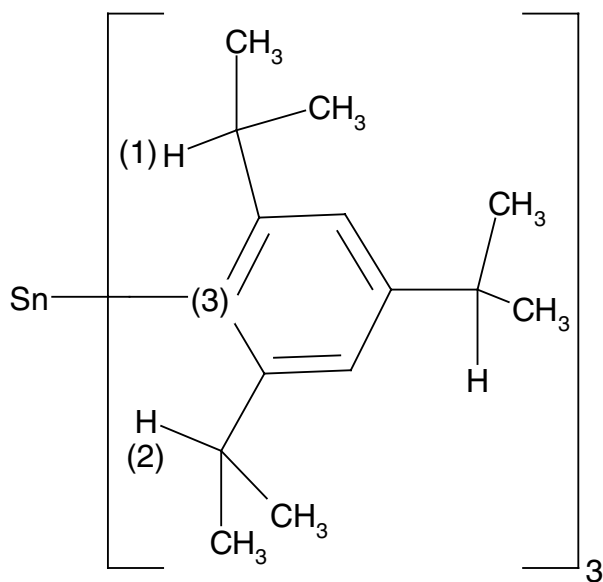


Table S2. Selected distances and dihedral angle for the Sn complex. Numbering of atoms corresponds to Figure A. CX(Y) is C atom number Y, from ligand X.

Bond Length in Å, between	Calculated structure
Sn- C1(3)	2.12
Sn- C2(3)	2.12
Sn- C3(3)	2.12
Atom Distance in Å, between	
Sn - H1(1)	2.57
Sn - H2(1)	2.57
Sn - H3(1)	2.58
Sn - H1(2)	2.57
Sn - H2(2)	2.58
Sn - H3(2)	2.57
Dihedral angle, between	
C1(3)-Sn-C2(3)-C2(4)	57.0
C2(3)-Sn-C3(3)-C3(4)	59.9
C3(3)-Sn-C1(3)-C1(4)	58.8

Bonding calculations:

In order to analyze the bonding in the Sn complex, we have used the “Atoms in Molecules” (AIM) method of Bader [Bader, 1991 #106], as implemented in the *Morphy* [Popelier, 1996 #110] program. A comprehensive explanation of the method was given by Popelier [Popelier, 1999 #107], and here only the main features of the method will be explained.

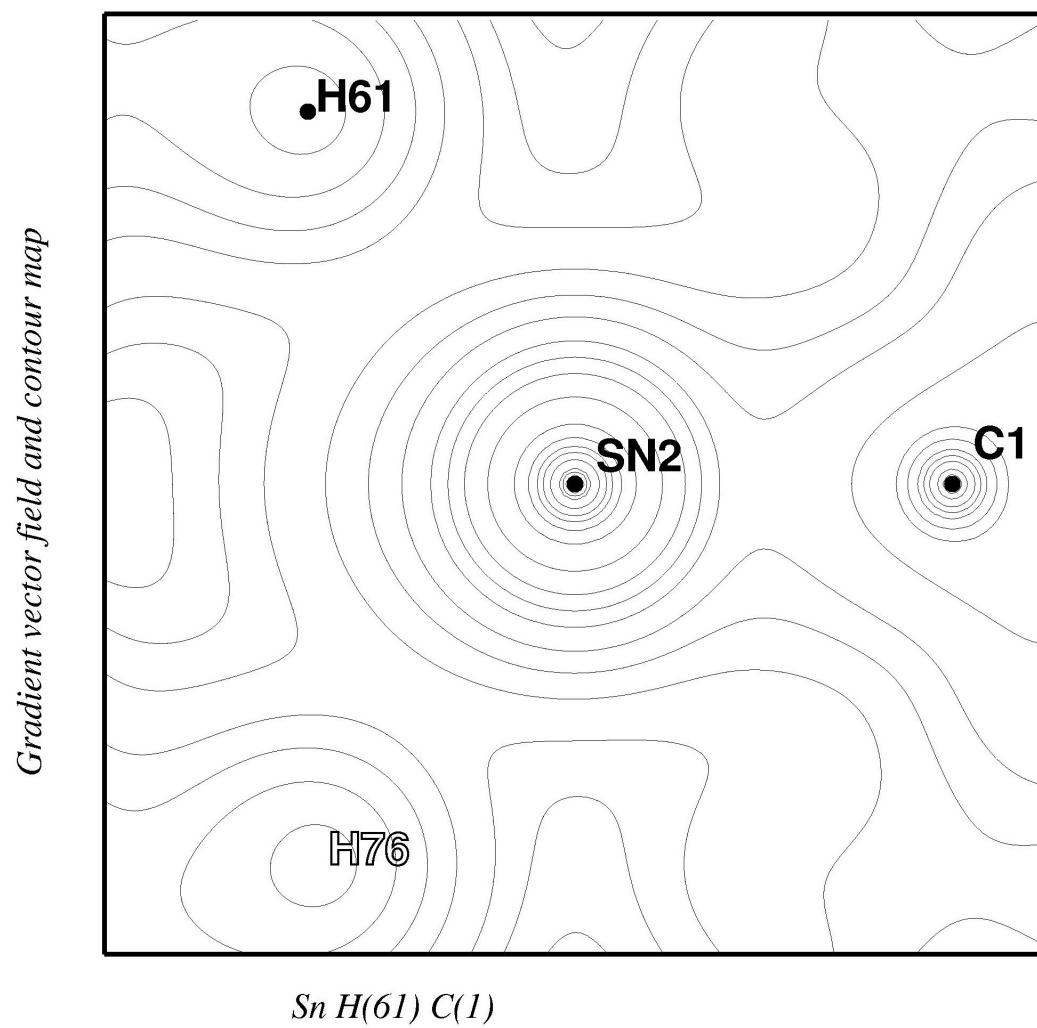
We have used The AIM method to discriminate whether or not there is a bond between the Sn center and the H (1 and 2) atoms that forms the trigonal prism around it. We have used the Huzinaga's full valence MIDI basis-set [Huzinaga, 1984 #109], as implemented in *GameSSUS* [Schmidt, 1993 #108] to calculate the electronic structure of the geometry-optimized complex, and then used it as an input for *Morphy*.

The only bond critical points (3, -1 critical points) between Sn and other atoms were for the Sn-C(3) bonds, with \mathbf{r} (au/bohr³) = 0.10143, 0.10157, 0.10132; \mathbf{r} (au/bohr³) = 0.19263, 0.19354, 0.19354. No bond critical points were found between the Hydrogens and Sn. Figure B displays the gradient vector field and contour map between Sn (numbered SN2 in Fig. 2), C(3) (numbered C1 in Fig. 2) and H(1) (numbered H61 in Fig. 2).

The **AIM** theory makes a link between quantum mechanics and standard chemical concepts such as an atom and a chemical bond. There is no explicit concept of an atom or a bond in the Schrödinger's equation. It is only concerned with particles (electrons and nuclei) in force fields. However, a lot of the standard chemical knowledge is based on the atomic model. AIM theory is unique in the sense that it provides a rigorous link between intuitive chemical concepts and quantum mechanics through analysis of the electron density $\rho(\mathbf{r})$ (\mathbf{r} is a space coordinate).

In AIM theory the *topology* of $\rho(\mathbf{r})$ is described by a set of *critical points* (CPs). These CPs are found where $\nabla \rho(\mathbf{r}) = 0$, where $\nabla \rho(\mathbf{r})$ is referred to as the gradient vector field. It should be mentioned that the $\rho(\mathbf{r})$ is only one of several possible scalar fields that can be subjected to localizing critical points. Another important scalar field is the *Laplacian* of $\rho(\mathbf{r})$: $\nabla^2 \rho(\mathbf{r})$. The CPs from this field satisfy $\nabla^2 \rho(\mathbf{r}) = 0$ and provide links to important chemical concepts such as those found in classical Lewis theory.

Figure B. Gradient vector field and contour map of the electronic density changes between atom Sn, C(3) and H(1).



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Using now 3 dimensions instead of two and the topology of the electron density, Bader describes 4 so called **critical points**.

(3, -3) critical point: The electron density falls down in all three perpendicular directions of space. This is a local maximum of electron density. This is the position of an atom. For all atoms except hydrogen it is also the position of the nuclei. The point therefore is also called an atomic critical point.

(3, -1) critical point: The electron density falls down in two perpendicular directions of space and rises in the third direction. This is a saddle point of electron density with a maximum of electron density in 2 directions of space and a minimum in the third one. This points are between two neighboring atoms defining a bond between them. This point is therefore also called a bond critical point.

(3, +1) critical point: The electron density falls in one direction of space and rises in the two other perpendicular directions of space. Again this is a saddle point with a maximum in one and a minimum in two directions of space. This point is to be found in the middle of several bonds forming a ring. It is also called a ring critical points.

(3, +3) critical point: This is a local minimum with electron density rising in all 3 directions of space. This point is found when several rings form a cage and is therefore called a cage critical point.

Connecting the critical points in space give again a space filling partitioning of space in atomic subunits. So in principle this model yields an exact quantum mechanic description where the molecule bonds are. The topology works equally well for coulomb bonds as for weak bonds.