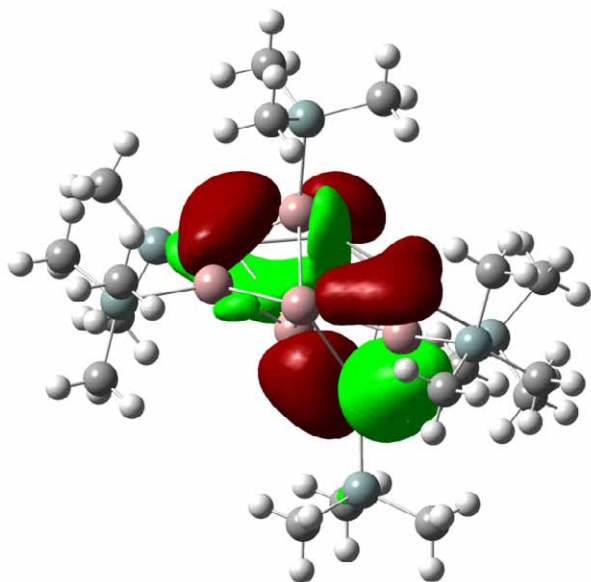


Results of DFT Calculations on **12a**:

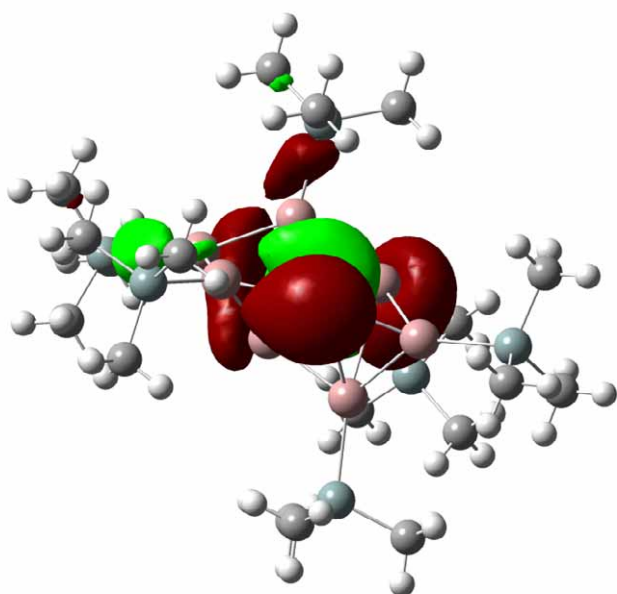
**Functional: BP86**

**Base set: def-Sv(P)**

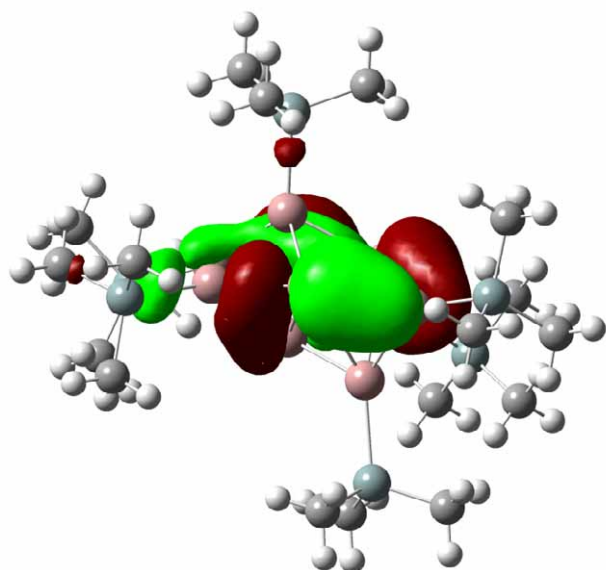
**Programms: Turbomole und Gaussian 03**



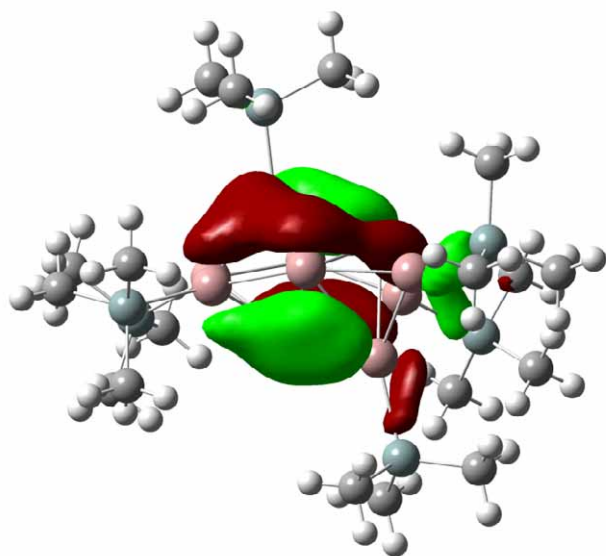
HOMO (-0.172 H)



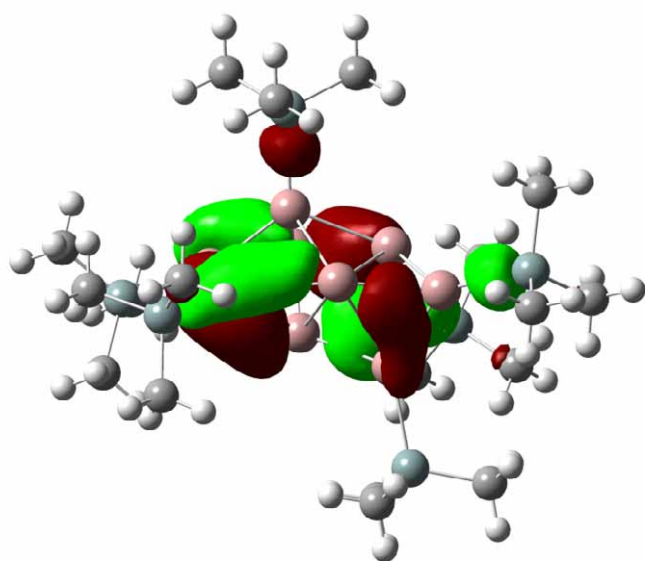
HOMO -1 (-0.188 H)



HOMO -2 ( -0.191 H)



HOMO -3 (-0.199 H)



HOMO -4 (-0.201 H)

**Table**

SEN	2-center SEN		2-center SEN	
figures	Ga(3)-Ga(4)	1.30	Ga(1)-Ga(9)	1.41
	Ga(2)-Ga(3)	1.43	Ga(1)-Ga(8)	1.52
	Ga(1)-Ga(2)	0.89	Ga(5)-Ga(8)	1.52
	Ga(1)-Ga(5)	0.64	Ga(7)-Ga(10)	1.55
	Ga(4)-Ga(5)	1.42	Ga(7)-Ga(8)	0.79
	Ga(4)-Ga(6)	1.41	Ga(1)-Ga(10)	1.05
	Ga(3)-Ga(6)	1.21	Ga(9)-Ga(10)	1.51
	Ga(1)-Ga(6)	0.95	Ga(6)-Ga(7)	0.91
	Ga(5)-Ga(6)	1.43		
	Ga(2)-Ga(6)	0.91		
	Ga(4)-Ga(7)	1.34	Ga(3)-Si(1)	1.18
	Ga(3)-Ga(7)	1.23	Ga(4)-Si(2)	1.15
	Ga(2)-Ga(7)	0.82	Ga(6)-Si(3)	0.99
	Ga(1)-Ga(7)	1.07	Ga(8)-Si(4)	1.21
	Ga(5)-Ga(7)	1.42	Ga(9)-Si(5)	1.19
	Ga(2)-Ga(9)	1.59	Ga(10)-Si(6)	1.17
	<i>n-o-p</i>	<i>3-center SEN</i>	<i>n-o-p</i>	<i>3-center SEN</i>
	<i>1-2-6</i>	<i>0.40</i>	<i>2-3-6</i>	<i>0.42</i>
	<i>1-2-7</i>	<i>0.30</i>	<i>2-3-7</i>	<i>0.40</i>
	<i>1-2-9</i>	<i>0.43</i>	<i>2-7-10</i>	<i>0.36</i>
<i>1-5-8</i>	<i>0.33</i>	<i>2-9-10</i>	<i>0.41</i>	
<i>1-6-7</i>	<i>0.44</i>	<i>3-4-6</i>	<i>0.45</i>	
<i>1-7-8</i>	<i>0.36</i>	<i>3-4-7</i>	<i>0.47</i>	
<i>1-8-10</i>	<i>0.33</i>	<i>3-6-7</i>	<i>0.31</i>	
<i>1-9-10</i>	<i>0.47</i>	<i>5-7-8</i>	<i>0.33</i>	
<i>1-10-7</i>	<i>0.44</i>	<i>8-7-10</i>	<i>0.30</i>	

SENs for **12a** as resulting from a Ahlrichs-Heinzmann population analysis; 2-center and 3-center SEN  $Ga(n)Ga(o)Ga(p)$  ( $\geq 0.30$ ) (numbering of atoms and bonds acc. to 1 and 3).