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Supporting Information

N,N-Dimethylaminopropylsilane – a Case-Study on the Nature of Weak Intramolecular Si···N Interactions

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Electronic Supplementary Information

GED Model for H3

The ratios of the four conformers shown in **Figure S1** were determined by three independent parameters: p_1, p_{56} and p_{57}. These were defined as the molar fraction of H3a (p_1), the fraction of H3c divided by the sum of the molar fractions of H3b, H3c and H3d (p_{56}) and finally, the fraction of H3b divided by the sum of the fractions of H3b and H3d (p_{57}).

The geometries of the four conformers of were described in terms of 55 independent parameters, p_2 to p_{55} and p_{58}, as shown in **Table S1**. All bonded distances were used in the models using a separate average distance for each atom pair type. Where the differences between bonded distances of the same type were calculated to be greater than *ca.* 0.002 Å, these were also included as parameters. The only exception being the C–H distances which, on the basis of the low scattering cross-section for hydrogen, were assumed to be identical.

The models for conformers H3b, H3c and H3d were built in the following way: Local C_3 symmetry was assumed for the SiH_3 group, the geometry of which was determined using the average H–Si–H angle, p_{50}, plus half the difference from the H3a conformer, p_{51}. The Si–H bond lengths in these conformers were equal in length and were defined by the average Si–H distance, p_{11}, minus a difference ($0.08333*p_{12}$). (The calculations predicted an elongation of one of the S–H bonds in H3a.) The heavy atom Si–C–C–C–N chains were positioned using a z-matrices, with independent Si–C–C–C and C–C–C–N dihedral angles for each conformer (p_{26} to p_{31}). The angles were defined in a different manner. An average Si–C–C angle was used, p_{18}, with a difference for conformer H3b, p_{19}. Due to the similarity of the non-bonded C···C and C···N distances, an average of the C–C–C and C–C–N angles was used, p_{20}, in conjunction with a difference, p_{21}. In addition, a second difference was used for the C–C–C angle in H3d, p_{22}. The methyl carbon atoms were placed using an average internal C–N–C angle, p_{14}. No local symmetry was assumed, as in each conformer one of the C–N–C angles was calculated to be appreciably different from the others. (The average angle was calculated to be similar for all conformers.) Two difference parameters were therefore included; one for H3a and one for H3b and H3d (p_{16} and p_{17}, respectively). The orientation of the methyl carbon atoms, relative to the rest of the molecule was defined using the C–C–N–C(28/51/73) dihedral angles, which were defined separately for each conformer (p_{32} to p_{34}).

The model for H3a was written in a different way to the models for conformers b, c and d. This made use of the Si–N distance (p_2) so that the Si–C–C–C–N chain was described in terms of a 5-membered ring, rather than by a z-matrix. The angles used to construct the ring were the C–Si···N and Si···N–C angles, p_{46} and p_{47}, and the C–Si···N–C and C(4)–C(1)···C(5)–N dihedral angles, p_{48} and p_{49}. Another difference between the model for H3a and those for the other conformers was that the orientation of the NMe_2 group with respect to the silicon atom was defined in terms of the difference between the Si···C3–N–C(7/8) dihedral angles, p_{55}, rather than the C–C–N–C(7) angle. The final point is that local C_s symmetry (rather than C_3) was assumed for the SiH_3 group, with the hydrogen atom facing away from the molecule being considered different to the other two atoms. This Si–H bond length was calculated to be longer than all the others ($= p_{11} + 0.91667*p_{12}$) and this hydrogen atom was positioned using the H–Si–C angle, p_{53}, and the H–Si–C···N dihedral angle, p_{54}. The two remaining hydrogen atoms were then placed using internal H–Si–H angles, which were derived from the average H–Si–H angle (p_{50}) minus half the difference between the average in H3a and the other conformers (p_{51}), and the difference between the angle spanning the local mirror plane (the larger one) and the two symmetrically equal angles, p_{52}.

The hydrogen atoms bonded to carbon were positioned in a similar manner in all four conformers. Those on the propylene chain were positioned using local C_s symmetry and local C_{2v} symmetry with respect to the bond angles. The only refining parameter was therefore the

H–C–H angle, which was defined in terms of an average of all H–C–H angles, p_{35}, and a difference between H–C–H in the chain and H–C–H in the methyl groups, p_{36}. All that remains is the orientation of the methyl groups. For these, local C_3 symmetry was assumed, making use of the internal H–C–H angle defined as above. For each conformer, separate C–N–C–H dihedral angles were used for the methyl groups, p_{38} to p_{45}, where the chosen hydrogen atoms were those farthest from Si. Finally, a tilt of the methyl groups was also employed, p_{37}. This was defined as an increase in the N–C–H angle, where the hydrogen was again the one farthest from Si.

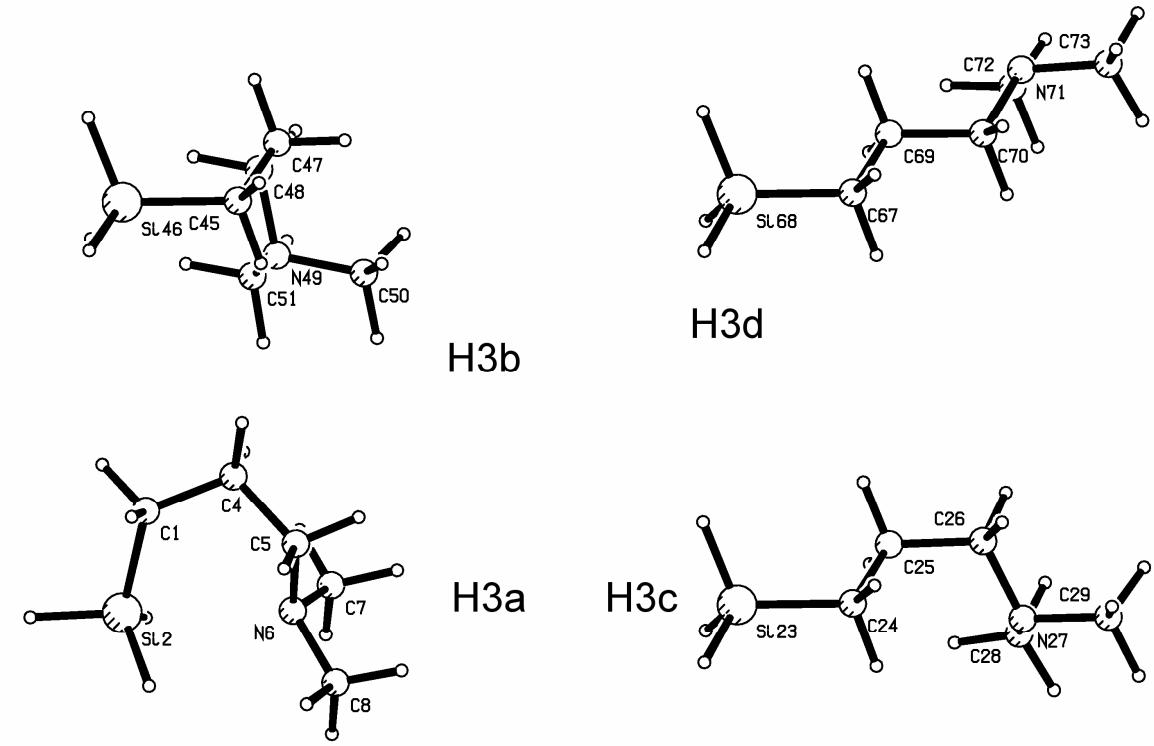


Figure S1 – Atom numbering used in the GED refinement.

Table S1 – Data analysis parameters. Units of s are nm^{-1}, nozzle-to-plate distances are mm and the electron wavelengths are Angstroms.

Dataset	Rg	Rd	Scale Factor	Corr. Parameter	Δs	s_{min}	s_{w1}	s_{w2}	s_{max}	Nozzle-to-plate distance	Electron wavelength
1	8.51%	4.80%	0.776(10)	0.4726	2	70	90	268	312	252.78	0.0535
2	2.20%	1.96%	0.755(8)	0.1197	2	70	90	194	226	252.78	0.0535
3	6.57%	4.41%	0.679(6)	0.3697	2	24	44	134	150	503.5	0.0534

Table S2 – Refined (r_{h1}) independent parameters, selected dependent parameters, corresponding calculated values and applied restraints.

Independent parameter	Description	Conformers	GED [a]	MP2/TZVPP [b]
p_1	Molar ratio of H3a	a /(a +b +c +d)	0.25(3)	0.48
p_2	*r* Si···N	a	2.912(35)	2.728
p_3	*r* Si–C average	a,b,c,d	1.888(2)	1.890
p_4	*r* Si–C difference	a - b,c,d	0.017(5)	0.016(5)
p_5	*r* C–C average	a,b,c,d	1.529(3)	1.526
p_6	*r* C–C difference [C(1)–C(4) - C(4)–C(5)] [c]	a,b,c,d	0.007(2)	0.007(2)
p_7	*r* C–C difference	b,c,d - a	0.002(1)	0.003(1)
p_8	*r* C–N average	a,b,c,d	1.461(1)	1.454
p_9	*r* C–N difference [C(5)–N - C(7/8)–N] [c]	a,b,c,d	0.004(2)	0.004(2)
p_{10}	*r* C(4)–N difference [c]	a - b,c,d	0.004(2)	0.004(2)
p_{11}	*r* Si–H average	a,b,c,d	1.491(7)	1.482
p_{12}	*r* Si–H difference	a	0.012(5)	0.012(5)
p_{13}	*r* C–H	a,b,c,d	1.105(1)	1.095
p_{14}	*a* C–N–C average	a,b,c,d	110.1(2)	110.4(10)
p_{15}	*a* C–N–C difference	a	1.7(5)	1.6(5)
p_{16}	*a* C–N–C difference	c	1.7(5)	1.6(5)
p_{17}	*a* C–N–C difference	b,d	2.0(5)	1.6(5)
p_{18}	*a* Si–C–C average	b,c,d	113.7(3)	113.5
p_{19}	*a* Si–C–C difference	b – c,d	2.1(5)	1.9(5)
p_{20}	*a* C–C–C, C–C–N average	b,c,d	113.2(3)	112.8
p_{21}	*a* C–C–C minus C–C–N	b,c,d	1.6(4)	1.0(5)
p_{22}	*a* C–C–C difference	d – b,c	1.6(5)	1.3(5)
p_{23}	*d* H–Si–C–C	c	180.0(20)	180.1(20)
p_{24}	*d* H–Si–C–C	b	188.4(20)	188.0(20)
p_{25}	*d* H–Si–C–C	d	180.1(20)	180.1(20)
p_{26}	*d* Si–C–C–C	c	180.9(17)	182.1(20)
p_{27}	*d* Si–C–C–C	b	300.3(16)	302.6(20)
p_{28}	*d* Si–C–C–C	d	180.1(20)	180.3(20)
p_{29}	*d* C–C–C–N	c	58.8(18)	55.6(20)
p_{30}	*d* C–C–C–N	b	310.3(14)	309.4(20)
p_{31}	*d* C–C–C–N	d	187.6(19)	186.9(20)
p_{32}	*d* C–C–N–C(28)	c	67.0(17)	65.9(20)
p_{33}	*d* C–C–N–C(51)	b	170.9(13)	171.4(20)
p_{34}	*d* C–C–N–C(73)	d	170.1(19)	171.3(20)
p_{35}	*a* H–C–H average	a,b,c,d	107.0(3)	107.5(5)
p_{36}	*a* H–C–H difference	a,b,c,d	1.9(5)	2.0(5)
p_{37}	*a* Methyl tilt	a,b,c,d	1.3(5)	1.5(5)
p_{38}	*d* H–C(7)–N–C(5)	a	64.3(20)	64.3(20)
p_{39}	*d* H–C(8)–N–C(5)	a	-61.3(20)	-61.5(20)
p_{40}	*d* H–C(28)–N–C(26)	c	56.8(20)	56.9(20)
p_{41}	*d* H–C(29)–N–C(26)	c	-61.2(20)	-61.4(20)
p_{42}	*d* H–C(51)–N–C(45)	b	60.8(20)	61.0(20)
p_{43}	*d* H–C(50)–N–C(45)	b	-57.6(19)	-58.0(20)
p_{44}	*d* H–C(73)–N–C(70)	d	61.2(20)	61.2(20)
p_{45}	*d* H–C(72)–N–C(70)	d	-57.4(20)	-57.5(20)
p_{46}	*a* C–Si···N	a	73.1(11)	76.3(100)
p_{47}	*a* Si···N–C	a	94.7(10)	97.4(100)
p_{48}	*d* C–Si···N–C4	a	2.5(35)	9.0(100)
p_{49}	*d* N–C5···C1–C4	a	124.3(21)	125.1(200)
p_{50}	*a* H–Si–H average	a,b,c,d	107.7(10)	108.1(10)
p_{51}	*a* H–Si–H difference of average angles	b,c,d - a	1.1(5)	1.1(5)

p_{52}	*a* H–Si–H difference in H3a	a	7.5(5)	7.5(5)
p_{53}	*a* H–Si–C	a	104.1(10)	104.2(10)
p_{54}	*d* H–Si–C···N	a	178.3(20)	178.4(20)
p_{55}	*d* Si···C–N–C(7/8) difference	a	2.9(19)	4.7(20)
p_{56}	Ratio of H3c	c /(b + c + d)	0.48(7)	0.29
p_{57}	Ratio of H3b	b / (b + d)	0.74(13)	0.68
p_{58}	*r* Si–C difference	b - c,d	0.004(2)	0.004(2)
	Dependant parameters			
d_1	*r* Si–H, C–N difference	a,b,c,d	0.030(8)	0.028(10)
d_2	*a* Si–C–C	a	117.7(5)	117.1
d_3	*a* C–C–C	a	110.3(6)	110.9
d_4	*a* C–C–N	a	111.7(5)	110.2
d_5	*a* Si–C–C	b	115.1(4)	114.8
d_6	*a* C–C–C	b	112.4(4)	112.9
d_7	*a* C–C–N	b	114.0(3)	113.0
d_8	*r* Si–C	a	1.897(4)	1.898
d_9	*r* Si–C	b	1.882(2)	1.885
d_{10}	*r* Si–C	c	1.878(2)	1.880
d_{11}	*r* Si–C	d	1.878(2)	1.882
d_{12}	*r* C(1)–C(4)	a	1.532(3)	1.528
d_{13}	*r* C(4)–C(5)	a	1.525(3)	1.520
d_{14}	*r* C(45)–C(47)	b	1.534(3)	1.531
d_{15}	*r* C(47)–C(48)	b	1.527(3)	1.524
d_{16}	*r* C(24)–C(25)	c	1.534(3)	1.529
d_{17}	*r* C(25)–C(26)	c	1.527(3)	1.524
d_{18}	*r* C(5)–N	a	1.465(2)	1.459
d_{19}	*r* C(7)–N	a	1.459(2)	1.453
d_{20}	*r* C(5)–N [c]	b,c,d	1.461(2)	1.455
d_{21}	*r* C(7)–N [c]	b,c,d	1.459(2)	1.452
d_{22}	*r* C–C–C–N difference	a,b,c,d	0.069(4)	0.072(5)
d_{23}	*d* Si–C–C–C	a	63.0(34)	52.9
d_{24}	*d* C–C–C–N	a	62.6(24)	60.6

[a] The numbers in parentheses are one standard deviation, obtained from the least-squares fit.
[b] Where the theoretical value is followed by a number in brackets, this value was used as a restraint in the GED refinement with an uncertainty equal to the number in parentheses.
[c] The atom numbers refer to those in Figure S1 for H3a and those in topologically equivalent positions in the other conformers.

Table S3 – Least-squares correlation matrix. All elements have been multiplied by 100 and only off-diagonal elements with greater than 50% correlation have been included. k_1, k_2 and k_3 are the scale factors for datasets 1, 2 and 3, respectively.

	p_4	p_{14}	p_{20}	p_{46}	p_{48}	p_{49}	u_{120}	u_{571}	k_2	k_3
p_2				-74	-51					
p_3	67									
p_5			-55				-73			
p_8		-80					54			
p_{14}							-52			
p_{18}								53		

p_{20}					-51		
p_{27}		-52	-50				
p_{46}			90	-50			
p_{47}			-65	86			
p_{48}				-77			
u_{55}						50	
u_{120}						62	53
k_1						59	
k_2							56

Table S4 – Selected inter-nuclear distances (r_a), refined (GED) and calculated (MP2/6-31G*) amplitudes of vibration (u), and distance corrections (k_{h1}) for curvilinear motion.

	Atom pair	Distance (r_a)	u	k_{h1}	u (MP2/6-31G*)
$u3$	C(1)-H(11)	1.103(1)	0.081(1)	0.004	0.076
$u466$	C(45)-H(56)	1.103(1)	0.081(Tied to $u3$)	0.004	0.076
$u4$	C(1)-H(12)	1.103(1)	0.081(Tied to $u3$)	0.004	0.076
$u465$	C(45)-H(55)	1.103(1)	0.081(Tied to $u3$)	0.004	0.076
$u697$	C(67)-H(78)	1.103(1)	0.081(Tied to $u3$)	0.004	0.076
$u696$	C(67)-H(77)	1.103(1)	0.081(Tied to $u3$)	0.004	0.076
$u238$	C(24)-H(42)	1.103(1)	0.081(Tied to $u3$)	0.004	0.076
$u18$	C(7)-H(22)	1.103(1)	0.082(Tied to $u3$)	0.004	0.077
$u20$	C(8)-H(18)	1.103(1)	0.082(Tied to $u3$)	0.004	0.077
$u237$	C(24)-H(41)	1.103(1)	0.081(Tied to $u3$)	0.004	0.076
$u709$	C(72)-H(79)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u712$	C(73)-H(82)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u713$	C(73)-H(83)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u252$	C(29)-H(35)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u479$	C(50)-H(65)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u481$	C(51)-H(61)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u19$	C(8)-H(17)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u247$	C(28)-H(30)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u478$	C(50)-H(64)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u250$	C(29)-H(33)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u249$	C(28)-H(32)	1.103(1)	0.082(Tied to $u3$)	0.004	0.077
$u710$	C(72)-H(80)	1.103(1)	0.082(Tied to $u3$)	0.004	0.077
$u21$	C(8)-H(19)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u483$	C(51)-H(63)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u16$	C(7)-H(20)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u248$	C(28)-H(31)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u482$	C(51)-H(62)	1.103(1)	0.082(Tied to $u3$)	0.004	0.077
$u480$	C(50)-H(66)	1.103(1)	0.082(Tied to $u3$)	0.004	0.077
$u714$	C(73)-H(84)	1.103(1)	0.082(Tied to $u3$)	0.004	0.077
$u251$	C(29)-H(34)	1.103(1)	0.082(Tied to $u3$)	0.004	0.077
$u711$	C(72)-H(81)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u17$	C(7)-H(21)	1.103(1)	0.080(Tied to $u3$)	0.004	0.075
$u10$	C(4)-H(14)	1.103(1)	0.081(Tied to $u3$)	0.004	0.076
$u471$	C(47)-H(57)	1.103(1)	0.081(Tied to $u3$)	0.004	0.076
$u240$	C(25)-H(39)	1.103(1)	0.081(Tied to $u3$)	0.004	0.076
$u12$	C(5)-H(15)	1.103(1)	0.082(Tied to $u3$)	0.004	0.077
$u474$	C(48)-H(59)	1.103(1)	0.083(Tied to $u3$)	0.004	0.078
$u703$	C(69)-H(86)	1.103(1)	0.081(Tied to $u3$)	0.004	0.076
$u706$	C(70)-H(88)	1.103(1)	0.083(Tied to $u3$)	0.004	0.078
$u243$	C(26)-H(43)	1.103(1)	0.083(Tied to $u3$)	0.004	0.078

*u*241	C(25)-H(40)	1.103(1)	0.081(Tied to *u*3)	0.004	0.076
*u*472	C(47)-H(58)	1.103(1)	0.081(Tied to *u*3)	0.004	0.076
*u*9	C(4)-H(13)	1.103(1)	0.081(Tied to *u*3)	0.004	0.076
*u*702	C(69)-H(85)	1.103(1)	0.081(Tied to *u*3)	0.004	0.076
*u*705	C(70)-H(87)	1.103(1)	0.081(Tied to *u*3)	0.004	0.076
*u*475	C(48)-H(60)	1.103(1)	0.081(Tied to *u*3)	0.004	0.076
*u*13	C(5)-H(16)	1.103(1)	0.081(Tied to *u*3)	0.004	0.076
*u*244	C(26)-H(44)	1.103(1)	0.081(Tied to *u*3)	0.004	0.076
*u*707	N(71)-C(72)	1.458(2)	0.053(Tied to *u*14)	0.001	0.048
*u*245	N(27)-C(28)	1.458(2)	0.053(Tied to *u*14)	0.001	0.048
*u*477	N(49)-C(51)	1.458(2)	0.053(Tied to *u*14)	0.001	0.048
*u*246	N(27)-C(29)	1.458(2)	0.053(Tied to *u*14)	0.001	0.048
*u*476	N(49)-C(50)	1.458(2)	0.053(Tied to *u*14)	0.001	0.048
*u*708	N(71)-C(73)	1.458(2)	0.053(Tied to *u*14)	0.001	0.048
*u*14	N(6)-C(7)	1.458(2)	0.053(1)	0.001	0.048
*u*15	N(6)-C(8)	1.458(2)	0.053(Tied to *u*14)	0.001	0.048
*u*704	C(70)-N(71)	1.460(2)	0.054(Tied to *u*14)	0.001	0.048
*u*242	C(26)-N(27)	1.460(2)	0.054(Tied to *u*14)	0.001	0.048
*u*473	C(48)-N(49)	1.460(2)	0.054(Tied to *u*14)	0.001	0.048
*u*11	C(5)-N(6)	1.465(2)	0.054(Tied to *u*14)	0.001	0.048
*u*469	Si(46)-H(54)	1.487(7)	0.096(Tied to *u*14)	0.003	0.087
*u*468	Si(46)-H(53)	1.487(7)	0.096(Tied to *u*14)	0.003	0.087
*u*233	Si(23)-H(36)	1.487(7)	0.096(Tied to *u*14)	0.003	0.087
*u*700	Si(68)-H(76)	1.487(7)	0.096(Tied to *u*14)	0.003	0.087
*u*699	Si(68)-H(75)	1.487(7)	0.096(Tied to *u*14)	0.003	0.087
*u*235	Si(23)-H(38)	1.487(7)	0.096(Tied to *u*14)	0.003	0.087
*u*234	Si(23)-H(37)	1.487(7)	0.096(Tied to *u*14)	0.003	0.087
*u*698	Si(68)-H(74)	1.487(7)	0.096(Tied to *u*14)	0.003	0.087
*u*467	Si(46)-H(52)	1.487(7)	0.096(Tied to *u*14)	0.003	0.086
*u*7	Si(2)-H(10)	1.487(7)	0.096(Tied to *u*14)	0.004	0.087
*u*5	Si(2)-H(3)	1.487(7)	0.096(Tied to *u*14)	0.004	0.087
*u*6	Si(2)-H(9)	1.499(8)	0.097(Tied to *u*14)	0.004	0.088
*u*8	C(4)-C(5)	1.524(3)	0.055(Tied to *u*14)	0.001	0.050
*u*470	C(47)-C(48)	1.526(3)	0.056(Tied to *u*14)	0.001	0.050
*u*239	C(25)-C(26)	1.526(3)	0.056(Tied to *u*14)	0.001	0.050
*u*701	C(69)-C(70)	1.526(3)	0.055(Tied to *u*14)	0.001	0.050
*u*2	C(1)-C(4)	1.531(3)	0.056(Tied to *u*14)	0.001	0.050
*u*695	C(67)-C(69)	1.533(3)	0.056(Tied to *u*14)	0.001	0.051
*u*464	C(45)-C(47)	1.533(3)	0.056(Tied to *u*14)	0.001	0.051
*u*236	C(24)-C(25)	1.533(3)	0.056(Tied to *u*14)	0.001	0.051
*u*694	C(67)-Si(68)	1.877(3)	0.055(Tied to *u*1)	0.001	0.052
*u*232	Si(23)-C(24)	1.877(2)	0.055(Tied to *u*1)	0.001	0.052
*u*463	C(45)-Si(46)	1.882(2)	0.056(Tied to *u*1)	0.001	0.052
*u*1	C(1)-Si(2)	1.896(4)	0.056(1)	0.001	0.053
*u*118	C(7)...C(8)	2.374(5)	0.063(Tied to *u*90)	0.000	0.068
*u*795	C(72)...C(73)	2.381(3)	0.063(Tied to *u*90)	0.000	0.068
*u*564	C(50)...C(51)	2.381(3)	0.063(Tied to *u*90)	0.000	0.068
*u*333	C(28)...C(29)	2.382(3)	0.063(Tied to *u*90)	0.000	0.068
*u*766	C(70)...C(73)	2.383(3)	0.064(Tied to *u*90)	0.000	0.069
*u*535	C(48)...C(51)	2.383(3)	0.062(Tied to *u*90)	0.000	0.068
*u*304	C(26)...C(29)	2.385(3)	0.064(Tied to *u*90)	0.001	0.069
*u*90	C(5)...C(7)	2.405(3)	0.062(2)	0.001	0.068
*u*91	C(5)...C(8)	2.405(3)	0.064(Tied to *u*90)	0.001	0.069
*u*303	C(26)...C(28)	2.409(5)	0.062(Tied to *u*90)	0.000	0.068
*u*765	C(70)...C(72)	2.411(5)	0.063(Tied to *u*90)	0.000	0.068

*u*534	C(48)...C(50)	2.412(5)	0.063(Tied to *u*90)	0.000	0.068
*u*507	Si(46)...H(56)	2.463(3)	0.110(Tied to *u*90)	-0.003	0.119
*u*506	Si(46)...H(55)	2.464(3)	0.110(Tied to *u*90)	-0.002	0.119
*u*45	Si(2)...H(12)	2.466(5)	0.112(Tied to *u*90)	-0.003	0.121
*u*737	Si(68)...H(77)	2.467(3)	0.110(Tied to *u*90)	-0.003	0.119
*u*267	Si(23)...H(42)	2.467(3)	0.110(Tied to *u*90)	-0.003	0.119
*u*738	Si(68)...H(78)	2.467(3)	0.110(Tied to *u*90)	-0.003	0.119
*u*266	Si(23)...H(41)	2.467(3)	0.110(Tied to *u*90)	-0.003	0.119
*u*44	Si(2)...H(11)	2.468(5)	0.110(Tied to *u*90)	-0.002	0.119
*u*75	C(4)...N(6)	2.470(7)	0.060(Tied to *u*90)	-0.003	0.065
*u*23	C(1)...C(5)	2.502(9)	0.066(Tied to *u*90)	-0.004	0.071
*u*287	C(25)...N(27)	2.503(4)	0.061(Tied to *u*90)	-0.002	0.066
*u*518	C(47)...N(49)	2.503(4)	0.061(Tied to *u*90)	-0.002	0.065
*u*749	C(69)...N(71)	2.504(4)	0.063(Tied to *u*90)	-0.002	0.068
*u*715	C(67)...C(70)	2.517(9)	0.068(Tied to *u*90)	-0.002	0.073
*u*484	C(45)...C(48)	2.540(6)	0.064(Tied to *u*90)	-0.003	0.070
*u*270	C(24)...C(26)	2.540(6)	0.065(Tied to *u*90)	-0.002	0.071
*u*253	Si(23)...C(25)	2.844(6)	0.097(Tied to *u*41)	-0.004	0.090
*u*732	Si(68)...C(69)	2.845(6)	0.097(Tied to *u*41)	-0.004	0.090
*u*501	Si(46)...C(47)	2.882(6)	0.091(Tied to *u*41)	-0.004	0.084
*u*41	Si(2)...N(6)	2.911(35)	0.205(6)	0.013	0.190
*u*39	Si(2)...C(4)	2.933(8)	0.082(Tied to *u*41)	-0.004	0.076
*u*24	C(1)...N(6)	2.963(23)	0.128(Tied to *u*41)	-0.009	0.119
*u*288	C(25)...C(28)	3.015(19)	0.147(Tied to *u*41)	-0.001	0.136
*u*271	C(24)...N(27)	3.019(17)	0.134(Tied to *u*41)	-0.002	0.124
*u*750	C(69)...C(72)	3.034(21)	0.159(Tied to *u*41)	0.000	0.148
*u*76	C(4)...C(7)	3.163(39)	0.121(Tied to *u*41)	-0.003	0.112
*u*502	Si(46)...C(48)	3.301(19)	0.145(Tied to *u*40)	-0.004	0.155
*u*40	Si(2)...C(5)	3.360(33)	0.119(6)	-0.002	0.128
*u*486	C(45)...C(50)	3.546(25)	0.133(Tied to *u*40)	-0.018	0.142
*u*272	C(24)...C(28)	3.662(41)	0.279(Tied to *u*42)	-0.019	0.273
*u*503	Si(46)...N(49)	3.672(37)	0.272(Tied to *u*42)	-0.014	0.266
*u*77	C(4)...C(8)	3.703(12)	0.077(Tied to *u*42)	-0.011	0.075
*u*42	Si(2)...C(7)	3.744(38)	0.236(10)	0.005	0.231
*u*751	C(69)...C(73)	3.753(4)	0.075(Tied to *u*42)	-0.017	0.073
*u*289	C(25)...C(29)	3.758(4)	0.073(Tied to *u*42)	-0.015	0.071
*u*520	C(47)...C(51)	3.767(4)	0.120(Tied to *u*42)	-0.002	0.118
*u*43	Si(2)...C(8)	3.784(39)	0.263(Tied to *u*42)	0.002	0.257
*u*25	C(1)...C(7)	3.938(28)	0.158(Tied to *u*42)	-0.017	0.154
*u*26	C(1)...C(8)	4.017(50)	0.167(Tied to *u*254)	-0.021	0.166
*u*733	Si(68)...C(70)	4.203(6)	0.083(Tied to *u*254)	-0.023	0.082
*u*254	Si(23)...C(26)	4.215(4)	0.082(3)	-0.025	0.082
*u*487	C(45)...C(51)	4.224(19)	0.203(Tied to *u*254)	-0.012	0.202
*u*273	C(24)...C(29)	4.271(19)	0.155(Tied to *u*254)	-0.023	0.154
*u*717	C(67)...C(72)	4.432(19)	0.122(Tied to *u*254)	-0.026	0.121
*u*505	Si(46)...C(51)	4.510(44)	0.267(Tied to *u*504)	-0.037	0.275
*u*255	Si(23)...N(27)	4.738(14)	0.149(Tied to *u*504)	-0.034	0.154
*u*504	Si(46)...C(50)	4.761(41)	0.330(15)	-0.022	0.341
*u*256	Si(23)...C(28)	5.072(44)	0.327(Tied to *u*504)	-0.036	0.337
*u*734	Si(68)...N(71)	5.323(7)	0.111(5)	-0.031	0.110
*u*735	Si(68)...C(72)	5.716(28)	0.199(10)	-0.028	0.204
*u*257	Si(23)...C(29)	6.059(16)	0.174(8)	-0.065	0.165
*u*736	Si(68)...C(73)	6.516(8)	0.105(5)	-0.052	0.105

Table S5 – Refined GED atomic coordinates (distances in Å).

Atom	X	Y	Z
C1	0.551413	0.078174	1.813064
Si2	0.000000	0.000000	0.000000
H3	0.375020	-1.250997	-0.716122
C4	1.888297	0.759530	2.121076
C5	3.033267	0.000000	1.460229
N6	2.912377	0.000000	0.000000
C7	3.510014	1.204395	-0.567031
C8	3.570064	-1.170265	-0.572002
H9	-1.499032	-0.040622	0.075352
H10	0.303837	1.218454	-0.800949
H11	-0.237640	0.592172	2.390624
H12	0.593229	-0.953974	2.204594
H13	1.871937	1.805669	1.766535
H14	2.046242	0.809650	3.213283
H15	3.998262	0.450048	1.754535
H16	3.055014	-1.039818	1.832625
H17	3.447600	-1.179572	-1.669859
H18	4.651851	-1.191869	-0.349192
H19	3.120523	-2.096144	-0.170709
H20	3.341247	1.237963	-1.658253
H21	3.050180	2.105282	-0.122814
H22	4.599081	1.253918	-0.388555
Si23	10.000000	0.000000	0.000000
C24	11.877908	0.000000	0.000000
C25	12.477911	1.411993	0.000000
C26	14.004706	1.395943	-0.022703
N27	14.575645	0.704981	-1.176579
C28	14.295158	1.423550	-2.415226
C29	16.018665	0.574889	-1.003287
H30	14.775468	0.914595	-3.270001
H31	13.206889	1.452245	-2.602899
H32	14.664028	2.464464	-2.386813
H33	16.458761	0.028294	-1.856471
H34	16.520740	1.556271	-0.931280
H35	16.243868	0.008051	-0.082226
H36	9.468276	0.695692	1.204885
H37	9.468276	-1.391307	0.000044
H38	9.468276	0.695615	-1.204929
H39	12.127343	1.962489	0.891308
H40	12.101216	1.973591	-0.873546
H41	12.244535	-0.554148	-0.882541
H42	12.244535	-0.554148	0.882541
H43	14.377674	2.435592	-0.002736
H44	14.375221	0.920724	0.903181
C45	1.882101	10.000000	0.000000
Si46	0.000000	10.000000	0.000000
C47	2.532930	11.389298	0.000000
C48	2.134619	12.218963	-1.218557
N49	2.284987	11.517377	-2.491348
C50	3.689484	11.273172	-2.802817
C51	1.680971	12.309500	-3.557634
H52	-0.531724	10.513065	-1.293251

H53	-0.531724	8.623479	0.202298
H54	-0.531724	10.863456	1.090953
H55	2.238616	9.439293	0.882541
H56	2.238616	9.439293	-0.882541
H57	2.252267	11.928864	0.922210
H58	3.632020	11.282507	0.031132
H59	2.740270	13.142576	-1.240924
H60	1.084947	12.544693	-1.106920
H61	0.607504	12.471263	-3.352997
H62	2.160529	13.298793	-3.665795
H63	1.768232	11.780620	-4.523576
H64	4.141412	10.613687	-2.040442
H65	3.782662	10.774238	-3.784018
H66	4.277979	12.207420	-2.837876
C67	11.877908	10.000000	0.000000
Si68	10.000000	10.000000	0.000000
C69	12.477911	11.411993	0.000000
C70	14.003867	11.354317	-0.003056
N71	14.649004	12.653252	0.174127
C72	14.444432	13.512938	-0.987058
C73	16.079121	12.460487	0.390616
H74	9.468276	8.608695	0.002136
H75	9.468276	10.697503	1.203838
H76	9.468276	10.693803	-1.205974
H77	12.244535	9.445853	-0.882541
H78	12.244535	9.445853	0.882541
H79	14.971670	14.473888	-0.849327
H80	14.815466	13.050776	-1.919321
H81	13.369117	13.729498	-1.118107
H82	16.575764	13.433445	0.555153
H83	16.249813	11.834761	1.284878
H84	16.568925	11.968410	-0.468644
H85	12.120077	11.973705	-0.881367
H86	12.123557	11.972226	0.883711
H87	14.341571	10.670712	0.796327
H88	14.346985	10.906631	-0.952910

Least-squares fitting procedure to determine the relative amount of *H3a* in *H3* by a combination of IR spectroscopy and first-principles computations

IR spectra based on the harmonic approximation of the PES have been calculated for eight conformers of **H3** (**H3a-h**) using the RI-MP2(fc)/TZVPP method and numerical gradient computations, (see Computational Part for references).

- In a first step the calculated IR intensities and wavelengths were tranformed into simulated, continuous IR spectra by a convolution procedure using Gaussian functions $[G(\bar{\nu}; w_i, n_i, h_i)]$ with fixed half-widths w_i, maxima n_i at the calculated frequencies and heights h_i of the calculated intensities

$$^{MP2}IR_{\mathbf{H3x}}(\bar{\nu}) \xrightarrow[w_i\, fixed]{convolution} {}^{sim}IR_{\mathbf{H3x}}(\bar{\nu}). \tag{1}$$

- A linear combination of all non-five-membered-ring conformers (**H3b-h**, each showing only one signal in the $\nu(SiH)$ region at similar wavelengths) with Boltzmann factors as conformer ratio coeffients was constructed

$$^{sim}IR_{open}(\bar{\nu}) = \sum_{x=b}^{h} {}^{sim}IR_{\mathbf{H3x}}(\bar{\nu}) \cdot e^{-\frac{^{MP2}\Delta G_0^{298.15}(\mathbf{H3a} \rightarrow \mathbf{H3x})}{RT}}. \tag{2}$$

- In a next step
  - a single Gaussian function $G_0 = G(\bar{\nu}; w_0, n_0, h_0)$, was fitted to the simulated open-ring conformer spectrum $[^{sim}IR_{open}(\bar{\nu})]$ in the Si-H stretching frequency region

$$^{sim}IR_{open}(\bar{\nu}) \xrightarrow[w_0,n_0,h_0]{fit} G_0, \quad \bar{\nu} \in [2000; 2400] \tag{3}$$

– and a linear combination of two Gaussian functions $G_1 = G(\bar{\nu}; w_1, n_1, h_1)$, $G_2 = G(\bar{\nu}; w_2, n_2, h_2)$ was fitted to the simulated IR spectrum ${}^{sim}IR_{\mathbf{H3a}}(\bar{\nu})$ of the five membered ring species **H3a** [showing one maximum n_1 for the $\nu_{as,sym}(SiH_2)$ and one n_2 for the $\nu_{trans}(SiH)$ vibrational mode]

$$ {}^{sim}IR_{\mathbf{H3a}}(\bar{\nu}) \xrightarrow[\substack{w_1\, n_1\, h_1 \\ w_2\, n_2\, h_2}]{fit} G_1 + G_2, \quad \bar{\nu} \in [2000; 2400]. \tag{4} $$

- Instead of fitting $aG_0 + b(G_1 + G_2)$ to the IR spectra via the parameters a and b, it was necessary to introduce further parameters and some assumptions on w_i, n_i and h_i for i = 0, ..., 2.

$$ -log[{}^{exp}IR(\bar{\nu})] \xrightarrow[\substack{a\, b\, c \\ n_0\, n_2}]{fit} a\,(\,b\, f_{\mathbf{H3a}} + (1-b)\, f_{open}), \quad \bar{\nu} \in [2050; 2250] \tag{5} $$

with

$$ f_{open} = G(\bar{\nu}; w_0 \cdot c, n_0, h_0) \tag{6} $$

$$ f_{\mathbf{H3a}} = G(\bar{\nu}; w_1 \cdot c, n_0, h_1) + G(\bar{\nu}; w_2 \cdot c, n_2, h2). \tag{7} $$

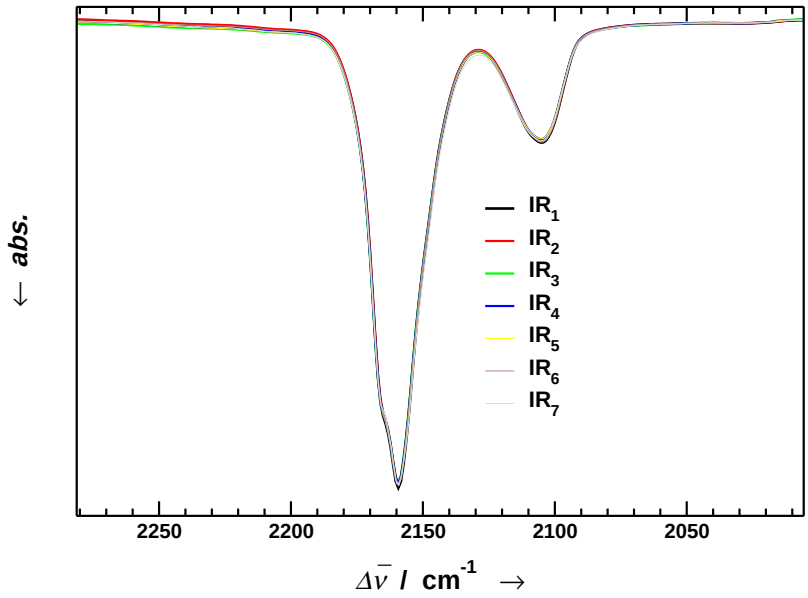
The parameters w_0, w_1, w_2 resulting from 3 and 4, are describing the width of the calculated peaks. They were kept at a constant ratio with respect to each others in f_{open} and $f_{\mathbf{H3a}}$, as well as the used peak heights h_0, h_1, h_2 within each of the two functions. This was necessary since all information about the relative calculated conformer- and peak-ratios is kept in these six parameters. In addition to a, b and c, the peak positions n_0 and n_2 were included as parameters into the fitting procedure, since the difference between the experimentally observed frequencies $\nu_{as,sym}(SiH_2) - \nu_{trans}(SiH)$ is considerably smaller than the calculated difference at the MP2 level of theory. In order to avoid a discrimination of wavelength differences within **H3a** and those between **H3b-h**, n_1 was not refined independently but was set to be equal n_0 in $f_{\mathbf{H3a}}$. The ratios b_i of conformere **H3a** resulting from the fitting procedure (applied to seven independently recorded IR spectra) are given in the following table:

i	b_i	σ^a
1	0.239305	0.005854
2	0.239157	0.005880
3	0.236933	0.005852
4	0.234722	0.005806
5	0.233105	0.005807
6	0.239305	0.005854
7	0.235645	0.005928
mean	0.236882	
max.		0.005928
σ^b	0.002494	

[a] asymptotic standard error

[b] standard deviation

After conversion into absorbances $\{-log[^{exp}IR(\bar{\nu})]\}$, all IR spectra are overlapping satisfactorily:



Cartesian Coordinates for Experimental and Calculated Structures in Atomic Units

DFT[a]/SV(P)

H3a

3.27215232611767	0.42116360200535	1.58779568378074	c
0.95214572994985	-0.29190081674796	3.19547798027996	c
-1.51460792265173	0.88787019178127	2.22682714032676	c
-2.14841947822118	0.03198326178200	-0.33206804816926	n
-3.69146145164985	1.83018984179622	-1.73183164825107	c
3.11857767736742	-0.15536773941154	-1.98353120210590	si
-3.23865228982316	-2.49577362618229	-0.39077086290114	c
1.85310690414652	1.90968571696504	-3.48338303560378	h

5.85408083841311	-0.13271023541135	-2.86244446431919	h
2.11081967567388	-2.72582606865758	-2.69299395404807	h
4.96221775793916	-0.62311827027119	2.28644633273164	h
3.72983684237382	2.46442219837306	1.85002097623432	h
0.75723691365680	-2.38695663772500	3.27184005936754	h
1.23721836502461	0.32066871204013	5.19155796584508	h
-3.10084200909895	0.51424347009062	3.59192344663596	h
-1.27248361293479	2.97690840720978	2.15441130016917	h
-3.97753277301189	1.14031276987421	-3.69629866189628	h
-5.60949493956593	2.13773319237998	-0.86588160365880	h
-2.71552397965009	3.68726982425225	-1.84052744637605	h
-3.44491346497740	-3.13667963311546	-2.38118419325518	h
-1.98299340092734	-3.86570695953677	0.58273368791628	h
-5.15089881745374	-2.58465208288305	0.53684411385035	h

H3b

2.71417569978841	1.61263865009877	1.02693014500181	c
4.75982000005389	-0.62808778729120	-0.92023827598647	si
0.61729781672058	0.40353224835598	2.65802830679799	c
-1.48177939552885	-1.12133602960081	1.32711494387297	c
-3.31433588684043	0.39090488869854	-0.10268419862608	n
-2.63029872662299	0.78349795882088	-2.73629658222399	c
-5.89033830917512	-0.54797590294689	0.11302650305767	c
3.37270431836960	-1.78230569505078	-3.12689425560966	h
7.00384294570833	0.79392149213991	-1.95889695657874	h
5.72915618325797	-2.75527556809218	0.71710146826077	h

4.04675147355196	2.63431662752350	2.30196682198440	h
1.92956376517602	3.09867486292919	-0.24117427726257	h
1.52999565031043	-0.89469790978572	4.04656438444043	h
-0.32834150240996	1.90954508732247	3.78585061750833	h
-2.54105072142687	-2.11809557561650	2.84327801226974	h
-0.63247304028463	-2.65888579637416	0.12353015458093	h
-7.20961948573759	0.77218227409325	-0.85661289357884	h
-6.17522251128418	-2.47675160894110	-0.74895467741320	h
-6.46551988954620	-0.65049637525686	2.13182258541093	h
-3.97662178801554	2.12880977135281	-3.63175067028752	h
-0.71206119680793	1.61069812007678	-2.89854179679157	h
-2.65038241746490	-1.01217790400411	-3.88434990844742	h

H3c

-5.69504866468237	-0.40462615017112	-0.38697002905296	si
-2.30707937838620	-0.74525928958178	0.74420613157924	c
-0.74796135918366	1.71407302542910	0.71668128355375	c
2.04499864328317	1.31051696391578	1.43861987561033	c
3.38550157095676	-0.47961139072955	-0.18395529427593	n
3.85083897747643	0.48661707829168	-2.71446847821698	c
5.69103744168083	-1.42316088120424	0.97616842871958	c
4.75500799953808	-1.00298661001043	-3.89011230615387	h
2.04978466022555	1.01964873223622	-3.65274119361913	h
5.12368783947872	2.19670863064989	-2.73641364482269	h
6.55729213388544	-2.89674994618589	-0.24881364564620	h
7.15969886956068	0.08710782348940	1.30086863278611	h

5.25641229219666	-2.30477954563742	2.83424853831580	h
-7.13981606037778	1.44989938325062	1.23284225831665	h
-7.05308838968696	-2.91087668414981	-0.29105016309046	h
-5.76879686624689	0.54665396152023	-3.07772921154553	h
-1.55737956824194	3.11222357781584	2.06724624245491	h
-0.87094093601019	2.63142986100723	-1.17587858466439	h
-1.33832554501857	-2.18539696600608	-0.44837763866440	h
-2.33975982801168	-1.55351750538952	2.69179165909890	h
3.02967553764093	3.20090864559867	1.49645541625589	h
2.11133886792333	0.54796695068044	3.39924851019594	h

H3d

3.04320796647078	-1.16878426786011	0.69903473270214	c
6.18073957272206	0.31409802606399	-0.23624082763876	si
0.69510877375609	0.24333066400431	-0.28989724334182	c
-1.79062231457118	-1.02554293237868	0.52810976281052	c
-4.05694240656760	0.10739154811188	-0.56753535392036	n
-4.60420180377369	2.62029443417054	0.40090890382285	c
-6.24300216527038	-1.54428904893829	-0.36377235202512	c
8.35837170280816	-1.18973166578992	0.82759041557401	h
6.45345345602450	0.40360536959311	-3.07409741413402	h
6.36630132404391	2.98351892176360	0.75539023534176	h
2.98968563048787	-1.28810685401052	2.80391397606857	h
3.03936460875451	-3.16278167875473	0.01256686839429	h
-6.27967816405193	3.41341906043902	-0.58998831090170	h
-5.01758096623278	2.64304180671949	2.49378493673059	h

-2.99643469876531	3.92346151109308	0.05070543346348	h
-7.88193252741087	-0.68840958572832	-1.36500277682594	h
-5.83554944008513	-3.39950144144359	-1.26557653118856	h
-6.84437847616422	-1.91872560868586	1.64739833367155	h
0.74865635994432	2.23510041915952	0.38901208985254	h
0.71771222340784	0.33620432157320	-2.39289914562255	h
-1.73064729437584	-3.03501778211735	-0.09589637712415	h
-1.88379837625326	-1.07383763352947	2.66120644430617	h

H3e

-1.01185639743571	-5.35561333117457	-0.16343565104834	si
1.83185788429116	-3.27234294995634	0.57928788683507	c
1.83184477170416	-0.57437368235228	-0.53474223208532	c
-0.18659595888625	1.16056889624026	0.63168130458303	c
-0.33448596345092	3.66215143156288	-0.52704165698329	n
-2.66562868113618	4.96283787672831	0.12315374428361	c
1.86228341782508	5.23798034261126	-0.03515198078268	c
-2.78811032883078	6.77877028483433	-0.92936602764186	h
-4.32423684011567	3.79034793378133	-0.41924801029076	h
-2.84005855302397	5.41135049243249	2.20055644075637	h
1.65955909359987	7.06969730480595	-1.04531801332952	h
2.14254369974561	5.66764972228591	2.03562991030533	h
3.61421705282992	4.32473227283682	-0.74395541936513	h
-3.43010285023918	-4.39103847718299	1.00132679301375	h
-0.55534966911066	-7.98397564294950	0.84623933244729	h
-1.40298808648823	-5.52966404580982	-2.98484219259433	h

1.52677783268363	-0.63316590268386	-2.61682261849025	h
3.74219502301672	0.26146842110153	-0.24576401270891	h
3.51614019906641	-4.32060849253146	-0.13094755324977	h
2.05949137148695	-3.19661070601683	2.67482835984400	h
-2.07144646666030	0.25702076643361	0.38895160398800	h
0.13264145385792	1.28720958380097	2.73974864785600	h

H3f

-0.79934965978936	5.20448910331221	0.86888705849182	si
1.01641987960871	3.34319994656662	-1.62736818438691	c
1.76018483154050	0.60271755691625	-0.95722364661256	c
-0.51943544173748	-1.13948546171350	-0.50580256153266	c
0.12589385445731	-3.81885457063102	-0.34975851495000	n
1.61522008288136	-4.46246344942459	1.86893461192210	c
-2.08909929563619	-5.42867158868576	-0.57382162386148	c
2.12217839331825	-6.50169763927179	1.81379868127693	h
3.40684333201569	-3.37075669604550	1.90697166808040	h
0.58998230813330	-4.09985433762214	3.70441342151902	h
-1.50304530937899	-7.44733584304969	-0.62564899167731	h
-3.47255965651871	-5.20106608458549	1.03211253035555	h
-3.11159347159288	-5.00853785874637	-2.36209356323446	h
-3.47976252551704	4.29040775317643	1.19622520766800	h
-0.91209372397967	7.95128265080330	0.10550450513784	h
0.51524914993980	5.03021490255061	3.39573799173521	h
3.00656941492887	0.62869591865046	0.73881665713673	h
2.90093656499364	-0.22753865455827	-2.52082324867738	h

2.75977133700033	4.45268741707180	-2.03888955531728	h
-0.11114204440367	3.38002945140744	-3.40934230784306	h
-1.58785998053278	-0.49185737689081	1.22785390075277	h
-1.84987166770593	-0.91297330096458	-2.12212084200369	h

H3g

-0.80565036384727	-5.34947820051213	0.26910689429009	si
1.88782981873998	-3.10381055996914	-0.55440215015032	c
1.17512812959804	-0.34514942455705	-1.18100540875527	c
0.14503544570775	1.14052662596912	1.12005229491542	c
-0.45716447697372	3.80506741807558	0.75147279454157	n
1.69075511054398	5.44019066790942	0.28065123638906	c
-2.59257625588719	4.30688564566389	-0.89105801010612	c
1.10813859247553	7.45264832713958	0.49022041220004	h
3.19948239167434	5.06200546199970	1.69629362106010	h
2.55846251291549	5.24403474904621	-1.65424874079346	h
-3.17455406142005	6.32097462654989	-0.70009139144421	h
-2.22887989672060	3.95816427849650	-2.95996348350646	h
-4.22749788993874	3.11220989851284	-0.32295038831975	h
-2.09567678351312	-4.69607256750711	2.72698481705306	h
0.20831357440726	-8.00511943784952	0.50350504732261	h
-2.77915153192890	-5.32138333435427	-1.79373498653264	h
-0.24371184479410	-0.31561735264230	-2.73890868708356	h
2.87853795106062	0.64281989195778	-1.92827072041156	h
2.87718155081350	-3.97056742694726	-2.20080716733627	h
3.28197699051508	-3.15176128616804	1.02890601879709	h

-1.59837727189470	0.19399426918373	1.83417932304644	h
1.55631187738352	1.01590886374289	2.68448299536376	h

H3h

-5.97001452294174	0.64968836112377	0.03426199899051	si
-3.00719103109404	-1.37465183097155	-0.08019207826492	c
-0.50550302910248	0.11962431375397	-0.02019085313230	c
1.83363163966214	-1.64584903909586	-0.07766805825869	c
4.32742146341592	-0.48395634182317	-0.00617492309069	n
5.02091503507872	0.93993961870018	-2.24164761100665	c
4.96588885281082	0.78455247115165	2.33701757993631	c
7.07894059938716	1.37961493506213	-2.19144324593150	h
4.65561198709884	-0.20951235735805	-3.96451371111241	h
3.99593989955176	2.79228367139341	-2.47116245759014	h
7.03526789748488	1.16728960386719	2.39976657201287	h
3.97824786932560	2.64627849195435	2.64295836326039	h
4.49917927220755	-0.45674645609721	3.96903425887795	h
-6.06310864324733	2.44440164397853	-2.18193457068526	h
-6.02783218659179	2.19570308431152	2.43256511954549	h
-8.31140948249415	-0.98006195126178	-0.03316608471741	h
-0.43907390167799	1.31437721686124	1.71418423183423	h
-0.42413016070149	1.44664401164997	-1.65274884939956	h
-3.09330474914965	-2.56107548537887	-1.82224144591086	h
-3.09135346071777	-2.72768801539829	1.53635275623046	h
1.70029571848443	-2.97623984042877	1.55497859911479	h
1.72460760536437	-2.83509645792167	-1.81625510602921	h

SCF/TZVPP

H3a

3.20314500756381	0.50728922999925	1.66646744502990	c
0.82259614978194	-0.35937046754832	3.07453790452023	c
-1.62223205049966	0.82328243859105	2.11581452848281	c
-2.28807693718746	0.02587515788458	-0.42309932980148	n
-3.84311582628656	1.85719345883769	-1.71959548439261	c
3.48913877840137	-0.16395655685546	-1.83994607777060	si
-3.42891139566666	-2.45508245891896	-0.49516095230674	c
2.22309768635120	1.72325620648182	-3.46120208584174	h
6.22677779337502	-0.04347418239479	-2.46837746348432	h
2.60644218960830	-2.73659198226481	-2.49170717550244	h
4.83741618309233	-0.37656229296726	2.54179458960269	h
3.46754965505953	2.52891169388252	1.93300851120527	h
0.68839123664739	-2.40233037663675	3.00464158921443	h
1.01053926830874	0.12193826568328	5.06076985618548	h
-3.15208238287433	0.42255433417714	3.44428970037930	h
-1.38814887481553	2.85776983648659	2.10067980489130	h
-4.20121391145898	1.23121396861607	-3.63347583926784	h
-5.66756631262440	2.15301988377525	-0.79634693483234	h
-2.87862546299576	3.65672446891797	-1.81766056858441	h
-3.68704374431938	-3.04262353507001	-2.43677872281660	h
-2.22767681930146	-3.83406794629871	0.41079361916214	h
-5.26982624105684	-2.49927975797483	0.44140204682118	h

H3b

2.51379751446168	0.89561978716692	1.64280178037420	c
4.67330506810218	0.25883047776132	-1.12531587418066	si
0.63538611837189	-1.19472250743011	2.35942675041399	c
-1.35105508262099	-1.79255152232387	0.35255442534730	c
-2.82530572570484	0.36548116058120	-0.46673870384512	n
-4.20103981188849	-0.16952855481445	-2.76202365401991	c
-4.47930201120085	1.34194543872326	1.47231703708969	c
3.29774717958369	0.08281244054602	-3.55500903560089	h
6.54459039462109	2.33043501561212	-1.33788685725072	h
6.06229657354576	-2.14806287183812	-0.74858507462799	h
3.73427580982762	1.27072019540077	3.25250763706121	h
1.50792508196203	2.64094822707086	1.26626077189849	h
1.64847592035810	-2.93711495545859	2.74612819254705	h
-0.28653169800009	-0.69419849312403	4.11937298559973	h
-2.57394627350675	-3.29877818258408	1.07140162337267	h
-0.41480777871677	-2.55700138480905	-1.29982041316433	h
-5.49409972523679	2.96583042443776	0.75479933778736	h
-5.87057745632505	-0.04978410961812	2.10617138102793	h
-3.41184542273468	1.95429113048588	3.10162914724152	h
-5.17864480746308	1.51185744189091	-3.39491394657356	h
-2.90706035559631	-0.73975337451878	-4.23868022279957	h
-5.60443323700929	-1.66914602528355	-2.52587701590835	h

DFT^b/TZVPP

H3a

3.22783788508821	0.44392341565082	1.56293142682030	c
0.94970671010960	-0.31799158986603	3.15455442371768	c
-1.49376241302302	0.85215370622215	2.21305250403102	c
-2.08831464653403	0.03514820739195	-0.33765529637978	n
-3.65943410753215	1.82291324650739	-1.67205212045628	c
3.05895316930069	-0.14657108320484	-1.96360257434564	si
-3.17368397763016	-2.46948139907615	-0.41194407350130	c
1.79919326432508	1.87988380822063	-3.45426162570717	h
5.75443579041831	-0.14617638720682	-2.85169222735338	h
2.03985610514082	-2.68651430381995	-2.62727795957175	h
4.91467903792923	-0.54446532559439	2.23500140950549	h
3.62787061794808	2.46025405122829	1.82099302253310	h
0.77452159693017	-2.37790238781108	3.17958553783825	h
1.23102510642441	0.24598990122498	5.12492974620350	h
-3.06007459418241	0.44366471222009	3.52778686468277	h
-1.27167959681989	2.90762356699281	2.17966898840741	h
-3.95220250347562	1.18143853113393	-3.61058607130945	h
-5.53077292419541	2.06956943049054	-0.78807000705792	h
-2.72754524267774	3.66072795837744	-1.74420085664889	h
-3.38969862326138	-3.07545614718616	-2.37122167065290	h
-1.93821132778170	-3.82518365871992	0.52407291489129	h
-5.04249705911561	-2.54824598108971	0.50872736490359	h

H3b

2.46053020781151	0.95222596170509	1.60465354212185	c
4.68698343952701	0.23753259229859	-1.07779217049820	si
0.63973109011602	-1.17153354694236	2.31754928903333	c
-1.30693523340984	-1.76595341837420	0.28620491413607	c
-2.82252010646167	0.39068314515702	-0.45634042932846	n
-4.18354865731142	-0.10390679616355	-2.76690832509997	c
-4.52071853999914	1.20659504219179	1.51543756100527	c
3.35125560127843	-0.17082647475343	-3.52500335086415	h
6.49202938459997	2.37204494054244	-1.42696672412124	h
6.17113029495998	-2.09591514608963	-0.51583111646444	h
3.63570331774448	1.44683535100216	3.23346252669964	h
1.39107534203765	2.64964138426319	1.10944642271442	h
1.68535416127626	-2.91269984693052	2.70948431742817	h
-0.32085518158989	-0.69577354779980	4.08606948202911	h
-2.51153847044098	-3.34602241703141	0.93804767307658	h
-0.33185034973998	-2.43929029334194	-1.40816816924838	h
-5.57642469124584	2.86065079183386	0.88055015398212	h
-5.89731670535349	-0.27064209054013	2.04987148671320	h
-3.47486676084003	1.74407199941999	3.20736848118867	h
-5.20847081268680	1.58814280889229	-3.35250439014154	h
-2.86170851698276	-0.60441666784568	-4.26893828850180	h
-5.56766804632740	-1.65641005511474	-2.57947293618134	h

MP2^b/TZVPP

H3a

3.23569003573404	0.42708232201529	1.50762987975374	c
1.00269464681409	-0.30237046356463	3.18663084513250	c
-1.42817881057433	0.89569794953834	2.23541293859710	c
-1.97572970920523	0.03310194917608	-0.32451737393200	n
-3.59969886855464	1.79801936705994	-1.66014159065191	c
2.89158470404515	-0.15443052899778	-2.01484756195090	si
-3.10906519987924	-2.46890639711356	-0.32567327720453	c
1.65221988966284	1.89873453151591	-3.45408585413700	h
5.54669637158782	-0.18470995955836	-2.97584273115908	h
1.85425655869188	-2.67493541603694	-2.65005266936388	h
4.93057908426718	-0.58583330852799	2.10551952102710	h
3.66501413840044	2.43440889865560	1.75509828060790	h
0.79842973783569	-2.35352754945276	3.23383925917782	h
1.32484758076542	0.29462543587163	5.13510275145345	h
-3.02177320843965	0.51750544380255	3.51670200714238	h
-1.16977274606425	2.94233612675982	2.16509500283486	h
-3.91464777731435	1.12284114683844	-3.57822647652313	h
-5.44476474700484	2.02126987278684	-0.73217663750416	h
-2.68361896121847	3.63645241934385	-1.76228616730676	h
-3.34412593379944	-3.11003107914079	-2.26620290233770	h
-1.88824864865969	-3.80967339892185	0.63887244471845	h
-4.96543579189458	-2.47138122527855	0.60777981361323	h

H3b

2.47819256396648	0.88819452951350	1.73402115681085	c
4.32456477568956	0.27221001461416	-1.24859614476728	si
0.65783168650812	-1.22906514465381	2.49183500843952	c
-1.26753813276989	-1.84176559047834	0.43947644717454	c
-2.56637592545423	0.38650924743709	-0.51125801837504	n
-4.07634359444298	-0.28041792746475	-2.70246500011246	c
-4.16779336914466	1.49666376524695	1.41990863887654	c
2.69107868302121	0.22957439578736	-3.51833055752062	h
6.26787959365503	2.25686154683050	-1.59624418865962	h
5.61849624301921	-2.20982293242424	-1.06549813668398	h
3.83776105506668	1.21608312346312	3.25208134896903	h
1.43664327719649	2.64729763695042	1.46858839493273	h
1.71225013889439	-2.95636045830138	2.89538242552467	h
-0.31296744445364	-0.73179057805081	4.24179624106038	h
-2.62956359854857	-3.24881665447577	1.15877227883927	h
-0.30247563784089	-2.71495819714807	-1.16289938774162	h
-5.15856701162060	3.11872463923499	0.63351400749367	h
-5.58452774484143	0.14811331805956	2.13445439755012	h
-3.03631828975280	2.14837606933080	3.00751360200344	h
-5.00858851514011	1.39935108752620	-3.43828281960446	h
-2.85778693481668	-1.04848062859347	-4.17136009195406	h
-5.53703987456476	-1.69422487023940	-2.25404743321542	h

H3c

-5.61523994663003	-0.30055887420465	-0.37769982611318	si
-2.24440521666848	-0.89858225191248	0.56990559945044	c
-0.72656869494349	1.53352018794595	0.93090255981337	c
2.02888857118553	1.03385596447380	1.60542461426994	c
3.32341053452769	-0.56658993939930	-0.21830787139909	n
3.55361839222367	0.68276622336670	-2.64986140689467	c
5.81716547780145	-1.21332736501936	0.72548356836904	c
4.61692130174353	-0.52174954105037	-3.93411697939392	h
1.69999037302221	1.01010237092267	-3.47520640399323	h
4.53905323954188	2.51179657373150	-2.50234950766193	h
6.76196228609145	-2.45977715481485	-0.61079506551006	h
7.01418658324427	0.46624230517275	1.00936190257922	h
5.64350906591171	-2.19486177066729	2.52477412055863	h
-6.91879129636914	1.23882880870200	1.56673686375449	h
-7.02720009391302	-2.69445910606155	-0.70779127239132	h
-5.68455750965175	1.11662591076403	-2.79386417460137	h
-1.54708545050317	2.66580940538393	2.44884223500317	h
-0.83359140616732	2.70066235310337	-0.76682949898573	h
-1.33306309584260	-2.07232601021586	-0.85982887176022	h
-2.21612621861041	-2.00246403369057	2.31511743273441	h
3.02939649518419	2.85167960886514	1.83212932050046	h
2.09820103133001	0.06856089860301	3.42842060744034	h

H3d

2.98943979980790	-1.24649592200703	0.62319232441543	c
6.07303312069451	0.33031201379190	-0.18733452689914	si

0.68963105990303	0.25259945266616	-0.28836845411554	c
-1.76896596608222	-1.06536896482156	0.40855512774852	c
-4.00237804688339	0.12166415227303	-0.67170770503026	n
-4.44465295249132	2.59765988414549	0.42891322685555	c
-6.19458358891304	-1.47143155652782	-0.23160522294397	c
8.25123320205193	-1.16942354941846	0.72839515294403	h
6.29461958341251	0.63128449909789	-2.96172276903540	h
6.17981111617816	2.87126207172585	0.98464698286073	h
2.89910382957233	-1.50560009273249	2.66991688881522	h
2.97419994906691	-3.13720769525142	-0.20648237536424	h
-6.17144449873516	3.39157881516427	-0.35727357409330	h
-4.65297587403270	2.50534006307577	2.49958849471085	h
-2.89939069169584	3.87499700880280	-0.01437068248915	h
-7.85755230303232	-0.61076428744799	-1.08329515102007	h
-5.89755034240916	-3.31461208697641	-1.09473090747090	h
-6.57207954329262	-1.75073878142200	1.79671000661005	h
0.73993932474471	2.14273228911946	0.53287355774027	h
0.74167393803776	0.48368587430986	-2.33755245108035	h
-1.69278222793242	-3.00174047209709	-0.30082690021837	h
-1.92061256667330	-1.18698526753252	2.48862123291406	h

H3e

-1.01986625328390	-5.21180308233204	-0.17625532545220	si
1.82411903411252	-3.22740398537119	0.64997672338944	c
1.86023079213914	-0.57297600822819	-0.51279092053545	c
-0.21272282880189	1.10414637113187	0.55956593744016	c

-0.34982284348012	3.57821261111926	-0.63399713051665	n
-2.61592879435510	4.87956539561371	0.20943177781729	c
1.84946535284348	5.10557596632170	-0.02833027395242	c
-2.74731971990423	6.71066284047841	-0.71839448489844	h
-4.27709972302680	3.77368565350841	-0.28868178161768	h
-2.62728565900953	5.18955944087424	2.26797404337449	h
1.63585578985819	6.96769890012447	-0.87535265118713	h
2.08917984331835	5.34746045050832	2.02667670586904	h
3.55694034894470	4.25639715298509	-0.78887239541880	h
-3.35740945552962	-4.27006490267553	1.04141100886250	h
-0.61679887220040	-7.85431568716367	0.65249910613981	h
-1.40472014959190	-5.18100294671118	-2.95015611624664	h
1.61974447665509	-0.67540261015639	-2.55864467312690	h
3.70025013107059	0.28535235870658	-0.16548072774089	h
3.48090711243265	-4.28169360791059	0.01438667679616	h
1.98484842026764	-3.10291150193466	2.70511852673914	h
-2.04000886880298	0.19105155763635	0.27264196881486	h
0.04630250427152	1.28622714422100	2.62537628185663	h

H3f

-0.96466891512939	5.00358576104989	0.76081021691064	si
1.29452626722157	3.32639248270247	-1.43054364093974	c
1.93515453592144	0.60171470769538	-0.68320335105491	c
-0.39782425057478	-1.07694535248013	-0.61421005952942	c
0.19458556823452	-3.75692952151221	-0.44406468651390	n
1.40628149753025	-4.35382262653532	1.94656679122610	c

-2.11451104739317	-5.22236410127037	-0.68690981314231	c
1.73449387179217	-6.38135053127332	2.05302119741554	h
3.22183122112410	-3.40592825312901	2.09350471942692	h
0.23553233326678	-3.79547821626906	3.57649990527677	h
-1.67033150747098	-7.22969466806508	-0.61712344512415	h
-3.47800727880777	-4.80194521085128	0.82909085760050	h
-3.00896766534425	-4.81198821593454	-2.49316685053090	h
-3.58468176392205	4.06059506324945	0.48702945174594	h
-0.96824992557286	7.74901507390420	0.21580863315915	h
-0.16198499107043	4.61381836600680	3.41706705176650	h
2.85696533772843	0.60993092826914	1.16046461948481	h
3.26865300659581	-0.21522390538811	-2.02723727787246	h
3.02328263455845	4.45175657651843	-1.49112971160097	h
0.51492395598436	3.36985316812285	-3.34230795955712	h
-1.64261991968033	-0.50056522403116	0.96150737391406	h
-1.47084615641933	-0.78963478733909	-2.35496153975217	h

H3g

-0.81000758943015	-5.16430226556918	0.28542197740582	si
1.91568526771055	-3.03961838763759	-0.59671691871579	c
1.19216746062382	-0.29761795136917	-1.19283006799781	c
0.10380853227319	1.04963248727764	1.12327359401988	c
-0.52516784403085	3.71434866488544	0.84639733605086	n
1.66170596641254	5.28271066222301	0.33269006321784	c
-2.49834437427326	4.14806715191085	-1.00461718874728	c
1.12001636339692	7.26383355136734	0.47365751895655	h

3.12172484707157	4.91166668304196	1.73549104358919	h
2.47659717262450	4.98496076764612	-1.55474321753443	h
-3.11435968098519	6.10913809199184	-0.89242766817650	h
-1.89612691665584	3.78525133931791	-2.95959023140500	h
-4.11168582771548	2.93891523999345	-0.58911845137884	h
-1.80045251229033	-4.61430035639829	2.84326313359025	h
0.00433394481534	-7.84107103500944	0.22715577193282	h
-2.89344856690619	-4.81421054783255	-1.55549935608286	h
-0.18291682791793	-0.26871068852417	-2.73018958864265	h
2.85720922587700	0.71867061145701	-1.86049535549674	h
2.82801355428816	-3.89428058539333	-2.23915377268076	h
3.31502430605406	-3.08599690105870	0.92197928163028	h
-1.61478140165945	0.08193238479832	1.73489683705574	h
1.45735316819470	0.88819645217971	2.67653881963865	h

H3h

-5.82152627983882	0.66846928092391	0.01057536301265	si
-2.94177637803488	-1.41763165499799	-0.02805519341502	c
-0.46717561511674	0.08107315232131	0.00207218516359	c
1.81716838344159	-1.69562609521996	-0.02538203071054	c
4.31725986825981	-0.54832309394982	-0.00487844384345	n
4.81596320298009	0.95265304842575	-2.24191015252548	c
4.80397250545590	0.89778475735569	2.27091499561013	c
6.79830943395025	1.50715352254368	-2.25708241887251	h
4.44750353206427	-0.17342483539099	-3.92505803874073	h
3.67580575437513	2.68591763339627	-2.35063150624920	h

6.79342516322056	1.42331618484347	2.32810735177190	h
3.68549801501447	2.64372116225619	2.40020326834771	h
4.39367849182800	-0.25850990026696	3.92363050349591	h
-5.80683111810531	2.35271931324015	-2.22616835173175	h
-5.80937631308020	2.26373043910015	2.31165597090362	h
-8.17876619755681	-0.83992567538962	-0.02036522447051	h
-0.40379396535206	1.27923471964245	1.68050849236831	h
-0.39944222007444	1.33843519153901	-1.63221356000192	h
-3.01533511656016	-2.62205718194800	-1.70412819150945	h
-3.01728768476600	-2.68443822859508	1.60139696954160	h
1.69344002524563	-2.94697906648230	1.61346808356198	h
1.69642697740511	-2.89369576456202	-1.70375578140342	h

***H3a* r(Si-N) = 2.50**

3.32225830675031	0.25725323020565	1.30294196136625	c
1.21177274477103	-0.17622766922719	3.22153808280726	c
-1.21666724135585	1.03076818362725	2.27798887224155	c
-1.82772127758265	0.02484005770221	-0.21985767693972	n
-3.55474471330376	1.68571145116071	-1.57069767251970	c
2.47386347979105	-0.12725416103842	-2.16892439017952	si
-2.91613727427187	-2.49845519403298	-0.05534588255136	c
1.26999480656675	2.07830244842356	-3.40886189247915	h
5.04835795865801	-0.15572982939841	-3.36342350748662	h
1.39560703237984	-2.59553518466915	-2.94190731857033	h
4.92525867038912	-0.98405780024373	1.67630926342665	h
4.05286094325417	2.18309868902838	1.48723572119063	h

0.92033237270150	-2.19544635709343	3.51141549903056	h
1.69096720754514	0.61093744486047	5.06625641739016	h
-2.79340548749299	0.76795221440240	3.60416342282637	h
-0.91268144118230	3.06136819321306	2.06659880800907	h
-3.92238991232994	0.91356928326894	-3.44230533400714	h
-5.36078097846177	1.89319464566093	-0.57269018405644	h
-2.69444747414413	3.53958813456770	-1.79115021812420	h
-3.20258598756103	-3.23572958392497	-1.95372741186855	h
-1.63714822392248	-3.76858057937916	0.92773800219911	h
-4.73567846483650	-2.47584063228852	0.94101903745591	h

H3a **r(Si-N) = 2.65**

3.27916574877107	0.41848016043471	1.54487099482654	c
1.09887732509929	-0.35767363814195	3.27153046390486	c
-1.47038828576786	0.93124334692657	2.21449167747488	c
-1.95079508614046	0.06387196770039	-0.35728023324253	n
-3.59384270479241	1.80326603863433	-1.70302383023342	c
2.78888522452974	-0.16976443104778	-1.95912817728256	si
-3.06513146551279	-2.44662844545558	-0.36790414735708	c
1.50795045347973	1.88293490505529	-3.36218229255292	h
5.40680756921560	-0.20160944012201	-3.01721174590630	h
1.74043276345564	-2.69498078068715	-2.55622751573618	h
5.00561946804510	-0.57648288230488	2.07923055578474	h
3.68496677574505	2.43174367349938	1.78366789926500	h
0.90620022392088	-2.41006485062297	3.31336383828684	h
1.42522430268102	0.25340882199615	5.21492635500241	h

-3.09212810368995	0.55101308999482	3.45934651832166	h
-1.20709932664677	2.97747357689286	2.15087551304263	h
-3.89347132059556	1.11871333498215	-3.62023493614075	h
-5.44474651779212	2.00434409766688	-0.78164468715559	h
-2.70209014970926	3.65350504379426	-1.80729831986275	h
-3.28564974752832	-3.08648963233347	-2.31055639563110	h
-1.83902558738385	-3.77962058493728	0.60069190291241	h
-4.92606421274901	-2.46459958426434	0.55625329103412	h

H3a **r(Si-N) = 2.80**

3.32619357267146	0.41207569490727	1.52850269886371	c
1.10481780841990	-0.33378851749612	3.21569016392257	c
-1.50043303255080	0.92401763174704	2.21053649816854	c
-2.05072990900222	0.05681087363116	-0.34724776766507	n
-3.69272723726415	1.80920998309357	-1.67730986213137	c
2.97374750778614	-0.17272386118910	-1.99260623732903	si
-3.16523167563658	-2.45363632607931	-0.34386723002054	c
1.71380267647365	1.87078096063774	-3.42772169182024	h
5.62552818749004	-0.18325386199111	-2.96318374141219	h
1.95309558343328	-2.70108214683058	-2.62361481440461	h
5.03079543745529	-0.58795966623470	2.12044509525140	h
3.74131727478381	2.42262300187293	1.77406378392751	h
0.91614009924075	-2.38640909052010	3.26399845366334	h
1.42951063070029	0.26600610741453	5.16287600289324	h
-3.08650433381726	0.53412575116160	3.49764209168155	h
-1.25766609119065	2.97252004955785	2.13892432877035	h

-4.00951907589563	1.13129582871581	-3.59412061605852	h
-5.53605251863672	2.01878346700980	-0.74272562409181	h
-2.79085842384524	3.65445353097268	-1.78308820250830	h
-3.40247577396580	-3.09690412116161	-2.28342135159538	h
-1.93090360968155	-3.78499548045483	0.61649676584573	h
-5.01814975033324	-2.46986602110416	0.59628798480404	h

H3a **r(Si-N) = 2.90**

3.35731777888284	0.40789015909409	1.51662961621415	c
1.10878427966384	-0.31774912646364	3.17643984083179	c
-1.51985393135014	0.91902224204494	2.20668651795290	c
-2.11733122423170	0.05205015398049	-0.34056981918871	n
-3.75877935214552	1.81299874971534	-1.65997541510971	c
3.09738646734226	-0.17427573441140	-2.01295045451944	si
-3.23212439580806	-2.45823548364829	-0.32741837358872	c
1.85195341399202	1.86301422773309	-3.46941034832634	h
5.77006268497138	-0.17073177933060	-2.92446656611707	h
2.09559729963448	-2.70458344195777	-2.66598886395243	h
5.04612770132659	-0.59576155852046	2.14650128344876	h
3.77882946364224	2.41645141531029	1.76750406237895	h
0.92272716831839	-2.37051391144360	3.22862867549954	h
1.43227262624587	0.27370585003132	5.12637522766002	h
-3.08125848942173	0.52278697480586	3.52171202307791	h
-1.29096371592435	2.96894844206019	2.13027912188816	h
-4.08748934719535	1.13934327482351	-3.57628076040378	h
-5.59673332307496	2.02838327609539	-0.71617906915328	h

-2.85014017521642	3.65483118878430	-1.76725205489168	h
-3.48101812151195	-3.10388121021559	-2.26472111657202	h
-1.99226561351419	-3.78857168410487	0.62722175264917	h
-5.07940384799076	-2.47303823672223	0.62379144897674	h

H3a **r(Si-N) = 3.00**

3.23455896882997	0.42100376571303	1.50737197143502	c
1.00095869140427	-0.29762029001085	3.19119442886724	c
-1.43054644725085	0.89523615176541	2.23723235561812	c
-1.97242033724503	0.03326063987028	-0.32399538430926	n
-3.59663502501417	1.79636020772597	-1.66169511708513	c
2.88764842788395	-0.15233456353884	-2.01627440646011	si
-3.10270947550918	-2.47036227739367	-0.32721897784655	c
1.64771593453059	1.90623339566164	-3.44768269696961	h
5.54299206407906	-0.17844389208589	-2.97902516820425	h
1.85060730015584	-2.67083253305071	-2.66089381915223	h
4.92545536844261	-0.59872260184592	2.10519097613293	h
3.67397770007564	2.42624694954341	1.75442195816779	h
0.79677270221232	-2.34838620261420	3.24840080137980	h
1.32683249255472	0.30719157478883	5.13654978761940	h
-3.02515618310472	0.51410987560170	3.51603699540750	h
-1.17560028443383	2.94218581664761	2.16754474978939	h
-3.90932807690463	1.12023092209068	-3.57988791511659	h
-5.44274453768905	2.01829315460407	-0.73567233278689	h
-2.68219958577528	3.63559436755820	-1.76405796166058	h
-3.33468992038032	-3.11184683277572	-2.26803936711178	h

-1.88125693456344	-3.81000803389622	0.63824224890456	h
-4.95989737531380	-2.47591952619409	0.60445458178907	h

GED/$\mathbf{r}_{h1}$

H3a

1.04202041562421	0.14772749219326	3.42619462756001	c1
0.00000000000000	0.00000000000000	0.00000000000000	si2
0.70868434848631	-2.36404295378942	-1.35327521567167	h3
3.56836556747188	1.43530314787266	4.00825462842248	c4
5.73204609436395	0.00000000000000	2.75943329818568	c5
5.50359552623086	0.00000000000000	0.00000000000000	n6
6.63296666714918	2.27597640003518	-1.07153322179159	c7
6.74644513123830	-2.21148154079090	-1.08092799789923	c8
-2.83276055088253	-0.07676390960712	0.14239373868550	h9
0.57416850231565	2.30254444514280	-1.51357392552126	h10
-0.44907426637126	1.11904302881157	4.51762515933703	h11
1.12103971400423	-1.80275010409559	4.16608025298753	h12
3.53744945028418	3.41221990991068	3.33826829152420	h13
3.86683882328535	1.53001624824780	6.07222675147710	h14
7.55562268704543	0.85046713854149	3.31559119361675	h15
5.77314103525198	-1.96497236671597	3.46316089363360	h16
6.51502107820018	-2.22906941582086	-3.15557764352068	h17
8.79072686937714	-2.25230662871138	-0.65987800000249	h18
5.89693589514255	-3.96113864043918	-0.32259316002852	h19
6.31404411219186	2.33941225645722	-3.13364434202798	h20

5.76400590758791	3.97840752960833	-0.23208489045236	h21
8.69100637128903	2.36956303434620	-0.73426198784959	h22

H3b

3.55665719901010	18.89726663510319	0.00000000000000	c45
0.00000000000000	18.89726663510319	0.00000000000000	si46
4.78654460191453	21.52266029823742	0.00000000000000	c47
4.03384606279040	23.09050037051871	-2.30274040979781	c48
4.31800029275646	21.76469403265516	-4.70796598779244	n49
6.97211572247671	21.30321389971062	-5.29655726194934	c50
3.17657534134227	23.26159036448027	-6.72295507292021	c51
-1.00481283145569	19.86682000160778	-2.44389108628405	h52
-1.00481283145569	16.29601819852130	0.38228773560214	h53
-1.00481283145569	20.52896189415316	2.06160335068191	h54
4.23037234456082	17.83768347781364	1.66776182625906	h55
4.23037234456082	17.83768347781364	-1.66776182625906	h56
4.25616975913506	22.54229161029770	1.74272558224652	h57
6.86352579229341	21.32085393119649	0.05883097048840	h58
5.17836204010809	24.83587553852013	-2.34500679224455	h59
2.05025308542286	23.70604103662392	-2.09177642734551	h60
1.14801650698917	23.56727727388636	-6.33624707767944	h61
4.08280850269662	25.13108277974106	-6.92735074343548	h62
3.34147534664485	22.26215078181961	-8.54832255956069	h63
7.82613668098160	20.05696788897085	-3.85587803069166	h64
7.14819799633794	20.36036388274276	-7.15075970980299	h65
8.08421079326455	23.06868631077847	-5.36280994493601	h66

H3c

18.89726663510319	0.00000000000000	0.00000000000000	si23
22.44599888740453	0.00000000000000	0.00000000000000	c24
23.57984074366338	2.66827987592659	0.00000000000000	c25
26.46506709871361	2.63795032989525	-0.04290246444167	c26
27.54398537230620	1.33222120399550	-2.22341214110831	n27
27.01394160963818	2.69012020286745	-4.56411621471271	c28
30.27089874228486	1.08638307185878	-1.89593781710794	c29
27.92159660133415	1.72833474678589	-6.17940845735074	h30
24.95741047429380	2.74434590947688	-4.91876688683368	h31
27.71100451708924	4.65716314308863	-4.51042378896772	h32
31.10256026593443	0.05346735929936	-3.50822255976100	h33
31.21968250097614	2.94092642640254	-1.75986408027589	h34
30.69647010019671	0.01521475628592	-0.15538466463380	h35
17.89245380364750	1.31466696610016	2.27690312199096	h36
17.89245380364750	-2.62918955708322	0.00008333694586	h37
17.89245380364750	1.31452259098306	-2.27698664790949	h38
22.91736247977189	3.70856703425504	1.68432849300006	h39
22.86799110301569	3.72954659070066	-1.65076354594812	h40
23.13882446075799	-1.04718730626758	-1.66776182625906	h41
23.13882446075799	-1.04718730626758	1.66776182625906	h42
27.16987410603173	4.60260314383243	-0.00517048112403	h43
27.16523747269014	1.73991650356121	1.70676446178525	h44

H3d

22.44599888740453	18.89726663510319	0.00000000000000	c67
18.89726663510319	18.89726663510319	0.00000000000000	si68
23.57984074366338	21.56554651102979	0.00000000000000	c69
26.46348067317960	21.45655539187583	-0.00577576057435	c70
27.68261420855999	23.91118749554261	0.32905224576440	n71
27.29602828966169	25.53575942993447	-1.86526982103117	c72
30.38514443539937	23.54691395730571	0.73815709244841	c73
17.89245380364750	16.26808029055530	0.00403702307126	h74
17.89245380364750	20.21535589619097	2.27492382228360	h75
17.89245380364750	20.20836371856331	-2.27896065638219	h76
23.13882446075799	17.85007932883561	-1.66776182625906	h77
23.13882446075799	17.85007932883561	1.66776182625906	h78
28.29236380730488	27.35169170031672	-1.60499512204856	h79
27.99718169944857	24.66239995361855	-3.62699188056262	h80
25.26397705146176	25.94499901412960	-2.11291585466687	h81
31.32366338782713	25.38553901032671	1.04908780437308	h82
30.70770509212928	22.36446285105405	2.42806878287581	h83
31.31074011409338	22.61702368579621	-0.88560849557613	h84
22.90363323761616	22.62702941053416	-1.66554347612877	h85
22.91020854154184	22.62423544966216	1.66997242851003	h86
27.10164949327169	20.16472841812153	1.50484036477318	h87
27.11187915061927	20.61055046490489	-1.80073905698029	h88