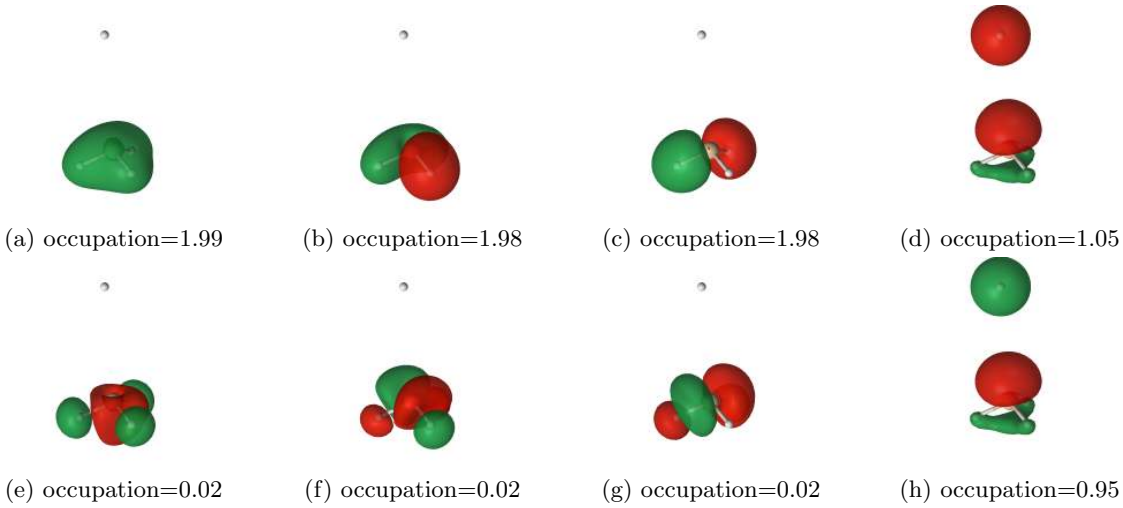
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplement 3: selection of active space in CASPT2 calculations

Different phases of all shown orbital wavefunctions are depicted in different colour. Electron occupations of each orbital are noted below each figure.

1 $\mathbf{SiH_4 \rightarrow SiH_3^{\cdot} + H^{\cdot}}$

symmetry: C_s
active space: (8,8)



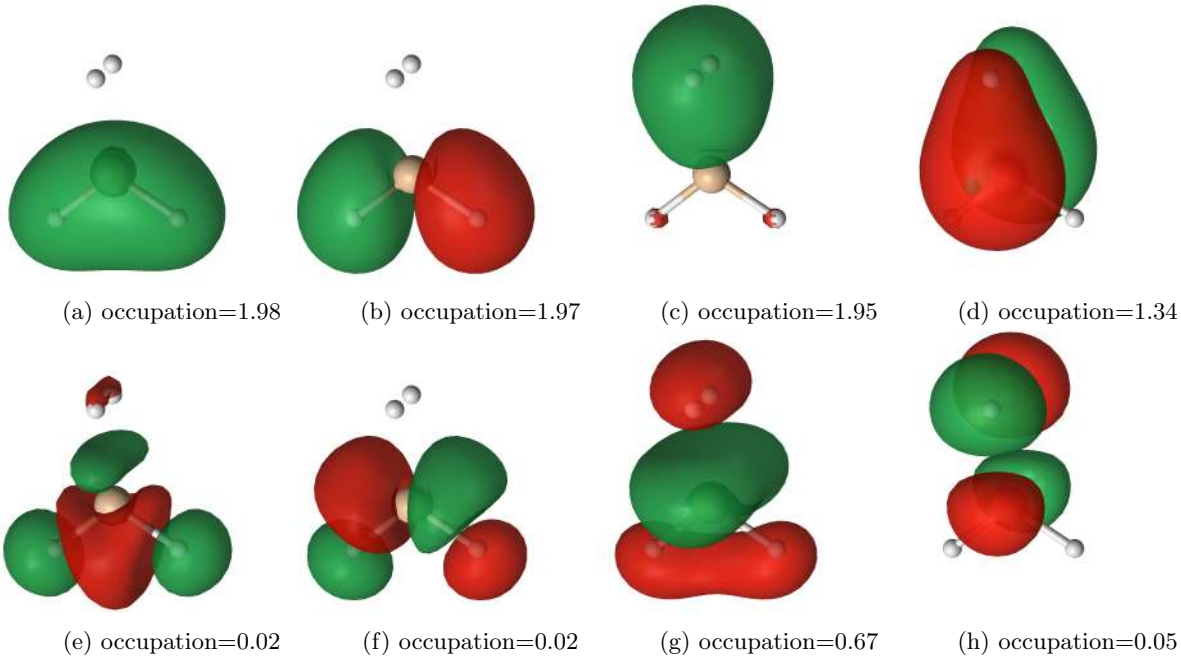
(a) occupation=1.99 (b) occupation=1.98 (c) occupation=1.98 (d) occupation=1.05

(e) occupation=0.02 (f) occupation=0.02 (g) occupation=0.02 (h) occupation=0.95

Figure 1: The active space used in CASPT2 calculations of SiH_4 dissociation energy. The active space includes 1s orbital on departing hydrogen, 3s orbital on silicon atom and three 2p orbitals on silicon atom and corresponding virtual orbitals. These orbitals are calculated on geometry, used for selection active space, in which separation between Si and H atoms is 5 Å. The final CASPT2 calculation for $SiH_3 + H$ system is done with the same active space, but on geometry with much larger separation (> 20 Å), that is too large to be suitable for visualisation.

2 $\mathbf{SiH_4 \longrightarrow SiH_2 + H_2}$

symmetry used: C_2v
active space: (8,8)



(a) occupation=1.98 (b) occupation=1.97 (c) occupation=1.95 (d) occupation=1.34

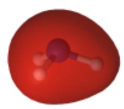
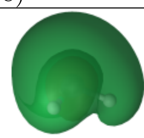
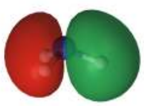
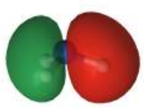
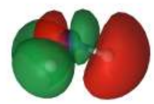
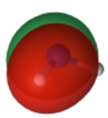
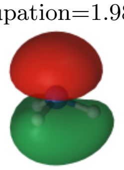
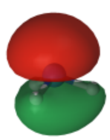
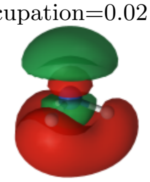
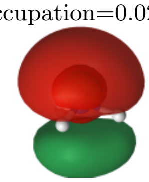
(e) occupation=0.02 (f) occupation=0.02 (g) occupation=0.67 (h) occupation=0.05

Figure 2: The active space used in CASPT2 calculations of $SiH_4 \longrightarrow SiH_2 + H_2$ dissociation energy. The active space includes 1s orbital on departing hydrogen atoms, 3s orbital on silicon atom and three 2p orbitals on silicon atom and corresponding virtual orbitals. These orbitals are calculated on geometry, used for selection active space, in which separation between Si and H_2 molecule is 2 Å. The final CASPT2 calculation for SiH_3+H system is done with the same active space, but on geometry with much larger separation ($>$ 20 Å), that is too large to be suitable for visualisation.

3 $\mathbf{NH_3 \xrightarrow{-e} NH_3^{+\cdot}}$

symmetry used: C_s

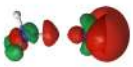
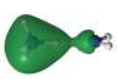
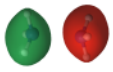
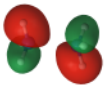
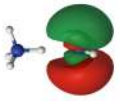
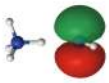
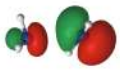
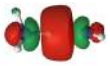
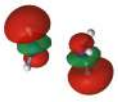
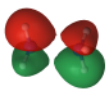
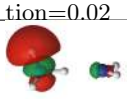
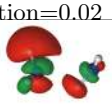
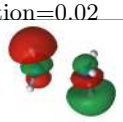
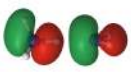
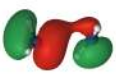
Table 1: The active space used in CASPT2 calculations of NH_3 ionisation.

NH_3 active space: (8,8)	NH_3 active space: (8,8)	$NH_3^{+\cdot}$ active space: (7,8)	$NH_3^{+\cdot}$ active space: (7,8)
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.00	 occupation=0.02	 occupation=0.01

4 $\mathbf{NH_3^{+\cdot} + NH_3 \longrightarrow NH_2^{\cdot} + NH_4^+}$

active space: (11,12)

Table 2: The active space used in CASPT2 calculations of the proton transfer between $NH_3^{+\cdot}$ and NH_3. Orbitals on pre–reaction complex, transition state and postreaction complex are shown. Energy of reactants and products are calculated with CASPT2 calculation on geometries in which molecular fragments are separated by large separation (> 20 Å). Separated reactants were subjected to optimisation in order allow breaking of symmetry of pre–reaction complex.

$NH_3^{+\cdot} + NH_3$ (pre–reaction complex)	transition state	$NH_2^{\cdot} + NH_4^+$ (postreaction complex)	$NH_3^{+\cdot} + NH_3$ (pre–reaction complex)	transition state	$NH_2^{\cdot} + NH_4^+$ (postreaction complex)
 occupation=1.99	 occupation=1.99	 occupation=1.99	 occupation=0.01	 occupation=0.01	 occupation=0.01
 occupation=1.99	 occupation=1.99	 occupation=1.99	 occupation=0.01	 occupation=0.01	 occupation=0.01
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.01	 occupation=0.01
 occupation=1.98	 occupation=1.00	 occupation=0.99	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.00	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.01

5 $\mathbf{NH_3 \rightarrow NH_2^{\cdot} + H^{\cdot}}$

symmetry: C_s
active space: (8,8)

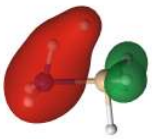
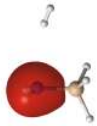
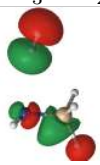
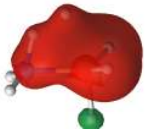
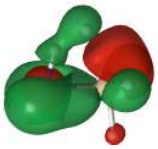
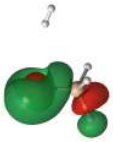
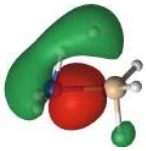
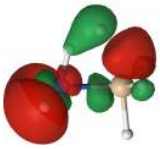
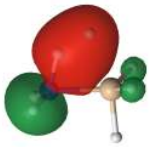
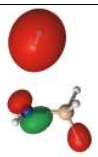
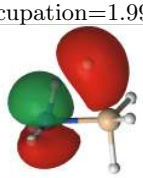
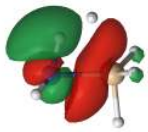
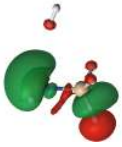
(a) occupation=1.99 (b) occupation=1.98 (c) occupation=1.01 (d) occupation=1.97

(e) occupation=0.01 (f) occupation=0.02 (g) occupation=0.99 (h) occupation=0.02

Figure 3: The active space used in CASPT2 calculations of NH_3 dissociation energy. The active space includes 1s orbital on departing hydrogen, 3s orbital on silicon atom and three 2p orbitals on silicon atom and corresponding virtual orbitals. These orbitals are calculated on geometry, used for selection active space, in which separation between Si and H atoms is 5 Å. The final CASPT2 calculation for $NH_2 + H$ system is done with the same active space, but on geometry with much larger separation (> 20 Å), that is too large to be suitable for visualisation.

6 $\mathbf{NH_3 + SiH_4 \rightarrow H_2NSiH_3 + H_2}$

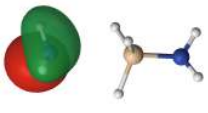
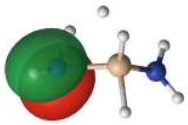
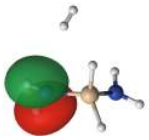
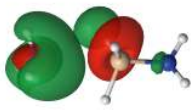
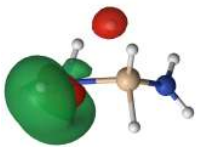
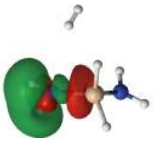
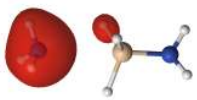
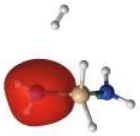
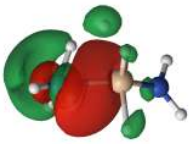
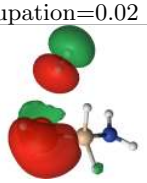
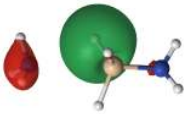
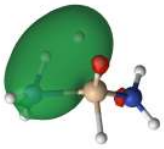
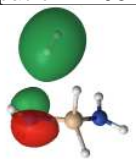
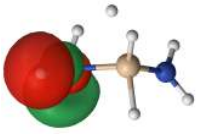
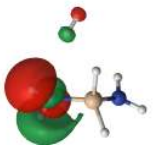
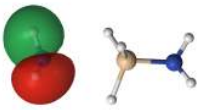
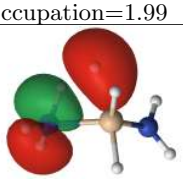
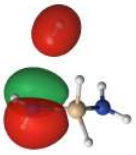
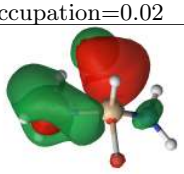
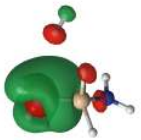
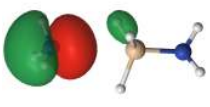
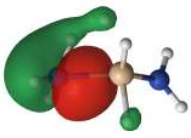
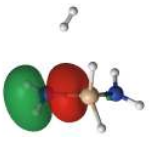
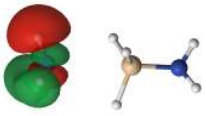
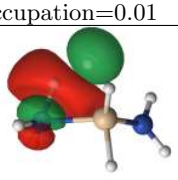
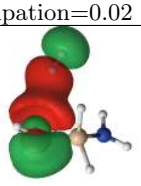
symmetry used: C_s
active space: (10,10)

$NH_3 + SiH_4$	transition state	$NH_2SiH_3 + H_2$	$NH_3 + SiH_4$	transition state	$NH_2SiH_3 + H_2$
 occupation=1.99	 occupation=1.99	 occupation=1.99	 occupation=0.02	 occupation=0.01	 occupation=0.02
 occupation=1.99	 occupation=1.99	 occupation=1.98	 occupation=0.01	 occupation=0.01	 occupation=0.01
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.99	 occupation=1.98	 occupation=0.02	 occupation=0.03	 occupation=0.03
 occupation=1.98	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.03	 occupation=0.01

7 $NH_2SiH_3 + NH_3 \rightarrow NH_2SiH_2NH_2 + H_2$

symmetry used: C_1
active space: (10,10)

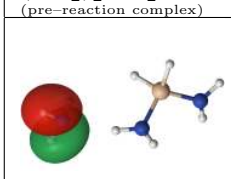
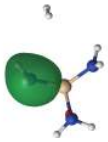
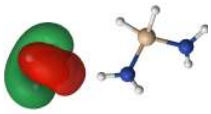
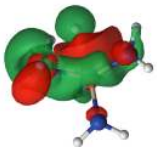
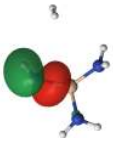
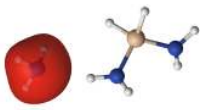
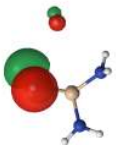
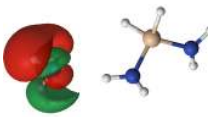
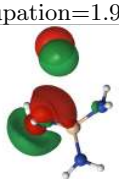
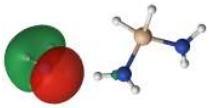
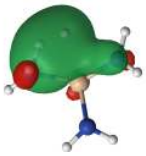
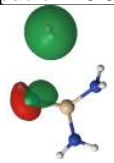
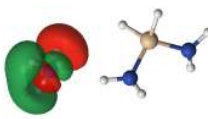
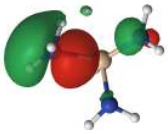
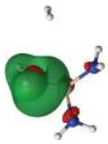
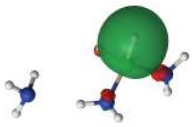
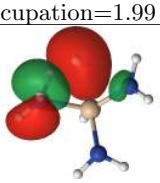
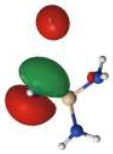
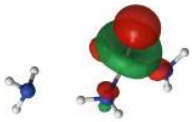
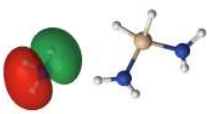
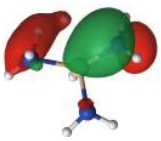
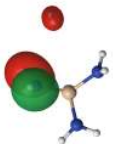
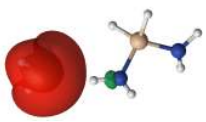
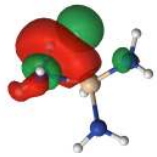
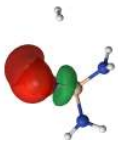
Table 4: The active space used in CASPT2 calculations for neutral–neutral eliminative association. Orbitals of pre–reaction complex, transition state and postreaction complex (shown below) are checked if they are converged into a desired state. In the CASPT2 calculations of energies of reactants (NH_2SiH_3+NH_3) and products ($NH_2SiH_2NH_2$+H_2), molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$NH_2SiH_3 + NH_3$ (pre–reaction complex)	transition state	$(NH_2)_2SiH_2 + H_2$ (postreaction complex)	$NH_2SiH_3 + NH_3$ (pre–reaction complex)	transition state	$(NH_2)_2SiH_2 + H_2$ (postreaction complex)
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.99	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.99	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.03	 occupation=0.03

8 $(NH_2)_2SiH_2 + NH_3 \rightarrow (NH_2)_3SiH + H_2$

symmetry used: C_1
active space: (10,10)

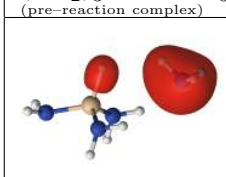
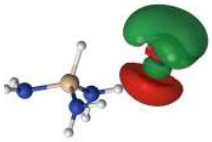
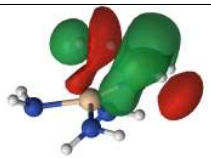
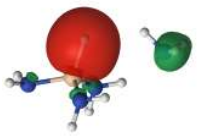
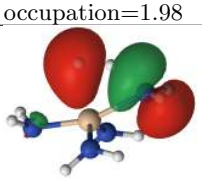
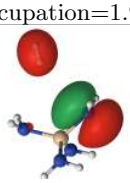
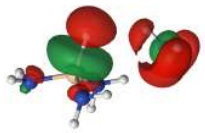
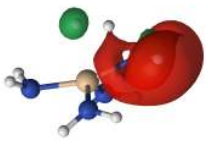
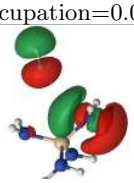
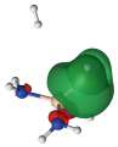
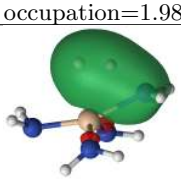
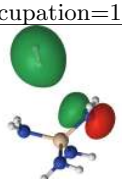
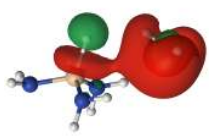
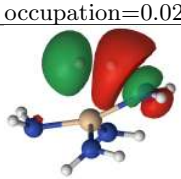
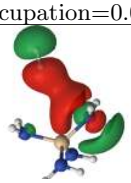
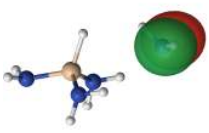
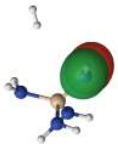
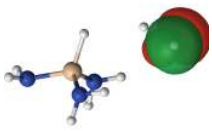
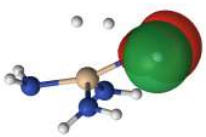
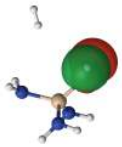
Table 5: The active space used in CASPT2 calculations for neutral–neutral eliminative association. Orbitals of pre–reaction complex, transition state and postreaction complex are shown below. These orbitals are checked if they are converged into a desired state. In the CASPT2 calculations of energies of reactants ($(NH_2)_2SiH_2 + NH_3$) and products ($(NH_2)_3SiH + H_2$), molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$(NH_2)_2SiH_2 + NH_3$ (pre–reaction complex)	transition state	$(NH_2)_3SiH + H_2$ (postreaction complex)	$(NH_2)_2SiH_2 + NH_3$ (pre–reaction complex)	transition state	$(NH_2)_3SiH + H_2$ (postreaction complex)
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.01	 occupation=1.98
 occupation=1.99	 occupation=0.02	 occupation=0.02	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.99	 occupation=1.98	 occupation=0.02	 occupation=1.98	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=1.98	 occupation=0.02	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.03	 occupation=0.02

9 $(NH_2)_3SiH + NH_3 \rightarrow (NH_2)_4Si + H_2$

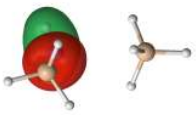
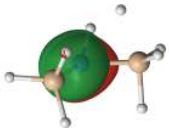
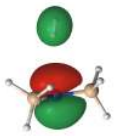
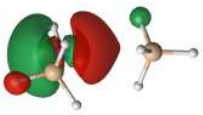
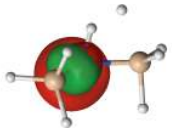
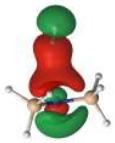
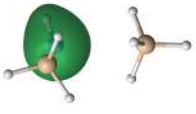
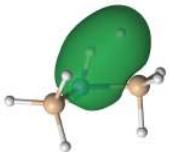
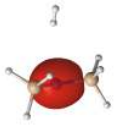
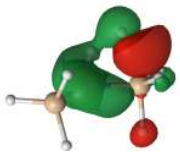
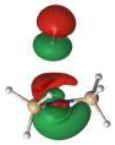
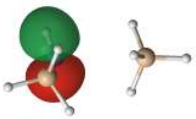
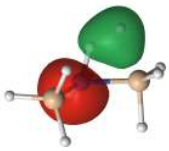
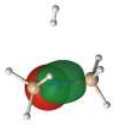
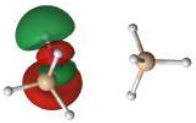
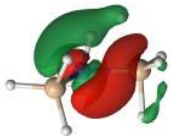
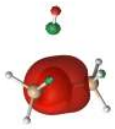
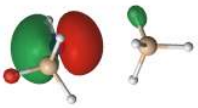
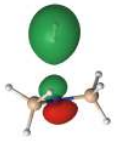
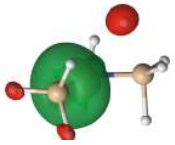
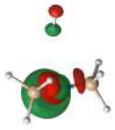
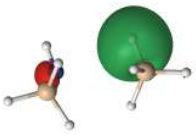
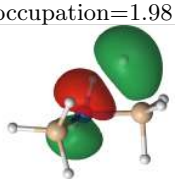
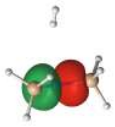
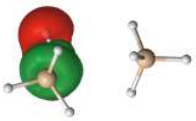
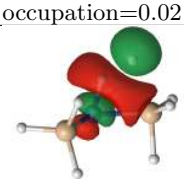
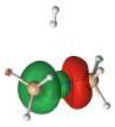
symmetry used: C_s
active space: (10,10)

Table 6: The active space used in CASPT2 calculations for neutral–neutral eliminative association. Orbitals of pre–reaction complex, transition state and postreaction complex are shown below. These orbitals are checked if they are converged into a desired state. In the CASPT2 calculations of energies of reactants ($(NH_2)_3SiH + NH_3$) and products ($(NH_2)_4Si + H_2$), molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$(NH_2)_3SiH + NH_3$ (pre–reaction complex)	transition state	$(NH_2)_4Si + H_2$ (postreaction complex)	$(NH_2)_3SiH + NH_3$ (pre–reaction complex)	transition state	$(NH_2)_4Si + H_2$ (postreaction complex)
 occupation=1.99	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.99	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02

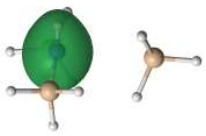
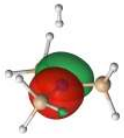
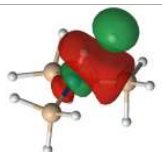
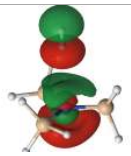
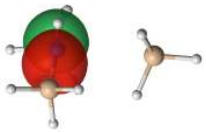
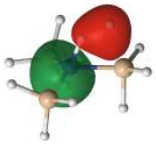
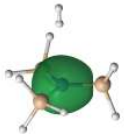
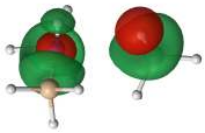
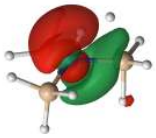
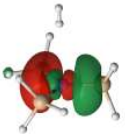
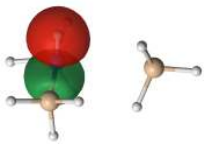
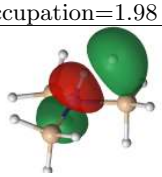
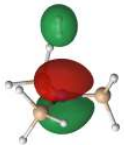
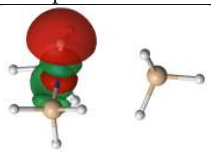
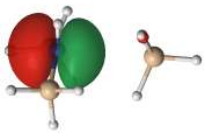
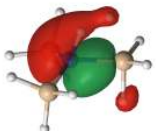
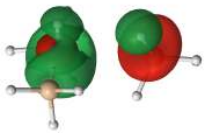
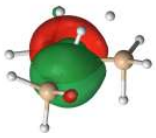
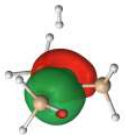
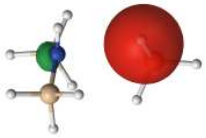
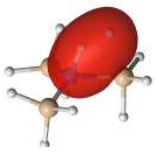
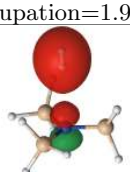
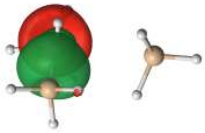
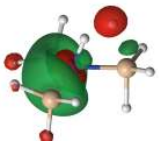
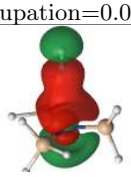
10 $\mathbf{NH_2SiH_3 + SiH_4 \rightarrow SiH_3NHSiH_3 + H_2}$

symmetry used: C_1
active space: (10,10)

$NH_2SiH_3 + SiH_4$ (pre–reaction complex)	transition state	$(SiH_3)_2NH + H_2$ (postreaction complex)	$NH_2SiH_3 + SiH_4$ (pre–reaction complex)	transition state	$(SiH_3)_2NH + H_2$ (postreaction complex)
 occupation=1.98	 occupation=1.98	 occupation=1.97	 occupation=0.02	 occupation=0.02	 occupation=0.03
 occupation=1.98	 occupation=1.99	 occupation=1.98	 occupation=0.02	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=1.98	 occupation=0.02	 occupation=0.03	 occupation=0.02

11 $(SiH_3)_2NH + SiH_4 \rightarrow (SiH_3)_3N + H_2$

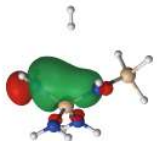
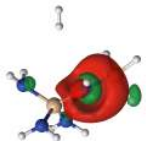
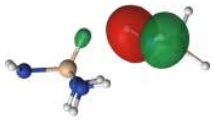
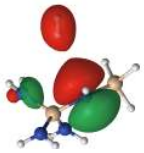
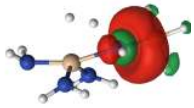
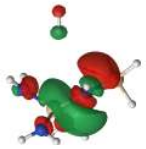
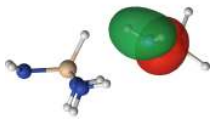
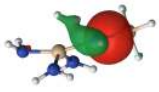
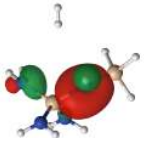
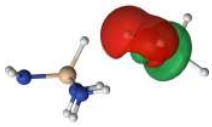
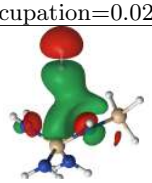
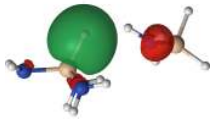
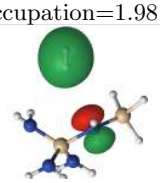
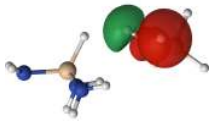
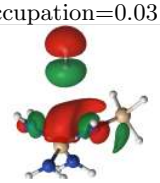
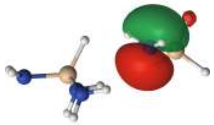
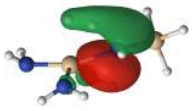
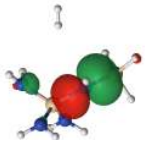
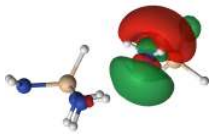
symmetry used: C_1
active space: (10,10)

$(SiH_3)_2NH + SiH_4$ (pre–reaction complex)	transition state	$(SiH_3)_3N + H_2$ (postreaction complex)	$(SiH_3)_2NH + SiH_4$ (pre–reaction complex)	transition state	$(SiH_3)_3N + H_2$ (postreaction complex)
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.03	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.03	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.01	 occupation=0.02
 occupation=1.97	 occupation=1.97	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.99	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.03

12 $(NH_2)_3SiH + NH_2SiH_3 \rightarrow (NH_2)_3SiNHSiH_3 + H_2$

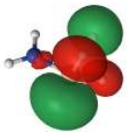
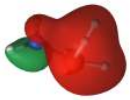
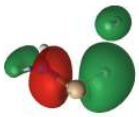
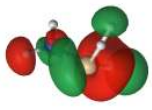
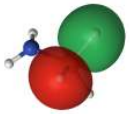
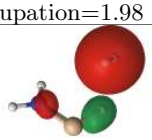
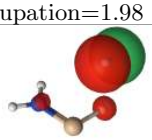
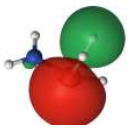
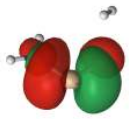
symmetry used: C_s
active space: (10,10)

Table 9: The active space used in CASPT2 calculations for neutral–neutral eliminative association. This reaction represents possible silicon nitride growth reaction. Orbitals of pre–reaction complex, transition state and postreaction complex are shown below. These orbitals are checked if they are converged into a desired state. In the CASPT2 calculations of energies of reactants ($(NH_2)_3SiH$+NH_2SiH_3) and products ($(NH_2)_3SiNHSiH_3$+H_2), molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$(NH_2)_3SiH + NH_2SiH_3$ (pre–reaction complex)	transition state	$(NH_2)_3Si NH_2SiH_3 + H_2$ (postreaction complex)	$(NH_2)_3SiH + NH_2SiH_3$ (pre–reaction complex)	transition state	$(NH_2)_3Si NH_2SiH_3 + H_2$ (postreaction complex)
 occupation=1.98	 occupation=1.99	 occupation=1.99	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.03	 occupation=0.03
 occupation=1.98	 occupation=1.99	 occupation=1.98	 occupation=0.02	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.01	 occupation=0.02

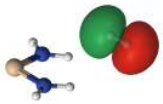
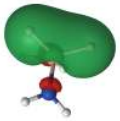
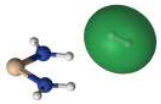
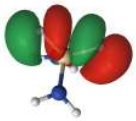
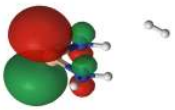
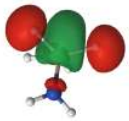
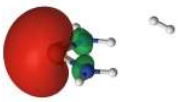
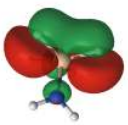
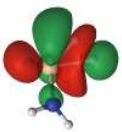
13 $NH_2SiH_3 \rightarrow NH_2SiH + H_2$

symmetry used: C_1v
active space: (10,10)

NH_2SiH_3	transition state	$NH_2SiH + H_2$	NH_2SiH_3	transition state	$NH_2SiH + H_2$
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.06	 occupation=0.02
 occupation=1.97	 occupation=1.99	 occupation=1.99	 occupation=1.93	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=1.98	 occupation=0.08	 occupation=0.01	 occupation=0.01
 occupation=0.02	 occupation=1.92	 occupation=0.03	 occupation=0.02	 occupation=0.02	 occupation=0.02

14 $(NH_2)_2SiH_2 \rightarrow (NH_2)_2Si + H_2$

symmetry used: C_s
active space: (8,8)

$(NH_2)_2SiH_2$	transition state	$(NH_2)_2Si + H_2$	$(NH_2)_2SiH_2$	transition state	$(NH_2)_2Si + H_2$
 occupation=2.00	 occupation=2.00	 occupation=1.99	 occupation=0.02	 occupation=0.13	 occupation=0.02
 occupation=1.97	 occupation=1.97	 occupation=1.98	 occupation=0.01	 occupation=0.01	 occupation=0.07
 occupation=2.00	 occupation=2.00	 occupation=1.99	 occupation=0.02	 occupation=0.01	 occupation=0.01
 occupation=1.97	 occupation=1.88	 occupation=1.94	 occupation=0.01	 occupation=0.01	 occupation=0.02

15 $\mathbf{NH_2SiH_3 \rightarrow SiH_3^{\cdot} + NH_2^{\cdot}}$

symmetry used: C_s
active space: (10,10)

Table 12: The active space used in CASPT2 calculations for dissociation of SiN bond.

NH_2SiH_3	$SiH_3^{\cdot} + NH_2^{\cdot}$	NH_2SiH_3	$SiH_3^{\cdot} + NH_2^{\cdot}$
 occupation=1.99	 occupation=1.99	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.01
 occupation=1.98	 occupation=1.00	 occupation=1.98	 occupation=1.98
 occupation=0.02	 occupation=1.00	 occupation=0.02	 occupation=0.02

16 $(NH_2)_2SiH_2 \rightarrow NH_2SiH_2^{\cdot} + NH_2^{\cdot}$

symmetry used: C_1
active space: (10,10)

Table 13: The active space used in CASPT2 calculations for dissociation of SiN bond.

$(NH_2)_2SiH_2$	$NH_2SiH_2^{\cdot} + NH_2^{\cdot}$	$(NH_2)_2SiH_2$	$NH_2SiH_2^{\cdot} + NH_2^{\cdot}$
 occupation=1.99	 occupation=1.99	 occupation=0.02	 occupation=1.00
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.01
 occupation=1.98	 occupation=1.00	 occupation=0.02	 occupation=0.02

17 $(NH_2)_3SiH \rightarrow (NH_2)_2SiH^{\cdot} + NH_2^{\cdot}$

symmetry used: C_1
active space: (10,10)

Table 14: The active space used in CASPT2 calculations for dissociation of SiN bond.

$(NH_2)_3SiH$	$(NH_2)_2SiH^{\cdot} + NH_2^{\cdot}$	$(NH_2)_3SiH$	$(NH_2)_2SiH^{\cdot} + NH_2^{\cdot}$
 occupation=1.99	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.00	 occupation=1.97	 occupation=1.98
 occupation=0.02	 occupation=0.99	 occupation=0.02	 occupation=0.02

18 $(NH_2)_4Si \rightarrow (NH_2)_3Si^{\cdot} + NH_2^{\cdot}$

symmetry used: C_s
active space: (10,10)

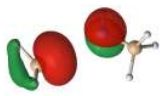
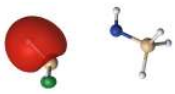
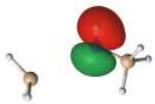
Table 15: The active space used in CASPT2 calculations for dissociation of SiN bond.

$(NH_2)_3SiH$	$(NH_2)_2SiH^{\cdot} + NH_2^{\cdot}$	$(NH_2)_3SiH$	$(NH_2)_2SiH^{\cdot} + NH_2^{\cdot}$
 occupation=1.98	 occupation=1.99	 occupation=0.02	 occupation=0.02
 occupation=0.02	 occupation=1.00	 occupation=0.03	 occupation=0.01
 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.01
 occupation=1.97	 occupation=1.00	 occupation=1.98	 occupation=1.98
 occupation=1.99	 occupation=1.98	 occupation=0.02	 occupation=0.02

19 $(SiH_3)_2NH \rightarrow SiH_3NH^{\cdot} + SiH_3^{\cdot}$

symmetry used: C_1
active space: (10,10)

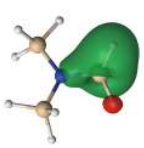
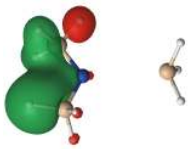
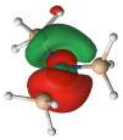
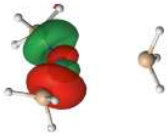
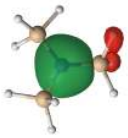
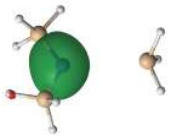
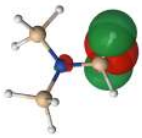
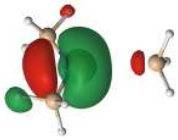
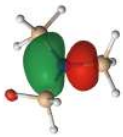
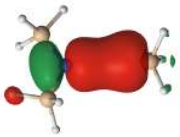
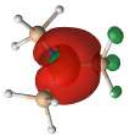
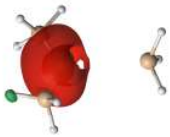
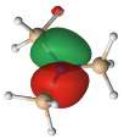
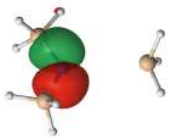
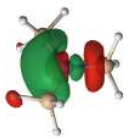
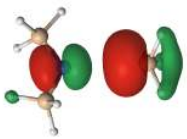
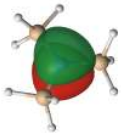
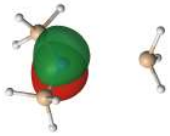
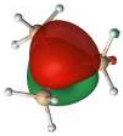
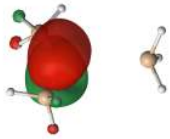
Table 16: The active space used in CASPT2 calculations for dissociation of SiN bond.

$(SiH_3)_2NH$	$SiH_3NH^{\cdot} + SiH_3^{\cdot}$	$(SiH_3)_2NH$	$SiH_3NH^{\cdot} + SiH_3^{\cdot}$
 occupation=1.99	 occupation=1.99	 occupation=0.02	 occupation=0.93
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.07	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.01

20 $(SiH_3)_3N \rightarrow (SiH_3)_2N^{\cdot} + SiH_3^{\cdot}$

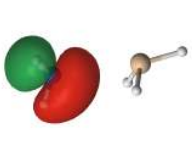
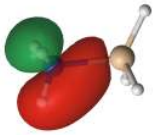
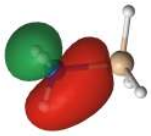
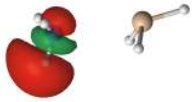
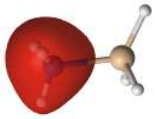
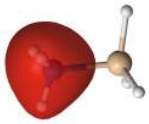
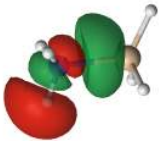
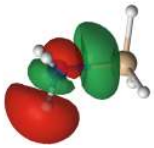
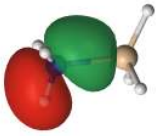
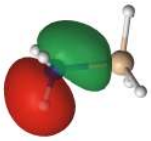
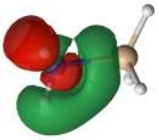
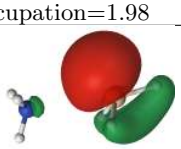
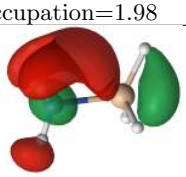
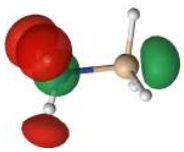
symmetry used: C_s
active space: (10,10)

Table 17: The active space used in CASPT2 calculations for dissociation of SiN bond.

$(SiH_3)_3N$	$(SiH_3)_2NH^{\cdot} + SiH_3^{\cdot}$	$(SiH_3)_3N$	$(SiH_3)_2NH^{\cdot} + SiH_3^{\cdot}$
 occupation=1.99	 occupation=2.00	 occupation=0.02	 occupation=0.02
 occupation=1.99	 occupation=1.98	 occupation=0.01	 occupation=0.01
 occupation=1.98	 occupation=1.55	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.44
 occupation=1.98	 occupation=1.97	 occupation=0.02	 occupation=0.03

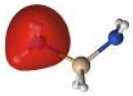
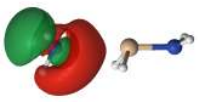
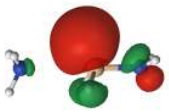
21 $\mathbf{NH_3 + SiH_3^{\cdot} \rightarrow NH_3SiH_3^{\cdot}}$

symmetry used: C_s
active space: (7,7)

$NH_3 + SiH_3^{\cdot}$	transition state	$NH_3SiH_3^{\cdot}$	$NH_3 + SiH_3^{\cdot}$	transition state	$NH_3SiH_3^{\cdot}$
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.01	 occupation=0.01
 occupation=1.99	 occupation=1.99	 occupation=1.99	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.00	 occupation=1.00	 occupation=1.00			

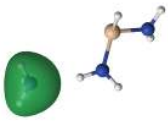
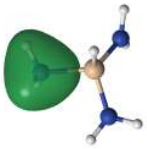
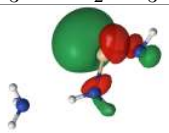
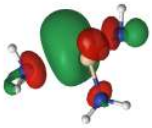
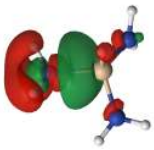
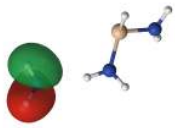
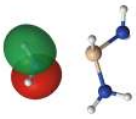
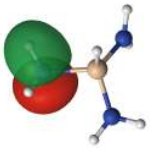
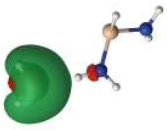
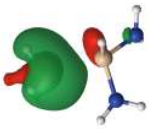
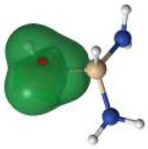
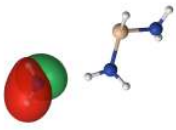
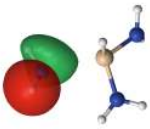
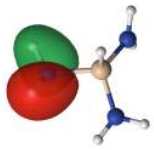
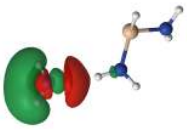
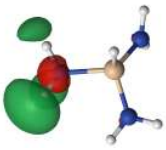
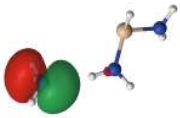
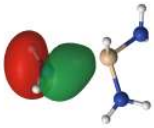
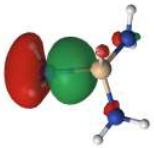
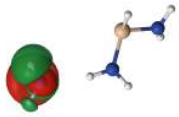
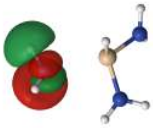
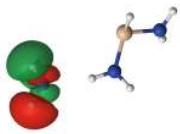
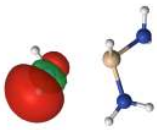
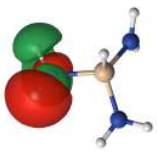
22 $NH_3 + NH_2SiH_3^{\cdot} \rightarrow NH_2SiH_2NH_3^{\cdot}$

symmetry used: C_s
active space: (7,7)

$NH_3 + NH_2SiH_3^{\cdot}$	transition state	$NH_2SiH_2NH_3^{\cdot}$	$NH_3 + NH_2SiH_3^{\cdot}$	transition state	$NH_2SiH_2NH_3^{\cdot}$
 occupation=1.99	 occupation=1.99	 occupation=1.99	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.01	 occupation=0.01
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.00	 occupation=1.00	 occupation=1.00			

23 $NH_3 + (NH_2)_2SiH^{\cdot} \rightarrow (NH_2)_2SiHNH_3^{\cdot}$

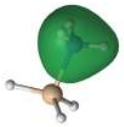
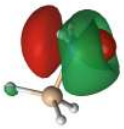
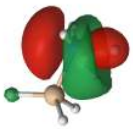
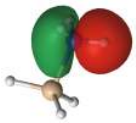
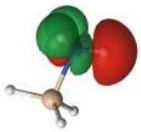
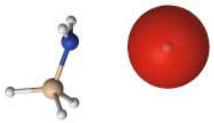
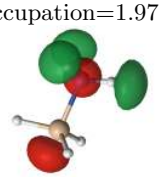
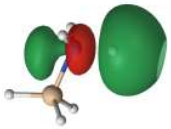
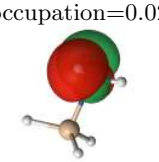
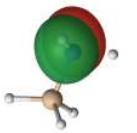
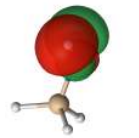
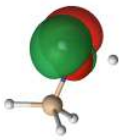
symmetry used: C_1
active space: (9,9)

$NH_3 + NH_2SiH_3^{\cdot}$	transition state	$NH_2SiH_2NH_3^{\cdot}$	$NH_3 + NH_2SiH_3^{\cdot}$	transition state	$NH_2SiH_2NH_3^{\cdot}$
 occupation=1.99	 occupation=1.98	 occupation=1.99	 occupation=1.00	 occupation=1.00	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=1.00
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=0.02	 occupation=0.03	 occupation=0.02			

24 $\mathbf{NH_3SiH_3^{\cdot} \rightarrow NH_2SiH_3 + H^{\cdot}}$

symmetry used: C_s
active space: (9,10)

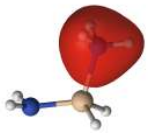
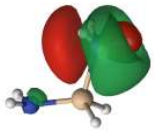
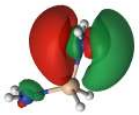
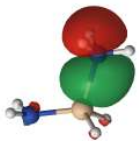
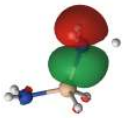
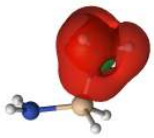
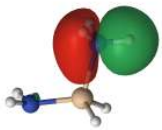
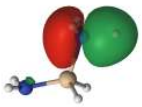
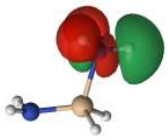
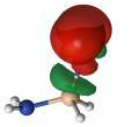
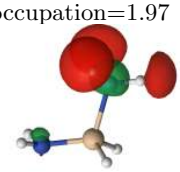
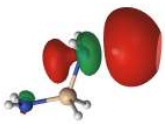
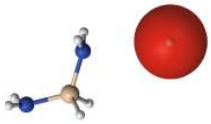
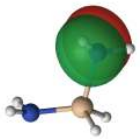
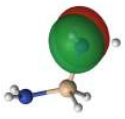
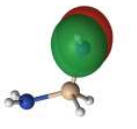
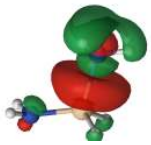
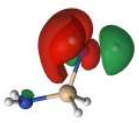
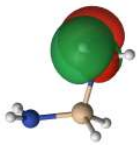
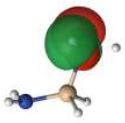
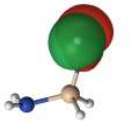
Table 21: The active space used in CASPT2 calculations for dissociation of NH bond.

$SiH_3NH_3^{\cdot}$ (pre–reaction complex)	transition state	$NH_2SiH_3 + H^{\cdot}$ (postreaction complex)	$SiH_3NH_3^{\cdot}$ (pre–reaction complex)	transition state	$NH_2SiH_3 + H^{\cdot}$ (postreaction complex)
 occupation=1.99	 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.00
 occupation=1.97	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.03	 occupation=1.00
 occupation=1.00	 occupation=1.00	 occupation=0.02	 occupation=0.02	 occupation=1.98	 occupation=0.02
 occupation=0.02	 occupation=0.02	 occupation=0.02	 occupation=1.98	 occupation=0.02	 occupation=1.97

25 $NH_2SiH_2NH_3^{\cdot} \rightarrow (NH_2)_2SiH_2 + H^{\cdot}$

symmetry used: C_s
active space: (9,10)

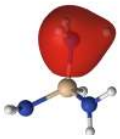
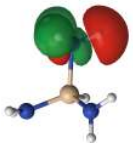
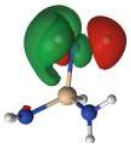
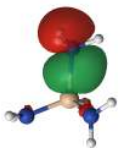
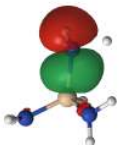
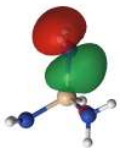
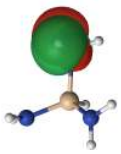
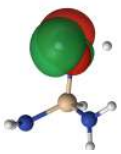
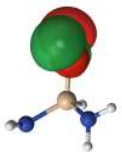
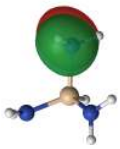
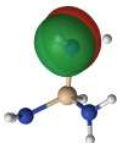
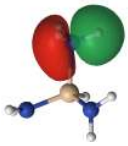
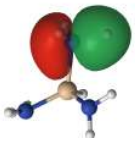
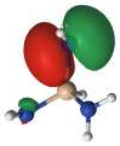
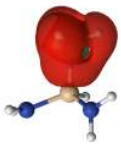
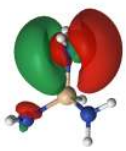
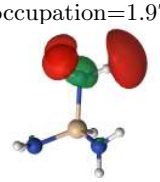
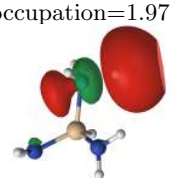
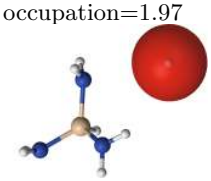
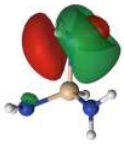
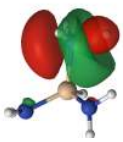
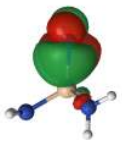
Table 22: The active space used in CASPT2 calculations for dissociation of NH bond.

$NH_2SiH_2NH_3^{\cdot}$ (pre–reaction complex)	transition state	$(NH_2)_2SiH_2 + H^{\cdot}$ (postreaction complex)	$NH_2SiH_2NH_3^{\cdot}$ (pre–reaction complex)	transition state	$(NH_2)_2SiH_2 + H^{\cdot}$ (postreaction complex)
 occupation=1.99	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.00
 occupation=1.97	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.00	 occupation=1.00	 occupation=1.00	 occupation=1.98	 occupation=1.98	 occupation=1.98
 occupation=0.02	 occupation=0.03	 occupation=0.02	 occupation=0.02	 occupation=0.02	 occupation=0.02

26 $(NH_2)_2SiHNH_3^{\cdot} \rightarrow (NH_2)_3SiH + H^{\cdot}$

symmetry used: C_1
active space: (9,10)

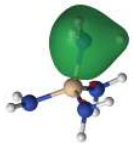
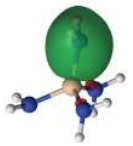
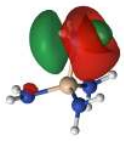
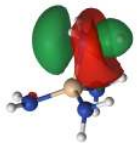
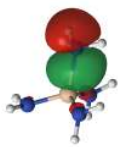
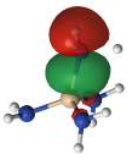
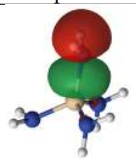
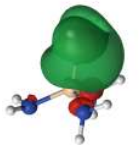
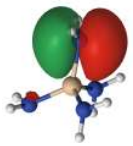
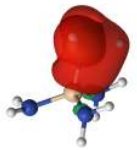
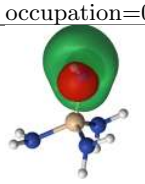
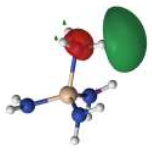
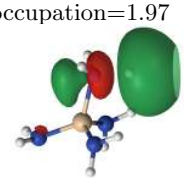
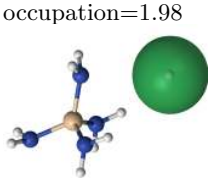
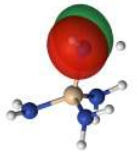
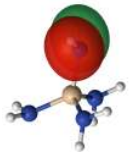
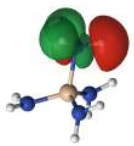
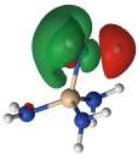
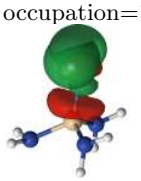
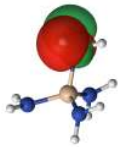
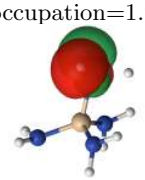
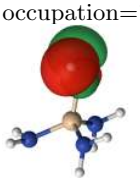
Table 23: The active space used in CASPT2 calculations for dissociation of NH bond.

$(NH_2)_2SiHNH_3^{\cdot}$ (reactant)	transition state	$(NH_2)_3SiH + H^{\cdot}$ (postreaction complex)	$(NH_2)_2SiHNH_3^{\cdot}$ (reactant)	transition state	$(NH_2)_3SiH + H^{\cdot}$ (postreaction complex)
 occupation=1.99	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.03	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.97	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.97	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.00	 occupation=1.00	 occupation=1.00	 occupation=0.01	 occupation=0.01	 occupation=0.01

27 $(NH_2)_3SiHNH_3^{\cdot} \rightarrow (NH_2)_4SiH + H^{\cdot}$

symmetry used: C_s
active space: (9,10)

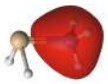
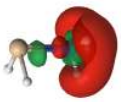
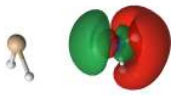
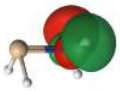
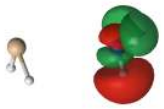
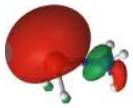
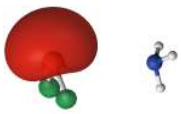
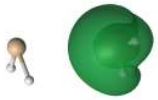
Table 24: The active space used in CASPT2 calculations for dissociation of NH bond.

$(NH_2)_3SiHNH_3^{\cdot}$ (reactant)	transition state	$(NH_2)_4SiH + H^{\cdot}$ (postreaction complex)	$(NH_2)_3SiHNH_3^{\cdot}$ (reactant)	transition state	$(NH_2)_4SiH + H^{\cdot}$ (postreaction complex)
 occupation=1.99	 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.97	 occupation=1.97	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.00
 occupation=1.00	 occupation=1.00	 occupation=1.00	 occupation=1.98	 occupation=1.98	 occupation=1.97
 occupation=0.02	 occupation=0.03	 occupation=0.02	 occupation=0.02	 occupation=0.02	 occupation=0.02

28 $NH_3 + SiH_2 \rightarrow NH_3SiH_2$

symmetry used: C_1v
active space: (10,10)

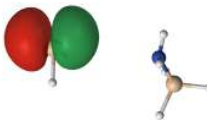
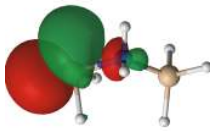
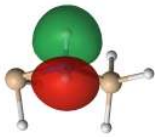
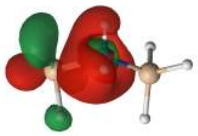
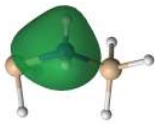
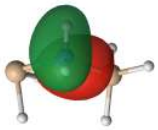
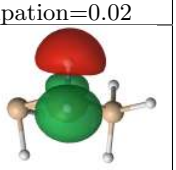
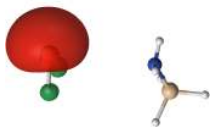
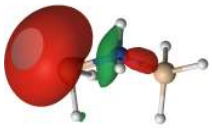
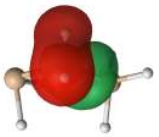
Table 25: Active orbitals, used in the calculation of dissociation curve of NH_3SiH_2. Shown orbitals are for the minimum energy geometry and for the geometry with Si—N separation of 4Å.

 occupation=1.99	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.05	 occupation=0.09
 occupation=1.95	 occupation=1.91	 occupation=0.01	 occupation=0.02

29 $SiH_2 + NH_2SiH_3 \rightarrow SiH_2NH_2SiH_3$

symmetry used: C_1v
active space: (10,10)

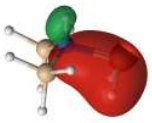
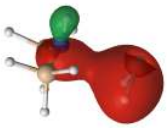
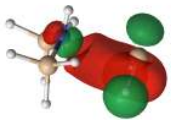
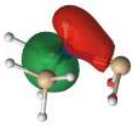
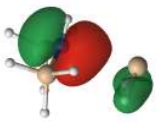
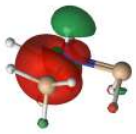
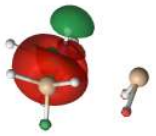
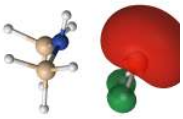
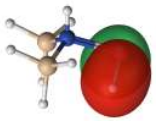
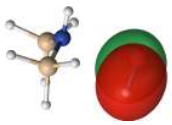
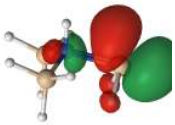
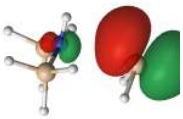
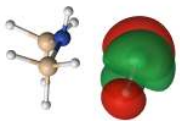
Table 26: Active orbitals, used in the calculation of dissociation curve of $SiH_2NH_2SiH_3$. Shown orbitals are for the minimum energy geometry and for the geometry with Si—N separation of 4.5Å.

 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.05
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.01
 occupation=1.98	 occupation=1.99	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.90	 occupation=1.96	 occupation=0.02	 occupation=0.02

30 $SiH_2 + NH(SiH_3)_2 \rightarrow SiH_2NH(SiH_3)_2$

symmetry used: C_1v
active space: (10,10)

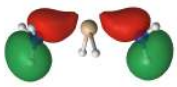
Table 27: Active orbitals, used in the calculation of dissociation curve of $SiH_2NH(SiH_3)_2$. Shown orbitals are for the minimum energy geometry and for the geometry with Si—N separation of 2.87Å.

 occupation=1.99	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02
 occupation=1.95	 occupation=1.92	 occupation=1.98	 occupation=1.98
 occupation=0.05	 occupation=0.08	 occupation=0.02	 occupation=0.02

31 $NH_3 + SiH_2NH_3 \rightarrow NH_3SiH_2NH_3$

symmetry used: C_1v
active space: (14,14)

Table 28: Active orbitals, used in the calculation of dissociation curve of $NH_3SiH_2NH_3$. Shown orbitals are for the minimum energy geometry and for the geometry with Si—N separation of 3.5Å.

 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=1.98	 occupation=1.98
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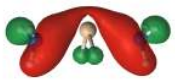
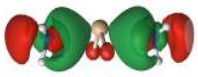
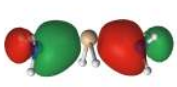
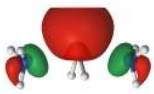
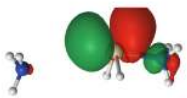
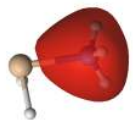
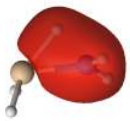
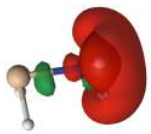
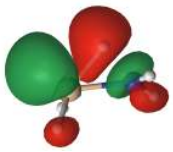
 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.01	 occupation=0.02	 occupation=0.02
 occupation=1.96	 occupation=1.95	 occupation=0.04	 occupation=0.05		

32 $NH_3SiH_2 \rightarrow NH_2SiH_3$

symmetry used: C_s
active space: (10,10)

NH_3SiH_2	transition state	NH_2SiH_3	NH_3SiH_2	transition state	NH_2SiH_3
					
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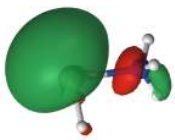	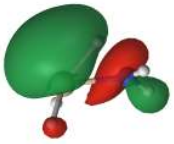		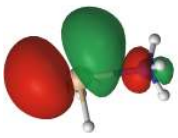		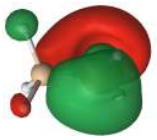
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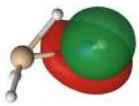
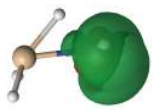
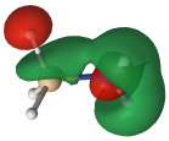
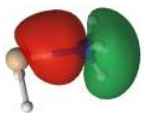
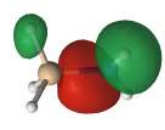
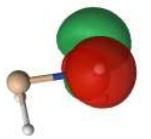
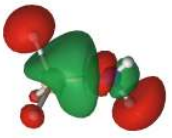
					
occupation=1.98	occupation=1.98	occupation=1.98	occupation=0.01	occupation=0.02	occupation=0.02
					
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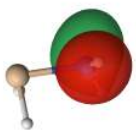
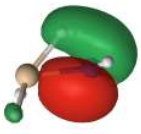
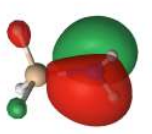
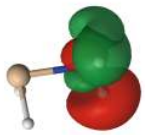
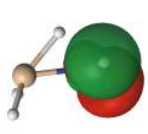
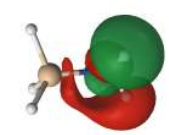
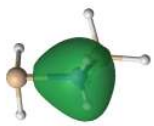
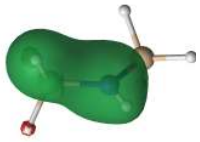
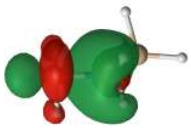
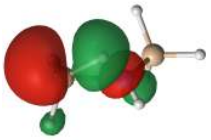
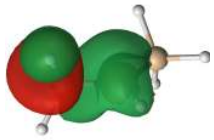
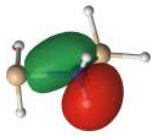
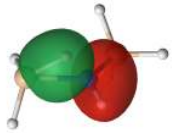
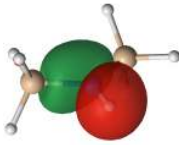
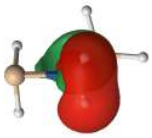
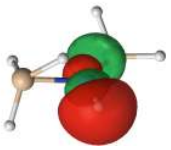
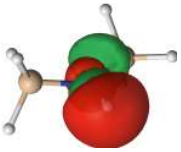
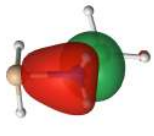
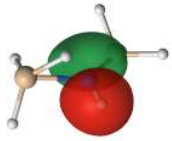
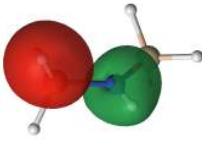
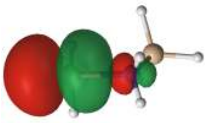
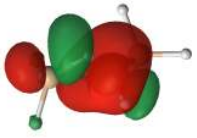
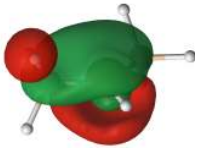
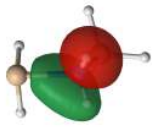
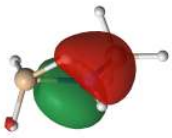
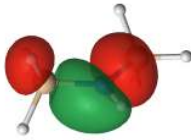
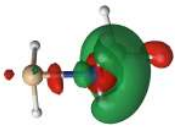
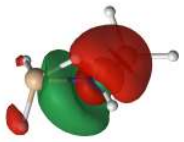
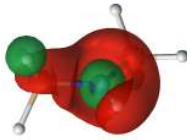
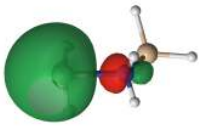
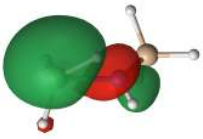
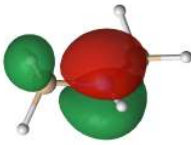
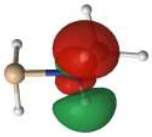
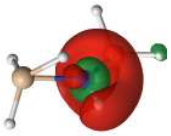
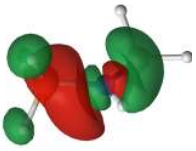
					
occupation=1.98	occupation=1.97	occupation=1.98	occupation=0.02	occupation=0.02	occupation=0.02

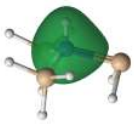
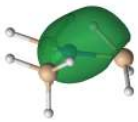
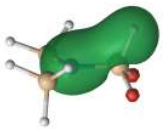
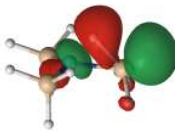
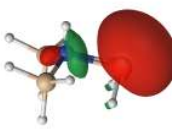
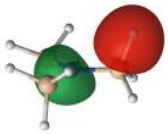
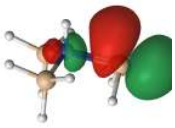
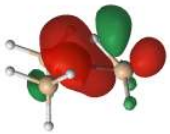
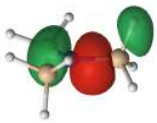
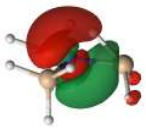
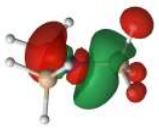
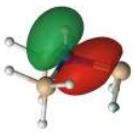
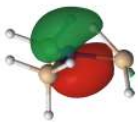
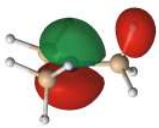
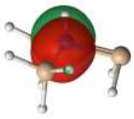
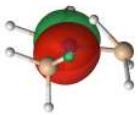
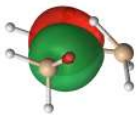
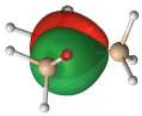
33 $SiH_2NH_2SiH_3 \rightarrow NH(SiH_3)_2$

symmetry used: C_1
active space: (10,10)

$SiH_2NH_2SiH_2$	transition state	SiH_3NHSiH_3	$SiH_2NH_2SiH_2$	transition state	SiH_3NHSiH_3
 occupation=1.98	 occupation=1.99	 occupation=1.98	 occupation=0.01	 occupation=0.08	 occupation=0.01
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.05	 occupation=0.01	 occupation=0.03
 occupation=1.98	 occupation=1.97	 occupation=1.98	 occupation=0.02	 occupation=0.03	 occupation=0.02
 occupation=1.95	 occupation=1.92	 occupation=1.97	 occupation=0.02	 occupation=0.02	 occupation=0.02

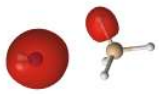
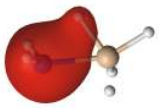
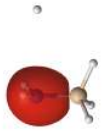
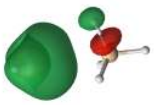
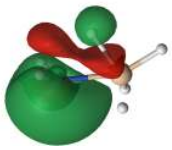
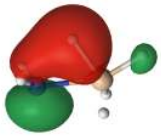
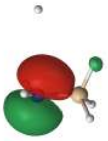
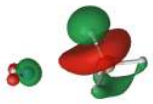
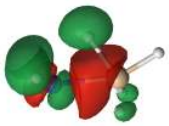
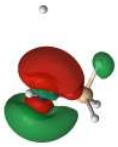
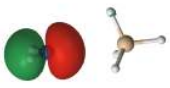
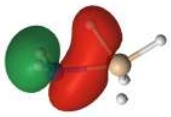
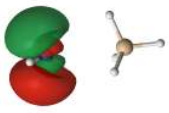
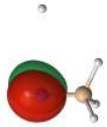
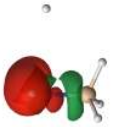
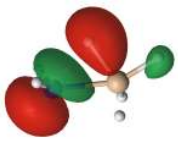
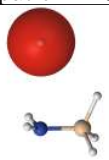
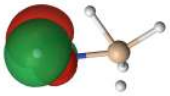
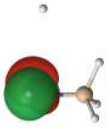
34 $\mathbf{SiH_2NH(SiH_3)_2 \rightarrow N(SiH_3)_3}$

symmetry used: C_s
active space: (10,10)

$SiH_2NH(SiH_3)_2$	transition state	$N(SiH_3)_3$	$SiH_2NH(SiH_3)_2$	transition state	$N(SiH_3)_3$
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.08	 occupation=0.01
 occupation=1.95	 occupation=1.92	 occupation=1.98	 occupation=0.05	 occupation=0.01	 occupation=0.03
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.03	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=1.97	 occupation=1.98	 occupation=1.98	 occupation=1.98
 occupation=0.02	 occupation=0.03	 occupation=0.02	 occupation=0.02	 occupation=0.02	 occupation=0.02

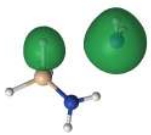
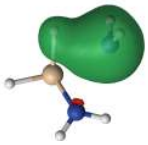
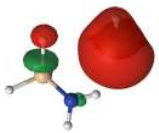
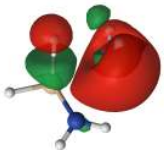
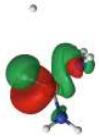
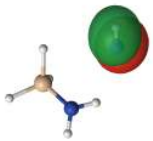
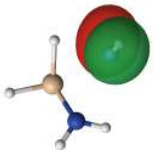
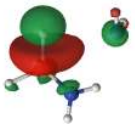
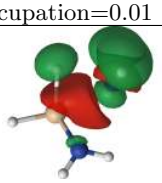
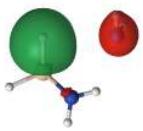
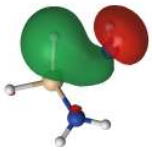
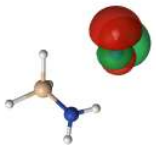
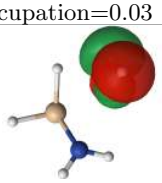
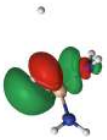
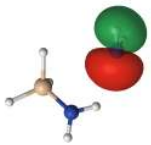
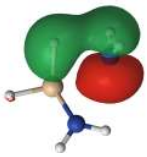
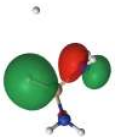
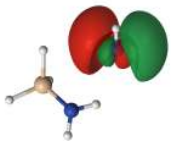
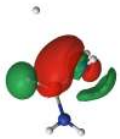
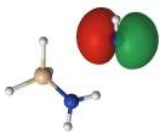
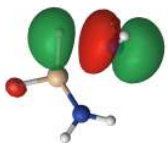
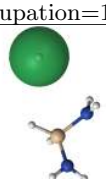
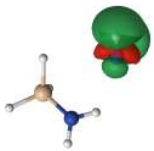
35 $\mathbf{NH_2^{\cdot} + SiH_4 \rightarrow NH_2SiH_3 + H^{\cdot}}$

symmetry used: C_s
active space: (9,10)

$NH_2^{\cdot} + SiH_4$	transition state	$NH_2SiH_3 + H^{\cdot}$	$NH_2^{\cdot} + SiH_4$	transition state	$NH_2SiH_3 + H^{\cdot}$
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.03	 occupation=0.02
 occupation=1.97	 occupation=1.97	 occupation=1.98	 occupation=0.01	 occupation=0.01	 occupation=0.00
 occupation=1.97	 occupation=1.97	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=0.99	 occupation=1.00	 occupation=1.00	 occupation=0.03	 occupation=0.02	 occupation=0.02

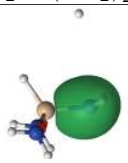
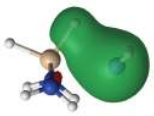
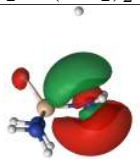
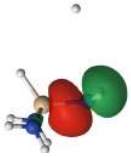
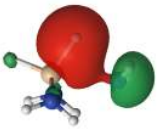
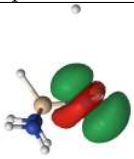
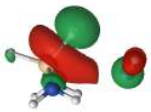
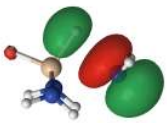
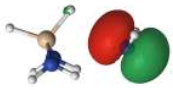
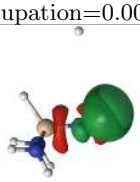
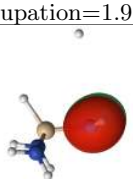
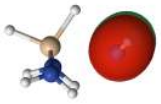
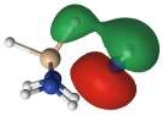
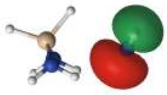
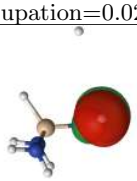
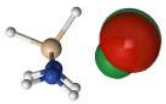
36 $\mathbf{NH_2^{\cdot} + NH_2SiH_3 \rightarrow NH_2SiH_2NH_2 + H^{\cdot}}$

symmetry used: C_1
active space: (9,10)

$NH_2^{\cdot} + NH_2SiH_3$	transition state	$SiH_2(NH_2)_2 + H^{\cdot}$	$NH_2^{\cdot} + NH_2SiH_3$	transition state	$SiH_2(NH_2)_2 + H^{\cdot}$
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.01	 occupation=0.01
 occupation=1.97	 occupation=1.97	 occupation=1.98	 occupation=0.02	 occupation=0.03	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.03	 occupation=0.02	 occupation=0.01
 occupation=1.97	 occupation=1.97	 occupation=1.97	 occupation=0.01	 occupation=0.01	 occupation=0.02
 occupation=0.99	 occupation=1.00	 occupation=1.00	 occupation=0.02	 occupation=0.02	 occupation=0.02

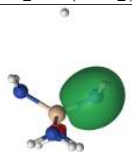
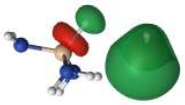
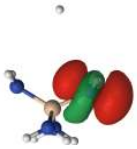
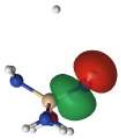
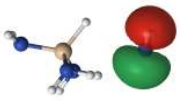
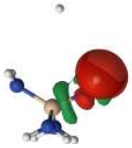
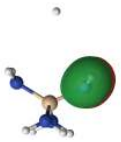
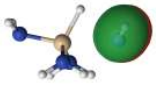
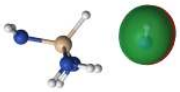
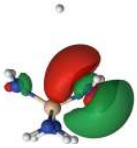
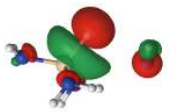
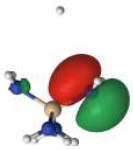
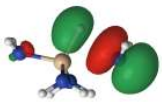
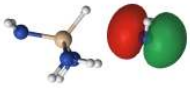
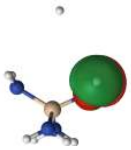
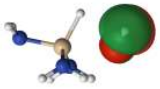
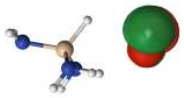
37 $\mathbf{NH_2^{\cdot} + (NH_2)_2SiH_2 \longrightarrow (NH_2)_3SiH + H^{\cdot}}$

symmetry used: C_s
active space: (9,10)

$NH_2^{\cdot} + (NH_2)_2SiH_2$	transition state	$(NH_2)_3SiH + H^{\cdot}$	$NH_2^{\cdot} + (NH_2)_2SiH_2$	transition state	$(NH_2)_3SiH + H^{\cdot}$
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.01	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.00	 occupation=0.03	 occupation=0.02
 occupation=1.97	 occupation=1.00	 occupation=0.99	 occupation=0.02	 occupation=0.01	 occupation=0.01
 occupation=1.98	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.00	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.03	 occupation=0.03

38 $\mathbf{NH_2^{\cdot} + (NH_2)_3SiH \rightarrow (NH_2)_4Si + H^{\cdot}}$

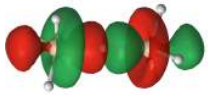
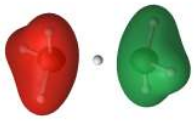
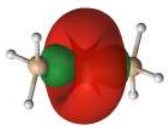
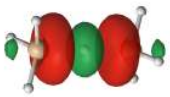
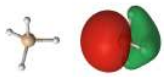
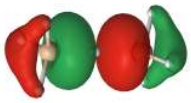
symmetry used: C_s
active space: (9,10)

$NH_2^{\cdot} + (NH_2)_3SiH$	transition state	$(NH_2)_4Si + H^{\cdot}$	$NH_2^{\cdot} + (NH_2)_3SiH$	transition state	$(NH_2)_4Si + H^{\cdot}$
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.01	 occupation=0.02
 occupation=1.00	 occupation=1.98	 occupation=1.98	 occupation=0.00	 occupation=0.01	 occupation=0.01
 occupation=1.98	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.03	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.97	 occupation=1.00	 occupation=0.99	 occupation=0.02	 occupation=0.03	 occupation=0.03

39 $SiH_3^{\cdot} + SiH_4 \rightarrow SiH_4 + SiH_3^{\cdot}$

symmetry used: C_s
active space: (7,7)

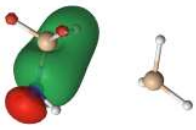
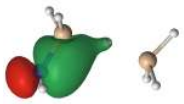
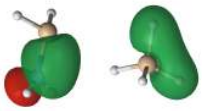
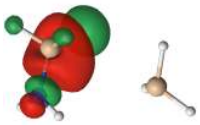
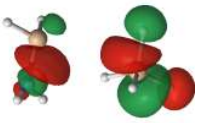
Table 36: The active space used in CASPT2 calculations for the proton transfer reaction. This reaction is symmetric, so only the pre–reaction complex and the transition state are calculated. The postreaction complex is symmetrically identical to the pre–reaction complex and, therefore their energies and orbitals should be equal. Energies of reactants are calculated on the geometry in which molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation. The Energy of products are taken as equal to the energy of reactant since in this case the symmetry applies too.

$SiH_4 + SiH_3^{\cdot}$	transition state	$SiH_4 + SiH_3^{\cdot}$	transition state
 occupation=2.00	 occupation=2.00	 occupation=0.01	 occupation=0.01
 occupation=1.99	 occupation=2.00	 occupation=0.01	 occupation=0.01
 occupation=1.98	 occupation=1.96	 occupation=0.02	 occupation=0.03
 occupation=1.00	 occupation=1.00		

40 $\mathbf{SiH_3^{\cdot} + SiH_3NH_2 \rightarrow SiH_4 + H_2SiNH_2^{\cdot}}$

symmetry used: C_1
active space: (7,7)

Table 37: The active space used in CASPT2 calculations for the proton transfer reaction. Energies of reactants and products are calculated on the geometry in which molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$SiH_3^{\cdot} + H_3SiNH_2$ (pre–reaction complex)	transition state	$SiH_4 + H_2SiNH_2^{\cdot}$ (postreaction complex)	$SiH_3^{\cdot} + H_3SiNH_2$ (pre–reaction complex)	transition state	$SiH_4 + H_2SiNH_2^{\cdot}$ (postreaction complex)
					
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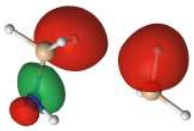		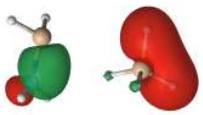			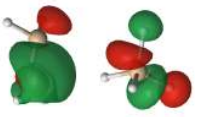
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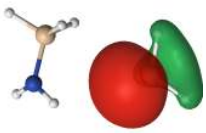	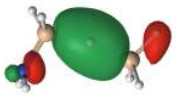	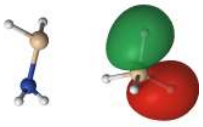	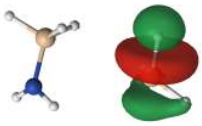		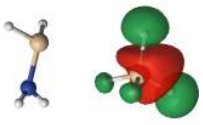
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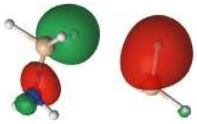	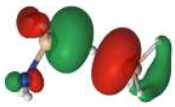	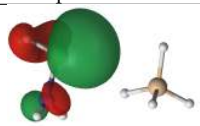			
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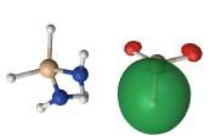
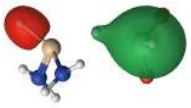
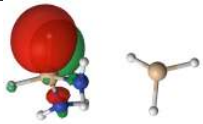
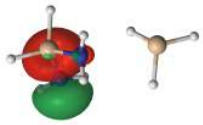
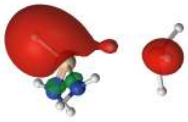
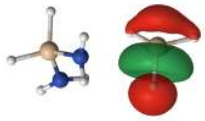
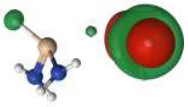
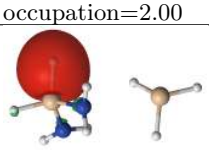
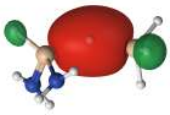
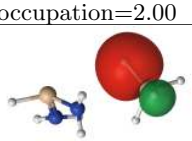
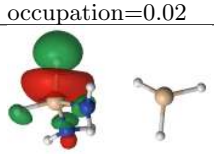
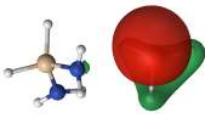
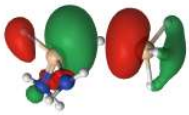
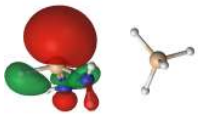
41 $\mathbf{SiH_3^{\cdot} + SiH_2(NH_2)_2 \rightarrow SiH_4 + SiH(NH_2)_2^{\cdot}}$

symmetry used: C_1
active space: (7,7)

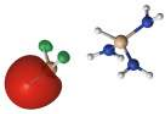
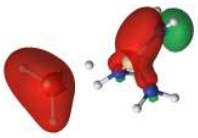
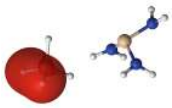
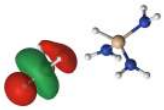
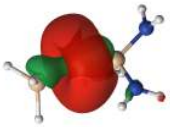
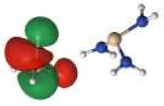
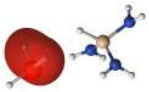
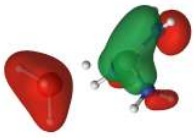
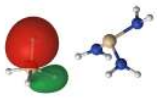
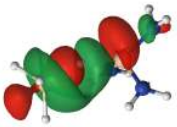
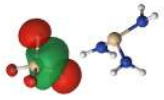
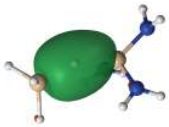
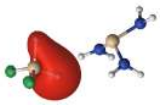
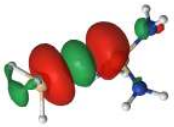
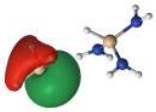
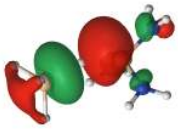
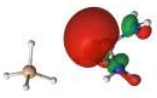
Table 38: The active space used in CASPT2 calculations for the proton transfer reaction. Energies of reactants and products are calculated on the geometry in which molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$SiH_3^{\cdot} + SiH_2(NH_2)_2$ (pre–reaction complex)	transition state	$SiH_4 + SiH(NH_2)_2^{\cdot}$ (postreaction complex)	$SiH_3^{\cdot} + SiH_2(NH_2)_2$ (pre–reaction complex)	transition state	$SiH_4 + SiH(NH_2)_2^{\cdot}$ (postreaction complex)
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.01	 occupation=0.02	 occupation=0.01
 occupation=2.00	 occupation=1.98	 occupation=2.00	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.97	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.03	 occupation=0.02
 occupation=1.00	 occupation=1.00	 occupation=1.00			

42 $\mathbf{SiH_3^{\cdot} + HSi(NH_2)_3 \rightarrow SiH_4 + Si(NH_2)_3^{\cdot}}$

symmetry used: C_s
active space: (7,7)

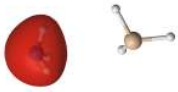
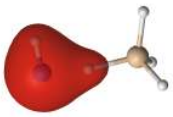
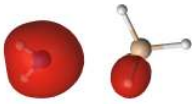
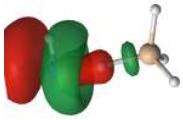
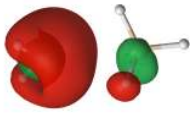
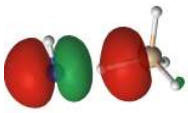
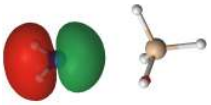
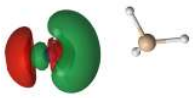
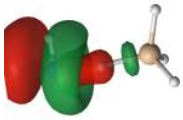
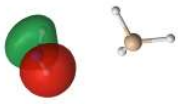
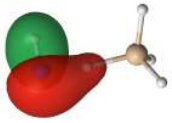
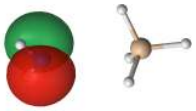
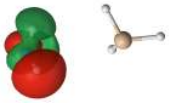
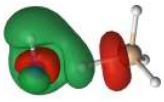
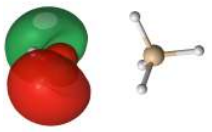
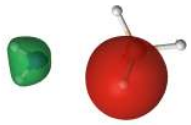
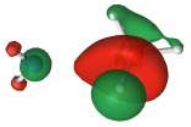
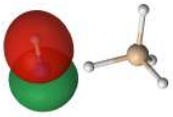
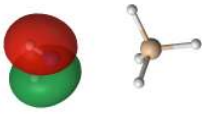
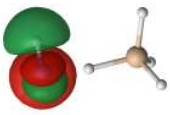
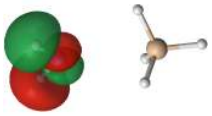
Table 39: The active space used in CASPT2 calculations for the proton transfer reaction. Energies of reactants and products are calculated on the geometry in which molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$SiH_3^{\cdot} + HSi(NH_2)_3$ (pre–reaction complex)	transition state	$SiH_4 + Si(NH_2)_3^{\cdot}$ (postreaction complex)	$SiH_3^{\cdot} + HSi(NH_2)_3$ (pre–reaction complex)	transition state	$SiH_4 + Si(NH_2)_3^{\cdot}$ (postreaction complex)
 occupation=1.98	 occupation=2.00	 occupation=2.00	 occupation=0.02	 occupation=0.00	 occupation=0.02
 occupation=2.00	 occupation=2.00	 occupation=1.98	 occupation=0.02	 occupation=0.01	 occupation=0.02
 occupation=1.97	 occupation=1.96	 occupation=1.97	 occupation=0.01	 occupation=0.03	 occupation=0.01
 occupation=1.00	 occupation=1.00	 occupation=1.00			

43 $\mathbf{NH_2^{\cdot} + SiH_4 \rightarrow NH_3 + SiH_3^{\cdot}}$

symmetry used: C_s
active space: (10,10)

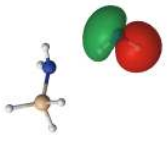
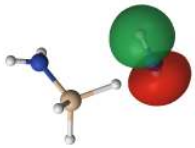
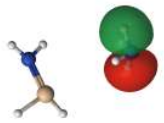
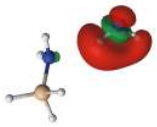
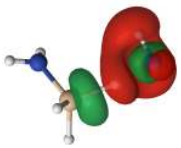
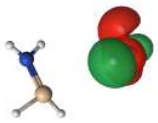
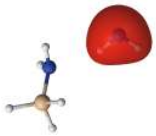
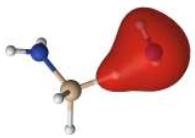
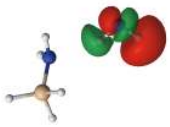
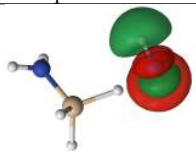
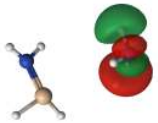
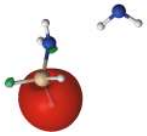
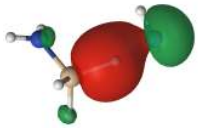
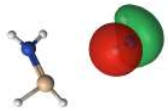
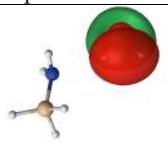
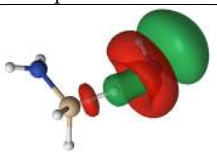
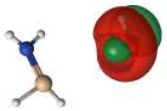
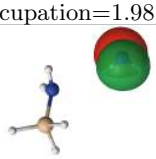
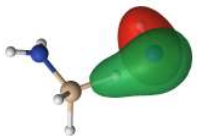
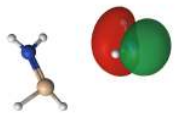
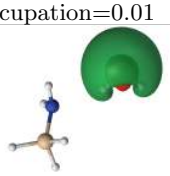
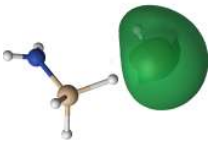
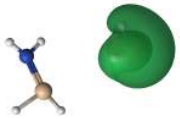
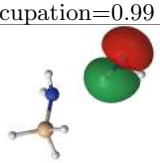
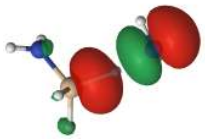
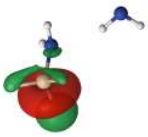
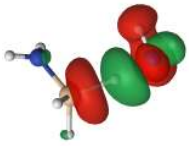
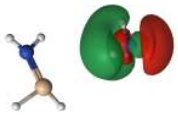
Table 40: The active space used in CASPT2 calculations for the proton transfer reaction. Energies of reactants and products are calculated on geometries in which molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$NH_2^{\cdot} + SiH_4$ (pre–reaction complex)	transition state	$NH_3 + SiH_3$ (postreaction complex)	$NH_2^{\cdot} + SiH_4$ (pre–reaction complex)	transition state	$NH_3 + SiH_3$ (postreaction complex)
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.00	 occupation=1.97	 occupation=0.02	 occupation=0.01	 occupation=0.02
 occupation=1.97	 occupation=1.97	 occupation=0.99	 occupation=0.01	 occupation=0.02	 occupation=0.01
 occupation=1.00	 occupation=1.97	 occupation=1.98	 occupation=0.02	 occupation=0.03	 occupation=0.02
 occupation=1.97	 occupation=1.97	 occupation=1.97	 occupation=0.03	 occupation=0.03	 occupation=0.03

44 $\mathbf{NH_2^{\cdot} + SiH_3NH_2 \rightarrow NH_3 + H_2SiNH_2^{\cdot}}$

symmetry used: C_1
active space: (10,10)

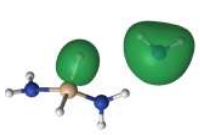
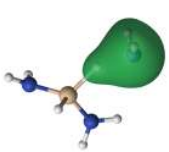
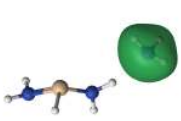
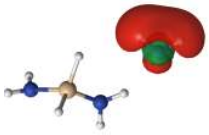
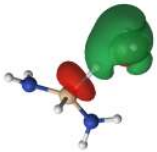
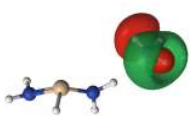
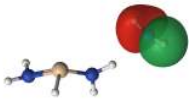
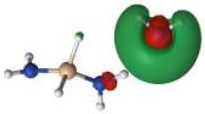
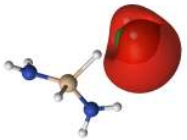
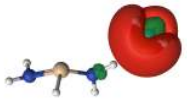
Table 41: The active space used in CASPT2 calculations for the proton transfer reaction. Energies of reactants and products are calculated on the geometry in which molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$NH_2^{\cdot} + H_3SiNH_2$ (pre–reaction complex)	transition state	$NH_3 + H_2SiNH_2^{\cdot}$ (postreaction complex)	$NH_2^{\cdot} + H_3SiNH_2$ (pre–reaction complex)	transition state	$NH_3 + H_2SiNH_2^{\cdot}$ (postreaction complex)
 occupation=1.97	 occupation=1.97	 occupation=1.97	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.03	 occupation=0.03	 occupation=0.02
 occupation=1.98	 occupation=1.97	 occupation=1.97	 occupation=0.01	 occupation=0.01	 occupation=0.01
 occupation=0.99	 occupation=1.97	 occupation=1.98	 occupation=0.02	 occupation=0.02	 occupation=0.02
 occupation=1.97	 occupation=1.00	 occupation=1.00	 occupation=0.02	 occupation=0.03	 occupation=0.02

45 $\mathbf{NH_2^{\cdot} + SiH_2(NH_2)_2 \rightarrow NH_3 + HSi(NH_2)_2^{\cdot}}$

symmetry used: C_1
active space: (10,10)

Table 42: The active space used in CASPT2 calculations for the proton transfer reaction. Energies of reactants and products are calculated on the geometry in which molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$NH_2^{\cdot}$+$SiH_2(NH_2)_2$ (pre–reaction complex)	transition state	$NH_3 + SiH(NH_2)_2^{\cdot}$ (postreaction complex)	$NH_2^{\cdot}$+$SiH_2(NH_2)_2$ (pre–reaction complex)	transition state	$NH_3 + SiH(NH_2)_2^{\cdot}$ (postreaction complex)
					
occupation=1.98	occupation=1.98	occupation=1.98	occupation=0.02	occupation=0.03	occupation=0.01
					
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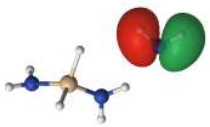
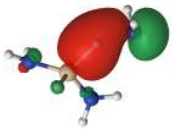
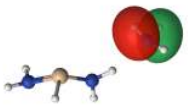
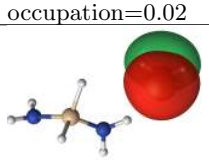
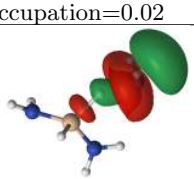
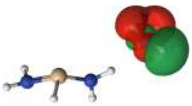
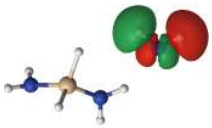
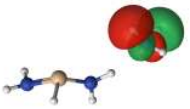
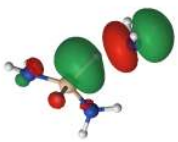
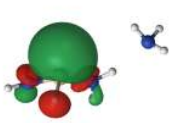
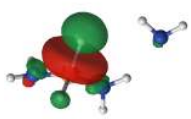
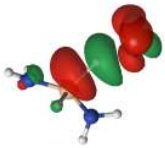
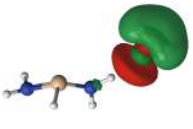
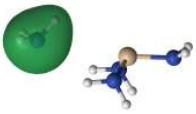
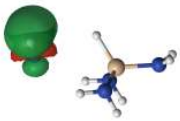
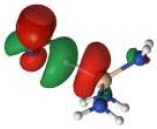
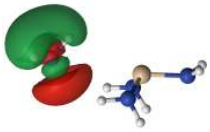
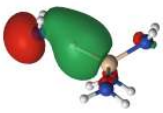
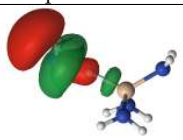
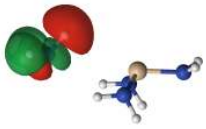
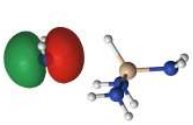
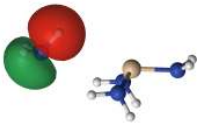
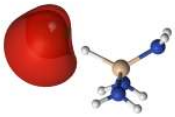
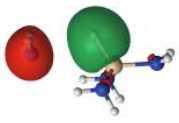
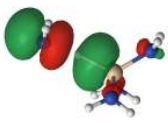
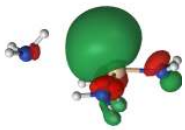
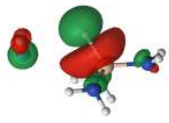
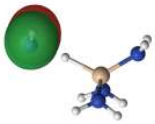
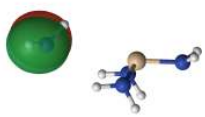
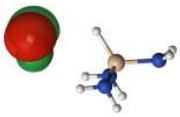
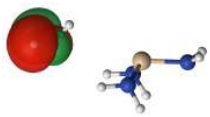
					
occupation=0.97	occupation=1.97	occupation=1.97	occupation=0.01	occupation=0.01	occupation=0.02
					
occupation=1.97	occupation=1.97	occupation=1.98	occupation=0.03	occupation=0.03	occupation=0.02
					
occupation=1.98	occupation=1.00	occupation=1.00	occupation=0.02	occupation=0.03	occupation=0.02

46 $\mathbf{NH_2^{\cdot} + SiH(NH_2)_3 \rightarrow NH_3 + Si(NH_2)_3^{\cdot}}$

symmetry used: C_s
active space: (10,10)

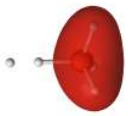
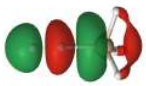
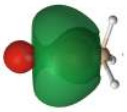
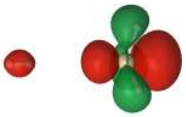
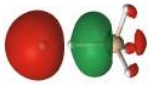
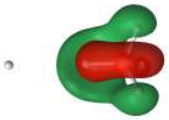
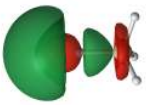
Table 43: The active space used in CASPT2 calculations for the proton transfer reaction. Energies of reactants and products are calculated on the geometry in which molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$NH_2^{\cdot} + SiH(NH_2)_3$ (pre–reaction complex)	transition state	$NH_3 + Si(NH_2)_3^{\cdot}$ (postreaction complex)	$NH_2^{\cdot} + SiH(NH_2)_3$ (pre–reaction complex)	transition state	$NH_3 + Si(NH_2)_3^{\cdot}$ (postreaction complex)
					
occupation=1.98	occupation=1.98	occupation=1.98	occupation=0.02	occupation=0.03	occupation=0.02
					
occupation=0.97	occupation=1.97	occupation=1.98	occupation=0.02	occupation=0.01	occupation=0.02
					
occupation=0.99	occupation=1.97	occupation=1.97	occupation=0.01	occupation=0.02	occupation=0.02
					
occupation=1.98	occupation=1.00	occupation=1.00	occupation=0.02	occupation=0.02	occupation=0.01
					
occupation=1.97	occupation=1.97	occupation=1.97	occupation=0.03	occupation=0.03	occupation=0.02

47 $\mathbf{H^{\cdot} + SiH_4 \rightarrow H_2 + SiH_3^{\cdot}}$

symmetry used: C_s
active space: (6,6)

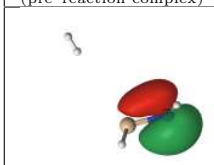
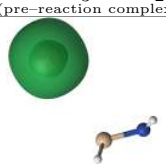
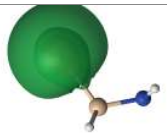
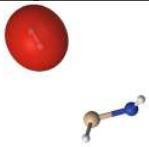
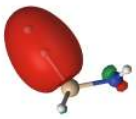
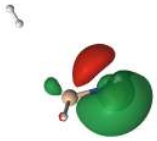
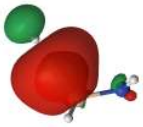
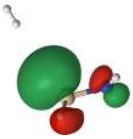
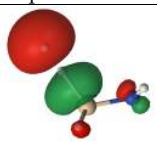
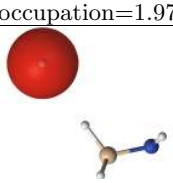
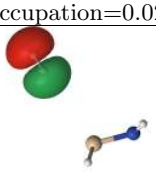
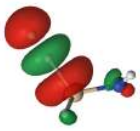
Table 44: The active space used in CASPT2 calculations for the proton transfer reaction. Energies of reactants and products are calculated on geometries in which molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$H^{\cdot} + SiH_4$ (pre–reaction complex)	transition state	$H_2 + SiH_3$ (postreaction complex)	$H^{\cdot} + SiH_4$ (pre–reaction complex)	transition state	$H_2 + SiH_3$ (postreaction complex)
 occupation=1.99	 occupation=2.00	 occupation=1.99	 occupation=0.02	 occupation=0.03	 occupation=0.02
 occupation=1.97	 occupation=1.96	 occupation=1.97	 occupation=0.01	 occupation=0.01	 occupation=0.01
 occupation=1.00	 occupation=1.00	 occupation=1.00	 occupation=0.01	 occupation=0.01	 occupation=0.01

48 $\mathbf{H^{\cdot} + SiH_3NH_2 \rightarrow H_2 + H_2SiNH_2^{\cdot}}$

symmetry used: C_1
active space: (6,6)

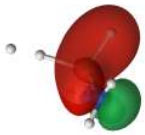
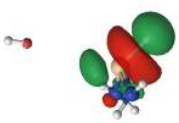
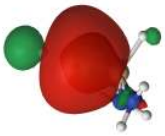
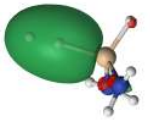
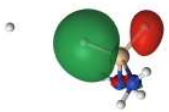
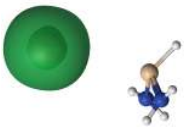
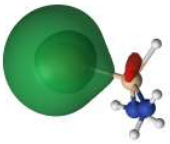
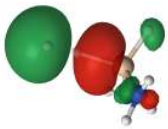
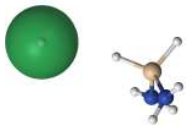
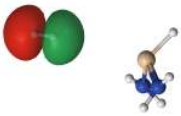
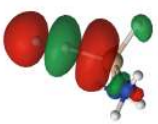
Table 45: The active space used in CASPT2 calculations for the proton transfer reaction. Energies of reactants and products are calculated on the geometry in which molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$H^{\cdot} + H_3SiNH_2$ (pre–reaction complex)	transition state	$H_2 + H_2SiNH_2^{\cdot}$ (postreaction complex)	$H^{\cdot} + H_3SiNH_2$ (pre–reaction complex)	transition state	$H_2 + H_2SiNH_2^{\cdot}$ (postreaction complex)
 occupation=1.98	 occupation=2.00	 occupation=1.98	 occupation=0.01	 occupation=0.01	 occupation=0.01
 occupation=1.97	 occupation=1.96	 occupation=1.97	 occupation=0.02	 occupation=0.01	 occupation=0.01
 occupation=1.00	 occupation=1.00	 occupation=1.00	 occupation=0.02	 occupation=0.03	 occupation=0.02

49 $\mathbf{H^{\cdot} + SiH_2(NH_2)_2 \rightarrow H_2 + HSi(NH_2)_2^{\cdot}}$

symmetry used: C_1
active space: (6,6)

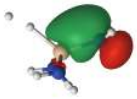
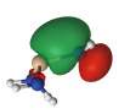
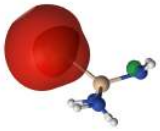
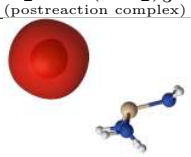
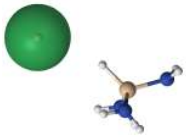
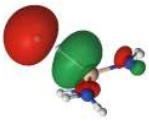
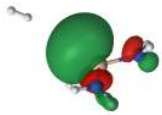
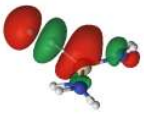
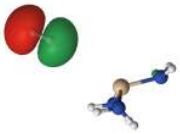
Table 46: The active space used in CASPT2 calculations for the proton transfer reaction. Energies of reactants and products are calculated on the geometry in which molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$H^{\cdot} + SiH_2(NH_2)_2$ (pre–reaction complex)	transition state	$H_2 + SiH(NH_2)_2^{\cdot}$ (postreaction complex)	$H^{\cdot} + SiH_2(NH_2)_2$ (pre–reaction complex)	transition state	$H_2 + SiH(NH_2)_2^{\cdot}$ (postreaction complex)
					
occupation=1.98	occupation=2.00	occupation=1.98	occupation=0.02	occupation=0.01	occupation=0.02
					
occupation=1.97	occupation=1.96	occupation=1.97	occupation=0.01	occupation=0.01	occupation=0.01
					
occupation=1.00	occupation=1.00	occupation=1.00	occupation=0.02	occupation=0.03	occupation=0.02

50 $\mathbf{H^{\cdot} + SiH(NH_2)_3 \rightarrow H_2 + Si(NH_2)_3^{\cdot}}$

symmetry used: C_1
active space: (6,6)

Table 47: The active space used in CASPT2 calculations for the proton transfer reaction. Energies of reactants and products are calculated on the geometry in which molecular fragments are placed on a much larger separation (> 20 Å), that is too large to be suitable for visualisation.

$H^{\cdot} + SiH(NH_2)_3$ (pre–reaction complex)	transition state	$H_2 + Si(NH_2)_3^{\cdot}$ (postreaction complex)	$H^{\cdot} + SiH(NH_2)_3$ (pre–reaction complex)	transition state	$H_2 + Si(NH_2)_3^{\cdot}$ (postreaction complex)
 occupation=1.98	 occupation=1.98	 occupation=1.98	 occupation=0.02	 occupation=0.01	 occupation=0.01
 occupation=1.00	 occupation=1.97	 occupation=1.97	 occupation=0.01	 occupation=0.01	 occupation=0.01
 occupation=1.97	 occupation=1.00	 occupation=1.00	 occupation=0.01	 occupation=0.03	 occupation=0.02