# Supporting Information:

# Quantitative Assessment of Tetrel Bonding Utilizing Vibrational Spectroscopy

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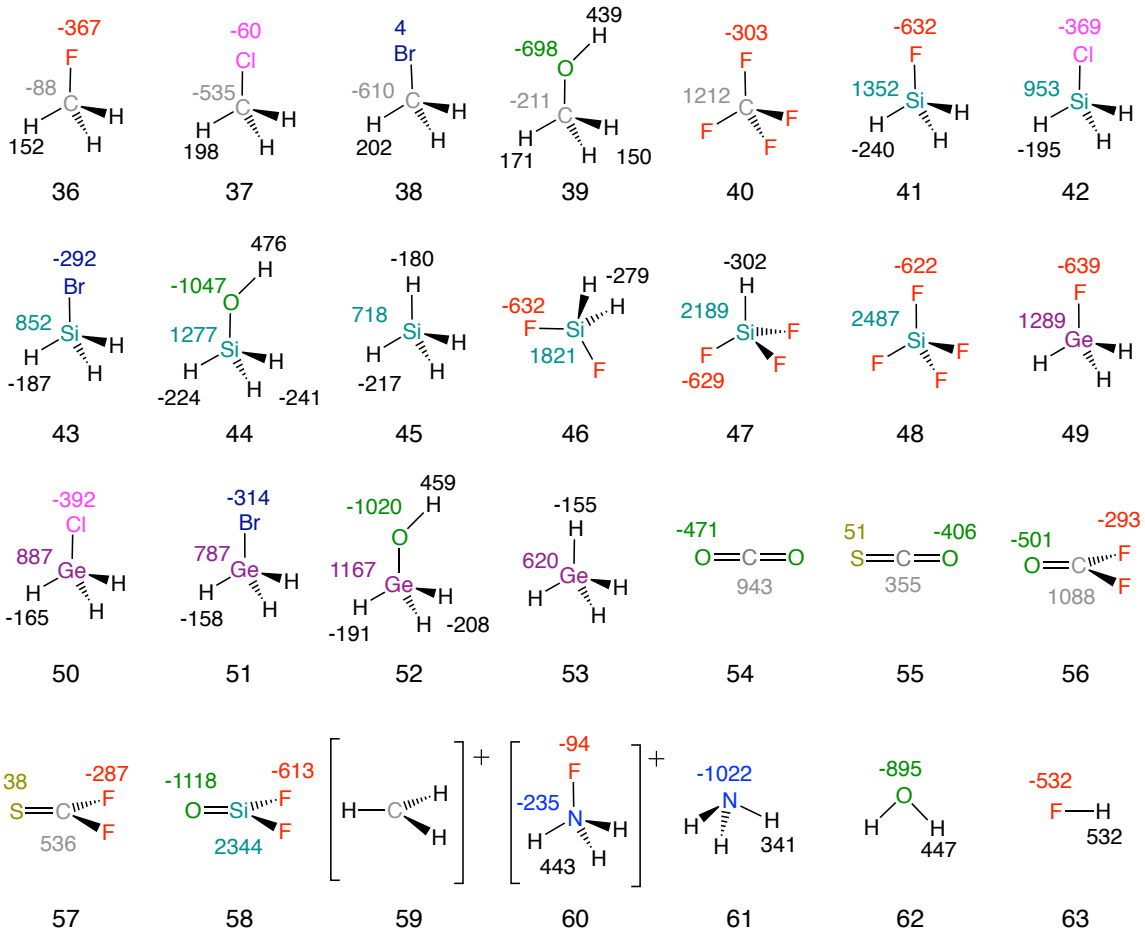


Figure S1: Schematic representation of monomers (**36-63**) with atomic charges from the natural population analysis calculated at CCSD(T)/aug-cc-pVTZ level of theory. Colors are used to correlate charges to specific atoms.

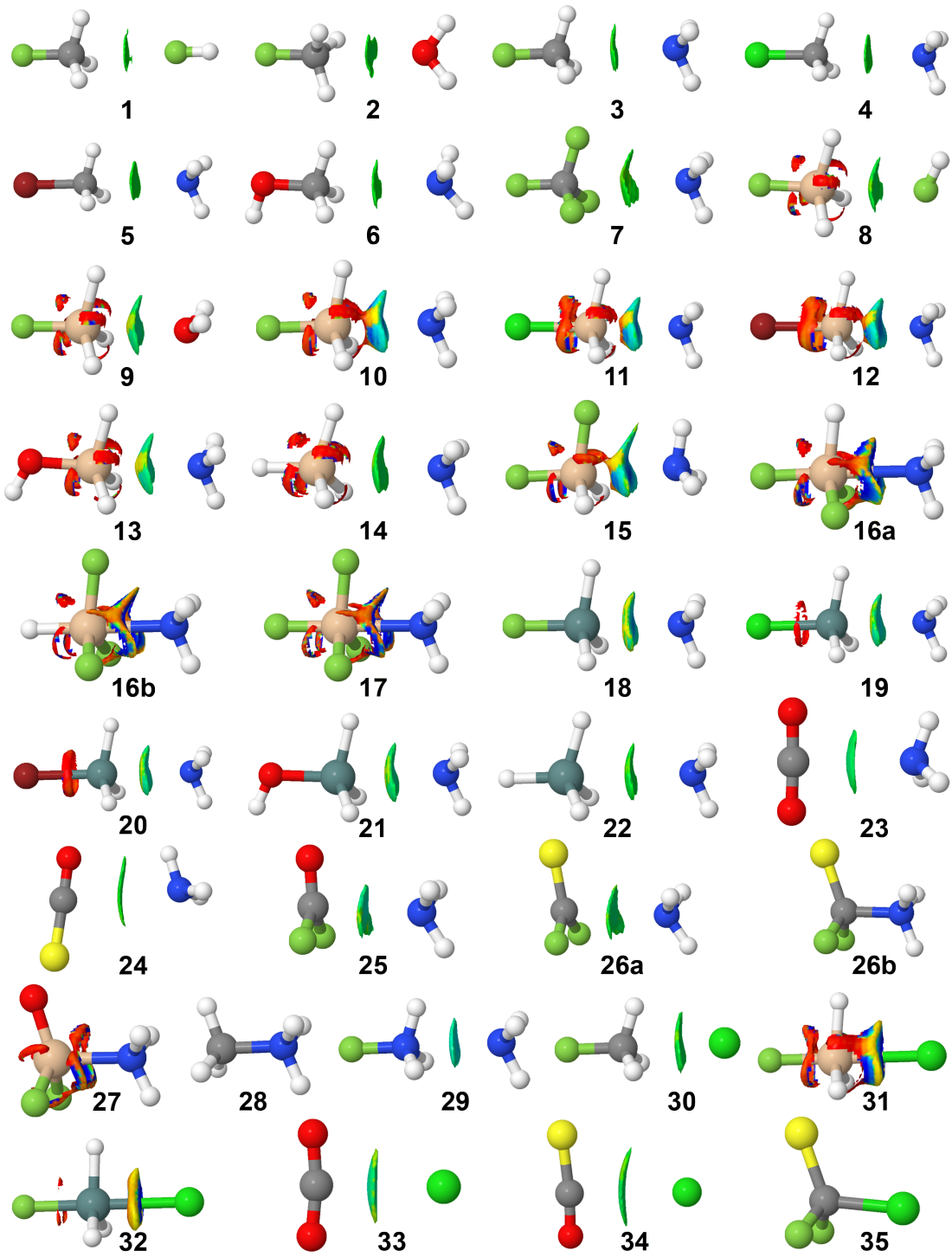


Figure S2: Noncovalent interactions (NCIs) plot of complexes **1-35** calculated at gradient isosurfaces $s = 0.5$ au., where green indicates weak attractive, blue indicates strong attractive, and red surface indicates repulsive noncovalent interactions.

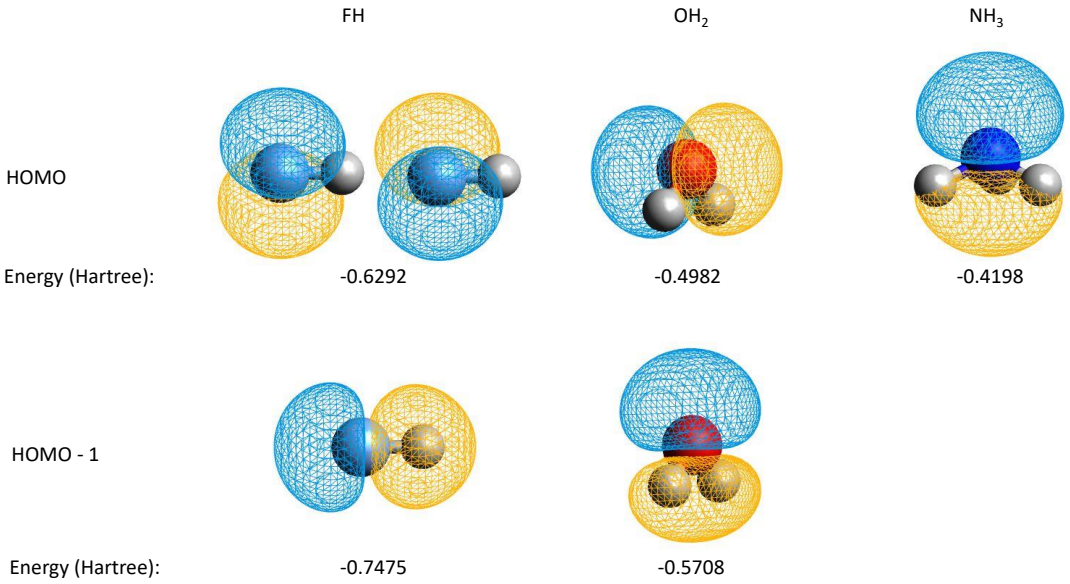


Figure S3: Selected molecular orbitals of the T-acceptors. Calculated at HF/6-31G(d) level of theory.

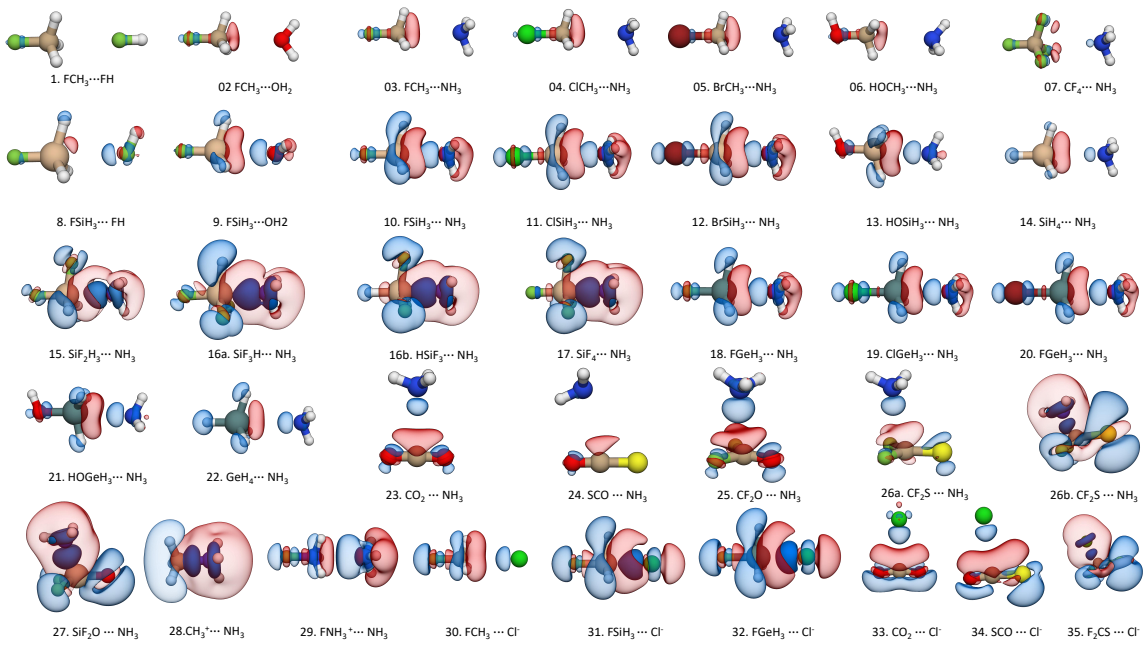


Figure S4: CCSD(T)/aug-cc-pVTZ electron difference density distributions $\Delta\rho(\mathbf{r})$ given for complexes **1-35**. $\Delta\rho(\mathbf{r})$ is plotted for an electron density surface with a constant density value of 0.001 a.u. Blue regions indicate an increase in the electron density, red regions indicate a density decrease relative to the superimposed density of the monomer.

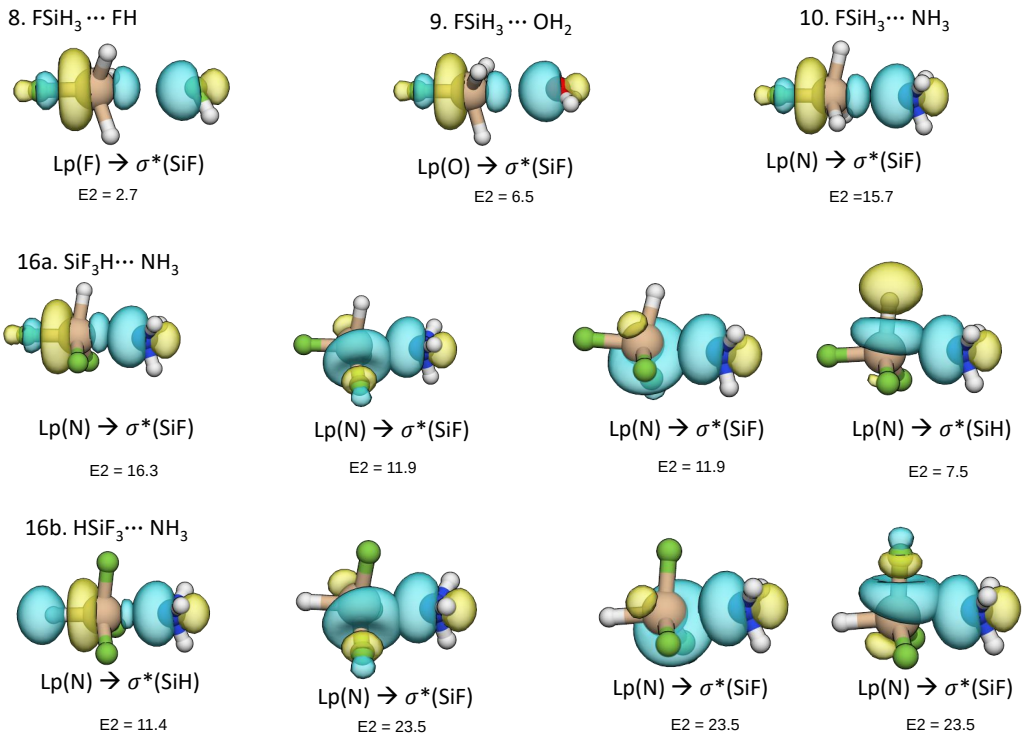


Figure S5: Combination of donor and acceptor NBO orbitals involved in the electron delocalization of selected complexes. Delocalization energies are given in kcal/mol

**Table S1: Comparion between DLPNO-CCSD(T)/aug-cc-pV5Z and CCSD(T)/aug-cc-pVTZ energies***

| # | Complex (symm.) | CCSD(T)/aug-cc-pVTZ $E_{int}$ | $E_{int}$(CP) | BSSE | CCSD(T)/aug-cc-pV5Z $E_{int}$ | $E_{int}$(CP) | BSSE |
|---|---|---|---|---|---|---|---|
| C - Tetrel bond | | | | | | | |
| **1** | $FCH_3\cdots FH$ ($C_{3v}$) | -1.51 | -1.30 | 0.21 | -1.36 | -1.33 | 0.03 |
| **2** | $FCH_3\cdots OH_2$ ($C_s$) | -2.11 | -1.89 | 0.22 | -1.96 | -1.93 | 0.03 |
| **3** | $FCH_3\cdots NH_3$ ($C_{3v}$) | -2.27 | -2.07 | 0.20 | -2.15 | -2.12 | 0.03 |
| **4** | $ClCH_3\cdots NH_3$ ($C_{3v}$) | -2.09 | -1.90 | 0.19 | -2.00 | -1.96 | 0.04 |
| **5** | $BrCH_3\cdots NH_3$ ($C_{3v}$) | -2.02 | -1.81 | 0.21 | -1.91 | -1.88 | 0.03 |
| **6** | $HOCH_3\cdots NH_3$ ($C_s$) | -1.39 | -1.23 | 0.16 | -1.27 | -1.25 | 0.02 |
| **7** | $CF_4\cdots NH_3$ ($C_{3v}$) | -1.69 | -1.30 | 0.39 | -1.38 | -1.32 | 0.06 |
| Si - Tetrel bond | | | | | | | |
| **8** | $FSiH_3\cdots FH$ ($C_s$) | -2.34 | -1.91 | 0.43 | -2.08 | -2.02 | 0.06 |
| **9** | $FSiH_3\cdots OH_2$ ($C_s$) | -4.55 | -3.96 | 0.59 | -4.31 | -4.24 | 0.07 |
| **10** | $FSiH_3\cdots NH_3$ ($C_{3v}$) | -8.91 | -8.06 | 0.85 | -8.81 | -8.72 | 0.09 |
| **11** | $ClSiH_3\cdots NH_3$ ($C_{3v}$) | -8.16 | -7.44 | 0.72 | -8.19 | -8.09 | 0.10 |
| **12** | $BrSiH_3\cdots NH_3$ ($C_{3v}$) | -8.35 | -7.58 | 0.77 | -8.39 | -8.30 | 0.09 |
| **13** | $HOSiH_3\cdots NH_3$ ($C_s$) | -4.81 | -4.29 | 0.52 | -4.70 | -4.64 | 0.06 |
| **14** | $SiH_4\cdots NH_3$ ($C_{3v}$) | -2.41 | -2.12 | 0.29 | -2.32 | -2.29 | 0.03 |
| **15** | $SiF_2H_2\cdots NH_3$ ($C_s$) | -11.73 | -10.47 | 1.26 | -11.46 | -11.32 | 0.14 |
| **16a** | $SiF_3H\cdots NH_3$ ($C_s$) | -19.43 | -17.54 | 1.89 | -19.06 | -18.84 | 0.22 |
| **16b** | $SiF_3H\cdots NH_3$ ($C_{3v}$) | -27.53 | -25.36 | 2.17 | -27.29 | -27.01 | 0.28 |
| **17** | $SiF_4\cdots NH_3$ ($C_{3v}$) | -32.55 | -30.00 | 2.55 | -32.05 | -31.75 | 0.30 |
| Ge - Tetrel bond | | | | | | | |
| **18** | $FGeH_3\cdots NH_3$ ($C_{3v}$) | -9.17 | -8.58 | 0.59 | -9.04 | -8.97 | 0.07 |
| **19** | $ClGeH_3\cdots NH_3$ ($C_{3v}$) | -7.29 | -6.82 | 0.47 | -7.28 | -7.20 | 0.08 |
| **20** | $BrGeH_3\cdots NH_3$ ($C_{3v}$) | -7.08 | -6.60 | 0.48 | -7.09 | -7.01 | 0.08 |
| **21** | $HOGeH_3\cdots NH_3$ ($C_s$) | -5.08 | -4.68 | 0.40 | -4.97 | -4.92 | 0.05 |
| **22** | $GeH_4\cdots NH_3$ ($C_{3v}$) | -2.08 | -1.88 | 0.20 | -2.01 | -1.99 | 0.02 |
| Double bond - Tetrel bond | | | | | | | |
| **23** | $CO_2\cdots NH_3$ ($C_s$) | -3.21 | -2.95 | 0.26 | -3.09 | -3.04 | 0.05 |
| **24** | $SCO\cdots NH_3$ ($C_s$) | -1.99 | -1.71 | 0.28 | -1.79 | -1.75 | 0.04 |
| **25** | $CF_2O\cdots NH_3$ ($C_s$) | -5.81 | -5.09 | 0.72 | -5.35 | -5.25 | 0.10 |
| **26a** | $CF_2S\cdots NH_3$ ($C_s$) | -4.02 | -3.34 | 0.68 | -3.53 | -3.44 | 0.09 |
| **26b** | $CF_2S\cdots NH_3$ ($C_s$) | -22.68 | -19.85 | 2.83 | -23.73 | -23.27 | 0.46 |
| **27** | $SiF_2O\cdots NH_3$ ($C_s$) | -52.10 | -50.12 | 1.98 | -53.34 | -53.07 | 0.27 |
| Anionic - Tetrel bond | | | | | | | |
| **28** | $CH_3^+\cdots NH_3$ ($C_{3v}$) | -135.20 | -133.96 | 1.24 | -135.92 | -135.74 | 0.18 |
| **29** | $FNH_3^+\cdots NH_3$ ($C_{3v}$) | -23.56 | -23.20 | 0.36 | -23.49 | -23.43 | 0.06 |
| **30** | $FCH_3\cdots Cl^-$ ($C_{3v}$) | -10.16 | -9.73 | 0.43 | -10.11 | -9.98 | 0.13 |
| **31** | $FSiH_3\cdots Cl^-$ ($C_{3v}$) | -32.76 | -31.52 | 1.24 | -33.42 | -33.14 | 0.28 |
| **32** | $FGeH_3\cdots Cl^-$ ($C_{3v}$) | -36.81 | -35.79 | 1.02 | -37.18 | -36.93 | 0.25 |
| **33** | $CO_2\cdots Cl^-$ ($C_s$) | -8.89 | -8.43 | 0.46 | -8.89 | -8.77 | 0.12 |
| **34** | $SCO\cdots Cl^-$ ($C_s$) | -5.88 | -5.48 | 0.40 | -5.85 | -5.75 | 0.10 |
| **35** | $CF_2S\cdots Cl^-$ ($C_s$) | -49.44 | -46.46 | 2.98 | -50.61 | -50.02 | 0.59 |

*Interaction energies ($E_{int}$), counterpoise (CP) corrected interaction energies and basis set superposition error calculated at CCSD(T)/aug-cc-pVTZ and DLPNO-CCSD(T)/aug-cc-pV5Z levels. All energies were obtained using CCSD(T)/aug-cc-pVTZ geometries. Values are given in kcal/mol.

## Table S2: Deviation from DLPNO-CCSD(T)/aug-cc-pV5Z interaction energies*

| # | Complex (symm.) | (a) | (b) | (c) |
|---|---|---|---|---|
| C - Tetrel bond | | | | |
| **1** | $FCH_3\cdots FH$ ($C_{3v}$) | -0.03 | 0.18 | 0.15 |
| **2** | $FCH_3\cdots OH_2$ ($C_s$) | -0.04 | 0.18 | 0.15 |
| **3** | $FCH_3\cdots NH_3$ ($C_{3v}$) | -0.05 | 0.15 | 0.12 |
| **4** | $ClCH_3\cdots NH_3$ ($C_{3v}$) | -0.06 | 0.13 | 0.09 |
| **5** | $BrCH_3\cdots NH_3$ ($C_{3v}$) | -0.07 | 0.14 | 0.11 |
| **6** | $HOCH_3\cdots NH_3$ ($C_s$) | -0.02 | 0.14 | 0.12 |
| **7** | $CF_4\cdots NH_3$ ($C_{3v}$) | -0.02 | 0.37 | 0.31 |
| Si - Tetrel bond | | | | |
| **8** | $FSiH_3\cdots FH$ ($C_s$) | -0.11 | 0.32 | 0.26 |
| **9** | $FSiH_3\cdots OH_2$ ($C_s$) | -0.28 | 0.31 | 0.24 |
| **10** | $FSiH_3\cdots NH_3$ ($C_{3v}$) | -0.66 | 0.19 | 0.10 |
| **11** | $ClSiH_3\cdots NH_3$ ($C_{3v}$) | -0.65 | 0.07 | -0.03 |
| **12** | $BrSiH_3\cdots NH_3$ ($C_{3v}$) | -0.72 | 0.05 | -0.04 |
| **13** | $HOSiH_3\cdots NH_3$ ($C_s$) | -0.35 | 0.17 | 0.11 |
| **14** | $SiH_4\cdots NH_3$ ($C_{3v}$) | -0.17 | 0.12 | 0.09 |
| **15** | $SiF_2H_2\cdots NH_3$ ($C_s$) | -0.85 | 0.41 | 0.27 |
| **16a** | $SiF_3H\cdots NH_3$ ($C_s$) | -1.30 | 0.59 | 0.37 |
| **16b** | $SiF_3H\cdots NH_3$ ($C_{3v}$) | -1.65 | 0.52 | 0.24 |
| **17** | $SiF_4\cdots NH_3$ ($C_{3v}$) | -1.75 | 0.80 | 0.50 |
| Ge - Tetrel bond | | | | |
| **18** | $FGeH_3\cdots NH_3$ ($C_{3v}$) | -0.39 | 0.20 | 0.13 |
| **19** | $ClGeH_3\cdots NH_3$ ($C_{3v}$) | -0.38 | 0.09 | 0.01 |
| **20** | $BrGeH_3\cdots NH_3$ ($C_{3v}$) | -0.41 | 0.07 | -0.01 |
| **21** | $HOGeH_3\cdots NH_3$ ($C_s$) | -0.24 | 0.16 | 0.11 |
| **22** | $GeH_4\cdots NH_3$ ($C_{3v}$) | -0.11 | 0.09 | 0.07 |
| Double bond - Tetrel bond | | | | |
| **23** | $CO_2\cdots NH_3$ ($C_s$) | -0.09 | 0.17 | 0.12 |
| **24** | $SCO\cdots NH_3$ ($C_s$) | -0.04 | 0.24 | 0.20 |
| **25** | $CF_2O\cdots NH_3$ ($C_s$) | -0.16 | 0.56 | 0.46 |
| **26a** | $CF_2S\cdots NH_3$ ($C_s$) | 0.10 | -0.58 | -0.49 |
| **26b** | $CF_2S\cdots NH_3$ ($C_s$) | -3.42 | -0.59 | -1.05 |
| **27** | $SiF_2O\cdots NH_3$ ($C_s$) | -2.95 | -0.97 | -1.24 |
| Anionic - Tetrel bond | | | | |
| **28** | $CH_3^+\cdots NH_3$ ($C_{3v}$) | -1.78 | -0.54 | -0.72 |
| **29** | $FNH_3^+\cdots NH_3$ ($C_{3v}$) | -0.23 | 0.13 | 0.07 |
| **30** | $FCH_3\cdots Cl^-$ ($C_{3v}$) | -0.25 | 0.18 | 0.05 |
| **31** | $FSiH_3\cdots Cl^-$ ($C_{3v}$) | -1.62 | -0.38 | -0.66 |
| **32** | $FGeH_3\cdots Cl^-$ ($C_{3v}$) | -1.14 | -0.12 | -0.37 |
| **33** | $CO_2\cdots Cl^-$ ($C_s$) | -0.34 | 0.12 | 0.00 |
| **34** | $SCO\cdots Cl^-$ ($C_s$) | -0.27 | 0.13 | 0.03 |
| **35** | $CF_2S\cdots Cl^-$ ($C_s$) | -3.56 | -0.58 | -1.17 |
| | MAD | 0.71 | 0.29 | 0.28 |

*Difference between DLPNO-CCSD(T)/aug-cc-pV5Z $E_{int}(CP)$ and CCSD(T)/aug-cc-pVTZ $E_{int}(CP)$ (a) and CCSD(T)/aug-cc-pVTZ $E_{int}$ (b). Difference between DLPNO-CCSD(T)/aug-cc-pVTZ $E_{int}$ and CCSD(T)/aug-cc-pVTZ $E_{int}$ (c). Energies and mean absolute deviation (MAD) given in kcal/mol.

**Table S3: Atomic Cartesian coordinates (in Å) of complexes 1-35 optimized at the CCSD(T)/aug-cc-pVTZ level of theory.**

| | | | |
|---|---|---|---|
| **1** | $FCH_3\cdots FH$, $C_{3v}$ | | |
| C | -0.64760 | 0.00000 | 0.00000 |
| F | -2.03974 | 0.00000 | 0.00000 |
| H | -0.29694 | 0.51589 | -0.89355 |
| H | -0.29694 | -1.03178 | 0.00000 |
| H | -0.29694 | 0.51589 | 0.89355 |
| F | 2.32388 | 0.00000 | 0.00000 |
| H | 3.24545 | 0.00000 | 0.00000 |
| **2** | $FCH_3\cdots OH_2$, $C_s$ | | |
| C | 0.58503 | -0.01958 | 0.00000 |
| F | 1.97844 | 0.01163 | 0.00000 |
| H | 0.25798 | -1.05889 | 0.00000 |
| H | 0.22171 | 0.48606 | -0.89362 |
| H | 0.22171 | 0.48606 | 0.89362 |
| O | -2.44987 | 0.00395 | 0.00000 |
| H | -3.06002 | -0.73963 | 0.00000 |
| H | -3.02146 | 0.77758 | 0.00000 |
| **3** | $FCH_3\cdots NH_3$, $C_{3v}$ | | |
| C | -0.59814 | 0.00000 | 0.00000 |
| F | -1.99271 | 0.00000 | 0.00000 |
| H | -0.24618 | -0.51535 | -0.89263 |
| H | -0.24618 | 1.03070 | 0.00000 |

| | | | |
|---|---|---|---|
| H | -0.24618 | -0.51535 | 0.89263 |
| N | 2.61945 | 0.00000 | 0.00000 |
| H | 3.00978 | 0.46868 | 0.81177 |
| H | 3.00978 | 0.46868 | -0.81177 |
| H | 3.00978 | -0.93735 | 0.00000 |

**4** $ClCH_3 \cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| C | 0.06943 | 0.00000 | 0.00000 |
| Cl | -1.72827 | 0.00000 | 0.00000 |
| H | 0.41195 | -0.51492 | -0.89188 |
| H | 0.41195 | 1.02985 | 0.00000 |
| H | 0.41195 | -0.51492 | 0.89188 |
| N | 3.35811 | 0.00000 | 0.00000 |
| H | 3.74840 | 0.46869 | 0.81179 |
| H | 3.74840 | 0.46869 | -0.81179 |
| H | 3.74840 | -0.93738 | 0.00000 |

**5** $BrCH_3 \cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| C | 0.86226 | 0.00000 | 0.00000 |
| Br | -1.09071 | 0.00000 | 0.00000 |
| H | 1.19569 | -0.51600 | -0.89374 |
| H | 1.19569 | 1.03200 | 0.00000 |
| H | 1.19569 | -0.51600 | 0.89374 |
| N | 4.16614 | 0.00000 | 0.00000 |
| H | 4.55633 | 0.46871 | 0.81183 |
| H | 4.55633 | 0.46871 | -0.81183 |

| | | | |
|---|---|---|---|
| H | 4.55633 | -0.93742 | 0.00000 |

**6** $(OH)CH_3\cdots NH_3$, $C_s$

| | | | |
|---|---|---|---|
| H | -2.49864 | 0.81659 | 0.00000 |
| O | -2.13732 | -0.07379 | 0.00000 |
| C | -0.71198 | 0.03232 | 0.00000 |
| H | -0.32011 | -0.98345 | 0.00000 |
| H | -0.33794 | 0.54691 | 0.88947 |
| H | -0.33794 | 0.54691 | -0.88947 |
| N | 2.65001 | 0.01052 | 0.00000 |
| H | 3.28000 | 0.80658 | 0.00000 |
| H | 2.89631 | -0.54671 | -0.81216 |
| H | 2.89631 | -0.54671 | 0.81216 |

**7** $CF_4\cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| C | -0.55900 | 0.00000 | 0.00000 |
| F | -1.88668 | 0.00000 | 0.00000 |
| F | -0.13050 | -0.62387 | -1.08058 |
| F | -0.13050 | 1.24774 | 0.00000 |
| F | -0.13050 | -0.62387 | 1.08058 |
| N | 2.86699 | 0.00000 | 0.00000 |
| H | 3.25551 | 0.46896 | 0.81227 |
| H | 3.25551 | 0.46896 | -0.81227 |
| H | 3.25551 | -0.93793 | 0.00000 |

**8** $FSiH_3\cdots FH$, $C_s$

| | | | |
|---|---|---|---|
| Si | 0.43320 | 0.01974 | 0.00000 |
| F | 2.04988 | -0.02546 | 0.00000 |
| H | -0.03966 | -1.38225 | 0.00000 |
| H | 0.00693 | 0.72855 | -1.22281 |
| H | 0.00693 | 0.72855 | 1.22281 |
| F | -2.53084 | 0.03461 | 0.00000 |
| H | -2.93319 | -0.79531 | 0.00000 |

**9** $FSiH_3 \cdots OH_2$, $C_s$

| | | | |
|---|---|---|---|
| Si | 0.01186 | 0.31211 | 0.00000 |
| F | -0.00996 | 1.93530 | 0.00000 |
| H | 1.43780 | -0.07630 | 0.00000 |
| H | -0.68509 | -0.11005 | -1.23076 |
| H | -0.68509 | -0.11005 | 1.23076 |
| O | -0.05586 | -2.46085 | 0.00000 |
| H | 0.33866 | -2.89719 | -0.76172 |
| H | 0.33866 | -2.89719 | 0.76172 |

**10** $FSiH_3 \cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| Si | -0.20928 | 0.00000 | 0.00000 |
| F | -1.84579 | 0.00000 | 0.00000 |
| H | 0.12338 | -0.72003 | -1.24713 |
| H | 0.12338 | 1.44006 | 0.00000 |
| H | 0.12338 | -0.72003 | 1.24713 |
| N | 2.31409 | 0.00000 | 0.00000 |
| H | 2.69382 | 0.47094 | 0.81569 |

| | | | |
|---|---|---|---|
| H | 2.69382 | 0.47094 | -0.81569 |
| H | 2.69382 | -0.94188 | 0.00000 |

**11** $ClSiH_3 \cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| Si | 0.33660 | 0.00000 | 0.00000 |
| Cl | -1.78021 | 0.00000 | 0.00000 |
| H | 0.66936 | -0.71839 | -1.24428 |
| H | 0.66936 | 1.43677 | 0.00000 |
| H | 0.66936 | -0.71839 | 1.24428 |
| N | 2.91649 | 0.00000 | 0.00000 |
| H | 3.29796 | 0.47068 | 0.81525 |
| H | 3.29796 | 0.47068 | -0.81525 |
| H | 3.29796 | -0.94136 | 0.00000 |

**12** $BrSiH_3 \cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| Si | 1.06281 | 0.00000 | 0.00000 |
| Br | -1.22723 | 0.00000 | 0.00000 |
| H | 1.38429 | -0.71948 | -1.24615 |
| H | 1.38429 | 1.43893 | 0.00000 |
| H | 1.38429 | -0.71948 | 1.24615 |
| N | 3.62836 | 0.00000 | 0.00000 |
| H | 4.00960 | 0.47077 | 0.81539 |
| H | 4.00960 | 0.47077 | -0.81539 |
| H | 4.00960 | -0.94154 | 0.00000 |

**13** $(HO)SiH_3 \cdots NH_3$, $C_s$

| | | | |
|---|---|---|---|
| H | -2.48714 | 0.75291 | 0.00000 |
| O | -2.00799 | -0.07791 | 0.00000 |
| Si | -0.33120 | 0.02073 | 0.00000 |
| H | 0.07573 | -1.39753 | 0.00000 |
| H | 0.10142 | 0.74724 | 1.21938 |
| H | 0.10142 | 0.74724 | -1.21938 |
| N | 2.49327 | -0.00992 | 0.00000 |
| H | 2.89338 | 0.92319 | 0.00000 |
| H | 2.86755 | -0.48701 | -0.81436 |
| H | 2.86755 | -0.48701 | 0.81436 |

**14** $SiH_4 \cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| Si | -1.13339 | 0.00000 | 0.00000 |
| H | -2.62311 | 0.00000 | 0.00000 |
| H | -0.67520 | -0.70437 | -1.22000 |
| H | -0.67520 | 1.40873 | 0.00000 |
| H | -0.67520 | -0.70437 | 1.22000 |
| N | 2.06884 | 0.00000 | 0.00000 |
| H | 2.45533 | 0.46945 | 0.81310 |
| H | 2.45533 | 0.46945 | -0.81310 |
| H | 2.45533 | -0.93887 | 0.00000 |

**15** $SiF_2H_2 \cdots NH_3$, $C_s$

| | | | |
|---|---|---|---|
| F | -0.12376 | 1.22628 | 0.00000 |
| Si | 0.25601 | -0.33778 | 0.00000 |
| F | 1.87344 | -0.28456 | 0.00000 |

| | | | |
|---|---|---|---|
| H | -0.05846 | -1.00506 | 1.26959 |
| H | -0.05846 | -1.00506 | -1.26959 |
| N | -2.29934 | -0.38588 | 0.00000 |
| H | -2.54738 | 0.59923 | 0.00000 |
| H | -2.73886 | -0.80171 | -0.81548 |
| H | -2.73886 | -0.80171 | 0.81548 |

**16a** $SiF_3H\cdots NH_3$, $C_s$

| | | | |
|---|---|---|---|
| H | 1.75218 | -0.00856 | 0.00000 |
| Si | 0.29667 | 0.17654 | 0.00000 |
| F | 0.24053 | 1.79282 | 0.00000 |
| F | -0.52830 | -0.08799 | -1.35509 |
| F | -0.52830 | -0.08799 | 1.35509 |
| N | 0.32143 | -2.02817 | 0.00000 |
| H | -0.63431 | -2.37362 | 0.00000 |
| H | 0.78216 | -2.40878 | 0.82139 |
| H | 0.78216 | -2.40878 | -0.82139 |

**16b** $HSiF_3\cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| Si | 0.47664 | 0.00000 | 0.00000 |
| H | 1.95077 | 0.00000 | 0.00000 |
| F | 0.23699 | 0.80167 | -1.38853 |
| F | 0.23699 | -1.60333 | 0.00000 |
| F | 0.23699 | 0.80167 | 1.38853 |
| N | -1.62736 | 0.00000 | 0.00000 |
| H | -1.99087 | -0.47405 | 0.82109 |

| | | | |
|---|---|---|---|
| H | -1.99087 | -0.47405 | -0.82109 |
| H | -1.99087 | 0.94811 | 0.00000 |

**17** $SiF_4 \cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| Si | -0.14293 | 0.00000 | 0.00000 |
| F | -1.75198 | 0.00000 | 0.00000 |
| F | 0.05853 | -0.79697 | -1.38040 |
| F | 0.05853 | 1.59395 | 0.00000 |
| F | 0.05853 | -0.79697 | 1.38040 |
| N | 1.92903 | 0.00000 | 0.00000 |
| H | 2.29379 | 0.47403 | 0.82104 |
| H | 2.29379 | 0.47403 | -0.82104 |
| H | 2.29379 | -0.94806 | 0.00000 |

**18** $FGeH_3 \cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| Ge | -0.10836 | 0.00000 | 0.00000 |
| F | -1.92384 | 0.00000 | 0.00000 |
| H | 0.18762 | -0.75421 | -1.30632 |
| H | 0.18762 | 1.50841 | 0.00000 |
| H | 0.18762 | -0.75421 | 1.30632 |
| N | 2.51587 | 0.00000 | 0.00000 |
| H | 2.89814 | 0.47046 | 0.81486 |
| H | 2.89814 | 0.47046 | -0.81486 |
| H | 2.89814 | -0.94092 | 0.00000 |

**19** $ClGeH_3 \cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| Ge | 0.21998 | 0.00000 | 0.00000 |
| Cl | -1.99578 | 0.00000 | 0.00000 |
| H | 0.56785 | -0.74722 | -1.29422 |
| H | 0.56785 | 1.49443 | 0.00000 |
| H | 0.56785 | -0.74722 | 1.29422 |
| N | 2.97467 | 0.00000 | 0.00000 |
| H | 3.35953 | 0.46997 | 0.81402 |
| H | 3.35953 | 0.46997 | -0.81402 |
| H | 3.35953 | -0.93995 | 0.00000 |

**20** $BrGeH_3 \cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| Ge | 0.79891 | 0.00000 | 0.00000 |
| Br | -1.57624 | 0.00000 | 0.00000 |
| H | 1.14870 | -0.74687 | -1.29360 |
| H | 1.14870 | 1.49372 | 0.00000 |
| H | 1.14870 | -0.74687 | 1.29360 |
| N | 3.56508 | 0.00000 | 0.00000 |
| H | 3.94994 | 0.46998 | 0.81403 |
| H | 3.94994 | 0.46998 | -0.81403 |
| H | 3.94994 | -0.93997 | 0.00000 |

**21** $(HO)GeH_3 \cdots NH_3$, $C_s$

| | | | |
|---|---|---|---|
| H | -2.43370 | 0.76387 | 0.00000 |
| O | -2.00116 | -0.09434 | 0.00000 |
| Ge | -0.18595 | 0.01398 | 0.00000 |
| H | 0.20520 | -1.47028 | 0.00000 |

| | | | |
|---|---|---|---|
| H | 0.22916 | 0.77228 | 1.27946 |
| H | 0.22916 | 0.77228 | -1.27946 |
| N | 2.72363 | -0.01997 | 0.00000 |
| H | 3.13198 | 0.90970 | 0.00000 |
| H | 3.09702 | -0.49920 | -0.81368 |
| H | 3.09702 | -0.49920 | 0.81368 |

**22** $GeH_4 \cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| Ge | -0.60690 | 0.00000 | 0.00000 |
| H | -2.15735 | 0.00000 | 0.00000 |
| H | -0.12312 | -0.73139 | -1.26680 |
| H | -0.12312 | 1.46278 | 0.00000 |
| H | -0.12312 | -0.73139 | 1.26680 |
| N | 2.71572 | 0.00000 | 0.00000 |
| H | 3.10263 | 0.46934 | 0.81291 |
| H | 3.10263 | 0.46934 | -0.81291 |
| H | 3.10263 | -0.93867 | 0.00000 |

**23** $CO_2 \cdots NH_3$, $C_s$

| | | | |
|---|---|---|---|
| H | -2.46031 | 0.93617 | 0.00000 |
| N | -2.10155 | -0.01349 | 0.00000 |
| C | 0.82078 | 0.00415 | 0.00000 |
| O | 0.83040 | 1.17131 | 0.00000 |
| O | 0.86401 | -1.16202 | 0.00000 |
| H | -2.50221 | -0.47280 | -0.81190 |
| H | -2.50221 | -0.47280 | 0.81190 |

**24** $SCO\cdots NH_3$, $C_s$

| | | | |
|---|---|---|---|
| H | -2.74176 | 0.25897 | 0.00000 |
| N | -2.51252 | -0.73021 | 0.00000 |
| C | 0.40035 | 0.61529 | 0.00000 |
| O | -0.30293 | 1.54197 | 0.00000 |
| S | 1.37539 | -0.61935 | 0.00000 |
| H | -2.97013 | -1.13168 | -0.81234 |
| H | -2.97013 | -1.13168 | 0.81234 |

**25** $CF_2O\cdots NH_3$, $C_s$

| | | | |
|---|---|---|---|
| N | -2.13545 | 0.02830 | 0.00000 |
| C | 0.54866 | 0.15032 | 0.00000 |
| O | 0.63058 | 1.32554 | 0.00000 |
| F | 0.54839 | -0.62376 | -1.06358 |
| F | 0.54839 | -0.62376 | 1.06358 |
| H | -2.68397 | -0.82584 | 0.00000 |
| H | -2.43069 | 0.56117 | -0.81244 |
| H | -2.43069 | 0.56117 | 0.81244 |

**26a** $CF_2S\cdots NH_3$, $C_s$

| | | | |
|---|---|---|---|
| N | -2.24144 | 1.00020 | 0.00000 |
| C | 0.28875 | -0.41164 | 0.00000 |
| S | 1.33700 | 0.80678 | 0.00000 |
| F | -0.18946 | -1.01830 | -1.05969 |
| F | -0.18946 | -1.01830 | 1.05969 |

| | | | |
|---|---|---|---|
| H | -3.16833 | 0.58588 | 0.00000 |
| H | -2.19908 | 1.60796 | -0.81245 |
| H | -2.19908 | 1.60796 | 0.81245 |

**26b** $CF_2S\cdots NH_3$, $C_s$

| | | | |
|---|---|---|---|
| N | -0.81775 | 1.37793 | 0.00000 |
| C | -0.18921 | -0.07947 | 0.00000 |
| S | 1.51010 | 0.00257 | 0.00000 |
| F | -0.83680 | -0.61886 | -1.08325 |
| F | -0.83680 | -0.61886 | 1.08325 |
| H | -1.83974 | 1.36073 | 0.00000 |
| H | -0.45152 | 1.84535 | -0.82816 |
| H | -0.45152 | 1.84535 | 0.82816 |

**27** $SiF_2O\cdots NH_3$, $C_s$

| | | | |
|---|---|---|---|
| N | -0.42376 | 1.66094 | 0.00000 |
| Si | 0.20327 | -0.15088 | 0.00000 |
| O | 1.73129 | -0.09429 | 0.00000 |
| F | -0.68147 | -0.62119 | -1.25214 |
| F | -0.68147 | -0.62119 | 1.25214 |
| H | -1.43724 | 1.75497 | 0.00000 |
| H | -0.05066 | 2.13614 | -0.81948 |
| H | -0.05066 | 2.13614 | 0.81948 |

**28** $CH_3^+\cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| N | 0.70513 | 0.00000 | 0.00000 |

| | | | |
|---|---|---|---|
| C | -0.80599 | 0.00000 | 0.00000 |
| H | -1.14296 | 0.51675 | -0.89504 |
| H | -1.14296 | -1.03351 | 0.00000 |
| H | -1.14296 | 0.51675 | 0.89504 |
| H | 1.07613 | -0.47653 | 0.82539 |
| H | 1.07613 | -0.47653 | -0.82539 |
| H | 1.07613 | 0.95307 | 0.00000 |

**29** $FNH_3^+\cdots NH_3$, $C_{3v}$

| | | | |
|---|---|---|---|
| N | -0.39134 | 0.00000 | 0.00000 |
| F | -1.76513 | 0.00000 | 0.00000 |
| H | -0.05710 | -0.48443 | -0.83905 |
| H | -0.05710 | 0.96885 | 0.00000 |
| H | -0.05710 | -0.48443 | 0.83905 |
| N | 2.22808 | 0.00000 | 0.00000 |
| H | 2.64176 | 0.46550 | 0.80625 |
| H | 2.64176 | 0.46550 | -0.80625 |
| H | 2.64176 | -0.93099 | 0.00000 |

**30** $FCH_3\cdots Cl^-$, $C_{3v}$

| | | | |
|---|---|---|---|
| C | -1.23588 | 0.00000 | 0.00000 |
| F | -2.65510 | 0.00000 | 0.00000 |
| H | -0.88447 | -0.51407 | -0.89040 |
| H | -0.88447 | 1.02814 | 0.00000 |
| H | -0.88447 | -0.51407 | 0.89040 |
| Cl | 1.94309 | 0.00000 | 0.00000 |

**31** $FSiH_3\cdots Cl^-$, $C_{3v}$

| | | | |
|---|---|---|---|
| Si | -0.65514 | 0.00000 | 0.00000 |
| F | -2.35776 | 0.00000 | 0.00000 |
| H | -0.50131 | -0.73709 | -1.27667 |
| H | -0.50131 | 1.47418 | 0.00000 |
| H | -0.50131 | -0.73709 | 1.27667 |
| Cl | 1.84845 | 0.00000 | 0.00000 |

**32** $FGeH_3\cdots Cl^-$, $C_{3v}$

| | | | |
|---|---|---|---|
| Ge | -0.41308 | 0.00000 | 0.00000 |
| F | -2.30517 | 0.00000 | 0.00000 |
| H | -0.31390 | -0.76825 | -1.33064 |
| H | -0.31390 | 1.53649 | 0.00000 |
| H | -0.31390 | -0.76825 | 1.33064 |
| Cl | 2.15274 | 0.00000 | 0.00000 |

**33** $CO_2\cdots Cl^-$, $C_s$

| | | | |
|---|---|---|---|
| Cl | 0.00000 | 0.00000 | 1.66499 |
| C | 0.00000 | 0.00000 | -1.25540 |
| O | 0.00000 | 1.16587 | -1.34912 |
| O | 0.00000 | -1.16587 | -1.34912 |

**34** $SCO\cdots Cl^-$, $C_s$

| | | | |
|---|---|---|---|
| Cl | 2.05468 | 0.23409 | 0.00000 |
| C | -0.96955 | -0.62147 | 0.00000 |

| | | | |
|---|---|---|---|
| O | -0.65121 | -1.73711 | 0.00000 |
| S | -1.55759 | 0.84626 | 0.00000 |

**35** $CF_2S\cdots Cl^-$, $C_s$

| | | | |
|---|---|---|---|
| Cl | -1.49219 | 0.66590 | 0.00000 |
| C | 0.15369 | -0.27857 | 0.00000 |
| S | 1.57057 | 0.70491 | 0.00000 |
| F | 0.00320 | -1.11800 | -1.07951 |
| F | 0.00320 | -1.11800 | 1.07951 |