# The nature of the intermolecular interaction in $(H_2X)_2$ (X = O, S, Se)

## Electronic Supplementary Information

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# 1 Computational Details

Geometry optimisations for the studied systems were performed at the CCSD/aug-cc-pDVZ[1;2] level of theory using the Psi4 code.[3] We considered uncorrected CounterPoise (CP) geometries because the CP correction is counterproductive for the attainment of intermolecular geometries consistent with experiment for $(H_2S)_2$. The uncorrected S···S distance in $(H_2S)_2$ (4.07 Å) is 0.04 Å too short when compared to the experimental value (4.11 Å) while the corrected value is 0.12 Å too long (4.23 Å). This situation for the H···S distance is even more consequential. The uncorrected value (2.71 Å) is 0.06 Å shorter than the corresponding experimental value (2.78 Å), but the corrected one (2.98 Å) is 0.20 Å longer. Furthermore, the uncorrected O···O distance (2.91 Å) is very similar to the experimental measurement (2.98 Å) in $(H_2O)_2$. For these equilibrium geometries, we determined the one- and two-electron density matrices at the CCSD/aug-cc-pDVZ[1;2] approximation. For this purpose, we have employed the package Mrcc.[5] The investigated potential energy curves were computed using the MP2/aug-cc-pVDZ methodology in combination with the Orca program.[4] These potential energy curves were computed as a function of the angle $\theta$ shown in Figure 3 of the main body of the paper. The QTAIM analyses, the IQA energy partition and the construction of the ELF isosurfaces were performed with the help of our in-house Promolden code.[6] The IQA integrations were carried out using $\beta$-spheres for all atoms, with a radius between 0.1 and 0.3 a.u. and Lebedev angular quadratures with 3074 points and 451 points. Gauss-Chebyshev mapped radial

grids were used within the $\beta$-spheres and the angular momentum number $L$ of the bipolar expansion employed to obtain the classic and exchange-correlation interaction energy terms was truncated at $L = 8$. Outside the $\beta$-spheres, extended 5810-point Lebedev and 551-mapped radial point trapezoidal quadratures were used, with $L$ expansions truncated at $L = 10$. Typical errors of IQA integrations are around $0.16\,\mathrm{m}E_\mathrm{h}$. The NCI calculations were completed with the help of the NCIPLOT code.[7] Density isosurfaces and electrostatic potential mappings were plotted using the AIMALL program.[8] The structure of the systems were visualised using the JMOL[9], VMD[10] and AVOGADRO [11] programs.

## 2 Dimer equilibrium geometries

Coordinates at the equilibrium geometry of the systems studied in this paper at the MP2/aug-cc-pVDZ level of theory, as implemented in the Psi4 code.

Table S1: Coordinates of the $H_2O$ dimer at the equilibrium geometry.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | 1.4316 | 0.0008 | 0.0000 |
| O | −1.5044 | −0.0021 | 0.0000 |
| H | −0.5397 | 0.0911 | 0.0000 |
| H | −1.8340 | 0.9028 | 0.0000 |
| H | 1.7645 | −0.487 25 | −0.7624 |
| H | 1.7645 | −0.487 25 | 0.7624 |

Table S2: Coordinates of the $H_2S$ dimer at the equilibrium the geometry.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | 2.0422 | 0.2292 | 0.0000 |
| S | −2.0873 | −0.2200 | 0.0000 |
| H | −0.7447 | −0.0447 | 0.0000 |
| H | −2.3283 | 1.1101 | 0.0000 |
| H | 2.2517 | −0.6793 | −0.9793 |
| H | 2.2517 | −0.6793 | 0.9793 |

Table S3: Coordinates of the $H_2Se$ dimer at the equilibrium geometry.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | 2.1674 | 0.2758 | 0.0000 |
| Se | −2.1864 | −0.2717 | 0.0000 |
| H | −0.7349 | −0.0308 | 0.0000 |
| H | −2.4744 | 1.1696 | 0.0000 |
| H | 2.3558 | −0.7303 | −1.0554 |
| H | 2.3558 | −0.7303 | 1.0554 |

# 3 Geometries computed for the potential energy curves

Geometries obtained by (i) freezing the angle, shown in Figure 3 in the main body of the paper to a specific value (between 0 and 350 degrees) and (ii) optimising the rest of the coordinates. All calculations were performed at the MP2/aug-cc-pVDZ level of theory, as implemented in the ORCA code.

## 3.1 $(H_2O)_2$

Table S4: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=0°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −2.243 056 | 0.000 130 | −0.324 547 |
| O | 5.178 017 | −0.000 153 | 0.308 789 |
| H | 4.212 326 | −0.000 121 | 0.318 211 |
| H | 5.419 445 | −0.000 647 | 1.244 065 |
| H | −1.650 608 | −0.760 958 | −0.273 986 |
| H | −1.650 674 | 0.761 269 | −0.273 991 |

Table S5: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=10°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −2.292 447 | 0.000 136 | −0.248 510 |
| O | 5.246 951 | −0.000 150 | 0.251 650 |
| H | 4.281 779 | −0.000 117 | 0.218 417 |
| H | 5.447 160 | −0.000 650 | 1.196 584 |
| H | −1.714 576 | −0.760 705 | −0.107 083 |
| H | −1.714 615 | 0.761 006 | −0.107 077 |

Table S6: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=20°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.861 472 | 0.000 054 | −0.066 630 |
| O | 3.810 939 | −0.000 052 | 0.073 123 |
| H | 2.845 461 | −0.000 032 | 0.077 682 |
| H | 4.049 763 | −0.000 548 | 1.009 218 |
| H | −0.312 638 | −0.763 527 | 0.153 191 |
| H | −0.312 625 | 0.763 624 | 0.153 195 |

Table S7: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=30°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.778 959 | 0.000 051 | −0.037 525 |
| O | 3.738 307 | −0.000 044 | 0.045 792 |
| H | 2.772 727 | −0.000 025 | 0.050 751 |
| H | 3.978 277 | −0.000 541 | 0.981 547 |
| H | −0.275 827 | −0.764 869 | 0.269 567 |
| H | −0.275 795 | 0.764 949 | 0.269 568 |

Table S8: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=40°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.511 284 | 0.112 810 | 0.275 159 |
| O | 3.639 493 | 0.151 775 | 0.781 211 |
| H | 2.743 238 | 0.554 020 | 0.634 808 |
| H | 3.543 733 | −0.576 342 | 0.055 596 |
| H | −0.134 525 | 0.401 571 | −0.583 321 |
| H | −0.212 466 | −0.644 314 | 0.577 628 |

Table S9: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=50°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.210 451 | −0.000 227 | 0.000 180 |
| O | 3.205 685 | 0.000 094 | 0.006 717 |
| H | 2.238 709 | 0.000 573 | 0.010 680 |
| H | 3.461 067 | −0.000 348 | 0.937 750 |
| H | 0.122 651 | −0.777 202 | 0.464 217 |
| H | 0.125 429 | 0.776 630 | 0.464 057 |

Table S10: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=60°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | 0.204 570 | −0.006 375 | 0.032 503 |
| O | 3.162 020 | 0.007 966 | −0.020 596 |
| H | 2.189 922 | −0.003 678 | −0.011 545 |
| H | 3.423 461 | 0.006 980 | 0.905 529 |
| H | −0.123 719 | −0.761 505 | 0.544 549 |
| H | −0.076 784 | 0.756 133 | 0.554 721 |

Table S11: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=70°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | 0.144 605 | −0.000 004 | 0.026 359 |
| O | 3.108 862 | −0.000 005 | −0.021 080 |
| H | 2.138 184 | −0.000 006 | 0.038 195 |
| H | 3.407 172 | −0.000 484 | 0.896 424 |
| H | −0.111 602 | −0.751 788 | 0.580 562 |
| H | −0.111 530 | 0.751 807 | 0.580 560 |

Table S12: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=80°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | 0.088 818 | −0.000 004 | 0.025 179 |
| O | 3.059 168 | −0.000 002 | −0.015 172 |
| H | 2.088 945 | −0.000 005 | 0.052 218 |
| H | 3.366 739 | −0.000 481 | 0.899 256 |
| H | −0.133 164 | −0.747 071 | 0.601 090 |
| H | −0.133 096 | 0.747 084 | 0.601 090 |

Table S13: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=90°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | 0.049 427 | −0.000 210 | 0.037 849 |
| O | 3.031 463 | 0.000 442 | 0.000 238 |
| H | 2.059 955 | −0.000 578 | −0.041 081 |
| H | 3.231 105 | −0.000 037 | 0.944 026 |
| H | −0.147 843 | −0.747 458 | 0.622 042 |
| H | −0.145 577 | 0.747 361 | 0.622 385 |

Table S14: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=100°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | 0.014 135 | −0.000 553 | 0.025 371 |
| O | 2.985 147 | 0.000 080 | 0.001 738 |
| H | 2.012 653 | 0.000 564 | 0.004 464 |
| H | 3.231 063 | −0.000 166 | 0.934 395 |
| H | −0.213 315 | −0.745 737 | 0.598 803 |
| H | −0.210 034 | 0.745 332 | 0.598 890 |

Table S15: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=110°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.010 113 | −0.000 187 | 0.013 410 |
| O | 2.949 885 | −0.000 007 | 0.006 338 |
| H | 1.977 406 | −0.000 124 | 0.015 516 |
| H | 3.204 960 | −0.000 406 | 0.936 112 |
| H | −0.270 315 | −0.752 711 | 0.564 679 |
| H | −0.270 452 | 0.752 956 | 0.564 965 |

Table S16: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=120°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.011 681 | 0.000 287 | 0.005 875 |
| O | 2.918 706 | 0.000 782 | 0.008 418 |
| H | 1.946 214 | −0.002 109 | 0.008 764 |
| H | 3.159 577 | −0.000 045 | 0.943 185 |
| H | −0.332 817 | −0.756 629 | 0.515 473 |
| H | −0.333 710 | 0.757 233 | 0.516 445 |

Table S17: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=130°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.019 005 | −0.000 122 | 0.005 038 |
| O | 2.924 540 | 0.000 045 | 0.008 651 |
| H | 1.952 241 | 0.000 070 | 0.013 270 |
| H | 3.169 982 | −0.000 406 | 0.940 574 |
| H | −0.407 227 | −0.760 440 | 0.457 997 |
| H | −0.406 561 | 0.760 373 | 0.458 069 |

Table S18: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=140°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.017 859 | −0.000 017 | 0.003 176 |
| O | 2.921 959 | 0.000 015 | 0.005 766 |
| H | 1.949 997 | 0.000 004 | 0.027 997 |
| H | 3.179 593 | −0.000 475 | 0.935 417 |
| H | −0.472 440 | −0.762 682 | 0.384 352 |
| H | −0.472 380 | 0.762 675 | 0.384 372 |

Table S19: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=150°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.013 768 | −0.000 017 | 0.004 382 |
| O | 2.922 478 | 0.000 014 | 0.004 334 |
| H | 1.951 076 | 0.000 003 | 0.035 623 |
| H | 3.187 737 | −0.000 475 | 0.931 857 |
| H | −0.524 625 | −0.763 886 | 0.301 743 |
| H | −0.524 568 | 0.763 881 | 0.301 762 |

Table S20: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=160°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.006 771 | −0.001 376 | 0.007 964 |
| O | 2.928 865 | 0.000 497 | 0.003 833 |
| H | 1.957 828 | −0.000 131 | 0.034 386 |
| H | 3.192 050 | 0.000 225 | 0.931 974 |
| H | −0.569 299 | −0.759 546 | 0.210 582 |
| H | −0.565 043 | 0.769 321 | 0.171 331 |

Table S21: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=170°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.005 107 | −0.000 016 | 0.009 447 |
| O | 2.930 784 | 0.000 015 | 0.004 203 |
| H | 1.959 744 | 0.000 004 | 0.028 171 |
| H | 3.186 890 | −0.000 480 | 0.934 338 |
| H | −0.584 770 | −0.764 986 | 0.113 903 |
| H | −0.584 730 | 0.764 983 | 0.113 919 |

Table S22: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=180°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.004 368 | 0.004 654 | 0.012 172 |
| O | 2.926 939 | −0.002 075 | 0.004 212 |
| H | 1.955 633 | 0.000 140 | 0.017 286 |
| H | 3.171 965 | −0.001 909 | 0.937 342 |
| H | −0.599 243 | −0.755 508 | 0.014 779 |
| H | −0.585 556 | 0.775 388 | 0.012 748 |

Table S23: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=190°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.001 131 | −0.000 056 | 0.013 792 |
| O | 2.933 209 | 0.000 204 | 0.004 991 |
| H | 1.961 955 | −0.000 341 | 0.009 858 |
| H | 3.169 550 | −0.000 375 | 0.940 402 |
| H | −0.580 507 | −0.765 483 | −0.088 038 |
| H | −0.580 265 | 0.765 571 | −0.087 905 |

Table S24: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=200°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.002 236 | −0.000 140 | 0.016 080 |
| O | 2.927 943 | 0.000 500 | 0.003 749 |
| H | 1.956 427 | −0.000 859 | 0.009 468 |
| H | 3.165 544 | −0.000 213 | 0.938 821 |
| H | −0.555 333 | −0.765 327 | −0.185 543 |
| H | −0.554 715 | 0.765 559 | −0.185 275 |

Table S25: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=210°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.006 239 | −0.000 003 | 0.017 777 |
| O | 2.918 908 | 0.000 011 | 0.001 108 |
| H | 1.947 230 | 0.000 006 | 0.020 402 |
| H | 3.170 712 | −0.000 487 | 0.932 455 |
| H | −0.516 136 | −0.765 161 | −0.277 186 |
| H | −0.516 144 | 0.765 154 | −0.277 176 |

Table S26: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=220°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.012 433 | −0.000 001 | 0.018 079 |
| O | 2.908 764 | 0.000 007 | −0.002 039 |
| H | 1.937 430 | 0.000 004 | 0.040 051 |
| H | 3.183 715 | −0.000 485 | 0.922 736 |
| H | −0.464 297 | −0.764 698 | −0.361 417 |
| H | −0.464 308 | 0.764 693 | −0.361 410 |

Table S27: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=230°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.019 315 | 0.000 001 | 0.014 876 |
| O | 2.898 821 | 0.000 002 | −0.004 661 |
| H | 1.929 059 | 0.000 001 | 0.069 443 |
| H | 3.205 829 | −0.000 481 | 0.909 967 |
| H | −0.400 207 | −0.763 792 | −0.438 073 |
| H | −0.400 217 | 0.763 790 | −0.438 073 |

Table S28: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=240°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.023 506 | 0.000 001 | 0.008 108 |
| O | 2.894 426 | −0.000 002 | −0.005 108 |
| H | 1.927 134 | −0.000 001 | 0.098 232 |
| H | 3.230 008 | −0.000 478 | 0.899 436 |
| H | −0.325 235 | −0.762 083 | −0.504 373 |
| H | −0.325 237 | 0.762 083 | −0.504 376 |

Table S29: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=250°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.023 177 | 0.000 007 | −0.007 290 |
| O | 2.890 640 | −0.000 012 | −0.002 129 |
| H | 1.929 547 | −0.000 006 | 0.148 983 |
| H | 3.273 301 | −0.000 474 | 0.883 497 |
| H | −0.244 468 | −0.759 704 | −0.563 494 |
| H | −0.244 474 | 0.759 708 | −0.563 506 |

Table S30: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=260°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.007 883 | 0.000 010 | −0.024 356 |
| O | 2.903 981 | −0.000 018 | 0.006 290 |
| H | 1.947 287 | −0.000 007 | 0.183 031 |
| H | 3.311 286 | −0.000 472 | 0.880 849 |
| H | −0.167 507 | −0.756 577 | −0.606 190 |
| H | −0.167 513 | 0.756 584 | −0.606 205 |

Table S31: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=270°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | 0.037 858 | 0.000 005 | −0.034 582 |
| O | 2.955 987 | −0.000 012 | 0.022 318 |
| H | 1.992 391 | −0.000 004 | 0.156 784 |
| H | 3.322 735 | −0.000 479 | 0.914 658 |
| H | −0.115 223 | −0.752 871 | −0.623 777 |
| H | −0.115 218 | 0.752 881 | −0.623 781 |

Table S32: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=280°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | 0.076 196 | 0.000 009 | −0.052 231 |
| O | 2.985 270 | −0.000 021 | 0.038 760 |
| H | 2.026 689 | −0.000 006 | 0.204 687 |
| H | 3.383 858 | −0.000 479 | 0.917 271 |
| H | −0.067 305 | −0.757 094 | −0.637 530 |
| H | −0.067 297 | 0.757 110 | −0.637 536 |

Table S33: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=290°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | 0.143 282 | 0.000 018 | −0.057 365 |
| O | 3.054 590 | −0.000 020 | 0.061 239 |
| H | 2.088 265 | −0.000 014 | 0.174 344 |
| H | 3.401 748 | −0.000 489 | 0.961 388 |
| H | −0.056 076 | −0.759 704 | −0.621 773 |
| H | −0.056 119 | 0.759 730 | −0.621 773 |

Table S34: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=300°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | 0.210 715 | 0.000 018 | −0.063 188 |
| O | 3.122 773 | −0.000 015 | 0.087 111 |
| H | 2.151 724 | −0.000 014 | 0.145 757 |
| H | 3.417 004 | −0.000 498 | 1.005 931 |
| H | −0.061 350 | −0.762 195 | −0.591 852 |
| H | −0.061 396 | 0.762 225 | −0.591 839 |

Table S35: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=310°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.104 837 | 0.000 039 | −0.140 748 |
| O | 2.801 052 | −0.000 132 | 0.069 152 |
| H | 2.047 553 | 0.000 012 | 0.677 737 |
| H | 3.579 039 | −0.000 423 | 0.640 528 |
| H | 0.310 147 | −0.762 350 | −0.566 541 |
| H | 0.310 136 | 0.762 374 | −0.566 649 |

Table S36: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=320°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.154 541 | 0.000 036 | −0.185 894 |
| O | 2.749 771 | −0.000 192 | 0.107 497 |
| H | 2.142 859 | 0.000 057 | 0.861 098 |
| H | 3.630 300 | −0.000 405 | 0.503 676 |
| H | 0.349 914 | −0.756 154 | −0.515 117 |
| H | 0.349 888 | 0.756 179 | −0.515 260 |

Table S37: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=330°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.208 104 | 0.000 023 | −0.243 566 |
| O | 2.703 582 | −0.000 265 | 0.172 890 |
| H | 2.290 008 | 0.000 113 | 1.047 107 |
| H | 3.651 775 | −0.000 381 | 0.356 604 |
| H | 0.360 754 | −0.751 748 | −0.457 749 |
| H | 0.360 716 | 0.751 777 | −0.457 906 |

Table S38: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=340°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −0.587 026 | −0.004 081 | −0.312 934 |
| O | 2.936 401 | 0.000 202 | 0.206 800 |
| H | 2.933 682 | −0.004 839 | 1.205 464 |
| H | 3.918 586 | 0.001 283 | 0.355 918 |
| H | 0.015 358 | −0.754 414 | −0.447 895 |
| H | 0.002 429 | 0.761 369 | −0.410 053 |

Table S39: Optimised geometry of the $H_2O$ dimer with a frozen angle $\theta$=350°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| O | −1.009 478 | 0.000 063 | −0.190 414 |
| O | 3.925 576 | −0.000 070 | 0.167 681 |
| H | 2.962 132 | −0.000 044 | 0.229 318 |
| H | 4.216 973 | −0.000 556 | 1.088 807 |
| H | −0.420 475 | −0.763 234 | −0.251 145 |
| H | −0.420 478 | 0.763 361 | −0.251 147 |

## 3.2 $(H_2S)_2$

Table S40: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=0°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.275 330 | 0.000 000 | −0.046 486 |
| S | 4.271 775 | 0.000 000 | 0.036 865 |
| H | 2.922 803 | 0.000 000 | 0.024 212 |
| H | 4.312 766 | 0.000 000 | 1.386 261 |
| H | 0.655 648 | −0.978 109 | −0.029 421 |
| H | 0.655 648 | 0.978 109 | −0.029 421 |

Table S41: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=10°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.019 420 | 0.000 000 | 0.158 548 |
| S | 4.202 631 | 0.000 000 | 0.208 353 |
| H | 3.163 895 | 0.000 000 | −0.654 686 |
| H | 3.386 989 | 0.000 000 | 1.284 424 |
| H | 0.897 188 | −0.976 329 | 0.331 706 |
| H | 0.897 188 | 0.976 329 | 0.331 706 |

Table S42: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=20°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.012 343 | 0.000 000 | 0.128 910 |
| S | 4.197 499 | 0.000 000 | 0.164 038 |
| H | 3.065 863 | 0.000 000 | −0.573 508 |
| H | 3.511 132 | 0.000 000 | 1.326 761 |
| H | 0.860 239 | −0.977 190 | 0.456 165 |
| H | 0.860 239 | 0.977 190 | 0.456 165 |

Table S43: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=30°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.002 347 | 0.000 000 | 0.096 588 |
| S | 4.190 619 | 0.000 000 | 0.126 910 |
| H | 2.988 953 | 0.000 000 | −0.490 735 |
| H | 3.626 858 | 0.000 000 | 1.353 692 |
| H | 0.798 624 | −0.978 231 | 0.570 668 |
| H | 0.798 624 | 0.978 231 | 0.570 668 |

Table S44: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=40°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | 0.008 895 | 0.000 000 | 0.064 179 |
| S | 4.182 074 | 0.000 000 | 0.095 882 |
| H | 2.927 382 | 0.000 000 | −0.406 698 |
| H | 3.735 645 | 0.000 000 | 1.369 968 |
| H | 0.711 147 | −0.979 772 | 0.672 529 |
| H | 0.711 147 | 0.979 772 | 0.672 529 |

Table S45: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=50°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | 0.019 352 | 0.000 000 | 0.042 952 |
| S | 4.168 268 | 0.000 000 | 0.062 613 |
| H | 2.872 844 | 0.000 000 | −0.325 020 |
| H | 3.838 919 | 0.000 000 | 1.371 712 |
| H | 0.598 953 | −0.982 150 | 0.765 846 |
| H | 0.598 953 | 0.982 150 | 0.765 846 |

Table S46: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=60°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | 0.023 015 | 0.000 000 | 0.028 958 |
| S | 4.154 247 | 0.000 000 | 0.034 899 |
| H | 2.830 980 | 0.000 000 | −0.245 939 |
| H | 3.933 157 | 0.000 000 | 1.366 510 |
| H | 0.454 876 | −0.984 559 | 0.845 821 |
| H | 0.454 876 | 0.984 559 | 0.845 821 |

Table S47: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=70°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | 0.029 075 | 0.000 000 | 0.013 600 |
| S | 4.143 365 | 0.000 000 | 0.009 484 |
| H | 2.799 508 | 0.000 000 | −0.149 688 |
| H | 4.044 522 | 0.000 000 | 1.355 632 |
| H | 0.256 660 | −0.989 388 | 0.903 281 |
| H | 0.256 660 | 0.989 388 | 0.903 281 |

Table S48: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=80°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | 0.060 816 | 0.000 000 | 0.007 935 |
| S | 4.164 541 | 0.000 000 | −0.041 943 |
| H | 2.812 643 | 0.000 000 | 0.018 968 |
| H | 4.287 180 | 0.000 000 | 1.302 139 |
| H | −0.093 775 | −0.975 042 | 0.929 036 |
| H | −0.093 775 | 0.975 042 | 0.929 036 |

Table S49: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=90°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.018 468 | 0.000 000 | 0.003 809 |
| S | 4.086 370 | 0.000 000 | −0.013 606 |
| H | 2.733 025 | 0.000 000 | −0.009 765 |
| H | 4.151 011 | 0.000 000 | 1.334 520 |
| H | −0.125 684 | −0.972 146 | 0.934 896 |
| H | −0.125 684 | 0.972 146 | 0.934 896 |

Table S50: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=100°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.072 855 | −0.000 032 | −0.015 646 |
| S | 4.030 955 | 0.000 040 | −0.006 164 |
| H | 2.677 952 | −0.000 059 | 0.021 308 |
| H | 4.119 476 | 0.000 025 | 1.340 596 |
| H | −0.246 131 | −0.974 518 | 0.902 559 |
| H | −0.245 888 | 0.979 243 | 0.897 497 |

Table S51: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=110°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.105 425 | 0.000 000 | −0.041 971 |
| S | 3.993 717 | 0.000 000 | −0.012 673 |
| H | 2.644 610 | 0.000 000 | 0.090 883 |
| H | 4.158 869 | 0.000 000 | 1.326 831 |
| H | −0.410 210 | −0.978 803 | 0.836 260 |
| H | −0.410 210 | 0.978 803 | 0.836 260 |

Table S52: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=120°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.118 791 | 0.000 000 | −0.060 494 |
| S | 3.973 473 | 0.000 000 | −0.021 796 |
| H | 2.632 596 | 0.000 000 | 0.156 671 |
| H | 4.213 089 | 0.000 000 | 1.306 404 |
| H | −0.575 189 | −0.979 945 | 0.747 643 |
| H | −0.575 189 | 0.979 945 | 0.747 643 |

Table S53: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=130°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.108 314 | −0.000 308 | −0.044 885 |
| S | 4.006 347 | 0.039 180 | −0.009 818 |
| H | 2.661 156 | −0.074 870 | 0.067 582 |
| H | 4.142 509 | 0.027 898 | 1.333 038 |
| H | −0.732 678 | −0.976 458 | 0.647 154 |
| H | −0.665 170 | 0.984 559 | 0.690 878 |

Table S54: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=140°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.103 321 | −0.003 925 | −0.038 213 |
| S | 4.020 167 | 0.044 867 | −0.010 653 |
| H | 2.677 039 | −0.086 636 | 0.064 386 |
| H | 4.153 036 | 0.032 491 | 1.332 509 |
| H | −0.847 655 | −0.973 265 | 0.534 192 |
| H | −0.774 417 | 0.986 468 | 0.586 169 |

Table S55: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=150°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.094 442 | −0.044 100 | −0.027 162 |
| S | 4.030 173 | 0.065 748 | −0.011 549 |
| H | 2.692 849 | −0.110 200 | 0.064 137 |
| H | 4.163 076 | 0.059 569 | 1.331 526 |
| H | −0.994 539 | −0.959 579 | 0.388 055 |
| H | −0.797 307 | 0.988 562 | 0.482 783 |

Table S56: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=160°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.090 224 | −0.008 064 | −0.016 485 |
| S | 4.060 940 | 0.034 947 | −0.004 920 |
| H | 2.714 750 | −0.065 471 | 0.034 776 |
| H | 4.156 702 | 0.023 435 | 1.341 421 |
| H | −0.986 088 | −0.971 546 | 0.283 627 |
| H | −0.937 570 | 0.986 699 | 0.320 111 |

Table S57: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=170°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.084 296 | −0.000 078 | −0.008 024 |
| S | 4.080 377 | 0.000 534 | 0.002 225 |
| H | 2.730 300 | −0.001 006 | 0.010 379 |
| H | 4.143 971 | 0.000 311 | 1.350 457 |
| H | −0.999 095 | −0.978 900 | 0.152 277 |
| H | −0.998 588 | 0.979 138 | 0.152 736 |

Table S58: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=180°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.082 776 | −0.000 005 | −0.007 376 |
| S | 4.083 417 | 0.000 011 | 0.004 819 |
| H | 2.733 453 | −0.000 017 | 0.011 695 |
| H | 4.147 003 | 0.000 006 | 1.353 064 |
| H | −1.011 642 | −0.978 705 | −0.010 099 |
| H | −1.011 626 | 0.978 711 | −0.010 092 |

Table S59: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=190°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.083 600 | −0.000 363 | −0.006 210 |
| S | 4.078 824 | 0.001 113 | 0.006 575 |
| H | 2.728 795 | −0.001 816 | 0.012 422 |
| H | 4.142 807 | 0.000 518 | 1.354 816 |
| H | −0.997 704 | −0.978 861 | −0.172 121 |
| H | −0.996 453 | 0.979 408 | −0.171 512 |

Table S60: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=200°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | 0.006 780 | 0.011 386 | 0.070 150 |
| S | 4.092 995 | −0.025 070 | 0.087 994 |
| H | 2.803 695 | −0.029 474 | −0.314 929 |
| H | 3.742 172 | 0.036 076 | 1.389 944 |
| H | −0.870 793 | −0.974 498 | −0.210 742 |
| H | −0.856 339 | 0.981 580 | −0.296 927 |

Table S61: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=210°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.065 654 | −0.075 551 | 0.018 237 |
| S | 4.050 414 | 0.111 661 | 0.020 305 |
| H | 2.721 875 | −0.113 374 | −0.075 739 |
| H | 4.027 566 | 0.028 875 | 1.367 308 |
| H | −0.984 537 | −0.949 003 | −0.443 703 |
| H | −0.749 854 | 0.997 392 | −0.430 178 |

Table S62: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=220°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.081 175 | −0.016 648 | 0.032 459 |
| S | 4.042 437 | 0.052 726 | 0.010 506 |
| H | 2.699 124 | −0.080 631 | −0.055 403 |
| H | 4.040 421 | 0.021 110 | 1.359 993 |
| H | −0.821 840 | −0.968 786 | −0.572 519 |
| H | −0.754 118 | 0.992 229 | −0.559 406 |

Table S63: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=230°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.088 747 | −0.010 700 | 0.039 342 |
| S | 4.028 462 | 0.038 505 | 0.004 151 |
| H | 2.681 059 | −0.061 287 | −0.047 926 |
| H | 4.039 071 | 0.016 925 | 1.353 762 |
| H | −0.703 784 | −0.973 153 | −0.679 487 |
| H | −0.652 211 | 0.989 709 | −0.669 771 |

Table S64: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=240°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.081 806 | 0.000 000 | 0.049 407 |
| S | 4.026 075 | 0.000 000 | 0.005 742 |
| H | 2.676 352 | 0.000 000 | −0.083 370 |
| H | 3.996 165 | 0.000 000 | 1.355 080 |
| H | −0.533 398 | −0.981 392 | −0.759 455 |
| H | −0.533 398 | 0.981 392 | −0.759 455 |

Table S65: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=250°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.102 419 | 0.000 000 | 0.022 307 |
| S | 4.001 094 | 0.000 000 | −0.011 164 |
| H | 2.648 498 | 0.000 000 | 0.020 086 |
| H | 4.093 638 | 0.000 000 | 1.335 253 |
| H | −0.384 730 | −0.982 381 | −0.859 026 |
| H | −0.384 730 | 0.982 381 | −0.859 026 |

Table S66: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=260°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.096 223 | 0.000 000 | 0.004 464 |
| S | 4.004 716 | 0.000 000 | −0.009 799 |
| H | 2.652 569 | 0.000 000 | 0.045 585 |
| H | 4.120 512 | 0.000 000 | 1.334 825 |
| H | −0.209 032 | −0.979 083 | −0.918 112 |
| H | −0.209 032 | 0.979 083 | −0.918 112 |

Table S67: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=270°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.053 061 | 0.000 000 | −0.032 531 |
| S | 4.042 823 | 0.000 000 | 0.009 236 |
| H | 2.692 938 | 0.000 000 | 0.105 233 |
| H | 4.200 227 | 0.000 000 | 1.349 622 |
| H | −0.091 178 | −0.974 814 | −0.966 145 |
| H | −0.091 178 | 0.974 814 | −0.966 145 |

Table S68: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=280°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.005 279 | 0.000 000 | −0.057 368 |
| S | 4.080 899 | 0.000 000 | 0.030 473 |
| H | 2.734 358 | 0.000 000 | 0.166 386 |
| H | 4.279 173 | 0.000 000 | 1.365 478 |
| H | 0.024 239 | −0.982 424 | −0.983 060 |
| H | 0.024 239 | 0.982 424 | −0.983 060 |

Table S69: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=290°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.046 707 | 0.000 000 | −0.075 161 |
| S | 4.023 879 | 0.000 000 | 0.014 568 |
| H | 2.700 693 | 0.000 000 | 0.297 195 |
| H | 4.367 891 | 0.000 000 | 1.319 447 |
| H | 0.242 017 | −0.983 707 | −0.953 810 |
| H | 0.242 017 | 0.983 707 | −0.953 810 |

Table S70: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=300°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.072 040 | 0.000 000 | −0.103 590 |
| S | 3.980 797 | 0.000 000 | 0.013 861 |
| H | 2.693 739 | 0.000 000 | 0.429 647 |
| H | 4.457 496 | 0.000 000 | 1.276 371 |
| H | 0.395 579 | −0.981 603 | −0.904 170 |
| H | 0.395 579 | 0.981 603 | −0.904 170 |

Table S71: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=310°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.101 834 | 0.000 000 | −0.144 896 |
| S | 3.904 909 | 0.000 000 | 0.015 284 |
| H | 2.694 082 | 0.000 000 | 0.615 865 |
| H | 4.566 232 | 0.000 000 | 1.191 544 |
| H | 0.516 950 | −0.979 410 | −0.838 863 |
| H | 0.516 950 | 0.979 410 | −0.838 863 |

Table S72: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=320°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.155 487 | 0.000 000 | −0.333 551 |
| S | 3.541 133 | 0.000 000 | 0.148 457 |
| H | 2.872 005 | 0.000 000 | 1.319 905 |
| H | 4.749 306 | 0.000 000 | 0.750 512 |
| H | 0.634 667 | −0.973 684 | −0.834 846 |
| H | 0.634 667 | 0.973 684 | −0.834 846 |

Table S73: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=330°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.184 948 | 0.000 000 | −0.379 265 |
| S | 3.522 200 | 0.000 000 | 0.178 393 |
| H | 2.927 193 | 0.000 000 | 1.389 475 |
| H | 4.764 122 | 0.000 000 | 0.706 995 |
| H | 0.686 382 | −0.973 990 | −0.719 684 |
| H | 0.686 382 | 0.973 990 | −0.719 684 |

Table S74: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=340°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.223 726 | 0.000 000 | −0.434 224 |
| S | 3.506 022 | 0.000 000 | 0.223 121 |
| H | 3.017 149 | 0.000 000 | 1.481 125 |
| H | 4.787 496 | 0.000 000 | 0.646 707 |
| H | 0.697 845 | −0.973 953 | −0.595 620 |
| H | 0.697 845 | 0.973 953 | −0.595 620 |

Table S75: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=350°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| S | −0.426 158 | −0.489 169 | 0.140 531 |
| S | 3.666 538 | −0.458 581 | 0.094 012 |
| H | 3.827 572 | 0.789 235 | −0.385 534 |
| H | 3.869 923 | −0.063 772 | 1.369 013 |
| H | 0.927 270 | −0.501 083 | 0.128 118 |
| H | −0.469 156 | 0.716 571 | 0.745 580 |

## 3.3 $(H_2Se)_2$

Table S76: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=0°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.331 657 | 0.000 000 | −0.063 710 |
| Se | 4.406 251 | 0.000 000 | 0.048 382 |
| H | 2.937 977 | 0.000 000 | 0.049 792 |
| H | 4.438 900 | 0.000 000 | 1.516 692 |
| H | 0.693 610 | −1.052 347 | −0.039 453 |
| H | 0.693 610 | 1.052 347 | −0.039 453 |

Table S77: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=10°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.061 246 | 0.000 000 | 0.181 301 |
| Se | 4.344 282 | 0.000 000 | 0.228 250 |
| H | 3.213 936 | 0.000 000 | −0.710 709 |
| H | 3.429 996 | 0.000 000 | 1.378 364 |
| H | 0.947 951 | −1.050 413 | 0.372 562 |
| H | 0.947 951 | 1.050 413 | 0.372 562 |

Table S78: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=20°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.056 052 | 0.000 000 | 0.147 131 |
| Se | 4.343 854 | 0.000 000 | 0.182 560 |
| H | 3.117 443 | 0.000 000 | −0.626 993 |
| H | 3.561 079 | 0.000 000 | 1.425 916 |
| H | 0.903 833 | −1.051 133 | 0.510 658 |
| H | 0.903 833 | 1.051 133 | 0.510 658 |

Table S79: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=30°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.052 603 | 0.000 000 | 0.109 893 |
| Se | 4.345 747 | 0.000 000 | 0.139 222 |
| H | 3.040 249 | 0.000 000 | −0.536 215 |
| H | 3.699 105 | 0.000 000 | 1.458 449 |
| H | 0.827 156 | −1.052 178 | 0.636 471 |
| H | 0.827 156 | 1.052 178 | 0.636 471 |

Table S80: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=40°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.057 342 | 0.000 000 | 0.068 739 |
| Se | 4.347 836 | 0.000 000 | 0.092 766 |
| H | 2.970 289 | 0.000 000 | −0.421 428 |
| H | 3.865 509 | 0.000 000 | 1.480 403 |
| H | 0.712 809 | −1.053 692 | 0.743 185 |
| H | 0.712 809 | 1.053 692 | 0.743 185 |

Table S81: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=50°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.061 860 | 0.000 000 | 0.036 416 |
| Se | 4.344 243 | 0.000 000 | 0.053 723 |
| H | 2.918 989 | 0.000 000 | −0.310 121 |
| H | 4.015 072 | 0.000 000 | 1.485 374 |
| H | 0.570 563 | −1.055 598 | 0.838 989 |
| H | 0.570 563 | 1.055 598 | 0.838 989 |

Table S82: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=60°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.370 802 | 0.390 839 | 0.288 976 |
| Se | 3.983 560 | 0.638 132 | 0.062 332 |
| H | 3.739 874 | −0.692 378 | −0.513 855 |
| H | 4.115 165 | 0.115 042 | 1.429 728 |
| H | −0.158 074 | −0.976 861 | 0.769 707 |
| H | 1.078 007 | 0.638 905 | 0.277 122 |

Table S83: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=70°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.066 591 | 0.000 000 | 0.010 125 |
| Se | 4.323 504 | 0.000 000 | −0.005 545 |
| H | 2.856 124 | 0.000 000 | −0.121 346 |
| H | 4.246 047 | 0.000 000 | 1.461 160 |
| H | 0.187 372 | −1.059 896 | 0.994 828 |
| H | 0.187 372 | 1.059 896 | 0.994 828 |

Table S84: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=80°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.067 274 | 0.000 000 | 0.009 554 |
| Se | 4.320 131 | 0.000 000 | −0.030 993 |
| H | 2.848 124 | 0.000 000 | −0.027 714 |
| H | 4.362 485 | 0.000 000 | 1.436 960 |
| H | −0.083 118 | −1.051 987 | 1.034 901 |
| H | −0.083 118 | 1.051 987 | 1.034 901 |

Table S85: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=90°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.160 371 | 0.000 000 | −0.001 857 |
| Se | 4.230 512 | 0.000 000 | −0.008 769 |
| H | 2.758 671 | 0.000 000 | −0.009 148 |
| H | 4.269 505 | 0.000 000 | 1.459 253 |
| H | −0.144 953 | −1.044 288 | 1.031 526 |
| H | −0.144 953 | 1.044 288 | 1.031 526 |

Table S86: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=100°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.220 719 | 0.000 000 | −0.028 121 |
| Se | 4.168 781 | 0.000 000 | 0.000 828 |
| H | 2.697 002 | 0.000 000 | 0.024 550 |
| H | 4.232 557 | 0.000 000 | 1.468 082 |
| H | −0.279 015 | −1.051 434 | 0.996 135 |
| H | −0.279 015 | 1.051 434 | 0.996 135 |

Table S87: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=110°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.226 531 | 0.000 000 | −0.045 445 |
| Se | 4.159 326 | 0.000 000 | 0.001 763 |
| H | 2.687 689 | 0.000 000 | 0.033 249 |
| H | 4.228 998 | 0.000 000 | 1.468 779 |
| H | −0.483 246 | −1.060 327 | 0.937 852 |
| H | −0.483 246 | 1.060 327 | 0.937 852 |

Table S88: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=120°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.228 394 | 0.003 023 | −0.056 570 |
| Se | 4.169 315 | 0.028 457 | −0.006 864 |
| H | 2.702 541 | −0.053 937 | 0.072 452 |
| H | 4.285 876 | 0.019 144 | 1.456 894 |
| H | −0.724 473 | −1.056 352 | 0.830 887 |
| H | −0.676 696 | 1.059 666 | 0.858 971 |

Table S89: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=130°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.222 417 | 0.000 556 | −0.056 793 |
| Se | 4.180 523 | 0.038 023 | −0.008 547 |
| H | 2.716 830 | −0.073 584 | 0.079 989 |
| H | 4.305 006 | 0.027 064 | 1.454 459 |
| H | −0.892 047 | −1.052 704 | 0.716 305 |
| H | −0.828 645 | 1.060 645 | 0.757 957 |

Table S90: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=140°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.210 834 | −0.003 434 | −0.048 722 |
| Se | 4.195 135 | 0.043 631 | −0.008 122 |
| H | 2.733 238 | −0.085 201 | 0.077 209 |
| H | 4.315 081 | 0.031 942 | 1.455 245 |
| H | −1.019 200 | −1.049 009 | 0.590 451 |
| H | −0.948 511 | 1.062 070 | 0.640 788 |

Table S91: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=150°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.193 855 | −0.047 091 | −0.036 145 |
| Se | 4.201 378 | 0.067 828 | −0.008 015 |
| H | 2.745 698 | −0.114 467 | 0.079 387 |
| H | 4.322 949 | 0.063 113 | 1.455 386 |
| H | −1.176 939 | −1.034 473 | 0.426 723 |
| H | −0.969 220 | 1.065 090 | 0.526 954 |

Table S92: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=160°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.180 492 | −0.000 140 | −0.019 940 |
| Se | 4.237 809 | 0.001 818 | 0.004 894 |
| H | 2.768 978 | −0.003 587 | 0.028 898 |
| H | 4.293 408 | 0.001 146 | 1.472 293 |
| H | −1.139 348 | −1.054 963 | 0.331 006 |
| H | −1.137 525 | 1.055 727 | 0.332 779 |

Table S93: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=170°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.174 341 | 0.000 168 | −0.015 059 |
| Se | 4.250 800 | 0.000 356 | 0.010 170 |
| H | 2.782 300 | −0.000 629 | 0.031 910 |
| H | 4.305 380 | 0.000 232 | 1.477 685 |
| H | −1.184 835 | −1.058 163 | 0.104 350 |
| H | −1.185 354 | 1.050 266 | 0.159 724 |

Table S94: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=180°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.174 940 | 0.000 031 | −0.015 116 |
| Se | 4.253 658 | −0.000 065 | 0.014 728 |
| H | 2.785 261 | 0.000 104 | 0.034 328 |
| H | 4.307 473 | −0.000 035 | 1.482 315 |
| H | −1.196 611 | −1.054 308 | −0.021 979 |
| H | −1.196 710 | 1.054 274 | −0.022 025 |

Table S95: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=190°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.176 080 | −0.000 668 | −0.014 092 |
| Se | 4.248 289 | 0.001 749 | 0.019 061 |
| H | 2.779 846 | −0.002 773 | 0.036 187 |
| H | 4.301 556 | 0.000 802 | 1.486 687 |
| H | −1.180 913 | −1.054 175 | −0.203 286 |
| H | −1.178 749 | 1.055 065 | −0.202 387 |

Table S96: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=200°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.181 683 | −0.001 227 | −0.008 366 |
| Se | 4.236 294 | 0.003 648 | 0.020 945 |
| H | 2.767 689 | −0.005 740 | 0.037 326 |
| H | 4.290 760 | 0.001 528 | 1.488 489 |
| H | −1.137 197 | −1.054 468 | −0.372 607 |
| H | −1.133 034 | 1.056 260 | −0.371 217 |

Table S97: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=210°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.100 209 | 0.005 878 | 0.078 909 |
| Se | 4.252 575 | −0.009 302 | 0.093 536 |
| H | 2.835 729 | −0.007 450 | −0.297 878 |
| H | 3.894 215 | 0.010 674 | 1.517 689 |
| H | −0.976 884 | −1.054 747 | −0.433 133 |
| H | −0.975 416 | 1.054 946 | −0.458 914 |

Table S98: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=220°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.171 433 | −0.064 615 | 0.031 335 |
| Se | 4.213 121 | 0.107 212 | 0.038 810 |
| H | 2.764 281 | −0.111 802 | −0.078 571 |
| H | 4.146 060 | 0.027 899 | 1.503 777 |
| H | −1.056 751 | −1.029 743 | −0.632 267 |
| H | −0.830 367 | 1.071 049 | −0.625 433 |

Table S99: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=230°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.200 089 | −0.013 041 | 0.037 516 |
| Se | 4.202 672 | 0.045 722 | 0.026 418 |
| H | 2.738 301 | −0.072 175 | −0.035 477 |
| H | 4.182 771 | 0.019 999 | 1.494 582 |
| H | −0.864 022 | −1.046 965 | −0.766 000 |
| H | −0.800 383 | 1.066 460 | −0.755 909 |

Table S100: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=240°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.213 899 | −0.005 940 | 0.034 874 |
| Se | 4.186 919 | 0.027 168 | 0.019 254 |
| H | 2.718 055 | −0.046 325 | −0.012 809 |
| H | 4.195 727 | 0.013 807 | 1.487 701 |
| H | −0.698 451 | −1.052 481 | −0.873 897 |
| H | −0.660 182 | 1.063 771 | −0.866 393 |

Table S101: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=250°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.233 305 | 0.000 000 | 0.019 566 |
| Se | 4.156 418 | 0.000 000 | 0.005 451 |
| H | 2.685 223 | 0.000 000 | 0.045 080 |
| H | 4.236 907 | 0.000 000 | 1.471 856 |
| H | −0.481 126 | −1.060 439 | −0.965 751 |
| H | −0.481 126 | 1.060 439 | −0.965 751 |

Table S102: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=260°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.242 709 | 0.000 000 | −0.000 485 |
| Se | 4.147 026 | 0.000 000 | 0.002 232 |
| H | 2.676 614 | 0.000 000 | 0.069 666 |
| H | 4.253 924 | 0.000 000 | 1.466 798 |
| H | −0.257 632 | −1.051 997 | −1.025 660 |
| H | −0.257 632 | 1.051 997 | −1.025 660 |

Table S103: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=270°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.175 910 | 0.000 000 | −0.040 443 |
| Se | 4.216 136 | 0.000 000 | 0.038 274 |
| H | 2.745 188 | 0.000 000 | 0.086 771 |
| H | 4.303 680 | 0.000 000 | 1.503 969 |
| H | −0.140 343 | −1.044 211 | −1.073 301 |
| H | −0.140 343 | 1.044 211 | −1.073 301 |

Table S104: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=280°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.096 846 | 0.000 000 | −0.075 424 |
| Se | 4.285 041 | 0.000 000 | 0.077 518 |
| H | 2.814 544 | 0.000 000 | 0.141 822 |
| H | 4.390 255 | 0.000 000 | 1.542 144 |
| H | −0.047 882 | −1.052 079 | −1.099 585 |
| H | −0.047 882 | 1.052 079 | −1.099 585 |

Table S105: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=290°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.123 367 | 0.000 000 | −0.091 062 |
| Se | 4.248 270 | 0.000 000 | 0.065 075 |
| H | 2.788 311 | 0.000 000 | 0.251 707 |
| H | 4.475 450 | 0.000 000 | 1.515 739 |
| H | 0.172 583 | −1.058 586 | −1.065 504 |
| H | 0.172 583 | 1.058 586 | −1.065 504 |

Table S106: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=300°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.153 144 | 0.000 000 | −0.116 814 |
| Se | 4.202 815 | 0.000 000 | 0.055 129 |
| H | 2.767 880 | 0.000 000 | 0.380 940 |
| H | 4.569 871 | 0.000 000 | 1.476 821 |
| H | 0.350 614 | −1.057 096 | −1.003 673 |
| H | 0.350 614 | 1.057 096 | −1.003 673 |

Table S107: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=310°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.185 148 | 0.000 000 | −0.153 486 |
| Se | 4.137 645 | 0.000 000 | 0.045 870 |
| H | 2.753 711 | 0.000 000 | 0.543 390 |
| H | 4.676 417 | 0.000 000 | 1.411 747 |
| H | 0.487 472 | −1.055 329 | −0.923 195 |
| H | 0.487 472 | 1.055 329 | −0.923 195 |

Table S108: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=320°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.207 226 | 0.000 000 | −0.280 130 |
| Se | 3.861 945 | 0.000 000 | 0.079 947 |
| H | 2.762 148 | 0.000 000 | 1.052 290 |
| H | 4.878 000 | 0.000 000 | 1.140 237 |
| H | 0.628 521 | −1.051 056 | −0.877 347 |
| H | 0.628 521 | 1.051 056 | −0.877 347 |

Table S109: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=330°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.263 169 | 0.000 000 | −0.460 530 |
| Se | 3.615 649 | 0.000 000 | 0.227 319 |
| H | 2.976 243 | 0.000 000 | 1.548 509 |
| H | 4.959 424 | 0.000 000 | 0.821 075 |
| H | 0.699 332 | −1.051 007 | −0.818 081 |
| H | 0.699 332 | 1.051 007 | −0.818 081 |

Table S110: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=340°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.291 447 | 0.000 000 | −0.488 705 |
| Se | 3.622 341 | 0.000 000 | 0.237 084 |
| H | 3.020 199 | 0.000 000 | 1.576 192 |
| H | 4.980 986 | 0.000 000 | 0.795 401 |
| H | 0.720 956 | −1.050 811 | −0.662 701 |
| H | 0.720 956 | 1.050 811 | −0.662 701 |

Table S111: Optimised geometry of the $H_2S$ dimer with a frozen angle $\theta$=350°.

| **Element** | $x$ | $y$ | $z$ |
|---|---|---|---|
| Se | −0.321 864 | 0.000 000 | −0.510 103 |
| Se | 3.630 139 | 0.000 000 | 0.253 017 |
| H | 3.091 014 | 0.000 000 | 1.619 183 |
| H | 5.011 922 | 0.000 000 | 0.751 044 |
| H | 0.705 829 | −1.050 395 | −0.495 486 |
| H | 0.705 829 | 1.050 395 | −0.495 486 |

# 4 Quantum theory of atoms in molecules

We report in this section the QTAIM analyses within the H-acceptor and H-donor molecules as well as the intermolecular interaction between monomers.

Table S112: Atomic charges and intermolecular delocalisation indices of the H-acceptor molecule in $(H_2O)_2$, $(H_2S)_2$ y $(H_2Se)_2$. The atomic labelling is shown in Figure 3 of the main body of the paper. Atomic units are used throughout.

| | $(H_2O)_2$ | $(H_2S)_2$ | $(H_2Se)_2$ |
|---|---|---|---|
| $q^{E1}$ | −1.254 | 0.608 | 0.385 |
| $q^{H5}$ | 0.633 | −0.297 | −0.184 |
| $q^{H6}$ | 0.633 | −0.297 | −0.184 |
| DI(E1,H5) | 0.607 | 1.143 | −0.262 |
| DI(E1,H6) | 0.607 | 1.143 | −0.262 |
| DI(H5,H6) | 0.006 | 0.084 | 0.055 |

Table S113: Atomic charges and intermolecular delocalisation indices of the H-donor molecule in $(H_2O)_2$, $(H_2S)_2$ y $(H_2Se)_2$. The atomic labelling is shown in Figure 3 of the main body of the paper. Atomic units are used throughout.

| | $(H_2O)_2$ | $(H_2S)_2$ | $(H_2Se)_2$ |
|---|---|---|---|
| $q^{E2}$ | −1.289 | 0.562 | 0.342 |
| $q^{H3}$ | 0.666 | −0.266 | −0.164 |
| $q^{H4}$ | 0.611 | −0.310 | −0.194 |
| DI(E2,H3) | 0.516 | 1.124 | 1.103 |
| DI(E2,H4) | 0.638 | 1.153 | 1.137 |
| DI(H3,H4) | 0.005 | 0.080 | 0.053 |

Table S114: Intermolecular delocalisation indices for $(H_2O)_2$, $(H_2S)_2$ and $(H_2Se)_2$ in their equilibrium configurations. The atomic labelling is shown in Figure 3 of the main body of the paper. Atomic units are used throughout.

| | $(H_2O)_2$ | $(H_2S)_2$ | $(H_2Se)_2$ |
|---|---|---|---|
| DI(E1,H3) | 0.053 | 0.064 | 0.070 |
| DI(E1,E2) | 0.057 | 0.024 | 0.030 |
| DI(E1,H4) | 0.001 | 0.002 | 0.002 |
| DI(E2,H5) | 0.001 | 0.001 | 0.001 |
| DI(E2,H6) | 0.001 | 0.001 | 0.001 |
| DI(H3,H5) | 0.001 | 0.003 | 0.002 |
| DI(H3,H6) | 0.001 | 0.003 | 0.002 |
| DI(H4,H5) | 0.000 | 0.000 | 0.000 |
| DI(H4,H6) | 0.000 | 0.000 | 0.000 |
| $\sum$DI($H_2X\cdots H_2X$) | 0.114 | 0.097 | 0.108 |

# 5 Interacting quantum atoms analyses

We report herein the results of the IQA analyses for the H-acceptor and H-donor molecules as well as the intermolecular interaction between monomers.

Table S115: Interacting quantum atoms energy partition scheme within the H-acceptor molecule in $(H_2O)_2$, $(H_2S)_2$ y $(H_2Se)_2$. Atomic units used throughout.

| | $(H_2O)_2$ | $(H_2S)_2$ | $(H_2Se)_2$ |
|---|---|---|---|
| $E_{\text{net}}^{\text{O1}}$ | −74.485 | −397.084 | −2399.549 |
| $E_{\text{net}}^{\text{H5}}$ | −0.270 | −0.339 | −0.402 |
| $E_{\text{net}}^{\text{H6}}$ | −0.270 | −0.339 | −0.402 |
| $E_{\text{class}}^{\text{E1-H5}}$ | −0.395 | −0.184 | −0.043 |
| $E_{\text{xc}}^{\text{E1-H5}}$ | −0.184 | −0.287 | −0.262 |
| $E_{\text{int}}^{\text{E1-H5}}$ | −0.579 | −0.472 | −0.306 |
| $E_{\text{class}}^{\text{E1-H6}}$ | −0.395 | −0.184 | −0.043 |
| $E_{\text{xc}}^{\text{E1-H6}}$ | −0.184 | −0.287 | −0.262 |
| $E_{\text{int}}^{\text{E1-H6}}$ | −0.579 | −0.472 | −0.306 |
| $E_{\text{class}}^{\text{H5-H6}}$ | 0.157 | 0.029 | 0.009 |
| $E_{\text{xc}}^{\text{H5-H6}}$ | −0.001 | −0.014 | −0.007 |
| $E_{\text{int}}^{\text{H5-H6}}$ | 0.157 | 0.016 | 0.001 |

Table S116: Interacting quantum atoms energy partition scheme within the H-donor molecule in $(H_2O)_2$, $(H_2S)_2$ y $(H_2Se)_2$.

| | $(H_2O)_2$ | $(H_2S)_2$ | $(H_2Se)_2$ |
|---|---|---|---|
| $E_{\text{net}}^{\text{O2}}$ | −74.485 | −397.109 | −2399.567 |
| $E_{\text{net}}^{\text{H3}}$ | −0.252 | −0.340 | −0.396 |
| $E_{\text{net}}^{\text{H4}}$ | −0.279 | −0.337 | −0.402 |
| $E_{\text{class}}^{\text{E2-H3}}$ | −0.432 | −0.158 | −0.035 |
| $E_{\text{xc}}^{\text{E2-H3}}$ | −0.163 | −0.287 | −0.261 |
| $E_{\text{int}}^{\text{E2-H3}}$ | −0.595 | −0.445 | −0.295 |
| $E_{\text{class}}^{\text{E2-H4}}$ | −0.386 | −0.187 | −0.044 |
| $E_{\text{xc}}^{\text{E2-H4}}$ | −0.192 | −0.288 | −0.263 |
| $E_{\text{int}}^{\text{E2-H4}}$ | −0.578 | −0.475 | −0.307 |
| $E_{\text{class}}^{\text{H3-H4}}$ | 0.159 | 0.027 | 0.008 |
| $E_{\text{xc}}^{\text{H3-H4}}$ | −0.001 | −0.013 | −0.007 |
| $E_{\text{int}}^{\text{H3-H4}}$ | 0.158 | 0.014 | 0.001 |

Table S117: Interacting quantum atomos energy partition for the intermolecular contacts in the $(H_2O)_2$, $(H_2S)_2$ and $(H_2Se)_2$ clusters. The atom labelling is shown in Figure 3 of the body of the manuscript. Atomic units used throughout.

| | $(H_2O)_2$ | $(H_2S)_2$ | $(H_2Se)_2$ |
|---|---|---|---|
| $E_{\text{class}}^{\text{E1-H3}}$ | −0.203 | −0.022 | −0.008 |
| $E_{\text{xc}}^{\text{E1-H3}}$ | −0.012 | −0.010 | −0.011 |
| $E_{\text{int}}^{\text{E1-H3}}$ | −0.215 | −0.032 | −0.019 |
| $E_{\text{class}}^{\text{E1-E2}}$ | 0.286 | 0.044 | 0.015 |
| $E_{\text{xc}}^{\text{E1-E2}}$ | −0.008 | −0.002 | −0.002 |
| $E_{\text{int}}^{\text{E1-E2}}$ | 0.278 | 0.042 | 0.013 |
| $E_{\text{class}}^{\text{E1-H4}}$ | −0.118 | −0.020 | −0.007 |
| $E_{\text{xc}}^{\text{E1-H4}}$ | 0.000 | 0.000 | 0.000 |
| $E_{\text{int}}^{\text{E1-H4}}$ | −0.118 | −0.020 | −0.007 |
| $E_{\text{class}}^{\text{E2-H5}}$ | −0.132 | −0.024 | −0.009 |
| $E_{\text{xc}}^{\text{E2-H5}}$ | 0.000 | 0.000 | 0.000 |
| $E_{\text{int}}^{\text{E2-H5}}$ | −0.132 | −0.024 | −0.009 |
| $E_{\text{class}}^{\text{E2-H6}}$ | −0.132 | −0.024 | −0.009 |
| $E_{\text{xc}}^{\text{E2-H6}}$ | 0.000 | 0.000 | 0.000 |
| $E_{\text{int}}^{\text{E2-H6}}$ | −0.132 | −0.024 | −0.009 |
| $E_{\text{class}}^{\text{H3-H5}}$ | 0.090 | 0.012 | 0.004 |
| $E_{\text{xc}}^{\text{H3-H5}}$ | 0.000 | 0.000 | 0.000 |
| $E_{\text{int}}^{\text{H3-H5}}$ | 0.090 | 0.012 | 0.004 |
| $E_{\text{class}}^{\text{H3-H6}}$ | 0.090 | 0.012 | 0.004 |
| $E_{\text{xc}}^{\text{H3-H6}}$ | 0.000 | 0.000 | 0.000 |
| $E_{\text{int}}^{\text{H3-H6}}$ | 0.090 | 0.012 | 0.004 |
| $E_{\text{class}}^{\text{H1-H5}}$ | 0.054 | 0.010 | 0.004 |
| $E_{\text{xc}}^{\text{H1-H5}}$ | 0.000 | 0.000 | 0.000 |
| $E_{\text{int}}^{\text{H1-H5}}$ | 0.054 | 0.010 | 0.004 |
| $E_{\text{class}}^{\text{H1-H6}}$ | 0.054 | 0.010 | 0.004 |
| $E_{\text{xc}}^{\text{H1-H6}}$ | 0.000 | 0.000 | 0.000 |
| $E_{\text{int}}^{\text{H1-H6}}$ | 0.054 | 0.010 | 0.004 |
| $\sum E_{\text{class}}$ | −0.011 | −0.002 | −0.001 |
| $\sum E_{\text{xc}}$ | −0.020 | −0.013 | −0.014 |
| $\sum E_{\text{int}}$ | −0.030 | −0.015 | −0.015 |

# 6 Dipole moments and interaction energy

The dipole moments of both acceptor and donor proton molecules were calculated within the dimer using the equation:

$$\boldsymbol{\mu}_{\text{frag}} = \sum_i \boldsymbol{\mu}_i + \sum_i q_i \boldsymbol{r}_i. \tag{1}$$

Here, the vector $\boldsymbol{\mu}_{\text{frag}}$ is the dipole moment of a fragment within a molecular cluster, $\sum_i \boldsymbol{\mu}_i$ is the sum of the atomic dipole moments within the monomer of interest and $\sum_i q_i \boldsymbol{r}_i$ is the sum of the multiplication of the atomic charge by the position vector of the nuclei of the considered moiety. All the vectors and scalars of the right side of equation (1) are obtained from the PROMOLDEN program.

In order to calculate the interaction energy between dipoles within the molecular cluster we employed the expression[12],

$$U_{\boldsymbol{\mu}_1\boldsymbol{\mu}_2} = \frac{R^2(\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2) - 3\,(\boldsymbol{\mu}_1 \cdot \boldsymbol{R})\,(\boldsymbol{\mu}_2 \cdot \boldsymbol{R})}{4\pi\epsilon_0 R^5}, \tag{2}$$

where all the parameters were computed with the aid of the PROMOLDEN[6] program.

Table S118: Magnitude of the dipole moment for H-acceptor and H-donor molecules and the corresponding interaction energy in $(H_2O)_2$, $(H_2S)_2$ and $(H_2Se)_2$. Dipole moments and $U_{\mu_1\mu_2}$ are reported in atomic units and kcal mol$^{-1}$ respectively.

| | $(H_2O)_2$ | $(H_2S)_2$ | $(H_2Se)_2$ |
|---|---|---|---|
| $\mu$ H-acceptor | 0.826 | 0.459 | 0.335 |
| $\mu$ H-donor | 0.873 | 0.510 | 0.391 |
| $U_{\mu_1\mu_2}$ | −3.557 | −0.274 | −0.090 |

# 7 Symmetry Adapted Perturbation Theory

The SAPT calculations were performed as is implemented in Psi4[3] program with the aug-cc-pVDZ basis set.

Table S119: Part 1 of the SAPT energy decompotition analyses for the $(H_2O)_2$, $(H_2S)_2$ and $(H_2S)_2$ complexes. We also present MP2 corrections for SAPT2+, SAPT2+(3) and SAPT2+3 terms. kcal mol$^{-1}$ are use throutghout.

| | $(H_2O)_2$ | $(H_2S)_2$ | $(H_2Se)_2$ |
|---|---|---|---|
| Electrostatics | −7.792 | −2.430 | −2.435 |
| Elst10,r | −8.020 | −2.530 | −2.501 |
| Elst12,r | 0.080 | 0.016 | −0.011 |
| Elst13,r | 0.148 | 0.083 | 0.077 |
| Exchange | 7.644 | 3.526 | 3.999 |
| Exch10 | 6.383 | 3.292 | 3.702 |
| Exch10($S^2$) | 6.341 | 3.273 | 3.676 |
| Exch11($S^2$) | 0.026 | 0.181 | 0.239 |
| Exch12($S^2$) | 1.235 | 0.053 | 0.058 |
| Induction | −2.293 | −0.907 | −0.854 |
| Ind20,r | −2.613 | −1.261 | −1.858 |
| Ind30,r | −2.739 | −2.796 | −9.269 |
| Ind22 | −0.464 | −0.078 | −0.121 |
| Exch-Ind20,r | 1.370 | 0.906 | 1.538 |
| Exch-Ind30,r | 2.408 | 2.726 | 9.215 |
| Exch-Ind22 | 0.243 | 0.056 | 0.100 |
| delta-HF,r (2) | −0.830 | −0.530 | −0.512 |
| delta-HF,r (3) | −0.500 | −0.460 | −0.459 |
| Dispersion | −2.151 | −1.715 | −1.949 |
| Disp20 | −2.101 | −1.907 | −2.182 |
| Disp30 | 0.035 | 0.045 | 0.057 |
| Disp21 | 0.071 | 0.171 | 0.207 |
| Disp22 (SDQ) | −0.105 | 0.077 | 0.076 |
| Disp22 (T) | −0.286 | −0.229 | −0.255 |
| Est. Disp22 (T) | −0.326 | −0.248 | −0.275 |
| Exch Disp20 | 0.371 | 0.254 | 0.299 |
| Exch Disp30 | −0.011 | −0.018 | −0.024 |
| Ind Disp30 | −0.515 | −0.362 | −0.454 |
| Exch Ind Disp30 | 0.430 | 0.272 | 0.348 |

Table S120: Part 2 of the SAPT energy decompotition analyses for the $(H_2O)_2$, $(H_2S)_2$ and $(H_2S)_2$ complexes. We also present MP2 corrections for SAPT2+, SAPT2+(3) and SAPT2+3 terms. $kcal\,mol^{-1}$ are use throutghout.

| | $(H_2O)_2$ | $(H_2S)_2$ | $(H_2Se)_2$ |
|---|---|---|---|
| Total HF | −3.710 | −0.123 | 0.369 |
| Total SAPT0 | −5.440 | −1.776 | −1.515 |
| Total SAPT2 | −4.320 | −1.548 | −1.249 |
| Total SAPT2+ | −4.679 | −1.548 | −1.242 |
| Total SAPT2+(3) | −4.496 | −1.419 | −1.107 |
| Total SAPT2+3 | −4.592 | −1.527 | −1.239 |
| | | | |
| Electrostatics sSAPT0 | −8.020 | −2.530 | −2.501 |
| Exchange sSAPT0 | 6.383 | 3.292 | 3.702 |
| Induction sSAPT0 | −2.045 | −0.869 | −0.800 |
| Dispersion sSAPT0 | −1.723 | −1.649 | −1.877 |
| Total sSAPT0 | −5.406 | −1.756 | −1.476 |

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