Characteristics of nonconventional hydrogen bonds and stability of dimers of chalcogenoaldehyde derivatives: a noticeable role of oxygen compared to other chalcogens

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SUPPORTING INFORMATION

Table S1. Interaction energy corrected both BSSE and ZPE of **2H-Z** dimers in two geometries including the hexagonal and perpendicular structures with Z= O, S, Se and Te

	2H-O	**2H-S**	**2H-Se**	**2H-Te**
$\Delta E^{*a)}$ (kJ.mol^{-1})	-10.3	-7.3	-7.9	-6.2
$\Delta E^{*b)}$ (kJ.mol^{-1})	-9.5	-2.9	-2.8	2.5

[a)] interaction energy of hexagonal structure
[b)] interaction energy of perpendicular structure

Table S2. The electron density [ρ(r)] and Laplacian electron density [$\nabla^2(\rho)$] at BCPs of C_{sp2}-H···H-C_{sp2} dihydrogen bond

	$2CH_3$-Se	**$2CH_3$-Te**	**$2NH_2$-Se**	**$2NH_2$-Te**
ρ(r) (au)	0.006	0.008	0.008	0.009
$\nabla^2(\rho)$ (au)	0.02	0.03	0.03	0.04

Table S3. The H···Z interaction distance ($r_{H\cdots Z}$ (Å)), the ratio between the intermolecular distance and the sum of van der Waals radii of the H and Z atoms ($r_{H\cdots Z}/\sum r_{vdW}$), the typical topological parameters at BCPs of **2R-Z** dimers, and individual enegy of nonconventional hydrogen bond (E_{HB}), with R= H, F, Cl, Br, CH_3, NH_2; and Z = O, S, Se, Te

	2H-O	**2H-S**	**2H-Se**	**2H-Te**
$r_{H\cdots Z}$ (Å)	2.50	2.82	2.96	3.12
$r_{H\cdots Z}/\sum r_{vdW}$	0.92	0.94	0.95	0.96
ρ(r) (au)	0.009	0.009	0.008	0.008
$\nabla^2(\rho)$ (au)	0.03	0.03	0.02	0.02
E_{HB} (kJ.mol^{-1})	-8.1	-6.3	-5.2	-4.8
	2F-O	**2F-S**	**2F-Se**	**2F-Te**
$r_{H\cdots Z}$ (Å)	2.48	2.86	2.98	3.15
$r_{H\cdots Z}/\sum r_{vdW}$	0.91	0.95	0.96	0.97
ρ(r) (au)	0.010	0.009	0.008	0.008

$\nabla^2(\rho)$ (au)	0.04	0.02	0.02	0.02
E_{HB} (kJ.mol^{-1})	-8.4	-5.6	-4.8	-4.7
	2Cl-O	**2Cl-S**	**2Cl-Se**	**2Cl-Te**
$r_{H\cdots Z}$ (Å)	2.47	2.76	2.86	3.02
$r_{H\cdots Z}/\sum r_{vdW}$	0.91	0.92	0.92	0.93
$\rho(r)$ (au)	0.010	0.010	0.010	0.010
$\nabla^2(\rho)$ (au)	0.04	0.03	0.03	0.02
E_{HB} (kJ.mol^{-1})	-8.6	-7.2	-6.4	-6.5
	2Br-O	**2Br-S**	**2Br-Se**	**2Br-Te**
$r_{H\cdots Z}$ (Å)	2.48	2.75	2.85	2.99
$r_{H\cdots Z}/\sum r_{vdW}$	0.91	0.92	0.92	0.92
$\rho(r)$ (au)	0.010	0.011	0.010	0.011
$\nabla^2(\rho)$ (au)	0.03	0.03	0.03	0.02
E_{HB} (kJ.mol^{-1})	-8.5	-7.4	-6.7	-6.7
	2CH$_3$-O	**2CH$_3$-S**	**2CH$_3$-Se**	**2CH$_3$-Te**
$r_{H\cdots Z}$ (Å)	2.46	2.78	2.91	3.06
$r_{H\cdots Z}/\sum r_{vdW}$	0.90	0.93	0.94	0.94
$\rho(r)$ (au)	0.010	0.010	0.009	0.009
$\nabla^2(\rho)$ (au)	0.03	0.03	0.02	0.02
E_{HB} (kJ.mol^{-1})	-8.7	-7.0	-5.9	-5.6
	2NH$_2$-O	**2NH$_2$-S**	**2NH$_2$-Se**	**2NH$_2$-Te**
$r_{H\cdots Z}$ (Å)	2.36	2.67	2.76	2.91
$r_{H\cdots Z}/\sum r_{vdW}$	0.87	0.89	0.89	0.89
$\rho(r)$ (au)	0.012	0.012	0.012	0.012
$\nabla^2(\rho)$ (au)	0.04	0.03	0.03	0.03
E_{HB} (kJ.mol^{-1})	-11.0	-9.3	-8.3	-8.0

Table S4. The minimum electrostatic potential ($V_{S,min}$) (kJ.mol^{-1}) in RCHZ monomer with R= H, F, Cl, Br, CH_3, NH_2 and Z= O, S, Se, Te

	HCHO	**HCHS**	**HCHSe**	**HCHTe**	**FCHO**	**FCHS**	**FCHSe**	**FCHTe**
$V_{S,min}$	-147.0	-88.7	-85.0	-80.4	-118.4	-74.3	-74.1	-71.4
	ClCHO	**ClCHS**	**ClCHSe**	**ClCHTe**	**BrCHO**	**BrCHS**	**BrCHSe**	**BrCHTe**
$V_{S,min}$	-114.5	-74.5	-74.7	-72.8	-108.3	-72.1	-71.1	-70.9
	CH$_3$CHO	**CH$_3$CHS**	**CH$_3$CHSe**	**CH$_3$CHTe**	**NH$_2$CHO**	**NH$_2$CHS**	**NH$_2$CHSe**	**NH$_2$CHTe**
$V_{S,min}$	-164.8	-104.5	-101.1	-95.6	-193.1	-131.0	-128.1	-120.9

Table S5. The charge of Z and H (C_{sp2}-H) atoms in **2R-Z** dimers with R= H, F, Cl, Br, CH_3, NH_2 and Z= O, S, Se, Te

	2H-O	**2H-S**	**2H-Se**	**2H-Te**
q(Z)	-0.62	-0.00	0.06	0.20
q(H)	0.12	0.18	0.19	0.18
	2F-O	**2F-S**	**2F-Se**	**2F-Te**
q(Z)	-0.65	-0.05	-0.00	0.11
q(H)	0.13	0.17	0.17	0.16
	2Cl-O	**2Cl-S**	**2Cl-Se**	**2Cl-Te**
q(Z)	-0.61	0.03	0.10	0.22
q(H)	0.16	0.20	0.20	0.19
	2Br-O	**2Br-S**	**2Br-Se**	**2Br-Te**

q(Z)	-0.61	0.06	0.13	0.26
q(H)	0.16	0.20	0.20	0.19
	$2CH_3$-O	**$2CH_3$-S**	**$2CH_3$-Se**	**$2CH_3$-Te**
q(Z)	-0.65	-0.06	-0.00	0.12
q(H)	0.12	0.18	0.18	0.17
	$2NH_2$-O	**$2NH_2$-S**	**$2NH_2$-Se**	**$2NH_2$-Te**
q(Z)	-0.75	-0.27	-0.24	-0.17
q(H)	0.13	0.19	0.19	0.18

Table S6. The percentage contribution (%) of energy components to total interaction energy of **2R-Z** dimers using SAPT2+ approach at def2-TZVPD, with R= H, F, Cl, Br, CH_3, NH_2 and Z= O, S, Se, Te

	2H-O	**2H-S**	**2H-Se**	**2H-Te**
%eles	53.2	40.6	35.5	45.6
%disp	26.4	31.8	32.4	0.2
%ind	16.3	20.6	22.4	54.2
$\%\delta E_{int,r}^{HF}$	4.1	7.0	9.7	0.0
	2F-O	**2F-S**	**2F-Se**	**2F-Te**
%eles	54.5	40.0	33.7	44.1
%disp	24.0	29.3	29.2	0.2
%ind	17.9	23.6	26.1	51.9
$\%\delta E_{int,r}^{HF}$	3.6	7.0	11.1	3.8
	2Cl-O	**2Cl-S**	**2Cl-Se**	**2Cl-Te**
%eles	50.6	37.9	32.0	45.7
%disp	27.0	30.5	30.3	0.3
%ind	18.2	23.9	26.6	53.9
$\%\delta E_{int,r}^{HF}$	4.2	7.7	11.0	0.1
	2Br-O	**2Br-S**	**2Br-Se**	**2Br-Te**
%eles	52.5	39.8	34.9	46.0
%disp	28.3	31.2	31.0	0.6
%ind	18.2	23.9	26.6	53.2
$\%\delta E_{int,r}^{HF}$	0.9	5.1	7.5	0.1
	2CH_3-O	**2CH_3-S**	**2CH_3-Se**	**2CH_3-Te**
%eles	50.2	39.4	34.4	46.7
%disp	28.0	32.2	32.7	1.0
%ind	17.4	21.4	23.9	51.7
$\%\delta E_{int,r}^{HF}$	4.4	7.0	8.9	0.6
	2NH_2-O	**2NH_2-S**	**2NH_2-Se**	**2NH_2-Te**
%eles	52.6	43.1	40.7	46.2
%disp	24.1	25.8	25.1	0.6
%ind	18.5	23.5	26.6	52.9
$\%\delta E_{int,r}^{HF}$	4.8	7.6	7.6	0.2

Table S7. The percentage contribution (%) of energy components to the total interaction energy of **2R-Te** dimers with R= H, F, Cl, Br, CH_3 and NH_2

	2H-Te	**2F-Te**	**2Br-Te**	**2Cl-Te**	**2CH_3-Te**	**2NH_2-Te**
%eles [a]	45.7	43.6	38.4	45.8	46.9	46.0
%disp [a]	0.2	0.3	1.7	0.5	1.5	0.8
%ind [a]	54.1	51.2	46.6	53.7	51.5	53.0
$\%\delta E_{int,r}^{HF}$ [a]	-	4.9	13.3	0.1	0.1	0.1
	2H-Te	**2F-Te**	**2Br-Te**	**2Cl-Te**	**2CH_3-Te**	**2NH_2-Te**
%eles [b]	45.6	24.3	46.6	48.2	47.7	46.9
%disp [b]	0.2	4.1	0.7	0.5	0.8	0.6
%ind [b]	54.2	32.7	52.5	51.4	51.5	52.4
$\%\delta E_{int,r}^{HF}$ [b]	0.0	39.0	0.0	0.3	-	0.2
	2H-Te	**2F-Te**	**2Br-Te**	**2Cl-Te**	**2CH_3-Te**	**2NH_2-Te**
%eles [c]	38.6	35.8	29.0	33.0	28.5	12.0
%disp [c]	15.1	10.8	14.5	13.4	17.1	20.4
%ind [c]	44.2	51.2	54.4	51.4	52.6	53.2
$\%\delta E_{int,r}^{HF}$ [c]	2.1	2.2	2.2	2.2	1.8	14.4

[a] using SAPT2+ appoach with def2-TZVPPD

[b] using SAPT2+ approach with def2-TZVPPD for Te atom and aug-cc-pVTZ for remaining atoms

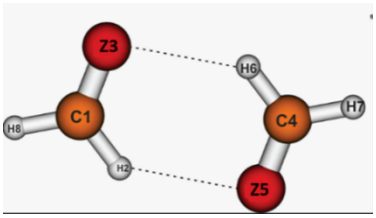
[c] using SAPT2 approach with basis set def2-QZVPPD

Table S8. The sign(λ_2)ρ(r) and reduced density gradient (RDG) values of C_{sp2}-H···Z interaction spikes in **2R-Z** dimers with R= H, F, Cl, Br, CH_3, NH_2 and Z= O, S, Se, Te

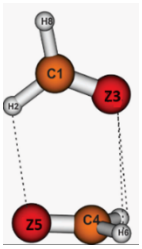
	2H-O	**2F-O**	**2Cl-O**	**2Br-O**	**2CH_3-O**	**2NH_2-O**
sign(λ_2)ρ(r) (au)	-0.0095	-0.01	-0.0105	-0.0102	-0.01	-0.0119
RDG (au)	0.105	0.124	0.136	0.109	0.148	0.106
	2H-S	**2F-S**	**2Cl-S**	**2Br-S**	**2CH_3-S**	**2NH_2-S**
sign(λ_2)ρ(r) (au)	-0.0089	-0.0085	-0.0101	-0.0101	-0.0096	-0.0112
RDG (au)	0.13	0.129	0.139	0.179	0.102	0.112
	2H-Se	**2F-Se**	**2Cl-Se**	**2Br-Se**	**2CH_3-Se**	**2NH_2-Se**
sign(λ_2)ρ(r) (au)	-0.0081	-0.0081	-0.001	-0.0101	-0.0082	-0.011
RDG (au)	0.119	0.152	0.086	0.116	0.105	0.122
	2H-Te	**2F-Te**	**2Cl-Te**	**2Br-Te**	**2CH_3-Te**	**2NH_2-Te**
sign(λ_2)ρ(r) (au)	-0.0075	-0.0076	-0.0095	-0.0099	-0.0084	-0.0113
RDG (au)	0.119	0.093	0.108	0.125	0.107	0.108

Table S9. Changes in C_{sp2}-H bond lengths ($\Delta r(C_{sp2}\text{-H})$, mÅ) and their corresponding stretching frequencies ($\Delta\nu(C_{sp2}\text{-H})$, cm^{-1}) in the **2R-Z** dimers with R= H, F, Cl, Br, CH_3, NH_2 and Z= O, S, Se, Te

	2H-O	**2H-S**	**2H-Se**	**2H-Te**
$\Delta\nu(C_{sp2}\text{-H})$	47.0	-6.0	-16.4	-22.5
$\Delta r(C_{sp2}\text{-H})$	-3.0	0.7	1.4	1.7
	2F-O	**2F-S**	**2F-Se**	**2F-Te**
$\Delta\nu(C_{sp2}\text{-H})$	25.5	-0.3	-8.4	-12.2
$\Delta r(C_{sp2}\text{-H})$	-1.5	0.3	0.8	0.8
	2Cl-O	**2Cl-S**	**2Cl-Se**	**2Cl-Te**
$\Delta\nu(C_{sp2}\text{-H})$	23.3	-13.8	-24.9	-33.4
$\Delta r(C_{sp2}\text{-H})$	-1.1	1.4	1.9	2.1
	2Br-O	**2Br-S**	**2Br-Se**	**2Br-Te**
$\Delta\nu(C_{sp2}\text{-H})$	21.3	-17.8	-29.5	-38.6
$\Delta r(C_{sp2}\text{-H})$	-0.9	1.7	2.2	2.4
	2CH_3-O	**2CH_3-S**	**2CH_3-Se**	**2CH_3-Te**
$\Delta\nu(C_{sp2}\text{-H})$	52.6	-2.3	-11.3	-10.6
$\Delta r(C_{sp2}\text{-H})$	-3.5	0.4	0.9	0.6
	2NH_2-O	**2NH_2-S**	**2NH_2-Se**	**2NH_2-Te**
$\Delta\nu(C_{sp2}\text{-H})$	43.1	-17.7	-31.5	-34.6
$\Delta r(C_{sp2}\text{-H})$	-2.5	1.3	2.0	1.9



2H-Z (I)



2H-Z (II)

Figure S1. Stable structures and interaction energies (given in parentheses, in kJ.mol^{-1}) of **2H-Z** dimer with Z= O, S, Se, Te

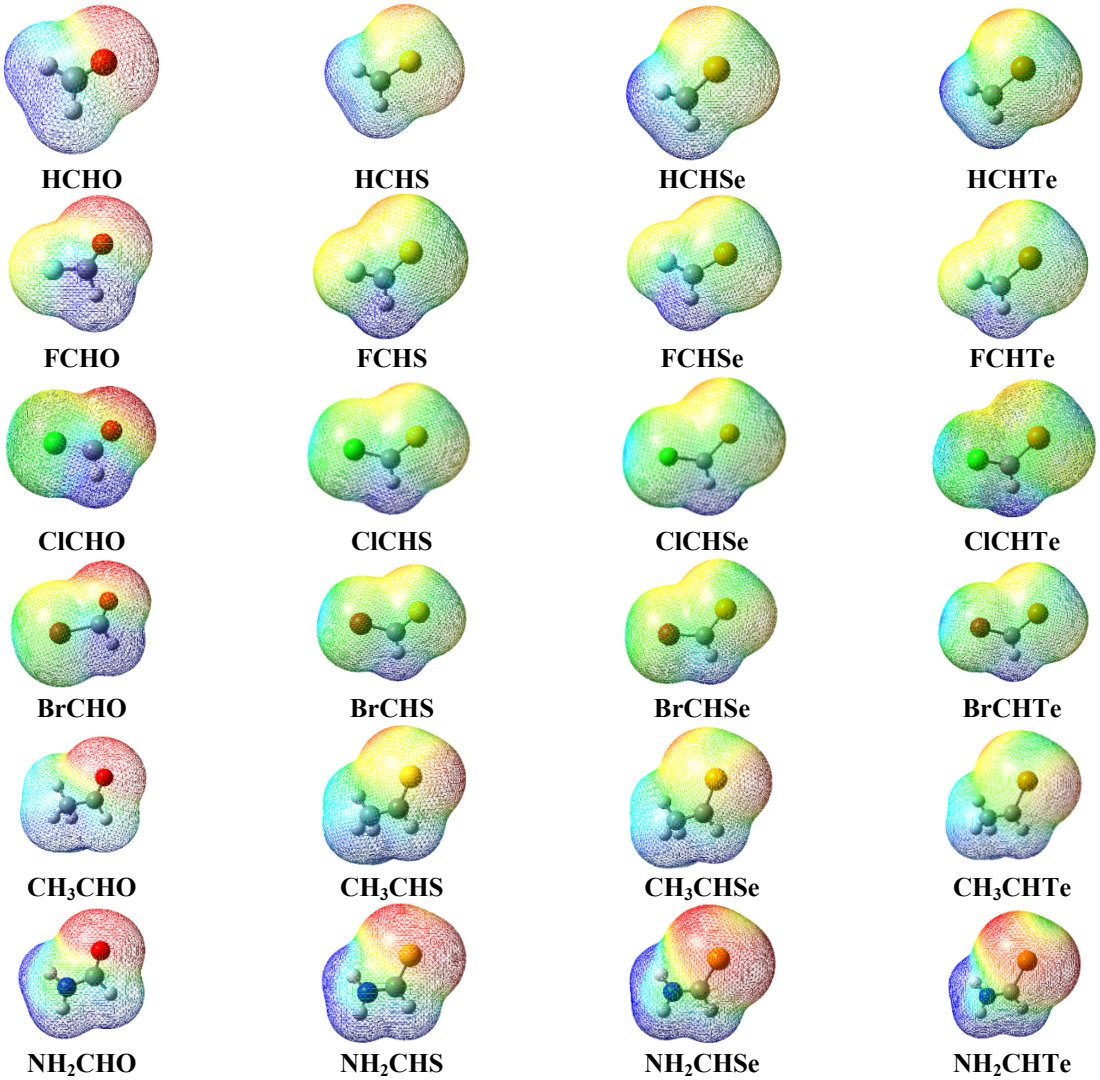
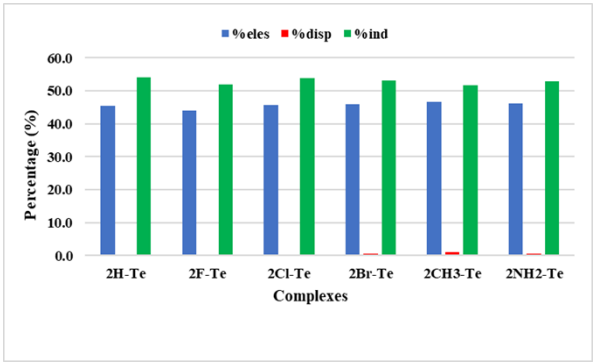
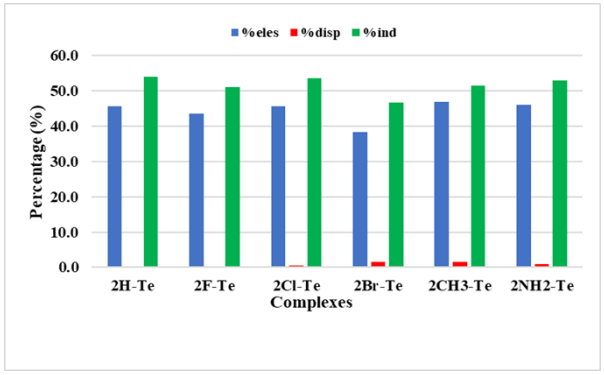


Figure S2. Molecular Electrostatic Potential (MEP) surface of monomers



(i)



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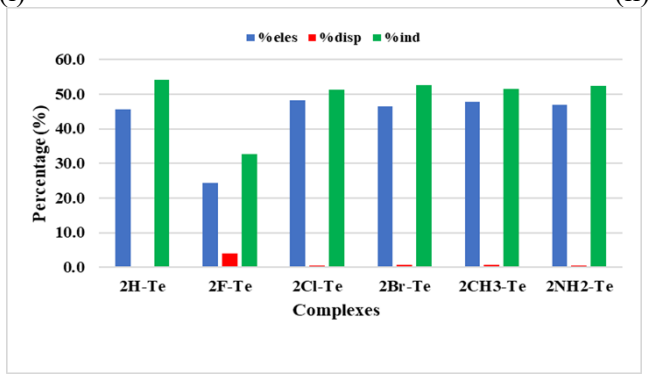

(iii)

Figure S3a. The percentage contribution (%) of energy components to the stability of **2R-Te** dimers using SAPT2+ approach at different level of theories: i) using def2-TZVPD; ii) using def2-TZVPPD; iii) using def2-TZVPPD for Te atom and aug-cc-pVTZ for remaining ones

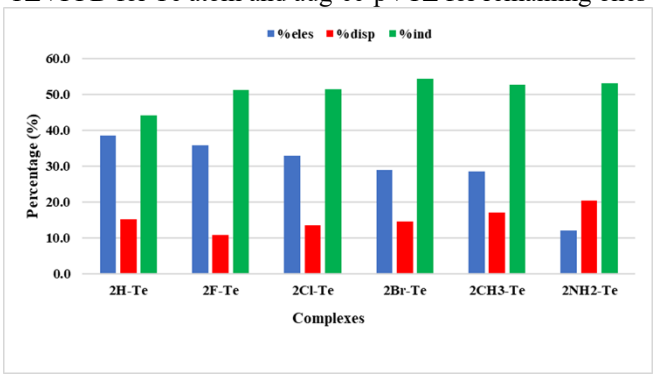

Figure S3b. The percentage contribution (%) of energy components to the stability of **2R-Te** dimers using SAPT2 approach with def2-QZVPPD

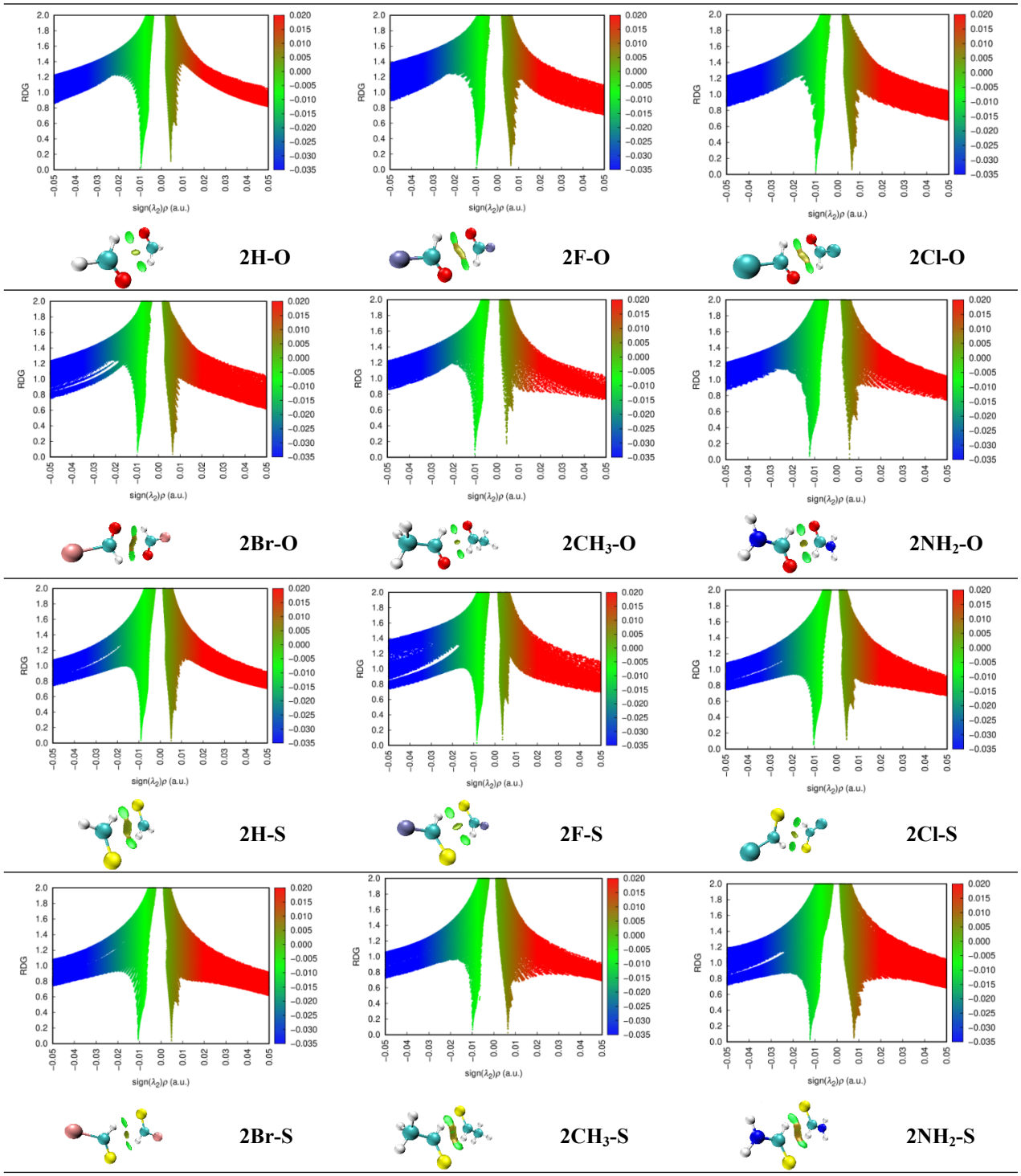

Figure S4a. Plots of the reduced density gradient (s, au) versus the electron density multiplied by the sign of the second Hessian eigenvalue (sign(λ_2)ρ, au) for the **2R-Z** dimers (R= H, F, Cl, Br, CH_3, NH_2; Z= O, S)

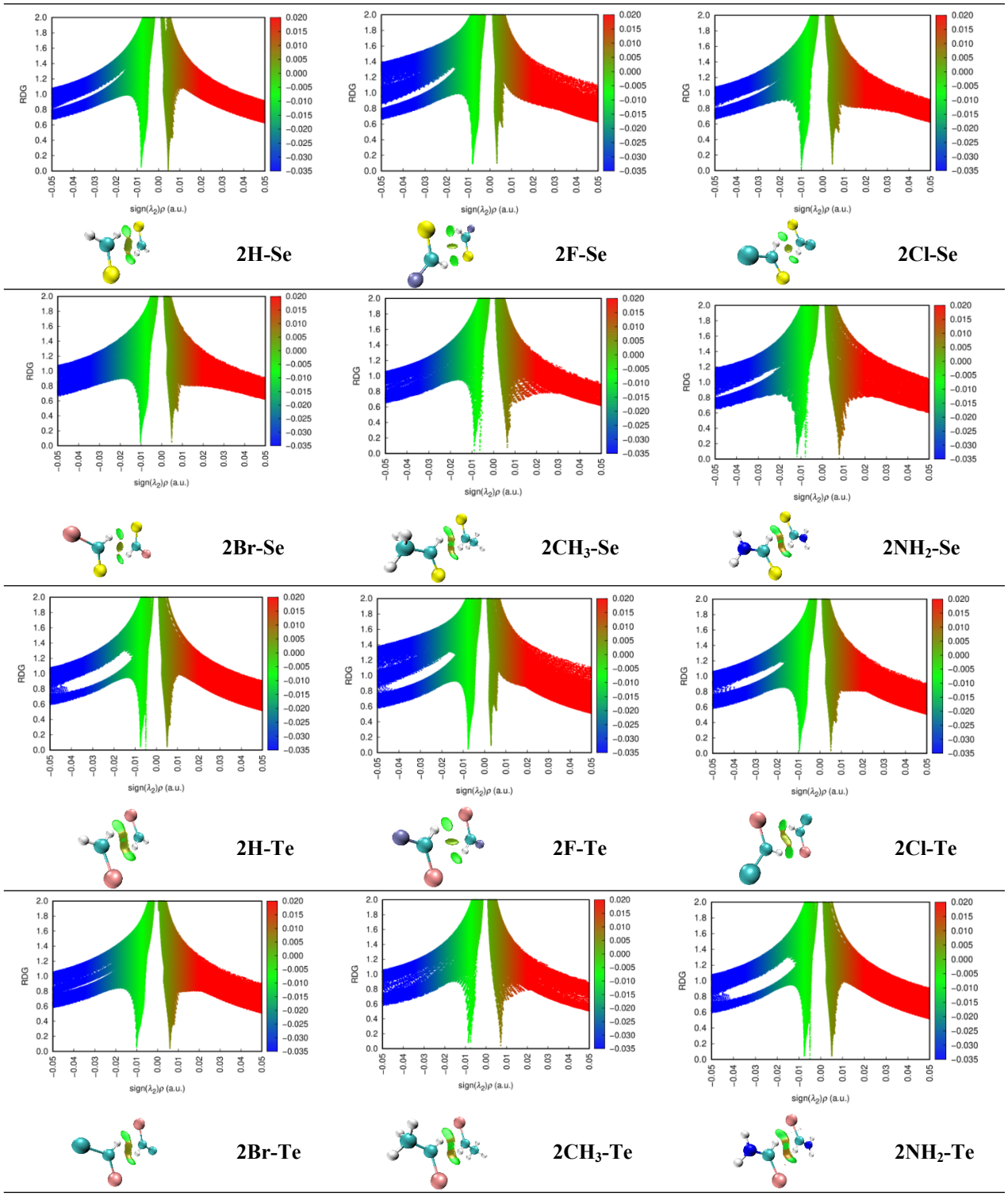

Figure S4b. Plots of the reduced density gradient (s, au) versus the electron density multiplied by the sign of the second Hessian eigenvalue (sign(λ_2)ρ, au) for the **2R-Z** dimers (R= H, F, Cl, Br, CH_3, NH_2; Z= Se, Te)

Table S10. XYZ coordinate of **2R-Z** dimers and **RCHZ** monomers with R= H, F, Cl, Br, CH_3, NH_2; Z= O, S, Se, Te optimized at MP2/aug-cc-pVTZ-PP for Te atom and MP2/6-311++G(3df,2pd) for remaining atoms

Dimer	Coordinate			
2H-O (hexagonal)	C	1.64728800	0.73447600	0.00000000
	O	1.64728800	-0.47790500	0.00000000
	H	0.70964100	1.30454500	0.00000000
	H	2.58978500	1.30271100	0.00000000
	C	-1.64728800	-0.73447600	0.00000000
	O	-1.64728800	0.47790500	0.00000000
	H	-0.70964100	-1.30454500	0.00000000
	H	-2.58978500	-1.30271100	0.00000000
2H-O (perpendicular)	C	-1.10336100	-1.00408500	0.00000000
	O	-0.08754400	-1.66491600	0.00000000
	H	-1.59277700	-0.69499300	0.93348200
	H	-1.59277700	-0.69499300	-0.93348200
	C	1.17517300	1.16529400	0.00000000
	O	0.00000000	1.46108100	0.00000000
	H	1.95607200	1.93850800	0.00000000
	H	1.49895600	0.11490400	0.00000000
2H-S (hexagonal)	C	-1.53942900	-1.04383400	-0.00000700
	H	-0.45690400	-1.14728900	-0.00000400
	S	-2.26208800	0.39576600	0.00000200
	C	1.53945100	1.04384600	-0.00000100
	S	2.26207500	-0.39577200	0.00000300
	H	0.45692900	1.14732500	0.00006600
	H	2.11642500	1.96484000	-0.00007300
	H	-2.11638000	-1.96484300	-0.00001600
2H-S (perpendicular)	C	0.90550900	-1.33161300	0.00000000
	H	0.53071200	-1.76640100	0.92158900
	H	0.53071200	-1.76640100	-0.92158900
	C	-1.09068500	1.46259800	0.00000000
	H	-1.60179200	2.42093200	0.00000000
	H	0.00000000	1.48687300	0.00000000
	S	-1.89660400	0.07382000	0.00000000
	S	1.99981800	-0.14637700	0.00000000
2H-Se (hexagonal)	C	-0.82888000	1.71827000	0.00000000
	H	-1.07139300	0.66002500	0.00000000
	Se	0.82888000	2.28528200	0.00000000
	C	0.82888000	-1.71827100	0.00000000
	Se	-0.82888000	-2.28528200	0.00000000
	H	1.07139300	-0.66002500	0.00000000
	H	1.65750600	-2.41833200	0.00000000
	H	-1.65750600	2.41833200	0.00000000
2H-Se (perpendicular)	C	0.85731800	-1.37536800	0.00000000
	H	0.47644300	-1.79539100	0.92361400
	H	0.47644300	-1.79539100	-0.92361400
	C	-1.08886500	1.55238100	0.00000000
	H	-1.55949800	2.52910900	0.00000000
	H	0.00000000	1.51861700	0.00000000
	Se	-2.03335700	0.08402100	0.00000000
	Se	2.09206000	-0.12869800	0.00000000
2H-Te (hexagonal)	C	1.92479800	0.17619000	0.00000000
	H	1.00235500	0.74713900	0.00000000
	Te	1.92479800	-1.76992600	0.00000000
	C	-1.92479800	-0.17619000	0.00000000
	Te	-1.92479800	1.76992600	0.00000000
	H	-1.00235500	-0.74713900	0.00000000

	H	-2.85536500	-0.73161200	0.00000000
	H	2.85536500	0.73161200	0.00000000
2H-Te (perpendicular)	C	0.81431000	-1.37859400	0.00000000
	H	0.47513500	-1.83134400	0.92328900
	H	0.47513500	-1.83134400	-0.92328900
	C	-1.09282500	1.57380300	0.00000000
	H	-1.57477300	2.54392900	0.00000000
	H	0.00000000	1.54745800	0.00000000
	Te	-2.11010500	-0.07205600	0.00000000
	Te	2.15425100	0.04128700	0.00000000
2F-O	C	-1.06861000	-1.37636700	0.00000000
	H	0.00000000	-1.58697300	0.00000000
	O	-1.59097100	-0.31243500	0.00000000
	C	1.06859900	1.37642600	0.00000000
	O	1.59080400	0.31241500	0.00000000
	H	0.00001300	1.58716500	0.00000000
	F	1.76878800	2.51730600	0.00000000
	F	-1.76863400	-2.51735000	0.00000000
2F-S	C	0.63618100	1.81632100	0.00000000
	H	-0.38212500	1.43745500	0.00000000
	S	1.96897200	0.93896400	0.00000000
	C	-0.63618100	-1.81632100	0.00000000
	S	-1.96897200	-0.93896400	0.00000000
	H	0.38212500	-1.43745500	0.00000000
	F	-0.63618100	-3.14786700	0.00000000
	F	0.63618100	3.14786700	0.00000000
2F-Se	C	1.75100400	0.92889400	0.00000000
	H	0.73696200	1.31939100	0.00000000
	Se	2.18673600	-0.75666600	0.00000000
	C	-1.75102500	-0.92890400	0.00000000
	Se	-2.18671600	0.75666400	0.00000000
	H	-0.73700000	-1.31944400	0.00000000
	F	-2.64163700	-1.91488300	0.00000000
	F	2.64158100	1.91490200	0.00000000
2F-Te	C	1.06832500	1.73658900	0.00000000
	H	0.00000000	1.53497100	0.00000000
	Te	2.45701200	0.38130900	0.00000000
	C	-1.06859400	-1.73693000	0.00000000
	Te	-2.45685100	-0.38121000	0.00000000
	H	-0.00018900	-1.53573500	0.00000000
	F	-1.31419900	-3.04530400	0.00000000
	F	1.31347200	3.04504300	0.00000000

2Cl-O	C	-1.07428000	-1.38652700	0.00000000
	H	0.00000000	-1.58251500	0.00000000
	O	-1.58262600	-0.30939800	0.00000000
	C	1.07413600	1.38669400	0.00000000
	O	1.58217500	0.30941700	0.00000000
	H	-0.00009700	1.58296400	0.00000000
	Cl	1.99412600	2.87920800	0.00000000
	Cl	-1.99385800	-2.87930200	0.00000000
2Cl-S	C	-1.85885100	0.02354200	0.00000500
	H	-1.09872700	-0.75359100	0.00001300
	S	-1.53146600	1.59373400	0.00000100
	C	1.85887600	-0.02350100	0.00000600
	S	1.53136700	-1.59366700	0.00000100
	H	1.09881300	0.75369100	0.00001500
	Cl	3.43904700	0.65822200	-0.00000400
	Cl	-3.43896800	-0.65830600	-0.00000300
2Cl-Se	C	0.82040300	1.70433200	0.00000000
	H	-0.18948500	1.30311600	0.00000000
	Se	2.24548400	0.68815800	0.00000000
	C	-0.82040300	-1.70433200	0.00000000
	Se	-2.24548400	-0.68815800	0.00000000
	H	0.18948500	-1.30311600	0.00000000
	Cl	-0.82040300	-3.41661200	0.00000000
	Cl	0.82040300	3.41661200	0.00000000
2Cl-Te	C	-1.03663200	-1.59744600	0.00000000
	H	0.00000000	-1.27070000	0.00000000
	Te	-2.52140300	-0.33438400	0.00000000
	C	1.03667300	1.59754800	0.00000000
	Te	2.52131800	0.33433800	0.00000000
	H	-0.00000600	1.27094900	0.00000000
	Cl	1.16305800	3.30250700	0.00000000
	Cl	-1.16281100	-3.30241800	0.00000000
2Br-O	C	1.15645300	-1.32586900	0.00000000
	H	1.57485100	-0.31621000	0.00000000
	O	-0.00050400	-1.60052500	0.00000000
	C	-1.15712200	1.32529800	0.00000000
	O	0.00000000	1.59927100	0.00000000
	H	-1.57614100	0.31589200	0.00000000
	Br	-2.55739400	2.65249200	0.00000000
	Br	2.55766100	-2.65209900	0.00000000
2Br-S	C	-1.82634100	0.24979400	-0.00004100
	H	-1.16256900	-0.61119600	-0.00005900
	S	-1.32677500	1.77183200	-0.00009200
	C	1.82632800	-0.24996200	-0.00011900
	S	1.32702200	-1.77208300	-0.00008900
	H	1.16241200	0.61091700	-0.00024200
	Br	3.63063900	0.31207600	0.00006300
	Br	-3.63074500	-0.31192400	0.00005500
2Br-Se	C	-1.87176100	0.05577300	-0.00002700
	H	-1.08671000	-0.69587900	-0.00006500
	Se	-1.54788400	1.77466800	-0.00001800
	C	1.87177500	-0.05575200	-0.00007900
	Se	1.54783900	-1.77463600	-0.00001600
	H	1.08675200	0.69592800	-0.00018300
	Br	3.57019100	0.74636600	0.00003200
	Br	-3.57015000	-0.74640200	0.00002700
2Br-Te	C	1.03683300	1.56007700	0.00000000

	H	-0.00000200	1.23321800	0.00000000
	Te	2.52782500	0.30507300	0.00000000
	C	-1.03683300	-1.56007400	0.00000000
	Te	-2.52782900	-0.30507500	0.00000000
	H	0.00000000	-1.23320800	0.00000000
	Br	-1.14859300	-3.42397600	0.00000000
	Br	1.14859800	3.42397900	0.00000000
$2CH_3$-O	C	-1.78360500	-0.00570900	0.00005000
	H	-1.06209700	0.82779600	0.00015300
	O	-1.38040600	-1.15278600	0.00006000
	C	1.78361100	0.00569800	0.00007000
	O	1.38037900	1.15276400	0.00006100
	H	1.06212500	-0.82782600	0.00020900
	C	-3.23381900	0.36802500	-0.00009700
	H	-3.86175100	-0.51744400	-0.00019900
	H	-3.44634600	0.98219100	0.87549500
	H	-3.44615200	0.98225400	-0.87569200
	C	3.23383500	-0.36799700	-0.00010500
	H	3.44639800	-0.98215000	0.87548700
	H	3.44616500	-0.98222800	-0.87570000
	H	3.86174300	0.51748900	-0.00022900
$2CH_3$-S	C	-1.81765900	0.30452600	0.00021500
	H	-0.84373500	0.79741300	0.00062300
	S	-1.89056300	-1.31008400	-0.00001100
	C	1.81766700	-0.30453100	-0.00025200
	S	1.89054700	1.31008000	0.00000400
	H	0.84374900	-0.79742900	-0.00074300
	C	-2.99165100	1.22273400	-0.00006500
	H	-3.92947700	0.67493800	-0.00045400
	H	-2.94396600	1.87415700	0.87485800
	H	-2.94337000	1.87438000	-0.87478800
	C	2.99167000	-1.22272300	0.00010900
	H	2.94332700	-1.87438400	0.87481900
	H	2.94406500	-1.87413400	-0.87482700
	H	3.92948900	-0.67491600	0.00058300

$2CH_3$-Se	C	-0.93691000	1.62583100	0.00000000
	H	0.04587200	1.15517500	0.00000000
	Se	-2.36471200	0.60104000	0.00000000
	C	0.93691000	-1.62583100	0.00000000
	Se	2.36471200	-0.60104000	0.00000000
	H	-0.04587200	-1.15517500	0.00000000
	C	-0.93691000	3.11437500	0.00000000
	H	-1.94411200	3.52161000	0.00000000
	H	-0.39383600	3.47995900	0.87463800
	H	-0.39383600	3.47995900	-0.87463800
	C	0.93691000	-3.11437500	0.00000000
	H	0.39383600	-3.47995900	0.87463800
	H	0.39383600	-3.47995900	-0.87463800
	H	1.94411200	-3.52161000	0.00000000
$2CH_3$-Te	C	-1.01729700	1.58651900	0.00000000
	H	-0.03422000	1.11843000	0.00000000
	Te	-2.58784000	0.43106000	0.00000000
	C	1.01729700	-1.58651900	0.00000000
	Te	2.58784000	-0.43106000	0.00000000
	H	0.03422000	-1.11843000	0.00000000
	C	-1.01729700	3.07531600	0.00000000
	H	-0.47490000	3.44436500	0.87456600
	H	-0.47490000	3.44436500	-0.87456600
	H	-2.02204200	3.48974200	0.00000000
	C	1.01729700	-3.07531600	0.00000000
	H	0.47490000	-3.44436500	0.87456600
	H	0.47490000	-3.44436500	-0.87456600
	H	2.02204200	-3.48974200	0.00000000
$2NH_2$-O	C	-1.69706300	-0.00489000	0.00001300
	H	-0.96887500	0.81679200	0.00004900
	O	-1.36058100	-1.17800900	0.00000100
	C	1.69706100	0.00489400	-0.00000500
	O	1.36059100	1.17801700	0.00000100
	H	0.96886400	-0.81678100	-0.00002600
	N	2.98628400	-0.41218200	-0.00002700
	N	-2.98629000	0.41217200	0.00001700
	H	3.72758700	0.26763900	0.00007400
	H	3.20991400	-1.39016100	0.00008400
	H	-3.72758700	-0.26765700	-0.00009500
	H	-3.20993100	1.39014900	-0.00008200
$2NH_2$-S	C	-1.71510000	0.38028200	-0.00012200
	H	-0.72935700	0.84712400	-0.00034100
	S	-1.90766300	-1.24448500	0.00000300
	C	1.71509900	-0.38028200	0.00019100
	S	1.90766400	1.24448600	0.00001100
	H	0.72935700	-0.84712300	0.00057800
	N	2.70902100	-1.27771700	-0.00008900
	N	-2.70902200	1.27771600	0.00000700
	H	3.66674000	-0.96393000	-0.00046900
	H	2.51312800	-2.26402000	0.00002000
	H	-3.66674100	0.96392800	0.00021800
	H	-2.51313000	2.26401900	-0.00006300
$2NH_2$-Se	C	-1.50760300	0.93023500	-0.00107900
	H	-0.42177100	1.01896500	-0.00420600
	Se	-2.31836900	-0.65665800	-0.00042300
	C	1.50761200	-0.93024300	0.00002000
	Se	2.31835900	0.65666000	-0.00041700

	H	0.42177700	-1.01898900	-0.00117600
	N	2.12246800	-2.11502500	0.00184100
	N	-2.12243600	2.11502500	0.00217800
	H	3.12980600	-2.16026700	0.00310000
	H	1.59271800	-2.97096900	0.00199700
	H	-3.12977000	2.16028200	0.00537200
	H	-1.59267300	2.97096000	0.00172300
$2NH_2$-Te	C	1.31779300	-1.17773900	-0.00088100
	H	0.23840900	-1.03286300	-0.00311600
	Te	2.56673600	0.36157600	-0.00040500
	C	-1.31770400	1.17763700	0.00269100
	Te	-2.56680400	-0.36155000	-0.00041600
	H	-0.23835500	1.03254000	0.00551800
	N	-1.65103500	2.46692700	0.00106900
	N	1.65134300	-2.46698000	0.00208300
	H	-2.62110300	2.74357900	-0.00190100
	H	-0.94105400	3.18245800	0.00247800
	H	2.62145800	-2.74347100	0.00475400
	H	0.94148300	-3.18263300	0.00204200
Monomer	**Coordinate**			
HCHO	C	0.00000000	0.00000000	-0.53209500
	O	0.00000000	0.00000000	0.67675400
	H	0.00000000	0.93593200	-1.11073200
	H	0.00000000	-0.93593200	-1.11073200
HCHS	C	0.00000000	0.00000000	-1.02440400
	S	0.00000000	0.00000000	0.58403200
	H	0.00000000	0.92238700	-1.59904100
	H	0.00000000	-0.92238700	-1.59904100
HCHSe	C	0.00000000	0.00000000	-1.39048600
	Se	0.00000000	0.00000000	0.36039000
	H	0.00000000	0.92564900	-1.95517500
	H	0.00000000	-0.92564900	-1.95517500
HCHTe	C	1.66859200	0.00000000	0.00003600
	H	2.23150200	-0.92570400	0.00001600
	H	2.23150200	0.92570400	0.00005400
	Te	-0.27835700	0.00000000	-0.00000500
FCHO	C	0.00000000	0.39750100	0.00000000
	O	1.14956500	0.12302900	0.00000000
	H	-0.45235100	1.38994600	0.00000000
	F	-0.97157400	-0.52879800	0.00000000
FCHS	C	0.00000000	0.63370800	0.00000000
	S	-0.71382500	-0.78914500	0.00000000
	H	-0.48892500	1.60366900	0.00000000
	F	1.32334700	0.80226700	0.00000000

FCHSe	C	0.43350600	-0.95722200	0.00000000
	Se	0.00000000	0.72573100	0.00000000
	H	1.44508200	-1.35184700	0.00000000
	F	-0.44956800	-1.95329700	0.00000000
FCHTe	C	-1.28586200	0.50590600	0.00003400
	H	-1.64491400	1.53119900	-0.00001300
	Te	0.57945800	-0.02742500	-0.00001000
	F	-2.30797100	-0.34894600	0.00003500
ClCHO	C	0.00000000	0.78814300	0.00000000
	O	1.13124600	1.14948500	0.00000000
	H	-0.88364200	1.43154700	0.00000000
	Cl	-0.48037200	-0.90331100	0.00000000
ClCHS	C	0.00000000	0.60771800	0.00000000
	S	1.51237300	0.08399200	0.00000000
	H	-0.28177600	1.65624000	0.00000000
	Cl	-1.40683500	-0.39096500	0.00000000
ClCHSe	C	0.00000000	0.81859000	0.00000000
	Se	-0.83457000	-0.71668900	0.00000000
	H	-0.52196200	1.76958300	0.00000000
	Cl	1.69984300	1.04037100	0.00000000
ClCHTe	C	-0.90470400	0.69168300	-0.00002000
	H	-1.08502600	1.76164500	0.00005200
	Te	0.89883700	-0.04901900	0.00000100
	Cl	-2.36625200	-0.19781000	0.00000200
BrCHO	C	0.37600500	-1.19155300	0.00000000
	O	-0.46418100	-2.02818900	0.00000000
	H	1.45741200	-1.35567200	0.00000000
	Br	0.00000000	0.70658600	0.00000000
BrCHS	C	0.00000000	0.94129300	0.00000000
	S	1.54457600	1.34984600	0.00000000
	H	-0.82196900	1.65028900	0.00000000
	Br	-0.68260700	-0.82558800	0.00000000
BrCHSe	C	0.00000000	0.73332300	0.00000000
	Se	1.63320000	0.11368700	0.00000000
	H	-0.23008900	1.79331300	0.00000000
	Br	-1.57996300	-0.28738900	0.00000000
BrCHTe	C	0.35773500	0.77566000	-0.00009300
	H	0.48591100	1.85282500	0.00025900
	Te	-1.40352700	-0.05923000	0.00004100
	Br	2.01003100	-0.09790900	-0.00005200
CH_3CHO	C	0.00000000	0.46100400	0.00000000
	H	-0.48062600	1.45696300	0.00000000
	O	1.20797400	0.37025400	0.00000000
	C	-0.93792900	-0.70702900	0.00000000
	H	-1.58425600	-0.65026400	0.87628800
	H	-1.58425600	-0.65026400	-0.87628800
	H	-0.38707800	-1.64231900	0.00000000
CH_3CHS	C	0.00000000	0.62198800	0.00000000
	H	0.51304800	1.58502200	0.00000000
	S	0.87625400	-0.73301200	0.00000000
	C	-1.48953100	0.69853800	0.00000000
	H	-1.82901500	1.25543900	0.87550900
	H	-1.82901500	1.25543900	-0.87550900
	H	-1.93790300	-0.29085900	0.00000000
CH_3CHSe	C	-0.48839400	-0.91198400	0.00000000
	H	-1.55310500	-1.13967000	0.00000000
	Se	0.00000000	0.77478800	0.00000000

	C	0.42631900	-2.08767100	0.00000000
	H	0.22796900	-2.71016900	0.87549900
	H	0.22796900	-2.71016900	-0.87549900
	H	1.46961600	-1.78483600	0.00000000
CH_3CHTe	C	-1.24017000	0.57212000	-0.00001400
	H	-1.41820300	1.64526600	0.00003100
	Te	0.61389700	-0.03521100	0.00000000
	C	-2.45373900	-0.29249900	0.00000200
	H	-2.20154800	-1.34972300	-0.00000400
	H	-3.06969500	-0.07113900	0.87555300
	H	-3.06971800	-0.07113400	-0.87553100
NH_2CHO	C	0.16001300	0.38881800	-0.00001200
	O	1.19477800	-0.24582400	-0.00002200
	H	0.13446000	1.48897900	-0.00003200
	N	-1.08169200	-0.15900100	0.00002700
	H	-1.17845800	-1.16018200	0.00005100
	H	-1.90246300	0.41788900	0.00004100
NH_2CHS	C	-0.40896800	0.48502100	0.00000300
	S	1.10870000	-0.10586000	0.00000100
	H	-0.60616400	1.55642200	-0.00000200
	N	-1.53734000	-0.24485600	-0.00001400
	H	-1.47520200	-1.25050600	0.00002800
	H	-2.44264200	0.19170700	0.00004400
NH_2CHSe	C	-0.92771500	0.51207500	-0.00000400
	Se	0.75570000	-0.04697200	0.00000000
	H	-1.16778200	1.57271800	0.00000100
	N	-2.01584100	-0.27068700	0.00000600
	H	-1.90587700	-1.27275900	-0.00001800
	H	-2.94295900	0.11944500	-0.00000500
NH_2CHTe	C	-1.29339400	0.52318000	-0.00002600
	H	-1.56357900	1.57566800	0.00005600
	Te	0.60261200	-0.02823300	0.00000100
	N	-2.35639700	-0.28979700	-0.00000700
	H	-2.22076500	-1.28933000	0.00001700
	H	-3.29633500	0.07128400	0.00007000