Supporting information :

Selective Sensing of NH₃ and NO₂ on WSe₂ Monolayer based on

Defect Concentration Regulation

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Figure s1. The WSe₂ monolayer after optimization ¹¹ (a) top view and (b) side view

Figure s2. Five optimized Se vacancy WSe_2 monolayers with (a) 2.000% (b) 3.125% (c) 5.556% (d) 8.333% (e) 12.500% V_{Se} concentration. The adsorption sites are also given, and the brown dotted circles represent the selenium vacancy.

Table s1 Defect formation energy ($E_{\rm f}/{\rm eV}$) of Se vacancy, W vacancy and Se on W antisite on WSe₂ monolayer ¹¹.

Table s2. Initial configuration, adsorption distance (d/Å), adsorption energy (E_{ads}/eV) , charge transfer number $(\Delta q/e)$ and final configurations of NO₂ on perfect and five Se vacancy WSe₂ monolayers with different Se vacancy concentration. N up, NO₂; N down, O₂N; Single O downward, ONO, and parallel, p.

Table s3. Initial configuration, adsorption distance (d/Å), adsorption energy (E_{ads}/eV) , charge transfer number $(\Delta q/e)$ and final configurations of NH₃ on perfect and five Se vacancy WSe₂ monolayers with different Se vacancy concentration. NH₃, treble H downward; HNH₂, double H downward; H₂NH, single H downward; and H₃N, treble H upward.

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Figure s1. The WSe₂ monolayer after optimization ¹¹(a) top view and (b) side view



Figure s2. Five optimized Se vacancy WSe₂ monolayers with (a) 2.000% (b) 3.125% (c) 5.556% (d) 8.333% (e) 12.500% V_{se} concentration. The adsorption sites are also given, and the brown dotted circles represent the selenium vacancy.

WSe ₂ monolayer ¹¹					
Defects	V_{Se}	$V_{\rm W}$	Sew	Ref	
F / M	2.70	4.95	4.72	This work	
<i>E</i> _f /ev	2.70			30	

Table s1 Defect formation energy $(E_{\rm f}/{\rm eV})$ of Se vacancy, W vacancy and Se on W antisite on

The calculated formation energy order is $E_{\rm f}$ (V_W) > $E_{\rm f}$ (Se_W) > $E_{\rm f}$ (V_{Se}) ¹¹. A single selenium vacancy has the lowest formation energy ^{11, 28-31}.

Table s2. Initial configuration, adsorption distance (d/Å), adsorption energy (E_{ads}/eV) , charge transfer number $(\Delta q/e)$ and final configurations of NO₂ on perfect and five Se vacancy WSe₂ monolayers with different Se vacancy concentration. N up, NO₂; N down, O₂N; Single O downward, ONO; and parallel, p.

Vacancy	Initial configuration	d/Å	$E_{\rm ads}/{\rm eV}$	Δq/e	Final
concentration					configuration
011	NO ₂ -hole	2.621	0.35	-0.205	N upward
	NO ₂ -hole p	2.686	0.33	-0.200	
	NO ₂ -W	2.687	0.33	-0.200	
	NO ₂ -W p	2.695	0.33	-0.201	
	NO ₂ -Se	2.798	0.29	-0.192	
	NO ₂ -Se p	2.696	0.33	-0.200	
	ONO-hole	2.721	0.26	-0.193	
	ONO-W	2.640	0.35	-0.205	
	ONO-Se	2.735	0.29	-0.192	
	O ₂ N-hole	2.688	0.24	-0.185	N downward
	O ₂ N-W	2.776	0.22	-0.182	
	O ₂ N-Se	2.998	0.17	-0.175	
2.000%	NO ₂ -hole ₂ p	2.631	0.40	-0.233	N upward
	NO ₂ -W ₂	2.601	0.38	-0.231	
	ONO-W ₂	2.607	0.38	-0.230	
	NO ₂ -W ₂ p	2.603	0.37	-0.231	
	ONO-Se ₁	2.637	0.37	-0.229	
	NO ₂ -W ₁	2.108	0.35	-0.223	
	NO ₂ -Se ₂ p	2.626	0.35	-0.233	
	ONO-hole ₂	2.505	0.34	-0.226	
	NO ₂ -V _{Se}	2.141	0.34	-0.225	
	NO ₂ -hole ₂	2.673	0.33	-0.223	
	ONO-Se ₂	2.785	0.32	-0.221	
	NO ₂ -Se ₂	2.815	0.32	-0.220	
	NO ₂ -Se ₁ p	2.728	0.32	-0.217	
	NO ₂ -V _{Se} p	2.264	0.30	-0.222	
	NO ₂ -Se ₁	2.759	0.30	-0.216	
	O_2N-W_1	1.615	0.41	-0.223	N downward
	O ₂ N-V _{Se}	1.668	0.40	-0.222	
	NO ₂ -W ₁ p	1.599	0.38	-0.222	
	O ₂ N-W ₂	2.703	0.25	-0.213	
	O ₂ N-hole ₂	2.709	0.25	-0.214	
	O ₂ N-Se ₁	2.979	0.19	-0.198	
	O ₂ N-hole ₁	2.979	0.19	-0.198	

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	O ₂ N-Se ₂	2.998	0.19	-0.199	
	ONO-V _{Se}	1.252	0.42	-0.221	Single O
	NO ₂ -hole ₁	1.860	0.37	-0.222	downward
	NO ₂ -hole ₁ p	1.912	0.33	-0.222	
	ONO-W ₁	2.959	0.12	-0.201	
	ONO-hole ₁	2.959	0.12	-0.201	
3.125% 11	NO ₂ -hole ₂	2.587	0.35	-0.209	N upward
	NO ₂ -hole ₁	2.641	0.35	-0.209	7
	NO ₂ -W ₂	2.608	0.35	-0.208	7
	ONO-hole ₂	2.607	0.35	-0.208	7
	NO ₂ -hole ₂ p	2.625	0.34	-0.206	7
	NO ₂ -hole ₁ p	2.645	0.33	-0.206	7
	NO ₂ -W ₂ p	2.652	0.33	-0.204	7
	ONO-W ₂	2.483	0.32	-0.200	7
	NO ₂ -V _{Se}	2.074	0.31	-0.202	7
	NO ₂ -Se	2.763	0.30	-0.198	7
	NO ₂ -V _{Se} p	2.262	0.30	-0.196	7
	ONO-Se	2.718	0.29	-0.198	1
	NO ₂ -Se p	2.715	0.28	-0.195	1
	ONO-hole ₁	2.844	0.22	-0.191	7
	NO ₂ -W ₁ p	2.965	0.20	-0.188	7
	O ₂ N-V _{Se}	1.582	0.40	-0.206	N downward
	ONO-W ₁	1.590	0.38	-0.204	-
	O ₂ N-hole ₂	2.606	0.26	-0.186	1
	O ₂ N-hole ₁	2.649	0.25	-0.186	1
	O ₂ N-W ₂	2.740	0.22	-0.186	7
	O ₂ N-Se	2.926	0.17	-0.178	7
	NO ₂ -W ₁	1.106	0.42	-0.208	Single O
	O_2N-W_1	1.097	0.42	-0.208	downward
	ONO-V _{Se}	1.567	0.40	-0.207	1
5.556%	NO ₂ -hole ₂	2.412	0.39	-0.141	N upward
	NO ₂ -Se	2.604	0.35	-0.197	-
	ONO-W ₂	2.617	0.33	-0.194	1
	NO ₂ -hole ₁	2.095	0.32	-0.187	1
	NO ₂ -W ₂	2.073	0.32	-0.186	1
	ONO-hole ₂	2.490	0.32	-0.191	1
	NO ₂ -hole ₂ p	2.417	0.32	-0.190	1
	NO ₂ -V _{Se}	2.048	0.31	-0.195	1
	NO ₂ -W ₂ p	2.610	0.30	-0.188	1
	ONO-Se	2.719	0.27	-0.184	1
	NO ₂ -Se p	2.757	0.27	-0.184	1
	O ₂ N-hole ₁	1.524	0.40	-0.199	N downward
	O_2N-W_1	1.519	0.40	-0.199	1
			1	1	

	O ₂ N-V _{Se}	2.318	0.27	-0.176	
	O ₂ N-hole ₂	2.712	0.21	-0.171	
	O ₂ N-W ₂	2.669	0.21	-0.167	
	O ₂ N-Se	2.955	0.15	-0.158	
	NO ₂ -W ₁	1.073	0.42	-0.205	Single O
	ONO-hole ₁	1.087	0.42	-0.204	downward
	NO ₂ -W ₁ p	1.110	0.42	-0.203	
	NO ₂ -V _{Se} p	1.071	0.41	-0.207	
	ONO-V _{Se}	1.104	0.41	-0.204	
	NO ₂ -hole ₁ p	1.102	0.41	-0.203	
	ONO-W ₁	2.065	0.32	-0.186	
8.333%	NO ₂ -W ₂ p	2.554	0.35	-0.185	N upward
	NO ₂ -V _{Se}	1.882	0.33	-0.190	
	NO ₂ -W ₂	2.285	0.31	-0.171	
	ONO-W ₂	2.409	0.31	-0.171	
	ONO-Se	2.719	0.28	-0.171	
	NO ₂ -Se	2.743	0.27	-0.170	
	NO ₂ -Se p	2.731	0.27	-0.169	
	NO ₂ -W ₁ p	1.288	0.44	-0.197	N downward
	O ₂ N-V _{Se}	1.297	0.44	-0.196	
	O_2N-W_1	1.312	0.44	-0.196	
	O ₂ N-hole	1.642	0.44	-0.146	
	O ₂ N-W ₂	2.659	0.21	-0.151	
	O ₂ N-Se	2.924	0.15	-0.144	
	NO ₂ -V _{Se} p	-0.686	3.43	-0.644	Single O
	NO ₂ -W ₁	-0.688	3.43	-0.643	downward
	ONO-V _{Se}	-0.685	3.43	-0.642	
	ONO-W ₁	-0.680	3.42	-0.644	
	ONO-hole	-0.679	3.42	-0.644	
	NO ₂ -hole	1.319	0.45	-0.151	
	NO ₂ -hole p	1.677	0.30	-0.170	
12.500%	NO ₂ -V _{Se}	1.979	0.42	-0.142	N upward
	NO ₂ -hole	2.158	0.39	-0.122	
	NO ₂ -Se ₁ p	2.849	0.34	-0.116	
	NO ₂ -W ₂ p	2.265	0.32	-0.162	
	NO ₂ -Se ₁	2.903	0.32	-0.113	
	ONO-Se ₂	2.702	0.29	-0.158	
	NO ₂ -Se ₂	2.700	0.29	-0.157	
	NO_2 -Se ₂ p	2.702	0.28	-0.157	
	ONO-Se ₁	2.677	0.26	-0.157	
	O ₂ N-hole	0.351	1.34	-0.228	N downward
	O ₂ N-V _{Se}	0.327	1.33	-0.229	
	O ₂ N-W ₂	1.819	0.28	-0.090	

	-0.085	0.23	3.118	O_2N -Se ₁
	-0.126	0.14	2.885	O ₂ N-Se ₂
Single	-0.638	3.48	-0.649	ONO-V _{Se}
downware	-0.638	3.48	-0.650	NO ₂ -W ₁ p
	-0.637	3.48	-0.649	NO ₂ -W ₁
	-0.637	3.48	-0.647	NO ₂ -W ₂
	-0.637	3.48	-0.649	ONO-hole
	-0.637	3.48	-0.648	ONO-W ₁
	-0.638	3.47	-0.650	O_2N-W_1
	-0.637	3.47	-0.647	NO ₂ -V _{Se} p
	-0.175	0.31	1.490	NO ₂ -hole p
7	-0.145	0.12	2.628	ONO-W ₂

Table s3. Initial configuration, adsorption distance (d/Å), adsorption energy (E_{ads}/eV) , charge transfer number $(\Delta q/e)$ and final configurations of NH₃ on perfect and five Se vacancy WSe₂ monolayers with different Se vacancy concentration. NH₃, treble H downward; HNH₂, double H downward; H₂NH, single H downward; and H₃N, treble H upward.

Vacancy	Initial	d/Å	E _{ads} /eV	Δq/e	Final
concentration	configuration				configuration
0	NH ₃ -hole	2.714	0.37	0.040	Treble H
	NH ₃ -W	2.745	0.36	0.048	downward
	NH ₃ -Se	3.094	0.29	0.028	
	HNH ₂ -W	2.608	0.33	0.015	Double H
	HNH ₂ -hole	2.640	0.33	0.011	downward
	HNH ₂ -Se	2.902	0.28	0.008	
	H ₂ NH-W	1.235	0.31	0.018	Single H
	H ₂ NH-hole	2.267	0.31	0.016	downward
	H ₂ NH-Se	2.704	0.27	-0.002	
	H ₃ N-hole	2.791	0.36	0.048	Treble H
	H ₃ N-W	2.813	0.35	0.045	upward
	H ₃ N-Se	3.389	0.26	0.018	
2.000%	NH ₃ -W ₂	2.623	0.36	0.047	Treble H
	NH ₃ -hole ₂	2.716	0.36	0.047	downward
	NH ₃ -W ₁	2.434	0.34	0.037	
	NH ₃ -Se ₁	3.028	0.29	0.029	
	NH ₃ -Se ₂	3.097	0.29	0.026	
	HNH ₂ -W ₂	2.606	0.56	0.013	Double H
	HNH ₂ -hole ₂	2.648	0.38	0.013	downward
	HNH ₂ -Se ₂	2.947	0.34	0.008	
	HNH ₂ -V _{Se}	1.246	0.29	0.076	
	HNH ₂ -Se ₁	2.946	0.29	0.007	
	H ₃ N-hole ₁	0.772	0.56	0.094	Single H
	NH ₃ -hole ₁	0.767	0.56	0.093	downward
	H_2NH-W_1	0.782	0.56	0.093	
	NH ₃ -V _{Se}	0.770	0.56	0.092	
	H ₂ NH-V _{Se}	0.769	0.56	0.092	
	H ₂ NH-hole ₂	2.272	0.56	0.017	
	HNH ₂ -W ₁	0.770	0.36	0.092	
	H ₂ NH-W ₂	2.216	0.31	0.018	
	HNH ₂ -hole ₁	0.770	0.30	0.091	
	H ₂ NH-hole ₁	2.322	0.28	0.007	
	H ₂ NH-Se ₁	2.676	0.26	-0.001	

	H ₂ NH-Se ₂	2.703	0.26	-0.001	
	H ₃ N-V _{Se}	1.806	0.38	0.046	Treble H
	H ₃ N-hole ₂	2.726	0.37	0.056	upward
	H ₃ N-W ₂	2.728	0.36	0.049	
	H_3N-W_1	2.665	0.32	0.039	
	H ₃ N-Se ₁	3.330	0.26	0.020	
	H ₃ N-Se ₂	3.388	0.26	0.019	
3.125%	NH ₃ -hole ₂	2.613	0.37	0.054	Treble H
	NH ₃ -hole ₁	2.622	0.36	0.057	downward
	H ₂ NH-hole ₁	2.655	0.36	0.057	
	NH ₃ -W ₂	2.727	0.36	0.041	
	NH ₃ -Se	3.028	0.29	0.029	
	HNH ₂ -hole ₂	2.600	0.33	0.020	Double H
	HNH ₂ -W ₂	2.666	0.33	0.010	downward
	HNH ₂ -W ₁	2.646	0.30	0.003	
	HNH ₂ -Se	2.904	0.27	0.007	
	H ₃ N-V _{Se}	0.736	0.57	0.099	Single H
	NH ₃ - W ₁	0.748	0.57	0.098	downward
	H ₂ NH-V _{Se}	0.753	0.57	0.096	
	H ₂ NH-W ₁	0.755	0.57	0.096	
	HNH ₂ -V _{Se}	1.029	0.57	0.096	
	NH ₃ -V _{Se}	0.762	0.57	0.095	
	H_3N-W_1	2.174	0.34	0.030	
	H ₂ NH-hole ₂	2.212	0.32	0.020	
	H ₂ NH-W ₂	2.215	0.31	0.020	
	H ₂ NH-Se	2.658	0.26	0.004	
	H ₃ N-hole ₁	2.688	0.37	0.057	Treble H
	HNH ₂ -hole ₁	2.700	0.37	0.055	upward
	H ₃ N-hole ₂	2.695	0.36	0.050	
	H ₃ N-W ₂	2.871	0.34	0.042	
	H ₃ N-Se	3.327	0.26	0.020	
5.556%	NH ₃ -hole ₂	2.666	0.36	0.052	Treble H
	NH ₃ -W ₂	2.651	0.36	0.047	downward
	NH ₃ -Se	2.973	0.28	0.033	
	HNH ₂ -V _{Se}	1.263	0.51	0.078	Double H
	HNH ₂ -hole ₂	2.666	0.33	0.014	downward
	HNH ₂ -W ₁	2.565	0.32	0.017	
	HNH ₂ -W ₂	2.614	0.32	0.017	
	HNH ₂ -hole ₁	2.588	0.31	0.015	
	HNH ₂ -Se	2.966	0.28	0.007	
	H ₃ N-V _{Se}	0.749	0.56	0.095	Single H
	NH ₃ -V _{Se}	2.669	0.56	0.092	downward
	NH ₃ -W ₁	0.760	0.56	0.092	

H2NH-Vac0.7670.560.092H3NF-Wi0.7640.560.091H3NF-Mole0.7690.560.090H3NF-Mole2.7160.360.001H3NF-Mole2.2860.290.010H3N-Mole2.2870.340.042H3N-Mole2.8290.340.042H3N-Mole2.8220.300.028H3N-Mole2.8220.300.028H3N-Mole2.8220.300.028H3N-Mole2.7280.250.004H3N-Mole2.7280.250.004H3N-Mole2.7280.330.011H3N-Ma2.7280.330.016H3N-Ma2.7280.330.010H3NH-M22.6260.350.004H3NH-Se3.1120.270.031M1H-Se3.1120.270.009HNH-W30.7640.560.091HNH-Sa0.7640.560.091HNH-Se0.7700.560.089HNH-Ma0.7610.560.089H2NH-W30.7620.560.089H2NH-W30.7620.560.089H3NH-Se0.7710.560.089H3NH-Se2.7940.320.044H3NH-Se3.0200.0341H3NH-Se3.0200.0341H3NH-Se3.0200.0341H3NH-Se3.0200.0341H3NH-Se3.0200.0361 <th></th> <th></th> <th></th> <th></th> <th></th> <th></th>						
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NH-hole;0.7690.560.090HNH-Se2.7160.360.050HNH-W;2.2520.310.014HNN-Nic2.2800.360.054HN-Nic2.8200.340.042HN-Nic2.8210.300.034HN-Nic2.8220.300.028HN-Nic2.8220.300.028HN-Se3.3870.250.017HNH-Se3.3870.250.017HNH-Se3.120.270.036downwatHNH-Se3.120.270.001downwatHNH-Se2.8930.270.009downwatHNH-Se0.7640.560.091downwatHNH-Se0.7640.560.091downwatHNH-Se0.7640.560.088downwatHNH-Vis0.7640.560.089downwatHNH-Vis0.7640.560.089downwatHNH-Vis0.7620.560.089downwatHNH-Vis0.7620.560.089downwatHNH-Vis0.7620.560.089HNH-Vis0.7640.560.089HNH-Vis0.7640.560.089HNH-Vis0.7640.560.089HNH-Vis0.7620.560.089HNH-Vis0.7640.560.089HNH-Vis0.7640.560.089HNH-Vis0.7640.560.089HNH-Vis0.7640.56 <td></td> <td>H_2NH-W_1</td> <td>0.764</td> <td>0.56</td> <td>0.091</td> <td></td>		H_2NH-W_1	0.764	0.56	0.091	
H2NH-Se2.7160.360.050H3NH-W22.2520.310.014H3NH-hole:2.2670.360.054H3N-hole:2.8670.360.054H3N-hole:2.8220.300.028H3N-W22.8220.300.028H3N-Se3.3870.250.017HSN-Se3.3870.250.004HN-hole:2.7280.250.004HSN-Se3.1120.270.031HNF-W22.6260.350.056HSN-Se3.1120.270.031HNF-Se2.8930.270.009HNH-Se2.8930.330.011Double7440.560.091HNH-Se0.7640.560.091HNH-Se0.7640.560.088HNH-V30.7640.560.088HNH-V30.7640.560.088HNH-Se0.7710.560.088HNH-V30.7620.560.088HNH-V30.7620.560.089HNH-W30.7640.560.089HNH-W40.7670.500.089HNH-W52.7310.260.031HNH-W62.7540.300.034HNH-Se3.0300.240.014HNH-Se3.0200.270.005HNH-Se3.0200.270.005HNH-Se3.0200.270.005HNH-Se3.0200.270.005HNH		NH ₃ -hole ₁	0.769	0.56	0.090	
H2NH-W22.2520.310.014H2NH-hole:2.2860.290.010H2N-hole:2.8670.360.054H3N-W22.8200.340.042H3N-N0ic.2.8250.300.034H3N-Wi2.8220.300.034H3N-Nie2.8250.300.034H3N-Nie2.8220.300.028H3N-Se3.3870.250.017H2NH-hole:2.7280.250.004NHz-Se3.1120.270.031NHz-Se3.1120.270.031HNH-Nie2.8890.330.011HNH-Nie0.7540.560.091HNH-Nie0.7640.560.091HNH-Nie0.7640.560.091HNH-Nie0.7640.560.089HNH-Nie0.7620.560.089HNH-Nie0.7620.560.089HNH-Nie0.7620.560.089HNH-Nie0.7620.560.089HNH-Ni0.7620.560.089HNH-Ni0.7620.560.089HNH-Ni0.7620.560.089HNH-Ni0.7620.560.089HNH-Ni0.7620.560.031HNH-Ni0.7620.560.039HNH-Ni0.7620.560.039HNH-Ni0.7620.560.039HNH-Ni0.7620.560.039HNH-Ni0.7620.560.031 </td <td></td> <td>H₂NH-Se</td> <td>2.716</td> <td>0.36</td> <td>0.050</td> <td></td>		H ₂ NH-Se	2.716	0.36	0.050	
H:NH-hole:2.2860.290.010H:N-hole:2.6970.360.054TrebleHH,N-W:2.8200.340.042upwardHH:N-W:2.8220.300.0340.042UpwardHH:N-W:2.8220.300.0280.017HHH:N-W:2.8220.300.028MHHH:N-W:2.7280.250.004MHH:N-W:2.6260.350.056TrebleHNH:-W:2.6260.350.056MMHNH:-Se3.1120.270.009downwardMHNH:-Se2.8930.270.009downwardMHNH:-Se2.8930.270.009downwardMHNH:-Se0.7660.560.091MMHNH:-Se0.7660.560.091MMHNH:-Nole0.7640.560.088MMH:NH-Se0.7710.560.088MMH:NH-Vs0.7670.500.089MMH:NH-Vs0.7670.500.089MMH:NH-Nole2.7540.300.043MMH:NH-Nole2.7540.300.043MMH:NH-Nole2.7540.300.034MMH:NH-Nole2.7540.300.034MMH:NH-Nole2.7540.300.039MM<		H ₂ NH-W ₂	2.252	0.31	0.014	
H3N-hole22.6970.360.054TrebleHH3N-W22.8200.340.042upwardupwardH3N-hole12.8250.300.0340.042H3N-W12.8220.300.0280.017H3N-W22.8220.300.0280.017H3N-Nole22.7280.250.0040.0094H3N-Nole22.7280.250.00617ebleNH3-W22.6260.350.056TrebleHNH3-W22.5890.330.011DoubleHHNH2-W22.5890.330.011DoubleHHNH2-W22.5890.330.011DoubleHHNH2-W22.5890.330.011DoubleHHNH2-W20.7660.560.091downwarddownwardHNH2-W30.7660.560.091downwardHHNH2-W30.7640.560.088HHNH2-W30.7710.560.088HHNH2-W30.7710.560.088HHNH2-W22.2500.310.014HHNH2-W22.2500.310.014HHNH2-W22.7740.320.043TrebleHHNH2-W30.7660.280.019HHNH2-W22.7540.300.034HHNH2-W22.7540.300.034HHNH2-W22.6220.320.016HHNH2-W2 <td< td=""><td></td><td>H₂NH-hole₁</td><td>2.286</td><td>0.29</td><td>0.010</td><td></td></td<>		H ₂ NH-hole ₁	2.286	0.29	0.010	
HiN-W22.8200.340.042upwardHiN-hole:2.8250.300.0340.044HiN-W12.8220.300.0280.028HiN-Se3.3870.250.0170.004HN-Se3.3870.250.0040.0048.33%NH:-W22.6260.350.056TrebleHNH:-Se3.1120.270.031downward1HNH22.5890.330.011DoubleHHNH2-Se2.8930.270.009downward1HNH2-Se2.8930.270.009downward1HNY-Se0.7660.560.091More1HNY-Se0.7660.560.091More1HNY-Se0.7710.560.088More1HNY-Vse0.7710.560.08811HNH-Vse0.7620.560.08111HNH-Vse0.7610.500.08911HNH-Vse0.7610.500.08911HNH-Vse0.7620.560.08111HNH-Vse0.7640.560.08111HNH-Vse0.7640.560.08111HNH-Vse0.7640.560.08111HNH-Vse0.7620.560.08111HNH-Vse0.7620.560.08111HNH-Vse0.7640.56 <td></td> <td>H₃N-hole₂</td> <td>2.697</td> <td>0.36</td> <td>0.054</td> <td>Treble H</td>		H ₃ N-hole ₂	2.697	0.36	0.054	Treble H
Handler Handler Handler Handler2.8250.300.034Handler Handler Handler2.8220.300.028Handler Handler2.7280.250.017Handler Handler2.7280.25-0.0048.33%NHa-Wa2.6260.350.056RNHa-Wa2.6260.350.056MMHandler Handler0.120.270.031downwardHNH2-Wa2.5890.330.011DoubleHHNH2-Wa2.5890.370.009downwardHNH2-Wa0.7640.560.091MHundler Handler0.7640.560.091MHundler Handler0.7640.560.088MHundler Handler0.7640.560.088MHundler Handler0.7620.560.088MHundler Handler0.7620.560.089MHandler Handler0.7620.560.089MHandler Handler0.7670.500.089MHandler Handler0.7640.560.089MHandler Handler0.7640.560.089MHandler Handler0.7620.560.089MHandler Handler0.7620.560.089MHandler Handler0.7640.560.089MHandler Handler0.7640.560.089MHandler Handler		H ₃ N-W ₂	2.820	0.34	0.042	upward
HaN-Wa2.8220.300.028HaN-Se3.3870.250.017HaNH-hole22.7280.25-0.0048.333%NH3-W22.6260.350.056TrebleHNH3-Se3.1120.270.031downwardHHNH2-W22.5890.330.011DoubleHHNH2-W22.5890.270.009downwardHHNH2-W22.8930.270.009downwardHHNH2-W20.7540.560.091downwardHH3N-V80.7660.560.091downwardHH3N-V80.7640.560.088HHH3N-V80.7710.560.088HH3H-V80.7710.560.089HH4NH2-V80.7710.560.089HH3N-V80.7620.560.089HH3N-W10.7670.500.089HH3N-W22.710.260.031HH3N-W12.9660.280.014HH3N-W22.7220.340.060HH3N-W12.9660.280.019HH3N-W22.7220.340.060HH3N-W22.6220.320.016HH3N-W22.6220.320.016HH3N-W22.6220.320.016HH3N-W22.6220.320.016HHM1-Se13.0190.27<		H ₃ N-hole ₁	2.825	0.30	0.034	
HaN-Se3.3870.250.017H2NH-hole:2.7280.25-0.0048.333%NH3-W22.6260.350.056TrebleHNH3-Se3.1120.270.031downwardHHM12-W22.5890.330.011DoubleHHNH2-W22.5890.270.009downwardHHNH2-W22.8930.270.009downwardHHNH2-W20.7540.560.091MHHNH2-W30.7660.560.091HHHN1-V60.7640.560.091HHHN1-V80.7640.560.088HHH2H-V30.7710.560.088HHH2H-V30.7710.560.088HHH2H-V30.7710.560.089HHH3H-W10.7670.500.089HHH3H-W10.7670.500.089HHH3H-W10.7670.500.031IrebleHH3H-W22.7210.340.014HH3N-W12.9660.280.019HH3N-W22.7220.340.060HH3N-W22.7220.340.060HH3N-Se13.0520.260.039HH3N-Se23.0100.270.005HH3N-Se23.0190.270.005HH3N-Se23.0190.27 </td <td></td> <td>H_3N-W_1</td> <td>2.822</td> <td>0.30</td> <td>0.028</td> <td></td>		H_3N-W_1	2.822	0.30	0.028	
H:NH-hole2 2.728 0.25 -0.004 8.333% NH-W2 2.626 0.35 0.056 Treble H NH-Se 3.112 0.27 0.031 downward H HNH-Se 2.589 0.33 0.011 Double H HNH-W2 2.589 0.27 0.009 downward H HNH-Se 2.893 0.27 0.009 downward H HNH-Se 0.766 0.56 0.091 downward H HNH-Se 0.764 0.56 0.090 M H NH-VSe 0.770 0.56 0.088 H H HNH-VSe 0.771 0.56 0.088 H H HNH-W1 0.767 0.50 0.089 H H HNH-W2 2.250 0.31 0.014 H H HNH-W2 2.734 0.32 0.043 H H HNH-Se 3.430 0.24		H ₃ N-Se	3.387	0.25	0.017	
8.333% NH-W2 2.626 0.35 0.056 Treble H NH-Se 3.112 0.27 0.031 downward HNH-Se 2.589 0.33 0.011 Double H HNH-Se 2.893 0.27 0.009 downward HNH-W1 0.754 0.56 0.093 Single H HNY-W1 0.766 0.56 0.091 downward H HNY-Se 0.764 0.56 0.090 M downward H HNY-Se 0.770 0.56 0.088 H M H HNH-Vse 0.764 0.56 0.088 H H M M M HNH-Vse 0.771 0.56 0.088 H H H M		H ₂ NH-hole ₂	2.728	0.25	-0.004	
NH-Se 3.112 0.27 0.031 downward HNH-W2 2.589 0.33 0.011 Double H HNH-W1 0.754 0.56 0.093 Single H HNH-W1 0.754 0.56 0.091 downward H HNH-W1 0.764 0.56 0.091 downward H HNH2-hole 0.764 0.56 0.091 downward H HNH2-bole 0.764 0.56 0.091 downward H HNH2-VSe 0.770 0.56 0.089 H H HNH2-VSe 0.771 0.56 0.088 H H HNH2-VSe 0.771 0.56 0.087 H HNH2-VSe 0.771 0.56 0.087 H HNH-W1 0.767 0.50 0.089 H HN-W2 2.250 0.31 0.014 H HNN-Se 2.731 0.26 0.003 H	8.333%	NH ₃ -W ₂	2.626	0.35	0.056	Treble H
HNH2-W12.5890.330.011DoubleHHNH2-Se2.8930.270.009downwardHNH2-W10.7540.560.091downwardHNH2-Na0.7660.560.091downwardHNH2-hole0.7640.560.091downwardHNH2-Nole0.7640.560.091downwardHNH2-Nole0.7640.560.091downwardH2NH-V30.7700.560.089downwardH2NH-V30.7710.560.088downwardH2NH-Na0.7620.560.087downwardH2NH-Na0.7620.560.087downwardH2NH-Na0.7670.500.089downwardH2NH-Na0.7670.500.089downwardH2NH-Na0.7670.500.031upwardH2NH-Na2.2500.310.014upwardH3N-Na2.9660.280.019upwardH3N-Na2.9660.280.019upwardH3N-Na2.9660.280.039downward12.500%NH3-Se13.0520.260.039downwardNH3-Se13.0520.260.039downwardHNH2-Se13.0200.270.006downwardHNH2-Se13.0200.270.006downwardHNH2-Se23.0190.270.005downwardHNH2-Se23.0190.570.089downwardHNH2-Se2 <t< td=""><td></td><td>NH₃-Se</td><td>3.112</td><td>0.27</td><td>0.031</td><td>downward</td></t<>		NH ₃ -Se	3.112	0.27	0.031	downward
HNH ₂ -Se 2.893 0.27 0.009 downward HNH ₂ -W1 0.754 0.56 0.093 Single H H ₃ N-Vs ₆ 0.766 0.56 0.091 downward H H ₃ N-Vs ₆ 0.764 0.56 0.091 downward H HNH ₂ -hole 0.764 0.56 0.090 downward H HNH ₂ -Nole 0.764 0.56 0.089 H H HNH ₂ -Vs ₆ 0.770 0.56 0.088 H H H HNH ₂ -Vs ₆ 0.771 0.56 0.088 H <td< td=""><td></td><td>HNH₂-W₂</td><td>2.589</td><td>0.33</td><td>0.011</td><td>Double H</td></td<>		HNH ₂ -W ₂	2.589	0.33	0.011	Double H
HNH:-W1 0.754 0.56 0.093 Single downward H H:N-Vs 0.766 0.56 0.091 downward H HNH:-hole 0.764 0.56 0.091 downward H NH3-hole 0.764 0.56 0.090 H H H HNH:-Vse 0.770 0.56 0.089 H		HNH ₂ -Se	2.893	0.27	0.009	downward
H.N-V ₅₆ 0.766 0.56 0.091 downward HNH ₂ -hole 0.764 0.56 0.091 NH NH ₃ -hole 0.764 0.56 0.090 NH NH ₃ -Nole 0.770 0.56 0.089 NH H2NH-V ₅₆ 0.784 0.56 0.088 NH H2NH-V ₅₆ 0.771 0.56 0.088 NH H2NH-V ₅₆ 0.771 0.56 0.088 NH H2NH-V ₅₆ 0.762 0.56 0.087 NH H2NH-W1 0.767 0.50 0.089 NH H2NH-W2 2.250 0.31 0.014 NH H2NH-W2 2.794 0.32 0.043 Treble H H3N-Nole 2.754 0.30 0.034 upward V H3N-Se1 3.052 0.26 0.039 downward N 12.500% NH ₃ -Se1 3.052 0.26 0.039 downward N 12.500%		HNH ₂ -W ₁	0.754	0.56	0.093	Single H
HNH2-hole 0.764 0.56 0.091 NH3-hole 0.764 0.56 0.090 NH3-VSe 0.770 0.56 0.089 H2NH-VSe 0.771 0.56 0.088 HNH2-VSe 0.771 0.56 0.088 HNH2-VSe 0.771 0.56 0.088 HNH2-VSe 0.771 0.56 0.088 H2NH-Nole 0.782 0.56 0.087 H3-W1 0.767 0.50 0.089 H2NH-W2 2.250 0.31 0.014 H2NH-W2 2.794 0.32 0.043 Treble H H3N-W2 2.794 0.32 0.043 upward Upward H3N-W1 2.966 0.28 0.019 Upward Upward Upward 12.500% NH3-W2 2.722 0.34 0.060 Treble H NH3-Se1 3.052 0.26 0.039 downward H NH3-Se2 3.081 0.26		H ₃ N-V _{Se}	0.766	0.56	0.091	downward
NH3-hole 0.764 0.56 0.090 NH3-VSe 0.770 0.56 0.089 H2NH-Vsc 0.784 0.56 0.088 HNH2-Vsc 0.771 0.56 0.088 HNH2-Vsc 0.771 0.56 0.088 H3NH-hole 0.782 0.56 0.087 H3NH3-N0 0.762 0.56 0.085 H2NH-W1 0.767 0.50 0.089 H2NH-W2 2.250 0.31 0.014 H3NH2-Se 2.731 0.26 -0.003 H3N-W2 2.794 0.32 0.043 upward H3N-W1 2.966 0.28 0.019 upward H3N-Se 3.430 0.24 0.014 0 12.500% NH3-Se1 3.052 0.26 0.039 0 NH3-Se2 3.081 0.26 0.039 0 0 12.500% NH3-Se2 3.019 0.27 0.006 0 NH3-Se2 3.020 </td <td></td> <td>HNH₂-hole</td> <td>0.764</td> <td>0.56</td> <td>0.091</td> <td></td>		HNH ₂ -hole	0.764	0.56	0.091	
$ \begin{array}{ c c c c c c c c } NH_3-VSe & 0.770 & 0.56 & 0.089 \\ \hline H_3NH-V_{Se} & 0.784 & 0.56 & 0.088 \\ \hline HNH_2-V_{Se} & 0.771 & 0.56 & 0.088 \\ \hline HNH_2-V_{Se} & 0.782 & 0.56 & 0.087 \\ \hline H_3NH-M_1 & 0.762 & 0.56 & 0.085 \\ \hline H_2NH-W_1 & 0.767 & 0.50 & 0.089 \\ \hline H_2NH-W_2 & 2.250 & 0.31 & 0.014 \\ \hline H_3NH-Se & 2.731 & 0.26 & -0.003 \\ \hline H_3N-W_2 & 2.794 & 0.32 & 0.043 \\ \hline H_3N-W_1 & 2.966 & 0.28 & 0.019 \\ \hline H_3N-Se & 3.430 & 0.24 & 0.014 \\ \hline H_3N-Se & 3.430 & 0.24 & 0.014 \\ \hline 12.500\% & NH_3-Se_1 & 3.052 & 0.26 & 0.039 \\ \hline NH_3-Se_1 & 3.052 & 0.26 & 0.039 \\ \hline NH_3-Se_1 & 3.052 & 0.26 & 0.039 \\ \hline NH_3-Se_1 & 3.020 & 0.27 & 0.006 \\ \hline NH_3-Se_1 & 3.020 & 0.27 & 0.006 \\ \hline NH_3-Se_1 & 3.020 & 0.27 & 0.006 \\ \hline NH_3-Se_1 & 3.020 & 0.27 & 0.006 \\ \hline NH_3-Se_1 & 3.019 & 0.27 & 0.005 \\ \hline NH_3-Se_1 & 3.020 & 0.27 & 0.005 \\ \hline NH_3-W_1 & 0.752 & 0.57 & 0.089 \\ \hline NH_3-N_1 & 0.752 & 0.57 & 0.089 \\ \hline NH_3-Ne_1 & 0.775 & 0.57 & 0.089 \\ \hline NH_3-Ne_1 & 0.775 & 0.57 & 0.089 \\ \hline NH_3-Ne_1 & 0.773 & 0.57 & 0.088 \\ \hline NH_3-Ne_1 & 0.$		NH ₃ -hole	0.764	0.56	0.090	
$ \begin{array}{ c c c c c c c c } \hline H_2NH-V_{Se} & 0.784 & 0.56 & 0.088 \\ \hline HNH_2-V_{Se} & 0.771 & 0.56 & 0.088 \\ \hline H2NH-hole & 0.782 & 0.56 & 0.087 \\ \hline H_2NH-hole & 0.762 & 0.56 & 0.085 \\ \hline H_2NH-W_1 & 0.767 & 0.50 & 0.089 \\ \hline H_2NH-W_2 & 2.250 & 0.31 & 0.014 \\ \hline H_2NH-Se & 2.731 & 0.26 & -0.003 \\ \hline H_3N-W_2 & 2.794 & 0.32 & 0.043 & \\ \hline H_3N-W_2 & 2.754 & 0.30 & 0.034 \\ \hline H_3N-W_1 & 2.966 & 0.28 & 0.019 \\ \hline H_3N-Se & 3.430 & 0.24 & 0.014 \\ \hline H_3N-Se & 3.430 & 0.24 & 0.014 \\ \hline H_{3N-Se_1} & 3.052 & 0.26 & 0.039 \\ \hline NH_3-Se_1 & 3.052 & 0.26 & 0.039 \\ \hline HNH_2-Se_2 & 3.081 & 0.26 & 0.039 \\ \hline HNH_2-Se_2 & 3.081 & 0.26 & 0.039 \\ \hline HNH_2-Se_2 & 3.081 & 0.26 & 0.016 \\ \hline HNH_2-Se_1 & 3.020 & 0.27 & 0.006 \\ \hline HNH_2-Se_2 & 3.019 & 0.27 & 0.005 \\ \hline HNH_2-Se_2 & 3.019 & 0.27 & 0.005 \\ \hline HNH_2-Se_2 & 3.019 & 0.27 & 0.005 \\ \hline HNH_2-V_1 & 0.752 & 0.57 & 0.089 \\ \hline HNH_2-V_1 & 0.775 & 0.57 & 0.089 \\ \hline HNH_2-W_1 & 0.768 & 0.57 & 0.089 \\ \hline HNH_2-W_1 & 0.768 & 0.57 & 0.088 \\ \hline H_3N-hole & 0.773 & 0.57 & 0.088 \\ \hline H_3N-hole & 0.773 & 0.57 & 0.088 \\ \hline \end{array}$		NH ₃ -VSe	0.770	0.56	0.089	
$ \begin{array}{ c c c c c c } HNH_2-V_{Se} & 0.771 & 0.56 & 0.088 \\ \hline H_2NH-hole & 0.782 & 0.56 & 0.087 \\ \hline H_2NH-Nu & 0.762 & 0.56 & 0.085 \\ \hline H_2NH-W_1 & 0.767 & 0.50 & 0.089 \\ \hline H_2NH-W_2 & 2.250 & 0.31 & 0.014 \\ \hline H_2NH-Se & 2.731 & 0.26 & -0.003 \\ \hline H_3N-W_2 & 2.794 & 0.32 & 0.043 & Treble & H \\ \hline H_3N-hole & 2.754 & 0.30 & 0.034 & 0.014 \\ \hline H_3N-M_1 & 2.966 & 0.28 & 0.019 \\ \hline H_3N-Se & 3.430 & 0.24 & 0.014 \\ \hline H_3N-Se & 3.430 & 0.24 & 0.014 \\ \hline H_3N-Se_1 & 3.052 & 0.26 & 0.039 \\ \hline NH_3-Se_1 & 3.052 & 0.26 & 0.039 \\ \hline NH_3-Se_2 & 3.081 & 0.26 & 0.039 \\ \hline HNH_2-Se_2 & 3.081 & 0.26 & 0.039 \\ \hline HNH_2-Se_2 & 3.019 & 0.27 & 0.006 & 0.0016 \\ \hline HNH_2-Se_2 & 3.019 & 0.27 & 0.005 \\ \hline HNH_2-Se_2 & 3.019 & 0.27 & 0.005 \\ \hline HNH_2-Se_2 & 3.019 & 0.27 & 0.005 \\ \hline HNH_2-Se_2 & 3.019 & 0.27 & 0.005 \\ \hline HNH_2-Se_2 & 0.759 & 0.57 & 0.089 \\ \hline HNH_2-V_{Se} & 0.769 & 0.57 & 0.089 \\ \hline HNH_2-V_{Se} & 0.768 & 0.57 & 0.088 \\ \hline HNH_2-W_1 & 0.755 & 0.57 & 0.088 \\ \hline HNH_2-W_1 & 0.773 & 0.57 & 0.088 \\ \hline HNH_2-W_1 & 0.773 & 0.57 & 0.088 \\ \hline HNH_2-W_1 & 0.773 & 0.57 & 0.087 \\ \hline \end{array}$		H ₂ NH-V _{Se}	0.784	0.56	0.088	
$ \begin{array}{ c c c c c c c c } \hline H_2 M H-hole & 0.782 & 0.56 & 0.087 \\ \hline M H_3 - W_1 & 0.762 & 0.56 & 0.085 \\ \hline H_2 M H- W_1 & 0.767 & 0.50 & 0.089 \\ \hline H_2 M H- W_2 & 2.250 & 0.31 & 0.014 \\ \hline H_2 M H- Se & 2.731 & 0.26 & -0.003 \\ \hline H_3 N- W_2 & 2.794 & 0.32 & 0.043 & Treble & H \\ \hline H_3 N-hole & 2.754 & 0.30 & 0.034 & 0.014 \\ \hline H_3 N- M_1 & 2.966 & 0.28 & 0.019 \\ \hline H_3 N-Se & 3.430 & 0.24 & 0.014 \\ \hline H_3 N-Se & 3.430 & 0.24 & 0.014 \\ \hline N H_3 - Se_1 & 3.052 & 0.26 & 0.039 \\ \hline N H_3 - Se_2 & 3.081 & 0.26 & 0.039 \\ \hline N H_3 - Se_2 & 3.081 & 0.26 & 0.039 \\ \hline H N H_2 - W_2 & 2.622 & 0.32 & 0.016 & 0.0016 \\ \hline H M H_2 - Se_1 & 3.020 & 0.27 & 0.006 \\ \hline M H_3 - Se_1 & 3.020 & 0.27 & 0.006 \\ \hline M H_3 - Se_2 & 3.019 & 0.27 & 0.005 \\ \hline H N H_2 - Se_2 & 3.019 & 0.27 & 0.005 \\ \hline M H_3 - W_1 & 0.752 & 0.57 & 0.089 \\ \hline M H_3 - M_1 & 0.755 & 0.57 & 0.089 \\ \hline M H_3 - hole & 0.768 & 0.57 & 0.088 \\ \hline H N H_2 - W_1 & 0.753 & 0.57 & 0.088 \\ \hline H N H_2 - W_1 & 0.773 & 0.57 & 0.087 \\ \hline \end{array}$		HNH ₂ -V _{Se}	0.771	0.56	0.088	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		H ₂ NH-hole	0.782	0.56	0.087	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		NH ₃ -W ₁	0.762	0.56	0.085	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		H ₂ NH-W ₁	0.767	0.50	0.089	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		H ₂ NH-W ₂	2.250	0.31	0.014	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		H ₂ NH-Se	2.731	0.26	-0.003	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		H ₃ N-W ₂	2.794	0.32	0.043	Treble H
$ \begin{array}{ c c c c c c c c } \hline H_3N-W_1 & 2.966 & 0.28 & 0.019 \\ \hline H_3N-Se & 3.430 & 0.24 & 0.014 \\ \hline H_3N-W_2 & 2.722 & 0.34 & 0.060 & Treble & H \\ \hline NH_3-Se_1 & 3.052 & 0.26 & 0.039 & \\ \hline NH_3-Se_2 & 3.081 & 0.26 & 0.039 & \\ \hline HNH_2-W_2 & 2.622 & 0.32 & 0.016 & Double & H \\ \hline HNH_2-Se_1 & 3.020 & 0.27 & 0.006 & \\ \hline HNH_2-Se_2 & 3.019 & 0.27 & 0.005 & \\ \hline NH_3-M_1 & 0.752 & 0.57 & 0.091 & Single & H \\ \hline HNH_2-V_{Se} & 0.769 & 0.57 & 0.089 & \\ \hline HNH_2-W_1 & 0.775 & 0.57 & 0.089 & \\ \hline HNH_2-W_1 & 0.768 & 0.57 & 0.089 & \\ \hline H_3-hole & 0.773 & 0.57 & 0.087 & \\ \hline \end{array} $		H ₃ N-hole	2.754	0.30	0.034	upward
H3N-Se 3.430 0.24 0.014 12.500%NH3-W2 2.722 0.34 0.060 TrebleHNH3-Se1 3.052 0.26 0.039 downwardHNH3-Se2 3.081 0.26 0.039 DoubleHHNH2-W2 2.622 0.32 0.016 DoubleHHNH2-Se1 3.020 0.27 0.006 downwardHHNH2-Se2 3.019 0.27 0.005 HdownwardHNH2-Se2 3.019 0.27 0.005 HdownwardHNH2-Vae 0.752 0.57 0.091 SingleHHNH2-Vae 0.769 0.57 0.089 MownwardHHNH2-Vae 0.768 0.57 0.089 HMownwardHNH2-N1 0.773 0.57 0.087 MM		H_3N-W_1	2.966	0.28	0.019	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		H ₃ N-Se	3.430	0.24	0.014	
$\begin{array}{ c c c c c c c } \hline NH_3-Se_1 & 3.052 & 0.26 & 0.039 & downward \\ \hline NH_3-Se_2 & 3.081 & 0.26 & 0.039 & & \\ \hline HNH_2-W_2 & 2.622 & 0.32 & 0.016 & Double & H \\ \hline HNH_2-Se_1 & 3.020 & 0.27 & 0.006 & & \\ \hline HNH_2-Se_2 & 3.019 & 0.27 & 0.005 & & \\ \hline NH_3-W_1 & 0.752 & 0.57 & 0.091 & Single & H \\ \hline HNH_2-V_{Se} & 0.769 & 0.57 & 0.089 & & \\ \hline HNH_2-W_1 & 0.775 & 0.57 & 0.089 & & \\ \hline HNH_2-W_1 & 0.768 & 0.57 & 0.088 & \\ \hline H_3N-hole & 0.773 & 0.57 & 0.087 & & \\ \hline \end{array}$	12.500%	NH ₃ -W ₂	2.722	0.34	0.060	Treble H
NH ₃ -Se2 3.081 0.26 0.039 HNH ₂ -W ₂ 2.622 0.32 0.016 Double H HNH ₂ -Se1 3.020 0.27 0.006 downward H HNH ₂ -Se2 3.019 0.27 0.005 H H HNH ₂ -Se2 3.019 0.27 0.005 H H H HNH ₂ -Se2 0.769 0.57 0.091 Single H HNH ₂ -V _{Se} 0.769 0.57 0.089 downward H HNH ₂ -W ₁ 0.775 0.57 0.089 H H HNH ₂ -hole 0.768 0.57 0.088 H H		NH ₃ -Se ₁	3.052	0.26	0.039	downward
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		NH ₃ -Se ₂	3.081	0.26	0.039	
HNH2-Se1 3.020 0.27 0.006 downward HNH2-Se2 3.019 0.27 0.005 NH3-W1 0.752 0.57 0.091 Single H HNH2-Vse 0.769 0.57 0.089 HNH2-W1 0.775 0.57 0.089 HNH2-W1 0.768 0.57 0.089 HNH2-W1 0.768 0.57 0.089		HNH ₂ -W ₂	2.622	0.32	0.016	Double H
HNH2-Se2 3.019 0.27 0.005 NH3-W1 0.752 0.57 0.091 Single H HNH2-Vse 0.769 0.57 0.089 downward HNH2-W1 0.775 0.57 0.089 H NH3-hole 0.768 0.57 0.088 H H3N-hole 0.773 0.57 0.087 H		HNH ₂ -Se ₁	3.020	0.27	0.006	downward
NH ₃ -W1 0.752 0.57 0.091 Single H HNH ₂ -V _{Se} 0.769 0.57 0.089 downward HNH ₂ -W1 0.775 0.57 0.089 downward NH ₃ -hole 0.768 0.57 0.088 H H ₃ N-hole 0.773 0.57 0.087 H		HNH ₂ -Se ₂	3.019	0.27	0.005	
$\begin{array}{c cccc} HNH_2\text{-}V_{Se} & 0.769 & 0.57 & 0.089 \\ HNH_2\text{-}W_1 & 0.775 & 0.57 & 0.089 \\ NH_3\text{-}hole & 0.768 & 0.57 & 0.088 \\ H_3N\text{-}hole & 0.773 & 0.57 & 0.087 \\ \end{array}$		NH ₃ -W ₁	0.752	0.57	0.091	Single H
HNH_2-W_1 0.7750.570.089 NH_3 -hole0.7680.570.088 H_3N -hole0.7730.570.087		HNH ₂ -V _{Se}	0.769	0.57	0.089	downward
NH3-hole0.7680.570.088H3N-hole0.7730.570.087		HNH ₂ -W ₁	0.775	0.57	0.089	
H ₃ N-hole 0.773 0.57 0.087		NH ₃ -hole	0.768	0.57	0.088	
		H ₃ N-hole	0.773	0.57	0.087	

H ₂ NH-V _{Se}	0.773	0.57	0.086		
H ₃ N-V _{Se}	0.771	0.56	0.090		
HNH ₂ -hole	0.771	0.56	0.090		
H ₂ NH-hole	0.774	0.56	0.089		
H_2NH-W_1	0.778	0.56	0.087		
NH ₃ -V _{Se}	0.903	0.55	0.080		
H_2NH-W_2	2.265	0.31	0.016		
H ₂ NH-Se ₁	2.755	0.26	0.000		
H ₃ N-Se ₁	2.779	0.26	-0.001		
H ₂ NH-Se ₂	2.753	0.26	-0.001		
H_3N-W_2	2.879	0.30	0.036	Treble	Н
H_3N-W_1	2.881	0.27	0.021	upward	
H ₃ N-Se ₂	3.445	0.22	0.013		