Table S1: Geometrical parameters for all the WH_n species computed at DFT/BP86/TZVPP and MP2/TZVPP levels of theory

Species	Method	W-H	W-H(H_2)	H-H
WH_2	DFT	1.72	--	--
	MP2	1.70	--	--
WH_4	DFT	1.72	--	--
	MP2	1.69	--	--
WH_6	DFT	1.67/1.71	--	--
	MP2	1.65/1.69	--	--
$WH_6(H_2)$	DFT	1.69/1.72	1.99	0.80
	MP2	1.67/1.70	1.97	0.79
$WH_6(H_2)_2$	DFT	1.70/1.71	1.95/1.97	0.82/0.83
	MP2	1.68/1.69	1.90/1.94	0.80/0.82
$WH_4(H_2)_3$	DFT	1.71/1.71	1.82/1.83	0.86/0.89
	MP2	1.68/1.68	1.80/1.81	0.87/0.90
$WH_4(H_2)_4$	DFT	1.74	1.85	0.88
	MP2	1.72	1.81	0.87

Table S2: Frequencies of $WH_4(H_2)_4$ at DFT/BP86/TZVPP and MP2/TZVPP levels of theory. Singlet state. D_{2d} symmetry.

Symm	Freq DFT/BP86/TZVPP	Int	Freq MP2/TZVPP	Int	Type
b_1	351	0	414	0	
b_2	414	171	389	217	Bending H-M-H (H of H2)
e	428	6	461	7	Bending H-M-H (H of H2)
e	428	6	461	7	Bending H-M-H (H of H2)
a_1	499	0	530	0	
a_2	539	0	571	0	
e	565	38	594	27	Bending H2-M-H2
e	565	38	594	27	Bending H2-M-H2
b_1	681	0	735	0	
e	748	8	724	22	Bending H-M-H2
e	748	8	724	22	Bending H-M-H2
a_2	775	0	800	0	
e	816	16	851	14	Bending H-M-H2
e	816	16	851	14	Bending H-M-H2
b_2	842	0	858	0	
a_1	871	0	881	0	
b_1	897	0	941	0	
e	1065	172	1178	276	Bend H2-M-H2+ sym str M-H2
e	1065	172	1178	276	Bend H2-M-H2+ sym str M-H2
b_2	1160	3	1289	11	Bend H2-M-H2+ sym str M-H2
a_1	1284	0	1413	0	
b_1	1741	0	1862	0	
a_2	1767	0	1894	0	
e	1790	40	1912	42	Asym stretch M-H2
e	1790	40	1912	42	Asym stretch M-H2
b_2	1844	212	1989	128	Symm Stretch M-H
e	1868	53	2017	30	Asym stretch M-H

e	1868	53	2017	30	Asym stretch M-H
a_1	1903	0	2021	0	
e	2657	208	2699	187	Stretch H-H
e	2657	208	2699	187	Stretch H-H
b_2	2683	11	2744	6	Stretch H-H
a_1	2740	0	2788	0	

Table S3: Frequencies of $WD_4(D_2)_4$ at DFT/BP86/TZVPP level of theory. Singlet state. D_{2d} symmetry.

Symm	Freq DFT/BP86/TZVPP	Int	Freq MP2/TZVPP	Int	Type
b_1	248	0	293	0	
b_2	299	89	281	113	Bending H-M-H (H of H2)
e	303	3	326	3	Bending H-M-H (H of H2)
e	303	3	326	3	Bending H-M-H (H of H2)
a_1	353	0	375	0	
a_2	381	0	404	0	
e	401	19	422	13	Bending H2-M-H2
e	401	19	422	13	Bending H2-M-H2
b_1	481	0	520	0	
e	530	4	512	11	Bending H-M-H2
e	530	4	512	11	Bending H-M-H2
a_2	548	0	566	0	
e	579	7	603	6	Bending H-M-H2
e	579	7	603	6	Bending H-M-H2
b_2	596	0	607	0	
a_1	616	0	623	0	
b_1	635	0	666	0	
e	767	93	849	147	Bend H2-M-H2 + sym str M-H2
e	767	93	849	147	Bend H2-M-H2+ sym str M-H2
b_2	823	2	914	7	Bend H2-M-H2+ sym str M-H2
a_1	908	0	1000	0	
b_1	1232	0	1318	0	
a_2	1250	0	1340	0	
e	1268	24	1354	24	Asym stretch M-H2
e	1268	24	1354	24	Asym stretch M-H2
b_2	1316	102	1420	60	Symm Stretch M-H
e	1324	23	1429	12	Asym stretch M-H
e	1324	23	1429	12	Asym stretch M-H
a_1	1347	0	1430	0	
e	1881	102	1912	91	Stretch H-H
e	1881	102	1912	91	Stretch H-H
b_2	1898	5	1942	3	Stretch H-H
a_1	1939	0	1973	0	

Table S4: Frequencies of $WH_2D_2(HD)_4$ at DFT/BP86/TZVPP level of theory. Singlet state. C_1 symmetry.

Symm	Freq DFT/BP86/TZVPP	Int	Freq MP2/TZVPP	Int	Type
a	262	0	321	3	
a	316	28	313	123	Bending H-M-H (H of H2)
a	325	61	352	5	Bending H-M-H (H of H2)
a	376	12	412	9	Bending H-M-H (H of H2)

a	432	1	460	10	Bending H2-M-H2
a	435	18	467	1	Bending H2-M-H2
a	457	29	484	20	Bending H2-M-H2
a	471	23	512	27	Bending H2-M-H2
a	552	0	579	2	Bending H2-M-H2
a	569	12	587	25	Bending H-M-H2
a	581	2	609	0	Bending H-M-H2
a	595	11	628	10	Bending H-M-H2
a	613	6	639	4	Bending H-M-H2
a	749	11	780	17	Bending H-M-H2
a	770	18	784	21	Bending H-M-H2
a	781	21	821	10	Bending H-M-H2
a	815	1	870	0	Bending H-M-H2
a	884	55	975	105	Bend H2-M-H2+ sym str M-H2
a	906	125	1008	213	Bend H2-M-H2+ sym str M-H2
a	938	12	1036	13	Bend H2-M-H2+ sym str M-H2
a	1015	0	1116	0	Bend H2-M-H2+ sym str M-H2
a	1319	60	1427	33	Bend H2-M-H2+ sym str M-H2
a	1332	8	1430	1	Bend H2-M-H2+ sym str M-H2
a	1501	116	1606	145	Asym stretch M-H2
a	1536	2	1652	4	Asym stretch M-H2
a	1541	0	1665	0	Symm Stretch M-H
a	1551	2	1657	9	Asym stretch M-H
a	1849	131	2001	79	Asym stretch M-H
a	1880	25	2019	16	Asym stretch M-H
a	2342	259	2381	234	Stretch H-H
a	2349	64	2386	49	Stretch H-H
a	2358	8	2408	4	Stretch H-H
a	2406	0	2445	0	Stretch H-H

Table S5: Frequencies of $WH_2D_2(H_2)_2(D_2)_4$ at DFT/BP86/TZVPP level of theory. Singlet state. C_1 symm.

Symm	Freq DFT/BP86/TZVPP	Int	Freq MP2/TZVPP	Int	Type
a	266	0	327	0	Bending H-M-H (H of H2)
a	303	5	335	4	Bending H-M-H (H of H2)
a	319	80	310	118	Bending H-M-H (H of H2)
a	394	5	431	4	Bending H-M-H (H of H2)
a	409	20	442	20	Bending H-M-H (H of H2)
a	447	38	463	34	Bending H-M-H (H of H2)
a	453	3	505	1	Bending H2-M-H2
a	514	18	525	1	Bending H2-M-H2
a	537	2	565	12	Bending H2-M-H2
a	553	8	581	15	Bending H-M-H2
a	596	5	618	11	Bending H-M-H2
a	634	6	671	7	Bending H-M-H2
a	642	7	682	1	Bending H-M-H2
a	715	49	752	52	Bending H-M-H2
a	760	10	801	6	Bending H-M-H2
a	795	11	811	13	Bending H-M-H2
a	811	13	870	15	Bending H-M-H
a	837	46	917	119	Bending H2-M-H2+ sym str M-H2
a	874	10	954	7	Bending H2-M-H2+ sym str M-H2
a	1045	160	1159	263	Bending H2-M-H2+ sym str M-H2
a	1223	2	1330	0	Bending H2-M-H2+ sym str M-H2
a	1233	0	1355	6	Bending H2-M-H2+ sym str M-H2

a	1262	18	1357	15	Bending H2-M-H2+ sym str M-H2
a	1320	62	1427	34	Asym stretch M-H2
a	1334	14	1432	8	Asym stretch M-H2
a	1741	0	1879	0	Symm stretch M-H
a	1773	65	1896	129	Asym stretch M-H
a	1848	127	1927	4	Asym stretch M-H
a	1878	13	1959	4	Asym stretch M-H
a	1896	105	2003	82	Stretch H-H
a	1929	1	2019	17	Stretch H-H
a	2669	212	2698	190	Stretch H-H
a	2725	6	2766	4	Stretch H-H

Table S6: Frequencies of WH_4 at DFT/BP86/TZVPP level of theory. Triplet state. T_d symmetry.

Symm	Freq DFT/BP86/TZVPP	Int	Freq MP2/TZVPP	Int	
t_2	568	90	597	109	Bending M-H-M
t_2	568	90	597	109	Bending M-H-M
t_2	568	90	597	109	Bending M-H-M
e	668	0	691	0	
e	668	0	691	0	
t_2	1930	159	2044	238	Asym stretch M-H
t_2	1930	159	2044	238	Asym stretch M-H
t_2	1930	159	2044	238	Asym stretch M-H
a_1	1964	0	2074	0	

Table S7: Frequencies of WH_6 at DFT/BP86/TZVPP level of theory. Singlet state.

Symm	Freq DFT/BP86/TZVPP	Int	Freq MP2/TZVPP	Int	
e	708	11	775	2	Bending M-H-M
e	708	11	775	2	Bending M-H-M
a_1	761	14	764	17	Bending M-H-M
a_2	816	0	804	0	
e	886	54	896	97	Bending M-H-M
e	886	54	896	97	Bending M-H-M
e	940	2	968	1	Bending M-H-M
e	940	2	968	1	Bending M-H-M
a_1	1131	84	1172	100	Bending M-H-M
e	1930	134	2042	189	Asym stretch M-H
e	1930	134	2042	189	Asym stretch M-H
a_1	1946	94	2046	69	Sym stretch M-H
e	2029	60	2152	41	Asym stretch M-H
e	2029	60	2152	41	Asym stretch M-H
a_1	2046	32	2137	46	Sym stretch M-H (3 of them)

Table S8: Frequencies of $WH_6(H_2)$ at DFT/BP86/TZVPP level of theory. Singlet state. C_s symmetry.

Symm	Freq DFT/BP86/TZVPP	Int	Freq MP2/TZVPP	Int	
a"	21	22	101	26	Bending M-H2
a"	401	1	476	3	
a'	441	11	455	16	Bending M-H2
a'	646	23	685	5	Bending M-H2 + M-H-M

a'	695	11	742	27	Bending M-H2 + M-H-M
a"	736	23	788	25	Bending M-H2 + M-H-M
a'	798	9	815	7	Bend M-H-M + str M-H2
a"	802	1	814	1	
a"	873	0	893	0	
a'	881	4	933	21	Bend M-H-M + sym str M-H2
a"	905	46	910	71	Bend M-H-M
a'	954	47	967	65	Bend M-H-M
a'	1058	43	1077	59	Bend M-H-M
a"	1333	21	1379	24	Asym str M-H2
a"	1915	140	2030	174	Asym str M-H
a'	1920	118	2030	91	Asym str M-H
a'	1939	89	2046	122	Asym str M-H
a'	1993	51	2097	47	Asym str M-H
a"	2003	22	2135	7	Asym str M-H
a'	2008	31	2121	21	Asym str M-H
a'	3510	46	3757	23	Str H-H

Table S9: Frequencies of $WH_6(H_2)_2$ at DFT/BP86/TZVPP level of theory. Singlet state. C_s symmetry.

Symm	Freq	Int	Freq	Int	
	DFT/BP86/TZVPP		MP2/TZVPP		
a"	245	25	229	29	Bending M-H2
a'	385	20	417	37	Bending M-H2
a"	388	13	367	15	Bending M-H2
a'	447	54	438	69	Bending M-H2
a"	478	2	455	5	Bending M-H2
a"	547	1	547	0	
a'	579	10	579	3	Bending M-H-M
a"	721	80	765	86	Bending M-H-M + bend M-H2
a'	794	54	788	61	Bending M-H-M
a'	823	29	882	20	Bend M-H-M + sym str M-H2
a"	835	1	860	1	
a'	876	3	940	4	sym str M-H2
a"	885	11	936	12	Bending M-H-M + bend M-H2
a'	954	25	1018	55	Bend M-H-M + sym str M-H2
a"	1014	59	1044	116	Bend M-H-M
a'	1026	30	1064	36	Bend M-H-M + sym str M-H2
a'	1077	6	1187	5	Bend M-H-M + sym str M-H2
a'	1454	16	1467	22	Asym str M-H2
a"	1489	9	1648	9	Asym str M-H2
a'	1818	135	1932	134	Str M-H
a"	1922	88	2048	94	Str M-H
a'	1925	48	2038	30	Str M-H
a'	1980	41	2079	32	Str M-H
a"	1982	34	2116	13	Asymm str M-H
a'	1999	12	2115	8	Str M-H
a'	3217	3	3226	1	Str H-H
a'	3303	75	3602	52	Str H-H

Table S10: Frequencies of $WH_4(H_2)_3$ at DFT/BP86/TZVPP level of theory. Singlet state. C_s symmetry.

Symm	Freq	Int	Freq	Int	
	DFT/BP86/TZVPP		MP2/TZVPP		

a'	297	25	151	43	Bending M-H2
a"	353	20	316	91	Bending M-H2
a"	492	6	526	12	Bending M-H2
a'	526	87	560	91	Bending M-H2
a"	541	29	612	24	Bending M-H2 + bend M-H-M
a'	570	67	594	112	Bending M-H2
a"	666	117	691	51	Bending M-H2 + bend M-H-M
a'	692	42	731	30	Bending M-H2 + bend M-H-M
a"	702	5	763	6	Bending M-H2 + bend M-H-M
a"	753	2	787	18	Bending M-H2 + bend M-H-M
a'	915	1	924	1	
a'	953	20	1015	30	bend M-H-M + str M-H2
a"	958	163	1044	126	bend M-H-M + str M-H2
a"	987	32	1064	179	bend M-H-M + str M-H2
a'	997	7	1021	48	bend M-H-M + str M-H2
a'	1039	52	1149	67	bend M-H-M
a'	1290	13	1414	15	str M-H2
a"	1633	17	1874	12	Asym str M-H2
a"	1769	0	1920	5	
a'	1823	99	1914	178	Str M-H + str M-H2
a'	1840	148	1940	86	Str M-H + str M-H2
a'	1935	137	2064	23	Str M-H
a"	1943	32	2098	16	Str M-H
a'	1952	19	2086	103	Str M-H
a"	2493	358	2644	343	Str H-H
a'	2576	20	2453	113	Str H-H
a'	2766	96	2746	6	Str H-H