Supplementary information for:

Direct Laser Cooling Schemes for the Triatomic SOH and SeOH Molecules Based on Ab Initio Calculations.

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This supplement provides further details of the supplementary data sets relevant to the text. In particular, the equilibrium geometrical structures and fundamental frequencies of the ground and low-lying excited states for 168 electronic states of 28 triatomic molecules containing OH are given by the new method, which can rapidly identify the preferable one among many candidate polyatomic molecules. And the equilibrium structures and fundamental frequencies for the screened molecules by MCSCF are also calculated by using TD/DFT method implemented in Gaussian 16. In addition, the fitting parameters and root mean square errors of two- and three-body terms for SOH and SeOH are listed.

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- Table S4. Fitting parameters and root mean square errors (in cm^{-1}) of the three-body terms for SOH and SeOH molecules.

Table S1 Calculated and experimental/theoretical molecular parameters for MOH (M is the second- to fifth-period elements of the first to the sixth main group in the periodic table, and includes Cs, Ba, Fr and Ra.). For the triatomic molecules (M=Li—Mg and Ca—Se, including H, P, S), the structural parameters are calculated by MCSCF/cc-pVTZ. For M=Rb and Sr, the basis set of ECP28MDF is used. For M=In—Te, including Si and Al, the cc-pVTZ-DK basis set is employed, while for M=K and Ba, def2-QZVP and ECP46MDF basis sets are adopted, respectively. And for M=Cs, Fr and Ra, ECP78MDF basis set is used. The blue part is the difference in bond lengths, bond angle, and vibrational frequencies between the lowest two electronic states of each molecule. Among them, the excited states are not optimized relative to the ground state of M = As, Sb, and Ga. The yellow mark is the molecules meeting the requirements of the laser cooling candidates. The internuclear distances R_i are given in Å and the harmonic frequencies of normal mode v_l in cm^{-1}. The X represents the symmetry of state because all the calculations are carried out without symmetry.

		$R_{O\text{-}H}$	$R_{O\text{-}M}$	∠ M-O-H	2	1	3	energy	
LiOH	1^1X	0.952	1.586	179.999	342.23	965.70	4010.34	-83.0829022	
		0.9499	1.5857	180	289	923	3831		Ref. [1]
		0.934	1.590	180	298	1014	4366		Exp. [2]
	2^1X	0.978	2.098	114.133	280.50	401.50	3679.24	-82.9445385	
	3^1X	0.973	2.094	180.000	244.2	491.16	3755.90	-82.94505605	
	1^3X	0.978	2.074	114.697	311.36	374.22	3682.25	-82.9551657	
	2^3X	0.973	2.067	179.989	270.99	365.05	3758.80	-82.9520152	
	3^3X	0.969	1.996	171.796	355.93	364.03	3790.84	-82.86923674	
difference		0.021	0.508	0.001	98.03	474.54	254.44	0.13784615	
BeOH	1^2X	0.958	1.421	129.053	494.93	1242.16	3928.80	-90.2321731	
		0.943	1.401	139.010					Ref. [3]
		0.934	1.399		306	1322	4377		Ref. [4]
		0.949	1.397	141.000	100.2	1263.4	38684		Ref. [5]
	2^2X	0.963	1.475	111.677	900.92	1115.69	3824.00	-90.0850508	
		0.949	1.446	118.160					Ref. [3]
	3^2X	0.959	1.481	120.314	580.06	1053.86	3875.23	-90.03029058	

	1^4X	0.982	1.842	102.965	437.11	605.70	3619.20	-89.9927095	
	2^4X	0.983	1.852	108.965	419.90	611.15	3609.70	-89.9944047	
	3^4X				Dissociation				
difference		0.005	0.054	17.376	405.99	126.47	104.8	0.1471223	
BOH	1^1X	0.970	1.315	115.864	703.59	1406.89	3815.20	-100.2465496	
		0.949/ 0.944	1.303/ 1.289	122.3/ 122.4					Ref. [6]
		0.964	1.312	117.0	671	1382	3881		Ref. [7]
	2^1X	1.557	1.263	111.398	618.54	1446.67	2739.30	-100.0980987	
	3^1X	0.974	1.431	106.853	822.00	1014.78	3699.52	-99.98977667	
	1^3X	0.969	1.355	110.900	1117.65	1350.31	3673.90	-100.1323634	
					1094	1328	3794		Ref. [7]
	2^3X	0.961	1.374	116.644	752.38	1275.10	3865.40	-100.1002726	
	3^3X				Dissociation				
difference		0.587	0.052	4.466	85.05	39.78	1075.9	0.1484509	
COH	1^2X	0.983	1.289	110.426	1189.84	1378.62	3415.20	-113.3280569	
		0.980	1.300	111.7	1167	1382	3613		Ref.[8]
		0.976	1.273	112.956	1146.6	1402.6	3489.1		Ref.[9]
	2^2X	0.969	1.327	111.540	802.58	1271.06	3776.60	-113.2893471	
		0.96211/ 0.96388	1.30507/ 1.31398	114.386/ 117.006	705.0/ 706.7	1317.7/ 1289.3	3847.4/ 3834.2		Ref.[9]
	3^2X				Non-convergence				
	1^4X	0.968	1.399	104.762	1067.07	1297.97	3717.90	-113.1976147	
	2^4X				Dissociation				
	3^4X				Dissociation				
difference		0.014	0.038	1.114	387.26	107.56	361.4	0.0387099	
NOH	1^1X	0.993	1.280	109.142	1206.69	1464.32	3197.50	-129.8904345	
		0.985/ 0.984/	1.263/ 1.265	110.42/ 110.30	1238	1430	2928		Ref.[10]
	2^1X	0.979	1.332	106.616	1119.80	1252.14	3528.40	-129.8600196	
	3^1X	0.972	1.380	106.581	856.96	1082.29	3726.01	-129.80783679	
	1^3X	0.972	1.353	104.990	1098.21	1272.63	3658.60	-129.9159503	
		0.968	1.326	107.47	1108	1215	3523		Ref.[10]
	2^3X				Dissociation				
	3^3X	0.976	2.205	104.644	180.46	290.24	3634.60	-129.8989907	
difference		0.004	0.852	0.346	917.75	982.39	24	0.0169596	
O2H	1^2X	0.974	1.360	102.699	1051.66	1423.81	3615.90	-150.3166449	
		0.971	1.330	104.3	1111.9	1413.3	3482.4		Exp.[11]
		0.954	1.370	104	1099.31	1381.1	3441.3		Ref.[12]
	2^2X	0.973	1.442	99.420	863.46	1261.05	3683.80	-150.2873047	
	3^2X				Dissociation				
	1^4X				Dissociation				
	2^4X				Dissociation				

	3^4X				Dissociation				
difference		0.001	0.082	3.279	188.2	162.76	67.9	0.0293402	
NaOH	1^1X	0.955	1.956	179.995	263.05	569.04	3915.10	-237.4269107	
		0.96	1.95			431			Exp.[13]
	2^1X	0.975	2.699	126.397	89.91	215.75	3716.83	-237.36880952	
	3^1X				virtual frequency				
	1^3X	0.976	2.631	119.020	120.66	245.80	3713.30	-237.3754286	
	2^3X	0.974	2.643	180.042	97.43	269.52	3741.50	-237.3742288	
	3^3X	0.973	2.359	179.734	212.53	268.28	3754.47	-237.28238159	
difference		0.02	0.743	53.598	173.14	353.29	198.27	0.05810118	
MgOH	1^2X	0.955	1.804	140.911	286.11	741.93	3949.30	-275.2102068	
		0.872	1.780						Exp.[14]
		0.941	1.773		389	785	4301		Ref.[4]
		0.9467	1.7745		160	747	3851		Ref.[15]
	2^2X	0.964	1.837	112.378	633.47	748.95	3828.80	-275.0890778	
	3^2X	0.982	2.105	103.944	265.10	881.45	3593.94	-275.07416817	
	1^4X	0.980	2.351	104.086	208.31	456.53	3636.60	-275.0231675	
	2^4X	0.979	2.363	116.352	198.09	428.22	3654.90	-275.0220575	
	3^4X	0.970	2.383	173.748	152.48	352.08	3739.89	-275.00315871	
difference		0.009	0.033	28.533	347.36	7.02	120.5	0.1211290	
AlOH	1^1X	0.951	1.686	172.055	144.54	836.33	4017.40	-317.5407782	
		0.950	1.691	162.26	98	834	4035		Exp.[16]
	2^1X	0.968	1.783	107.585	609.78	932.90	3773.90	-317.3601877	
					654.2	825.2	3258.4		Exp.[17]
	3^1X				Dissociation				
	1^3X	0.963	1.730	114.555	739.09	834.02	3820.00	-317.4208038	
	2^3X	0.956	1.718	126.175	506.17	824.74	3920.20	-317.4085655	
	3^3X	0.986	1.703	115.910	576.87	756.11	3332.44	-317.29772882	
difference		0.017	0.097	64.47	465.24	96.57	243.50	0.1805905	
SiOH	1^2X	0.966	1.671	114.330	827.12	879.39	3771.10	-364.4664058	
		0.969	1.647	118.5					Exp.[18]
		0.9603	1.6508	118.57					Ref.[18]
	2^2X	0.959	1.666	125.933	532.87	852.32	3890.00	-364.4503606	
		0.9532	1.6380	137.90					Ref.[18]
	3^2X				virtual frequency				
	1^4X	0.966	1.712	108.245	737.31	1008.65	3762.90	-364.3484888	
	2^4X	0.971	3.037	171.796	81.69	160.70	3711.28	-364.30612696	
	3^4X				Dissociation				
difference		0.007	0.005	11.603	294.25	27.07	118.9	0.0160452	
POH	1^1X	0.969	1.643	109.272	868.09	1112.09	3704.90	-416.2345280	
	2^1X	0.967	1.657	111.738	820.45	982.15	3747.00	-416.2187978	
	3^1X	0.963	1.664	117.814	674.08	847.20	3835.31	-416.18754847	
	1^3X	0.962	1.671	111.470	773.38	1014.92	3848.80	-416.2428944	

	2^3X	0.983	2.212	97.903	300.18	566.41	3577.20	-416.0896498	
	3^3X				Dissociation				
difference		0.021	0.541	13.567	473.2	448.51	271.6	0.1532446	
SOH	1^2X	0.968	1.663	105.981	805.92	1232.95	3722.70	-473.0346473	
		0.963	1.647	107.4					Ref.[19]
		0.963	1.645	106.4	821	1202	3729		Ref.[20]
	2^2X	0.968	1.700	106.080	721.39	1105.29	3738.80	-473.0131165	
	3^2X				Dissociation				
	1^4X				Dissociation				
	2^4X				Dissociation				
	3^4X				Dissociation				
difference		0.000	-0.037	-0.099	84.53	127.66	-16.1	-0.0215308	
KOH	1^1X	0.959	2.222	179.993	328.12	461.29	3797.30	-674.6497061	
		0.912	2.2115		300	408			Exp.[21]
					320	390			Exp.[22]
	2^1X	0.973	3.014	179.982	85.40	503.53	3681.46	-674.6041247	
	3^1X	0.951	2.936	180.245	106.53	601.10	4036.86	-674.57738291	
	1^3X	0.975	2.998	127.865	101.15	193.30	3658.50	-674.6053536	
	2^3X	0.973	2.970	180.001	95.84	238.63	3680.07	-674.5191102	
	3^3X	0.953	2.803	123.825	161.07	330.02	4005.28	-674.53872446	
difference		0.014	0.792	0.013	242.84	41.26	115.6	0.0455814	
CaOH	1^2X	0.932	2.005	179.995	402.46	626.90	4294.40	-752.2877004	
		0.930	1.976		339	606.1			Exp.[21]
		0.922	1.985						Exp.[14]
		9.333	2.0038	179.97	411/408	622	4276		Ref.[23]
		0.9562	1.9746	180.00					Exp.[24]
	2^2X	0.932	1.977	180.000	383.77	652.80	4298.40	-752.2178303	
		0.932	1.956						Exp.[21]
		0.9332	1.9769	179.9	402/386	646	4279		Ref.[23]
		0.9572	1.9532	180.00					Exp.[24]
	3^2X				Non-convergence				
	1^4X				Dissociation				
	2^4X				Dissociation				
	3^4X				Dissociation				
difference		0	0.028	0.005	18.69	25.9	4.0	0.0698701	
GaOH	1^1X	0.964	1.828	121.577	550.30	639.99	3830.30	-1998.8943855	
		0.969	1.832	126.1	497	613.2	3767.1		Exp.[25]
	2^1X				Dissociation				
	3^1X				Dissociation				
	1^3X	0.966	1.814	108.431	642.32	917.31	3766.80	-1998.7633443	
	2^3X	0.965	1.827	111.634	600.09	807.75	3789.30	-1998.7473206	
	3^3X	0.980	2.315	101.364	548.66	1489.92	3625.48	-1998.72203955	
difference		/	/	/	/	/	/	/	

GeOH	1^2X	0.967	1.796	111.530	679.86	866.80	3748.90	-2150.9455931	
		0.964	1.812	117.0	638.5				Exp.[26]
		0.951	1.769	116.59	716	808	4026		Ref.[27]
	2^2X	0.963	1.800	119.354	608.19	691.21	3824.90	-2150.9291853	
	3^2X	1.009	1.895	180.025	300.26	688.06	2700.01	-2150.80638820	
	1^4X	0.971	1.862	103.656	519.40	1033.53	3697.50	-2150.8216064	
	2^4X				Non-convergence				
	3^4X				Dissociation				
difference		0.004	0.004	7.824	71.67	175.59	76.0	0.0164078	
AsOH	1^1X	0.969	1.782	107.740	706.21	1049.48	3718.40	-2309.7373966	
	2^1X	0.968	1.797	110.096	671.57	946.93	3743.70	-2309.7242295	
	3^1X	0.965	1.806	114.550	632.09	775.88	3791.33	-2309.694079	
	1^3X	0.966	1.824	108.672	611.29	979.05	3771.90	-2309.7468493	
	2^3X				Dissociation				
	3^3X				Non-convergence				
difference		/	/	/	/	/	/	/	
SeOH	1^2X	0.968	1.804	105.321	662.77	1159.24	3729.10	-2475.3875138	
		0.966	1.766	105.900					Ref.[28]
	2^2X	0.969	1.839	105.698	600.38	1056.74	3731.40	-2475.3698670	
	3^2X				Dissociation				
	1^4X				Dissociation				
	2^4X	1.572	2.069	90.569	338.83	684.69	3047.98	-2475.17412838	
	3^4X				Dissociation				
difference		0.001	0.035	0.377	62.39	102.5	2.3	0.0176468	
RbOH	1^1X	0.959	2.327	180.000	297.54	403.28	3789.26	-99.27645737	
		0.957	2.301	180.000	309	354.4	3600		Ref.[29]
		0.965	2.305	180.000					Exp.[30]
		0.956	2.488	180.000	277	369	3902		Ref.[31]
	2^1X	0.973	3.217	180.000	68.82	427.22	3683.05	-99.23207614	
	3^1X	0.951	3.200	180.006	68.49	685.96	4036.86	-99.20640565	
	1^3X	0.952	3.164	132.343	87.12	159.16	4034.32	-99.21061136	
	2^3X				virtual frequency				
	3^3X	0.953	2.965	122.825	138.11	317.87	3997.24	-99.16917874	
difference		0.014	0.89	0	228.72	23.94	106.21	0.04438123	
SrOH	1^2X	0.933	2.140	180.000	366.20	536.08	4293.51	-105.85742286	
		0.922	2.111	180.000	361	528			Exp.[32]
		0.945	2.102	180.000	360	522	3700		Exp.[33]
	2^2X	0.932	2.115	180.000	389.41	550.56	4288.43	-105.78827317	
		0.946	2.088	180.000					Exp.[33]
						544			Exp.[34]
	3^2X				Non-convergence				
	1^4X	0.955	2.763	111.858	168.29	383.31	3985.05	-105.72724307	
	2^4X				virtual frequency				

	3^4X				Dissociation				
difference		0.001	0.025	0	23.21	14.48	5.08	0.06914969	
InOH	1^1X	0.940	2.038	129.331	472.22	589.54	4178.10	-5815.7581042	
		0.911/ 0.980	2.0167/ 2.031	132/ 127.7					Exp.[35]
				132	378	542			Exp.[36]
	2^1X	0.964	2.056	121.096	519.42	576.95	3821.70	-5815.7888674	
	3^1X				Dissociation				
	1^3X	0.971	2.016	109.564	575.97	815.77	3717.00	-5815.6557034	
				105	496	829			Exp.[36]
	2^3X	0.963	2.015	117.549	569.75	694.10	3833.60	-5815.6586702	
	3^3X				Dissociation				
difference		0.024	0.018	8.235	47.2	12.59	356.4	0.0307632	
SnOH	1^2X	0.962	1.981	117.608	634.10	744.63	3840.40	-6098.4930371	
	2^2X	0.940	2.000	126.927	524.31	629.73	4184.50	-6098.4888271	
	3^2X				Dissociation				
	1^4X	0.943	2.037	108.688	530.41	975.83	4138.50	-6098.4001203	
	2^4X				Dissociation				
	3^4X				Dissociation				
difference		0.022	0.019	9.319	109.79	114.90	344.1	0.0042100	
SbOH	1^1X	0.943	1.982	111.811	624.30	966.19	4137.40	-6388.9727957	
	2^1X	0.943	1.989	114.637	607.69	865.10	4135.90	-6388.9672654	
	3^1X	0.942	1.987	120.259	586.22	745.49	4155.72	-6388.94491042	
	1^3X	0.942	2.014	112.280	552.93	908.86	4153.50	-6388.9852139	
	2^3X				Dissociation				
	3^3X				Non-convergence				
difference		/	/	/	/	/	/	/	
TeOH	1^2X	0.943	1.985	108.866	608.83	1087.87	4130.10	-6687.2972143	
		0.9525	1.984	108	582	959	3655		Ref.[37]
	2^2X	0.944	2.001	110.772	577.78	977.33	4119.10	-6687.2859932	
				113					Ref.[37]
	3^2X				Dissociation				
	1^4X	0.949	2.379	102.972	386.46	717.83	4059.50	-6687.2052910	
	2^4X				Dissociation				
	3^4X				Dissociation				
difference		0.001	0.016	1.906	31.05	110.54	11	0.0112211	
BaOH	1^2X	0.934	2.275	180.001	335.31	487.37	4267.44	-100.61899699	
		0.923	2.201		341.6	492.4			Exp.[32]
		0.927	2.200						Exp.[38]
	2^2X	0.934	2.259	180.000	373.23	493.78	4253.75	-100.57513127	
	3^2X				Non-convergence				
	1^4X	0.956	2.953	112.026	157.65	355.53	3961.38	-100.49023407	
	2^4X	0.962	2.953	154.142	137.94	486.21	3905.63	-100.48812360	

	3^4X				Dissociation				
difference		0	0.016	0.001	37.92	6.41	13.69	0.04386572	
RaOH	1^2X	0.934	2.362	179.999	386.84	457.00	4252.83	-99.1881411	
		0.94	2.38	180.0	366	437	4243		Ref.[39]
	2^2X	0.934	2.338	179.999	396.95	476.20	4259.38	-99.1327616	
		0.94	2.35	180.0	383	461	4248		Ref.[39]
	3^2X				Non-convergence				
	1^4X	0.955	3.082	111.776	137.18	349.46	3968.80	-99.0606957	
	2^4X	0.960	3.040	154.813	134.01	461.18	3921.30	-99.0588003	
	3^4X				Dissociation				
difference		0.000	0.024	0.000	10.11	32.58	19.2	0.0553795	
CsOH	1^1X	0.960	2.446	180.000	280.88	304.43	3768.69	-95.33595961	
		0.960	2.391	180.000	306	335.6	3600		Ref.[29]
		0.957	2.658	180.000	327	336	3887		Ref.[31]
		0.969	2.395	180.000					Exp.[40]
					304.2	335.6			Exp.[41]
	2^1X	0.973	3.424	180.000	66.67	342.83	3682.63	-95.28852669	
	3^1X				Non-convergence				
	1^3X				virtual frequency				
	2^3X	0.973	3.384	180.000	72.62	175.22	3682.48	-95.28901199	
	3^3X				Dissociation				
difference		0.013	0.978	0.000	214.21	38.4	86.06	0.04743292	
FrOH	1^1X	0.964	2.515	180.000	207.85	355.62	3717.24	-94.31469397	
		0.958	2.500	180.000	313	351	3878		Ref.[31]
	2^1X	0.976	3.90	140.932	23.56	89.01	3606.11	-94.28059596	
	3^1X								
	1^3X				virtual frequency				
	2^3X				virtual frequency				
	3^3X				virtual frequency				
difference		0.012	1.385	39.068	184.29	266.61	111.13	0.03409801	

Table S2 By using TD/DFT method implemented in Gaussian 16, the equilibrium structures and fundamental frequencies for the screened molecules (CaOH, SrOH, BaOH, RaOH, SOH, and SeOH) by MCSCF are calculated and list corresponding experimental and theoretical molecular parameters. For the H, O, S, Se and Ca, the structural parameters are calculated by B3LYP/cc-pVTZ. For Sr, B3LYP/cc-pVTZ-X2C is employed, while for Ba and Ra, B3LYP/def-SVP is

adopted, respectively. The blue part is the difference in bond lengths, bond angle, and vibrational frequencies between the lowest two electronic states of each molecule. The internuclear distances R_i are given in Å and the harmonic frequencies of normal mode v_l in cm^{-1}. The X represents the symmetry of state because all the calculations are carried out without symmetry.

		R_{O-H}	R_{O-M}	∠ M-O-H	2	1	3	energy	
SOH	1^2X	0.967	1.648	108.412	842.50	1179.27	3744.25	-474.0258564	
		0.963	1.647	107.4					Ref.[19]
		0.963	1.645	106.4	821	1202	3729		Ref.[20]
	2^2X	0.966	1.674	109.907	771.41	1018.94	3780.70	-474.0028341	
	3^2X				Non-convergence				
	1^4X	0.972	2.085	102.317	391.39	642.49	3702.73	-473.9298231	
	2^4X	1.298	1.768	91.984	661.95	968.59	2863.36	-473.81618	
	3^4X				Non-convergence				
difference		0.001	0.026	1.495	71.09	160.33	36.45	0.0230223	
CaOH	1^2X	0.955	1.971	180.000	334.93	633.29	3935.25	-753.5083407	
		0.930	1.976		339	606.1			Exp.[21]
		0.922	1.985						Exp.[14]
		9.333	2.0038	179.97	411/408	622	4276		Ref.[23]
		0.9562	1.9746	180.00					Exp.[24]
	2^2X	0.955	1.963	180.000	305.67	612.94	3940.70	-753.4342936	
		0.932	1.956						Exp.[21]
		0.9332	1.9769	179.9	402/386	646	4279		Ref.[23]
		0.9572	1.9532	180.00					Exp.[24]
	3^2X	0.955	1.963	180.000	306.08	612.51	3940.76	-753.4342936	
	1^4X				virtual frequency				
	2^4X				Non-convergence				
	3^4X				Non-convergence				
difference		0	0.008	0	29.26	20.35	5.45	0.0740471	
SeOH	1^2X	0.966	1.793	107.445	697.20	1104.43	3778.11	-2477.446099	
		0.966	1.766	105.900					Ref.[28]
	2^2X	0.966	1.817	108.786	649.68	983.89	3790.55	-2477.428654	
	3^2X	0.970	2.157	112.755	325.61	428.73	3721.85	-2477.361816	
	1^4X				Non-convergence				
	2^4X	1.336	1.888	92.605	590.08	889.38	2756.13	-2477.244162	
	3^4X				Non-convergence				
difference		0	0.024	1.341	47.52	120.54	12.44	0.017445	
SrOH	1^2X	0.955	2.112	175.974	314.06	532.55	3934.30	-3180.5297843	
		0.922	2.111	180.000	361	528			Exp.[32]
		0.945	2.102	180.000	360	522	3700		Exp.[33]
	2^2X	0.955	2.103	176.789	314.06	532.55	3934.30	-3180.4659659	

		0.946	2.088	180.000					Exp.[33]
						544			Exp.[34]
	3^2X	0.955	2.103	176.789	348.99	532.76	3934.35	-3180.4659618	
	1^4X				virtual frequency				
	2^4X				Non-convergence				
	3^4X	0.984	2.667	179.578	194.44	310.18	3388.23	-3180.332551	
difference		0	0.009	0.815	0	0	0	0.0638184	
BaOH	1^2X	0.956	2.268	180.000	333.35	492.66	3910.18	-101.3022346	
		0.923	2.201		341.6	492.4			Exp.[32]
		0.927	2.200						Exp.[38]
	2^2X	0.956	2.294	180.000	288.51	465.38	3909.37	-101.2566596	
	3^2X	0.956	2.294	180.000	288.82	464.93	3909.36	-101.2566594	
	1^4X				virtual frequency				
	2^4X				virtual frequency				
	3^4X				virtual frequency				
difference		0	0.026	0	44.84	27.28	0.81	0.045575	
RaOH	1^2X	0.957	2.305	180.000	347.17	464.28	3907.73	-99.8862797	
		0.94	2.38	180.0	366	437	4243		Ref.[39]
	2^2X	0.956	2.308	180.000	318.43	459.14	3915.16	-99.8213846	
		0.94	2.35	180.0	383	461	4248		Ref.[39]
	3^2X	0.956	2.309	180.000	318.29	458.90	3915.19	-99.82138469	
	1^4X				virtual frequency				
	2^4X				Non-convergence				
	3^4X	0.9818	2.976	180.000	135.1901	1840.7436	3430.6424	-99.69457468	
difference		0.001	0.003	0	28.74	5.14	7.43	0.0648951	

Table S3 Fitting parameters and root mean square errors (in cm^{-1}) of the two-body terms for SOH and SeOH molecules.

	OH	OS	HS	OSe	HSe
w_{31}	1.06591068E+00	1.00574608E+00	1.28941611E+00	1.15047659E+00	8.54717421E-01
w_{32}	2.21143445E+00	2.36936228E+00	1.28322974E+00	2.74767195E+00	2.04487456E+00
w_{33}	1.07000000E+04	1.07000000E+04	1.07000000E+04	1.07000000E+04	1.07000000E+04
w_{34}	2.13000000E+04	2.13000000E+04	2.13000000E+04	2.13000000E+04	2.13000000E+04
w_{35}	2.21545177E+00	-7.77371197E+02	-7.77371197E+02	-7.77371197E+02	-7.77371197E+02
b_{21}	-5.71811388E-01	4.66510320E-05	-2.49254323E+00	-1.06317888E+00	-1.88023664E+00
b_{22}	-7.70304074E-01	-2.12340593E+00	1.36005536E+00	-3.18955667E+00	1.80319024E-01
b_{23}	-1.39000000E+05	-1.39000000E+05	-1.39000000E+05	-1.39000000E+05	-1.39000000E+05
b_{24}	1.07000000E+04	1.07000000E+04	1.07000000E+04	1.07000000E+04	1.07000000E+04
b_{25}	1.53066123E-01	6.91500843E+03	6.91500843E+03	6.91500843E+03	6.91500843E+03

w_{211}	1.95713733E+06	3.60000000E+05	3.60000000E+05	3.59988035E+05	3.60000000E+05
w_{221}	-3.32648081E+06	-3.43000000E+06	-3.43000000E+06	-3.43001117E+06	-3.43000000E+06
w_{231}	-1.17737612E+05	2.22000000E+04	2.22000000E+04	2.22053930E+04	2.22000000E+04
w_{241}	6.84871222E+04	7.97000000E+04	7.97000000E+04	7.96946072E+04	7.97000000E+04
w_{251}	1.46416448E+06	1.71000000E+06	1.71000000E+06	1.70999471E+06	1.71000000E+06
w_{212}	3.63000000E+02	3.63000000E+02	3.63000000E+02	3.63000000E+02	3.63000000E+02
w_{222}	-8.83000000E+01	-8.83000000E+01	-8.83000000E+01	-8.83000000E+01	-8.83000000E+01
w_{232}	3.39000000E+02	3.39000000E+02	3.39000000E+02	3.39000000E+02	3.39000000E+02
w_{242}	-3.87000000E+02	-3.87000000E+02	-3.87000000E+02	-3.87000000E+02	-3.87000000E+02
w_{252}	1.76000000E+02	1.76000000E+02	1.76000000E+02	1.76000000E+02	1.76000000E+02
w_{213}	-2.15000000E+02	-2.15000000E+02	-4.46405211E+00	-2.15000000E+02	5.91244302E-01
w_{223}	1.21000000E+02	1.21000000E+02	-2.46497333E-01	1.21000000E+02	-7.21582735E+00
w_{233}	6.09000000E+02	6.09000000E+02	5.51477515E+02	6.09000000E+02	5.48594146E+02
w_{243}	2.16000000E+02	2.16000000E+02	2.73766667E+02	2.16000000E+02	2.76640773E+02
w_{253}	5.52000000E+02	5.52000000E+02	6.09872377E+02	5.52000000E+02	6.12790058E+02
w_{214}	-8.64588828E-02	-1.33582659E+00	-8.28774067E-02	-1.31219360E+00	-4.20118859E-01
w_{224}	-2.80589749E-01	4.85828089E-01	8.37718861E+00	1.23138091E+00	6.92831183E+00
w_{234}	-2.61314134E+00	-2.78522735E+00	-3.07971188E-01	1.04355742E+00	-6.56828289E-01
w_{244}	-3.86364216E+00	-3.96550923E+00	-6.37434225E+00	-2.55025995E+00	-6.10868815E+00
w_{254}	2.47421861E+00	2.98003812E+00	4.47546797E-01	4.39551727E+00	8.50251489E-01
w_{215}	8.22953580E+00	5.00425433E+01	1.95944107E-01	1.86209760E+01	1.28588870E+00
w_{225}	1.35435209E+02	6.65205071E+02	5.70957924E+02	1.17032296E+03	5.71359212E+02
w_{235}	1.02571829E+02	2.48085737E+02	2.10601378E+02	3.70297201E+02	2.10982772E+02
w_{245}	3.39889419E+02	1.90664772E+02	2.28618845E+02	6.69954563E+01	2.28247063E+02
w_{255}	-2.25825705E+02	-3.52482538E+02	-3.20312874E+02	-4.59539455E+02	-3.20674569E+02
b_{11}	-2.80943919E+05	-2.93000000E+05	-2.93000000E+05	-2.93005390E+05	-2.93000000E+05
b_{12}	2.12000000E+02	2.12000000E+02	2.12000000E+02	2.12000000E+02	2.12000000E+02
b_{13}	-3.94000000E+02	-3.94000000E+02	-3.37415679E+02	-3.94000000E+02	-3.34541340E+02
b_{14}	2.08477430E+00	2.27035492E+00	-3.90562152E-05	3.14744177E+00	4.46946859E-01
b_{15}	-1.59709070E+02	-3.09697301E+02	-2.71718613E+02	-4.30631042E+02	-2.72135799E+02
w_{11}	-2.42397439E+07	-2.42521021E+07	-2.40216785E+07	-2.41961889E+07	-2.38374814E+07
w_{12}	-4.07397430E+07	-4.07505024E+07	-4.05220676E+07	-4.07097815E+07	-4.03446903E+07
w_{13}	-4.59933523E+04	-2.63714055E+05	-8.64622576E+05	-5.89301148E+05	-2.53335992E+06
w_{14}	-1.18960173E+08	-1.18937246E+08	-1.19194641E+08	-1.18658558E+08	-1.19368457E+08
w_{15}	-2.84400943E+07	-2.84497067E+07	-2.82232051E+07	-2.82605113E+07	-2.79915772E+07
b_0	2.48397436E+07	2.48515863E+07	2.46219755E+07	2.48058139E+07	2.44213675E+07
RMS	2.478	14.930	5.125	12.757	15.830

Table S4 Fitting parameters and root mean square errors (in cm^{-1}) of the three-body terms of the X^2A'' and $1^2A'$ states for SOH and SeOH molecules.

	SOH	SeOH

	X^2A''	$1^2A'$	X^2A''	$1^2A'$
p_{311}	-5.13000015E+04	-5.13000000E+04	-3.92387256E+04	-4.54119603E+04
p_{321}	-9.03000265E+03	-9.03000000E+03	-7.43863342E+03	-8.14093313E+03
p_{331}	-5.96000026E+04	-5.96000000E+04	-5.73850061E+04	-5.83829127E+04
p_{341}	1.95459486E-01	2.41560916E-01	2.40454166E-01	2.42999039E-01
p_{351}	-2.09244555E-02	-3.91773924E-02	-3.51879729E-02	-4.08748796E-02
p_{361}	2.61671642E-04	1.78326436E-02	5.60913455E-03	1.53287211E-02
p_{371}	1.17655033E-01	4.48557432E-02	3.17124070E-02	-4.74199164E-03
p_{381}	-1.53545652E-01	1.51777740E-01	4.57883608E-01	3.42070857E-01
p_{391}	1.22109322E-01	4.51849634E-02	-1.92560228E-01	1.77675892E-04
p_{3101}	2.13462582E-01	1.65000400E+00	4.07111477E+05	4.07111477E+05
p_{312}	-8.66580468E-02	3.33394749E-01	3.82330362E+05	3.82330362E+05
p_{322}	-1.43045120E-01	-1.73833935E+00	-9.58973619E+05	-9.58973619E+05
p_{332}	2.39087693E-01	-1.47639703E-02	8.93789108E-02	-3.57952786E-03
p_{342}	2.15163222E-01	1.80552802E-02	9.88243926E-03	-4.57625239E-03
p_{352}	-2.69838673E-01	-3.37904008E-02	-1.10706372E-01	-7.25819206E-02
p_{362}	-3.27506461E-01	-2.72316219E-01	-3.93904709E-01	-3.03719897E-01
p_{372}	-1.56509564E+00	-5.08728564E-02	-1.71164569E-01	-5.46126337E-02
p_{382}	2.00710197E+00	6.33516889E-02	2.68573199E-01	1.01476413E-01
p_{392}	-7.71233712E-02	-5.06422352E-08	-1.76097700E-01	-8.02747396E-02
p_{3102}	-7.89962270E-03	-4.40014689E-02	-9.93604088E-03	-2.74329287E-02
p_{313}	2.77287445E-02	5.19071635E-02	1.40494047E-01	1.31107988E-01
p_{323}	2.19411294E-01	2.43174172E-01	2.43309026E-01	2.42997723E-01
p_{333}	-2.71830898E-02	-3.43940729E-02	-3.42934188E-02	-3.58679621E-02
p_{343}	1.81683799E-02	1.35024912E-02	9.36785440E-03	1.15878828E-02
p_{353}	1.84986067E+01	1.85000000E+01	1.84992936E+01	1.84992936E+01
p_{363}	1.13981795E+01	1.14000000E+01	1.13994682E+01	1.13994682E+01
p_{373}	-1.68173240E+00	-1.68000000E+00	-1.68038432E+00	-1.68038432E+00
p_{383}	-2.23865478E-01	-2.22000000E-01	-2.22424441E-01	-2.22424441E-01
p_{393}	-1.82014316E+01	-1.82000000E+01	-1.82004699E+01	-1.82004699E+01
p_{3103}	-7.53184176E+00	-7.53000000E+00	-7.53073822E+00	-7.53073822E+00
a_{21}	2.38999998E+05	2.39000000E+05	2.44901141E+05	2.40884758E+05
a_{22}	-3.38130717E-01	-3.59342578E-01	-3.72991040E-01	-3.61540728E-01
a_{23}	-1.06906696E-01	-1.31332871E+00	-6.51995990E-01	-1.65718190E+00
a_{24}	-3.01925490E-01	-4.32372445E+00	-3.95443834E+05	-3.95443834E+05
a_{25}	-3.03686562E-01	-3.34628856E-01	-2.77412678E-01	-8.02846103E-03
a_{26}	9.94503179E-02	4.21527554E-01	3.79456501E-01	3.98490426E-01
a_{27}	-1.18745892E-01	1.58918897E-02	7.20339877E-02	-2.95434510E-01
a_{28}	-3.91855582E-01	-3.61773995E-01	-3.91715272E-01	-3.57679121E-01
a_{29}	1.16997616E+02	1.17000000E+02	1.16999403E+02	1.16999403E+02
a_{30}	-1.17175856E+00	-1.17000000E+00	-1.17069910E+00	-1.17069910E+00
p_{211}	-9.05216279E+00	-9.05000000E+00	-9.05040958E+00	-9.05040958E+00
p_{221}	-1.41002326E+02	-1.41000000E+02	-1.41000694E+02	-1.41000694E+02

p_{231}	-1.47002670E+02	-1.47000000E+02	-1.47000570E+02	-1.47000570E+02
p_{241}	1.24997306E+02	1.25000000E+02	1.24999384E+02	1.24999384E+02
p_{251}	-1.29002142E+02	-1.29000000E+02	-1.29000676E+02	-1.29000676E+02
p_{261}	6.45979926E+01	6.46000000E+01	6.45995207E+01	6.45995207E+01
p_{271}	1.30998475E+02	1.31000000E+02	1.30999297E+02	1.30999297E+02
p_{281}	6.51824524E+00	6.52000000E+00	6.51934260E+00	6.51934260E+00
p_{291}	-1.74001749E+02	-1.74000000E+02	-1.74000753E+02	-1.74000753E+02
p_{2101}	1.26998063E+02	1.27000000E+02	1.26999503E+02	1.26999503E+02
p_{212}	1.03195072E-01	1.64000000E+01	1.63993623E+01	1.63993623E+01
p_{222}	1.05917895E+03	-6.56000000E+01	-6.56006402E+01	-6.56006402E+01
p_{232}	-3.30710535E+02	2.20000000E+01	2.19995933E+01	2.19995933E+01
p_{242}	6.24511949E+01	1.39000000E+02	1.38999351E+02	1.38999351E+02
p_{252}	-1.24092047E+02	-4.03000000E+02	-4.03000599E+02	-4.03000599E+02
p_{262}	-3.79852711E-01	9.73000000E+01	9.72993258E+01	9.72993258E+01
p_{272}	8.64832775E+02	3.00000000E+02	2.99999572E+02	2.99999572E+02
p_{282}	-4.07905866E+02	1.15000000E+02	1.14999339E+02	1.14999339E+02
p_{292}	5.03522682E+01	8.26000000E+01	8.25993157E+01	8.25993157E+01
p_{2102}	-4.95940901E+01	-6.60000000E+01	-6.60006240E+01	-6.60006240E+01
p_{213}	-2.25452199E+05	-1.86175928E+03	-1.06533508E+03	-2.01954135E+03
p_{223}	4.78998532E+02	-1.21401185E+03	-1.25781650E+04	-2.73034768E+03
p_{233}	1.30999760E+03	1.81764286E+02	-4.84387478E+02	-8.14081022E+01
p_{243}	2.32174857E+05	9.41258108E+02	3.09413471E+03	7.87130003E+02
p_{253}	2.08201286E+05	1.02561441E+03	-2.30646810E+03	9.08870854E+02
p_{263}	1.54275873E+05	4.52216743E+02	-7.60953945E+02	1.27839137E+03
p_{273}	-9.61821637E+04	-1.34770953E+02	-7.79690908E+02	8.37921589E+03
p_{283}	9.02981447E+01	1.74250644E+03	1.12216799E+04	-7.52804092E+01
p_{293}	-2.12841277E+05	-1.09065538E+02	-8.52793680E+02	4.85885108E+01
p_{2103}	1.73513895E+05	1.82324798E+02	-1.20637159E+03	2.42289820E+01
p_{214}	1.28999791E+03	1.29000000E+03	1.28999925E+03	1.28999925E+03
p_{224}	-2.00000225E+03	-2.00000000E+03	-2.00000076E+03	-2.00000076E+03
p_{234}	9.29997473E+02	9.30000000E+02	9.29999552E+02	9.29999552E+02
p_{244}	2.20999848E+03	2.21000000E+03	2.20999925E+03	2.20999925E+03
p_{254}	-2.55000231E+03	-2.55000000E+03	-2.55000048E+03	-2.55000048E+03
p_{264}	1.36999784E+03	1.37000000E+03	1.36999939E+03	1.36999939E+03
p_{274}	2.98999791E+03	2.99000000E+03	2.98999939E+03	2.98999939E+03
p_{284}	-2.34000243E+03	-2.34000000E+03	-2.34000071E+03	-2.34000071E+03
p_{294}	-1.31000268E+03	-1.31000000E+03	-1.31000041E+03	-1.31000041E+03
p_{2104}	3.04999858E+03	3.05000000E+03	3.04999952E+03	3.04999952E+03
p_{215}	5.62004630E+01	5.26968962E+02	5.28347806E+02	5.26264892E+02
p_{225}	3.13201978E+03	5.33400207E+02	5.24133397E+02	5.01818095E+02
p_{235}	1.96301594E+02	1.24811501E+01	3.27665190E+01	2.22660312E+01
p_{245}	-2.18413251E+02	1.84896523E+03	1.84761080E+03	1.84969710E+03
p_{255}	2.96961808E+00	-1.71670618E+02	-1.65378673E+02	-1.83294599E+02

p_{265}	-7.20905628E-02	7.36636468E+01	7.11721584E+01	7.33917212E+01
p_{275}	-1.33924327E+02	-2.71612267E+02	-1.95502261E+02	-1.77579540E+02
p_{285}	-2.74397953E+03	-4.54517368E+02	-4.95231402E+02	-4.69212039E+02
p_{295}	-5.51916623E+01	4.16902119E+02	4.18285710E+02	4.16199364E+02
p_{2105}	2.09309631E+01	-4.47292552E+02	-4.48676008E+02	-4.46589677E+02
p_{216}	1.01999984E+04	1.02000000E+04	1.01999994E+04	1.01999994E+04
p_{226}	-6.91000224E+03	-6.91000000E+03	-6.91000048E+03	-6.91000048E+03
p_{236}	-3.46000017E+04	-3.46000000E+04	-3.46000006E+04	-3.46000006E+04
p_{246}	2.34999977E+04	2.35000000E+04	2.34999996E+04	2.34999996E+04
p_{256}	-7.24000257E+03	-7.24000000E+03	-7.24000074E+03	-7.24000074E+03
p_{266}	-1.07000021E+04	-1.07000000E+04	-1.07000007E+04	-1.07000007E+04
p_{276}	-7.24000181E+03	-7.24000000E+03	-7.24000070E+03	-7.24000070E+03
p_{286}	-7.80000258E+03	-7.80000000E+03	-7.80000043E+03	-7.80000043E+03
p_{296}	-6.27000261E+03	-6.27000000E+03	-6.27000042E+03	-6.27000042E+03
p_{2106}	8.49999983E+04	8.50000000E+04	8.49999995E+04	8.49999995E+04
p_{217}	7.28719030E+05	5.57427587E+03	5.57427520E+03	5.57427520E+03
p_{227}	-6.69552708E+06	1.99000000E+02	1.98999523E+02	1.98999523E+02
p_{237}	-1.83151856E+06	-5.31631035E+02	-5.31631579E+02	-5.31631579E+02
p_{247}	7.95741338E+05	2.42449500E+03	2.42449454E+03	2.42449454E+03
p_{257}	-1.87459949E+06	1.32811596E+03	1.32811554E+03	1.32811554E+03
p_{267}	-1.69279576E+06	5.85282446E+02	5.85281835E+02	5.85281835E+02
p_{277}	3.01497081E+06	-7.21000000E+01	-7.21007502E+01	-7.21007502E+01
p_{287}	-1.21892719E+07	5.81000000E+01	5.80995769E+01	5.80995769E+01
p_{297}	-8.25293976E+05	2.91000000E+01	2.90995811E+01	2.90995811E+01
p_{2107}	2.20331198E+04	-4.88147365E+03	-4.88147435E+03	-4.88147435E+03
p_{218}	-1.18020823E+01	-1.18000000E+01	-1.18007285E+01	-1.18007285E+01
p_{228}	3.45998064E+02	3.46000000E+02	3.45999570E+02	3.45999570E+02
p_{238}	4.82983377E+01	4.83000000E+01	4.82993736E+01	4.82993736E+01
p_{248}	4.37923782E+05	-7.44000000E+01	-7.44007480E+01	-7.44007480E+01
p_{258}	4.39998169E+02	4.40000000E+02	4.39999410E+02	4.39999410E+02
p_{268}	3.74455196E+05	-8.38000000E+01	-8.38004916E+01	-8.38004916E+01
p_{278}	8.14982376E+01	8.15000000E+01	8.14992592E+01	8.14992592E+01
p_{288}	-2.54613001E+05	-3.83000000E+02	-3.83000449E+02	-3.83000449E+02
p_{298}	1.29986371E+01	1.30000000E+01	1.29994920E+01	1.29994920E+01
p_{2108}	4.84860982E+05	6.86000000E+01	6.85994985E+01	6.85994985E+01
p_{219}	-2.78542487E-02	-1.30431723E-01	1.27701103E-01	3.17128608E-02
p_{229}	1.73593721E+02	5.68536126E+01	-1.00839664E+02	1.04222688E+01
p_{239}	8.61256126E+01	1.13203995E+01	-2.36987651E+00	-2.04356476E+00
p_{249}	-2.19538327E+01	-2.81679738E+01	-2.93386395E+01	-2.20492064E+01
p_{259}	4.85803517E+01	9.30368064E+01	1.52631104E+02	3.36020386E+01
p_{269}	-2.98625199E-01	-3.48842625E+01	-9.85126348E+00	-3.00768619E+01
p_{279}	1.26837587E+02	9.98669234E+01	1.25153623E+02	4.84806612E+01
p_{289}	-1.98062741E+02	-9.39485828E+01	1.27332515E+02	-3.08033763E+01

p_{299}	1.52902950E+01	1.42556847E+01	1.57903299E+01	8.25783251E+00
p_{2109}	6.01915374E+00	6.99693573E+00	5.87029200E+00	1.29951406E+01
p_{2110}	2.19367752E-02	1.68302259E-01	2.96330277E-01	1.48301241E-01
p_{2210}	8.18165181E+01	9.92451539E+00	7.30020963E+00	4.87515329E+00
p_{2310}	-9.11825669E+01	-1.29057077E+01	-1.15183131E+01	-1.47021438E+01
p_{2410}	9.46042279E+00	1.70370467E+01	1.64610386E+01	1.72850669E+01
p_{2510}	-5.47545742E+01	-3.43409516E+01	-4.22683588E+01	-3.64929247E+01
p_{2610}	-1.14619294E+00	-3.60853861E+00	-2.13023214E+01	-6.46013481E+00
p_{2710}	-4.68143496E+01	-1.44256434E+01	2.41166375E-05	-1.14977181E+01
p_{2810}	1.36446992E+01	-1.20998250E+01	-2.67208636E+01	-1.90040054E+01
p_{2910}	1.44097266E+00	-1.05337750E+00	-4.83242286E-01	-1.31387465E+00
p_{21010}	-1.55827979E+00	7.99086904E-01	2.81721672E-01	1.06161788E+00
p_{2111}	7.12187932E+06	2.68000000E+06	2.68000000E+06	2.68000000E+06
p_{2211}	-1.26123623E+07	-1.65000000E+07	-1.65000000E+07	-1.65000000E+07
p_{2311}	-2.37575409E+07	-2.07000000E+07	-2.07000000E+07	-2.07000000E+07
p_{2411}	-6.68056101E+05	-2.96000000E+05	-2.96000001E+05	-2.96000001E+05
p_{2511}	-4.51594565E+06	-1.43000000E+07	-1.43000000E+07	-1.43000000E+07
p_{2611}	-3.91080675E+06	1.70000000E+05	1.69999999E+05	1.69999999E+05
p_{2711}	1.88419836E+07	-1.13000000E+06	-1.13000000E+06	-1.13000000E+06
p_{2811}	2.33156156E+07	-1.81000000E+07	-1.81000000E+07	-1.81000000E+07
p_{2911}	1.24225079E+07	1.71000000E+05	1.70999999E+05	1.70999999E+05
p_{21011}	-9.08706607E+06	-1.43000000E+05	-1.43000001E+05	-1.43000001E+05
p_{2112}	-1.62302854E-02	-1.59859337E-01	-2.95498785E-01	-1.01043214E-01
p_{2212}	7.64645470E+01	6.20645117E+01	8.86669925E+01	7.03608653E+01
p_{2312}	7.36021947E+01	1.28258481E+01	1.04720707E+01	1.23482733E+01
p_{2412}	-1.22297144E+01	-1.96903235E+01	-1.94109603E+01	-1.95179336E+01
p_{2512}	4.33845125E+01	4.83784066E+01	6.41039084E+01	4.50850961E+01
p_{2612}	1.06916789E+00	-7.05324315E+00	1.69812497E+01	-5.69021186E+00
p_{2712}	7.23596767E+01	3.20927775E+01	2.38707564E+01	2.52688501E+01
p_{2812}	-1.20968979E+02	-7.05673472E+01	-6.46822058E+01	-6.66068403E+01
p_{2912}	3.74079635E+00	4.03630747E+00	3.76142021E+00	3.86896942E+00
p_{21012}	1.28664736E+00	9.30456689E-01	1.20666828E+00	1.09749242E+00
p_{2113}	1.18998016E+02	1.48643926E+02	1.47275435E+02	1.48349423E+02
p_{2213}	2.01998157E+02	-5.84517071E+02	-5.20534418E+02	-5.64628224E+02
p_{2313}	1.58351072E-01	-1.16164092E+01	-3.31324407E+01	-2.22876908E+01
p_{2413}	-4.77022120E+01	6.27998798E+01	6.41032600E+01	6.30343142E+01
p_{2513}	5.73976614E+01	2.00931060E+02	2.02996662E+02	2.01708483E+02
p_{2613}	-5.04215981E+00	-8.06136709E+01	-7.25205432E+01	-7.63812283E+01
p_{2713}	1.15998290E+02	3.02342147E+02	2.23731558E+02	1.91856011E+02
p_{2813}	-1.61001882E+02	4.99254980E+02	4.97132284E+02	5.33056867E+02
p_{2913}	5.77985976E+01	8.74222235E+01	8.60613407E+01	8.71348413E+01
p_{21013}	3.36837173E+06	2.08165234E+02	2.09526855E+02	2.08453036E+02
p_{2114}	8.02984474E+01	8.03000000E+01	8.02993217E+01	8.02993217E+01

p_{2214}	5.01983161E+01	5.02000000E+01	5.01994377E+01	5.01994377E+01
p_{2314}	2.68983149E+01	2.69000000E+01	2.68995063E+01	2.68995063E+01
p_{2414}	1.24616137E-01	1.26000000E-01	1.25397896E-01	1.25397896E-01
p_{2514}	8.68985394E+01	8.69000000E+01	8.68993755E+01	8.68993755E+01
p_{2614}	6.34985638E+01	6.35000000E+01	6.34995342E+01	6.34995342E+01
p_{2714}	-3.72020552E+01	-3.72000000E+01	-3.72005947E+01	-3.72005947E+01
p_{2814}	4.23981273E+01	4.24000000E+01	4.23994693E+01	4.23994693E+01
p_{2914}	2.67639491E-01	2.70000000E-01	2.69359614E-01	2.69359614E-01
p_{21014}	-8.32021433E+01	-8.32000000E+01	-8.32007422E+01	-8.32007422E+01
p_{2115}	5.79999983E+04	5.80000000E+04	5.79999995E+04	5.79999995E+04
p_{2215}	6.76998557E+02	6.77000000E+02	6.76999405E+02	6.76999405E+02
p_{2315}	-9.21001733E+02	-9.21000000E+02	-9.21000474E+02	-9.21000474E+02
p_{2415}	-3.21001698E+02	-3.21000000E+02	-3.21000527E+02	-3.21000527E+02
p_{2515}	-9.99000223E+03	-9.99000000E+03	-9.99000074E+03	-9.99000074E+03
p_{2615}	-7.09000183E+03	-7.09000000E+03	-7.09000048E+03	-7.09000048E+03
p_{2715}	-3.73025275E+01	-3.73000000E+01	-3.73005605E+01	-3.73005605E+01
p_{2815}	-1.35000145E+03	-1.35000000E+03	-1.35000057E+03	-1.35000057E+03
p_{2915}	3.71997371E+02	3.72000000E+02	3.71999259E+02	3.71999259E+02
p_{21015}	4.21999978E+04	4.22000000E+04	4.21999993E+04	4.21999993E+04
a_{11}	-2.00002079E+02	-2.00000000E+02	-2.00000551E+02	-2.00000551E+02
a_{12}	1.50233558E+02	8.16000000E+01	8.15995124E+01	8.15995124E+01
a_{13}	-2.09494079E+05	-1.13256173E+02	2.92692794E+03	4.40831145E+01
a_{14}	-1.31000167E+03	-1.31000000E+03	-1.31000046E+03	-1.31000046E+03
a_{15}	-5.38087189E+01	4.15616894E+02	4.16999548E+02	4.14913515E+02
a_{16}	-6.29000244E+03	-6.29000000E+03	-6.29000068E+03	-6.29000068E+03
a_{17}	1.54643201E+05	1.61000000E-01	1.60588192E-01	1.60588192E-01
a_{18}	1.40981227E+01	1.41000000E+01	1.40994733E+01	1.40994733E+01
a_{19}	5.04855538E+00	3.85103664E+00	6.36042462E+00	-2.26809967E+00
a_{110}	-8.81544446E-04	-2.42170622E+00	-1.85909286E+00	-2.68296963E+00
a_{111}	-5.59928116E+06	1.71000000E+05	1.70999999E+05	1.70999999E+05
a_{112}	2.86439498E+00	3.16618309E+00	2.89437136E+00	2.99925644E+00
a_{113}	5.78980555E+01	8.75618496E+01	8.61995087E+01	8.72736666E+01
a_{114}	3.11997810E+02	3.12000000E+02	3.11999569E+02	3.11999569E+02
a_{115}	5.93997544E+02	5.94000000E+02	5.93999601E+02	5.93999601E+02
p_{11}	-1.59183382E+03	-2.96653904E+03	-1.58736061E+03	-3.16996900E+03
p_{12}	6.41659752E+02	3.56254595E+03	2.17350501E+03	3.75621884E+03
p_{13}	-3.33516947E+02	-6.39194578E+02	-3.35463393E+00	-9.77425317E+02
p_{14}	5.35210000E+02	-9.40935198E+02	5.65686845E+02	-1.17177588E+03
p_{15}	-6.74001926E+02	1.84959300E+04	1.76199409E+04	1.65108201E+04
p_{16}	-1.90273613E+02	-1.77211040E+03	-3.01392393E+02	-1.96421196E+03
p_{17}	4.00098985E-01	-9.57823769E+03	-8.81983319E+03	-8.75337145E+03
p_{18}	1.34685794E+03	-1.34829295E+02	1.20952637E+03	-3.10041470E+02
p_{19}	1.10072705E+03	-4.12726207E+03	-3.45816420E+02	-3.79211370E+02

p_{110}	4.27099347E+03	1.36116279E+04	1.39105947E+04	1.58084468E+04
p_{111}	-3.98485954E-01	1.82665122E+03	7.39075116E+01	2.04192763E+03
p_{112}	4.26139359E+03	1.77780623E+04	2.94878426E+04	1.73030534E+04
p_{113}	2.64767073E+03	1.62163022E+04	1.97435829E+04	1.88592962E+04
p_{114}	4.02595213E+02	1.72789961E+03	3.33380766E+02	1.92054081E+03
p_{115}	-9.02542655E-02	-9.55917140E+03	-8.80054443E+03	-8.73390162E+03
a_0	1.72234080E+03	3.17784139E+03	1.78139394E+03	3.36982493E+03
RMS	336.205	260.777	183.486	250.742

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