

Table 1: Average residuals of energy levels calculated with this PES, the POKAZATEL PES (Polyansky et al., 2018) and the PES15K PES (Mizus et al., 2018) compared to MARVEL levels (Furtenbacher et al., 2020) with $J \leq 20$.

PES	This Work		POKAZATEL		PES15K	
J	N_J	σ (cm $^{-1}$)	N_J	σ (cm $^{-1}$)	N_J	σ (cm $^{-1}$)
E \leq 15 000 cm $^{-1}$						
0	50	0.03946	50	0.02923	50	0.01523
1	149	0.02973	151	0.02539	151	0.01084
2	258	0.02956	256	0.02118	257	0.01054
3	360	0.02843	363	0.01828	365	0.01126
4	461	0.02703	460	0.01640	461	0.00705
5	564	0.02665	566	0.02410	563	0.00831
6	641	0.02651	640	0.03322	639	0.01049
7	700	0.02872	703	0.04919	698	0.01473
8	729	0.02697	730	0.06102	729	0.01820
9	735	0.02912	737	0.07750	736	0.03304
10	707	0.03212	704	0.08884	708	0.02740
11	662	0.03254	661	0.09984	664	0.03033
12	641	0.03651	632	0.10682	640	0.03185
13	603	0.03847	589	0.11009	603	0.03735
14	554	0.03894	535	0.11618	557	0.04162
15	502	0.03957	473	0.12102	508	0.04691
16	480	0.03931	433	0.11932	482	0.04944
17	464	0.04322	414	0.12201	461	0.05870
18	439	0.04474	390	0.12950	438	0.06495
19	425	0.04872	363	0.12984	421	0.06882
20	402	0.05577	338	0.12996	399	0.07676
Total	10526	0.03453	10191	0.08047	10530	0.03160
E \leq 26 000 cm $^{-1}$						
0	82	0.04560	82	0.03184	-	-
1	273	0.03683	276	0.02976	-	-
2	485	0.03799	485	0.02704	-	-
3	679	0.03949	683	0.02594	-	-
4	832	0.03583	849	0.02888	-	-
5	993	0.03511	1007	0.03557	-	-
6	1061	0.03574	1074	0.04327	-	-
7	1105	0.03687	1123	0.06028	-	-
8	1049	0.03376	1049	0.07379	-	-
9	981	0.03447	981	0.08988	-	-
10	880	0.03580	870	0.10130	-	-
11	772	0.03340	765	0.11047	-	-
12	703	0.03821	688	0.11478	-	-
13	643	0.03940	621	0.11491	-	-
14	599	0.04112	568	0.12002	-	-
15	540	0.04059	488	0.12256	-	-
16	508	0.04026	447	0.12119	-	-

(To be continued)

PES J	This Work		POKAZATEL		PES15K	
	N_J	σ (cm $^{-1}$)	N_J	σ (cm $^{-1}$)	N_J	σ (cm $^{-1}$)
17	484	0.04403	420	0.12342	-	-
18	469	0.04581	400	0.13151	-	-
19	456	0.05064	375	0.13184	-	-
20	436	0.05621	431	0.13117	-	-
Total	14030	0.03833	13682	0.07989		
<hr/> <hr/> E \leq 37 000 cm $^{-1}$ <hr/> <hr/>						
0	98	0.15349	96	0.08515	-	-
1	312	0.10341	315	0.08023	-	-
2	564	0.12777	572	0.10604	-	-
3	727	0.07496	738	0.06679	-	-
4	873	0.07327	890	0.05624	-	-
5	1032	0.06786	1052	0.06131	-	-
6	1073	0.04407	1088	0.05067	-	-
7	1113	0.04561	1131	0.06486	-	-
8	1051	0.03535	1060	0.07391	-	-
Total	6843	0.06475	6942	0.06695		

References

- 5 Furtenbacher, T., Tóbiás, R., Tennyson, J., Polyansky, O. L., and Császár, A. G.: W2020: A Database of Validated Rovibrational Experimental Transitions and Empirical Energy Levels of H₂O, *Journal of Physical and Chemical Reference Data*, 49, 033 101, <https://doi.org/10.1063/5.0008253>, 2020.
- Mizus, I. I., Kyuberis, A. A., Zobov, N. F., Makhnev, V. Y., Polyansky, O. L., and Tennyson, J.: High accuracy water potential energy surface for the calculation of infrared spectra, *Phil. Trans. Royal Soc. London A*, 376, 20170 149, <https://doi.org/10.1098/rsta.2017.0149>, 2018.
- Polyansky, O. L., Kyuberis, A. A., Zobov, N. F., Tennyson, J., Yurchenko, S. N., and Lodi, L.: ExoMol molecular line lists XXX: a complete high-accuracy line list for water, *Mon. Not. R. Astron. Soc.*, 480, 2597–2608, <https://doi.org/10.1093/mnras/sty1877>, 2018.