Table S3. Total energies (in a.u.) as function of the internuclear distances (in a_0) for the potential energy curves of the Λ + S states of OH^+.

R	$X\ ^3\Sigma^+$	$1\ ^1\Delta$	$1\ ^3\Pi$	$1\ ^1\Sigma^+$	$1\ ^1\Pi$
1.20	-74.90935398	-74.82936749	-74.74399057	-74.77480887	-74.63782677
1.30	-75.01350719	-74.93374970	-74.85141752	-74.87945492	-74.74971321
1.40	-75.08389375	-75.00428938	-74.92536504	-74.95022849	-74.82810188
1.50	-75.13061156	-75.05109827	-74.97594508	-74.99724461	-74.88304405
1.60	-75.16063334	-75.08116031	-75.01012523	-75.02749249	-74.92144561
1.70	-75.17884126	-75.09936589	-75.03276239	-75.04586927	-74.94810528
1.80	-75.18869387	-75.10918080	-75.04727225	-75.05585075	-74.96638818
1.90	-75.19265861	-75.11307605	-75.05606567	-75.05991666	-74.97866567
2.00	-75.19250114	-75.11281956	-75.06084484	-75.05984197	-74.98661454
2.10	-75.18948955	-75.10968070	-75.06281247	-75.05690129	-74.99142707
2.20	-75.18453857	-75.10457401	-75.06282241	-75.05201341	-74.99395919
2.30	-75.17831038	-75.09816317	-75.06148412	-75.04584677	-74.99483032
2.40	-75.17128448	-75.09092859	-75.05923485	-75.03888633	-74.99449206
2.50	-75.16380650	-75.08321765	-75.05638938	-75.03148449	-74.99327582
2.80	-75.14079352	-75.05938515	-75.04625439	-75.00884447	-74.98651452
3.20	-75.11255288	-75.02990701	-75.03284394	-74.98181577	-74.97469683
3.50	-75.09439520	-75.01087109	-75.02443579	-74.96551820	-74.96584236
3.70	-75.08375624	-74.99974006	-75.01982863	-74.95674322	-74.96037277
3.90	-75.07421070	-74.98981580	-75.01601869	-74.94962170	-74.95538409
4.10	-75.06567104	-74.98103772	-75.01294945	-74.94405441	-74.95093675
4.20	-75.06175025	-74.97705701	-75.01166643	-74.94180204	-74.94892545
4.30	-75.05804749	-74.97333655	-75.01053530	-74.93986839	-74.94705722
4.40	-75.05455218	-74.96986729	-75.00954236	-74.93822350	-74.94533126
4.50	-75.05125410	-74.96663981	-75.00867503	-74.93683619	-74.94374534
4.60	-75.04811815	-74.96364461	-75.00792062	-74.93567529	-74.94229622
4.70	-75.04518243	-74.96087231	-75.00726688	-74.93471075	-74.94098035
4.80	-75.04241620	-74.95831329	-75.00670228	-74.93391458	-74.93979029
4.90	-75.03981049	-74.95595776	-75.00621608	-74.93326132	-74.93872067
5.00	-75.03735749	-74.95379552	-75.00579844	-74.93272825	-74.93776425
5.10	-75.03504946	-74.95181684	-75.00544048	-74.93229566	-74.93691412
5.20	-75.03287905	-74.95001100	-75.00513422	-74.93194630	-74.93616155
5.30	-75.03083925	-74.94836789	-75.00487259	-74.93166617	-74.93549872

5.40	-75.02892337	-74.94687671	-75.00464937	-74.93144281	-74.93491748
5.50	-75.02712501	-74.94552687	-75.00445911	-74.93126612	-74.93440983
5.60	-75.02543802	-74.94430709	-75.00429709	-74.93112738	-74.93396806
6.00	-75.01968979	-74.94053403	-75.00385762	-74.93083423	-74.93272093
6.50	-75.01437200	-74.93771864	-75.00359377	-74.93074429	-74.93192310
7.00	-75.01062196	-74.93599223	-75.00348134	-74.93067487	-74.93155345
7.50	-75.00800388	-74.93490262	-75.00343951	-74.93070358	-74.93138223
8.00	-75.00618644	-74.93416867	-75.00342963	-74.93079351	-74.93130318
8.50	-75.00493683	-74.93363993	-75.00343711	-74.93089730	-74.93126809
9.00	-75.00411531	-74.93324636	-75.00345204	-74.93099801	-74.93125481
10.00	-75.00338637	-74.93270675	-75.00348354	-74.93117232	-74.93125548
11.00	-75.00319850	-74.93235712	-75.00350733	-74.93129949	-74.93126863
15.00	-75.00306154	-74.93173891	-75.00355710	-74.93154329	-74.93126147
20.00	-75.00303005	-74.93154179	-75.00360622	-74.93166332	-74.93145192
50.00	-75.00301615	-74.93141805	-75.00364840	-74.93175432	-74.93148712
100.00	-75.00301582	-74.93141135	-75.00365150	-74.93176035	-74.93148982
200.00	-75.00301579	-74.93141054	-75.00365192	-74.93176113	-74.93149019
300.00	-75.00301579	-74.93141046	-75.00365196	-74.93176121	-74.93149022
500.00	-75.00301579	-74.93141044	-75.00365197	-74.93176124	-74.93149024

Table S4. Total energies (in a.u.) as function of the internuclear distances (in a_0) for the potential energy curves of selected Λ + S states of OH^{2+}.

R	$1\ ^2\Delta$	$1\ ^2\Sigma^+$	$2\ ^2\Sigma^+$	$2\ ^2\Delta$	$1\ ^2\Pi$
1.70	-73.89962466	-73.82794535	-73.29446871	-73.24774089	-74.00365450
2.00	-73.96941976	-73.90084657	-73.38353288	-73.35928622	-74.05026142
2.10	-73.98489670	-73.91715774	-73.40155295	-73.38942843	-74.05829406
2.40	-74.02033770	-73.95454681	-73.46818428	-73.44048741	-74.07321016
2.80	-74.05572635	-73.99152264	-73.54315472	-73.50619433	-74.08697121
3.20	-74.08583578	-74.02249640	-73.58849713	-73.56968062	-74.10275876
3.50	-74.10620643	-74.04324806	-73.60884426	-73.59803950	-74.11658633
3.70	-74.11877663	-74.05599574	-73.61783903	-73.61047135	-74.12628089
3.90	-74.13053501	-74.06789000	-73.62412725	-73.61917572	-74.13601099
4.10	-74.14149517	-74.07895577	-73.62835348	-73.62509707	-74.14554727
4.20	-74.14668633	-74.08419112	-73.62985931	-73.62724936	-74.15019424

4.30	-74.15169170	-74.08923606	-73.63103389	-73.62896434	-74.15474255
4.40	-74.15651669	-74.09409662	-73.63192400	-73.63030532	-74.15918258
4.50	-74.16116710	-74.09877912	-73.63257065	-73.63132732	-74.16350770
4.60	-74.16564908	-74.10329023	-73.63301023	-73.63207800	-74.16771388
4.70	-74.16996902	-74.10763649	-73.63327439	-73.63259943	-74.17179911
4.80	-74.17413341	-74.11182482	-73.63339097	-73.63292760	-74.17576299
4.90	-74.17814870	-74.11586198	-73.63338433	-73.63309390	-74.17960633
5.00	-74.18202124	-74.11975438	-73.63327588	-73.63312558	-74.18333086
5.10	-74.18575731	-74.12350877	-73.63308383	-73.63304626	-74.18693900
5.20	-74.18936295	-74.12713123	-73.63286090	-73.63283785	-74.19043366
5.30	-74.19284402	-74.13062781	-73.63261840	-73.63252479	-74.19381806
5.40	-74.19620610	-74.13400421	-73.63231807	-73.63217051	-74.19709568
5.50	-74.19945464	-74.13726596	-73.63197298	-73.63178538	-74.20027010
5.60	-74.20259480	-74.14041833	-73.63159431	-73.63137829	-74.20334495
6.00	-74.21416546	-74.15202983	-73.62991544	-73.62966554	-74.21472095
6.50	-74.22671006	-74.16461209	-73.62785095	-73.62764992	-74.22711761
7.00	-74.23751816	-74.17544766	-73.62612243	-73.62599849	-74.23783583
7.50	-74.24691913	-74.18486919	-73.62479670	-73.62475756	-74.24717927
8.00	-74.25516669	-74.19313244	-73.62396025	-73.62386623	-74.25538807
8.50	-74.26245819	-74.20043607	-73.62322636	-73.62307770	-74.26265251
9.00	-74.26894915	-74.20693658	-73.62258860	-73.62168979	-74.26912400
10.00	-74.28000110	-74.21800241	-73.62197259	-73.61657182	-74.28015085
11.00	-74.28905684	-74.22706737	-73.62162327	-73.62161303	-74.28919160
15.00	-74.31324790	-74.25127552	-73.68054458	-73.67999655	-74.31335920
20.00	-74.32990203	-74.26793608	-73.69710071	-73.69673583	-74.33000548
50.00	-74.35990018	-74.29793795	-73.72705247	-73.72680492	-74.35999618
100.00	-74.36990020	-74.30793822	-73.73704854	-73.73680930	-74.36999590
200.00	-74.37490021	-74.31293827	-73.74204928	-73.74180874	-74.37499588
300.00	-74.37656688	-74.31460494	-73.74371601	-73.74347538	-74.37666254

Table S5. Total energies (in a.u.) as function of the internuclear distances (in a_0) for the potential energy curves of selected Λ + S states of OH^{2+}.

R	$2\,^2\Pi$	$3\,^2\Pi$	$4\,^2\Pi$	$1\,^2\Sigma^-$	$2\,^2\Sigma^-$
1.70	-73.71424623	-73.16992345	-73.09887558	-73.90003273	-73.29411203
2.00	-73.81894894	-73.31748581	-73.26882341	-73.97249437	-73.38322312
2.10	-73.84477094	-73.36533622	-73.30415239	-73.98947360	-73.40144403
2.40	-73.90696689	-73.48227134	-73.40592273	-74.02707863	-73.45270397
2.80	-73.96748682	-73.58340778	-73.51426406	-74.06191364	-73.57800067
3.20	-74.01185891	-73.64588314	-73.57703143	-74.09019563	-73.65027798
3.50	-74.03784011	-73.67612833	-73.60322237	-74.10932663	-73.68216004
3.70	-74.05262283	-73.69035338	-73.61432190	-74.12125167	-73.69629912
3.90	-74.06581710	-73.70086135	-73.62191902	-74.13250640	-73.70633534
4.10	-74.07770672	-73.70843455	-73.62697174	-74.14308197	-73.71329541
4.20	-74.08323367	-73.71133485	-73.62877171	-74.14811831	-73.71587797
4.30	-74.08851219	-73.71374290	-73.63018303	-74.15298995	-73.71797315
4.40	-74.09356043	-73.71572284	-73.63126429	-74.15769935	-73.71965033
4.50	-74.09839423	-73.71733182	-73.63206579	-74.16224970	-73.72096990
4.60	-74.10302768	-73.71862061	-73.63263092	-74.16664493	-73.72198446
4.70	-74.10747340	-73.71963413	-73.63299707	-74.17088949	-73.72273979
4.80	-74.11174278	-73.72041198	-73.63319656	-74.17498820	-73.72327569
4.90	-74.11584618	-73.72098894	-73.63325731	-74.17894609	-73.72362672
5.00	-74.11979302	-73.72139549	-73.63320341	-74.18276833	-73.72382283
5.10	-74.12359200	-73.72165827	-73.63305568	-74.18646013	-73.72389001
5.20	-74.12725110	-73.72180056	-73.63283208	-74.19002664	-73.72385075
5.30	-74.13077774	-73.72184259	-73.63254809	-74.19347298	-73.72372451
5.40	-74.13417881	-73.72180202	-73.63221701	-74.19680414	-73.72352806
5.50	-74.13746073	-73.72169397	-73.63185023	-74.20002498	-73.72327587
5.60	-74.14062950	-73.72153166	-73.63145751	-74.20314020	-73.72298033
6.00	-74.15227986	-73.72054326	-73.62977429	-74.21463260	-73.72155460
6.50	-74.16487550	-73.71904465	-73.62776237	-74.22711134	-73.71968154
7.00	-74.17570667	-73.71766076	-73.62610137	-74.23787426	-73.71805976
7.50	-74.18511663	-73.71653794	-73.62484512	-74.24724310	-73.71678982
8.00	-74.19336569	-73.71568216	-73.62403625	-74.25546670	-73.71584495
8.50	-74.20065515	-73.71504900	-73.62305433	-74.26273953	-73.71515826
9.00	-74.20714242	-73.71458552	-73.62263567	-74.26921590	-73.71466282

10.00	-74.21818589	-73.71399276	-73.62204642	-74.28024743	-73.71403894
11.00	-74.22723360	-73.71365688	-73.62170989	-74.28928938	-73.71369084
15.00	-74.25140559	-73.71317987	-73.68010901	-74.31345452	-73.71320337
20.00	-74.26805047	-73.71305463	-73.69680137	-74.33009881	-73.71307679
50.00	-74.29803944	-73.72604599	-73.71313920	-74.36008793	-73.72606188
100.00	-74.30803903	-73.73629702	-73.71309299	-74.37008755	-73.73626994
200.00	-74.31303899	-73.74142186	-73.71307048	-74.37508751	-73.74137551
300.00	-74.31470565	-73.74313009	-73.71306300	-74.37675417	-73.74307748

Table S6. Total energies (in a.u.) as function of the internuclear distances (in a_0) for the potential energy curves of selected Λ + S states of OH^{2+}.

R	$1\,^4\Pi$	$2\,^4\Pi$	$X\,^4\Sigma^-$	$2\,^4\Sigma^-$	$3\,^4\Sigma^-$
1.70	-73.37702036	-73.15814026	-74.03704189	-73.49863113	
2.00	-73.48713900	-73.36441585	-74.10102058	-73.59195574	-73.27000829
2.10	-73.51317208	-73.41497307	-74.11501326	-73.61105261	-73.33196784
2.40	-73.57731185	-73.52312363	-74.14725216	-73.64905776	-73.47568371
2.80	-73.64623463	-73.59742271	-74.18051285	-73.67694542	-73.59470988
3.20	-73.69000155	-73.64168996	-74.20977243	-73.69582533	-73.66075694
3.50	-73.70909134	-73.66751295	-74.22985465	-73.70828690	-73.68927958
3.70	-73.71746267	-73.68235955	-74.24230545	-73.71611602	-73.70206504
3.90	-73.72349924	-73.69550961	-74.25397655	-73.72371246	-73.71130405
4.10	-73.72815272	-73.70685402	-74.26487017	-73.73141063	-73.71760354
4.20	-73.73032498	-73.71169469	-74.27003321	-73.73531658	-73.71983830
4.30	-73.73265166	-73.71581785	-74.27501297	-73.73922157	-73.72158188
4.40	-73.73533247	-73.71908912	-74.27981442	-73.74309786	-73.72291647
4.50	-73.73846736	-73.72146987	-74.28444311	-73.74692466	-73.72391180
4.60	-73.74199680	-73.72307038	-74.28890504	-73.75068739	-73.72462563
4.70	-73.74577069	-73.72407837	-74.29320643	-73.75437538	-73.72510573
4.80	-73.74964722	-73.72466674	-74.29735362	-73.75798155	-73.72539185
4.90	-73.75352835	-73.72496152	-74.30135295	-73.76150152	-73.72551741
5.00	-73.75735552	-73.72504785	-74.30521069	-73.76493253	-73.72551069
5.10	-73.76109780	-73.72498280	-74.30893297	-73.76827335	-73.72539580
5.20	-73.76474124	-73.72480581	-74.31252577	-73.77152385	-73.72519329
5.30	-73.76827815	-73.72454552	-74.31599486	-73.77468443	-73.72492080

5.40	-73.77170690	-73.72422343	-74.31934580	-73.77775630	-73.72460176
5.50	-73.77502835	-73.72385667	-74.32258391	-73.78074111	-73.72423238
5.60	-73.77824411	-73.72345836	-74.32571428	-73.78364075	-73.72383200
6.00	-73.79011085	-73.72173332	-74.33725188	-73.79443269	-73.72208658
6.50	-73.80296724	-73.71967453	-74.34976565	-73.80629041	-73.71997255
7.00	-73.81401598	-73.71798384	-74.36055105	-73.81661088	-73.71821682
7.50	-73.82360039	-73.71669912	-74.36993507	-73.82565224	-73.71687466
8.00	-73.83198852	-73.71576061	-74.37816970	-73.83362668	-73.71589208
8.50	-73.83938916	-73.71508647	-74.38545103	-73.84070592	-73.71518636
9.00	-73.84596580	-73.71460305	-74.39193368	-73.84702910	-73.71468132
10.00	-73.85713834	-73.71399641	-74.40297456	-73.85783880	-73.71405053
11.00	-73.86627567	-73.71365760	-74.41202314	-73.86673235	-73.71370095
15.00	-73.89061017	-73.71317987	-74.43619966	-73.89062353	-73.71321305
20.00	-73.90731903	-73.71305463	-74.45284886	-73.90716404	-73.71308647
50.00	-73.93735127	-73.71299925	-74.48284105	-73.93708099	-73.71303081
100.00	-73.94735343	-73.71299790	-74.49284086	-73.94707622	-73.71302946
200.00	-73.95235371	-73.71299781	-74.49784085	-73.95207563	-73.71302937
300.00	-73.95402041	-73.71299781	-74.49950751	-73.95374224	-73.71302937

Table S7. Transition dipole moment (in a.u.) as function of the internuclear distances (in a_0) for selected pair of Λ + S states of OH^{2+}.

R	$3\,^2\Pi - 2\,^2\Pi$	$3\,^2\Pi - 1\,^2\Sigma^+$	$3\,^2\Pi - 1\,^2\Sigma^-$	$3\,^2\Pi - 1\,^2\Delta$	$3\,^2\Pi - 1\,^2\Pi$
2.00	0.14428	0.07152	0.16605	0.17404	0.17744
2.10	0.11140	0.04285	0.10598	0.14281	0.25026
2.40	0.10766	0.00198	0.03886	0.09912	0.38421
2.80	0.18185	0.02213	0.00687	0.08056	0.54530
3.20	0.27813	0.03281	0.01098	0.06959	0.61670
3.50	0.32371	0.03551	0.01769	0.06271	0.58587
3.70	0.33498	0.03591	0.01996	0.05872	0.54170
3.90	0.33282	0.03562	0.02108	0.05511	0.49003
4.10	0.32061	0.03486	0.02143	0.05176	0.43721
4.20	0.31184	0.03435	0.02139	0.05017	0.41156
4.30	0.30182	0.03377	0.02125	0.04861	0.38679
4.40	0.29089	0.03313	0.02102	0.04709	0.36305
4.50	0.27933	0.03243	0.02072	0.04559	0.34043

4.60	0.26738	0.03169	0.02036	0.04412	0.31898
4.70	0.25525	0.03092	0.01996	0.04267	0.29870
4.80	0.24309	0.03011	0.01951	0.04124	0.27958
4.90	0.23102	0.02928	0.01902	0.03983	0.26158
5.00	0.21916	0.02842	0.01851	0.03843	0.24466
5.10	0.20756	0.02755	0.01798	0.03706	0.22877
5.20	0.19629	0.02667	0.01744	0.03570	0.21385
5.30	0.18538	0.02577	0.01688	0.03436	0.19986
5.40	0.17487	0.02487	0.01631	0.03303	0.18674
5.50	0.16477	0.02397	0.01574	0.03173	0.17443
5.60	0.15510	0.02307	0.01516	0.03045	0.16290
6.00	0.12066	0.01954	0.01288	0.02556	0.12358
6.50	0.08664	0.01545	0.01021	0.02007	0.08688
7.00	0.06122	0.01187	0.00786	0.01538	0.06056
7.50	0.04271	0.00893	0.00592	0.01155	0.04188
8.00	0.02943	0.00657	0.00436	0.00850	0.02870

Table S8. Transition dipole moment (in a.u.) as function of the internuclear distances (in a_0) for selected pair of Λ + S states of OH^{2+}.

R	$3\ ^4\Sigma^- - X\ ^4\Sigma^-$	$2\ ^4\Pi - X\ ^4\Sigma^-$	$2\ ^2\Sigma^- - 2\ ^2\Pi$	$2\ ^2\Sigma^- - 1\ ^2\Sigma^-$	$2\ ^2\Sigma^- - 1\ ^2\Pi$
2.00	0.62012	0.08392	0.00096		
2.10	0.64774	0.11319	0.00212		
2.40	0.70239	0.24786	0.03962	0.64641	0.02449
2.80	0.71229	0.39309	0.04603	0.69918	0.00591
3.20	0.67774	0.43085	0.04858	0.65640	0.01983
3.50	0.63673	0.43710	0.04808	0.59085	0.02613
3.70	0.59363	0.43443	0.04691	0.54073	0.02896
3.90	0.52562	0.42362	0.04529	0.48973	0.03084
4.10	0.43984	0.39593	0.04337	0.44020	0.03190
4.20	0.39924	0.36971	0.04234	0.41644	0.03217
4.30	0.36329	0.33081	0.04127	0.39351	0.03228
4.40	0.33221	0.27917	0.04017	0.37147	0.03226
4.50	0.30539	0.22181	0.03905	0.35036	0.03211
4.60	0.28204	0.16903	0.03791	0.33020	0.03184
4.70	0.26147	0.12652	0.03676	0.31099	0.03148

4.80	0.24310	0.09442	0.03561	0.29273	0.03103
4.90	0.22652	0.07060	0.03445	0.27538	0.03051
5.00	0.21142	0.05287	0.03329	0.25892	0.02992
5.10	0.19756	0.03951	0.03213	0.24333	0.02927
5.20	0.18476	0.02930	0.03097	0.22857	0.02857
5.30	0.17288	0.02139	0.02983	0.21461	0.02783
5.40	0.16183	0.01522	0.02869	0.20140	0.02706
5.50	0.15150	0.01034	0.02756	0.18893	0.02626
5.60	0.14186	0.00648	0.02645	0.17714	0.02543
6.00	0.10887	0.00257	0.02218	0.13626	0.02200
6.50	0.07766	0.00643	0.01735	0.09711	0.01774
7.00	0.05481	0.00692	0.01323	0.06837	0.01384
7.50	0.04622	0.00616	0.00987	0.04758	0.01049
8.00	0.03825	0.00499	0.00722	0.03279	0.00778