Table. Compared with spectroscopic parameters for the Λ- S states of OH^- anion at spin free MRCI+Q level based on different basis sets.

states	basis sets	R_e (Å)	ω_e (cm^{-1})	$\omega_e\chi_e$ (cm^{-1})	B_e (cm^{-1})	D_e (eV)	T_e (cm^{-1})	ν (cm^{-1})
$X^1\Sigma^+$	basis1[a]	0.9645	3722.10	87.93	19.1111	4.9857	0	3555.932
	basis2[b]	0.9645	3722.20	87.93	19.1113	4.9858	0	3556.033
	basis3[c]	0.9636	3727.96	87.40	19.1417	5.0193	0	3559.882
	basis4[d]	0.9636	3728.64	87.43	19.1430	5.0203	0	3560.636
	Expt.[23]		3680 ± 37		19.13	4.981[22] [e]		
	Expt.[24]	0.9643	3738.44	91.42	19.1209			3555.605
$a^3\Pi$	basis1[a]	0.9790	3402.39	146.44	18.5735	2.6693	18674.86	3318.210
	basis2[b]	0.9789	3402.48	146.45	18.5737	2.6693	18675.81	3318.298
	basis3[c]	0.9782	3403.47	145.96	18.5989	2.6893	18789.31	3319.562
	basis4[d]	0.9781	3404.28	145.99	18.6004	2.6900	18791.46	3320.332
$A^1\Pi$	basis1[a]	0.9763	3864.48	177.96	18.6615	2.6128	19130.88	3410.554
	basis2[b]	0.9763	3864.56	177.97	18.6617	2.6128	19131.80	3410.638
	basis3[c]	0.9755	3868.36	177.06	18.6882	2.6326	19246.12	3412.515
	basis4[d]	0.9754	3869.14	177.08	18.6896	2.6333	19248.20	3413.255

[a] At AV5Z-DK for H and ACV5Z-DK for O level;

[b] At AV5Z for H and ACV5Z for O level;

[c] At AV5Z-DK for H and O level;

[d] At AV5Z for H and O level;

[e] D_e (OH^-) = 0.36 eV + 4.921 eV. Where 4.921 eV was the D_e for the ground state $X^2\Pi$ of OH molecule.[48]

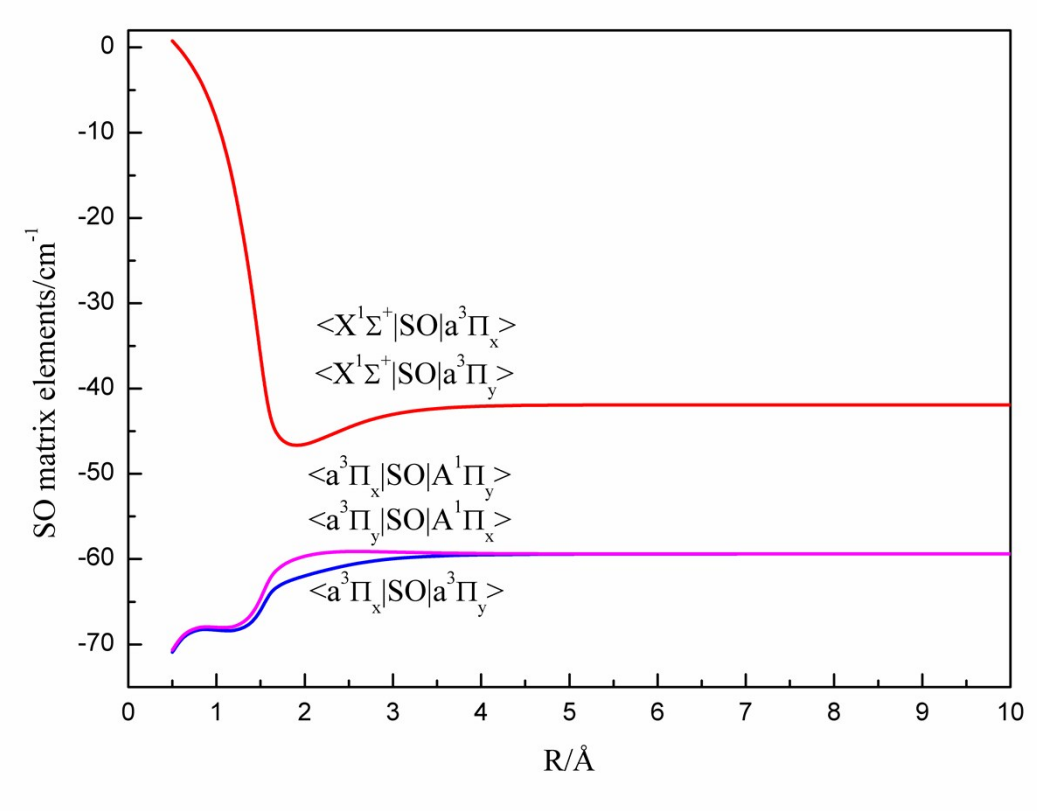

Figure. The SO matrix elements of OH^- anion.