

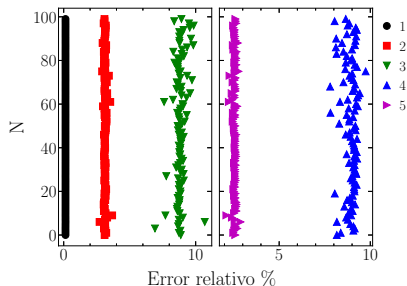
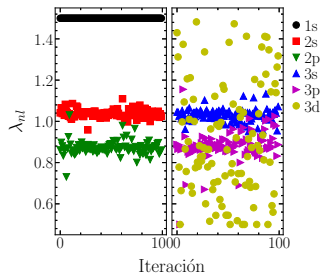
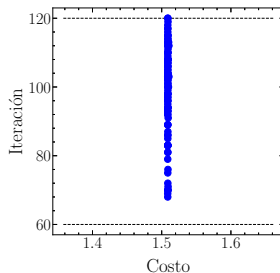
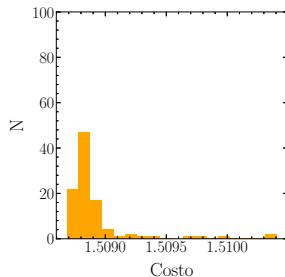
Optimización de la estructura electrónica del átomo de O^{6+}

A. Mendez

November 27, 2019

Minimización de E_j :

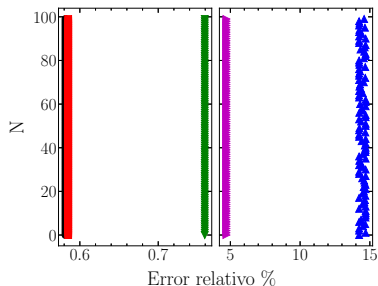
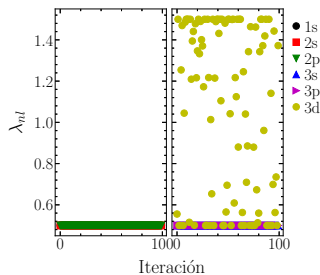
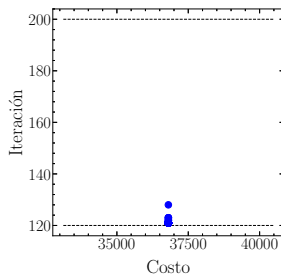
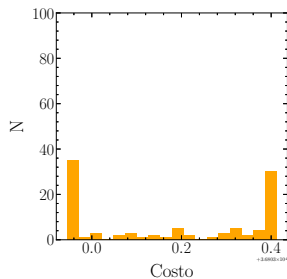
initer=60, maxevals=60



	i	er%	observed	computed	acc
	1	0.152386	-118.386965	-118.206560	0
	2	0.139040	-77.155412	-77.048135	0
	3	0.118636	-76.596450	-76.505579	0
	4	0.126675	-76.574570	-76.477569	0
	5	0.134440	-76.202582	-76.100135	0
	6	0.147771	-69.736057	-69.633007	0
	7	0.140538	-69.582509	-69.484719	0
	8	0.141154	-69.575674	-69.477465	0
	9	0.139684	-69.502749	-69.405665	0
	10	0.132023	-69.493205	-69.401458	0
	11	0.136336	-69.465138	-69.370432	0
	1	3.235E+00	3.309E+12	3.416E+12	1.0000
	2	8.756E+00	9.365E+11	1.018E+12	1.0000
	3	8.851E+00	1.451E+08	1.323E+08	1.0000
	4	2.467E+00	3.310E+05	3.228E+05	3.0000
	5	1.290E+05	3.310E+05	4.274E+08	3.0000

Minimización de A_{ki} :

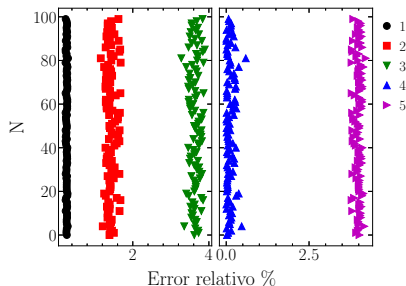
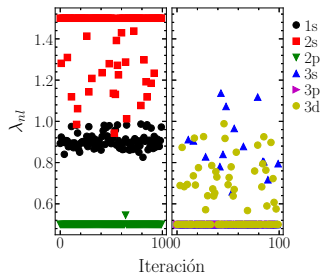
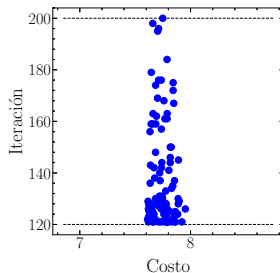
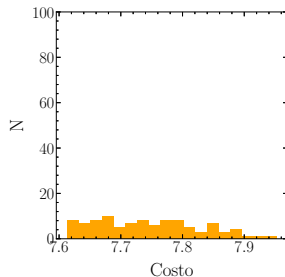
initer=120, maxevals=80



i	er%	observed	computed	acc
1	0.222437	-118.386965	-118.123629	0
2	0.473400	-77.155412	-76.790158	0
3	0.404711	-76.596450	-76.286456	0
4	0.377540	-76.574570	-76.285470	0
5	0.439635	-76.202582	-75.867569	0
6	0.583576	-69.736057	-69.329094	0
7	0.578243	-69.582509	-69.180153	0
8	0.590571	-69.575674	-69.164780	0
9	0.584637	-69.502749	-69.096410	0
10	0.578513	-69.493205	-69.091178	0
11	0.581660	-69.465138	-69.061087	0
1	5.851E-01	3.309E+12	3.328E+12	1.0000
2	7.594E-01	9.365E+11	9.294E+11	1.0000
3	1.423E+01	1.451E+08	1.657E+08	1.0000
4	4.713E+00	3.310E+05	3.154E+05	3.0000
5	1.104E+05	3.310E+05	3.656E+08	3.0000

Minimización de $E_j + A_{ki}$:

initer=120, maxevals=80



i	er%	observed	computed	acc
1	0.138697	-118.386965	-118.222766	0
2	0.211036	-77.155412	-76.992586	0
3	0.197012	-76.596450	-76.445546	0
4	0.207541	-76.574570	-76.415646	0
5	0.211158	-76.202582	-76.041674	0
6	0.286920	-69.736057	-69.535970	0
7	0.269438	-69.582509	-69.395027	0
8	0.267581	-69.575674	-69.389503	0
9	0.269706	-69.502749	-69.315296	0
10	0.262683	-69.493205	-69.310658	0
11	0.265320	-69.465138	-69.280833	0
1	1.394E+00	3.309E+12	3.355E+12	1.0000
2	3.627E+00	9.365E+11	9.705E+11	1.0000
3	4.135E-03	1.451E+08	1.451E+08	1.0000
4	4.016E+00	3.310E+05	3.177E+05	3.0000