Excitation into high-lying states in Li^{3+}-H collisions.

Aicha Ibaaz,[1] Rosa Esteban Hernandez,[1] Alain Dubois,[1] and Nicolas Sisourat[1]

[1]*Sorbonne Universités, UPMC Univ Paris 06, CNRS,*

Laboratoire de Chimie Physique Matière et Rayonnement, F-75005, Paris, France

*

(Dated: May 11, 2016)

* Nicolas.Sisourat@upmc.fr

I. SUPPLEMENTARY DATA

The target and projectile states are described as linear combinations of Gaussian-type orbitals (GTO):

$$\chi_k(\vec{r}) = N x^{u_k} y^{v_k} z^{w_k} e^{-\alpha_k r^2} \tag{1}$$

where N_k is a normalization factor and u_k, v_k and w_k are integers. In the following, we use the notation l_k=u_k+v_k+w_k for simplicity. The exponents α_k are chosen to provide even-tempered basis sets, ensuring thus an even coverage of the Hilbert space [1]. The basis sets used to describe hydrogen atomic states in this work are given in Tab. I, II, III and IV. The numbers of GTO and their exponents for l_k =0-3 are identical in all basis sets. For l_k =4-5, we fix the largest and smallest exponents for all basis sets, and then increase the number of GTO from B7 to B10 according to the even-tempered formulae [1].

These basis sets are compared by detailed inspection of the energy of the states of importance in the present work: the relative energy difference between the orbitals in each basis set and the exact ones are given in Tab. V. It is seen that the description of each state, in particular of the high-lying ones, is systematically improved at each level from B7 to B10. Such construction of the basis sets allows to check the convergence of the results in a systematic fashion.

Finally, it should be noted that the basis sets for the Li^{2+} projectile states are constructed from that of the hydrogen ones (B7 to B10) : the exponents are just modified according to the scaling law [2] $\alpha_Z = \alpha_H * Z^2$, where α_H are the exponents for hydrogen atomic states and Z is the nuclear charge of the projectile.

---

[1] Cherkes I, Klaiman S and Moiseyev N 2009 *Int. J. of Quant. Chem.* **109** 2996

[2] Pye C C and Mercer C J 2012 *J. Chem. Educ.* **89** 1405

l_k=0	l_k=1	l_k=2	l_k=3	l_k=4	l_k=5
10.00000000	3.00000000	1.00000000	0.30000000	0.10000000	0.03000000
6.30957365	1.89287210	0.63095737	0.18928722	0.06652696	0.01240556
3.98107196	1.19432159	0.39810720	0.11943216	0.04425837	0.00512993
2.51188668	0.75356600	0.25118867	0.07535660	0.02944375	0.00212132
1.58489340	0.47546802	0.15848934	0.04754680	0.01958803	0.00087721
-	-	-	-	0.01303132	0.00036274
-	-	-	-	0.00866934	0.00015000
-	-	-	-	0.00576745	-
-	-	-	-	0.00383691	-
-	-	-	-	0.00255258	-
-	-	-	-	0.00169815	-
-	-	-	-	0.00112973	-
-	-	-	-	0.00075157	-
-	-	-	-	0.00050000	-

Table I. Exponents of the GTO basis set labeled B7

l_k=0	l_k=1	l_k=2	l_k=3	l_k=4	l_k=5
10.00000000	3.00000000	1.00000000	0.30000000	0.10000000	0.03000000
6.30957365	1.89287210	0.63095737	0.18928722	0.07024219	0.01407352
3.98107196	1.19432159	0.39810720	0.11943216	0.04933965	0.00660213
2.51188668	0.75356600	0.25118867	0.07535660	0.03465724	0.00309717
1.58489340	0.47546802	0.15848934	0.04754680	0.02434401	0.00145294
-	-	-	-	0.01709976	0.00068160
-	-	-	-	0.01201125	0.00031975
-	-	-	-	0.00843696	0.00015000
-	-	-	-	0.00592631	-
-	-	-	-	0.00416277	-
-	-	-	-	0.00292402	-
-	-	-	-	0.00205389	-
-	-	-	-	0.00144270	-
-	-	-	-	0.00101338	-
-	-	-	-	0.00071182	-
-	-	-	-	0.00050000	-

Table II. Exponents of the GTO basis set labeled B8

l_k=0	l_k=1	l_k=2	l_k=3	l_k=4	l_k=5
10.00000000	3.00000000	1.00000000	0.30000000	0.10000000	0.03000000
6.30957365	1.89287210	0.63095737	0.18928722	0.07322263	0.01547008
3.98107196	1.19432159	0.39810720	0.11943216	0.05361553	0.00797744
2.51188668	0.75356600	0.25118867	0.07535660	0.03925870	0.00411372
1.58489340	0.47546802	0.15848934	0.04754680	0.02874625	0.00212132
-	-	-	-	0.02104876	0.00109390
-	-	-	-	0.01541245	0.00056409
-	-	-	-	0.01128540	0.00029088
-	-	-	-	0.00826347	0.00015000
-	-	-	-	0.00605073	-
-	-	-	-	0.00443050	-
-	-	-	-	0.00324413	-
-	-	-	-	0.00237544	-
-	-	-	-	0.00173936	-
-	-	-	-	0.00127360	-
-	-	-	-	0.00093257	-
-	-	-	-	0.00068285	-
-	-	-	-	0.00050000	-

Table III. Exponents of the GTO basis set labeled B9

l_k=0	l_k=1	l_k=2	l_k=3	l_k=4	l_k=5
10.00000000	3.00000000	1.00000000	0.30000000	0.10000000	0.03000000
6.30957365	1.89287210	0.63095737	0.18928722	0.07566468	0.01665142
3.98107196	1.19432159	0.39810720	0.11943216	0.05725143	0.00924233
2.51188668	0.75356600	0.25118867	0.07535660	0.04331911	0.00512993
1.58489340	0.47546802	0.15848934	0.04754680	0.03277726	0.00284735
-	-	-	-	0.02480081	0.00158042
-	-	-	-	0.01876545	0.00087721
-	-	-	-	0.01419882	0.00048689
-	-	-	-	0.01074349	0.00027025
-	-	-	-	0.00812903	0.00015000
-	-	-	-	0.00615080	-
-	-	-	-	0.00465398	-
-	-	-	-	0.00352142	-
-	-	-	-	0.00266447	-
-	-	-	-	0.00201606	-
-	-	-	-	0.00152545	-
-	-	-	-	0.00115423	-
-	-	-	-	0.00087334	-
-	-	-	-	0.00066081	-
-	-	-	-	0.00050000	-

Table IV. Exponents of the GTO basis set labeled B10

Orbitals	B7	B8	B9	B10
1s	7.933 (-2)	7.931 (-2)	7.928 (-2)	7.926 (-2)
2s	4.017 (-2)	3.990 (-2)	3.975 (-2)	3.970 (-2)
2p	1.173 (-3)	7.928 (-4)	8.472 (-4)	9.017 (-4)
3s	2.687 (-2)	2.665 (-2)	2.653 (-2)	2.648 (-2)
3p	1.514 (-1)	1.905 (-2)	2.037 (-3)	9.335 (-4)
3d	1.466 (-4)	8.053 (-5)	4.067 (-5)	2.146 (-5)
4s	2.017 (-2)	1.999 (-2)	1.990 (-2)	1.986 (-2)
4p	5.447 (-1)	7.008 (-2)	7.909 (-3)	1.557 (-3)
4d	1.502 (-4)	8.263 (-5)	4.192 (-5)	2.233 (-5)
4f	8.624 (-2)	7.165 (-3)	6.475 (-4)	1.687 (-4)
5s	1.614 (-2)	1.600 (-2)	1.592 (-2)	1.589 (-2)
5p	1.407	2.607 (-1)	3.888 (-2)	4.287 (-3)
5d	1.353 (-4)	7.434 (-5)	3.778 (-5)	2.018 (-5)
5f	5.213 (-1)	4.380 (-2)	7.608 (-3)	6.203 (-4)
5g	5.543 (-7)	4.079 (-7)	3.144 (-7)	1.182 (-8)
6s	1.346 (-2)	1.333 (-2)	1.327 (-2)	1.324 (-2)
6p	3.752	7.427 (-1)	1.683 (-1)	2.508 (-2)
6d	1.204 (-4)	6.558 (-5)	3.335 (-5)	1.776 (-5)
6f	2.305	1.588 (-1)	6.151 (-2)	4.573 (-3)
6g	9.998 (-7)	6.710 (-7)	4.997 (-7)	1.274 (-7)
6h	8.693 (-2)	1.941 (-2)	2.171 (-3)	1.676 (-4)

Table V. Relative energy difference (in percentages) of the hydrogen atomic state with respect to the exact one for the 5 different basis sets considered. The numbers in parentheses give the power of 10 by which the preceding number should be multiplied.