Supporting Information for Photoabsorption Spectra of Small Na Clusters: TDHF and BSE versus CI and experiment

C. H. Patterson
School of Physics, Trinity College Dublin, Dublin 2, Ireland

(Dated: February 2, 2019)

This document contains time-dependent Hartree-Fock (TDHF), Bethe-Salpeter equation (BSE) and full CI (FCI) or quadruples CI (QCI, Ref. [1]) and multi-reference doubles CI (MRD-CI, Ref. [2]) excitation energies and oscillator strengths for D_{3h} Na_5^+, D_{3h} and D_{4h} Na_6 and D_{4d} Na_8 clusters. It also contains a density of HF energy levels for a C_3 Na_{20} cluster.

TABLE I. Na_5^+ D_{3h} excitation energies in eV and oscillator strengths, f.

State	TDHF	f	BSE	f	FCI[a]	f[a]
$1^1E'$ (x,y)	2.58	0.47	2.58	0.05	-	-
$2^1E'$ (x,y)	3.15	1.89	2.97	2.11	3.16	2.14
1^1A_2" z	2.02	0.67	2.15	0.91	2.23	0.96
2^1A_2" z	2.39	0.53	2.54	0.24	-	-

[a] Ref.[1]

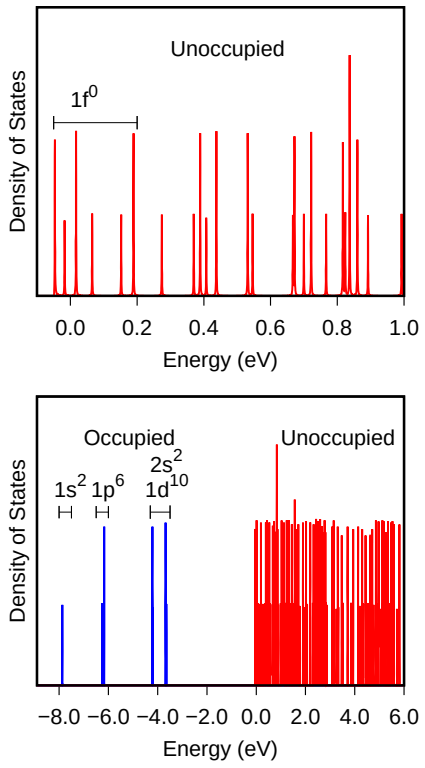

FIG. 1. Energy levels of Na_{20} C_3 cluster indicated by vertical sticks. Upper panel shows virtual states up to 1 eV above the vacuum level and lower panel shows the shell structure in occupied and low energy virtual states.

TABLE II. Na_6 D_{3h} excitation energies in eV and oscillator strengths, f.

State	TDHF	f	BSE	f	QCI[a]	f[a]
$^1E'$ (x,y)	1.62	0.81	1.68	0.71	1.36	0.14[a]
$^1E'$ (x,y)	2.07	2.28	2.12	2.20	1.94	2.64[a]
$^1E'$ (x,y)	2.62	0.31	2.80	0.27	2.49	0.15
$^1A_2''$ z	2.62	0.93	2.80	0.99	2.81	0.81
$^1A_2''$ z	3.33	0.29	3.28	0.25	-	-
$^1A_2''$ z	3.43	0.14	-	-	-	-
$^1A_2''$ z	3.49	0.31	3.51	0.33	-	-
$^1A_2''$ z	4.99	0.19	4.87	0.27	-	-

[a] Ref.[1]
[b] Values corrected from those published in Ref. [1]. D. Rai (private communication).

TABLE III. Na_6 D_{4h} excitation energies in eV and oscillator strengths, f.

State	TDHF	f	BSE	f	QCI[a]	f[a]
^1E_u (x,y)	1.54	0.45	1.77	0.44	1.65	0.28
^1E_u (x,y)	1.96	0.27	2.17	0.66	1.90	0.04
^1E_u (x,y)	2.23	2.22	2.40	1.89	2.34	1.30
^1E_u (x,y)	3.06	0.32	3.16	0.29	-	-
$^1A_{2u}$ z	2.39	0.70	2.71	1.12	2.71	0.80
$^1A_{2u}$ z	3.26	0.84	3.29	0.45	-	-
$^1A_{2u}$ z	3.40	0.13	-	-	-	-
$^1A_{2u}$ z	4.76	0.17	4.72	0.26	-	-

[a] Ref.[1]

TABLE IV. Na_8 D_{4d} excitation energies in eV and oscillator strengths, f.

State	TDHF[a]	f	BSE[a]	f	MRD-CI[b]	f
$^1E_1$ (x,y)	1.29	0.03	1.33	0.01	1.45	0.46
$^1E_1$ (x,y)	1.76	0.00	1.81	0.09	1.86	0.02
$^1E_1$ (x,y)	1.90	0.47	2.04	0.30	1.97	0.29
$^1E_1$ (x,y)	2.42	3.43	2.36	3.28	2.70	4.36
$^1E_1$ (x,y)	2.94	0.18	3.14	0.12	-	-
$^1E_1$ (x,y)	3.15	0.32	3.17	0.18	-	-
$^1E_1$ (x,y)	3.32	0.14	3.50	0.29	-	-
$^1E_1$ (x,y)	3.33	0.11	3.55	0.27	-	-
$^1B_2$	z 1.47	0.01	1.60	0.01	-	-
$^1B_2$	z 1.54	0.13	1.73	0.10	-	-
$^1B_2$	z 2.39	1.62	2.39	1.62	-	-
$^1B_2$	z 2.82	0.19	2.86	0.11	-	-
$^1B_2$	z 2.97	0.12	3.01	0.08	-	-
$^1B_2$	z 3.07	0.09	3.13	0.13	-	-
$^1B_2$	z 3.33	0.21	3.51	0.27	-	-
$^1B_2$	z 4.46	0.14	4.45	0.14	-	-

[a] This work
[b] Ref.[2]

[1] P. K. Priya, D. K. Rai, and A. Shukla, Eur. Phys. J. D **71**, 116 (2017).

[2] V. Bonačić-Koutecký, P. Fantucci, and J. Koutecký, Chem. Phys. Lett. **166**, 32 (1990).