GAP_hcp_bcc_varcell8

<command_line><![CDATA[at_file=Ti_hcp_bcc_varcell_k8_labelled_v3.xyz gap="distance_Nb order=2 cutoff=9.0
covariance_type=ard_se n_sparse=20 theta_uniform=1.0 delta=0.003 compact_clusters=T :soap cutoff=4.0
covariance_type=dot_product n_sparse=2000 delta=0.095 sparse_method=cur_points l_max=10 n_max=10 zeta=4 atom_sigma=0.5"
e0=-4.42384810052 sparse_separate_file=F gp_file=gp_soap_hcp_bcc_varcell_k8_labelled.xml default_sigma={0.005 0.5 0.5 0.0}]]></command_line>

	-	GAP_hcp_bcc_varcell8	NRLTB8
0	bcc_c12	90.09	7%
1	bcc_c11	120.99	-2%
2	bcc_c44	59.93	-54%
3	hcp_c44	34.37	-4%
4	hcp_c13	74.85	-12%
5	hcp_c12	80.83	6%
6	hcp_c11	159.74	-8%
7	hcp_c66	39.36	19%
8	hcp_c33	198.79	-9%











