GAP_hcp_bcc_varcell16

<command_line><![CDATA[at_file=Ti_hcp_bcc_varcell_k16_labelled.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_k16_labelled.xml default_sigma={0.005 0.5 0.0}]]></command_line>

	-	GAP_hcp_bcc_varcell16	NRLTB16
0	bcc_c12	89.96	11%
1	bcc_c11	111.53	-5%
2	bcc_c44	56.04	-30%
3	hcp_c44	34.17	0%
4	hcp_c13	74.46	-8%
5	hcp_c12	81.39	-29%
6	hcp_c11	163.51	7%
7	hcp_c66	41.40	35%
8	hcp_c33	188.59	-9%











