

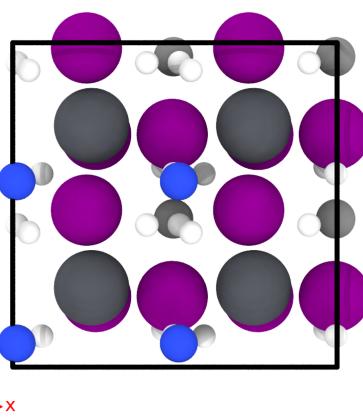
[1/1] ML_ABCAR-MAPbI3 (Cubic-(SSHS-MAPbI3))

file

name ML_ABCAR-MAPbI3
 structure groups 1
 total structures 777

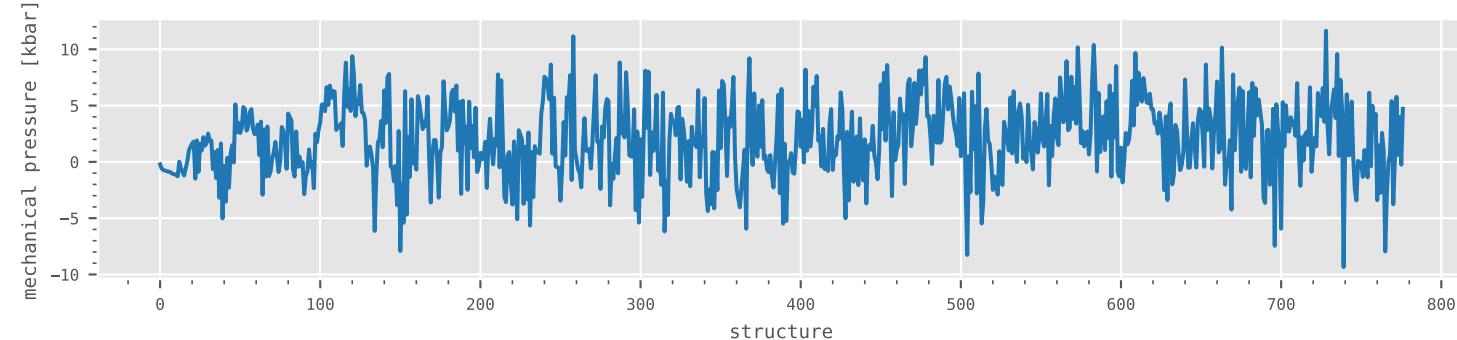
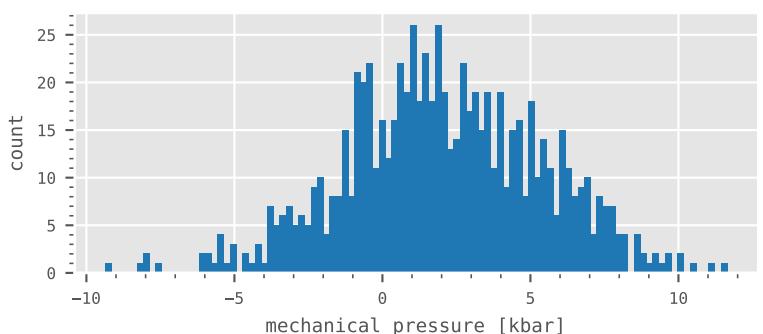
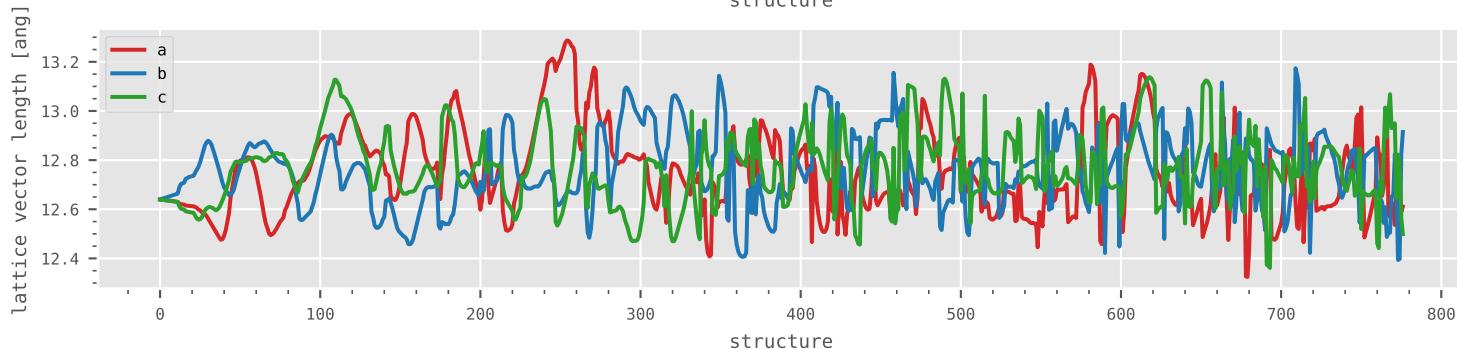
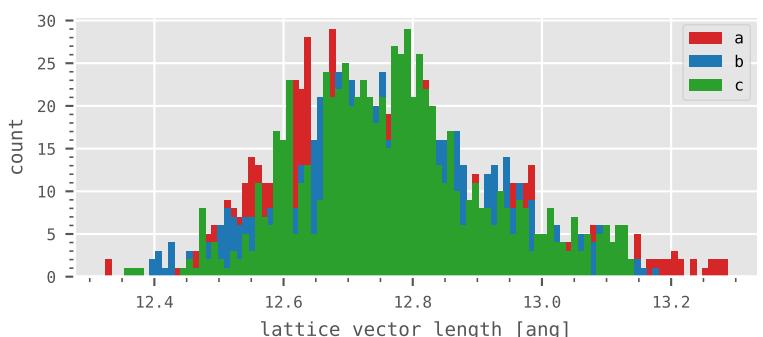
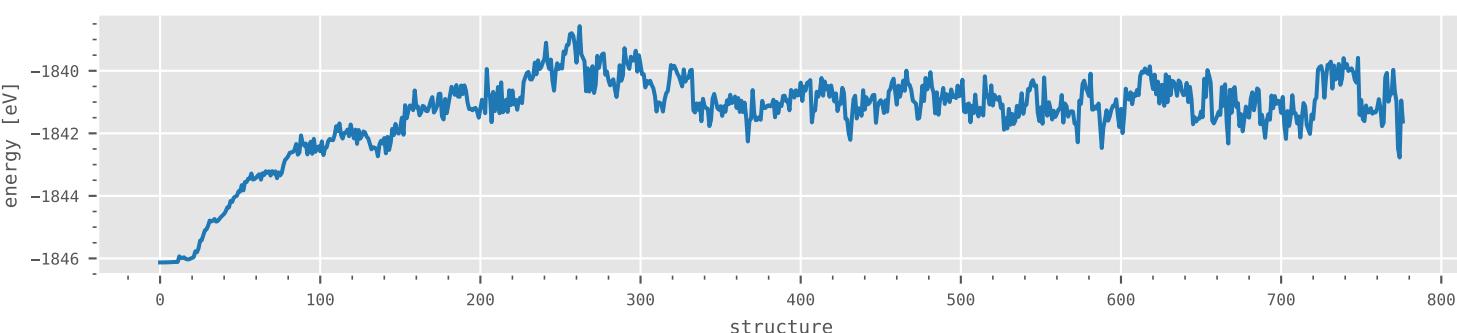
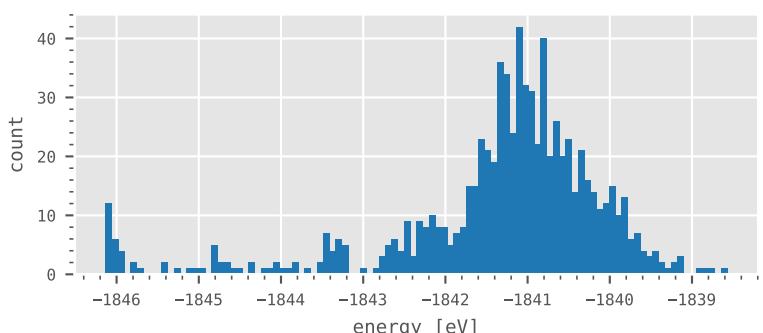
overview

energy	-1841.3 ± 1.36	eV
volume	2078.3 ± 40.40	ang^3
lattice vector a	12.7 ± 0.17	ang
lattice vector b	12.8 ± 0.15	ang
lattice vector c	12.8 ± 0.15	ang
non-periodic radius	6.2 (min. for group)	ang

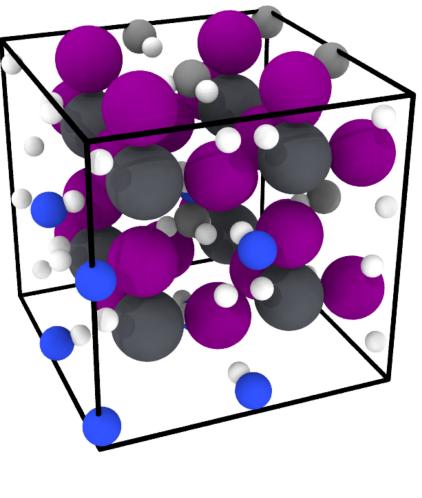


current structure group

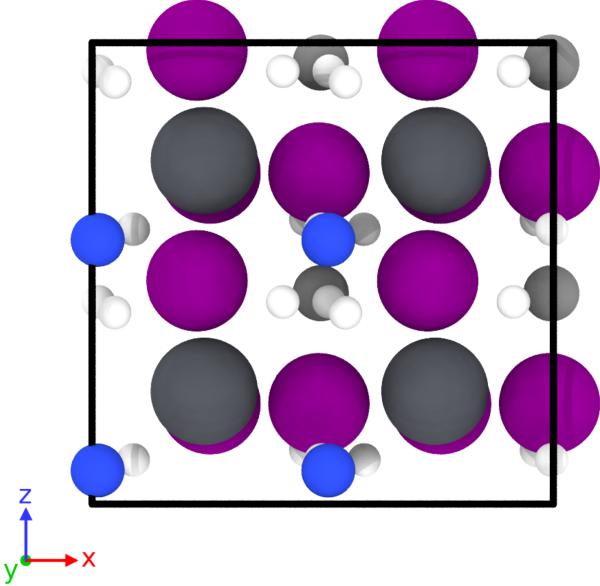
name Cubic-(SSHS-MAPbI3)
 structure group 1 (of 1 in file)
 structures 777 (of 777 in file)
 atoms Pb (8), I (24), C (8), N (8), H (48)
 96 total



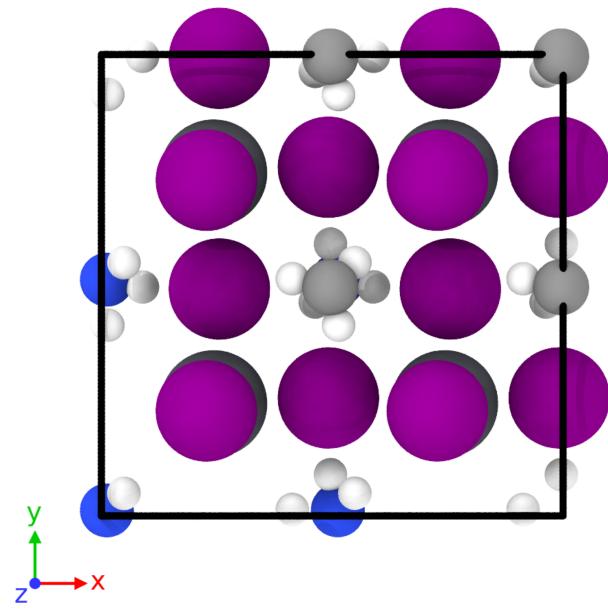
minimum energy configuration (structure 4)



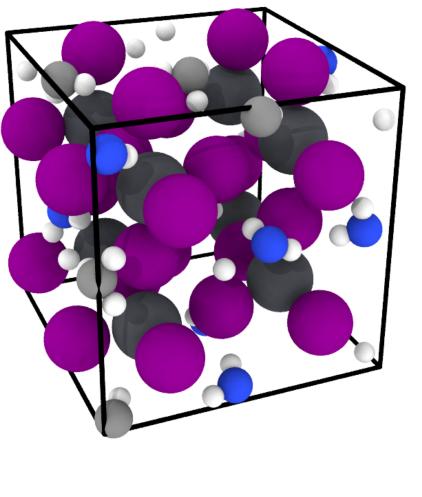
front



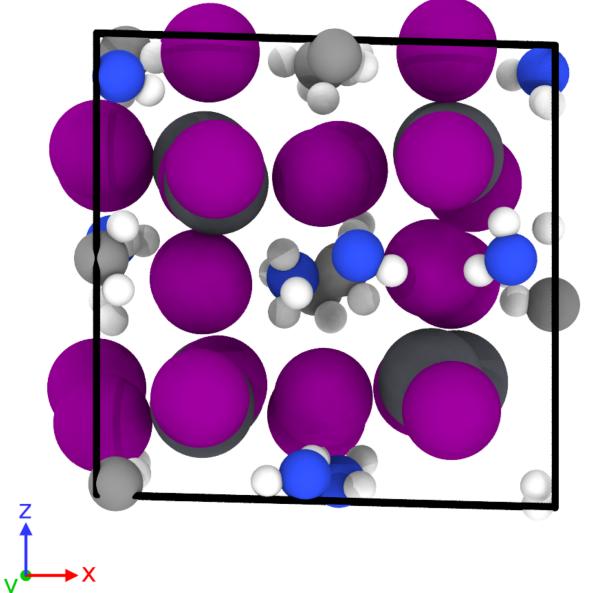
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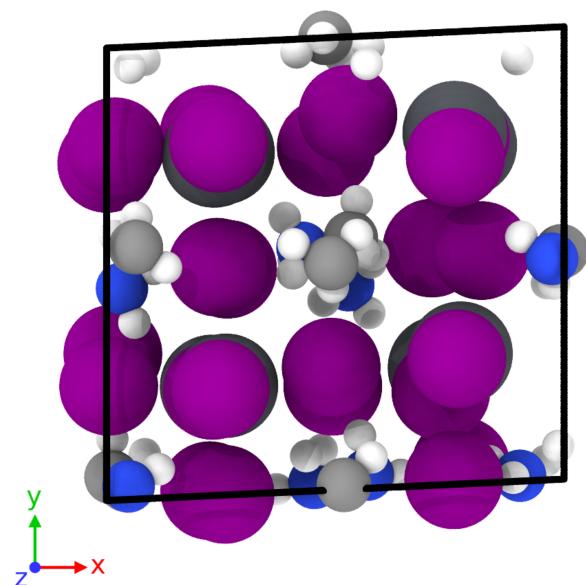
maximum energy configuration (structure 263)



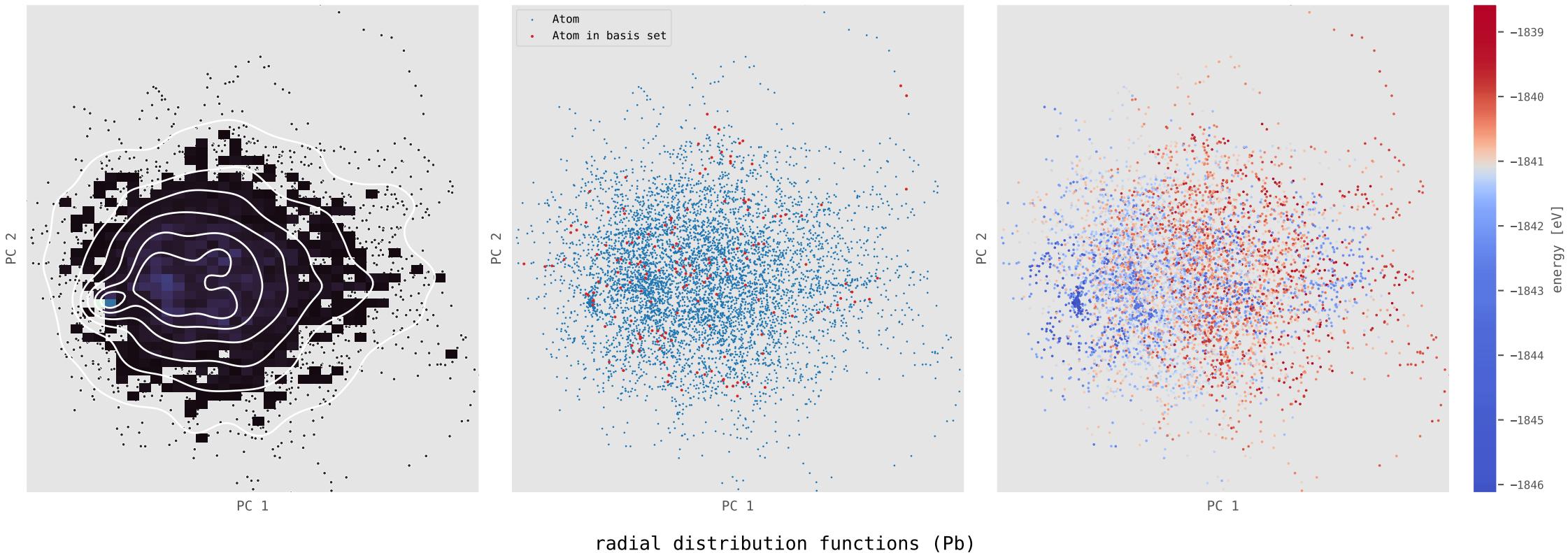
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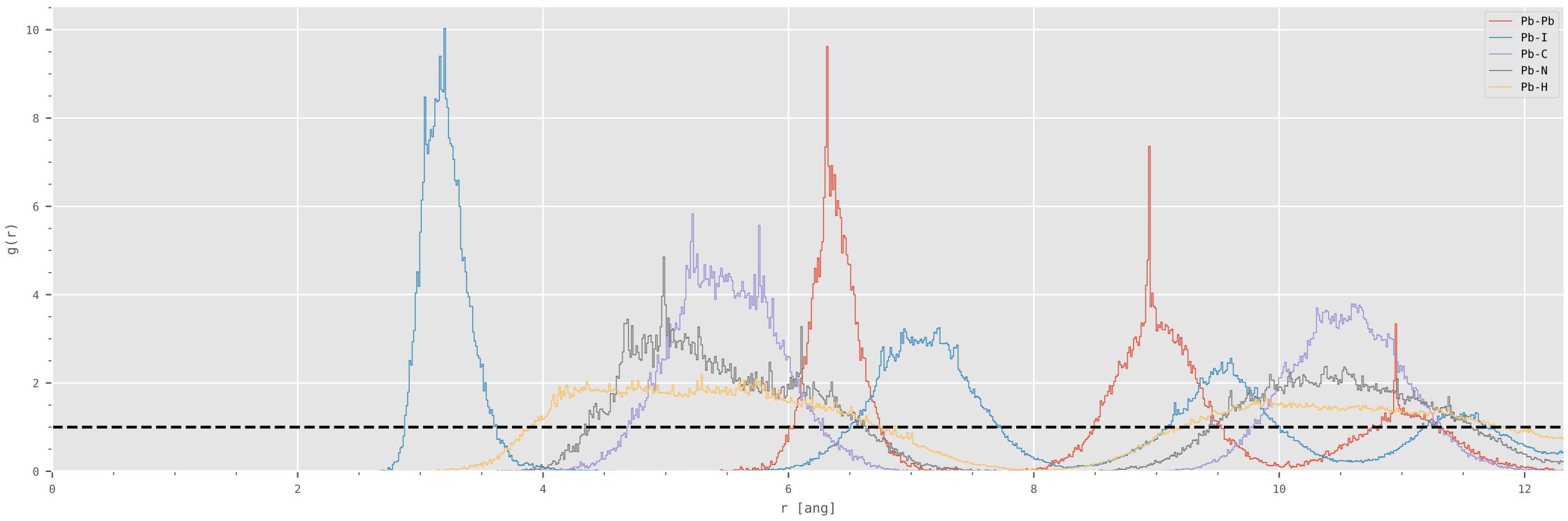
top



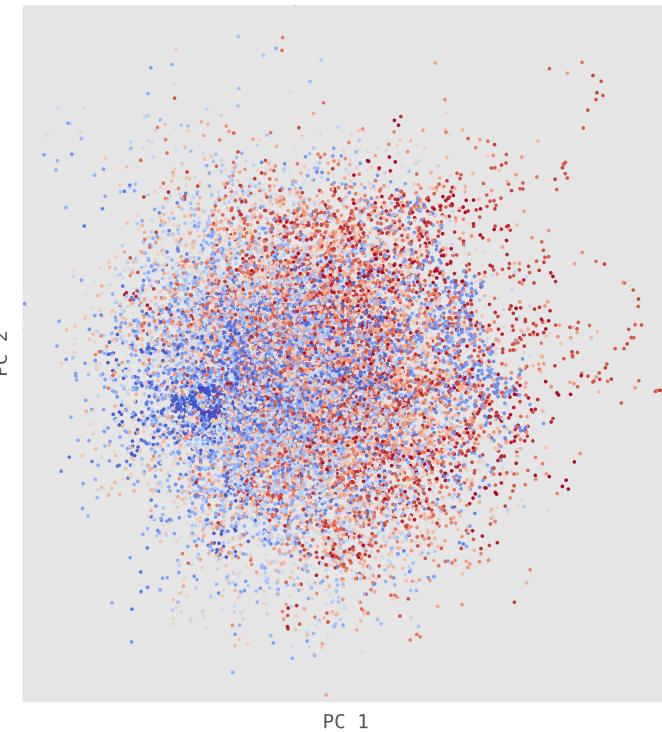
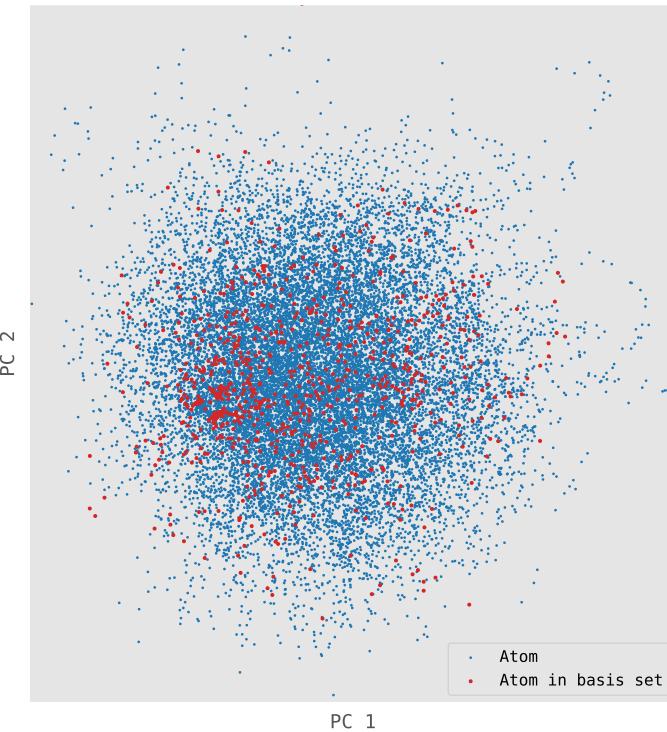
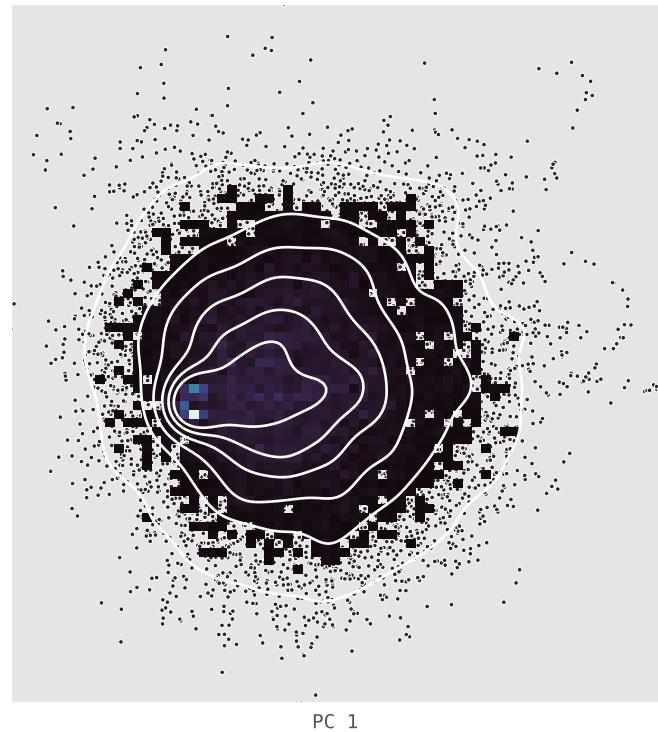
principal component analysis of descriptors (Pb)



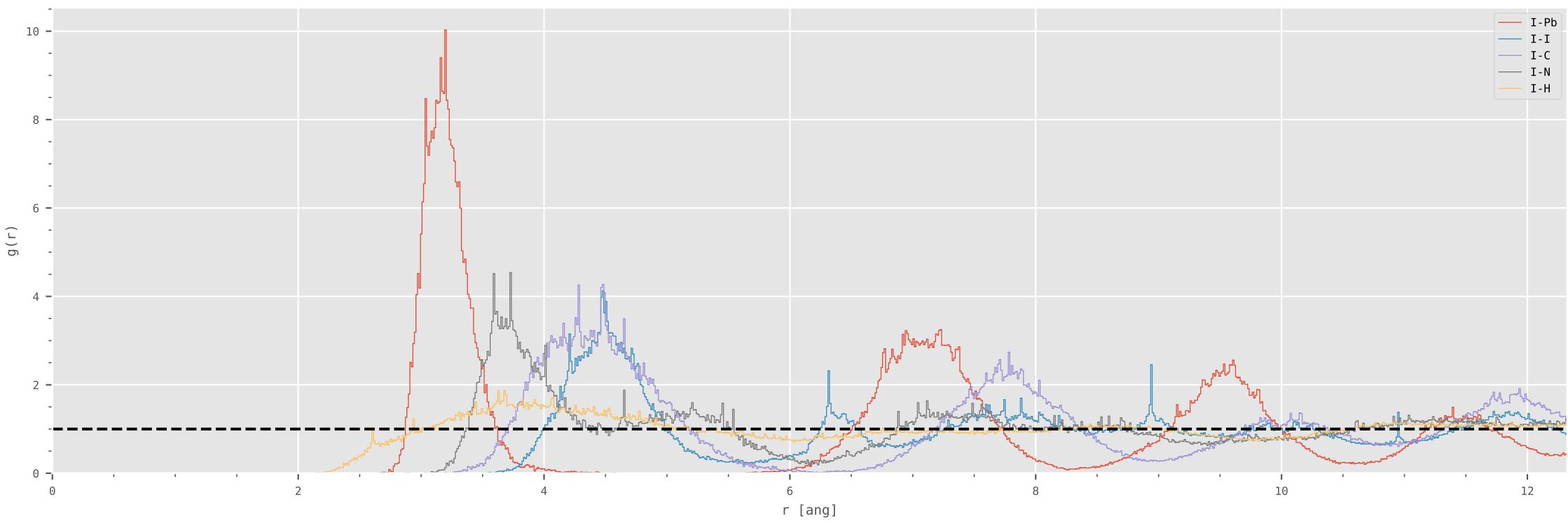
radial distribution functions (Pb)



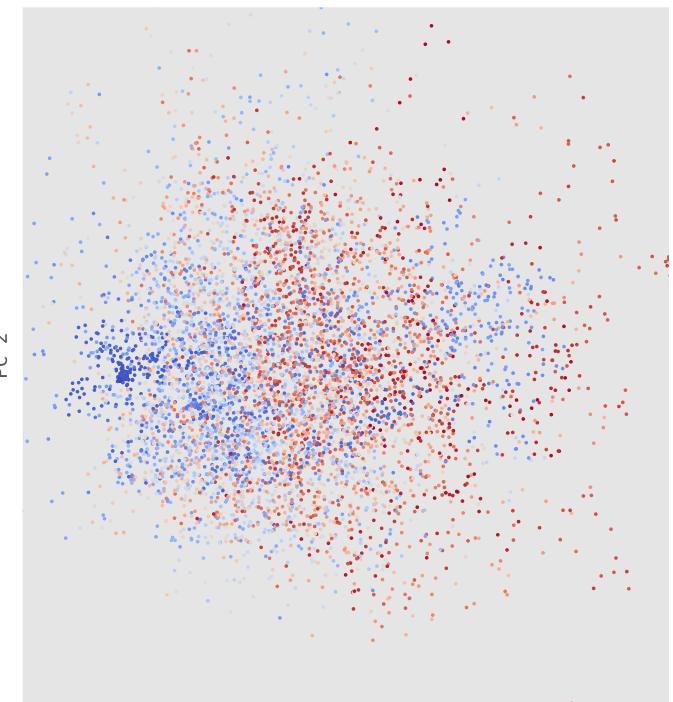
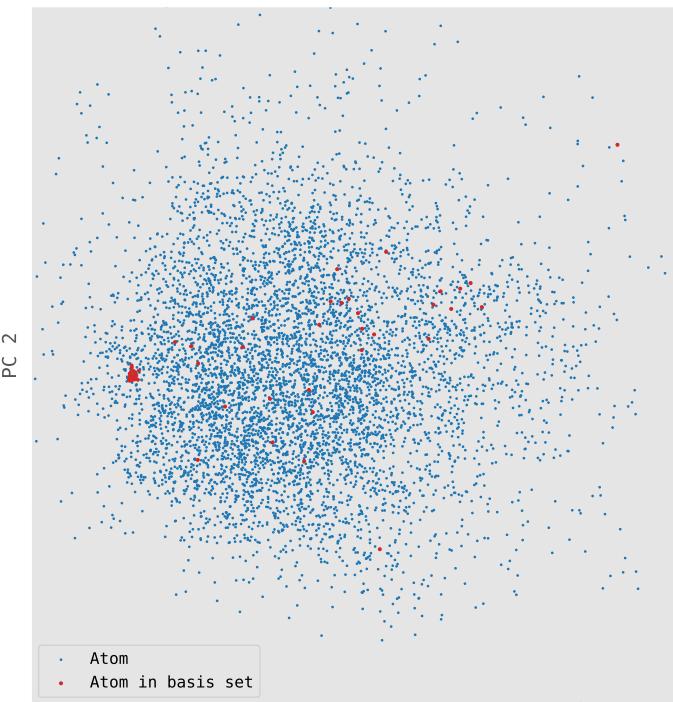
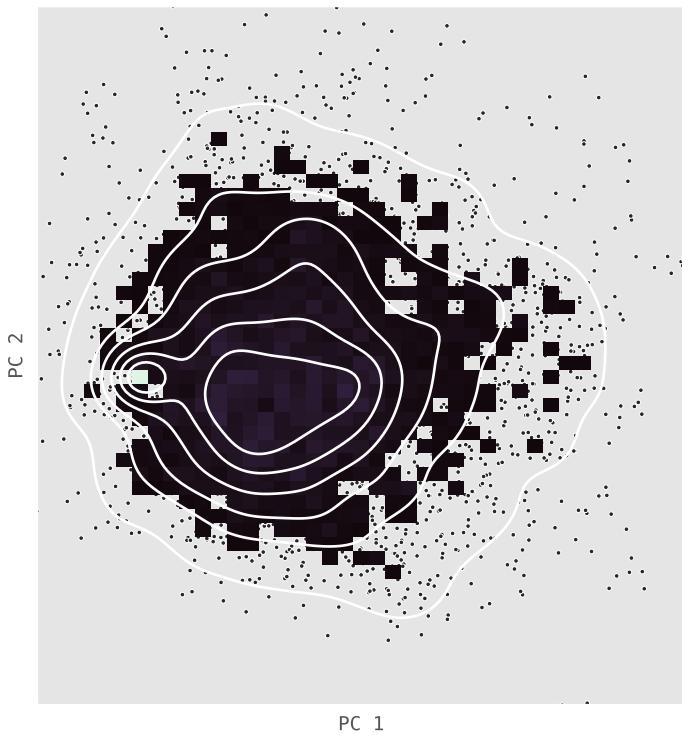
principal component analysis of descriptors (I)



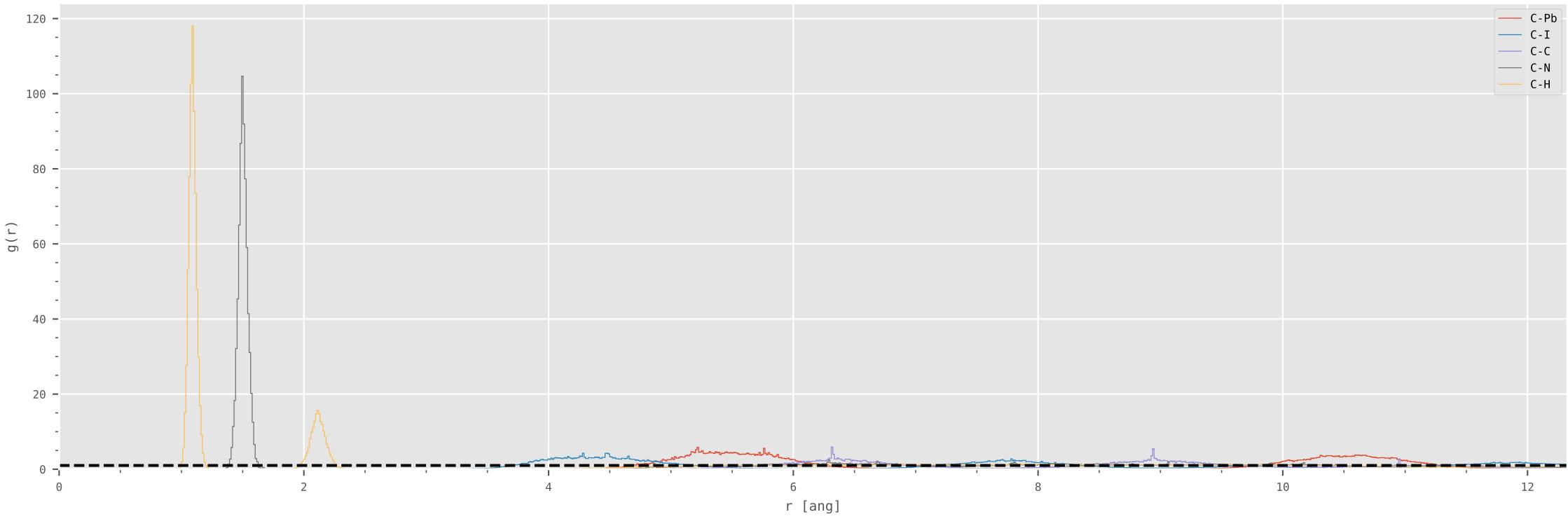
radial distribution functions (I)



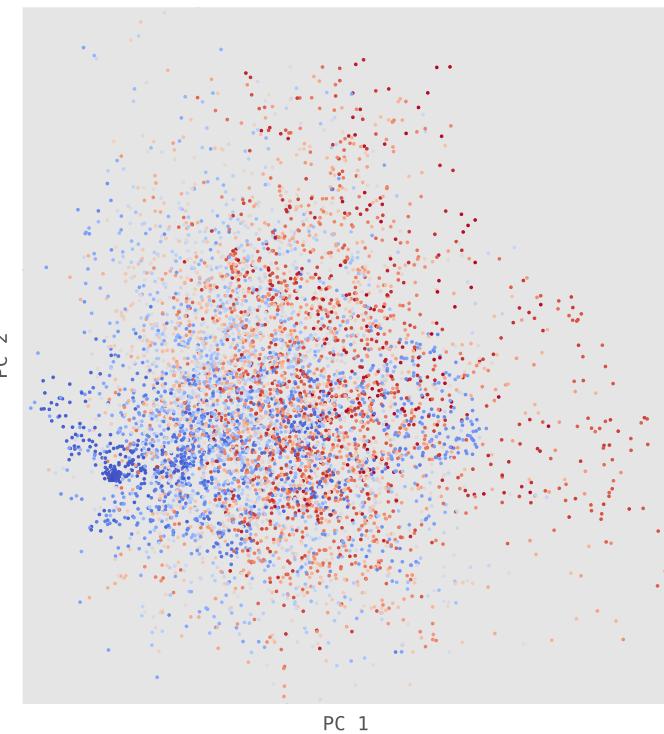
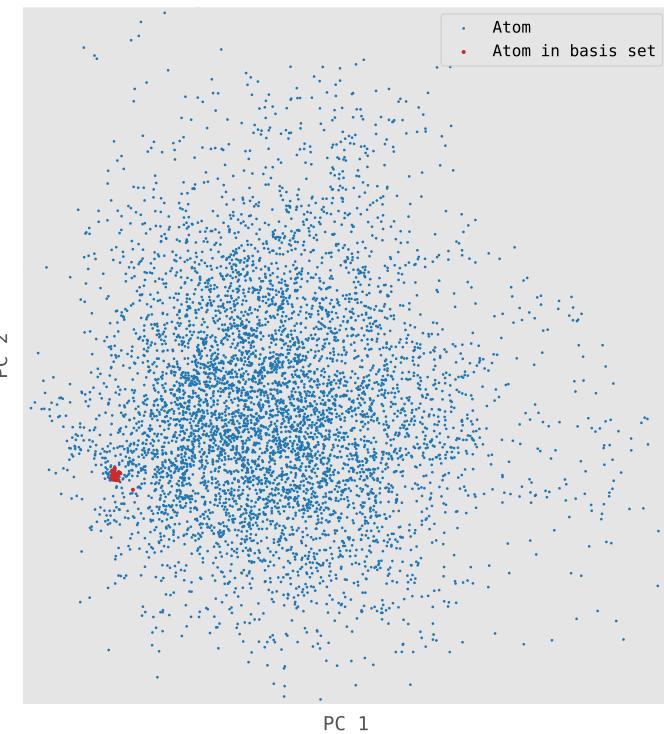
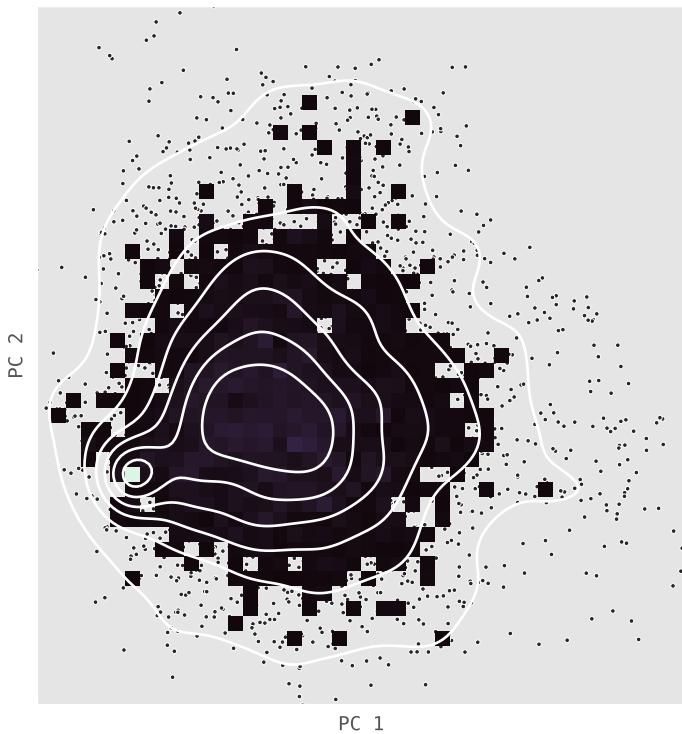
principal component analysis of descriptors (C)



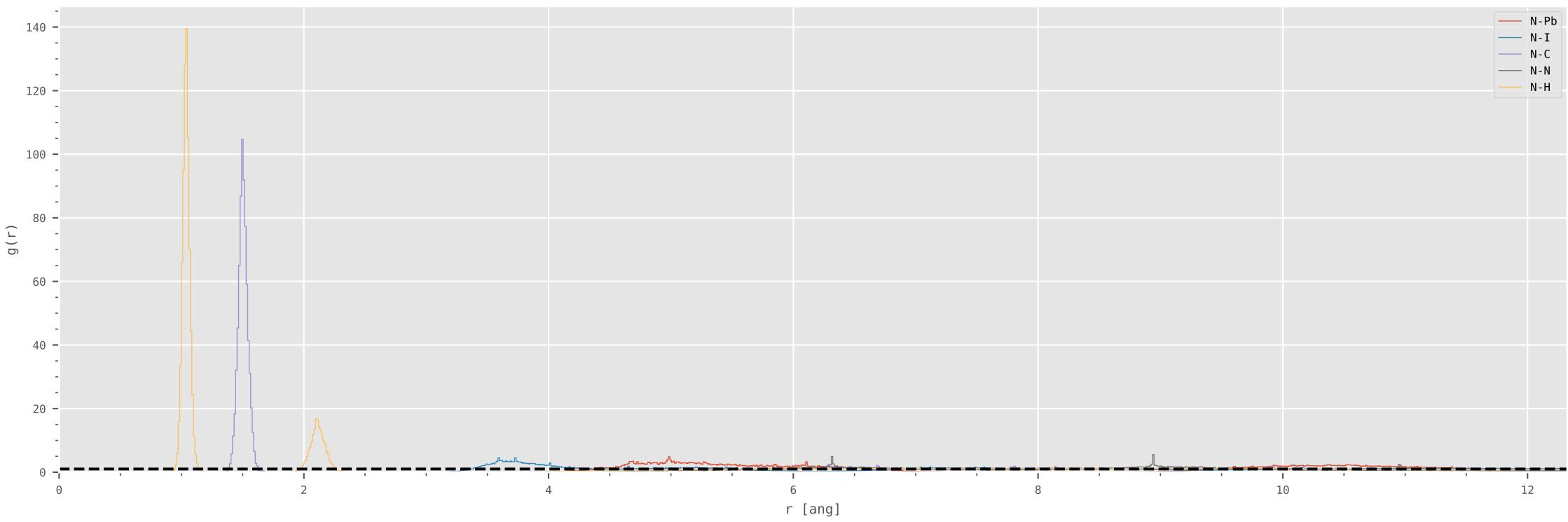
radial distribution functions (C)



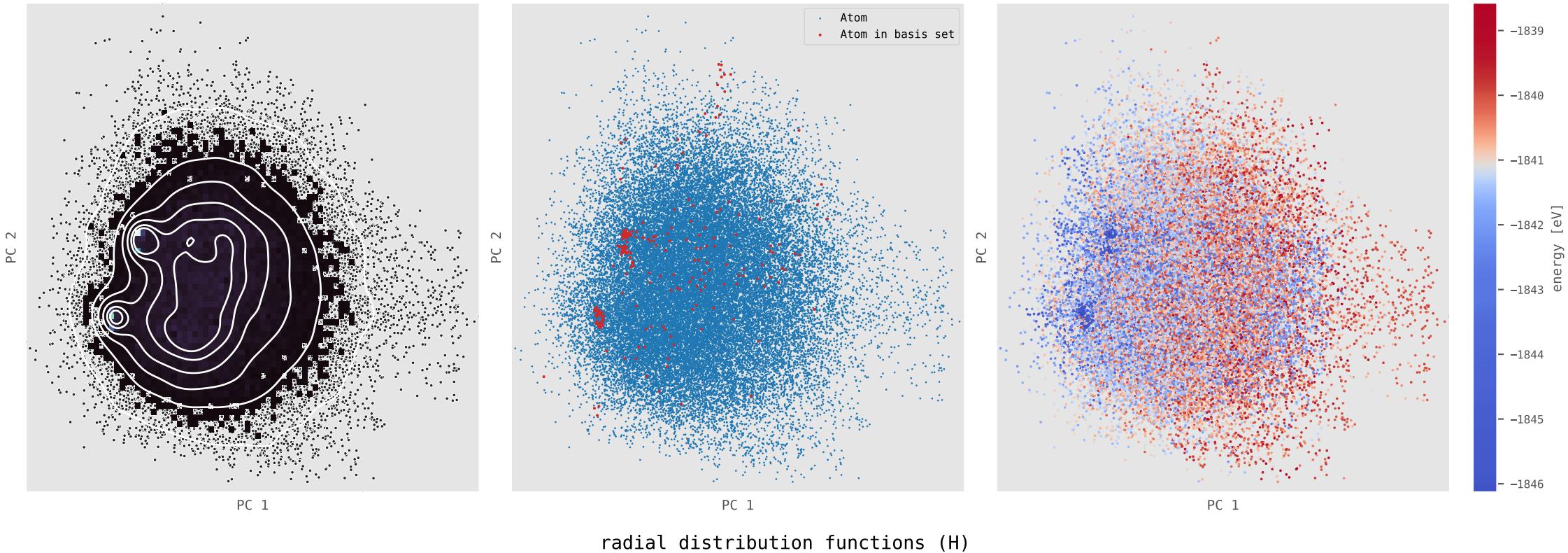
principal component analysis of descriptors (N)



radial distribution functions (N)



principal component analysis of descriptors (H)



radial distribution functions (H)

