

<b>all_gradient</b>	<b>compiled binary</b>	<b>fortran unit test</b>	<b>C API</b>
hl_gap	12.391144584175	12.391144584178	n/a
energy	-20.323978512118	-20.323978512117	n/a
gradient_norm	0.007811924008	0.007811923956	n/a
gradient(1,5)	-0.002219212304	-0.002219212205	n/a
gradient(2,2)	0.002219212304	0.002219212205	n/a
gradient(1,4)	0.000956216022	0.000956215978	n/a
gradient(3,6)	-0.001190415424	-0.001190415384	n/a

<b>atomic_symbols</b>	<b>compiled binary</b>	<b>fortran unit test</b>	<b>C API</b>
hl_gap	12.520985724004	12.718203165741	n/a
energy	-10.155934021424	-10.160927754235	-10.160927754235
gradient_norm	0.024959693923	0.021549557655	n/a
gradient(1,5)	-0.002315603938	-0.002032674926	-0.002032675005
gradient(2,2)	0.002594449909	0.003312545972	0.003312546032
gradient(1,4)	0.000847029764	-0.001192940566	-0.001192940535
gradient(3,6)	-0.001471110650	-0.001660768275	-0.001660768316
pcgradient(1,5)	-0.000366987011	-0.000248319580	-0.000248319582
pcgradient(2,2)	-0.001293800068	0.001420844472	0.001420844475
pcgradient(1,4)	0.001577640256	0.003746685270	0.003746685275
pcgradient(3,6)	0.000184214174	0.000651613443	0.000651613444

<b>point_charge_99</b>	<b>compiled binary</b>	<b>fortran unit test</b>	<b>C API</b>
hl_gap	12.620038103611	13.024345612330	n/a
energy	-10.157418280497	-10.168788268962	-10.152737646640
gradient_norm	0.024086791687	0.018113624401	n/a
gradient(1,5)	-0.001994597749	-0.000506462895	-0.002702555136
gradient(2,2)	0.002098856519	0.002546832066	0.003733296658
gradient(1,4)	-0.000645240452	-0.007492788009	0.002167306942
gradient(3,6)	-0.001260948864	-0.001324851465	-0.001930216404
pcgradient(1,5)	-0.000806213820	-0.002157370323	0.001719768278
pcgradient(2,2)	-0.001675533707	0.002565366215	0.000013639209
pcgradient(1,4)	0.002470474973	0.012124342986	-0.002684282199
pcgradient(3,6)	0.000233497343	0.001214057506	0.000020147962

*C API: <https://github.com/pultar/xtb-example>*

*compiled binary: master branch, but conda release gives same result*

*comparison fortran unit tests: <https://github.com/grimme-lab/xtb/blob/36202cd82313559dd9d7ec11936dec!>*

identical results

fortran unit tests and C API agree with each other, compiled binary differs (!)

compiled binary differs (!), difference to C API was discussed already here: <https://github.com/grimme-lab/>