

Supplementary_Electronic_Information_PCCP.txt

Supplementary Electronic Information
for the paper:

"Are ab initio quantum chemistry methods able to predict vibrational states up to the dissociation limit for multi-electron molecules close to spectroscopic accuracy?"

by

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Table A1

Potential energy curve data used to produce the final vibrational levels of LiH. The function is composed of the B0 (calculated at the MRCISD+QP/(56) level), MVD relativistic correction (obtained at icMR-CISD/cc-pwCV5Z level) and DBOC (calculated at the MRCISD/cc-pwCVTZ level) contributions.

R	PEC (final)
Bohr	(Hartree)

1.850	-7.96651541
1.875	-7.97298958
1.900	-7.97913828
1.925	-7.98497334
1.950	-7.99051096
1.975	-7.99576266
2.000	-8.00074224
2.025	-8.00546043
2.050	-8.00992964
2.075	-8.01416162
2.100	-8.01816503
2.130	-8.02268399
2.150	-8.02553007
2.160	-8.02690550
2.200	-8.03209955
2.230	-8.03568801
2.250	-8.03794235
2.260	-8.03902945
2.300	-8.04312099
2.350	-8.04769282
2.400	-8.05170994
2.450	-8.05522046
2.500	-8.05826790
2.550	-8.06089203
2.600	-8.06312939
2.650	-8.06501339
2.700	-8.06657411
2.750	-8.06784009
2.800	-8.06883697
2.850	-8.06958796
2.900	-8.07011467
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3.000	-8.07057275
3.050	-8.07053903
3.100	-8.07035117
3.150	-8.07002304

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