

Supporting Information

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<b>Molecule</b>	<b>Converged</b>	<b>Number of vectors in Newton-Raphson procedure</b>	<b>Number of linearly independent vectors in the Newton-Raphson procedure.</b>
Propane	yes	11	9
Butane	no	40	20
Pentane	yes	15	14
Hexane	no	40	10
Heptane	yes	15	14
Octane	no	40	8

Table 1: The Newton-Raphson approach for solving the ACPF equations is not stable for CD-LACPF. Large numbers of linearly dependent vectors indicate a failure of the solver.