Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

New tuned range-separated density functional for the accurate calculation of electronic second hyperpolarizabilities (SI1)

Pau Besalú-Sala[§], Sebastian P. Sitkiewicz[§‖], Pedro Salvador*[§], Eduard Matito*[‖‡], Josep M. Luis*[§]

[§] Departament de Química and Institut de Química Computacional i Catàlisi (IQCC), University of Girona, Campus Montilivi, Girona 17003, Spain.

[‖] Kimika Fakultatea, Euskal Herriko Unibertsitatea, UPV/EHU and Donostia International Physics Center (DIPC), P.K. 1072, 20080 Donostia, Euskadi, Spain.

[‡] Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain.

Contents

This document contains the information (γ_{zzzz} values, Cartesian coordinates and field-dependent CCSD(T) energies) regarding the 60 molecules that form the γ-NLO set.

1. γ_{zzzz} values at the following levels of theory: CCSD(T), B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD, CAM-B3LYP, LC-BLYP, OT-LC-BLYP and Tα-LC-BLYP for the γ-NLO set

SI1.1 Values of the second hyperpolarizabilities (γ_{zzzz}) for γ-NLO set using LC-BLYP, T_α-LC-BLYP, CAM-B3LYP, OT-LC-BLYP, B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD density functionals as well as CCSD(T) method. aug-cc-pVDZ basis set used in all cases.

	Electronic second hyperpolarizabilities (zzzz element of the tensor) (a.u.)										
System	**CCSD(T)**	**LC-BLYP**	**Tα-LC-BLYP**	**CAM-B3LYP**	**OT-LC-BLYP**	**B3LYP**	**BH&HLYP**	**PBE0**	**M06-2X**	**MN15**	**wB97XD**
Hydrogen fluoride	2.880E+02	2.857E+02	2.811E+02	3.088E+02	2.515E+02	3.249E+02	2.726E+02	3.052E+02	2.428E+02	3.348E+02	3.040E+02
Nitric acid	4.032E+03	2.932E+03	3.296E+03	3.629E+03	3.074E+03	4.341E+03	2.968E+03	3.896E+03	2.969E+03	3.242E+03	3.381E+03
Carbonic acid	4.690E+03	3.163E+03	3.682E+03	4.294E+03	3.435E+03	5.576E+03	3.385E+03	4.792E+03	3.426E+03	3.756E+03	4.012E+03
Boric acid	3.465E+03	2.949E+03	3.376E+03	3.603E+03	3.092E+03	4.237E+03	2.952E+03	3.824E+03	2.863E+03	3.477E+03	3.486E+03
Dioxygen	4.097E+02	3.877E+02	4.632E+02	4.430E+02	3.617E+02	4.992E+02	2.501E+02	4.368E+02	4.083E+02	4.279E+02	4.040E+02
Water	4.740E+02	4.369E+02	4.757E+02	5.015E+02	4.179E+02	5.472E+02	4.598E+02	5.178E+02	4.832E+02	5.496E+02	5.188E+02
Hydrogen peroxide	1.557E+03	1.372E+03	1.555E+03	1.574E+03	1.342E+03	1.741E+03	1.363E+03	1.579E+03	1.290E+03	1.514E+03	1.442E+03
Dinitrogen	1.130E+03	1.067E+03	1.293E+03	1.216E+03	1.051E+03	1.328E+03	9.561E+02	1.210E+03	1.148E+03	1.127E+03	1.135E+03
Carbon monoxide	1.657E+03	1.404E+03	1.703E+03	1.680E+03	1.363E+03	1.880E+03	1.399E+03	1.764E+03	1.652E+03	1.583E+03	1.651E+03
Nitroxyl	1.504E+03	1.124E+03	1.375E+03	1.331E+03	1.326E+03	1.561E+03	1.043E+03	1.441E+03	1.228E+03	1.354E+03	1.353E+03
Cyanic fluoride	2.047E+03	1.564E+03	1.891E+03	1.780E+03	1.521E+03	1.973E+03	1.432E+03	1.834E+03	1.642E+03	1.708E+03	1.719E+03
Carbon dioxide	7.705E+02	8.026E+02	9.795E+02	9.146E+02	7.643E+02	9.913E+02	7.402E+02	9.254E+02	8.204E+02	8.980E+02	8.670E+02
Nitrous acid	5.117E+03	3.282E+03	4.266E+03	4.248E+03	4.068E+03	5.486E+03	3.383E+03	4.815E+03	3.521E+03	3.706E+03	3.863E+03
Ammonia	1.049E+03	9.405E+02	1.125E+03	1.129E+03	9.405E+02	1.301E+03	1.021E+03	1.199E+03	1.142E+03	1.182E+03	1.173E+03
Formaldehyde	2.259E+03	1.822E+03	2.347E+03	2.251E+03	1.849E+03	2.785E+03	1.811E+03	2.480E+03	2.115E+03	2.276E+03	2.358E+03
1-Pentanoic acid	2.087E+04	1.514E+04	2.103E+04	2.150E+04	1.847E+04	3.013E+04	1.872E+04	2.681E+04	2.108E+04	2.110E+04	2.043E+04
Cyclohexane	1.670E+04	1.125E+04	1.446E+04	1.457E+04	1.286E+04	1.823E+04	1.322E+04	1.683E+04	1.554E+04	1.479E+04	1.456E+04
1-Pentanamide	2.569E+04	1.776E+04	2.488E+04	2.570E+04	1.839E+04	3.699E+04	2.228E+04	3.297E+04	2.564E+04	2.570E+04	2.469E+04
Dinitrogen oxide	1.939E+03	1.463E+03	2.342E+03	2.146E+03	1.984E+03	2.344E+03	1.815E+03	2.140E+03	1.977E+03	2.120E+03	2.025E+03
Pentanal	1.872E+04	1.349E+04	1.849E+04	1.867E+04	1.575E+04	2.593E+04	1.670E+04	2.357E+04	1.972E+04	1.923E+04	1.802E+04
n-Butanol	1.504E+04	1.002E+04	1.355E+04	1.386E+04	1.100E+04	1.896E+04	1.262E+04	1.715E+04	1.438E+04	1.396E+04	1.334E+04

Hydrogen cyanide	2.350E+03	1.884E+03	2.462E+03	2.247E+03	1.861E+03	2.586E+03	1.884E+03	2.376E+03	2.129E+03	2.233E+03	2.221E+03
Hydrogen isocyanide	5.503E+03	3.542E+03	5.015E+03	4.741E+03	1.861E+03	2.586E+03	1.884E+03	2.376E+03	2.129E+03	2.233E+03	2.221E+03
Methane	1.720E+03	1.595E+03	1.968E+03	1.867E+03	1.612E+03	2.073E+03	1.686E+03	1.982E+03	1.925E+03	1.985E+03	2.070E+03
n-Butylamine	1.636E+04	1.550E+04	1.667E+04	1.713E+04	1.454E+04	2.364E+04	1.568E+04	2.139E+04	1.795E+04	1.734E+04	1.654E+04
Propane	9.545E+03	7.547E+03	1.002E+04	9.977E+03	8.096E+03	1.271E+04	9.098E+03	1.171E+04	1.063E+04	1.008E+04	1.002E+04
Ethane	5.178E+03	4.533E+03	5.858E+03	5.767E+03	4.705E+03	6.942E+03	5.281E+03	6.573E+03	6.304E+03	5.904E+03	6.096E+03
Butane	1.424E+04	1.096E+04	1.465E+04	1.487E+04	1.217E+04	1.964E+04	1.366E+04	1.795E+04	1.615E+04	1.512E+04	1.465E+04
Pentane	1.954E+04	1.406E+04	1.934E+04	1.937E+04	1.513E+04	2.628E+04	1.787E+04	2.392E+04	2.099E+04	1.976E+04	1.879E+04
Hexane	2.447E+04	1.749E+04	2.416E+04	2.434E+04	1.799E+04	3.356E+04	2.250E+04	3.064E+04	2.665E+04	2.506E+04	2.354E+04
PMI1	4.167E+03	2.991E+03	4.198E+03	3.746E+03	3.324E+03	4.564E+03	3.042E+03	4.151E+03	3.619E+03	3.801E+03	3.871E+03
Heptane	2.869E+04	2.075E+04	2.867E+04	2.898E+04	2.048E+04	4.032E+04	2.682E+04	3.688E+04	3.188E+04	3.011E+04	2.798E+04
Octane	3.319E+04	2.428E+04	3.360E+04	3.402E+04	2.311E+04	4.760E+04	3.148E+04	4.369E+04	3.767E+04	3.564E+04	3.287E+04
Benzene	1.340E+04	9.858E+03	1.215E+04	1.179E+04	1.235E+04	1.371E+04	1.104E+04	1.262E+04	1.219E+04	1.254E+04	1.189E+04
1-Butene	1.726E+04	1.348E+04	1.836E+04	1.870E+04	2.374E+04	2.559E+04	1.780E+04	2.267E+04	1.952E+04	1.846E+04	1.802E+04
PMI2	1.459E+04	1.150E+04	1.425E+04	1.368E+04	1.363E+04	1.568E+04	1.235E+04	1.465E+04	1.363E+04	1.382E+04	1.376E+04
PA1	4.055E+03	2.719E+03	3.635E+03	3.337E+03	3.190E+03	3.881E+03	2.843E+03	3.687E+03	3.730E+03	3.541E+03	3.711E+03
Acetylene	3.259E+03	2.728E+03	3.301E+03	3.151E+03	2.857E+03	3.484E+03	2.915E+03	3.212E+03	3.153E+03	3.378E+03	3.267E+03
PMI3	6.048E+04	4.862E+04	6.038E+04	6.179E+04	5.769E+04	7.614E+04	5.811E+04	7.120E+04	6.092E+04	6.397E+04	6.063E+04
PA2	3.160E+04	2.380E+04	2.847E+04	2.743E+04	2.780E+04	3.022E+04	2.530E+04	2.815E+04	2.764E+04	2.721E+04	2.765E+04
PMI4	1.940E+05	1.476E+05	1.877E+05	2.085E+05	1.994E+05	2.956E+05	2.008E+05	2.726E+05	2.064E+05	2.269E+05	1.990E+05
PDA1	1.133E+05	9.602E+04	1.142E+05	1.201E+05	1.158E+05	1.456E+05	1.159E+05	1.347E+05	1.198E+05	1.232E+05	2.639E+00
PMI5	4.518E+05	3.430E+05	4.454E+05	5.408E+05	5.199E+05	9.105E+05	5.310E+05	8.204E+05	5.426E+05	6.236E+05	5.004E+05
PA3	1.501E+05	1.192E+05	1.364E+05	1.379E+05	1.420E+05	1.525E+05	1.295E+05	1.434E+05	1.385E+05	1.368E+05	1.350E+05
PMI6	9.884E+05	6.565E+05	8.613E+05	1.144E+06	1.062E+06	2.326E+06	1.142E+06	2.035E+06	1.168E+06	1.401E+06	1.024E+06
PA4	4.890E+05	4.007E+05	4.532E+05	4.821E+05	5.010E+05	5.521E+05	4.557E+05	5.221E+05	4.881E+05	4.920E+05	4.652E+05
PDA2	7.606E+05	6.680E+05	7.997E+05	9.656E+05	9.172E+05	1.393E+06	1.592E+03	1.274E+06	1.662E+03	1.072E+06	8.969E+05
PA5	1.240E+06	1.035E+06	1.147E+06	1.319E+06	1.364E+06	1.594E+06	1.257E+06	1.509E+06	1.349E+06	1.391E+06	1.256E+06
PDA3	2.443E+06	2.231E+06	2.579E+06	3.778E+06	2.230E+06	6.738E+06	3.779E+06	6.011E+06	3.893E+06	4.554E+06	3.380E+06

PA6	2.482E+06	2.223E+06	2.429E+06	3.027E+06	3.136E+06	3.914E+06	2.916E+06	3.692E+06	3.127E+06	3.300E+06	2.838E+06
PDA4	5.299E+06	4.955E+06	5.621E+06	9.638E+06	9.249E+06	2.127E+07	9.847E+06	1.841E+07	1.010E+07	1.250E+07	8.325E+06
H_2	1.398E+03	1.465E+03	1.567E+03	1.634E+03	1.255E+03	1.720E+03	1.455E+03	1.632E+03	1.323E+03	1.759E+03	1.748E+03
PDA5	1.110E+07	8.676E+06	9.538E+06	1.883E+07	1.861E+07	5.039E+07	1.960E+07	4.229E+07	2.000E+07	2.594E+07	1.580E+07
$(H_2)_2$	1.257E+04	1.304E+04	1.275E+04	1.591E+04	1.289E+04	1.877E+04	1.444E+04	1.780E+04	1.654E+04	1.713E+04	1.603E+04
$(H_2)_3$	3.536E+04	3.977E+04	3.643E+04	5.281E+04	4.140E+04	7.041E+04	4.820E+04	6.593E+04	5.485E+04	6.217E+04	5.252E+04
$(H_2)_4$	7.404E+04	8.629E+04	7.583E+04	1.235E+05	9.340E+04	1.840E+05	1.122E+05	1.693E+05	1.257E+05	1.557E+05	1.202E+05
$(H_2)_5$	1.251E+05	1.492E+05	1.259E+05	2.264E+05	1.660E+05	3.694E+05	2.048E+05	3.352E+05	2.266E+05	2.997E+05	2.167E+05
$(H_2)_7$	2.059E+05	2.241E+05	1.837E+05	3.551E+05	2.512E+05	6.221E+05	3.200E+05	5.579E+05	3.509E+05	4.887E+05	3.353E+05
$(H_2)_6$	2.498E+05	3.067E+05	2.492E+05	5.016E+05	3.457E+05	9.277E+05	4.506E+05	8.245E+05	4.912E+05	7.105E+05	4.690E+05
$(H_2)_8$	3.165E+05	3.944E+05	3.099E+05	6.604E+05	4.364E+05	1.272E+06	5.915E+05	1.122E+06	6.421E+05	9.561E+05	6.128E+05

SI1.2 Absolute errors of the second hyperpolarizabilities (γ_{zzzz}) respect to CCSD(T) benchmark values for γ-NLO set obtained using LC-BLYP, T_{α}-LC-BLYP, CAM-B3LYP, OT-LC-BLYP, B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD density functionals. aug-cc-pVDZ basis set used in all cases.

	Absolute errors respect to CCSD(T) (a.u.)									
System	**LC-BLYP**	**Tα-LC-BLYP**	**CAM-B3LYP**	**OT-LC-BLYP**	**B3LYP**	**BH&HLYP**	**PBE0**	**M06-2X**	**MN15**	**wB97XD**
Hydrogen fluoride	2.222E+00	6.835E+00	2.088E+01	3.644E+01	3.691E+01	1.537E+01	1.727E+01	4.520E+01	4.685E+01	1.602E+01
Nitric acid	1.100E+03	7.361E+02	4.028E+02	9.578E+02	3.092E+02	1.064E+03	1.359E+02	1.063E+03	7.900E+02	6.509E+02
Carbonic acid	1.526E+03	1.008E+03	3.960E+02	1.255E+03	8.860E+02	1.304E+03	1.026E+02	1.264E+03	9.334E+02	6.778E+02
Boric acid	5.153E+02	8.876E+01	1.385E+02	3.726E+02	7.725E+02	5.126E+02	3.590E+02	6.021E+02	1.257E+01	2.130E+01
Dioxygen	2.201E+01	5.353E+01	3.329E+01	4.798E+01	8.955E+01	1.596E+02	2.707E+01	1.420E+00	1.825E+01	5.727E+00
Water	3.718E+01	1.639E+00	2.743E+01	5.613E+01	7.315E+01	1.426E+01	4.372E+01	9.200E+00	7.558E+01	4.474E+01
Hydrogen peroxide	1.846E+02	1.336E+00	1.671E+01	2.144E+02	1.845E+02	1.943E+02	2.266E+01	2.665E+02	4.272E+01	1.152E+02
Dinitrogen	6.211E+01	1.637E+02	8.659E+01	7.856E+01	1.986E+02	1.734E+02	8.090E+01	1.879E+01	2.257E+00	5.316E+00
Carbon monoxide	2.526E+02	4.633E+01	2.336E+01	2.936E+02	2.233E+02	2.578E+02	1.074E+02	4.651E+00	7.328E+01	6.086E+00
Nitroxyl	3.807E+02	1.293E+02	1.732E+02	1.786E+02	5.615E+01	4.612E+02	6.345E+01	2.762E+02	1.505E+02	1.514E+02
Cyanic fluoride	4.826E+02	1.561E+02	2.662E+02	5.254E+02	7.347E+01	6.142E+02	2.123E+02	4.045E+02	3.387E+02	3.278E+02
Carbon dioxide	3.202E+01	2.090E+02	1.440E+02	6.230E+00	2.208E+02	3.030E+01	1.549E+02	4.984E+01	1.275E+02	9.647E+01
Nitrous acid	1.835E+03	8.515E+02	8.697E+02	1.050E+03	3.683E+02	1.734E+03	3.026E+02	1.596E+03	1.411E+03	1.255E+03
Ammonia	1.087E+02	7.586E+01	7.938E+01	1.087E+02	2.520E+02	2.832E+01	1.495E+02	9.259E+01	1.332E+02	1.235E+02
Formaldehyde	4.377E+02	8.739E+01	8.403E+00	4.098E+02	5.255E+02	4.483E+02	2.205E+02	1.438E+02	1.678E+01	9.897E+01
1-Pentanoic acid	5.730E+03	1.604E+02	6.334E+02	2.397E+03	9.263E+03	2.154E+03	5.940E+03	2.143E+02	2.320E+02	4.395E+02
Cyclohexane	5.457E+03	2.241E+03	2.133E+03	3.841E+03	1.530E+03	3.487E+03	1.298E+02	1.168E+03	1.913E+03	2.142E+03
1-Pentanamide	7.931E+03	8.141E+02	4.988E+00	7.307E+03	1.130E+04	3.417E+03	7.272E+03	5.295E+01	4.256E+00	1.004E+03
Dinitrogen oxide	4.759E+02	4.029E+02	2.066E+02	4.525E+01	4.044E+02	1.245E+02	2.013E+02	3.730E+01	1.806E+02	8.596E+01
Pentanal	5.225E+03	2.349E+02	5.101E+01	2.975E+03	7.213E+03	2.018E+03	4.855E+03	9.973E+02	5.120E+02	7.035E+02
n-Butanol	5.024E+03	1.491E+03	1.184E+03	4.041E+03	3.916E+03	2.417E+03	2.107E+03	6.588E+02	1.084E+03	1.706E+03
Hydrogen cyanide	4.660E+02	1.121E+02	1.033E+02	4.896E+02	2.362E+02	4.667E+02	2.556E+01	2.211E+02	1.174E+02	1.295E+02
Hydrogen isocyanide	1.961E+03	4.883E+02	7.624E+02	3.643E+03	2.917E+03	3.620E+03	3.128E+03	3.374E+03	3.271E+03	3.283E+03

Methane	1.249E+02	2.482E+02	1.471E+02	1.085E+02	3.524E+02	3.464E+01	2.622E+02	2.051E+02	2.644E+02	3.501E+02
n-Butylamine	8.556E+02	3.136E+02	7.756E+02	1.819E+03	7.282E+03	6.813E+02	5.035E+03	1.588E+03	9.822E+02	1.773E+02
Propane	1.998E+03	4.711E+02	4.314E+02	1.449E+03	3.163E+03	4.474E+02	2.161E+03	1.082E+03	5.388E+02	4.758E+02
Ethane	6.445E+02	6.803E+02	5.890E+02	4.725E+02	1.764E+03	1.036E+02	1.396E+03	1.126E+03	7.259E+02	9.187E+02
Butane	3.287E+03	4.066E+02	6.241E+02	2.068E+03	5.400E+03	5.834E+02	3.712E+03	1.908E+03	8.820E+02	4.088E+02
Pentane	5.477E+03	2.027E+02	1.727E+02	4.413E+03	6.737E+03	1.674E+03	4.384E+03	1.446E+03	2.161E+02	7.463E+02
Hexane	6.970E+03	3.100E+02	1.239E+02	6.480E+03	9.099E+03	1.961E+03	6.170E+03	2.185E+03	5.975E+02	9.253E+02
PMI1	1.176E+03	3.109E+01	4.217E+02	8.432E+02	3.962E+02	1.125E+03	1.614E+01	5.484E+02	3.660E+02	2.963E+02
Heptane	7.934E+03	1.524E+01	2.937E+02	8.204E+03	1.163E+04	1.865E+03	8.196E+03	3.196E+03	1.424E+03	7.028E+02
Octane	8.907E+03	4.121E+02	8.285E+02	1.007E+04	1.442E+04	1.711E+03	1.050E+04	4.479E+03	2.458E+03	3.170E+02
Benzene	3.542E+03	1.249E+03	1.607E+03	1.047E+03	3.138E+02	2.361E+03	7.839E+02	1.207E+03	8.557E+02	1.510E+03
1-Butene	3.778E+03	1.108E+03	1.439E+03	6.478E+03	8.332E+03	5.438E+02	5.412E+03	2.261E+03	1.200E+03	7.630E+02
PMI2	3.099E+03	3.488E+02	9.133E+02	9.603E+02	1.088E+03	2.244E+03	5.730E+01	9.602E+02	7.705E+02	8.307E+02
PA1	1.336E+03	4.201E+02	7.180E+02	8.652E+02	1.737E+02	1.212E+03	3.678E+02	3.253E+02	5.138E+02	3.437E+02
Acetylene	5.308E+02	4.244E+01	1.082E+02	4.023E+02	2.251E+02	3.436E+02	4.681E+01	1.060E+02	1.194E+02	7.876E+00
PMI3	1.186E+04	1.064E+02	1.304E+03	2.793E+03	1.566E+04	2.368E+03	1.072E+04	4.357E+02	3.491E+03	1.442E+02
PA2	7.795E+03	3.125E+03	4.165E+03	3.792E+03	1.372E+03	6.291E+03	3.450E+03	3.954E+03	4.390E+03	3.945E+03
PMI4	4.641E+04	6.321E+03	1.450E+04	5.430E+03	1.017E+05	6.788E+03	7.860E+04	1.243E+04	3.295E+04	5.060E+03
PDA1	1.724E+04	9.873E+02	6.816E+03	2.556E+03	3.234E+04	2.618E+03	2.143E+04	6.511E+03	9.968E+03	1.133E+05
PMI5	1.088E+05	6.422E+03	8.901E+04	6.810E+04	4.587E+05	7.922E+04	3.686E+05	9.082E+04	1.717E+05	4.857E+04
PA3	3.088E+04	1.368E+04	1.221E+04	8.103E+03	2.430E+03	2.066E+04	6.752E+03	1.165E+04	1.327E+04	1.514E+04
PMI6	3.320E+05	1.271E+05	1.558E+05	7.330E+04	1.337E+06	1.538E+05	1.047E+06	1.797E+05	4.122E+05	3.592E+04
PA4	8.826E+04	3.580E+04	6.848E+03	1.201E+04	6.317E+04	3.323E+04	3.315E+04	8.560E+02	3.034E+03	2.381E+04
PDA2	9.254E+04	3.916E+04	2.051E+05	1.567E+05	6.329E+05	7.590E+05	5.136E+05	7.589E+05	3.116E+05	1.363E+05
PA5	2.049E+05	9.339E+04	7.875E+04	1.238E+05	3.535E+05	1.677E+04	2.681E+05	1.085E+05	1.502E+05	1.528E+04
PDA3	2.121E+05	1.368E+05	1.336E+06	2.121E+05	4.295E+06	1.337E+06	3.569E+06	1.450E+06	2.112E+06	9.378E+05
PA6	2.596E+05	5.315E+04	5.444E+05	6.531E+05	1.432E+06	4.337E+05	1.209E+06	6.441E+05	8.180E+05	3.551E+05
PDA4	3.434E+05	3.223E+05	4.339E+06	3.950E+06	1.597E+07	4.548E+06	1.311E+07	4.801E+06	7.199E+06	3.027E+06

H_2	6.744E+01	1.696E+02	2.358E+02	1.423E+02	3.225E+02	5.733E+01	2.341E+02	7.473E+01	3.609E+02	3.499E+02
PDA5	2.419E+06	1.557E+06	7.733E+06	7.513E+06	3.929E+07	8.502E+06	3.120E+07	8.903E+06	1.485E+07	4.705E+06
$(H_2)_2$	4.628E+02	1.742E+02	3.333E+03	3.148E+02	6.198E+03	1.865E+03	5.222E+03	3.963E+03	4.556E+03	3.457E+03
$(H_2)_3$	4.412E+03	1.071E+03	1.745E+04	6.041E+03	3.505E+04	1.284E+04	3.057E+04	1.950E+04	2.681E+04	1.716E+04
$(H_2)_4$	1.225E+04	1.796E+03	4.949E+04	1.936E+04	1.100E+05	3.819E+04	9.523E+04	5.165E+04	8.165E+04	4.619E+04
$(H_2)_5$	2.414E+04	8.362E+02	1.013E+05	4.091E+04	2.443E+05	7.974E+04	2.101E+05	1.015E+05	1.746E+05	9.157E+04
$(H_2)_7$	1.826E+04	2.219E+04	1.492E+05	4.533E+04	4.163E+05	1.141E+05	3.521E+05	1.451E+05	2.829E+05	1.294E+05
$(H_2)_6$	5.694E+04	5.956E+02	2.519E+05	9.594E+04	6.780E+05	2.008E+05	5.747E+05	2.414E+05	4.608E+05	2.193E+05
$(H_2)_8$	7.795E+04	6.527E+03	3.439E+05	1.200E+05	9.557E+05	2.751E+05	8.060E+05	3.256E+05	6.397E+05	2.964E+05
MAE (a.u.)[a)]	**7.43E+04**	**4.07E+04**	**2.58E+05**	**2.20E+05**	**1.11E+06**	**2.78E+05**	**8.93E+05**	**2.98E+05**	**4.63E+05**	**1.71E+05**
RMSD (a.u.)	**3.23E+05**	**2.07E+05**	**1.16E+06**	**1.10E+06**	**5.51E+06**	**1.26E+06**	**4.40E+06**	**1.33E+06**	**2.15E+06**	**7.36E+05**
MAX (a.u.)	**2.42E+06**	**1.56E+06**	**7.73E+06**	**7.51E+06**	**3.93E+07**	**8.50E+06**	**3.12E+07**	**8.90E+06**	**1.48E+07**	**4.70E+06**

a) MAE: Mean Absolute Error.

b) RMSD: Root-Mean-Square Deviation.

c) MAX: Maximum absolute error.

SI1.3 Absolute values of the relative errors of the second hyperpolarizabilities (γ_{zzzz}) respect to CCSD(T) benchmark values for γ-NLO set obtained using LC-BLYP, T_{α}-LC-BLYP, CAM-B3LYP, OT-LC-BLYP, B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD density functionals. aug-cc-pVDZ basis set used in all cases.

	Absolute values for the relative errors respect to CCSD(T) (%)									
System	**LC-BLYP**	**Tα-LC-BLYP**	**CAM-B3LYP**	**OT-LC-BLYP**	**B3LYP**	**BH&HLYP**	**PBE0**	**M06-2X**	**MN15**	**wB97XD**
Hydrogen fluoride	0.77	2.37	7.25	12.65	12.82	5.34	6.00	15.70	16.27	5.56
Nitric acid	27.29	18.25	9.99	23.76	7.67	26.40	3.37	26.37	19.59	16.14
Carbonic acid	32.54	21.49	8.44	26.75	18.89	27.82	2.19	26.95	19.90	14.45
Boric acid	14.87	2.56	4.00	10.75	22.29	14.79	10.36	17.38	0.36	0.61
Dioxygen	5.37	13.06	8.13	11.71	21.86	38.96	6.61	0.35	4.45	1.40
Water	7.84	0.35	5.79	11.84	15.43	3.01	9.22	1.94	15.94	9.44
Hydrogen peroxide	11.86	0.09	1.07	13.77	11.85	12.48	1.46	17.12	2.74	7.40
Dinitrogen	5.50	14.49	7.67	6.95	17.59	15.36	7.16	1.66	0.20	0.47
Carbon monoxide	15.25	2.80	1.41	17.72	13.48	15.56	6.48	0.28	4.42	0.37
Nitroxyl	25.30	8.60	11.51	11.87	3.73	30.65	4.22	18.36	10.01	10.06
Cyanic fluoride	23.58	7.63	13.01	25.67	3.59	30.01	10.37	19.76	16.55	16.02
Carbon dioxide	4.16	27.12	18.69	0.81	28.65	3.93	20.10	6.47	16.55	12.52
Nitrous acid	35.86	16.64	16.99	20.51	7.20	33.88	5.91	31.19	27.58	24.52
Ammonia	10.36	7.23	7.57	10.36	24.02	2.70	14.25	8.82	12.70	11.77
Formaldehyde	19.37	3.87	0.37	18.14	23.26	19.84	9.76	6.37	0.74	4.38
1-Pentanoic acid	27.46	0.77	3.04	11.49	44.38	10.32	28.46	1.03	1.11	2.11
Cyclohexane	32.67	13.41	12.77	23.00	9.16	20.87	0.78	6.99	11.45	12.82
1-Pentanamide	30.87	3.17	0.02	28.44	43.97	13.30	28.30	0.21	0.02	3.91
Dinitrogen oxide	24.54	20.77	10.65	2.33	20.85	6.42	10.38	1.92	9.31	4.43
Pentanal	27.91	1.25	0.27	15.89	38.53	10.78	25.93	5.33	2.74	3.76
n-Butanol	33.40	9.92	7.87	26.87	26.03	16.07	14.01	4.38	7.20	11.34
Hydrogen cyanide	19.83	4.77	4.39	20.83	10.05	19.86	1.09	9.41	4.99	5.51
Hydrogen isocyanide	35.63	8.87	13.85	66.19	53.00	65.78	56.83	61.31	59.43	59.65

Methane	7.26	14.43	8.55	6.31	20.49	2.01	15.24	11.92	15.37	20.35
n-Butylamine	5.23	1.92	4.74	11.12	44.52	4.17	30.78	9.71	6.00	1.08
Propane	20.93	4.94	4.52	15.18	33.14	4.69	22.63	11.34	5.64	4.98
Ethane	12.45	13.14	11.38	9.13	34.07	2.00	26.95	21.75	14.02	17.74
Butane	23.08	2.86	4.38	14.52	37.91	4.10	26.07	13.39	6.19	2.87
Pentane	28.03	1.04	0.88	22.58	34.48	8.57	22.44	7.40	1.11	3.82
Hexane	28.49	1.27	0.51	26.49	37.19	8.02	25.22	8.93	2.44	3.78
PMI1	28.22	0.75	10.12	20.23	9.51	27.00	0.39	13.16	8.78	7.11
Heptane	27.66	0.05	1.02	28.60	40.54	6.50	28.57	11.14	4.97	2.45
Octane	26.84	1.24	2.50	30.35	43.45	5.16	31.64	13.50	7.41	0.96
Benzene	26.43	9.32	11.99	7.81	2.34	17.62	5.85	9.01	6.39	11.27
1-Butene	21.89	6.42	8.34	37.54	48.28	3.15	31.36	13.10	6.95	4.42
PMI2	21.24	2.39	6.26	6.58	7.46	15.37	0.39	6.58	5.28	5.69
PA1	32.96	10.36	17.71	21.34	4.28	29.88	9.07	8.02	12.67	8.48
Acetylene	16.29	1.30	3.32	12.34	6.91	10.54	1.44	3.25	3.66	0.24
PMI3	19.61	0.18	2.16	4.62	25.90	3.91	17.72	0.72	5.77	0.24
PA2	24.67	9.89	13.18	12.00	4.34	19.91	10.92	12.51	13.89	12.49
PMI4	23.92	3.26	7.47	2.80	52.40	3.50	40.52	6.41	16.99	2.61
PDA1	15.22	0.87	6.02	2.26	28.55	2.31	18.92	5.75	8.80	100.00
PMI5	24.09	1.42	19.70	15.07	101.52	17.54	81.59	20.10	38.01	10.75
PA3	20.57	9.11	8.13	5.40	1.62	13.76	4.50	7.76	8.84	10.08
PMI6	33.58	12.86	15.76	7.42	135.29	15.56	105.88	18.18	41.70	3.63
PA4	18.05	7.32	1.40	2.46	12.92	6.80	6.78	0.18	0.62	4.87
PDA2	12.17	5.15	26.96	20.60	83.21	99.79	67.53	99.78	40.97	17.92
PA5	16.52	7.53	6.35	9.98	28.50	1.35	21.61	8.75	12.11	1.23
PDA3	8.68	5.60	54.69	8.68	175.85	54.73	146.11	59.38	86.46	38.39
PA6	10.46	2.14	21.93	26.31	57.69	17.47	48.71	25.95	32.95	14.30
PDA4	6.48	6.08	81.88	74.55	301.33	85.83	247.37	90.61	135.86	57.12

H_2	4.82	12.13	16.87	10.18	23.07	4.10	16.75	5.35	25.82	25.04
PDA5	21.80	14.04	69.70	67.72	354.12	76.63	281.17	80.24	133.82	42.40
$(H_2)_2$	3.68	1.39	26.51	2.50	49.29	14.83	41.53	31.52	36.24	27.50
$(H_2)_3$	12.48	3.03	49.35	17.09	99.13	36.32	86.46	55.14	75.83	48.53
$(H_2)_4$	16.55	2.43	66.84	26.15	148.53	51.58	128.63	69.76	110.29	62.39
$(H_2)_5$	19.30	0.67	80.97	32.70	195.24	63.74	167.94	81.13	139.56	73.20
$(H_2)_7$	8.87	10.78	72.49	22.02	202.21	55.44	171.02	70.46	137.41	62.88
$(H_2)_6$	22.80	0.24	100.83	38.41	271.43	80.39	230.09	96.65	184.48	87.78
$(H_2)_8$	24.63	2.06	108.67	37.91	301.99	86.92	254.70	102.89	202.13	93.66
MAPE (%)	**19.47**	**6.65**	**18.81**	**18.92**	**58.95**	**23.42**	**45.96**	**23.35**	**31.00**	**18.85**
RMSD (%)	**21.57**	**9.08**	**31.98**	**24.14**	**99.89**	**33.86**	**82.15**	**36.60**	**56.49**	**31.05**
MAX (%)	**35.86**	**27.12**	**108.67**	**74.55**	**354.12**	**99.79**	**281.17**	**102.89**	**202.13**	**100.00**

[a] MAPE: Mean Absolute Percentage Error.

[b] RMSD: Root-Mean-Square Deviation.

[c] MAX: Maximum absolute percentage error.

2. μ_{zz}, α_{zz} and β_{zzz} values at the following levels of theory: CCSD(T), B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD, CAM-B3LYP, LC-BLYP, OT-LC-BLYP and Tα-LC-BLYP for the γ-NLO set

SI1.4 Values of the dipole moment (μ_z) for γ-NLO set (only molecules with non-zero dipole moment) using LC-BLYP, T_α-LC-BLYP, CAM-B3LYP, OT-LC-BLYP, B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD density functionals as well as CCSD(T) method. aug-cc-pVDZ basis set used in all cases.

	μ_z (a.u.)										
System	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**	**CCSD(T)**
1-Butene	-1.63E-01	-1.60E-01	-1.61E-01	-1.59E-01	-1.57E-01	-1.61E-01	-1.61E-01	-1.61E-01	-1.65E-01	-1.65E-01	-1.34E-01
1-Pentanal	5.19E-01	5.19E-01	5.15E-01	5.15E-01	5.08E-01	5.07E-01	5.15E-01	5.14E-01	5.19E-01	5.16E-01	4.68E-01
1-Pentanamide	-1.69E-01	-2.05E-01	-1.81E-01	-1.99E-01	-1.82E-01	-1.69E-01	-1.73E-01	-1.96E-01	-1.66E-01	-1.76E-01	-1.53E-01
1-Pentanoic acid	-1.79E-01	-2.00E-01	-1.84E-01	-1.91E-01	-1.90E-01	-1.70E-01	-1.80E-01	-1.83E-01	-1.74E-01	-1.79E-01	-1.62E-01
n-Butylamine	-1.99E-02	-1.96E-02	-1.71E-02	-1.40E-02	-1.98E-02	-2.87E-02	-1.43E-02	-1.40E-02	-2.47E-02	-1.72E-02	-1.71E-02
n-Butanol	3.75E-02	4.20E-02	4.30E-02	5.16E-02	3.58E-02	2.81E-02	4.59E-02	4.99E-02	3.11E-02	3.72E-02	3.47E-02
Carbon monoxide	4.58E-03	-5.74E-02	-7.72E-03	-2.06E-02	-1.59E-02	-1.30E-02	9.13E-03	-2.61E-02	1.05E-02	9.24E-04	2.78E-02
Cyanic fluoride	8.57E-01	8.55E-01	8.63E-01	8.71E-01	8.31E-01	8.39E-01	8.75E-01	8.71E-01	8.61E-01	8.70E-01	8.18E-01
Formaldehyde	9.78E-01	1.06E+00	1.01E+00	1.07E+00	1.00E+00	9.92E-01	1.01E+00	1.06E+00	9.77E-01	1.01E+00	9.48E-01
Carbonic acid	3.88E-08	4.11E-08	4.00E-08	3.98E-08	3.94E-08	4.06E-08	3.98E-08	3.99E-08	3.94E-08	4.02E-08	3.89E-08
Boric acid	-1.65E-01	-1.70E-01	-1.68E-01	-1.74E-01	-1.67E-01	-1.68E-01	-1.71E-01	-1.73E-01	-1.65E-01	-1.67E-01	-1.64E-01
Hydrogen cyanide	1.20E+00	1.25E+00	1.22E+00	1.26E+00	1.20E+00	1.20E+00	1.22E+00	1.26E+00	1.20E+00	1.22E+00	1.18E+00
Hydrogen fluoride	-7.09E-01	-7.35E-01	-7.18E-01	-7.34E-01	-7.19E-01	-7.21E-01	-7.37E-01	-7.54E-01	-7.12E-01	-7.18E-01	-7.08E-01
Hydrogen isocyanide	1.20E+00	1.25E+00	1.22E+00	1.26E+00	1.20E+00	1.20E+00	1.22E+00	1.26E+00	1.20E+00	1.22E+00	-1.21E+00
Nitroxyl	4.31E-01	4.84E-01	4.54E-01	4.88E-01	4.54E-01	4.54E-01	4.56E-01	4.62E-01	4.32E-01	4.49E-01	4.10E-01
Nitrous acid	6.35E-01	6.37E-01	6.38E-01	6.48E-01	6.20E-01	6.40E-01	6.44E-01	6.44E-01	6.36E-01	6.41E-01	5.75E-01
Nitric acid	8.46E-01	8.98E-01	8.65E-01	8.90E-01	8.70E-01	8.61E-01	8.74E-01	8.83E-01	8.51E-01	8.62E-01	8.15E-01
Dinitrogen oxide	2.01E-02	-6.80E-02	-1.49E-02	-6.15E-02	-5.24E-02	-3.25E-02	4.00E-03	-4.53E-02	1.70E-02	-3.16E-03	-5.42E-03
PMI1	5.74E-01	6.10E-01	5.95E-01	6.26E-01	5.76E-01	5.72E-01	5.92E-01	6.15E-01	5.72E-01	5.95E-01	5.57E-01

PMI2	-7.26E-01	-7.99E-01	-7.60E-01	-8.00E-01	-7.28E-01	-7.21E-01	-7.44E-01	-7.54E-01	-7.31E-01	-7.64E-01	-6.71E-01
PMI3	1.14E+00	1.27E+00	1.20E+00	1.25E+00	1.15E+00	1.14E+00	1.17E+00	1.18E+00	1.15E+00	1.21E+00	1.02E+00
PMI4	-1.68E+00	-1.88E+00	-1.78E+00	-1.85E+00	-1.70E+00	-1.69E+00	-1.74E+00	-1.72E+00	-1.71E+00	-1.80E+00	-1.49E+00
PMI5	2.31E+00	2.60E+00	2.45E+00	2.53E+00	2.34E+00	2.33E+00	2.40E+00	2.36E+00	2.36E+00	2.48E+00	2.02E+00
PMI6	-3.02E+00	-3.39E+00	-3.19E+00	-3.28E+00	-3.05E+00	-3.04E+00	-3.14E+00	-3.08E+00	-3.09E+00	-3.24E+00	-2.61E+00

SI1.5 Absolute errors of the dipolar moment (μ_z) respect to CCSD(T) benchmark values for γ-NLO set obtained using LC-BLYP, T_α-LC-BLYP, CAM-B3LYP, OT-LC-BLYP, B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD density functionals. aug-cc-pVDZ basis set used in all cases.

	Absolute values for absolute errors (a.u.)									
System	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**
1-Butene	2.90E-02	2.63E-02	2.67E-02	2.54E-02	2.30E-02	2.70E-02	2.75E-02	2.69E-02	3.09E-02	3.11E-02
1-Pentanal	5.08E-02	5.17E-02	4.75E-02	4.76E-02	4.02E-02	3.96E-02	4.74E-02	4.61E-02	5.10E-02	4.85E-02
1-Pentanamide	1.61E-02	5.15E-02	2.76E-02	4.60E-02	2.88E-02	1.59E-02	1.99E-02	4.26E-02	1.30E-02	2.26E-02
1-Pentanoic acid	1.62E-02	3.75E-02	2.20E-02	2.92E-02	2.80E-02	7.91E-03	1.75E-02	2.10E-02	1.18E-02	1.62E-02
n-Butylamine	2.82E-03	2.50E-03	3.70E-05	3.06E-03	2.72E-03	1.16E-02	2.83E-03	3.11E-03	7.55E-03	8.91E-05
n-Butanol	2.83E-03	7.33E-03	8.30E-03	1.69E-02	1.10E-03	6.58E-03	1.12E-02	1.52E-02	3.56E-03	2.49E-03
Carbon monoxide	2.32E-02	2.96E-02	2.00E-02	7.13E-03	1.18E-02	1.47E-02	1.86E-02	1.69E-03	1.73E-02	2.68E-02
Cyanic fluoride	3.94E-02	3.75E-02	4.51E-02	5.36E-02	1.33E-02	2.17E-02	5.73E-02	5.29E-02	4.30E-02	5.27E-02
Formaldehyde	3.01E-02	1.09E-01	6.63E-02	1.19E-01	5.31E-02	4.46E-02	6.30E-02	1.15E-01	2.95E-02	5.90E-02
Carbonic acid	1.38E-10	2.14E-09	1.05E-09	8.87E-10	4.77E-10	1.69E-09	8.64E-10	9.28E-10	4.57E-10	1.30E-09
Boric acid	1.05E-03	6.52E-03	4.35E-03	1.03E-02	3.12E-03	4.18E-03	7.71E-03	9.40E-03	1.35E-03	3.17E-03
Hydrogen cyanide	1.94E-02	6.62E-02	4.44E-02	8.12E-02	2.31E-02	2.24E-02	4.36E-02	8.32E-02	2.00E-02	4.11E-02
Hydrogen fluoride	6.35E-04	2.70E-02	1.04E-02	2.61E-02	1.10E-02	1.29E-02	2.86E-02	4.61E-02	3.62E-03	9.99E-03
Hydrogen isocyanide	7.05E-03	3.97E-02	1.80E-02	5.47E-02	3.33E-03	4.05E-03	1.71E-02	5.67E-02	6.48E-03	1.46E-02
Nitroxyl	2.09E-02	7.42E-02	4.43E-02	7.85E-02	4.37E-02	4.45E-02	4.64E-02	5.20E-02	2.22E-02	3.90E-02

Nitrous acid	5.98E-02	6.25E-02	6.30E-02	7.33E-02	4.48E-02	6.52E-02	6.92E-02	6.95E-02	6.13E-02	6.59E-02
Nitric acid	3.18E-02	8.35E-02	5.06E-02	7.50E-02	5.55E-02	4.62E-02	5.93E-02	6.84E-02	3.61E-02	4.77E-02
Dinitrogen oxide	1.47E-02	6.26E-02	9.47E-03	5.61E-02	4.70E-02	2.70E-02	1.42E-03	3.99E-02	1.16E-02	2.26E-03
PMI1	1.73E-02	5.29E-02	3.79E-02	6.91E-02	1.94E-02	1.55E-02	3.50E-02	5.80E-02	1.52E-02	3.77E-02
PMI2	5.58E-02	1.29E-01	8.93E-02	1.29E-01	5.76E-02	5.08E-02	7.30E-02	8.30E-02	6.00E-02	9.30E-02
PMI3	1.14E-01	2.44E-01	1.74E-01	2.28E-01	1.21E-01	1.12E-01	1.44E-01	1.58E-01	1.30E-01	1.85E-01
PMI4	1.92E-01	3.95E-01	2.87E-01	3.57E-01	2.06E-01	1.97E-01	2.48E-01	2.30E-01	2.23E-01	3.08E-01
PMI5	2.91E-01	5.77E-01	4.26E-01	5.08E-01	3.13E-01	3.06E-01	3.79E-01	3.35E-01	3.40E-01	4.60E-01
PMI6	4.15E-01	7.85E-01	5.89E-01	6.75E-01	4.40E-01	4.36E-01	5.31E-01	4.73E-01	4.83E-01	6.35E-01
MAE (a.u.)	**6.05E-02**	**1.23E-01**	**8.80E-02**	**1.15E-01**	**6.63E-02**	**6.39E-02**	**8.12E-02**	**8.70E-02**	**6.75E-02**	**9.17E-02**
RMSD (a.u.)	**1.16E-01**	**2.27E-01**	**1.67E-01**	**2.01E-01**	**1.24E-01**	**1.21E-01**	**1.50E-01**	**1.40E-01**	**1.34E-01**	**1.80E-01**
MAX (a.u.)	**4.15E-01**	**7.85E-01**	**5.89E-01**	**6.75E-01**	**4.40E-01**	**4.36E-01**	**5.31E-01**	**4.73E-01**	**4.83E-01**	**6.35E-01**
DFA	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**

SI1.6 Relative errors of the dipolar moment (μ_z) respect to CCSD(T) benchmark values for γ-NLO set obtained using LC-BLYP, T_α-LC-BLYP, CAM-B3LYP, OT-LC-BLYP, B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD density functionals. aug-cc-pVDZ basis set used in all cases.

	Absolute values for relative errors (%)									
System	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**
1-Butene	22	20	20	19	17	20	21	20	23	23
1-Pentanal	11	11	10	10	9	8	10	10	11	10
1-Pentanamide	11	34	18	30	19	10	13	28	9	15
1-Pentanoic acid	10	23	14	18	17	5	11	13	7	10
n-Butylamine	16	15	0	18	16	68	17	18	44	1
n-Butanol	8	21	24	49	3	19	32	44	10	7
Carbon monoxide	83	107	72	26	43	53	67	6	62	97
Cyanic fluoride	5	5	6	7	2	3	7	6	5	6

Formaldehyde	3	11	7	13	6	5	7	12	3	6
Carbonic acid	0	5	3	2	1	4	2	2	1	3
Boric acid	1	4	3	6	2	3	5	6	1	2
Hydrogen cyanide	2	6	4	7	2	2	4	7	2	3
Hydrogen fluoride	0	4	1	4	2	2	4	7	1	1
Hydrogen isocyanide	1	3	1	5	0	0	1	5	1	1
Nitroxyl	5	18	11	19	11	11	11	13	5	10
Nitrous acid	10	11	11	13	8	11	12	12	11	11
Nitric acid	4	10	6	9	7	6	7	8	4	6
Dinitrogen oxide	270	1155	175	1035	867	499	26	736	213	42
PMI1	3	9	7	12	3	3	6	10	3	7
PMI2	8	19	13	19	9	8	11	12	9	14
PMI3	11	24	17	22	12	11	14	15	13	18
PMI4	13	27	19	24	14	13	17	15	15	21
PMI5	14	29	21	25	15	15	19	17	17	23
PMI6	16	30	23	26	17	17	20	18	19	24
MAPE (%)	**22**	**67**	**20**	**59**	**46**	**33**	**14**	**43**	**20**	**15**
RMSD (%)	**59**	**237**	**41**	**212**	**177**	**104**	**20**	**151**	**47**	**25**
MAX (%)	**270**	**1155**	**175**	**1035**	**867**	**499**	**67**	**736**	**213**	**97**
DFA	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**

SI1.7 Values of the polarizability (α_{zz}) for γ-NLO set using LC-BLYP, T_{α}-LC-BLYP, CAM-B3LYP, OT-LC-BLYP, B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD density functionals as well as CCSD(T) method. aug-cc-pVDZ basis set used in all cases.

	α_{zz} (a.u.)										
System	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**	**CCSD(T)**
1-Butene	6.81E+01	6.62E+01	6.68E+01	6.51E+01	6.65E+01	6.79E+01	6.73E+01	6.70E+01	6.74E+01	6.68E+01	6.43E+01
Water	1.02E+01	9.68E+00	1.00E+01	9.85E+00	9.68E+00	1.00E+01	1.01E+01	9.70E+00	9.97E+00	9.95E+00	9.94E+00
Ammonia	1.38E+01	1.32E+01	1.36E+01	1.33E+01	1.33E+01	1.36E+01	1.38E+01	1.33E+01	1.36E+01	1.36E+01	1.35E+01
Benzene	8.39E+01	8.22E+01	8.29E+01	8.14E+01	8.21E+01	8.41E+01	8.36E+01	8.37E+01	8.29E+01	8.28E+01	8.14E+01
Butane	6.29E+01	6.05E+01	6.16E+01	6.00E+01	6.24E+01	6.30E+01	6.26E+01	6.09E+01	6.24E+01	6.17E+01	6.07E+01
1-Pentanal	8.04E+01	7.65E+01	7.84E+01	7.59E+01	7.87E+01	7.99E+01	7.96E+01	7.78E+01	7.98E+01	7.86E+01	7.75E+01
1-Pentanamide	9.25E+01	8.75E+01	8.98E+01	8.65E+01	9.00E+01	9.13E+01	9.08E+01	8.70E+01	9.16E+01	9.00E+01	8.94E+01
1-Pentanoic acid	8.84E+01	8.36E+01	8.60E+01	8.31E+01	8.59E+01	8.72E+01	8.73E+01	8.57E+01	8.75E+01	8.60E+01	8.54E+01
n-butylamine	7.55E+01	7.23E+01	7.37E+01	7.14E+01	7.43E+01	7.50E+01	7.47E+01	7.33E+01	7.48E+01	7.37E+01	7.29E+01
n-butanol	7.00E+01	6.71E+01	6.85E+01	6.65E+01	6.87E+01	6.95E+01	6.95E+01	6.75E+01	6.94E+01	6.84E+01	6.76E+01
Acetylene	3.33E+01	3.28E+01	3.30E+01	3.25E+01	3.26E+01	3.34E+01	3.33E+01	3.27E+01	3.27E+01	3.29E+01	3.18E+01
Cyclohexane	7.64E+01	7.39E+01	7.51E+01	7.33E+01	7.57E+01	7.68E+01	7.58E+01	7.47E+01	7.58E+01	7.53E+01	7.43E+01
Carbon monoxide	1.58E+01	1.53E+01	1.57E+01	1.55E+01	1.53E+01	1.55E+01	1.59E+01	1.54E+01	1.57E+01	1.58E+01	1.61E+01
Carbon dioxide	2.67E+01	2.58E+01	2.67E+01	2.67E+01	2.61E+01	2.65E+01	2.73E+01	2.65E+01	2.65E+01	2.67E+01	2.79E+01
Ethane	3.22E+01	3.11E+01	3.17E+01	3.10E+01	3.19E+01	3.23E+01	3.21E+01	3.11E+01	3.18E+01	3.18E+01	3.11E+01
Cyanic fluoride	2.68E+01	2.57E+01	2.65E+01	2.62E+01	2.58E+01	2.62E+01	2.69E+01	2.61E+01	2.65E+01	2.66E+01	2.64E+01
H_2	1.20E+01	1.19E+01	1.21E+01	1.21E+01	1.12E+01	1.24E+01	1.22E+01	1.19E+01	1.19E+01	1.18E+01	1.11E+01
$(H_2)_2$	3.48E+01	3.33E+01	3.40E+01	3.31E+01	3.37E+01	3.52E+01	3.29E+01	3.30E+01	3.44E+01	3.35E+01	2.98E+01
Formaldehyde	2.31E+01	2.23E+01	2.28E+01	2.25E+01	2.23E+01	2.27E+01	2.32E+01	2.25E+01	2.28E+01	2.27E+01	2.26E+01
Carbonic acid	3.11E+01	2.90E+01	3.04E+01	2.95E+01	2.95E+01	3.01E+01	3.03E+01	3.00E+01	3.06E+01	3.02E+01	3.06E+01
Hydrogen peroxide	1.92E+01	1.91E+01	1.91E+01	1.88E+01	1.87E+01	1.88E+01	1.90E+01	1.88E+01	1.89E+01	1.88E+01	1.87E+01
$(H_2)_3$	6.51E+01	6.06E+01	6.20E+01	5.92E+01	6.08E+01	6.51E+01	5.82E+01	5.97E+01	6.40E+01	6.11E+01	5.26E+01

Boric acid	3.13E+01	2.91E+01	3.07E+01	3.00E+01	2.96E+01	3.04E+01	3.09E+01	3.03E+01	3.08E+01	3.05E+01	3.08E+01
$(H_2)_4$	9.98E+01	9.10E+01	9.34E+01	8.80E+01	9.10E+01	9.91E+01	8.57E+01	8.95E+01	9.80E+01	9.20E+01	7.73E+01
$(H_2)_5$	1.37E+02	1.23E+02	1.27E+02	1.18E+02	1.23E+02	1.35E+02	1.14E+02	1.21E+02	1.34E+02	1.25E+02	1.03E+02
$(H_2)_6$	1.76E+02	1.56E+02	1.61E+02	1.49E+02	1.56E+02	1.73E+02	1.43E+02	1.53E+02	1.72E+02	1.58E+02	1.29E+02
$(H_2)_7$	2.15E+02	1.89E+02	1.95E+02	1.80E+02	1.89E+02	2.11E+02	1.73E+02	1.85E+02	2.11E+02	1.92E+02	1.56E+02
$(H_2)_8$	2.56E+02	2.23E+02	2.30E+02	2.11E+02	2.22E+02	2.50E+02	2.01E+02	2.16E+02	2.49E+02	2.26E+02	1.82E+02
Hydrogen cyanide	2.40E+01	2.35E+01	2.38E+01	2.34E+01	2.34E+01	2.38E+01	2.41E+01	2.34E+01	2.37E+01	2.38E+01	2.34E+01
Heptane	1.14E+02	1.10E+02	1.12E+02	1.08E+02	1.13E+02	1.15E+02	1.13E+02	1.08E+02	1.14E+02	1.12E+02	1.10E+02
Hexane	9.68E+01	9.31E+01	9.46E+01	9.19E+01	9.60E+01	9.70E+01	9.61E+01	9.23E+01	9.63E+01	9.48E+01	9.34E+01
Hydrogen fluoride	6.51E+00	6.10E+00	6.44E+00	6.37E+00	6.16E+00	6.31E+00	6.32E+00	6.04E+00	6.36E+00	6.33E+00	6.28E+00
Hydrogen isocyanide	2.40E+01	2.35E+01	2.38E+01	2.34E+01	2.34E+01	2.38E+01	2.41E+01	2.34E+01	2.37E+01	2.38E+01	2.47E+01
Nitroxyl	1.94E+01	1.89E+01	1.92E+01	1.89E+01	1.87E+01	1.89E+01	1.93E+01	1.92E+01	1.91E+01	1.91E+01	1.88E+01
Nitrous acid	3.14E+01	2.96E+01	3.08E+01	3.00E+01	2.97E+01	3.02E+01	3.12E+01	3.10E+01	3.08E+01	3.06E+01	3.14E+01
Nitric acid	3.05E+01	2.86E+01	2.99E+01	2.91E+01	2.89E+01	2.94E+01	2.98E+01	2.94E+01	3.00E+01	2.98E+01	3.04E+01
Methane	1.72E+01	1.67E+01	1.71E+01	1.69E+01	1.72E+01	1.74E+01	1.75E+01	1.69E+01	1.70E+01	1.71E+01	1.67E+01
Dinitrogen	1.53E+01	1.50E+01	1.52E+01	1.51E+01	1.48E+01	1.51E+01	1.54E+01	1.51E+01	1.51E+01	1.53E+01	1.50E+01
Dinitrogen oxide	3.37E+01	3.31E+01	3.38E+01	3.40E+01	3.30E+01	3.37E+01	3.45E+01	3.42E+01	3.34E+01	3.37E+01	3.44E+01
Dioxygen	1.51E+01	1.55E+01	1.51E+01	1.51E+01	1.49E+01	1.50E+01	1.51E+01	1.51E+01	1.51E+01	1.52E+01	1.52E+01
Octane	1.32E+02	1.27E+02	1.29E+02	1.25E+02	1.31E+02	1.33E+02	1.31E+02	1.24E+02	1.32E+02	1.29E+02	1.28E+02
PA5	4.33E+02	4.03E+02	3.96E+02	3.61E+02	3.88E+02	4.06E+02	3.69E+02	3.96E+02	4.23E+02	3.92E+02	3.28E+02
PA6	6.14E+02	5.59E+02	5.48E+02	4.89E+02	5.37E+02	5.66E+02	4.99E+02	5.52E+02	5.98E+02	5.41E+02	4.41E+02
PA1	3.65E+01	3.62E+01	3.63E+01	3.60E+01	3.56E+01	3.67E+01	3.66E+01	3.63E+01	3.59E+01	3.62E+01	3.44E+01
PA2	8.85E+01	8.72E+01	8.67E+01	8.44E+01	8.52E+01	8.74E+01	8.63E+01	8.60E+01	8.71E+01	8.65E+01	7.97E+01
PA3	1.71E+02	1.65E+02	1.64E+02	1.56E+02	1.60E+02	1.66E+02	1.60E+02	1.62E+02	1.68E+02	1.63E+02	1.45E+02
PA4	2.85E+02	2.71E+02	2.67E+02	2.49E+02	2.62E+02	2.72E+02	2.56E+02	2.67E+02	2.80E+02	2.66E+02	2.28E+02
PDA1	1.52E+02	1.44E+02	1.44E+02	1.35E+02	1.41E+02	1.46E+02	1.41E+02	1.42E+02	1.49E+02	1.44E+02	1.30E+02
PDA2	3.66E+02	3.31E+02	3.29E+02	2.97E+02	3.24E+02	3.39E+02	3.11E+02	3.26E+02	3.56E+02	3.28E+02	2.82E+02

PDA3	6.61E+02	5.72E+02	5.66E+02	4.93E+02	5.59E+02	5.92E+02	5.11E+02	4.93E+02	6.39E+02	5.62E+02	4.65E+02
PDA4	1.02E+03	8.47E+02	8.36E+02	7.08E+02	8.26E+02	8.85E+02	7.29E+02	8.43E+02	9.78E+02	8.26E+02	6.66E+02
PDA5	1.42E+03	1.14E+03	1.13E+03	9.33E+02	1.11E+03	1.20E+03	9.53E+02	1.15E+03	1.36E+03	1.11E+03	8.75E+02
Pentane	7.93E+01	7.62E+01	7.76E+01	7.54E+01	7.85E+01	7.94E+01	7.88E+01	7.62E+01	7.87E+01	7.77E+01	7.65E+01
PMI1	3.02E+01	2.97E+01	2.99E+01	2.95E+01	2.94E+01	2.99E+01	3.03E+01	2.97E+01	2.98E+01	2.98E+01	2.91E+01
PMI2	6.97E+01	6.81E+01	6.82E+01	6.61E+01	6.71E+01	6.85E+01	6.82E+01	6.77E+01	6.87E+01	6.79E+01	6.49E+01
PMI3	1.28E+02	1.23E+02	1.23E+02	1.17E+02	1.21E+02	1.24E+02	1.22E+02	1.21E+02	1.26E+02	1.22E+02	1.14E+02
PMI4	2.06E+02	1.92E+02	1.92E+02	1.79E+02	1.89E+02	1.96E+02	1.88E+02	1.91E+02	2.01E+02	1.91E+02	1.76E+02
PMI5	3.00E+02	2.74E+02	2.74E+02	2.51E+02	2.70E+02	2.80E+02	2.65E+02	2.74E+02	2.92E+02	2.72E+02	2.47E+02
PMI6	4.09E+02	3.64E+02	3.64E+02	3.29E+02	3.60E+02	3.75E+02	3.48E+02	3.64E+02	3.96E+02	3.60E+02	3.25E+02
Propane	4.63E+01	4.46E+01	4.55E+01	4.43E+01	4.58E+01	4.64E+01	4.61E+01	4.48E+01	4.59E+01	4.55E+01	4.47E+01

SI1.8 Absolute errors of the polarizability (α_{zz}) respect to CCSD(T) benchmark values for γ-NLO set obtained using LC-BLYP, T_{α}-LC-BLYP, CAM-B3LYP, OT-LC-BLYP, B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD density functionals. aug-cc-pVDZ basis set used in all cases.

	Absolute values for absolute errors (a.u.)									
System	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**
1-Butene	3.83E+00	1.97E+00	2.49E+00	8.54E-01	2.26E+00	3.60E+00	3.06E+00	2.72E+00	3.10E+00	2.55E+00
Water	2.23E-01	2.67E-01	1.03E-01	9.03E-02	2.69E-01	5.30E-02	1.69E-01	2.43E-01	2.15E-02	6.37E-03
Ammonia	3.19E-01	2.40E-01	1.51E-01	1.33E-01	1.30E-01	1.82E-01	3.84E-01	1.33E-01	8.82E-02	1.07E-01
Benzene	2.50E+00	8.52E-01	1.53E+00	2.28E-02	6.73E-01	2.72E+00	2.20E+00	2.36E+00	1.48E+00	1.42E+00
Butane	2.18E+00	1.84E-01	8.92E-01	7.55E-01	1.62E+00	2.26E+00	1.92E+00	1.84E-01	1.70E+00	9.88E-01
1-Pentanal	2.92E+00	9.51E-01	8.78E-01	1.58E+00	1.22E+00	2.41E+00	2.14E+00	2.95E-01	2.28E+00	1.10E+00
1-Pentanamide	3.15E+00	1.88E+00	3.86E-01	2.86E+00	5.85E-01	1.92E+00	1.44E+00	2.41E+00	2.24E+00	6.63E-01
1-Pentanoic acid	2.98E+00	1.79E+00	6.01E-01	2.29E+00	4.72E-01	1.79E+00	1.87E+00	2.85E-01	2.11E+00	5.58E-01
n-butylamine	2.54E+00	6.42E-01	7.47E-01	1.52E+00	1.32E+00	2.02E+00	1.72E+00	3.21E-01	1.90E+00	7.34E-01
n-butanol	2.41E+00	5.33E-01	8.58E-01	1.11E+00	1.12E+00	1.91E+00	1.86E+00	1.54E-01	1.79E+00	7.79E-01

Acetylene	1.44E+00	1.00E+00	1.19E+00	7.08E-01	7.72E-01	1.54E+00	1.49E+00	8.91E-01	8.87E-01	1.09E+00
Cyclohexane	2.08E+00	4.53E-01	7.45E-01	1.03E+00	1.31E+00	2.43E+00	1.47E+00	3.41E-01	1.51E+00	9.59E-01
Carbon monoxide	2.38E-01	7.82E-01	3.51E-01	5.96E-01	7.83E-01	5.16E-01	1.90E-01	6.61E-01	3.55E-01	2.27E-01
Carbon dioxide	1.12E+00	2.10E+00	1.17E+00	1.18E+00	1.77E+00	1.32E+00	6.17E-01	1.32E+00	1.40E+00	1.18E+00
Ethane	1.08E+00	1.40E-02	5.76E-01	1.18E-01	8.12E-01	1.20E+00	1.06E+00	6.66E-02	7.68E-01	6.83E-01
Cyanic fluoride	3.96E-01	6.33E-01	1.49E-01	1.79E-01	5.97E-01	1.37E-01	5.08E-01	2.80E-01	1.20E-01	2.19E-01
H_2	9.21E-01	8.08E-01	9.91E-01	9.89E-01	1.01E-01	1.26E+00	1.10E+00	7.53E-01	7.63E-01	7.24E-01
$(H_2)_2$	4.98E+00	3.52E+00	4.13E+00	3.23E+00	3.85E+00	5.35E+00	3.10E+00	3.16E+00	4.53E+00	3.64E+00
Formaldehyde	5.01E-01	3.14E-01	2.09E-01	1.64E-01	3.46E-01	7.21E-02	5.14E-01	1.23E-01	1.56E-01	9.75E-02
Carbonic acid	5.52E-01	1.60E+00	1.47E-01	1.05E+00	1.09E+00	5.05E-01	2.83E-01	6.27E-01	2.39E-03	3.46E-01
Hydrogen peroxide	4.72E-01	4.52E-01	3.97E-01	1.06E-01	1.75E-02	1.24E-01	3.25E-01	7.10E-02	1.63E-01	1.40E-01
$(H_2)_3$	1.25E+01	8.02E+00	9.42E+00	6.62E+00	8.24E+00	1.25E+01	5.57E+00	7.13E+00	1.15E+01	8.51E+00
Boric acid	4.83E-01	1.67E+00	6.95E-02	8.43E-01	1.16E+00	4.40E-01	9.40E-02	5.06E-01	1.22E-03	2.86E-01
$(H_2)_4$	2.25E+01	1.37E+01	1.61E+01	1.06E+01	1.37E+01	2.18E+01	8.32E+00	1.22E+01	2.06E+01	1.46E+01
$(H_2)_5$	3.40E+01	2.00E+01	2.35E+01	1.50E+01	1.98E+01	3.23E+01	1.10E+01	1.78E+01	3.13E+01	2.15E+01
$(H_2)_6$	4.66E+01	2.67E+01	3.14E+01	1.96E+01	2.62E+01	4.36E+01	1.37E+01	2.34E+01	4.28E+01	2.88E+01
$(H_2)_7$	5.97E+01	3.36E+01	3.97E+01	2.43E+01	3.29E+01	5.54E+01	1.68E+01	2.91E+01	5.47E+01	3.63E+01
$(H_2)_8$	7.31E+01	4.07E+01	4.80E+01	2.90E+01	3.97E+01	6.74E+01	1.90E+01	3.38E+01	6.70E+01	4.39E+01
Hydrogen cyanide	5.74E-01	1.23E-01	4.02E-01	5.59E-02	2.53E-02	4.15E-01	6.80E-01	2.59E-02	2.82E-01	4.05E-01
Heptane	4.02E+00	5.13E-01	1.35E+00	1.95E+00	3.00E+00	4.24E+00	3.10E+00	2.17E+00	3.39E+00	1.59E+00
Hexane	3.40E+00	3.90E-01	1.20E+00	1.53E+00	2.55E+00	3.56E+00	2.70E+00	1.15E+00	2.82E+00	1.35E+00
Hydrogen fluoride	2.21E-01	1.85E-01	1.60E-01	8.16E-02	1.26E-01	2.96E-02	4.00E-02	2.45E-01	7.30E-02	4.98E-02
Hydrogen isocyanide	6.98E-01	1.15E+00	8.71E-01	1.22E+00	1.30E+00	8.58E-01	5.93E-01	1.25E+00	9.90E-01	8.68E-01
Nitroxyl	6.16E-01	1.60E-01	4.17E-01	1.09E-01	1.15E-01	1.10E-01	5.26E-01	4.45E-01	3.29E-01	3.36E-01
Nitrous acid	2.80E-02	1.77E+00	6.25E-01	1.38E+00	1.66E+00	1.18E+00	1.44E-01	3.46E-01	5.86E-01	7.93E-01
Nitric acid	7.98E-02	1.73E+00	4.93E-01	1.24E+00	1.51E+00	1.00E+00	5.76E-01	9.67E-01	4.25E-01	5.87E-01
Methane	5.38E-01	1.34E-02	4.09E-01	1.66E-01	4.66E-01	7.17E-01	7.92E-01	1.99E-01	3.44E-01	4.05E-01

Dinitrogen	2.54E-01	1.57E-02	2.26E-01	9.56E-02	2.37E-01	1.23E-01	3.66E-01	7.44E-02	9.48E-02	2.46E-01
Dinitrogen oxide	6.79E-01	1.30E+00	5.65E-01	3.59E-01	1.36E+00	7.37E-01	1.15E-01	2.14E-01	1.03E+00	6.74E-01
Dioxygen	9.11E-02	2.99E-01	1.91E-02	7.05E-02	2.50E-01	1.94E-01	6.66E-02	5.98E-02	9.99E-02	1.00E-02
Octane	4.69E+00	6.35E-01	1.51E+00	2.40E+00	3.58E+00	4.99E+00	3.52E+00	3.35E+00	4.03E+00	1.81E+00
PA5	1.05E+02	7.48E+01	6.80E+01	3.31E+01	6.00E+01	7.80E+01	4.15E+01	6.86E+01	9.54E+01	6.46E+01
PA6	1.72E+02	1.18E+02	1.06E+02	4.78E+01	9.58E+01	1.24E+02	5.74E+01	1.10E+02	1.57E+02	9.98E+01
PA1	2.00E+00	1.79E+00	1.85E+00	1.54E+00	1.17E+00	2.21E+00	2.10E+00	1.81E+00	1.49E+00	1.72E+00
PA2	8.74E+00	7.46E+00	6.98E+00	4.69E+00	5.45E+00	7.69E+00	6.59E+00	6.23E+00	7.42E+00	6.75E+00
PA3	2.57E+01	2.04E+01	1.87E+01	1.10E+01	1.54E+01	2.07E+01	1.52E+01	1.74E+01	2.28E+01	1.81E+01
PA4	5.68E+01	4.25E+01	3.88E+01	2.05E+01	3.32E+01	4.36E+01	2.76E+01	3.85E+01	5.12E+01	3.72E+01
PDA1	2.18E+01	1.39E+01	1.37E+01	5.30E+00	1.15E+01	1.63E+01	1.14E+01	1.20E+01	1.89E+01	1.36E+01
PDA2	8.42E+01	4.94E+01	4.75E+01	1.51E+01	4.27E+01	5.79E+01	2.96E+01	4.41E+01	7.49E+01	4.62E+01
PDA3	1.96E+02	1.07E+02	1.02E+02	2.80E+01	9.40E+01	1.28E+02	4.60E+01	2.80E+01	1.75E+02	9.69E+01
PDA4	3.52E+02	1.81E+02	1.71E+02	4.18E+01	1.60E+02	2.19E+02	6.32E+01	1.77E+02	3.12E+02	1.60E+02
PDA5	5.45E+02	2.68E+02	2.51E+02	5.75E+01	2.37E+02	3.28E+02	7.78E+01	2.75E+02	4.80E+02	2.32E+02
Pentane	2.75E+00	2.81E-01	1.04E+00	1.11E+00	1.99E+00	2.87E+00	2.29E+00	2.89E-01	2.21E+00	1.15E+00
PMI1	1.15E+00	6.15E-01	8.56E-01	4.02E-01	2.96E-01	8.32E-01	1.19E+00	6.24E-01	7.45E-01	7.33E-01
PMI2	4.80E+00	3.21E+00	3.25E+00	1.21E+00	2.17E+00	3.61E+00	3.25E+00	2.75E+00	3.80E+00	3.01E+00
PMI3	1.40E+01	8.61E+00	8.50E+00	2.49E+00	6.49E+00	9.78E+00	7.48E+00	6.21E+00	1.17E+01	8.02E+00
PMI4	3.02E+01	1.68E+01	1.66E+01	3.80E+00	1.38E+01	1.99E+01	1.27E+01	1.55E+01	2.57E+01	1.56E+01
PMI5	5.37E+01	2.70E+01	2.70E+01	4.40E+00	2.36E+01	3.36E+01	1.80E+01	2.77E+01	4.57E+01	2.49E+01
PMI6	8.45E+01	3.88E+01	3.93E+01	4.60E+00	3.57E+01	5.08E+01	2.30E+01	3.97E+01	7.17E+01	3.57E+01
Propane	1.58E+00	8.47E-02	7.44E-01	3.62E-01	1.11E+00	1.68E+00	1.42E+00	1.09E-01	1.16E+00	7.85E-01
MAE (a.u.)	**3.44E+01**	**1.92E+01**	**1.86E+01**	**7.03E+00**	**1.70E+01**	**2.39E+01**	**9.38E+00**	**1.71E+01**	**3.05E+01**	**1.75E+01**
RMSD (a.u.)	**9.45E+01**	**4.96E+01**	**4.67E+01**	**1.44E+01**	**4.34E+01**	**5.99E+01**	**1.89E+01**	**4.73E+01**	**8.37E+01**	**4.36E+01**
MAX (a.u.)	**5.45E+02**	**2.68E+02**	**2.51E+02**	**5.75E+01**	**2.37E+02**	**3.28E+02**	**7.78E+01**	**2.75E+02**	**4.80E+02**	**2.32E+02**
DFA	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**

SI1.9 Relative errors of the polarizability (α_{zz}) respect to CCSD(T) benchmark values for γ-NLO set obtained using LC-BLYP, T_{α}-LC-BLYP, CAM-B3LYP, OT-LC-BLYP, B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD density functionals. aug-cc-pVDZ basis set used in all cases.

	Absolute values for relative errors (%)									
System	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**
1-Butene	6	3	4	1	4	6	5	4	5	4
Water	2	3	1	1	3	1	2	2	0	0
Ammonia	2	2	1	1	1	1	3	1	1	1
Benzene	3	1	2	0	1	3	3	3	2	2
Butane	4	0	1	1	3	4	3	0	3	2
1-Pentanal	4	1	1	2	2	3	3	0	3	1
1-Pentanamide	4	2	0	3	1	2	2	3	3	1
1-Pentanoic acid	3	2	1	3	1	2	2	0	2	1
n-butylamine	3	1	1	2	2	3	2	0	3	1
n-butanol	4	1	1	2	2	3	3	0	3	1
Acetylene	5	3	4	2	2	5	5	3	3	3
Cyclohexane	3	1	1	1	2	3	2	0	2	1
Carbon monoxide	1	5	2	4	5	3	1	4	2	1
Carbon dioxide	4	8	4	4	6	5	2	5	5	4
Ethane	3	0	2	0	3	4	3	0	2	2
Cyanic fluoride	2	2	1	1	2	1	2	1	0	1
H_2	8	7	9	9	1	11	10	7	7	7
$(H_2)_2$	17	12	14	11	13	18	10	11	15	12
Formaldehyde	2	1	1	1	2	0	2	1	1	0
Carbonic acid	2	5	0	3	4	2	1	2	0	1
Hydrogen peroxide	3	2	2	1	0	1	2	0	1	1
$(H_2)_3$	24	15	18	13	16	24	11	14	22	16

Boric acid	2	5	0	3	4	1	0	2	0	1
$(H_2)_4$	29	18	21	14	18	28	11	16	27	19
$(H_2)_5$	33	19	23	15	19	31	11	17	30	21
$(H_2)_6$	36	21	24	15	20	34	11	18	33	22
$(H_2)_7$	38	22	25	16	21	36	11	19	35	23
$(H_2)_8$	40	22	26	16	22	37	10	19	37	24
Hydrogen cyanide	2	1	2	0	0	2	3	0	1	2
Heptane	4	0	1	2	3	4	3	2	3	1
Hexane	4	0	1	2	3	4	3	1	3	1
Hydrogen fluoride	4	3	3	1	2	0	1	4	1	1
Hydrogen isocyanide	3	5	4	5	5	3	2	5	4	4
Nitroxyl	3	1	2	1	1	1	3	2	2	2
Nitrous acid	0	6	2	4	5	4	0	1	2	3
Nitric acid	0	6	2	4	5	3	2	3	1	2
Methane	3	0	2	1	3	4	5	1	2	2
Dinitrogen	2	0	2	1	2	1	2	0	1	2
Dinitrogen oxide	2	4	2	1	4	2	0	1	3	2
Dioxygen	1	2	0	0	2	1	0	0	1	0
Octane	4	0	1	2	3	4	3	3	3	1
PA5	32	23	21	10	18	24	13	21	29	20
PA6	39	27	24	11	22	28	13	25	36	23
PA1	6	5	5	4	3	6	6	5	4	5
PA2	11	9	9	6	7	10	8	8	9	8
PA3	18	14	13	8	11	14	10	12	16	12
PA4	25	19	17	9	15	19	12	17	22	16
PDA1	17	11	11	4	9	13	9	9	15	11
PDA2	30	18	17	5	15	21	11	16	27	16

PDA3	42	23	22	6	20	27	10	6	38	21
PDA4	53	27	26	6	24	33	9	27	47	24
PDA5	62	31	29	7	27	37	9	31	55	27
Pentane	4	0	1	1	3	4	3	0	3	2
PMI1	4	2	3	1	1	3	4	2	3	3
PMI2	7	5	5	2	3	6	5	4	6	5
PMI3	12	8	7	2	6	9	7	5	10	7
PMI4	17	10	9	2	8	11	7	9	15	9
PMI5	22	11	11	2	10	14	7	11	19	10
PMI6	26	12	12	1	11	16	7	12	22	11
Propane	4	0	2	1	2	4	3	0	3	2
MAPE (%)	**1.25E+01**	**7.77E+00**	**7.63E+00**	**4.28E+00**	**7.11E+00**	**1.00E+01**	**5.21E+00**	**6.63E+00**	**1.08E+01**	**7.12E+00**
RMSD (%)	**1.94E+01**	**1.14E+01**	**1.15E+01**	**6.12E+00**	**1.02E+01**	**1.50E+01**	**6.46E+00**	**1.01E+01**	**1.73E+01**	**1.07E+01**
MAX (%)	**6.22E+01**	**3.06E+01**	**2.87E+01**	**1.59E+01**	**2.71E+01**	**3.75E+01**	**1.30E+01**	**3.14E+01**	**5.49E+01**	**2.66E+01**
DFA	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**

SI1.10 Values of the first hyperpolarizability (β_{zzz}) for γ-NLO set (only molecules with non-zero value of beta) using LC-BLYP, T_{α}-LC-BLYP, CAM-B3LYP, OT-LC-BLYP, B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD density functionals as well as CCSD(T) method. aug-cc-pVDZ basis set used in all cases.

	β_{zzz} (a.u.)										
System	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**	**CCSD(T)**
1-Butene	1.06E+01	1.31E+01	2.58E+01	3.23E+01	2.13E+01	3.41E+01	3.78E+01	3.74E+01	1.69E+01	3.46E+01	-2.92E+01
1-Pentanal	-1.58E+01	-5.47E+00	-1.26E+01	-9.13E+00	-1.22E+01	-1.00E+01	-1.70E+01	-1.32E+01	-1.51E+01	-9.10E+00	5.43E+00
1-Pentanamida	8.69E+01	3.87E+01	5.56E+01	3.16E+01	4.10E+01	4.39E+01	5.72E+01	3.40E+01	7.54E+01	4.83E+01	-4.28E+01
1-Pentanoic acid	5.65E+01	1.57E+01	3.00E+01	1.03E+01	7.48E+00	1.23E+01	3.32E+01	2.34E+01	4.35E+01	1.73E+01	-2.09E+01
n-butylamine	1.65E+01	1.72E+01	1.74E+01	1.78E+01	2.46E+01	2.47E+01	1.83E+01	1.80E+01	1.68E+01	2.18E+01	-1.51E+01
n-butanol	2.91E+01	3.25E+01	3.26E+01	3.23E+01	4.12E+01	4.08E+01	3.44E+01	3.29E+01	3.01E+01	3.82E+01	-3.22E+01
Carbon monoxide	-3.31E+01	-3.14E+01	-3.28E+01	-3.08E+01	-2.77E+01	-3.37E+01	-3.32E+01	-3.05E+01	-3.21E+01	-3.31E+01	3.06E+01
Cyanic fluoride	-5.26E+01	-4.65E+01	-5.35E+01	-5.38E+01	-4.96E+01	-5.53E+01	-5.84E+01	-5.31E+01	-5.03E+01	-5.41E+01	5.08E+01
Formaldehyde	4.35E+01	3.69E+01	3.68E+01	3.17E+01	3.53E+01	4.08E+01	3.46E+01	3.18E+01	4.19E+01	4.05E+01	-3.28E+01
Boric acid	-2.85E+01	-2.55E+01	-2.72E+01	-2.54E+01	-2.54E+01	-2.93E+01	-2.66E+01	-2.58E+01	-2.72E+01	-2.72E+01	2.87E+01
Hydrogen cyanide	1.26E+01	1.10E+01	8.54E+00	5.38E+00	6.77E+00	1.04E+01	5.21E+00	5.46E+00	1.16E+01	8.16E+00	-9.99E+00
Hydrogen fluoride	-1.15E+01	-1.07E+01	-1.10E+01	-1.02E+01	-9.41E+00	-1.17E+01	-1.01E+01	-9.62E+00	-1.10E+01	-1.13E+01	1.19E+01
Hydrogen isocyanide	1.26E+01	1.10E+01	8.54E+00	5.38E+00	6.77E+00	1.04E+01	5.21E+00	5.46E+00	1.16E+01	8.16E+00	-1.82E+01
Nytroxyl	2.28E+01	1.81E+01	1.97E+01	1.76E+01	1.97E+01	2.16E+01	1.96E+01	1.91E+01	2.17E+01	2.07E+01	-1.80E+01
Nitrous acid	3.86E+01	1.76E+01	2.13E+01	6.70E+00	1.26E+01	1.45E+01	1.72E+01	1.47E+01	3.13E+01	1.77E+01	-9.46E+00

Nitric acid	5.72E+00	3.57E+00	-4.17E-01	-5.62E+00	9.96E-01	-2.34E+00	-6.03E+00	-5.88E+00	3.47E+00	-1.32E+00	-2.62E+00
Dinitrogen oxide	-5.19E+01	-5.52E+01	-5.44E+01	-5.85E+01	-5.39E+01	-5.42E+01	-5.62E+01	-5.79E+01	-5.05E+01	-5.29E+01	5.80E+01
PMI1	2.39E+01	2.11E+01	1.77E+01	1.40E+01	1.66E+01	2.19E+01	1.39E+01	1.33E+01	2.25E+01	1.99E+01	-8.99E+00
PMI2	-9.62E+01	-9.82E+01	-7.66E+01	-5.64E+01	-6.74E+01	-8.57E+01	-5.86E+01	-5.61E+01	-9.31E+01	-7.80E+01	-1.10E+01
PMI3	4.23E+02	3.52E+02	2.67E+02	1.37E+02	2.36E+02	3.03E+02	1.74E+02	1.57E+02	3.95E+02	2.63E+02	9.11E+01
PMI4	-1.36E+03	-9.22E+02	-6.90E+02	-2.38E+02	-6.23E+02	-8.28E+02	-3.66E+02	-4.38E+02	-1.23E+03	-6.48E+02	-2.83E+02
PMI5	3.35E+03	1.87E+03	1.36E+03	2.77E+02	1.26E+03	1.76E+03	5.38E+02	8.99E+02	2.95E+03	1.21E+03	7.34E+02
PMI6	-6.81E+03	-3.13E+03	-2.20E+03	-1.35E+02	-2.07E+03	-3.10E+03	-5.28E+02	-1.28E+03	-5.81E+03	-1.82E+03	-1.64E+03

SI1.11 Absolute errors of the first hyperpolarizability (β_{zzz}) respect to CCSD(T) benchmark values for γ-NLO set (only molecules with non-zero value of beta) obtained using LC-BLYP, T_{α}-LC-BLYP, CAM-B3LYP, OT-LC-BLYP, B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD density functionals. aug-cc-pVDZ basis set used in all cases.

	Absolute values for absolute errors (a.u.)									
System	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**
1-Butene	1.86E+01	1.61E+01	3.33E+00	3.12E+00	7.88E+00	4.93E+00	8.60E+00	8.29E+00	1.22E+01	5.48E+00
1-Pentanal	1.03E+01	4.61E-02	7.17E+00	3.70E+00	6.73E+00	4.61E+00	1.15E+01	7.73E+00	9.64E+00	3.67E+00
1-Pentanamida	4.41E+01	4.11E+00	1.28E+01	1.12E+01	1.86E+00	1.06E+00	1.44E+01	8.87E+00	3.26E+01	5.43E+00
1-Pentanoic acid	3.55E+01	5.23E+00	9.13E+00	1.06E+01	1.34E+01	8.63E+00	1.23E+01	2.50E+00	2.26E+01	3.62E+00
n-butylamine	1.35E+00	2.08E+00	2.27E+00	2.73E+00	9.46E+00	9.64E+00	3.18E+00	2.89E+00	1.70E+00	6.71E+00
n-butanol	3.12E+00	2.48E-01	3.57E-01	1.46E-01	9.00E+00	8.61E+00	2.23E+00	6.70E-01	2.13E+00	6.03E+00
Carbon monoxide	2.44E+00	7.31E-01	2.14E+00	1.76E-01	2.93E+00	3.03E+00	2.55E+00	1.39E-01	1.45E+00	2.46E+00

Cyanic fluoride	1.87E+00	4.22E+00	2.79E+00	3.05E+00	1.14E+00	4.50E+00	7.64E+00	2.31E+00	4.38E-01	3.38E+00
Formaldehyde	1.07E+01	4.15E+00	4.04E+00	1.08E+00	2.47E+00	7.98E+00	1.79E+00	1.00E+00	9.07E+00	7.67E+00
Boric acid	1.49E-01	3.12E+00	1.42E+00	3.21E+00	3.29E+00	6.82E-01	2.11E+00	2.81E+00	1.41E+00	1.45E+00
Hydrogen cyanide	2.60E+00	1.02E+00	1.45E+00	4.61E+00	3.22E+00	4.23E-01	4.78E+00	4.53E+00	1.63E+00	1.83E+00
Hydrogen fluoride	3.36E-01	1.14E+00	8.61E-01	1.72E+00	2.47E+00	1.71E-01	1.80E+00	2.26E+00	8.40E-01	6.08E-01
Hydrogen isocyanide	5.58E+00	7.16E+00	9.63E+00	1.28E+01	1.14E+01	7.75E+00	1.30E+01	1.27E+01	6.55E+00	1.00E+01
Nytroxyl	4.73E+00	8.96E-02	1.64E+00	4.25E-01	1.71E+00	3.55E+00	1.58E+00	1.13E+00	3.64E+00	2.65E+00
Nitrous acid	2.91E+01	8.11E+00	1.18E+01	2.76E+00	3.16E+00	5.00E+00	7.70E+00	5.22E+00	2.18E+01	8.20E+00
Nitric acid	3.11E+00	9.58E-01	2.20E+00	3.00E+00	1.62E+00	2.79E-01	3.41E+00	3.26E+00	8.55E-01	1.29E+00
Dinitrogen oxide	6.15E+00	2.83E+00	3.60E+00	4.62E-01	4.16E+00	3.86E+00	1.85E+00	9.70E-02	7.55E+00	5.11E+00
PMI1	1.49E+01	1.21E+01	8.72E+00	5.04E+00	7.65E+00	1.29E+01	4.87E+00	4.28E+00	1.35E+01	1.09E+01
PMI2	8.52E+01	8.72E+01	6.56E+01	4.54E+01	5.64E+01	7.47E+01	4.76E+01	4.51E+01	8.21E+01	6.70E+01
PMI3	3.32E+02	2.61E+02	1.76E+02	4.54E+01	1.45E+02	2.12E+02	8.30E+01	6.61E+01	3.04E+02	1.72E+02
PMI4	1.08E+03	6.38E+02	4.07E+02	4.49E+01	3.39E+02	5.45E+02	8.22E+01	1.54E+02	9.49E+02	3.65E+02
PMI5	2.62E+03	1.13E+03	6.30E+02	4.57E+02	5.26E+02	1.03E+03	1.96E+02	1.65E+02	2.21E+03	4.75E+02
PMI6	5.17E+03	1.49E+03	5.62E+02	1.50E+03	4.37E+02	1.46E+03	1.11E+03	3.61E+02	4.17E+03	1.86E+02
MAE (a.u.)	**4.12E+02**	**1.60E+02**	**8.37E+01**	**9.41E+01**	**6.94E+01**	**1.48E+02**	**7.06E+01**	**3.75E+01**	**3.42E+02**	**5.88E+01**
RMSD (a.u.)	**1.23E+03**	**4.17E+02**	**1.99E+02**	**3.28E+02**	**1.62E+02**	**3.93E+02**	**2.36E+02**	**9.04E+01**	**1.01E+03**	**1.36E+02**
MAX (a.u.)	**5.17E+03**	**1.49E+03**	**6.30E+02**	**1.50E+03**	**5.26E+02**	**1.46E+03**	**1.11E+03**	**3.61E+02**	**4.17E+03**	**4.75E+02**
DFA	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**

SI1.12 Relative errors of the first hyperpolarizability (β_{zzz}) respect to CCSD(T) benchmark values for γ-NLO set (only molecules with non-zero value of beta) obtained using LC-BLYP, T_{α}-LC-BLYP, CAM-B3LYP, OT-LC-BLYP, B3LYP, BH&HLYP, PBE0, M06-2X, MN15, ωB97XD density functionals. aug-cc-pVDZ basis set used in all cases.

	Absolute values for relative errors (%)									
System	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**
1-Butene	64	55	11	11	27	17	29	28	42	19
1-Pentanal	190	1	132	68	124	85	212	142	178	68
1-Pentanamida	103	10	30	26	4	2	34	21	76	13
1-Pentanoic acid	170	25	44	51	64	41	59	12	108	17
n-butylamine	9	14	15	18	63	64	21	19	11	44
n-butanol	10	1	1	0	28	27	7	2	7	19
Carbon monoxide	8	2	7	1	10	10	8	0	5	8
Cyanic fluoride	4	8	6	6	2	9	15	5	1	7
Formaldehyde	33	13	12	3	8	24	5	3	28	23
Boric acid	1	11	5	11	11	2	7	10	5	5
Hydrogen cyanide	26	10	14	46	32	4	48	45	16	18
Hydrogen fluoride	3	10	7	14	21	1	15	19	7	5
Hydrogen isocyanide	31	39	53	70	63	43	71	70	36	55
Nytroxyl	26	0	9	2	9	20	9	6	20	15
Nitrous acid	308	86	125	29	33	53	81	55	231	87

Nitric acid	119	37	84	115	62	11	130	125	33	49
Dinitrogen oxide	11	5	6	1	7	7	3	0	13	9
PMI1	166	135	97	56	85	143	54	48	150	121
PMI2	776	794	597	413	514	680	433	411	747	610
PMI3	365	286	193	50	159	233	91	73	334	189
PMI4	380	225	144	16	120	192	29	54	335	129
PMI5	356	154	86	62	72	140	27	23	301	65
PMI6	316	91	34	92	27	89	68	22	255	11
MAE (%)	**151**	**87**	**74**	**51**	**67**	**83**	**63**	**52**	**128**	**69**
RMSD (%)	**240**	**190**	**144**	**98**	**124**	**164**	**112**	**100**	**216**	**142**
MAX (%)	**776**	**794**	**597**	**413**	**514**	**680**	**433**	**411**	**747**	**610**
DFA	**B3LYP**	**BHandHLYP**	**CAM-B3LYP**	**LC-BLYP**	**M06-2X**	**MN15**	**Tα-LC-BLYP**	**OT-LC-BLYP**	**PBE0**	**wB97XD**

3. Geometry RMSD respect to MP2 values for: B3LYP, LC-BLYP and Tα-LC-BLYP

SI1.13 RMSD of geometries (distances, angles and dihedral angles) for all compounds of the γ-NLO set. Reference geometry MP2. DFA tested B3LYP, LC-BLYP and Tα-LC-BLYP.

	RMSD OF GEOMETRY B3LYP			RMSD OF GEOMETRY LC-BLYP			RMSD OF GEOMETRY Tα-LC-BLYP		
Compound	**DISTANCES**	**ANGLES**	**DIHEDRALS**	**DISTANCES**	**ANGLES**	**DIHEDRALS**	**DISTANCES**	**ANGLES**	**DIHEDRALS**
Water	1.000E-03	8.722E-01	-	3.000E-03	2.227E+00	-	1.600E-03	1.75E+00	NaN
Ammonia	1.600E-03	4.641E-01	9.474E-01	5.900E-03	2.294E+00	4.947E+00	8.000E-04	1.54E+00	3.25E+00
Benzene	6.671E-03	2.013E-03	0.000E+00	1.667E-02	6.671E-04	0.000E+00	1.023E-02	8.14E-04	0.00E+00
1-Pentanal	4.389E-03	4.007E-01	3.345E-01	1.196E-02	1.805E-01	2.113E-01	7.294E-03	1.90E-01	2.33E-01
1-Pentanamida	4.027E-03	7.554E-01	1.235E+01	1.221E-02	1.007E+00	2.520E+01	7.694E-03	7.33E-01	1.60E+01
1-Pentanoic acid	3.791E-03	3.716E-01	3.048E-01	1.286E-02	4.140E-01	2.324E-01	7.726E-03	2.99E-01	2.36E-01
n-Butylamine	2.591E-03	3.694E-01	5.499E-01	1.102E-02	7.245E-01	1.195E+00	6.337E-03	5.13E-01	8.46E-01
n-Butanol	2.711E-03	3.227E-01	2.711E-01	1.153E-02	4.511E-01	2.563E-01	6.799E-03	3.00E-01	2.12E-01
Butane	2.327E-03	2.937E-01	2.701E-01	9.585E-03	1.396E-01	1.631E-01	5.338E-03	1.19E-01	1.49E-01
1-Butene	4.688E-03	5.012E-01	1.578E+00	1.184E-02	3.456E-01	2.108E+00	7.287E-03	2.88E-01	2.09E+00
Acetylene	1.313E-02	0.000E+00	-	2.004E-02	0.000E+00	-	1.369E-02	0.00E+00	-
Cyclohexane	2.814E-03	2.796E-01	1.791E+00	1.132E-02	1.549E-01	8.889E-01	6.353E-03	1.21E-01	5.93E-01
Carbon dioxide	1.280E-02	0.000E+00	-	2.330E-02	0.000E+00	-	1.570E-02	0.00E+00	-
Carbon monoxide	1.610E-02	-	-	2.630E-02	-	-	1.970E-02	-	-
Ethane	1.815E-03	9.563E-02	0.000E+00	7.698E-03	1.181E-01	0.000E+00	4.169E-03	1.30E-01	0.00E+00
Cyanic fluoride	2.002E-02	2.554E-03	-	3.277E-02	2.554E-03	-	2.477E-02	2.55E-03	-
Carbonic acid	5.736E-03	7.613E-01	1.358E-03	1.744E-02	1.463E+00	1.751E-03	1.389E-02	1.20E+00	1.66E-03
Formaldehyde	9.581E-03	1.810E-01	2.900E-02	1.489E-02	2.055E-01	5.000E-04	1.109E-02	3.04E-01	2.90E-02
Hydrogen peroxide	1.133E-02	1.601E+00	3.266E-01	3.703E-02	3.141E+00	1.618E-01	2.809E-02	2.51E+00	5.70E-03
Boric acid	7.227E-03	8.357E-01	4.123E-04	1.609E-02	1.654E+00	3.559E-04	1.332E-02	1.35E+00	5.83E-04
Hydrogen cyanide	1.856E-02	0.000E+00	-	2.781E-02	0.000E+00	-	2.005E-02	0.00E+00	-

Heptane	2.492E-03	2.814E-01	2.856E-01		1.043E-02	1.761E-01	2.209E-01		5.949E-03	1.61E-01	2.11E-01
Hexane	2.390E-03	2.818E-01	2.801E-01		1.024E-02	1.729E-01	2.130E-01		5.761E-03	1.29E-01	1.66E-01
Hydrogen fluoride	8.000E-04	-	-		1.900E-03	-	-		1.000E-03	-	-
Hydrogen isocyanide	1.856E-02	0.000E+00	-		2.781E-02	0.000E+00	-		2.005E-02	0.00E+00	-
Nitrous acid	1.136E-02	9.681E-01	0.000E+00		4.583E-02	2.062E+00	0.000E+00		2.980E-02	1.37E+00	0.00E+00
Nitric acid	7.473E-03	5.871E-01	7.874E-04		3.114E-02	1.240E+00	1.136E-03		2.470E-02	9.89E-01	2.19E-03
Nitroxyl	2.026E-02	1.261E+00	-		2.917E-02	1.264E+00	-		2.283E-02	1.07E+00	-
Methane	1.400E-03	0.000E+00	0.000E+00		4.200E-03	0.000E+00	0.000E+00		2.300E-03	0.00E+00	0.00E+00
Dinitrogen oxide	2.843E-02	0.000E+00	-		4.077E-02	0.000E+00	-		3.064E-02	0.00E+00	-
Dinitrogen	0.000E+00	-	-		1.060E-02	-	-		3.300E-03	-	-
Dioxygen	0.000E+00	-	-		2.090E-02	-	-		1.220E-02	-	-
Octane	2.501E-03	2.923E-01	2.951E-01		1.056E-02	1.819E-01	2.292E-01		6.047E-03	1.68E-01	2.19E-01
PA5	0.000E+00	0.000E+00	0.000E+00		6.296E-03	1.813E-01	0.000E+00		0.000E+00	0.00E+00	0.00E+00
PA6	0.000E+00	0.000E+00	0.000E+00		0.000E+00	0.000E+00	0.000E+00		0.000E+00	0.00E+00	0.00E+00
PA1	3.560E-03	1.114E-01	0.000E+00		4.079E-03	6.788E-02	0.000E+00		3.600E-03	5.53E-02	0.00E+00
PA2	4.323E-03	1.896E-01	0.000E+00		4.842E-03	1.515E-01	0.000E+00		3.473E-03	1.93E-01	0.00E+00
PA3	5.146E-03	1.859E-01	0.000E+00		5.413E-03	1.562E-01	0.000E+00		3.024E-03	1.87E-01	0.00E+00
PA4	5.934E-03	2.170E-01	0.000E+00		5.913E-03	1.731E-01	0.000E+00		3.055E-03	1.80E-01	0.00E+00
PDA1	1.729E-02	8.425E-01	0.000E+00		1.211E-02	5.136E-01	0.000E+00		1.788E-02	6.09E-01	0.00E+00
PDA2	1.860E-02	6.786E-01	0.000E+00		1.136E-02	4.826E-01	0.000E+00		1.601E-02	5.40E-01	0.00E+00
PDA3	0.000E+00	8.941E-03	0.000E+00		0.000E+00	0.000E+00	0.000E+00		2.949E-05	1.23E-03	0.00E+00
PDA4	0.000E+00	0.000E+00	0.000E+00		0.000E+00	0.000E+00	0.000E+00		0.000E+00	1.59E-03	0.00E+00
PDA5	0.000E+00	2.896E-03	0.000E+00		0.000E+00	0.000E+00	0.000E+00		2.390E-05	1.36E-03	0.00E+00
Pentane	2.370E-03	2.837E-01	2.724E-01		9.980E-03	1.695E-01	2.017E-01		5.635E-03	1.52E-01	1.91E-01
PMI1	8.771E-03	7.953E-01	0.000E+00		1.582E-02	1.026E+00	0.000E+00		1.045E-02	7.41E-01	0.00E+00
PMI2	8.971E-03	8.630E-01	0.000E+00		1.811E-02	1.110E+00	0.000E+00		1.167E-02	7.83E-01	0.00E+00
PMI3	9.317E-03	9.317E-01	0.000E+00		1.901E-02	1.138E+00	0.000E+00		1.220E-02	8.04E-01	0.00E+00

PMI4	9.583E-03	9.592E-01	0.000E+00		1.939E-02	1.156E+00	0.000E+00		1.278E-02	8.46E-01	0.00E+00
PMI5	9.817E-03	9.815E-01	0.000E+00		1.955E-02	1.175E+00	0.000E+00		1.317E-02	8.82E-01	0.00E+00
PMI6	1.012E-02	1.001E+00	0.000E+00		1.963E-02	1.188E+00	0.000E+00		1.357E-02	9.16E-01	0.00E+00
Propane	2.138E-03	2.907E-01	2.552E-01		8.898E-03	1.672E-01	1.821E-01		4.941E-03	1.30E-01	1.59E-01
SUMMATION (a.u.)	**3.645E-01**	**2.012E+01**	**2.014E+01**		**7.652E-01**	**2.847E+01**	**3.642E+01**		**5.280E-01**	**2.23E+01**	**2.46E+01**
RMSD (a.u.)	**9.656E-03**	**5.791E-01**	**2.002E+00**		**1.809E-02**	**9.463E-01**	**4.083E+00**		**1.304E-02**	**7.25E-01**	**2.60E+00**
MAX (a.u.)	**2.843E-02**	**1.601E+00**	**1.235E+01**		**4.583E-02**	**3.141E+00**	**2.520E+01**		**3.064E-02**	**2.51E+00**	**1.60E+01**

SI1.14 Comparison of summation, RMSD and MAX of RMSDs of table SI1.13 by functional.

Summary of SUMMATION			
	Distances	**Angles**	**Dihedral**
B3LYP	**3.645E-01**	**2.012E+01**	**2.014E+01**
LC-BLYP	**7.652E-01**	**2.847E+01**	**3.642E+01**
Tα-LC-BLYP	**5.280E-01**	**2.225E+01**	**2.455E+01**
Summary of RMSD			
	Distances	**Angles**	**Dihedral**
B3LYP	**9.656E-03**	**5.791E-01**	**2.002E+00**
LC-BLYP	**1.809E-02**	**9.463E-01**	**4.083E+00**
Tα-LC-BLYP	**1.304E-02**	**7.251E-01**	**2.604E+00**
Summary of MAX			
	Distances	**Angles**	**Dihedral**
B3LYP	**2.843E-02**	**1.601E+00**	**1.235E+01**
LC-BLYP	**4.583E-02**	**3.141E+00**	**2.520E+01**
Tα-LC-BLYP	**3.064E-02**	**2.512E+00**	**1.597E+01**

4. Analytical vibrational frequency RMSD respect to MP2 values for: B3LYP, LC-BLYP and Tα-LC-BLYP

SI1.15 Comparison RMSD and MAX of RMSDs for vibrational frequency calculations.

	B3LYP	**LC-BLYP**	**Tα-LC-BLYP**
Water	1.99E+01	5.63E+01	1.70E+01
Ammonia	3.23E+01	6.23E+01	2.07E+01
Benzene	4.06E+01	6.39E+01	6.62E+01
1-Pentanal	2.60E+01	3.45E+01	3.76E+01
1-Pentanamida	2.39E+01	3.39E+01	4.01E+01
1-Pentanoic acid	2.04E+01	3.27E+01	3.58E+01
n-Butylamine	2.32E+01	2.90E+01	3.45E+01
n-Butanol	2.30E+01	2.80E+01	3.76E+01
Butane	2.56E+01	2.29E+01	3.30E+01
1-Butene	2.49E+01	3.10E+01	4.06E+01
Acetylene	9.89E+01	1.80E+02	1.90E+02
Cyclohexane	1.96E+01	3.00E+01	2.76E+01
Carbon dioxide	2.62E+01	7.97E+01	6.34E+01
Carbon monoxide	1.13E+02	2.13E+02	1.62E+02
Ethane	3.30E+01	1.80E+01	2.90E+01
Cyanic fluoride	9.62E+01	1.74E+02	1.49E+02
Carbonic acid	3.11E+00	4.83E+01	4.01E+01
Formaldehyde	6.16E+01	6.72E+01	6.04E+01
Hydrogen peroxide	3.05E+01	9.95E+01	8.40E+01
Boric acid	7.49E+00	4.36E+01	4.15E+01
Hydrogen cyanide	1.00E+02	1.64E+02	1.37E+02
Heptane	2.27E+01	2.55E+01	3.35E+01
Hexane	2.35E+01	2.48E+01	3.31E+01
Hydrogen fluoride	2.16E+01	2.36E+01	3.74E+01
Hydrogen isocyanide	1.00E+02	1.64E+02	1.37E+02
Nitrous acid	5.52E+01	1.44E+02	1.12E+02
Nitric acid	3.46E+01	7.92E+01	6.91E+01
Nitroxyl	1.17E+02	1.57E+02	1.25E+02
Methane	4.14E+01	1.72E+01	2.72E+01
Dinitrogen oxide	7.42E+01	1.57E+02	1.14E+02
Dinitrogen	3.84E+01	1.62E+02	9.80E+01
Dioxygen	5.87E+01	2.21E+02	1.67E+02
Octane	2.28E+01	2.57E+01	3.34E+01
PA5	4.52E+01	5.55E+01	6.45E+01
PA6	4.83E+01	5.89E+01	6.53E+01
PA1	3.43E+01	2.45E+01	4.35E+01
PA2	4.49E+01	4.09E+01	6.21E+01
PA3	5.13E+01	4.94E+01	6.63E+01
PA4	5.29E+01	5.29E+01	6.70E+01
PDA1[a]	2.03E+02	1.96E+02	2.32E+02
PDA2[a]	2.00E+02	1.93E+02	2.23E+02
PDA3[a]	9.70E+01	1.10E+02	1.24E+02
PDA4[a]	9.65E+01	1.10E+02	1.21E+02
PDA5[a]	9.65E+01	1.11E+02	1.19E+02
Pentane	2.44E+01	2.39E+01	3.43E+01
PMI1	3.94E+01	5.71E+01	5.20E+01
PMI2	2.85E+01	6.43E+01	5.93E+01
PMI3	2.58E+01	6.54E+01	5.97E+01
PMI4	2.44E+01	6.57E+01	5.98E+01
PMI5	2.42E+01	6.51E+01	5.92E+01
PMI6	2.40E+01	6.43E+01	5.87E+01
Propane	2.77E+01	2.03E+01	3.25E+01
RMSD	**6.59E+01**	**9.92E+01**	**9.18E+01**
MAX	**2.03E+02**	**2.21E+02**	**2.32E+02**

[a] All PDA geometries are taken from M. B. Oviedo et al. *Journal of Chemical Theory and Computation*, **2016**, 12, 3593-3602.

5. Cartesian coordinates of the γ-NLO set (Å)

C_4H_8

6	-0.29528	-0.09454	1.82007
1	-1.19281	0.52845	1.88929
6	0.43449	-0.14001	0.684
1	1.32731	-0.77952	0.65409
1	-0.0121	-0.67359	2.70254
6	0.09863	0.60686	-0.58025
1	0.94448	1.26167	-0.85629
1	-0.7727	1.25931	-0.39972
6	-0.1949	-0.35466	-1.74505
1	-1.05961	-0.99439	-1.50834
1	0.66946	-1.01066	-1.93852
1	-0.4154	0.19865	-2.6716

C_2H_2

6	0.000000000	0.000000000	0.615743000
6	0.000000000	0.000000000	-0.615743000
1	0.000000000	0.000000000	-1.690998000
1	0.000000000	0.000000000	1.690998000

H_2O

8	0.000000000	0.066647332	0.000000000
1	0.000000000	-0.528870783	0.760506888
1	0.000000000	-0.528870783	-0.760506888

NH_3

7	0.069271254	0.000000000	0.000000000
1	-0.320826353	0.942677685	0.000000000
1	-0.320826353	-0.471338843	-0.816382824
1	-0.320826353	-0.471338843	0.816382824

C_6H_6

6	0.000000000	1.407956951	-0.000000322
6	0.000000000	0.703979492	1.219328702
6	0.000000000	0.703979492	-1.219329044
1	0.000000000	1.251082573	2.166937948
1	0.000000000	1.251082245	-2.166938439
6	0.000000000	-0.703979051	1.219328363
6	0.000000000	-0.703979062	-1.219327906
1	0.000000000	-1.251082047	2.166937890
1	0.000000000	-1.251082470	-2.166937200
6	0.000000000	-1.407957791	0.000000214
1	0.000000000	-2.502163158	0.000000113
1	0.000000000	2.502162478	-0.000000406

C_6H_{12}

6	-0.236914753	0.806433475	-1.219493089
6	0.236914755	1.459328726	0.088645339
6	-0.236914754	0.652895247	1.308138425
6	0.236914753	-0.806433475	1.219493089
6	-0.236914755	-1.459328726	-0.088645339
6	0.236914754	-0.652895247	-1.308138425
1	0.126607312	1.381163141	-2.088602381
1	-1.342457344	0.831248369	-1.257018293
1	-0.126607315	2.499364279	0.151821170
1	1.342457349	1.504233942	0.091373058
1	0.126607307	1.118201172	2.240423546
1	-1.342457348	0.672985593	1.348391339
1	-0.126607312	-1.381163141	2.088602381
1	1.342457344	-0.831248369	1.257018293
1	0.126607315	-2.499364279	-0.151821170
1	-1.342457349	-1.504233942	-0.091373058
1	-0.126607307	-1.118201172	-2.240423546
1	1.342457348	-0.672985593	-1.348391339

C_4H_9CHO

6	0.000000000	-0.891602281	-0.708944628
1	0.879324204	-1.560933888	-0.637022666
1	-0.879324204	-1.560933888	-0.637022666
6	0.000000000	0.149910062	0.408589951
1	0.881779475	0.803724590	0.295765953
1	-0.881779475	0.803724590	0.295765953
6	0.000000000	-0.490479742	1.801295984
1	-0.885189620	-1.143761461	1.903846343
1	0.885189620	-1.143761461	1.903846343
6	0.000000000	0.556358175	2.921327009
1	-0.890536432	1.202225730	2.852522914
1	0.000000000	0.083468227	3.915888426
1	0.890536432	1.202225730	2.852522914
6	0.000000000	-0.310687235	-2.104657168
8	0.000000000	0.889513711	-2.356870375
1	0.000000000	-1.057107982	-2.936268149

$C_4H_9CONH_2$

6	-0.655690191	-0.424609631	0.319169396
1	-0.711238149	-1.526474450	0.295180465
1	-1.681450382	-0.028849998	0.237608473
6	0.188303776	0.089831055	-0.859146715
1	1.218224677	-0.301009832	-0.768071802
1	0.253752959	1.188337102	-0.785893583
6	-0.396886854	-0.312586835	-2.216738506
1	-1.425657804	0.081693579	-2.296002350
1	-0.476160194	-1.413293283	-2.271146416
6	0.447532116	0.203348435	-3.387832787
1	0.516445090	1.303053069	-3.364224697
1	0.014209328	-0.088951430	-4.357176342
1	1.472340807	-0.199896723	-3.339236365
6	-0.080908814	0.074649131	1.635640884
8	-0.055984480	1.272624008	1.931408468
7	0.465876781	-0.888208156	2.451473485
1	0.821449723	-0.600482719	3.355085330
1	0.338976154	-1.872517792	2.266183755

C_4H_9COOH

6	0.000000000	-0.672737294	0.303232887
1	0.880928066	-1.337927148	0.313005285
1	-0.880928066	-1.337927148	0.313005285
6	0.000000000	0.230262649	-0.929887814
1	0.882611490	0.891319980	-0.897956475
1	-0.882611490	0.891319980	-0.897956475
6	0.000000000	-0.577913920	-2.232123403
1	-0.885212724	-1.238672590	-2.252739985
1	0.885212724	-1.238672590	-2.252739985
6	0.000000000	0.322911542	-3.472585768
1	0.890616306	0.972205441	-3.484136653
1	-0.890616306	0.972205441	-3.484136653
1	0.000000000	-0.269324624	-4.400954392
6	0.000000000	0.098616624	1.602606005
8	0.000000000	1.313474390	1.722045670
8	0.000000000	-0.746514199	2.681130148
1	0.000000000	-0.172068500	3.467525115

$C_4H_9NH_2$

6	-0.014180539	0.515563704	-1.259765683
1	0.867668785	1.178169122	-1.278477477
1	-0.911376991	1.167148243	-1.243248387
6	0.015602311	-0.326165457	0.015477483
1	0.924046258	-0.953183946	0.002910524
1	-0.848339065	-1.018012807	0.013003010
6	-0.021422372	0.524697968	1.289748467
1	-0.931410912	1.150900018	1.287218374
1	0.837808336	1.219019102	1.287368339
6	0.011326840	-0.328922555	2.563165194
1	-0.853620208	-1.011579038	2.598888194
1	-0.013341525	0.295878711	3.469882901
1	0.926146870	-0.942785945	2.599064089
7	0.059442062	-0.355454849	-2.447184859
1	-0.777502987	-0.939489203	-2.495746621
1	0.057289599	0.206553035	-3.299276525

C_4H_9OH

6	0.000000000	0.520199718	-1.233917537
1	0.895894738	1.168557292	-1.254900835
1	-0.895894738	1.168557292	-1.254900835
6	0.000000000	-0.326571917	0.029780813
1	0.887636763	-0.982528505	0.014712675
1	-0.887636763	-0.982528505	0.014712675
6	0.000000000	0.528374835	1.302470817
1	-0.885481594	1.188790629	1.302239661
1	0.885481594	1.188790629	1.302239661
6	0.000000000	-0.327804301	2.574547327
1	0.890514837	-0.976389337	2.609116604
1	-0.890514837	-0.976389337	2.609116604
1	0.000000000	0.296800926	3.481595538
8	0.000000000	-0.374592047	-2.361655819
1	0.000000000	0.157734640	-3.168280267

CH_4

6	0.000000000	0.000000000	0.000000000
1	0.634026715	0.634026715	0.634026715
1	-0.634026715	-0.634026715	0.634026715
1	0.634026715	-0.634026715	-0.634026715
1	-0.634026715	0.634026715	-0.634026715

C_2H_6

6	0.000000000	0.000000000	0.766784047
1	-0.889223057	0.513393172	1.164717200
1	0.889223057	0.513393172	1.164717200
1	0.000000000	-1.026786344	1.164717200
6	0.000000000	0.000000000	-0.766797751
1	0.000000000	1.026801379	-1.164662809
1	0.889236080	-0.513400690	-1.164662809
1	-0.889236080	-0.513400690	-1.164662809

C_3H_8

6	0.000000000	0.271608577	1.271827791
1	0.890318274	0.921251107	1.306218243
1	-0.890318274	0.921251107	1.306218243
1	0.000000000	-0.350425710	2.180800854
6	0.000000000	-0.584725065	0.000000143
1	-0.884234000	-1.244931845	0.000004336
1	0.884234000	-1.244931845	0.000004336
6	0.000000000	0.271603702	-1.271828559
1	0.890319173	0.921246243	-1.306214962
1	-0.890319173	0.921246243	-1.306214962
1	0.000000000	-0.350419667	-2.180808649

C_4H_{10}

6	0.000002259	-0.516278918	0.566586241
1	0.884924916	-1.169399792	0.460475662
1	-0.884916902	-1.169404315	0.460472288
6	-0.000002607	0.131856888	1.955851982
1	0.890516314	0.767624127	2.091443824
1	-0.890531521	0.767610129	2.091447439
1	0.000005358	-0.624586648	2.756445231
6	0.000002985	0.516279470	-0.566586951
1	-0.884920765	1.169398808	-0.460478085
1	0.884920434	1.169407980	-0.460472438
6	-0.000000997	-0.131857560	-1.955851790
1	-0.890529076	-0.767615869	-2.091434926
1	0.890519770	-0.767619116	-2.091448253
1	-0.000008056	0.624586132	-2.756444564

C_5H_{12}

6	0.000000000	0.335246001	2.551237655
1	0.890580497	0.984210668	2.586064127
1	-0.890580497	0.984210668	2.586064127
1	0.000000000	-0.287715664	3.459645948
6	0.000000000	-0.521544559	1.279628985
1	-0.885039837	-1.182760335	1.276945760
1	0.885039837	-1.182760335	1.276945760
6	0.000000000	0.322144931	0.000000058
1	0.885597949	0.985366354	-0.000000436
1	-0.885597949	0.985366354	-0.000000436
6	0.000000000	-0.521551478	-1.279627594
1	0.885039503	-1.182768690	-1.276940215
1	-0.885039503	-1.182768690	-1.276940215
6	0.000000000	0.335227401	-2.551239508
1	-0.890580957	0.984192088	-2.586066409
1	0.000000000	-0.287735120	-3.459646780
1	0.890580957	0.984192088	-2.586066409

C_6H_{14}

6	0.000000000	-0.221710606	3.212391803
1	0.890593917	-0.866930782	3.289801326
1	-0.890593917	-0.866930782	3.289801326
1	0.000000000	0.459740220	4.077787977
6	0.000000000	0.549241874	1.886959063
1	-0.885069280	1.208654426	1.840132364
1	0.885069280	1.208654426	1.840132364
6	0.000000000	-0.378216212	0.666301654
1	0.885738837	-1.039453797	0.711017932
1	-0.885738837	-1.039453797	0.711017932
6	0.000000000	0.378213659	-0.666298885
1	0.885737705	1.039453733	-0.711009149
1	-0.885737705	1.039453733	-0.711009149
6	0.000000000	-0.549242747	-1.886962952
1	-0.885067883	-1.208658711	-1.840145644
1	0.885067883	-1.208658711	-1.840145644
6	0.000000000	0.221712828	-3.212391142
1	0.890594430	0.866934008	-3.289788832
1	0.000000000	-0.459723654	-4.077798500
1	-0.890594430	0.866934008	-3.289788832

C_7H_{16}

6	0.000000000	0.493989584	2.558662080
1	0.885065988	1.155054828	2.555408211
1	-0.885065988	1.155054828	2.555408211
6	0.000000000	-0.350588480	1.279275605
1	-0.885761703	-1.013216538	1.279632615
1	0.885761703	-1.013216538	1.279632615
6	0.000000000	0.493408429	-0.000000842
1	0.885893664	1.155673685	0.000012421
1	-0.885893664	1.155673685	0.000012421
6	0.000000000	-0.350571701	-1.279282460
1	0.885771726	-1.013184581	-1.279679380
1	-0.885771726	-1.013184581	-1.279679380
6	0.000000000	0.494038186	-2.558655583
1	-0.885086764	1.155072481	-2.555403726
1	0.885086764	1.155072481	-2.555403726
6	0.000000000	-0.362873650	-3.830232312
1	0.890622598	-1.011756358	-3.864773171
1	0.000000000	0.259875331	-4.738762527
1	-0.890622598	-1.011756358	-3.864773171
6	0.000000000	-0.362927558	3.830241777
1	-0.890622381	-1.011806370	3.864753659
1	0.000000000	0.259828138	4.738762864
1	0.890622381	-1.011806370	3.864753659

C_8H_{18}

6	0.000000000	0.350476857	-1.932946382
1	0.885780759	1.012614750	-1.957528062
1	-0.885780759	1.012614750	-1.957528062
6	0.000000000	-0.445795861	-0.623466192
1	-0.885914064	-1.107465421	-0.598569399
1	0.885914064	-1.107465421	-0.598569399
6	0.000000000	0.445797476	0.623459069
1	0.885915683	1.107465900	0.598567243
1	-0.885915683	1.107465900	0.598567243
6	0.000000000	-0.350475082	1.932943719
1	0.885783378	-1.012611334	1.957522145
1	-0.885783378	-1.012611334	1.957522145
6	0.000000000	0.540396026	3.180557439
1	-0.885109439	1.200814203	3.153138485
1	0.885109439	1.200814203	3.153138485
6	0.000000000	-0.269574178	4.482562068
1	0.890629917	-0.916750772	4.540699957
1	0.000000000	0.385863001	5.367790258
1	-0.890629917	-0.916750772	4.540699957

6 0.000000000 -0.540400769 -3.180554298
1 -0.885108217 -1.200817481 -3.153141753
1 0.885108217 -1.200817481 -3.153141753
6 0.000000000 0.269574845 -4.482556623
1 0.890630843 0.916749736 -4.540682066
1 0.000000000 -0.385853993 -5.367789079
1 -0.890630843 0.916749736 -4.540682066

CO_2
6 0.000000000 0.000000000 0.000000000
8 0.000000000 0.000000000 1.180223701
8 0.000000000 0.000000000 -1.180223701

CO
6 0.000000000 0.000000000 -0.657250000
8 0.000000000 0.000000000 0.492938000

FCN
6 -1.442228000 0.000002000 -2.761158000
7 -1.442189000 -0.000001000 -3.948346000
9 -1.442190000 -0.000001000 -1.476439000

H_2CO_3
8 0.000000066 1.320180049 -0.000000067
6 -0.000000301 0.102261320 0.000000001
8 0.000000035 -0.692811704 1.091882042
1 0.000000721 -0.089486379 1.852916048
8 0.000000035 -0.692811799 -1.091881977
1 0.000000721 -0.089486523 -1.852916026

H_2CO
8 -1.725356000 -0.000006000 -4.524494000
6 -1.726219000 0.000000000 -3.300784000
1 -1.726640000 0.946255000 -2.717664000
1 -1.726624000 -0.946248000 -2.717652000

H_2O_2
8 -0.058888000 0.000000000 0.735118000
8 -0.058888000 0.000000000 -0.735118000
1 0.471103000 -0.799591000 -0.889536000
1 0.471103000 0.799591000 0.889536000

H_3BO_3
5 0.000000481 0.002471736 0.009342940
8 0.000000662 0.151535903 1.386658725
1 -0.000000100 1.068426994 1.683087340
8 -0.000001512 -1.296696006 -0.450867024
1 0.000009424 -1.317972016 -1.416471716
8 0.000000080 1.038037613 -0.924862692
1 -0.000002364 1.922655913 -0.542127581

$(H_2)_1$
1 0.000000000 0.000000000 0.000000000
1 0.000000000 0.000000000 1.058354498

$(H_2)_2$
1 0.000000000 0.000000000 0.000000000
1 0.000000000 0.000000000 1.058354498
1 0.000000000 0.000000000 2.645886245
1 0.000000000 0.000000000 3.704240743

$(H_2)_3$
1 0.000000000 0.000000000 0.000000000
1 0.000000000 0.000000000 1.058354498
1 0.000000000 0.000000000 2.645886245
1 0.000000000 0.000000000 3.704240743
1 0.000000000 0.000000000 5.291772490
1 0.000000000 0.000000000 6.350126988

$(H_2)_4$
1 0.000000000 0.000000000 0.000000000
1 0.000000000 0.000000000 1.058354498
1 0.000000000 0.000000000 2.645886245
1 0.000000000 0.000000000 3.704240743
1 0.000000000 0.000000000 5.291772490
1 0.000000000 0.000000000 6.350126988
1 0.000000000 0.000000000 7.937658735
1 0.000000000 0.000000000 8.996013233

$(H_2)_5$
1 0.000000000 0.000000000 0.000000000
1 0.000000000 0.000000000 1.058354498
1 0.000000000 0.000000000 2.645886245
1 0.000000000 0.000000000 3.704240743
1 0.000000000 0.000000000 5.291772490
1 0.000000000 0.000000000 6.350126988
1 0.000000000 0.000000000 7.937658735
1 0.000000000 0.000000000 8.996013233
1 0.000000000 0.000000000 10.583544980
1 0.000000000 0.000000000 11.641899478

$(H_2)_6$
1 0.000000000 0.000000000 0.000000000
1 0.000000000 0.000000000 1.058354498
1 0.000000000 0.000000000 2.645886245
1 0.000000000 0.000000000 3.704240743
1 0.000000000 0.000000000 5.291772490
1 0.000000000 0.000000000 6.350126988
1 0.000000000 0.000000000 7.937658735
1 0.000000000 0.000000000 8.996013233
1 0.000000000 0.000000000 10.583544980
1 0.000000000 0.000000000 11.641899478
1 0.000000000 0.000000000 13.229431225
1 0.000000000 0.000000000 14.287785723

$(H_2)_7$
1 0.000000000 0.000000000 0.000000000
1 0.000000000 0.000000000 1.058354498
1 0.000000000 0.000000000 2.645886245
1 0.000000000 0.000000000 3.704240743
1 0.000000000 0.000000000 5.291772490
1 0.000000000 0.000000000 6.350126988
1 0.000000000 0.000000000 7.937658735
1 0.000000000 0.000000000 8.996013233
1 0.000000000 0.000000000 10.583544980
1 0.000000000 0.000000000 11.641899478
1 0.000000000 0.000000000 13.229431225
1 0.000000000 0.000000000 14.287785723
1 0.000000000 0.000000000 15.875317470
1 0.000000000 0.000000000 16.933671968

$(H_2)_8$
1 0.000000000 0.000000000 0.000000000
1 0.000000000 0.000000000 1.058354498
1 0.000000000 0.000000000 2.645886245
1 0.000000000 0.000000000 3.704240743
1 0.000000000 0.000000000 5.291772490
1 0.000000000 0.000000000 6.350126988
1 0.000000000 0.000000000 7.937658735
1 0.000000000 0.000000000 8.996013233
1 0.000000000 0.000000000 10.583544980
1 0.000000000 0.000000000 11.641899478
1 0.000000000 0.000000000 13.229431225
1 0.000000000 0.000000000 14.287785723
1 0.000000000 0.000000000 15.875317470
1 0.000000000 0.000000000 16.933671968
1 0.000000000 0.000000000 18.521203715
1 0.000000000 0.000000000 19.579558213

HCN
6 0.155374000 -0.500466000 -4.204967000
7 0.155374000 -0.500466000 -5.387793000
1 0.155374000 -0.500466000 -3.127037000

HF
1 0.000000000 0.000000000 0.087594000
9 0.000000000 0.000000000 1.012406000

HNC

6	0.155374000	-0.500466000	-4.204967000
7	0.155374000	-0.500466000	-5.387793000
1	0.155374000	-0.500466000	-3.127037000

HNO_2

8	0.000000000	-0.243968018	-1.071911208
7	0.000000000	0.503816188	-0.150414664
8	0.000000000	-0.228370327	1.093594898
1	0.000000000	0.496154057	1.745778100

HNO_3

7	0.000000312	0.025759999	-0.125408252
8	0.000001458	-0.394131443	1.227229249
1	-0.000012927	0.457918197	1.705430353
8	-0.000001145	-0.890984981	-0.917062213
8	0.000000228	1.233711301	-0.307833443

HNO

7	0.000000000	0.085465752	0.620560625
8	0.000000000	-0.018397094	-0.607614485
1	0.000000000	-0.895515843	1.020996556

N_2O

7	0.000000000	0.000000000	-0.079147000
7	0.000000000	0.000000000	1.094369000
8	0.000000000	0.000000000	2.284778000

N_2

7	0.000000000	0.000000000	0.552204000
7	0.000000000	0.000000000	-0.552204000

O_2

8	0.000000000	0.000000000	0.604263000
8	0.000000000	0.000000000	-0.604263000

PA1

6	0.000000000	0.000000000	0.664070000
1	0.000000000	0.931000000	1.237110000
1	0.000000000	-0.931000000	1.237110000
6	0.000000000	0.000000000	-0.664070000
1	0.000000000	-0.931000000	-1.237110000
1	0.000000000	0.931000000	-1.237110000

PA2

6	0.00000	0.11956	-1.84254
1	0.00000	-0.51542	-2.72994
1	0.00000	1.20142	-2.00164
6	0.00000	-0.39856	-0.61186
1	0.00000	-1.48640	-0.48228
6	0.00000	0.39856	0.61186
1	0.00000	1.48640	0.48228
6	0.00000	-0.11956	1.84254
1	0.00000	-1.20142	2.00164
1	0.00000	0.51542	2.72994

PA3

6	0.00000	-0.17822	3.06677
6	0.00000	0.41497	1.86864
6	0.00000	-0.29953	0.60150
6	0.00000	0.29953	-0.60150
6	0.00000	-0.41497	-1.86864
6	0.00000	0.17822	-3.06677
1	0.00000	-0.40203	-3.99063
1	0.00000	1.26758	-3.15971
1	0.00000	-1.50880	-1.80948
1	0.00000	1.39435	-0.65242
1	0.00000	-1.39435	0.65242
1	0.00000	1.50880	1.80948
1	0.00000	-1.26758	3.15971
1	0.00000	0.40203	3.99063

PA4

6	0.00000	0.20777	-4.29804
6	0.00000	-0.40727	-3.11036
6	0.00000	0.28260	-1.83126
6	0.00000	-0.34131	-0.63848
6	0.00000	0.34131	0.63848
6	0.00000	-0.28260	1.83126
6	0.00000	0.40727	3.11036
6	0.00000	-0.20777	4.29804
1	0.00000	0.35569	5.23217
1	0.00000	-1.29859	4.37098
1	0.00000	1.50205	3.07166
1	0.00000	-1.37810	1.86014
1	0.00000	1.43698	0.61321
1	0.00000	-1.43698	-0.61321
1	0.00000	1.37810	-1.86014
1	0.00000	-1.50205	-3.07166
1	0.00000	1.29859	-4.37098
1	0.00000	-0.35569	-5.23217

PA5

6	0.00000	0.28119	-3.06419
6	0.00000	-0.35233	-1.87561
6	0.00000	0.31835	-0.59439
6	0.00000	-0.31835	0.59439
6	0.00000	0.35233	1.87561
6	0.00000	-0.28119	3.06419
6	0.00000	0.39872	4.34803
6	0.00000	-0.22493	5.53144
1	0.00000	0.33186	6.46954
1	0.00000	-1.31625	5.59668
1	0.00000	1.49377	4.31754
1	0.00000	-1.37687	3.08438
1	0.00000	1.44820	1.85967
1	0.00000	-1.41409	0.60873
1	0.00000	1.41409	-0.60873
1	0.00000	-1.44820	-1.85967
1	0.00000	1.37687	-3.08438
6	0.00000	-0.39872	-4.34803
6	0.00000	0.22493	-5.53144
1	0.00000	-1.49377	-4.31754
1	0.00000	1.31625	-5.59668
1	0.00000	-0.33186	-6.46954

PA6

6	0.000000000	0.310420000	-1.828270000
6	0.000000000	-0.331680000	-0.641370000
6	0.000000000	0.331680000	0.641370000
6	0.000000000	-0.310420000	1.828270000
6	0.000000000	0.354860000	3.111500000
6	0.000000000	-0.283230000	4.298010000
6	0.000000000	0.391920000	5.584110000
6	0.000000000	-0.235920000	6.765420000
1	0.000000000	0.317580000	7.705460000
1	0.000000000	-1.327450000	6.826730000
1	0.000000000	1.487090000	5.557580000
1	0.000000000	-1.378960000	4.314010000
1	0.000000000	1.450810000	3.099980000
1	0.000000000	-1.406180000	1.837720000
1	0.000000000	1.427510000	0.632530000
1	0.000000000	-1.427510000	-0.632530000
1	0.000000000	1.406180000	-1.837720000
6	0.000000000	-0.354860000	-3.111500000
6	0.000000000	0.283230000	-4.298010000
1	0.000000000	-1.450810000	-3.099980000
1	0.000000000	1.378960000	-4.314010000
6	0.000000000	-0.391920000	-5.584110000
6	0.000000000	0.235920000	-6.765420000
1	0.000000000	-1.487090000	-5.557580000
1	0.000000000	1.327450000	-6.826730000
1	0.000000000	-0.317580000	-7.705460000

All PDA geometries are taken from M. B. Oviedo et al. *Journal of Chemical Theory and Computation*, 2016, **12**, 3593-3602.

PDA1

6	-0.489644000	-0.448409000	0.000000000
6	0.489644000	0.448409000	0.000000000
1	-1.517940000	-0.144205000	0.000000000
1	-0.293691000	-1.503025000	0.000000000
1	0.252110000	1.496882000	0.000000000
6	1.883890000	0.125653000	0.000000000
6	3.056632000	-0.125653000	0.000000000
6	4.450879000	-0.448409000	0.000000000
6	5.430166000	0.448409000	0.000000000
1	4.688413000	-1.496882000	0.000000000
1	6.458462000	0.144205000	0.000000000
1	5.234214000	1.503025000	0.000000000

PDA2

6	-0.489376000	-0.448848000	0.000000000
6	0.489376000	0.448848000	0.000000000
1	-1.517737000	-0.145137000	0.000000000
1	-0.292819000	-1.503313000	0.000000000
1	0.252303000	1.497299000	0.000000000
6	1.882858000	0.125579000	0.000000000
6	3.056092000	-0.125355000	0.000000000
6	4.443410000	-0.454338000	0.000000000
6	5.422643000	0.454338000	0.000000000
1	4.688808000	-1.499988000	0.000000000
1	5.177246000	1.499988000	0.000000000
6	6.809961000	0.125355000	0.000000000
6	7.983196000	-0.125579000	0.000000000
6	9.376677000	-0.448848000	0.000000000
6	10.355430000	0.448848000	0.000000000
1	9.613750000	-1.497299000	0.000000000
1	11.383791000	0.145137000	0.000000000
1	10.158872000	1.503313000	0.000000000

PDA3

6	-0.489039000	-0.449220000	0.000000000
6	0.489039000	0.449220000	0.000000000
1	-1.517595000	-0.146239000	0.000000000
1	-0.291738000	-1.503539000	0.000000000
1	0.251579000	1.497539000	0.000000000
6	1.882574000	0.126253000	0.000000000
6	3.055853000	-0.124497000	0.000000000
6	4.442747000	-0.453331000	0.000000000
6	5.422195000	0.455608000	0.000000000
1	4.688265000	-1.498966000	0.000000000
1	5.177802000	1.501397000	0.000000000
6	6.808405000	0.125447000	0.000000000
6	7.982141000	-0.125447000	0.000000000
6	9.368351000	-0.455608000	0.000000000
6	10.347799000	0.453331000	0.000000000
1	9.612744000	-1.501397000	0.000000000
1	10.102281000	1.498966000	0.000000000
6	11.734693000	0.124497000	0.000000000
6	12.907972000	-0.126253000	0.000000000
6	14.301507000	-0.449220000	0.000000000
6	15.279585000	0.449220000	0.000000000
1	14.538967000	-1.497539000	0.000000000
1	16.308141000	0.146239000	0.000000000
1	15.082284000	1.503539000	0.000000000

PDA4

6	-0.488743000	-0.449538000	0.000000000
6	0.488743000	0.449538000	0.000000000
1	-1.517486000	-0.147214000	0.000000000
1	-0.290778000	-1.503730000	0.000000000
1	0.250767000	1.497722000	0.000000000
6	1.882429000	0.127169000	0.000000000
6	3.055797000	-0.123101000	0.000000000
6	4.442723000	-0.451380000	0.000000000
6	5.421921000	0.457864000	0.000000000
1	4.688602000	-1.496940000	0.000000000
1	5.177595000	1.503631000	0.000000000
6	6.808037000	0.127400000	0.000000000
6	7.981720000	-0.123805000	0.000000000
6	9.367373000	-0.454378000	0.000000000
6	10.347451000	0.454378000	0.000000000
1	9.611447000	-1.500258000	0.000000000
1	10.103377000	1.500258000	0.000000000
6	11.733105000	0.123805000	0.000000000
6	12.906788000	-0.127400000	0.000000000
6	14.292904000	-0.457864000	0.000000000
6	15.272101000	0.451380000	0.000000000
1	14.537230000	-1.503631000	0.000000000
1	15.026223000	1.496940000	0.000000000
6	16.659027000	0.123101000	0.000000000
6	17.832395000	-0.127169000	0.000000000
6	19.226081000	-0.449538000	0.000000000
6	20.203567000	0.449538000	0.000000000
1	19.464057000	-1.497722000	0.000000000
1	21.232310000	0.147214000	0.000000000
1	20.005602000	1.503730000	0.000000000

PDA5

6	-0.488502000	-0.449799000	0.000000000
6	0.488502000	0.449799000	0.000000000
1	-1.517400000	-0.148019000	0.000000000
1	-0.289984000	-1.503887000	0.000000000
1	0.250038000	1.497864000	0.000000000
6	1.882335000	0.128035000	0.000000000
6	3.055802000	-0.121735000	0.000000000
6	4.442828000	-0.449434000	0.000000000
6	5.421693000	0.460169000	0.000000000
1	4.689112000	-1.494903000	0.000000000
1	5.177148000	1.505868000	0.000000000
6	6.807874000	0.129899000	0.000000000
6	7.981577000	-0.121152000	0.000000000
6	9.367177000	-0.451554000	0.000000000
6	10.347275000	0.457213000	0.000000000
1	9.611313000	-1.497431000	0.000000000
1	10.103576000	1.503142000	0.000000000
6	11.732746000	0.125929000	0.000000000
6	12.906301000	-0.125929000	0.000000000
6	14.291773000	-0.457213000	0.000000000
6	15.271871000	0.451554000	0.000000000
1	14.535471000	-1.503142000	0.000000000
1	15.027735000	1.497431000	0.000000000
6	16.657471000	0.121152000	0.000000000
6	17.831174000	-0.129899000	0.000000000
6	19.217354000	-0.460169000	0.000000000
6	20.196219000	0.449434000	0.000000000
1	19.461900000	-1.505868000	0.000000000
1	19.949936000	1.494903000	0.000000000
6	21.583246000	0.121735000	0.000000000
6	22.756713000	-0.128035000	0.000000000
6	24.150546000	-0.449799000	0.000000000
6	25.127550000	0.449799000	0.000000000
1	24.389009000	-1.497864000	0.000000000
1	26.156448000	0.148019000	0.000000000
1	24.929031000	1.503887000	0.000000000

PMI1

6	0.000000000	-0.017867000	0.639709000
7	0.000000000	0.081906000	-0.646190000
1	0.000000000	0.904785000	1.233451000
1	0.000000000	-0.971511000	1.191819000
1	0.000000000	-0.858565000	-1.063790000

PMI2

6	0.000000000	0.152520511	-1.721498927
7	0.000000000	-0.168299939	1.720003776
6	0.000000000	0.363370826	0.548847249
1	0.000000000	1.456824484	0.355118738
7	0.000000000	-0.480388867	-0.595049845
1	0.000000000	-0.425174851	-2.651286820
1	0.000000000	1.256247027	-1.794101992
1	0.000000000	0.582582912	2.422329093

PMI3

6	0.000000000	0.389757403	-1.698311961
6	0.000000000	0.272391198	2.839546733
7	0.000000000	-0.162599782	-2.861952306
7	0.000000000	-0.433336479	-0.547049153
6	0.000000000	0.217082475	0.567905597
1	0.000000000	0.577554289	-3.575673069
1	0.000000000	1.487060603	-1.531571753
1	0.000000000	1.330287112	0.618867614
7	0.000000000	-0.486737637	1.791409499
1	0.000000000	-0.197414771	3.827884612
1	0.000000000	1.376709090	2.785439831

PMI4

6	0.000000000	0.426522079	2.828877273
6	0.000000000	0.401495609	-3.955827391
7	0.000000000	-0.090944580	4.008864293
7	0.000000000	-0.428354381	1.702593082
6	0.000000000	0.192782077	0.568576596
1	0.000000000	0.670307646	4.699977089
1	0.000000000	1.518873188	2.630631466
1	0.000000000	1.304474703	0.496870690
7	0.000000000	-0.541806369	-0.628051431
6	0.000000000	0.188591648	-1.695669349
1	0.000000000	1.302188948	-1.665307445
7	0.000000000	-0.428381314	-2.961970800
1	0.000000000	0.000312044	-4.973810859
1	0.000000000	1.499275882	-3.825820957

PMI5

6	0.000000000	0.555626452	5.063591187
7	0.000000000	0.031933531	-5.149093133
6	0.000000000	0.499035456	-3.948130145
1	0.000000000	1.582296983	-3.704482590
7	0.000000000	-0.401350005	-2.858548275
6	0.000000000	0.172773763	-1.699558276
1	0.000000000	1.281111563	-1.583937017
7	0.000000000	-0.607535239	-0.534134152
6	0.000000000	0.083250882	0.562253919
1	0.000000000	1.196914816	0.564393209
7	0.000000000	-0.578909491	1.796595173
6	0.000000000	0.213023742	2.820510209
1	0.000000000	1.322794967	2.724714177
7	0.000000000	-0.330148175	4.118908227
1	0.000000000	0.213284862	6.102768690
1	0.000000000	1.644020352	4.870778871
1	0.000000000	0.821893463	-5.807138073

PMI6

6	0.000000000	0.611261359	5.054980697
6	0.000000000	0.741788272	-6.158483764
7	0.000000000	0.202168654	6.276992378
7	0.000000000	-0.339270108	4.009223456
6	0.000000000	0.179946954	2.824492516
1	0.000000000	1.022840058	6.896252585
1	0.000000000	1.681840184	4.760240674
1	0.000000000	1.281975659	2.658060619
7	0.000000000	-0.652176601	1.696261212
6	0.000000000	-0.011167783	0.569507089
1	0.000000000	1.101737229	0.519359644
7	0.000000000	-0.724738574	-0.633712494
6	0.000000000	0.025728975	-1.691298642
1	0.000000000	1.137721042	-1.631479123
7	0.000000000	-0.568175648	-2.958273147
6	0.000000000	0.278518965	-3.937906248
1	0.000000000	1.381361855	-3.781593003
7	0.000000000	-0.193862632	-5.263011833
1	0.000000000	0.455927661	-7.214552479
1	0.000000000	1.818116943	-5.907156244

6. Field dependent CCSD(T) energies for the γ-NLO set (all values in a.u.)

Electronic energies computed at CCSD(T)/aug-cc-pVDZ level of theory, with the required convergence criterion to achieve a change in the energy below 10^{-8} atomic units (a.u.)

C_4H_8

Field along Z	CCSD(T) energy
0	-1.56784341873796E+02
0.0001	-1.56784355597067E+02
0.0002	-1.56784369959756E+02
0.0004	-1.56784400618234E+02
0.0008	-1.56784469645816E+02
0.0016	-1.56784638569697E+02
0.0032	-1.56785099978884E+02
0.0064	-1.56786518247362E+02
0.0128	-1.56791352358949E+02
-0.0001	-1.56784328794511E+02
-0.0002	-1.56784316358021E+02
-0.0004	-1.56784293413733E+02
-0.0008	-1.56784255233796E+02
-0.0016	-1.56784209714635E+02
-0.0032	-1.56784242030692E+02
-0.0064	-1.56784800466316E+02
-0.0128	-1.56787903358608E+02

C_2H_2

Field along Z	CCSD(T) energy
0	-7.71213617644029E+01
0.0001	-7.71213619235575E+01
0.0002	-7.71213624010940E+01
0.0004	-7.71213643112302E+01
0.0008	-7.71213719518149E+01
0.0016	-7.71214025147154E+01
0.0032	-7.71215247761464E+01
0.0064	-7.71220141118256E+01
0.0128	-7.71239734680086E+01
0.0256	-7.71318518352783E+01
0.0512	-7.71640840108516E+01
0.1024	-7.75690005383098E+01
-0.0001	-7.71213619235575E+01
-0.0002	-7.71213624010940E+01
-0.0004	-7.71213643112302E+01
-0.0008	-7.71213719518149E+01
-0.0016	-7.71214025147154E+01
-0.0032	-7.71215247761464E+01
-0.0064	-7.71220141118256E+01
-0.0128	-7.71239734680086E+01
-0.0256	-7.71318518352783E+01
-0.0512	-7.71640840108516E+01
-0.1024	-7.75690005383098E+01

H_2O

Field along Z	CCSD(T) energy
0	-7.62739028815543E+01
0.0001	-7.62739029312691E+01
0.0002	-7.62739030804456E+01
0.0004	-7.62739036771275E+01
0.0008	-7.62739060638762E+01
0.0016	-7.62739156112341E+01
0.0032	-7.62739538070188E+01
0.0064	-7.62741066000862E+01
0.0128	-7.62747181582168E+01
0.0256	-7.62771706331507E+01
0.0512	-7.62870861598157E+01
0.1024	-7.63295090589653E+01
-0.0001	-7.62739029312691E+01
-0.0002	-7.62739030804456E+01
-0.0004	-7.62739036771275E+01
-0.0008	-7.62739060638762E+01
-0.0016	-7.62739156112341E+01
-0.0032	-7.62739538070188E+01
-0.0064	-7.62741066000862E+01
-0.0128	-7.62747181582168E+01
-0.0256	-7.62771706331507E+01
-0.0512	-7.62870861598157E+01
-0.1024	-7.63295090589653E+01

NH_3

Field along Z	CCSD(T) energy
0	-5.64254918018114E+01
0.0001	-5.64254918691292E+01
0.0002	-5.64254920711755E+01
0.0004	-5.64254928790975E+01
0.0008	-5.64254961103955E+01

0.0016	-5.64255090355912E+01
0.0032	-5.64255607396086E+01
0.0064	-5.64257676086109E+01
0.0128	-5.64265959418657E+01
0.0256	-5.64299233752804E+01
0.0512	-5.64435067386899E+01
0.1024	-5.66504165758845E+01
-0.0001	-5.64254918691292E+01
-0.0002	-5.64254920711755E+01
-0.0004	-5.64254928790975E+01
-0.0008	-5.64254961103955E+01
-0.0016	-5.64255090355912E+01
-0.0032	-5.64255607396086E+01
-0.0064	-5.64257676086109E+01
-0.0128	-5.64265959418657E+01
-0.0256	-5.64299233752804E+01
-0.0512	-5.64435067386899E+01
-0.1024	-5.66504165758845E+01

C_6H_6

Field along Z	CCSD(T) energy
0	-2.31617067523284E+02
0.0001	-2.31617067920663E+02
0.0002	-2.31617069150676E+02
0.0004	-2.31617074032006E+02
0.0008	-2.31617093562461E+02
0.0016	-2.31617171689334E+02
0.0032	-2.31617484234651E+02
0.0064	-2.31618735075780E+02
0.0128	-2.31623749249742E+02
0.0256	-2.31643989146892E+02
0.0512	-2.31789354859830E+02
0.1024	-2.33123354917622E+02
-0.0001	-2.31617067920663E+02
-0.0002	-2.31617069150676E+02
-0.0004	-2.31617074032006E+02
-0.0008	-2.31617093562461E+02
-0.0016	-2.31617171689334E+02
-0.0032	-2.31617484234651E+02
-0.0064	-2.31618735075780E+02
-0.0128	-2.31623749249742E+02
-0.0256	-2.31643989146892E+02
-0.0512	-2.31789354859830E+02
-0.1024	-2.33123354917622E+02

C_6H_{12}

Field along Z	CCSD(T) energy
0	-2.35230825386088E+02
0.0001	-2.35230825757310E+02
0.0002	-2.35230826872921E+02
0.0004	-2.35230831333494E+02
0.0008	-2.35230849177318E+02
0.0016	-2.35230920556061E+02
0.0032	-2.35231206116608E+02
0.0064	-2.35232349049317E+02
0.0128	-2.35236932372349E+02
-0.0001	-2.35230825757310E+02
-0.0002	-2.35230826872921E+02
-0.0004	-2.35230831333494E+02
-0.0008	-2.35230849177318E+02
-0.0016	-2.35230920556061E+02
-0.0032	-2.35231206116608E+02
-0.0064	-2.35232349049317E+02
-0.0128	-2.35236932372349E+02

C_4H_9CHO

Field along Z	CCSD(T) energy
0	-2.71081037737039E+02
0.0001	-2.71080991349766E+02
0.0002	-2.71080945737100E+02
0.0004	-2.71080856837189E+02
0.0008	-2.71080688337690E+02
0.0016	-2.71080388538372E+02
0.0032	-2.71079937780789E+02
0.0064	-2.71079632356552E+02
0.0128	-2.71081419014598E+02
-0.0001	-2.71081084899454E+02
-0.0002	-2.71081132836370E+02
-0.0004	-2.71081231036013E+02
-0.0008	-2.71081436734546E+02
-0.0016	-2.71081885337633E+02
-0.0032	-2.71082931423451E+02
-0.0064	-2.71085619985969E+02
-0.0128	-2.71093395916542E+02

$C_4H_9CO_2H$

Field along Z	CCSD(T) energy
0	-3.46190971974346E+02
0.0001	-3.46190988631664E+02

0.0002	-3.46191006142904E+02
0.0004	-3.46191043727776E+02
0.0008	-3.46191129151724E+02
0.0016	-3.46191341017045E+02
0.0032	-3.46191928916980E+02
0.0064	-3.46193762646361E+02
0.0128	-3.46200080632245E+02
-0.0001	-3.46190956171205E+02
-0.0002	-3.46190941223431E+02
-0.0004	-3.46190913889257E+02
-0.0008	-3.46190869471099E+02
-0.0016	-3.46190821634394E+02
-0.0032	-3.46190889980781E+02
-0.0064	-3.46191683370050E+02
-0.0128	-3.46195909469300E+02

$C_4H_9NH_2$

Field along Z	CCSD(T) energy
0	-2.13234051199701E+02
0.0001	-2.13234053274533E+02
0.0002	-2.13234056079114E+02
0.0004	-2.13234063876063E+02
0.0008	-2.13234088224320E+02
0.0016	-2.13234171942930E+02
0.0032	-2.13234479541100E+02
0.0064	-2.13235656344354E+02
0.0128	-2.13240270623997E+02
-0.0001	-2.13234049854170E+02
-0.0002	-2.13234049238208E+02
-0.0004	-2.13234050194004E+02
-0.0008	-2.13234060858155E+02
-0.0016	-2.13234117195065E+02
-0.0032	-2.13234369921354E+02
-0.0064	-2.13235436105864E+02
-0.0128	-2.13239821903765E+02

C_4H_9OH

Field along Z	CCSD(T) energy
0	-2.33077559773463E+02
0.0001	-2.33077556644335E+02
0.0002	-2.33077554192412E+02
0.0004	-2.33077551320302E+02
0.0008	-2.33077553704082E+02
0.0016	-2.33077590565557E+02
0.0032	-2.33077795317374E+02
0.0064	-2.33078726602161E+02
0.0128	-2.33082689924040E+02
0.0256	-2.33099253001542E+02
0.0512	-2.33425807023617E+02
0.1024	-2.35176123483830E+02
-0.0001	-2.33077563152371E+02
-0.0002	-2.33077567635864E+02
-0.0004	-2.33077578633994E+02
-0.0008	-2.33077608754700E+02
-0.0016	-2.33077701488462E+02
-0.0032	-2.33078016904452E+02
-0.0064	-2.33079167651069E+02
-0.0128	-2.33083554676302E+02
-0.0256	-2.33100834059620E+02
-0.0512	-2.33512497602314E+02
-0.1024	-2.34980116255639E+02

CH_4

Field along Z	CCSD(T) energy
0	-4.03957699730404E+01
0.0001	-4.03957700564441E+01
0.0002	-4.03957703066675E+01
0.0004	-4.03957713077219E+01
0.0008	-4.03957753126795E+01
0.0016	-4.03957913353452E+01
0.0032	-4.03958554278664E+01
0.0064	-4.03961118828247E+01
0.0128	-4.03971390726931E+01
0.0256	-4.04012703031965E+01
0.0512	-4.04181965451696E+01
0.1024	-4.05024137016487E+01
-0.0001	-4.03957700564441E+01
-0.0002	-4.03957703066675E+01
-0.0004	-4.03957713077219E+01
-0.0008	-4.03957753126795E+01
-0.0016	-4.03957913353452E+01
-0.0032	-4.03958554278664E+01
-0.0064	-4.03961118828247E+01
-0.0128	-4.03971390726931E+01
-0.0256	-4.04012703031965E+01
-0.0512	-4.04181965451696E+01
-0.1024	-4.05024137016487E+01

C_2H_6

Field along Z	CCSD(T) energy
0	-7.95978766851569E+01
0.0001	-7.95978768410752E+01
0.0002	-7.95978773075923E+01
0.0004	-7.95978791729791E+01
0.0008	-7.95978866329309E+01
0.0016	-7.95979164721665E+01
0.0032	-7.95980358412197E+01
0.0064	-7.95985135903591E+01
0.0128	-7.96004291835346E+01
0.0256	-7.96081716349198E+01
0.0512	-7.96412551076081E+01
0.1024	-8.00619828043353E+01
-0.0001	-7.95978768410752E+01
-0.0002	-7.95978773075923E+01
-0.0004	-7.95978791729791E+01
-0.0008	-7.95978866329309E+01
-0.0016	-7.95979164721665E+01
-0.0032	-7.95980358412197E+01
-0.0064	-7.95985135903591E+01
-0.0128	-7.96004291835346E+01
-0.0256	-7.96081716349198E+01
-0.0512	-7.96412551076081E+01
-0.1024	-8.00619828043353E+01

C_3H_8

Field along Z	CCSD(T) energy
0	-1.18803648922288E+02
0.0001	-1.18803649145326E+02
0.0002	-1.18803649817782E+02
0.0004	-1.18803652498820E+02
0.0008	-1.18803663228018E+02
0.0016	-1.18803706148896E+02
0.0032	-1.18803877860741E+02
0.0064	-1.18804565180795E+02
0.0128	-1.18807322258305E+02
0.0256	-1.18818495210731E+02
0.0512	-1.19009556945203E+02
0.1024	-1.19858310788221E+02
-0.0001	-1.18803649145326E+02
-0.0002	-1.18803649817782E+02
-0.0004	-1.18803652498820E+02
-0.0008	-1.18803663228018E+02
-0.0016	-1.18803706148896E+02
-0.0032	-1.18803877860741E+02
-0.0064	-1.18804565180795E+02
-0.0128	-1.18807322258305E+02
-0.0256	-1.18818495210731E+02
-0.0512	-1.19009556945203E+02
-0.1024	-1.19858310788221E+02

C_4H_{10}

Field along Z	CCSD(T) energy
0	-1.58009684928599E+02
0.0001	-1.58009685232837E+02
0.0002	-1.58009686142928E+02
0.0004	-1.58009689787372E+02
0.0008	-1.58009704363876E+02
0.0016	-1.58009762671957E+02
0.0032	-1.58009995946600E+02
0.0064	-1.58010929761073E+02
0.0128	-1.58014677095033E+02
0.0256	-1.58029903660809E+02
0.0512	-1.58258949203492E+02
0.1024	-1.59530294167756E+02
-0.0001	-1.58009685232837E+02
-0.0002	-1.58009686142928E+02
-0.0004	-1.58009689787372E+02
-0.0008	-1.58009704363876E+02
-0.0016	-1.58009762671957E+02
-0.0032	-1.58009995946600E+02
-0.0064	-1.58010929761073E+02
-0.0128	-1.58014677095033E+02
-0.0256	-1.58029903660809E+02
-0.0512	-1.58258949203492E+02
-0.1024	-1.59530294167756E+02

C_5H_{12}

Field along Z	CCSD(T) energy
0	-1.972157870274890E+02
0.0001	-1.972157874119960E+02
0.0002	-1.972157885591290E+02
0.0004	-1.972157931495170E+02
0.0008	-1.972158115146560E+02
0.0016	-1.972158849811240E+02
0.0032	-1.972161789059260E+02

0.0064	-1.972173555573320E+02
0.0128	-1.972220781525410E+02
0.0256	-1.972413199543720E+02
0.0512	-1.988928366152960E+02
0.1024	-1.995918154939200E+02
-0.0001	-1.972157874119960E+02
-0.0002	-1.972157885591290E+02
-0.0004	-1.972157931495170E+02
-0.0008	-1.972158115146560E+02
-0.0016	-1.972158849811240E+02
-0.0032	-1.972161789059260E+02
-0.0064	-1.972173555573320E+02
-0.0128	-1.972220781525410E+02
-0.0256	-1.972413199543720E+02
-0.0512	-1.988928366152960E+02
-0.1024	-1.995918154939200E+02

C_6H_{14}

Field along Z	CCSD(T) energy
0	-2.36421978906774E+02
0.0001	-2.36421979372471E+02
0.0002	-2.36421980767399E+02
0.0004	-2.36421986377265E+02
0.0008	-2.36422008807022E+02
0.0016	-2.36422098517516E+02
0.0032	-2.36422457438087E+02
0.0064	-2.36423894335083E+02
0.0128	-2.36429662447380E+02
0.0256	-2.36453296892652E+02
0.0512	-2.36952175716076E+02
0.1024	-2.39568853368632E+02
-0.0001	-2.36421979372471E+02
-0.0002	-2.36421980767399E+02
-0.0004	-2.36421986377265E+02
-0.0008	-2.36422008807022E+02
-0.0016	-2.36422098517516E+02
-0.0032	-2.36422457438087E+02
-0.0064	-2.36423894335083E+02
-0.0128	-2.36429662447380E+02
-0.0256	-2.36453296892652E+02
-0.0512	-2.36952175716076E+02
-0.1024	-2.39568853368632E+02

C_7H_{16}

Field along Z	CCSD(T) energy
0	-2.75628185703428E+02
0.0001	-2.75628186256219E+02
0.0002	-2.75628187910321E+02
0.0004	-2.75628194526489E+02
0.0008	-2.75628220988926E+02
0.0016	-2.75628326848416E+02
0.0032	-2.75628750369966E+02
0.0064	-2.75630445907599E+02
0.0128	-2.75637252758564E+02
0.0256	-2.82006321683693E+02
0.0512	-2.76442983602518E+02
0.1024	-2.79704094756947E+02
-0.0001	-2.75628186256219E+02
-0.0002	-2.75628187910321E+02
-0.0004	-2.75628194526489E+02
-0.0008	-2.75628220988926E+02
-0.0016	-2.75628326848416E+02
-0.0032	-2.75628750369966E+02
-0.0064	-2.75630445907599E+02
-0.0128	-2.75637252758564E+02
-0.0256	-2.82006321683693E+02
-0.0512	-2.76442983602518E+02
-0.1024	-2.79704094756947E+02

C_8H_{18}

Field along Z	CCSD(T) energy
0	-3.14834403041984E+02
0.0001	-3.14834403681752E+02
0.0002	-3.14834405595373E+02
0.0004	-3.14834413257066E+02
0.0008	-3.14834443901049E+02
0.0016	-3.14834566483148E+02
0.0032	-3.14835056916780E+02
0.0064	-3.14837020362766E+02
0.0128	-3.14844903456956E+02
0.0256	-3.15090068235795E+02
0.0512	-3.15903932340044E+02
0.1024	-3.20015214851159E+02
-0.0001	-3.14834403681752E+02
-0.0002	-3.14834405595373E+02
-0.0004	-3.14834413257066E+02

-0.0008	-3.14834443901049E+02
-0.0016	-3.14834566483148E+02
-0.0032	-3.14835056916780E+02
-0.0064	-3.14837020362766E+02
-0.0128	-3.14844903456956E+02
-0.0256	-3.15090068235795E+02
-0.0512	-3.15903932340044E+02
-0.1024	-3.20015214851159E+02

CO_2

Field along Z	CCSD(T) energy
0	-1.88186027767428E+02
0.0001	-1.88186027904713E+02
0.0002	-1.88186028322846E+02
0.0004	-1.88186029995179E+02
0.0008	-1.88186036650158E+02
0.0016	-1.88186063439308E+02
0.0032	-1.88186170462517E+02
0.0064	-1.88186598583213E+02
0.0128	-1.88188311680543E+02
0.0256	-1.88195174011239E+02
0.0512	-1.88222798980373E+02
0.1024	-1.88338288943040E+02
-0.0001	-1.88186027904713E+02
-0.0002	-1.88186028322846E+02
-0.0004	-1.88186029995179E+02
-0.0008	-1.88186036650158E+02
-0.0016	-1.88186063439308E+02
-0.0032	-1.88186170462517E+02
-0.0064	-1.88186598583213E+02
-0.0128	-1.88188311680543E+02
-0.0256	-1.88195174011239E+02
-0.0512	-1.88222798980373E+02
-0.1024	-1.88338288943040E+02

CO

Field along Z	CCSD(T) energy
0	-1.13074035500878E+02
0.0001	-1.13074032805288E+02
0.0002	-1.13074030270267E+02
0.0004	-1.13074025681935E+02
0.0008	-1.13074018430896E+02
0.0016	-1.13074011625710E+02
0.0032	-1.13074028751267E+02
0.0064	-1.13074185578204E+02
0.0128	-1.13074987129833E+02
0.0256	-1.13078531443472E+02
0.0512	-1.13093477865794E+02
0.1024	-1.13182708527980E+02
-0.0001	-1.13074038357177E+02
-0.0002	-1.13074041374055E+02
-0.0004	-1.13074047889911E+02
-0.0008	-1.13074062850915E+02
-0.0016	-1.13074100497094E+02
-0.0032	-1.13074206745206E+02
-0.0064	-1.13074543576655E+02
-0.0128	-1.13075719297471E+02
-0.0256	-1.13080127941412E+02
-0.0512	-1.13097822655310E+02
-0.1024	-1.13186501135704E+02

FCN

Field along Z	CCSD(T) energy
0	-1.92235731195694E+02
0.0001	-1.92235649563644E+02
0.0002	-1.92235568195726E+02
0.0004	-1.92235406250513E+02
0.0008	-1.92235085523498E+02
0.0016	-1.92234456709972E+02
0.0032	-1.92233249562419E+02
0.0064	-1.92231036540010E+02
0.0128	-1.92227411127022E+02
0.0256	-1.92223338164515E+02
0.0512	-1.92227940649841E+02
0.1024	-1.92592218893216E+02
-0.0001	-1.92235813091009E+02
-0.0002	-1.92235895250731E+02
-0.0004	-1.92236060361707E+02
-0.0008	-1.92236393752387E+02
-0.0016	-1.92237073219878E+02
-0.0032	-1.92238482997287E+02
-0.0064	-1.92241506739089E+02
-0.0128	-1.92248378238206E+02
-0.0256	-1.92265488587169E+02
-0.0512	-1.92314033216566E+02
-0.1024	-1.92488794591493E+02

H_2CO_3

Field along Z	CCSD(T) energy
0	-2.64453306579753E+02
0.0002	-2.64453307189507E+02
0.0004	-2.64453309022667E+02
0.0008	-2.64453316360549E+02
0.0016	-2.64453345716745E+02
0.0032	-2.64453463156069E+02
0.0064	-2.64453933126012E+02
0.0128	-2.64455816372158E+02
0.0256	-2.64463410180515E+02
0.0512	-2.64625108918666E+02
0.1024	-2.65121516154372E+02
-0.0002	-2.64453307189432E+02
-0.0004	-2.64453309022635E+02
-0.0008	-2.64453316360679E+02
-0.0016	-2.64453345717077E+02
-0.0032	-2.64453463156328E+02
-0.0064	-2.64453933126578E+02
-0.0128	-2.64455816373416E+02
-0.0256	-2.64463410182508E+02
-0.0512	-2.64625108803911E+02
-0.1024	-2.65121516149746E+02

H_2CO

Field along Z	CCSD(T) energy
0	-1.14245192890312E+02
0.0001	-1.14245098246566E+02
0.0002	-1.14245003829284E+02
0.0004	-1.14244815673900E+02
0.0008	-1.14244442081878E+02
0.0016	-1.14243705778757E+02
0.0032	-1.14242276137162E+02
0.0064	-1.14239593660381E+02
0.0128	-1.14234932598323E+02
0.0256	-1.14228490424385E+02
0.0512	-1.14228023341989E+02
0.1024	-1.14349054316662E+02
-0.0001	-1.14245287760374E+02
-0.0002	-1.14245382856875E+02
-0.0004	-1.14245573728649E+02
-0.0008	-1.14245958187002E+02
-0.0016	-1.14246737955470E+02
-0.0032	-1.14248340847378E+02
-0.0064	-1.14251719675554E+02
-0.0128	-1.14259167233765E+02
-0.0256	-1.14276814999193E+02
-0.0512	-1.14323252392266E+02
-0.1024	-1.14467010540948E+02

H_2O_2

Field along Z	CCSD(T) energy
0	-1.51243286241833E+02
0.0001	-1.51243286335383E+02
0.0002	-1.51243286615796E+02
0.0004	-1.51243287737449E+02
0.0008	-1.51243292224055E+02
0.0016	-1.51243310170793E+02
0.0032	-1.51243381962512E+02
0.0064	-1.51243669205006E+02
0.0128	-1.51244819413868E+02
0.0256	-1.51249440729772E+02
0.0512	-1.51268309078240E+02
0.1024	-1.52482720881697E+02
-0.0001	-1.51243286335373E+02
-0.0002	-1.51243286615785E+02
-0.0004	-1.51243287737441E+02
-0.0008	-1.51243292224049E+02
-0.0016	-1.51243310170806E+02
-0.0032	-1.51243381962509E+02
-0.0064	-1.51243669205016E+02
-0.0128	-1.51244819413867E+02
-0.0256	-1.51249440729763E+02
-0.0512	-1.51268309078260E+02
-0.1024	-1.52482720954808E+02

$B(OH)_3$

Field along Z	CCSD(T) energy
0	-2.51946686240623E+02
0.0002	-2.51946719584080E+02
0.0004	-2.51946754159247E+02
0.0008	-2.51946827004659E+02
0.0016	-2.51946987469416E+02
0.0032	-2.51947367452919E+02
0.0064	-2.51948363372355E+02
0.0128	-2.51951298181460E+02
0.0256	-2.51960954394789E+02
0.0512	-2.51996188525699E+02

0.1024	-2.52555771045761E+02
-0.0002	-2.51946654129733E+02
-0.0004	-2.51946623251200E+02
-0.0008	-2.51946565191983E+02
-0.0016	-2.51946463872496E+02
-0.0032	-2.51946320492352E+02
-0.0064	-2.51946271331530E+02
-0.0128	-2.51947129187787E+02
-0.0256	-2.51952738240036E+02
-0.0512	-2.51980702846292E+02
-0.1024	-2.52507931841824E+02

$(H_2)_1$

Field along Z	CCSD(T) energy
0	-1.13258838500230E+00
0.0001	-1.13258844040383E+00
0.0002	-1.13258860674703E+00
0.0004	-1.13258927262188E+00
0.0008	-1.13259193694745E+00
0.0016	-1.13260259813888E+00
0.0032	-1.13264524212822E+00
0.0064	-1.13281588673857E+00
0.0128	-1.13349956991679E+00
0.0256	-1.13625232377268E+00
0.0512	-1.14757556958525E+00
-0.0001	-1.13258844040383E+00
-0.0002	-1.13258860674703E+00
-0.0004	-1.13258927262188E+00
-0.0008	-1.13259193694745E+00
-0.0016	-1.13260259813888E+00
-0.0032	-1.13264524212822E+00
-0.0064	-1.13281588673857E+00
-0.0128	-1.13349956991679E+00
-0.0256	-1.13625232377268E+00
-0.0512	-1.14757556958525E+00

$(H_2)_2$

Field along Z	CCSD(T) energy
0	-2.26161249280880E+00
0.0001	-2.26161264197439E+00
0.0002	-2.26161308944469E+00
0.0004	-2.26161487933559E+00
0.0008	-2.26162203887341E+00
0.0016	-2.26165067910584E+00
0.0032	-2.26176517604759E+00
0.0064	-2.26222413491908E+00
0.0128	-2.26406982493089E+00
0.0256	-2.27162442872898E+00
0.0512	-2.31195878912303E+00
0.1024	-2.86550767163557E+00
-0.0001	-2.26161264197439E+00
-0.0002	-2.26161308944469E+00
-0.0004	-2.26161487933559E+00
-0.0008	-2.26162203887341E+00
-0.0016	-2.26165067910584E+00
-0.0032	-2.26176517604759E+00
-0.0064	-2.26222413491908E+00
-0.0128	-2.26406982493089E+00
-0.0256	-2.27162442872898E+00
-0.0512	-2.31195878912303E+00
-0.1024	-2.86550767163557E+00

$(H_2)_3$

Field along Z	CCSD(T) energy
0	-3.39090999302700E+00
0.0001	-3.39091025595882E+00
0.0002	-3.39091104488202E+00
0.0004	-3.39091420051319E+00
0.0008	-3.39092682273449E+00
0.0016	-3.39097731889090E+00
0.0032	-3.39117941278525E+00
0.0064	-3.39198955342858E+00
0.0128	-3.39525946177879E+00
0.0256	-3.40891134549976E+00
0.0512	-3.68679897037435E+00
0.1024	-4.97069005241339E+00
-0.0001	-3.39091025595882E+00
-0.0002	-3.39091104488202E+00
-0.0004	-3.39091420051319E+00
-0.0008	-3.39092682273449E+00
-0.0016	-3.39097731889090E+00
-0.0032	-3.39117941278525E+00
-0.0064	-3.39198955342858E+00
-0.0128	-3.39525946177879E+00
-0.0256	-3.40891134549976E+00
-0.0512	-3.68679897037435E+00
-0.1024	-4.97069005241339E+00

$(H_2)_4$

Field along Z	CCSD(T) energy
0	-4.52026322505225E+00
0.0001	-4.52026361165548E+00
0.0002	-4.52026477158816E+00
0.0004	-4.52026941158364E+00
0.0008	-4.52028797242650E+00
0.0016	-4.52036223009364E+00
0.0032	-4.52065948915261E+00
0.0064	-4.52185224478660E+00
0.0128	-4.52668617902223E+00
0.0256	-4.54758999798255E+00
0.0512	-5.08168860870813E+00
0.1024	-7.33548283076086E+00
-0.0001	-4.52026361165548E+00
-0.0002	-4.52026477158816E+00
-0.0004	-4.52026941158364E+00
-0.0008	-4.52028797242650E+00
-0.0016	-4.52036223009364E+00
-0.0032	-4.52065948915261E+00
-0.0064	-4.52185224478660E+00
-0.0128	-4.52668617902223E+00
-0.0256	-4.54758999798255E+00
-0.0512	-5.08168860870813E+00
-0.1024	-7.33548283076086E+00

$(H_2)_5$

Field along Z	CCSD(T) energy
0	-5.64960420847806E+00
0.0001	-5.64960472349960E+00
0.0002	-5.64960626917403E+00
0.0004	-5.64961245201521E+00
0.0008	-5.64963718491277E+00
0.0016	-5.64973614010691E+00
0.0032	-5.65013234733161E+00
0.0064	-5.65172347989115E+00
0.0128	-5.65819709026428E+00
0.0256	-5.83576794610809E+00
0.0512	-6.65246977742253E+00
0.1024	-9.90813998756452E+00
-0.0001	-5.64960472349960E+00
-0.0002	-5.64960626917403E+00
-0.0004	-5.64961245201521E+00
-0.0008	-5.64963718491277E+00
-0.0016	-5.64973614010691E+00
-0.0032	-5.65013234733161E+00
-0.0064	-5.65172347989115E+00
-0.0128	-5.65819709026428E+00
-0.0256	-5.83576794610809E+00
-0.0512	-6.65246977742253E+00
-0.1024	-9.90813998756452E+00

$(H_2)_6$

Field along Z	CCSD(T) energy
0	-6.77897008775868E+00
0.0001	-6.77897073425048E+00
0.0002	-6.77897267320997E+00
0.0004	-6.77898042978255E+00
0.0008	-6.77901145800321E+00
0.0016	-6.77913560667646E+00
0.0032	-6.77963277235822E+00
0.0064	-6.78163078293914E+00
0.0128	-6.78978806718628E+00
0.0256	-7.04376426033474E+00
0.0512	-8.30653538771142E+00
0.1024	
-0.0001	-6.77897073425048E+00
-0.0002	-6.77897267320997E+00
-0.0004	-6.77898042978255E+00
-0.0008	-6.77901145800321E+00
-0.0016	-6.77913560667646E+00
-0.0032	-6.77963277235822E+00
-0.0064	-6.78163078293914E+00
-0.0128	-6.78978806718628E+00
-0.0256	-7.04376426033474E+00
-0.0512	-8.30653538771142E+00

$(H_2)_7$

Field along Z	CCSD(T) energy
0	-7.90831231577732E+00
0.0001	-7.90831309449879E+00
0.0002	-7.90831543099234E+00
0.0004	-7.90832477743450E+00
0.0008	-7.90836216572066E+00
0.0016	-7.90851176677914E+00
0.0032	-7.90911094343528E+00
0.0064	-7.91152034058704E+00
0.0128	-7.92138709728912E+00
0.0256	-8.32104933767100E+00

0.0512	-1.00111717233688E+01
0.1024	-1.65031024122524E+01
-0.0001	-7.90831309449879E+00
-0.0002	-7.90831543099234E+00
-0.0004	-7.90832477743450E+00
-0.0008	-7.90836216572066E+00
-0.0016	-7.90851176677914E+00
-0.0032	-7.90911094343528E+00
-0.0064	-7.91152034058704E+00
-0.0128	-7.92138709728912E+00
-0.0256	-8.32104933767100E+00
-0.0512	-1.00111717233688E+01
-0.1024	-1.65031024122524E+01

$(H_2)_8$

Field along Z	CCSD(T) energy
0	-9.03768008790902E+00
0.0001	-9.03768100012687E+00
0.0002	-9.03768373640850E+00
0.0004	-9.03769468234782E+00
0.0008	-9.03773846976372E+00
0.0016	-9.03791368035137E+00
0.0032	-9.03861550768863E+00
0.0064	-9.04143904010104E+00
0.0128	-9.05303240546807E+00
0.0256	-9.56386193271060E+00
0.0512	-1.19342836249596E+01
-0.0001	-9.03768100012687E+00
-0.0002	-9.03768373640850E+00
-0.0004	-9.03769468234782E+00
-0.0008	-9.03773846976372E+00
-0.0016	-9.03791368035137E+00
-0.0032	-9.03861550768863E+00
-0.0064	-9.04143904010104E+00
-0.0128	-9.05303240546807E+00
-0.0256	-9.56386193271060E+00
-0.0512	-1.19342836249596E+01

HCN

Field along Z	CCSD(T) energy
0	-9.32046012734320E+01
0.0001	-9.32044834509469E+01
0.0002	-9.32043658621041E+01
0.0004	-9.32041313866818E+01
0.0008	-9.32036652428458E+01
0.0016	-9.32027441870988E+01
0.0032	-9.32009470282222E+01
0.0064	-9.31975327653004E+01
0.0128	-9.31914272935885E+01
0.0256	-9.31821468070988E+01
0.0512	-9.31761476805395E+01
0.1024	-9.40156467769195E+01
-0.0001	-9.32047193300768E+01
-0.0002	-9.32048376202936E+01
-0.0004	-9.32050749026470E+01
-0.0008	-9.32055522734843E+01
-0.0016	-9.32065182384665E+01
-0.0032	-9.32084950484340E+01
-0.0064	-9.32126281483121E+01
-0.0128	-9.32216127341787E+01
-0.0256	-9.32424272217233E+01
-0.0512	-9.32961661693630E+01
-0.1024	-9.34675105232167E+01

HF

Field along Z	CCSD(T) energy
0	-1.00263640590702E+02
0.0001	-1.00263711422793E+02
0.0002	-1.00263782317717E+02
0.0004	-1.00263924296028E+02
0.0008	-1.00264209006166E+02
0.0016	-1.00264781437881E+02
0.0032	-1.00265938326468E+02
0.0064	-1.00268300045749E+02
0.0128	-1.00273214081605E+02
0.0256	-1.00283796792899E+02
0.0512	-1.00307941848477E+02
0.1024	-1.00368280702142E+02
-0.0001	-1.00263569821461E+02
-0.0002	-1.00263499115082E+02
-0.0004	-1.00263357890948E+02
-0.0008	-1.00263076197535E+02
-0.0016	-1.00262515832825E+02
-0.0032	-1.00261407214035E+02
-0.0064	-1.00259238602494E+02
-0.0128	-1.00255097475173E+02
-0.0256	-1.00247613787865E+02
-0.0512	-1.00235986172880E+02

-0.1024	-1.00227930090158E+02

HNC

Field along Z	CCSD(T) energy
0	-9.31814388735475E+01
0.0001	-9.31815595814463E+01
0.0002	-9.31816805359870E+01
0.0004	-9.31819231850916E+01
0.0008	-9.31824114438533E+01
0.0016	-9.31833998085269E+01
0.0032	-9.31854239726216E+01
0.0064	-9.31896625220296E+01
0.0128	-9.31989062168303E+01
0.0256	-9.32205394164819E+01
0.0512	-9.32779048131514E+01
0.1024	-9.35089808955191E+01
-0.0001	-9.31813184122471E+01
-0.0002	-9.31811981975631E+01
-0.0004	-9.31809585079534E+01
-0.0008	-9.31804820872589E+01
-0.0016	-9.31795410768606E+01
-0.0032	-9.31777063617626E+01
-0.0064	-9.31742261728183E+01
-0.0128	-9.31680241410423E+01
-0.0256	-9.31587055959028E+01
-0.0512	-9.31588090675687E+01
-0.1024	-9.73678349213012E+01

HNO_2

Field along Z	CCSD(T) energy
0	-2.05283660966570E+02
0.0002	-2.05283546627731E+02
0.0004	-2.05283433544425E+02
0.0008	-2.05283211142960E+02
0.0016	-2.05282781408680E+02
0.0032	-2.05281982243994E+02
0.0064	-2.05280625487563E+02
0.0128	-2.05278883491311E+02
0.0256	-2.05279373326531E+02
0.0512	-2.05299700923638E+02
0.1024	-2.05646357397461E+02
-0.0002	-2.05283776560496E+02
-0.0004	-2.05283893409703E+02
-0.0008	-2.05284130872945E+02
-0.0016	-2.05284620859794E+02
-0.0032	-2.05285661063882E+02
-0.0064	-2.05287982472327E+02
-0.0128	-2.05293591376174E+02
-0.0256	-2.05308713320117E+02
-0.0512	-2.05355271254866E+02
-0.1024	-2.05587155615197E+02

HNO_3

Field along Z	CCSD(T) energy
0	-2.80312550112624E+02
0.0002	-2.80312387815305E+02
0.0004	-2.80312226733414E+02
0.0008	-2.80311908215106E+02
0.0016	-2.80311285761400E+02
0.0032	-2.80310099197346E+02
0.0064	-2.80307959620081E+02
0.0128	-2.80304617685993E+02
0.0256	-2.80301737103477E+02
0.0512	-2.80312737311108E+02
-0.0002	-2.80312713624787E+02
-0.0004	-2.80312878351975E+02
-0.0008	-2.80313211452398E+02
-0.0016	-2.80313892236093E+02
-0.0032	-2.80315312144141E+02
-0.0064	-2.80318385495034E+02
-0.0128	-2.80325468998369E+02
-0.0256	-2.80343425795092E+02
-0.0512	-2.80395237133837E+02

HNO

Field along Z	CCSD(T) energy
0	-1.30203832148296E+02
0.0002	-1.30203750542734E+02
0.0004	-1.30203669688099E+02
0.0008	-1.30203510233084E+02
0.0016	-1.30203200343017E+02
0.0032	-1.30202616680154E+02
0.0064	-1.30201594146922E+02
0.0128	-1.30200131395048E+02
0.0256	-1.30199569590583E+02

0.0512	-1.30208363179698E+02
0.1024	-1.30432245451494E+02
-0.0002	-1.30203914504971E+02
-0.0004	-1.30203997612471E+02
-0.0008	-1.30204166079345E+02
-0.0016	-1.30204512017329E+02
-0.0032	-1.30205239881310E+02
-0.0064	-1.30206839378206E+02
-0.0128	-1.30210612362661E+02
-0.0256	-1.30220454360015E+02
-0.0512	-1.30249466612332E+02
-0.1024	-1.30571563676166E+02

N_2O

Field along Z	CCSD(T) energy
0	-1.84269605955331E+02
0.0001	-1.84269606669523E+02
0.0002	-1.84269607727959E+02
0.0004	-1.84269610874538E+02
0.0008	-1.84269621292922E+02
0.0016	-1.84269658614491E+02
0.0032	-1.84269799096773E+02
0.0064	-1.84270342663791E+02
0.0128	-1.84272474822001E+02
0.0256	-1.84280885605360E+02
0.0512	-1.84314179125953E+02
0.1024	-1.84456566524710E+02
-0.0001	-1.84269605585135E+02
-0.0002	-1.84269605559693E+02
-0.0004	-1.84269606539599E+02
-0.0008	-1.84269612631168E+02
-0.0016	-1.84269641350548E+02
-0.0032	-1.84269765043345E+02
-0.0064	-1.84270278366268E+02
-0.0128	-1.84272376851634E+02
-0.0256	-1.84280939511308E+02
-0.0512	-1.84316467381900E+02
-0.1024	-1.84457831167706E+02

N_2

Field along Z	CCSD(T) energy
0	-1.09294603587159E+02
0.0001	-1.09294603662105E+02
0.0002	-1.09294603887210E+02
0.0004	-1.09294604788040E+02
0.0008	-1.09294608391622E+02
0.0016	-1.09294622804695E+02
0.0032	-1.09294680467759E+02
0.0064	-1.09294911155612E+02
0.0128	-1.09295834824686E+02
0.0256	-1.09299544704037E+02
0.0512	-1.09314667589791E+02
0.1024	-1.09390977961320E+02
-0.0001	-1.09294603662105E+02
-0.0002	-1.09294603887210E+02
-0.0004	-1.09294604788040E+02
-0.0008	-1.09294608391622E+02
-0.0016	-1.09294622804695E+02
-0.0032	-1.09294680467759E+02
-0.0064	-1.09294911155612E+02
-0.0128	-1.09295834824686E+02
-0.0256	-1.09299544704037E+02
-0.0512	-1.09314667589791E+02
-0.1024	-1.09390977961320E+02

O_2

Field along Z	CCSD(T) energy
0	-1.50020885530207E+02
0.0001	-1.50020885605138E+02
0.0002	-1.50020885833460E+02
0.0004	-1.50020886741171E+02
0.0008	-1.50020890381163E+02
0.0016	-1.50020904940354E+02
0.0032	-1.50020963184477E+02
0.0064	-1.50021196170170E+02
0.0128	-1.50022128392510E+02
0.0256	-1.50025862586139E+02
0.0512	-1.50040888640871E+02
0.1024	-1.50103026380412E+02
-0.0001	-1.50020885605138E+02
-0.0002	-1.50020885833460E+02
-0.0004	-1.50020886741171E+02
-0.0008	-1.50020890381163E+02
-0.0016	-1.50020904940354E+02
-0.0032	-1.50020963184477E+02
-0.0064	-1.50021196170170E+02
-0.0128	-1.50022128392510E+02
-0.0256	-1.50025862586139E+02
-0.0512	-1.50040888640871E+02

-0.1024	-1.50103026380412E+02

PA1

Field along Z	CCSD(T) energy
0.0000	-7.83688442603742E+01
0.0008	-7.83688552844304E+01
0.0016	-7.83688883571352E+01
0.0032	-7.83690206604508E+01
0.0064	-7.83695500737932E+01
0.0128	-7.83716709480397E+01
0.0256	-7.83802073999594E+01
-0.0008	-7.83688552844304E+01
-0.0016	-7.83688883571352E+01
-0.0032	-7.83690206604508E+01
-0.0064	-7.83695500737932E+01
-0.0128	-7.83716709480397E+01
-0.0256	-7.83802073999594E+01

PA2

Field along Z	CCSD(T) energy
0	-1.55563446381697E+02
0.0008	-1.55563471894747E+02
0.0016	-1.55563548440333E+02
0.0032	-1.55563854720015E+02
0.0064	-1.55565081406100E+02
0.0128	-1.55570013696015E+02
0.0256	-1.55590185334619E+02
-0.0008	-1.55563471894747E+02
-0.0016	-1.55563548440333E+02
-0.0032	-1.55563854720015E+02
-0.0064	-1.55565081406100E+02
-0.0128	-1.55570013696015E+02
-0.0256	-1.55590185334619E+02

PA3

Field along Z	CCSD(T) energy
0	-2.32759454680080E+02
0.0008	-2.32759501063892E+02
0.0016	-2.32759640226481E+02
0.0032	-2.32760197340939E+02
0.0064	-2.32762433311530E+02
0.0128	-2.32771502998842E+02
0.0256	-2.32810253549305E+02
-0.0008	-2.32759501063892E+02
-0.0016	-2.32759640226481E+02
-0.0032	-2.32760197340939E+02
-0.0064	-2.32762433311530E+02
-0.0128	-2.32771502998842E+02
-0.0256	-2.32810253549305E+02

PA4

Field along Z	CCSD(T) energy
0	-3.09955989007618E+02
0.0008	-3.09956062076287E+02
0.0016	-3.09956281392192E+02
0.0032	-3.09957160166865E+02
0.0064	-3.09960700105690E+02
0.0128	-3.09975296667372E+02
0.0256	-3.10043261228925E+02
-0.0008	-3.09956062076287E+02
-0.0016	-3.09956281392192E+02
-0.0032	-3.09957160166865E+02
-0.0064	-3.09960700105690E+02
-0.0128	-3.09975296667372E+02
-0.0256	-3.10043261228925E+02

PA5

Field along Z	CCSD(T) energy
0	-3.87152695268084E+02
0.0008	-3.87152800167412E+02
0.0016	-3.87153115127097E+02
0.0032	-3.87154378818410E+02
0.0064	-3.87159497841270E+02
0.0128	-3.87181200858548E+02
0.0256	-3.87429740376604E+02
-0.0008	-3.87152800167412E+02
-0.0016	-3.87153115127097E+02
-0.0032	-3.87154378818410E+02
-0.0064	-3.87159497841270E+02
-0.0128	-3.87181200858548E+02
-0.0256	-3.87429740376604E+02

PA6

Field along Z	CCSD(T) energy
0	-4.64349479752374E+02
0.0008	-4.64349620982260E+02
0.0016	-4.64350044924609E+02
0.0032	-4.64351748915321E+02
0.0064	-4.64358707476886E+02

0.0128	-4.64389603819957E+02
-0.0008	-4.64349620982260E+02
-0.0016	-4.64350044924609E+02
-0.0032	-4.64351748915321E+02
-0.0064	-4.64358707476886E+02
-0.0128	-4.64389603819957E+02

PDA1

Field along X	CCSD(T) energy
0	-2.31504885448926E+02
0.0001	-2.31504886098835E+02
0.0002	-2.31504888047518E+02
0.0004	-2.31504895845131E+02
0.0008	-2.31504927015546E+02
0.0016	-2.31505051740160E+02
0.0032	-2.31505550985152E+02
0.0064	-2.31507553542112E+02
0.0128	-2.31515656853987E+02
0.0256	-2.31549919177047E+02
-0.0001	-2.31504886098835E+02
-0.0002	-2.31504888047518E+02
-0.0004	-2.31504895845131E+02
-0.0008	-2.31504927015546E+02
-0.0016	-2.31505051740160E+02
-0.0032	-2.31505550985152E+02
-0.0064	-2.31507553542112E+02
-0.0128	-2.31515656853987E+02
-0.0256	-2.31549919177047E+02

PDA2

Field along X	CCSD(T) energy
0	-3.84644730227448E+02
0.0001	-3.84644731634220E+02
0.0002	-3.84644735860899E+02
0.0004	-3.84644752746189E+02
0.0008	-3.84644820326159E+02
0.0016	-3.84645090773445E+02
0.0032	-3.84646174933886E+02
0.0064	-3.84650550920023E+02
0.0128	-3.84668793148365E+02
0.0256	-3.84872675923382E+02
0.0512	-3.86180621941716E+02
-0.0001	-3.84644731634220E+02
-0.0002	-3.84644735860899E+02
-0.0004	-3.84644752746189E+02
-0.0008	-3.84644820326159E+02
-0.0016	-3.84645090773445E+02
-0.0032	-3.84646174933886E+02
-0.0064	-3.84650550920023E+02
-0.0128	-3.84668793148365E+02
-0.0256	-3.84872675923382E+02
-0.0512	-3.86180621941716E+02

PDA3

Field along X	CCSD(T) energy
0	-5.37784724528857E+02
0.0001	-5.37784726852202E+02
0.0002	-5.37784733824333E+02
0.0004	-5.37784761708501E+02
0.0008	-5.37784873280431E+02
0.0016	-5.37785320147635E+02
0.0032	-5.37787115308832E+02
0.0064	-5.37794436205454E+02
0.0128	-5.37827247272289E+02
0.0256	-5.38434335391203E+02
0.0512	-5.40816217114377E+02
-0.0001	-5.37784726852202E+02
-0.0002	-5.37784733824333E+02
-0.0004	-5.37784761708501E+02
-0.0008	-5.37784873280431E+02
-0.0016	-5.37785320147635E+02
-0.0032	-5.37787115308832E+02
-0.0064	-5.37794436205454E+02
-0.0128	-5.37827247272289E+02
-0.0256	-5.38434335391203E+02
-0.0512	-5.40816217114377E+02

PDA4 (warning. F=+-0.0128 was not converged).

Field along X	CCSD(T) energy
0	-6.91E+02
0.0001	-6.91E+02
0.0002	-6.91E+02
0.0004	-6.91E+02
0.0008	-6.91E+02
0.0016	-6.91E+02
0.0032	-6.91E+02
0.0064	-6.91E+02

0.0256	-6.92E+02
-0.0001	-6.91E+02
-0.0002	-6.91E+02
-0.0004	-6.91E+02
-0.0008	-6.91E+02
-0.0016	-6.91E+02
-0.0032	-6.91E+02
-0.0064	-6.91E+02
-0.0256	-6.92E+02

PDA5

Field along X	CCSD(T) energy
0	-8.44064740339387E+02
0.0001	-8.44064744695533E+02
0.0002	-8.44064757836571E+02
0.0004	-8.44064810344704E+02
0.0008	-8.44065020535084E+02
0.0016	-8.44065863380674E+02
0.0032	-8.44069267978299E+02
0.0064	-8.44083562661894E+02
0.0128	-8.44351631891559E+02
-0.0001	-8.44064744695533E+02
-0.0002	-8.44064757836571E+02
-0.0004	-8.44064810344704E+02
-0.0008	-8.44065020535084E+02
-0.0016	-8.44065863380674E+02
-0.0032	-8.44069267978299E+02
-0.0064	-8.44083562661894E+02
-0.0128	-8.44351631891559E+02

PMI1

Field along Z	CCSD(T) energy
0	-9.43846187126045E+01
0.0001	-9.43845619427640E+01
0.0002	-9.43845054619756E+01
0.0004	-9.43843933673909E+01
0.0008	-9.43841726470458E+01
0.0016	-9.43837450830631E+01
0.0032	-9.43829454816111E+01
0.0064	-9.43815686269292E+01
0.0128	-9.43797076496310E+01
0.0256	-9.43796091730600E+01
0.0512	-9.43958630227364E+01
0.1024	-9.47240749990062E+01
-0.0001	-9.43846757730000E+01
-0.0002	-9.43847331210000E+01
-0.0004	-9.43848486830000E+01
-0.0008	-9.43850832770000E+01
-0.0016	-9.43855663370000E+01
-0.0032	-9.43865879440000E+01
-0.0064	-9.43888531960000E+01
-0.0128	-9.43942738270000E+01
-0.0256	-9.44087134870000E+01
-0.0512	-9.44528083080000E+01
-0.1024	-9.47508833530000E+01

PMI2

Field along Z	CCSD(T) energy
0	-1.87586232454433E+02
0.0001	-1.87586163450825E+02
0.0002	-1.87586095090199E+02
0.0004	-1.87585960297965E+02
0.0008	-1.87585698428734E+02
0.0016	-1.87585205548090E+02
0.0032	-1.87584343204456E+02
0.0064	-1.87583112388489E+02
0.0128	-1.87582632925686E+02
0.0256	-1.87589753802061E+02
0.0512	-1.87783405874361E+02
0.1024	-1.88760736382845E+02
-0.0001	-1.87586302101212E+02
-0.0002	-1.87586372391024E+02
-0.0004	-1.87586514900062E+02
-0.0008	-1.87586807636493E+02
-0.0016	-1.87587423991041E+02
-0.0032	-1.87588780312302E+02
-0.0064	-1.87591988351602E+02
-0.0128	-1.87600397962352E+02
-0.0256	-1.87625356993092E+02
-0.0512	-1.87818311382595E+02
-0.1024	-1.88962845240812E+02

PMI3

Field along Z	CCSD(T) energy
0	-2.80830737544802E+02
0.0001	-2.80830635655837E+02
0.0002	-2.80830534909884E+02
0.0004	-2.80830336848975E+02
0.0008	-2.80829954447122E+02
0.0016	-2.80829244513666E+02
0.0032	-2.80828044130651E+02
0.0064	-2.80826522691206E+02
0.0128	-2.80827032712879E+02
0.0256	-2.80843116832729E+02
0.0512	-2.81214678885062E+02
-0.0001	-2.80830840578085E+02
-0.0002	-2.80830944754984E+02
-0.0004	-2.80831156540533E+02
-0.0008	-2.80831593841916E+02
-0.0016	-2.80829244510000E+02
-0.0032	-2.80834602636342E+02
-0.0064	-2.80839645480397E+02
-0.0128	-2.80867704632777E+02
-0.0256	-2.80895763785156E+02
-0.0512	-2.81328790435726E+02

PMI4 (warning. F=+-0.0256 was not converged).

Field along Z	CCSD(T) energy
0.0000	-3.74047785070649E+02
0.0001	-3.74047934722371E+02
0.0002	-3.74048086245135E+02
0.0004	-3.74048394696908E+02
0.0008	-3.74049032443666E+02
0.0016	-3.74050392410263E+02
0.0032	-3.74053451240503E+02
0.0064	-3.74060936617678E+02
0.0128	-3.74081537864506E+02
0.0512	-3.74845261717853E+02
0.1024	-3.77736784381592E+02
-0.0001	-3.74047636969528E+02
-0.0002	-3.74047490707080E+02
-0.0004	-3.74047203449123E+02
-0.0008	-3.74046649993850E+02
-0.0016	-3.74045627291071E+02
-0.0032	-3.74043918689669E+02
-0.0064	-3.74041853218781E+02
-0.0128	-3.74043249251091E+02
-0.0512	-3.74986238917788E+02
-0.1024	-3.77938824171198E+02

PMI5 (warning. F=+-0.0256 was not converged).

Field along Z	CCSD(T) energy
0	-4.6726510199E+02
0.0001	-4.6726490104E+02
0.0002	-4.6726470238E+02
0.0004	-4.6726431271E+02
0.0008	-4.6726356273E+02
0.0016	-4.6726218083E+02
0.0032	-4.6725988922E+02
0.0064	-4.6725720580E+02
0.0128	-4.6725976895E+02
0.0512	-4.6845208165E+02
0.1024	-4.7292486399E+02
-0.0001	-4.6726530550E+02
-0.0002	-4.6726551147E+02
-0.0004	-4.6726593080E+02
-0.0008	-4.6726679908E+02
-0.0016	-4.6726865440E+02
-0.0032	-4.6727284230E+02
-0.0064	-4.6728315752E+02
-0.0128	-4.6731194663E+02
-0.0512	-4.6858171031E+02
-0.1024	-4.7262708616E+02

PMI6

Field along Z	CCSD(T) energy
0	-5.6048257816E+02
0.0001	-5.6048284029E+02
0.0002	-5.6048310567E+02
0.0004	-5.6048364618E+02
0.0008	-5.6048476627E+02
0.0016	-5.6048716319E+02
0.0032	-5.6049258966E+02
0.0064	-5.6050603275E+02
0.0128	-5.6054414528E+02

0.0256	-5.6087818557E+02
0.0512	-5.6227576377E+02
0.1024	-5.6815023876E+02
-0.0001	-5.6048231931E+02
-0.0002	-5.6048206367E+02
-0.0004	-5.6048156211E+02
-0.0008	-5.6048059790E+02
-0.0016	-5.6047882483E+02
-0.0032	-5.6047589989E+02
-0.0064	-5.6047255740E+02
-0.0128	-5.6047669781E+02
-0.0256	-5.6069743071E+02
-0.0512	-5.6230063611E+02
-0.1024	-5.6867708479E+02