Supplemental material: The orbital-specific virtual local triples correction: OSV-L(T)

Martin Schütz*
Institut für Physikalische und Theoretische Chemie
Universität Regensburg
Regensburg, D-93040, Germany

Jun Yang† and Garnet Kin-Lic Chan‡
Department of Chemistry
Princeton University
Princeton, New Jersey 08544, USA

Frederick R. Manby§
Center for Computational Chemistry
School of Chemistry
University of Bristol
Bristol BS8 1TS, United Kingdom

Hans-Joachim Werner¶
Institut für Theoretische Chemie
Universität Stuttgart
Stuttgart D-70569, Germany
(Dated: January 9, 2013)

In the following the geometries of the individual glycine peptide chains (section III.A) and of the guanine-cytosine dimers (section III.C) are given. Additional timings, Hartree-Fock reference, and correlation energies are also provided.

XYZ inputs (in Angstrom) for glycine peptide chains. The structures are not fully optimized.

Gly1:

```
   10
 DF-HF/VTZ Energy=-282.94971136
 H           0.0000000000       -0.1061597829       -2.3510046258
 O           0.0000000000       -0.6780750342       -1.5910464079
 C           0.0000000000        0.0823670137       -0.5009090248
 O           0.0000000000        1.2677910334       -0.5437527942
 C           0.0000000000       -0.7442212482        0.7651366511
 H          -0.8704158024       -1.4023240162        0.7258639905
 H           0.8704158024       -1.4023240162        0.7258639905
 N           0.0000000000        0.0135391781        1.9877130330
 H           0.7992326054        0.6243970256        2.0075525810
 H          -0.7992326054        0.6243970256        2.0075525810
```

Average domain sizes (AVD) and correlation energies (in Hartree).

METHOD	OSVSEL	AVD	EC_LCCSD	EC_LCCSD(T0)	EC_LCCSD(T1)	EC_LCCSD(T)
OSV	1.00D-04	49.1	-1.016167	-1.054480	-1.055387	-1.055562
OSV	3.20D-05	62.6	-1.021133	-1.060449	-1.061435	-1.061627
OSV	1.00D-05	77.0	-1.023387	-1.063164	-1.064192	-1.064392
Canonical			-1.024627			-1.066265

Gly2:

```
   17
 DF-HF/VTZ Energy=-489.84108308
 H           0.0000000000       -0.0901752637       -4.1503406681
 O           0.0000000000       -0.6376184604       -3.3723044072
 C           0.0000000000        0.1490669303       -2.3091193487
 O           0.0000000000        1.3340923892       -2.3746868713
 C           0.0000000000       -0.6451506810       -1.0323136341
 H          -0.8736447751       -1.2989498850       -1.0356348259
 H           0.8736447751       -1.2989498850       -1.0356348259
 N           0.0000000000        0.2479698325        0.0910178353
 H           0.0000000000        1.2273975368       -0.1036238496
 C           0.0000000000       -0.2165188180        1.3610447202
 O           0.0000000000       -1.3899441029        1.6130326803
 C           0.0000000000        0.8541039574        2.4453598994
 H           0.8735158156        1.4933414143        2.2922353148
 H          -0.8735158156        1.4933414143        2.2922353148
 N           0.0000000000        0.3493895269        3.7934111672
 H          -0.7962843174       -0.2528035542        3.9201918563
 H           0.7962843174       -0.2528035542        3.9201918563
```

Average domain sizes (AVD) and correlation energies (in Hartree).

METHOD	OSVSEL	AVD	EC_LCCSD	EC_LCCSD(T0)	EC_LCCSD(T1)	EC_LCCSD(T)
OSV	1.00D-04	51.4	-1.769389	-1.838765	-1.840330	-1.840638
OSV	3.20D-05	65.7	-1.779308	-1.850717	-1.852434	-1.852772
OSV	1.00D-05	81.9	-1.784246	-1.856696	-1.858504	-1.858859
Canonical			-1.786898			-1.863319

Gly3:

```
   24
 DF-HF/VTZ Energy=-696.73406643
 H           0.0000000000        0.2557044471       -5.9356629691
 O           0.0000000000       -0.3753968005       -5.2238022438
 C           0.0000000000        0.2873226768       -4.0792327759
 O           0.0000000000        1.4722393313       -4.0117275157
 C           0.0000000000       -0.6448377834       -2.8993635784
 H          -0.8736447751       -1.2941554868       -2.9758550776
 H           0.8736447751       -1.2941554868       -2.9758550776
 N           0.0000000000        0.1169145385       -1.6831106270
 H           0.0000000000        1.1119753300       -1.7668843387
 C           0.0000000000       -0.4868307236       -0.4730653166
 O           0.0000000000       -1.6810894227       -0.3540233448
 C           0.0000000000        0.4556758788        0.7242875301
 H           0.8769989824        1.1046987468        0.6630938683
 H          -0.8769989824        1.1046987468        0.6630938683
 N           0.0000000000       -0.3142378624        1.9353906111
 H           0.0000000000       -1.3087128233        1.8449275488
 C           0.0000000000        0.2813568504        3.1494684228
 O           0.0000000000        1.4747880552        3.2765384458
 C           0.0000000000       -0.6691799916        4.3404563518
 H          -0.8735158156       -1.3209844465        4.2554703692
 H           0.8735158156       -1.3209844465        4.2554703692
 N           0.0000000000       -0.0253699122        5.6278908001
 H           0.7962843174        0.5868229375        5.6905786360
 H          -0.7962843174        0.5868229375        5.6905786360

 Average domain sizes (AVD) and correlation energies (in Hartree).

 METHOD     OSVSEL   AVD      EC_LCCSD     EC_LCCSD(T0)   EC_LCCSD(T1)  EC_LCCSD(T)
 OSV      1.00D-04   52.3    -2.522960      -2.623497      -2.625708     -2.626151
 OSV      3.20D-05   67.3    -2.537997      -2.641643      -2.644081     -2.644567
 OSV      1.00D-05   83.6    -2.545215      -2.650396      -2.652968     -2.653477
 Canonical                   -2.549422                                   -2.660735
```

Gly4:

```
   31
 DF-HF/VTZ Energy=-903.62725584
 H           0.0000000000        0.1232859298       -7.7484537562
 O           0.0000000000       -0.4843918564       -7.0164959808
 C           0.0000000000        0.2151064181       -5.8940261431
 O           0.0000000000        1.4015892456       -5.8649927437
 C           0.0000000000       -0.6782908855       -4.6845404240
 H          -0.8736447751       -1.3297481169       -4.7399290966
 H           0.8736447751       -1.3297481169       -4.7399290966
 N           0.0000000000        0.1225133869       -3.4936372544
 H           0.0000000000        1.1143330746       -3.6096446702
 C           0.0000000000       -0.4416626943       -2.2646444375
 O           0.0000000000       -1.6314314295       -2.1069257382
 C           0.0000000000        0.5391876547       -1.0984947354
 H           0.8769989824        1.1858839735       -1.1807092030
 H          -0.8769989824        1.1858839735       -1.1807092030
 N           0.0000000000       -0.1910351473        0.1369454701
 H           0.0000000000       -1.1879212067        0.0787888009
 C           0.0000000000        0.4436283993        1.3310644664
 O           0.0000000000        1.6405534585        1.4193550876
```

C	0.0000000000	-0.4677749460	2.5522591590
H	-0.8769989824	-1.1181568470	2.5077762379
H	0.8769989824	-1.1181568470	2.5077762379
N	0.0000000000	0.3330293264	3.7431623286
H	0.0000000000	1.3248490141	3.6271549128
C	0.0000000000	-0.2311467549	4.9721551455
O	0.0000000000	-1.4209154900	5.1298738448
C	0.0000000000	0.7497035942	6.1383048477
H	0.8735158156	1.3991069546	6.0365849367
H	-0.8735158156	1.3991069546	6.0365849367
N	0.0000000000	0.1392145576	7.4418699642
H	-0.7962843174	-0.4711637249	7.5202804368
H	0.7962843174	-0.4711637249	7.5202804368

Average domain sizes (AVD) and correlation energies (in Hartree).

METHOD	OSVSEL	AVD	EC_LCCSD	EC_LCCSD(T0)	EC_LCCSD(T1)	EC_LCCSD(T)
OSV	1.00D-04	52.8	-3.276588	-3.408304	-3.411160	-3.411737
OSV	3.20D-05	68.0	-3.296611	-3.432487	-3.435643	-3.436276
OSV	1.00D-05	84.6	-3.306242	-3.444172	-3.447507	-3.448170
Canonical			-3.312013			-3.458241

Elapsed times in seconds [OSV-LCCSD(T); 7 cores on Intel(R) Xeon(R) CPU X5690@3.47GHz]

Note: local fitting was not enabled, and therefore several parts of the program
scale cubically. For more timings and details see
J. Chem. Phys. 136, 144105 (2012); doi: 10.1063/1.3696963

OSVSEL=1.0d-4:

	Gly1	Gly2	Gly3	Gly4
DF-2ext transformation	1.56	11.20	37.24	84.17
DF-3ext transformations	12.32	48.22	110.23	263.51
DF-4ext transformations	6.86	32.03	87.19	181.26
LMP2 (7 iterations)	0.43	1.81	4.29	8.42
LCCSD (13 iterations)	36.15	181.88	450.48	748.24
LT(0)	11.39	33.78	79.56	128.14
L(T) (7 iterations)	446.86	1168.74	1942.84	2783.11

OSVSEL=3.2d-5:

	Gly1	Gly2	Gly3	Gly4
DF-2ext transformation	2.21	17.02	56.37	125.84
DF-3ext transformations	21.15	91.08	233.01	808.10
DF-4ext transformations	14.26	70.59	172.10	359.81
LMP2 (7 iterations)	0.87	3.35	8.46	16.69
LCCSD (13 iterations)	71.72	336.13	798.61	1561.60
LT(0)	27.89	99.60	225.74	363.75
L(T) (7 iterations)	1078.67	2966.86	5308.34	7257.70

OSVSEL=1.0d-5:

DF-2ext transformation	2.92	24.17	82.06	179.13
DF-3ext transformations	30.52	170.14	689.27	1485.66
DF-4ext transformations	31.19	136.98	377.12	739.65
LMP2 (7 iterations)	1.38	6.09	15.17	31.30

```
LCCSD (13 iterations)      131.40    662.90   3234.08   7787.13
LT(0)                       65.69    281.19    581.37    941.34
L(T) (7 iterations)       2487.34   7423.34  12476.69  17508.74


guanine-cytosine Watson-Crick dimer
-----------------------------------
XYZ input (in Angstrom, taken from Ref. 66)
29
G-C Watson-Crick
 C1    -1.0398599    -0.0950435     2.9628987
 N1    -0.8760506    -0.1198953     4.3522101
 C1     0.3372729    -0.0573522     4.9526643
 C1     1.4603152     0.0294729     4.2021231
 C1     1.2876371     0.0522766     2.7771415
 N1     0.0866353    -0.0006919     2.2061593
 O1    -2.1779850    -0.1592983     2.4996990
 N1     2.3517978     0.1313296     1.9777210
 H1    -1.7254816    -0.1869061     4.8897274
 H1     0.3482118    -0.0833071     6.0321432
 H1     2.4345221     0.0778275     4.6597911
 H1     3.2714721     0.1534551     2.3764404
 H1     2.2350290     0.1077513     0.9551229
 O2     2.0171439     0.0263963    -0.7905108
 C2     0.9445057     0.0313388    -1.4013109
 N2    -0.2671137     0.0963439    -0.7051367
 C2    -1.5207327     0.1136461    -1.2552546
 N2    -1.7528129     0.0544172    -2.5494108
 C2    -0.6040129    -0.0113445    -3.2574879
 C2     0.7161247    -0.0244271    -2.8113172
 N2     1.6041685    -0.0981114    -3.8601422
 C2     0.8295480    -0.1292217    -4.9265187
 N2    -0.5075993    -0.0802063    -4.6198760
 N2    -2.5513427     0.2447649    -0.3850923
 H2    -0.1820496     0.1041077     0.3219703
 H2     1.1760819    -0.1871623    -5.9443460
 H2    -1.2844954    -0.0872596    -5.2590531
 H2    -3.4573855     0.0691895    -0.7801319
 H2    -2.4169221     0.0545062     0.6045745

Basis: AVTZ,H=VTZ, OSVSEL=3.2d-5:
DF-HF Reference energy:            -932.390543885613
LCCSD|LRPA total energy            -935.891703351165
LCCSD(T0)|LRPA total energy        -936.064136580488

guanine-cytosine stacked dimer:
-------------------------------
XYZ input (in Angstrom, taken from Ref. 66)
29
G-C stacked
 O1    -1.2390176    -2.5490521     0.6548924
 C1    -1.0284571    -1.3714583     0.9008651
 N1    -0.0318511    -0.9949528     1.8248233
 C1     0.3841646     0.2706806     2.1182164
 N1    -0.1910285     1.3513281     1.6527710
 C1    -1.2092305     1.0513624     0.8089237
 C1    -1.6565083    -0.1915101     0.3706051
 N1    -2.6541580    -0.0639048    -0.5661534
```

```
 C1    -2.8177333     1.2431899    -0.6803818
 N1    -1.9753657     1.9574414     0.1290579
 N1     1.4525454     0.3558875     2.9872621
 H1     0.4866119    -1.7695272     2.2174674
 H1    -3.5338415     1.7253425    -1.3240899
 H1    -1.9138820     2.9580997     0.2181746
 H1     1.7298659     1.3225221     3.0797421
 H1     2.2376547    -0.1901480     2.6476325
 C2     2.2123373    -0.0590839    -0.4645529
 N2     2.1205577     1.1822577    -1.1169007
 C2     1.2003987     1.4553092    -2.0711004
 C2     0.3300220     0.4917324    -2.4615962
 C2     0.4626198    -0.7818118    -1.8195186
 N2     1.3658705    -1.0412675    -0.8919664
 O2     3.0203933    -0.1851683     0.4516286
 N2    -0.3645719    -1.7922584    -2.1870353
 H2     2.7522574     1.8928231    -0.7832658
 H2     1.2077958     2.4531651    -2.4849122
 H2    -0.4090987     0.6756472    -3.2236499
 H2    -1.2619684    -1.5144746    -2.5505972
 H2    -0.4171470    -2.5417743    -1.5096178

Basis: AVTZ,H=VTZ, OSVSEL=3.2d-5:
DF-HF Reference energy:            -932.360995678131
LCCSD|LRPA total energy            -935.873396673906
LCCSD(T0)|LRPA total energy        -936.047406432852
```