Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Effects of London Dispersion Correction in Density Functional Theory on the Structures of Organic Molecules in the Gas Phase [†]

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Cartesian coordinates (in Bohr, B3LYP-D3/QZVP optimized)

1

2.23667541170500	-0.67283503250531	2.38568253922519	c
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-0.48012069646097	0.30917220842204	-2.39577441887601	c
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3.65336800636983	0.13835609685104	-0.00000247800079	c
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-1.48975622300485	-0.35008848481785	4.06555981754143	h
-0.48073227764683	2.37263715331778	2.47267448384796	h
-1.99248067933607	-2.59225689996747	-0.00000954734425	h
-1.48975628032267	-0.35005117125012	-4.06556831579173	h
-0.48071136805865	2.37265288635679	-2.47265501683762	h
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-3.37828801149758	-2.45514491321885	-1.02287596022842	c
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3.78994224845693	-3.68556703260052	1.33343411046377	h
6.17280798866797	-1.86737863628852	-0.13719529733109	h
4.86868305246601	-0.89924718066069	2.78493488760499	h
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-5.06518001489220	-2.37461080830829	-2.20062436925793	h
-1.95970634286911	-3.56506740153556	-2.02199126023895	h
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3

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0.48788150518592	4.22320819051619	2.98719656860429	n
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1.55464995470395	4.13416804827663	-1.98405649822160	h
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0.53772597311340	5.08344156542256	4.69274596546400	h
-0.09340990085838	2.42446878489274	3.28170621648915	h

4

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-1.63124790216423	-2.08143536615466	-0.83796002133030	c
-1.33726541567622	-4.43816359893985	0.78976370678445	c
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-3.58329095128877	-1.44518152272503	-0.71189182232791	h
-1.30246217017328	-2.54988615657418	-2.84246709656944	h
-1.76878758432381	-4.00348072406042	2.75489425917973	h
-2.61944658262279	-5.91734777642599	0.14532865054929	h
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5

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-1.81446878891090	-0.40807341370678	-1.65367933398115	o
-3.24830486762866	-1.97805724849264	-0.16325726188248	c
-4.14178688274172	-2.35032952667043	4.39469057834902	o
-4.50377584984800	-3.68312556601839	-0.98119475204270	o
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2.64920916770516	-0.82143055883507	-4.63614586965221	o
-0.48482768707666	2.12649711861197	4.48971673844929	o
-5.12960865294101	-3.72141526622181	3.70425692915641	h
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3.28468940900946	-1.22306539337173	0.49768918450208	o
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6

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4.18095655653149	-3.64450336980226	-0.17180707458534	c
-7.94943232687465	2.85932253413066	-2.25496553847782	h
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7

1.90219350738625	0.46935577298065	-0.21549312786882	c
0.01411604521985	-1.18146158988767	0.63785286592999	c
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4.63070441591528	-3.15002128025948	-0.89729874489995	c
4.20794523579647	-0.57017535562216	-0.98584493661925	c
1.51893263836457	3.24554953447912	-0.26691720221544	c
-2.27848491956402	-0.31974227626569	1.53079690051046	o
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3.53981783733124	4.49321305068223	-1.23077156975762	o
-3.97029964063373	0.66936547421167	-0.18110945246392	c
3.11088180700024	6.26720510957193	-1.18521887756988	h
-3.69598781339924	0.49330456365879	-2.41578467122196	o
-6.10640680107258	1.92441277285982	1.18039357993873	c
-1.06996114072974	-4.96866121262034	1.40167137738583	h
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-6.76448643390937	0.76105933089058	2.74226870383192	h
-7.63225535934796	2.30701864869044	-0.13386275195093	h
-5.39919710824368	3.69431920651840	1.96014035778375	h

8

-0.00001095420643	2.41481241505571	-0.45939834899309	c
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-2.32993070143681	-1.25489425302257	-1.65137986571612	c
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2.32992311359333	-1.25486289927325	-1.65140607152503	c
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-0.00001628597443	-1.45894005910310	2.35663627311871	c
-0.00002429815492	4.46592452162169	-0.53802516201334	h
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1.66144752676063	2.19945428118544	3.31762984522282	h
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9

1.63251988428858	-1.48163225438175	-0.88545662903816	o
-0.19919692211995	0.33334882879082	0.02616350323115	c
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3.83258566707193	2.10464659100899	0.29743442124667	c
4.16500223779708	-0.57804455348259	-0.55933205998089	c
-2.17952516090773	0.80746251310652	-2.13041654773403	c
5.66632437564117	-0.90680710432944	-2.98972192807093	c
-0.86536377512846	1.97170946148085	-4.43927916560056	c
-4.25855730643417	2.62450430499735	-1.23529096556692	c
-3.39034943881196	-1.69830015870271	-2.95638102367303	c
-1.43709716221995	-0.68992997342248	2.46127250826185	c
0.41497642929310	-1.62211713028167	4.46815781501658	c
-0.94083845285099	-2.55849491333281	6.83706083786618	c
0.62113591137646	4.39144362307642	1.22945898338534	h
5.40081900253571	3.36871033253171	0.62235726125853	h
5.07811260878145	-1.69519045319314	0.93372527524219	h
4.88153327646677	0.25246526585197	-4.49666548565664	h
7.63118569223145	-0.35895386333074	-2.69253679032811	h
5.62718423418492	-2.87756529488321	-3.58166379247351	h
-0.01773154077982	3.79482753306639	-4.00076411257370	h
0.61208395518427	0.72993997722622	-5.14428649627586	h
-2.23645363716566	2.25561017749351	-5.95038967474291	h
-3.48263979824429	4.41990764552974	-0.58749428567721	h
-5.53643255084777	3.03496231777277	-2.79856403602587	h
-5.38424799888054	1.82319470605940	0.28801149404660	h

-1.94986190970079	-3.05882914424238	-3.50343343843965	h
-4.54286939644145	-2.53569401480093	-1.47244645666780	h
-4.62053987666476	-1.36970209789259	-4.57677232106005	h
-2.70090679707975	-2.24000563484840	1.97012636046867	h
-2.61496803889068	0.79627078333323	3.27330778204226	h
1.55151088925955	-3.14543437225674	3.67400978195634	h
1.72184691988486	-0.10997972139231	4.97475869260535	h
-2.22671114475496	-4.10899749037939	6.39464359067923	h
0.39630861737606	-3.23811129419355	8.24923102155808	h
-2.05652213026735	-1.05495261019709	7.70255844256369	h

Rotational constants (in MHz) for all methods and molecules

If not mentioned otherwise, results refer to the QZVP AO basis set

		B_e(reference)	B_e(calc.)	deviation	relative deviation in %
HF-D3					
	A	4293.9	4309.9	-16.0	-0.37
1	B	1395.9	1403.7	-7.8	-0.56
	C	1130.2	1134.9	-4.7	-0.42
	A	3322.5	3333.4	-10.9	-0.33
2	B	719.8	725.6	-5.8	-0.81
	C	698.0	704.4	-6.4	-0.91
	A	3071.1	3094.0	-22.9	-0.75
3	B	1285.0	1293.8	-8.8	-0.69
	C	1248.7	1245.6	3.1	0.25
	A	2755.9	2760.3	-4.4	-0.16
4	B	2675.6	2698.8	-23.2	-0.87
	C	2653.3	2677.2	-23.9	-0.90
5	A	2336.9	2342.4	-5.5	-0.23
	A	1464.2	1504.8	-40.6	-2.77
6	B	768.2	763.7	4.5	0.58
	C	580.6	580.7	-0.1	-0.01
	A	1165.7	1179.6	-13.9	-1.19
7	B	661.2	662.8	-1.6	-0.24
	C	454.0	456.8	-2.8	-0.63
	A	1166.3	1171.0	-4.7	-0.40
8	B	767.6	776.5	-8.9	-1.16
	C	513.0	515.7	-2.7	-0.52
	A	862.5	869.5	-7.0	-0.82
9	B	754.2	754.7	-0.5	-0.07
	C	513.7	515.5	-1.8	-0.34
HF-D3/def2-TZVP					
	A	4293.9	4304.6	-10.7	-0.25
1	B	1395.9	1401.7	-5.8	-0.42
	C	1130.2	1133.5	-3.3	-0.29
	A	3322.5	3325.1	-2.6	-0.08
2	B	719.8	727.7	-7.9	-1.10
	C	698.0	706.0	-8.0	-1.15
	A	3071.1	3087.0	-15.9	-0.52
3	B	1285.0	1293.9	-8.9	-0.69

	C	1248.7	1243.3	5.4	0.43
	A	2755.9	2755.3	0.6	0.02
4	B	2675.6	2694.0	-18.4	-0.69
	C	2653.3	2673.2	-19.9	-0.75
5	A	2336.9	2338.1	-1.2	-0.05
	A	1464.2	1498.9	-34.7	-2.37
6	B	768.2	767.4	0.8	0.10
	C	580.6	582.7	-2.1	-0.37
	A	1165.7	1176.3	-10.6	-0.91
7	B	661.2	664.1	-2.9	-0.44
	C	454.0	456.8	-2.8	-0.62
	A	1166.3	1170.1	-3.8	-0.33
8	B	767.6	774.5	-6.9	-0.90
	C	513.0	514.1	-1.1	-0.22
	A	862.5	868.3	-5.8	-0.67
9	B	754.2	754.5	-0.3	-0.04
	C	513.7	515.3	-1.6	-0.31

HF-D3/SV(P)

	A	4293.9	4274.5	19.4	0.45
1	B	1395.9	1389.3	6.6	0.47
	C	1130.2	1123.7	6.5	0.58
	A	3322.5	3299.2	23.3	0.70
2	B	719.8	730.9	-11.1	-1.55
	C	698.0	707.9	-9.9	-1.41
	A	3071.1	3071.4	-0.3	-0.01
3	B	1285.0	1282.4	2.6	0.21
	C	1248.7	1240.6	8.1	0.65
	A	2755.9	2734.5	21.4	0.78
4	B	2675.6	2675.1	0.5	0.02
	C	2653.3	2651.3	2.0	0.07
5	A	2336.9	2328.9	8.0	0.34
	A	1464.2	1497.4	-33.2	-2.26
6	B	768.2	775.1	-6.9	-0.90
	C	580.6	587.5	-6.9	-1.18
	A	1165.7	1164.5	1.2	0.10
7	B	661.2	664.1	-2.9	-0.44
	C	454.0	454.1	-0.1	-0.02
	A	1166.3	1171.2	-4.9	-0.42
8	B	767.6	769.7	-2.1	-0.27
	C	513.0	512.3	0.7	0.14
	A	862.5	866.4	-3.9	-0.45

9	B	754.2	750.5	3.7	0.49
	C	513.7	514.2	-0.5	-0.10

HF

	A	4293.9	4284.2	9.7	0.23
1	B	1395.9	1393.7	2.2	0.16
	C	1130.2	1125.8	4.4	0.39
	A	3322.5	3323.5	-1.0	-0.03
2	B	719.8	707.0	12.8	1.77
	C	698.0	682.7	15.3	2.19
	A	3071.1	3077.7	-6.6	-0.22
3	B	1285.0	1280.8	4.2	0.33
	C	1248.7	1227.4	21.3	1.70
	A	2755.9	2746.0	9.9	0.36
4	B	2675.6	2685.3	-9.7	-0.36
	C	2653.3	2669.8	-16.5	-0.62
5	A	2336.9	2319.2	17.7	0.76
	A	1464.2	1505.5	-41.3	-2.82
6	B	768.2	747.8	20.4	2.66
	C	580.6	570.1	10.5	1.80
	A	1165.7	1177.4	-11.7	-1.00
7	B	661.2	644.5	16.7	2.52
	C	454.0	447.8	6.2	1.38
	A	1166.3	1147.0	19.3	1.65
8	B	767.6	768.7	-1.1	-0.14
	C	513.0	506.6	6.4	1.26
	A	862.5	856.7	5.8	0.68
9	B	754.2	745.1	9.1	1.20
	C	513.7	507.7	6.0	1.17

MP2

	A	4293.9	4303.0	-9.1	-0.21
1	B	1395.9	1399.7	-3.8	-0.27
	C	1130.2	1134.4	-4.2	-0.37
	A	3322.5	3319.1	3.4	0.10
2	B	719.8	727.1	-7.3	-1.02
	C	698.0	705.7	-7.7	-1.11
	A	3071.1	3078.6	-7.5	-0.24
3	B	1285.0	1292.6	-7.6	-0.59
	C	1248.7	1253.0	-4.3	-0.34
	A	2755.9	2769.0	-13.1	-0.48

4	B	2675.6	2684.6	-9.0	-0.33
	C	2653.3	2658.5	-5.2	-0.20
5	A	2336.9	2345.9	-9.0	-0.38
	A	1464.2	1459.2	5.0	0.34
6	B	768.2	775.7	-7.5	-0.97
	C	580.6	585.5	-4.9	-0.84
	A	1165.7	1175.7	-10.0	-0.86
7	B	661.2	661.0	0.2	0.03
	C	454.0	456.9	-2.9	-0.64
	A	1166.3	1175.6	-9.3	-0.80
8	B	767.6	768.0	-0.4	-0.05
	C	513.0	515.9	-2.9	-0.56
	A	862.5	864.9	-2.4	-0.27
9	B	754.2	758.5	-4.3	-0.57
	C	513.7	516.0	-2.3	-0.45

MP2/TZVPP

	A	4293.9	4292.8	1.1	0.02
1	B	1395.9	1395.7	0.2	0.01
	C	1130.2	1131.1	-0.9	-0.08
	A	3322.5	3310.7	11.8	0.36
2	B	719.8	728.6	-8.8	-1.22
	C	698.0	707.6	-9.6	-1.38
	A	3071.1	3071.7	-0.6	-0.02
3	B	1285.0	1290.9	-5.9	-0.46
	C	1248.7	1249.9	-1.2	-0.10
	A	2755.9	2762.5	-6.6	-0.24
4	B	2675.6	2677.8	-2.2	-0.08
	C	2653.3	2651.7	1.6	0.06
5	A	2336.9	2340.5	-3.6	-0.15
	A	1464.2	1453.7	10.5	0.72
6	B	768.2	775.2	-7.0	-0.91
	C	580.6	585.1	-4.5	-0.78
	A	1165.7	1170.8	-5.1	-0.44
7	B	661.2	660.6	0.6	0.10
	C	454.0	455.6	-1.6	-0.34
	A	1166.3	1163.1	3.2	0.27
8	B	767.6	766.7	0.9	0.12
	C	513.0	512.6	0.4	0.07
	A	862.5	862.9	-0.4	-0.04
9	B	754.2	757.6	-3.4	-0.45
	C	513.7	515.2	-1.5	-0.30

SCS-MP2

	A	4293.9	4278.8	15.1	0.35
1	B	1395.9	1390.9	5.0	0.36
	C	1130.2	1126.7	3.5	0.31
	A	3322.5	3308.8	13.7	0.41
2	B	719.8	717.2	2.6	0.36
	C	698.0	695.6	2.4	0.34
	A	3071.1	3060.8	10.3	0.34
3	B	1285.0	1281.5	3.5	0.27
	C	1248.7	1240.1	8.6	0.69
	A	2755.9	2750.4	5.5	0.20
4	B	2675.6	2669.7	5.9	0.22
	C	2653.3	2647.5	5.8	0.22
5	A	2336.9	2327.0	9.9	0.42
	A	1464.2	1458.1	6.1	0.42
6	B	768.2	763.8	4.4	0.57
	C	580.6	577.7	2.9	0.50
	A	1165.7	1169.4	-3.7	-0.32
7	B	661.2	654.2	7.0	1.06
	C	454.0	452.6	1.4	0.32
	A	1166.3	1156.6	9.7	0.83
8	B	767.6	764.8	2.8	0.36
	C	513.0	509.9	3.1	0.61
	A	862.5	858.0	4.5	0.52
9	B	754.2	751.9	2.3	0.30
	C	513.7	511.4	2.3	0.44

B2PLYP-D3

	A	4293.9	4288.7	5.2	0.12
1	B	1395.9	1396.1	-0.2	-0.02
	C	1130.2	1129.5	0.7	0.07
	A	3322.5	3293.5	29.0	0.87
2	B	719.8	716.8	3.0	0.41
	C	698.0	694.7	3.3	0.47
	A	3071.1	3063.3	7.8	0.25
3	B	1285.0	1285.3	-0.3	-0.03
	C	1248.7	1244.4	4.3	0.35
	A	2755.9	2755.7	0.2	0.01
4	B	2675.6	2677.9	-2.3	-0.08
	C	2653.3	2658.0	-4.7	-0.18

5	A	2336.9	2330.9	6.0	0.26
	A	1464.2	1460.5	3.7	0.25
6	B	768.2	765.6	2.6	0.33
	C	580.6	578.7	1.9	0.32
	A	1165.7	1166.1	-0.4	-0.04
7	B	661.2	659.1	2.1	0.32
	C	454.0	453.4	0.6	0.12
	A	1166.3	1164.4	1.9	0.16
8	B	767.6	763.5	4.1	0.53
	C	513.0	510.9	2.1	0.40
	A	862.5	862.4	0.1	0.01
9	B	754.2	750.5	3.7	0.49
	C	513.7	511.8	1.9	0.37

B2PLYP

	A	4293.9	4284.4	9.5	0.22
1	B	1395.9	1393.3	2.6	0.19
	C	1130.2	1127.0	3.2	0.28
	A	3322.5	3306.6	15.9	0.48
2	B	719.8	708.4	11.4	1.58
	C	698.0	684.2	13.8	1.97
	A	3071.1	3061.4	9.7	0.32
3	B	1285.0	1280.9	4.1	0.32
	C	1248.7	1239.7	9.0	0.72
	A	2755.9	2753.1	2.8	0.10
4	B	2675.6	2675.1	0.5	0.02
	C	2653.3	2656.9	-3.6	-0.14
5	A	2336.9	2324.6	12.3	0.53
	A	1464.2	1462.8	1.4	0.09
6	B	768.2	759.5	8.7	1.13
	C	580.6	574.8	5.8	1.00
	A	1165.7	1165.5	0.2	0.02
7	B	661.2	653.9	7.3	1.11
	C	454.0	450.6	3.4	0.75
	A	1166.3	1156.5	9.8	0.84
8	B	767.6	761.4	6.2	0.80
	C	513.0	508.1	4.9	0.95
	A	862.5	857.4	5.1	0.59
9	B	754.2	748.6	5.6	0.75
	C	513.7	509.4	4.3	0.83

PW6B95-D3

	A	4293.9	4322.7	-28.8	-0.67
1	B	1395.9	1404.6	-8.7	-0.63
	C	1130.2	1136.7	-6.5	-0.57
	A	3322.5	3321.2	1.3	0.04
2	B	719.8	721.9	-2.1	-0.29
	C	698.0	699.7	-1.7	-0.24
	A	3071.1	3079.2	-8.1	-0.26
3	B	1285.0	1286.8	-1.8	-0.14
	C	1248.7	1260.8	-12.1	-0.97
	A	2755.9	2774.7	-18.8	-0.68
4	B	2675.6	2701.0	-25.4	-0.95
	C	2653.3	2677.8	-24.5	-0.92
5	A	2336.9	2345.2	-8.3	-0.35
	A	1464.2	1477.6	-13.4	-0.91
6	B	768.2	770.4	-2.2	-0.29
	C	580.6	583.7	-3.1	-0.54
	A	1165.7	1174.6	-8.9	-0.77
7	B	661.2	663.9	-2.7	-0.41
	C	454.0	457.1	-3.1	-0.69
	A	1166.3	1187.9	-21.6	-1.85
8	B	767.6	768.5	-0.9	-0.11
	C	513.0	518.5	-5.5	-1.06
	A	862.5	864.2	-1.7	-0.20
9	B	754.2	761.2	-7.0	-0.93
	C	513.7	517.0	-3.3	-0.64

PW6B95

	A	4293.9	4321.7	-27.8	-0.65
1	B	1395.9	1403.2	-7.3	-0.52
	C	1130.2	1135.5	-5.3	-0.47
	A	3322.5	3339.1	-16.6	-0.50
2	B	719.8	714.3	5.5	0.77
	C	698.0	690.2	7.8	1.12
	A	3071.1	3079.3	-8.2	-0.27
3	B	1285.0	1284.0	1.0	0.07
	C	1248.7	1258.6	-9.9	-0.80
	A	2755.9	2774.2	-18.3	-0.66
4	B	2675.6	2700.2	-24.6	-0.92
	C	2653.3	2677.6	-24.3	-0.92
5	A	2336.9	2342.0	-5.1	-0.22
	A	1464.2	1479.8	-15.6	-1.07

6	B	768.2	766.6	1.6	0.20
	C	580.6	581.3	-0.7	-0.13
	A	1165.7	1174.4	-8.7	-0.74
7	B	661.2	660.7	0.5	0.08
	C	454.0	455.2	-1.2	-0.27
	A	1166.3	1184.3	-18.0	-1.55
8	B	767.6	767.4	0.2	0.03
	C	513.0	517.0	-4.0	-0.79
	A	862.5	861.4	1.1	0.12
9	B	754.2	760.2	-6.0	-0.79
	C	513.7	515.6	-1.9	-0.37

M06

	A	4293.9	4313.8	-19.9	-0.46
1	B	1395.9	1406.0	-10.1	-0.73
	C	1130.2	1138.4	-8.2	-0.72
	A	3322.5	3333.8	-11.3	-0.34
2	B	719.8	726.8	-7.0	-0.97
	C	698.0	704.6	-6.6	-0.95
	A	3071.1	3105.0	-33.9	-1.10
3	B	1285.0	1307.4	-22.4	-1.74
	C	1248.7	1242.7	6.0	0.48
	A	2755.9	2771.1	-15.2	-0.55
4	B	2675.6	2697.4	-21.8	-0.82
	C	2653.3	2671.9	-18.6	-0.70
5	A	2336.9	2345.0	-8.1	-0.35
	A	1464.2	1473.7	-9.5	-0.65
6	B	768.2	771.9	-3.7	-0.48
	C	580.6	583.2	-2.6	-0.45
	A	1165.7	1179.7	-14.0	-1.20
7	B	661.2	657.0	4.2	0.63
	C	454.0	455.9	-1.9	-0.43
	A	1166.3	1158.6	7.7	0.66
8	B	767.6	769.1	-1.5	-0.20
	C	513.0	510.5	2.5	0.49
	A	862.5	871.6	-9.1	-1.06
9	B	754.2	751.2	3.0	0.40
	C	513.7	514.1	-0.4	-0.08

M06-2X

	A	4293.9	4284.2	9.7	0.23

1	B	1395.9	1397.0	-1.1	-0.08
	C	1130.2	1130.3	-0.1	-0.01
	A	3322.5	3220.5	102.0	3.07
2	B	719.8	746.4	-26.6	-3.70
	C	698.0	721.9	-23.9	-3.43
	A	3071.1	3094.7	-23.6	-0.77
3	B	1285.0	1294.9	-9.9	-0.77
	C	1248.7	1240.2	8.5	0.68
	A	2755.9	2750.8	5.1	0.19
4	B	2675.6	2677.3	-1.7	-0.06
	C	2653.3	2656.7	-3.4	-0.13
5	A	2336.9	2330.5	6.4	0.27
	A	1464.2	1463.1	1.1	0.08
6	B	768.2	781.1	-12.9	-1.68
	C	580.6	589.5	-8.9	-1.53
	A	1165.7	1167.8	-2.1	-0.18
7	B	661.2	666.6	-5.4	-0.81
	C	454.0	458.8	-4.8	-1.06
	A	1166.3	1171.8	-5.5	-0.47
8	B	767.6	766.6	1.0	0.13
	C	513.0	512.3	0.7	0.14
	A	862.5	858.6	3.9	0.45
9	B	754.2	756.1	-1.9	-0.26
	C	513.7	514.6	-0.9	-0.17

B3LYP-NL

	A	4293.9	4265.1	28.8	0.67
1	B	1395.9	1391.1	4.8	0.35
	C	1130.2	1124.6	5.6	0.50
	A	3322.5	3275.6	46.9	1.41
2	B	719.8	713.6	6.2	0.86
	C	698.0	691.1	6.9	0.99
	A	3071.1	3052.1	19.0	0.62
3	B	1285.0	1279.2	5.8	0.45
	C	1248.7	1239.0	9.7	0.78
	A	2755.9	2741.2	14.7	0.53
4	B	2675.6	2666.5	9.1	0.34
	C	2653.3	2647.9	5.4	0.20
5	A	2336.9	2319.8	17.1	0.73
	A	1464.2	1457.1	7.1	0.49
6	B	768.2	765.1	3.1	0.41
	C	580.6	578.2	2.4	0.42

	A	1165.7	1160.6	5.1	0.44
7	B	661.2	658.5	2.7	0.41
	C	454.0	452.0	2.0	0.44
	A	1166.3	1166.4	-0.1	-0.01
8	B	767.6	761.2	6.4	0.83
	C	513.0	510.1	2.9	0.56
	A	862.5	858.8	3.7	0.42
9	B	754.2	745.7	8.5	1.12
	C	513.7	509.1	4.6	0.90

B3LYP-D3

	A	4293.9	4261.3	32.6	0.76
1	B	1395.9	1390.3	5.6	0.40
	C	1130.2	1123.5	6.7	0.60
	A	3322.5	3271.1	51.4	1.55
2	B	719.8	710.1	9.7	1.34
	C	698.0	687.7	10.3	1.47
	A	3071.1	3043.8	27.3	0.89
3	B	1285.0	1277.1	7.9	0.62
	C	1248.7	1235.3	13.4	1.08
	A	2755.9	2738.2	17.7	0.64
4	B	2675.6	2664.7	10.9	0.41
	C	2653.3	2648.0	5.3	0.20
5	A	2336.9	2315.4	21.5	0.92
	A	1464.2	1455.5	8.7	0.59
6	B	768.2	759.2	9.0	1.17
	C	580.6	574.4	6.2	1.07
	A	1165.7	1158.5	7.2	0.62
7	B	661.2	656.7	4.5	0.68
	C	454.0	451.1	2.9	0.65
	A	1166.3	1156.1	10.2	0.87
8	B	767.6	759.0	8.6	1.12
	C	513.0	507.5	5.5	1.08
	A	862.5	859.9	2.6	0.30
9	B	754.2	742.9	11.3	1.50
	C	513.7	507.9	5.8	1.13

B3LYP

	A	4293.9	4249.5	44.4	1.03
1	B	1395.9	1383.7	12.2	0.87
	C	1130.2	1117.7	12.5	1.10

	A	3322.5	3288.8	33.7	1.01
2	B	719.8	696.0	23.8	3.31
	C	698.0	669.6	28.4	4.06
	A	3071.1	3037.5	33.6	1.09
3	B	1285.0	1267.7	17.3	1.34
	C	1248.7	1224.4	24.3	1.95
	A	2755.9	2731.6	24.3	0.88
4	B	2675.6	2657.9	17.7	0.66
	C	2653.3	2645.2	8.1	0.31
5	A	2336.9	2300.9	36.0	1.54
	A	1464.2	1459.6	4.6	0.32
6	B	768.2	746.3	21.9	2.86
	C	580.6	566.1	14.5	2.49
	A	1165.7	1158.2	7.5	0.65
7	B	661.2	644.3	16.9	2.55
	C	454.0	444.8	9.2	2.02
	A	1166.3	1138.2	28.1	2.41
8	B	767.6	754.1	13.5	1.75
	C	513.0	501.0	12.0	2.34
	A	862.5	849.1	13.4	1.56
9	B	754.2	738.2	16.0	2.12
	C	513.7	502.6	11.1	2.16

B3LYP/6-31G*

	A	4293.9	4219.7	74.2	1.73
1	B	1395.9	1372.9	23.0	1.65
	C	1130.2	1109.6	20.6	1.82
	A	3322.5	3235.4	87.1	2.62
2	B	719.8	701.6	18.2	2.54
	C	698.0	677.3	20.7	2.96
	A	3071.1	3019.5	51.6	1.68
3	B	1285.0	1260.2	24.8	1.93
	C	1248.7	1219.0	29.7	2.38
	A	2755.9	2712.6	43.3	1.57
4	B	2675.6	2640.1	35.5	1.33
	C	2653.3	2622.3	31.0	1.17
5	A	2336.9	2290.1	46.8	2.00
	A	1464.2	1448.2	16.0	1.09
6	B	768.2	758.6	9.6	1.25
	C	580.6	574.1	6.5	1.12
	A	1165.7	1140.1	25.6	2.20
7	B	661.2	653.9	7.3	1.10

	C	454.0	444.1	9.9	2.18
	A	1166.3	1140.4	25.9	2.22
8	B	767.6	750.4	17.2	2.24
	C	513.0	500.4	12.6	2.47
	A	862.5	848.3	14.2	1.65
9	B	754.2	734.4	19.8	2.62
	C	513.7	502.0	11.7	2.28

TPSS-D3

	A	4293.9	4239.8	54.1	1.26
1	B	1395.9	1383.0	12.9	0.92
	C	1130.2	1118.3	11.9	1.05
	A	3322.5	3220.2	102.3	3.08
2	B	719.8	709.8	10.0	1.38
	C	698.0	687.2	10.8	1.55
	A	3071.1	3020.5	50.6	1.65
3	B	1285.0	1267.7	17.3	1.34
	C	1248.7	1232.8	15.9	1.28
	A	2755.9	2729.1	26.8	0.97
4	B	2675.6	2653.1	22.5	0.84
	C	2653.3	2632.8	20.5	0.77
5	A	2336.9	2307.1	29.8	1.27
	A	1464.2	1435.2	29.0	1.98
6	B	768.2	764.6	3.6	0.47
	C	580.6	577.3	3.3	0.58
	A	1165.7	1157.2	8.5	0.73
7	B	661.2	652.3	8.9	1.35
	C	454.0	449.9	4.1	0.91
	A	1166.3	1158.7	7.6	0.65
8	B	767.6	753.3	14.3	1.86
	C	513.0	507.0	6.0	1.18
	A	862.5	854.2	8.3	0.96
9	B	754.2	741.8	12.4	1.65
	C	513.7	506.3	7.4	1.43

TPSS-D3(0)

	A	4293.9	4232.5	61.4	1.43
1	B	1395.9	1380.3	15.6	1.12
	C	1130.2	1116.0	14.2	1.25
	A	3322.5	3217.3	105.2	3.17
2	B	719.8	709.1	10.7	1.48

	C	698.0	686.7	11.3	1.61
	A	3071.1	3019.8	51.3	1.67
3	B	1285.0	1267.3	17.7	1.38
	C	1248.7	1227.8	20.9	1.68
	A	2755.9	2724.6	31.3	1.14
4	B	2675.6	2649.0	26.6	0.99
	C	2653.3	2630.4	22.9	0.86
5	A	2336.9	2300.1	36.8	1.57
	A	1464.2	1434.6	29.6	2.02
6	B	768.2	761.9	6.3	0.82
	C	580.6	575.7	4.9	0.84
	A	1165.7	1155.6	10.1	0.86
7	B	661.2	650.5	10.7	1.61
	C	454.0	448.8	5.2	1.15
	A	1166.3	1154.0	12.3	1.05
8	B	767.6	751.8	15.8	2.06
	C	513.0	505.6	7.4	1.45
	A	862.5	854.2	8.3	0.96
9	B	754.2	741.8	12.4	1.65
	C	513.7	506.3	7.4	1.43

TPSS

	A	4293.9	4231.6	62.3	1.45
1	B	1395.9	1378.2	17.7	1.27
	C	1130.2	1114.1	16.1	1.43
	A	3322.5	3259.6	62.9	1.89
2	B	719.8	695.0	24.8	3.44
	C	698.0	668.4	29.6	4.24
	A	3071.1	3017.3	53.8	1.75
3	B	1285.0	1260.3	24.7	1.92
	C	1248.7	1224.0	24.7	1.98
	A	2755.9	2724.7	31.2	1.13
4	B	2675.6	2648.3	27.3	1.02
	C	2653.3	2631.0	22.3	0.84
5	A	2336.9	2295.9	41.0	1.76
	A	1464.2	1439.5	24.7	1.69
6	B	768.2	752.9	15.3	1.99
	C	580.6	569.7	10.9	1.88
	A	1165.7	1156.3	9.4	0.81
7	B	661.2	641.7	19.5	2.94
	C	454.0	444.3	9.7	2.15
	A	1166.3	1144.9	21.4	1.83

8	B	767.6	749.5	18.1	2.35
	C	513.0	502.1	10.9	2.12
	A	862.5	845.4	17.1	1.99
9	B	754.2	738.2	16.0	2.12
	C	513.7	502.1	11.6	2.26

PBE-D3

	A	4293.9	4242.8	51.1	1.19
1	B	1395.9	1382.7	13.2	0.95
	C	1130.2	1118.1	12.1	1.07
	A	3322.5	3245.0	77.5	2.33
2	B	719.8	705.1	14.7	2.04
	C	698.0	682.0	16.0	2.29
	A	3071.1	3022.7	48.4	1.58
3	B	1285.0	1270.9	14.1	1.10
	C	1248.7	1232.8	15.9	1.28
	A	2755.9	2731.3	24.6	0.89
4	B	2675.6	2652.5	23.1	0.86
	C	2653.3	2631.2	22.1	0.83
5	A	2336.9	2308.0	28.9	1.24
	A	1464.2	1437.6	26.6	1.82
6	B	768.2	757.4	10.8	1.40
	C	580.6	572.5	8.1	1.40
	A	1165.7	1152.4	13.3	1.15
7	B	661.2	652.2	9.0	1.36
	C	454.0	448.3	5.7	1.26
	A	1166.3	1153.6	12.7	1.09
8	B	767.6	751.4	16.2	2.10
	C	513.0	505.6	7.4	1.45
	A	862.5	853.3	9.2	1.07
9	B	754.2	740.8	13.4	1.77
	C	513.7	505.4	8.3	1.62

PBE

	A	4293.9	4235.8	58.1	1.35
1	B	1395.9	1378.9	17.0	1.22
	C	1130.2	1114.7	15.5	1.37
	A	3322.5	3272.1	50.4	1.52
2	B	719.8	694.3	25.5	3.54
	C	698.0	668.3	29.7	4.26
	A	3071.1	3019.4	51.7	1.68

3	B	1285.0	1264.9	20.1	1.57
	C	1248.7	1226.0	22.7	1.81
	A	2755.9	2727.5	28.4	1.03
4	B	2675.6	2648.5	27.1	1.01
	C	2653.3	2629.6	23.7	0.89
5	A	2336.9	2299.1	37.8	1.62
	A	1464.2	1440.7	23.5	1.61
6	B	768.2	748.8	19.4	2.53
	C	580.6	566.9	13.7	2.36
	A	1165.7	1151.8	13.9	1.19
7	B	661.2	644.3	16.9	2.55
	C	454.0	444.2	9.8	2.16
	A	1166.3	1142.4	23.9	2.05
8	B	767.6	748.7	18.9	2.46
	C	513.0	501.7	11.3	2.21
	A	862.5	846.6	15.9	1.85
9	B	754.2	737.9	16.3	2.16
	C	513.7	502.1	11.6	2.26

B97-D3

	A	4293.9	4240.7	53.2	1.24
1	B	1395.9	1383.1	12.8	0.92
	C	1130.2	1118.1	12.1	1.07
	A	3322.5	3243.8	78.7	2.37
2	B	719.8	704.2	15.6	2.17
	C	698.0	682.9	15.1	2.17
	A	3071.1	3021.6	49.5	1.61
3	B	1285.0	1273.5	11.5	0.89
	C	1248.7	1223.9	24.8	1.99
	A	2755.9	2726.6	29.3	1.06
4	B	2675.6	2650.2	25.4	0.95
	C	2653.3	2632.4	20.9	0.79
5	A	2336.9	2302.1	34.8	1.49
	A	1464.2	1440.1	24.1	1.64
6	B	768.2	752.5	15.7	2.05
	C	580.6	569.8	10.8	1.86
	A	1165.7	1155.2	10.5	0.90
7	B	661.2	649.7	11.5	1.75
	C	454.0	448.5	5.5	1.22
	A	1166.3	1145.6	20.7	1.78
8	B	767.6	751.2	16.4	2.13
	C	513.0	504.9	8.1	1.58

	A	862.5	854.9	7.6	0.88
9	B	754.2	738.2	16.0	2.12
	C	513.7	504.2	9.5	1.84

B97

	A	4293.9	4211.2	82.7	1.93
1	B	1395.9	1371.7	24.2	1.74
	C	1130.2	1107.6	22.6	2.00
	A	3322.5	3264.7	57.8	1.74
2	B	719.8	683.0	36.8	5.12
	C	698.0	656.8	41.2	5.90
	A	3071.1	3003.3	67.8	2.21
3	B	1285.0	1257.7	27.3	2.12
	C	1248.7	1203.0	45.7	3.66
	A	2755.9	2712.2	43.7	1.59
4	B	2675.6	2635.2	40.4	1.51
	C	2653.3	2626.2	27.1	1.02
5	A	2336.9	2274.3	62.6	2.68
	A	1464.2	1443.8	20.4	1.39
6	B	768.2	730.9	37.3	4.85
	C	580.6	556.0	24.6	4.23
	A	1165.7	1157.9	7.8	0.67
7	B	661.2	625.9	35.3	5.33
	C	454.0	437.8	16.2	3.57
	A	1166.3	1109.2	57.1	4.90
8	B	767.6	743.2	24.4	3.17
	C	513.0	492.6	20.4	3.97
	A	862.5	838.2	24.3	2.82
9	B	754.2	727.6	26.6	3.53
	C	513.7	494.8	18.9	3.68

LDA

	A	4293.9	4336.7	-42.8	-1.00
1	B	1395.9	1411.7	-15.8	-1.13
	C	1130.2	1143.5	-13.3	-1.18
	A	3322.5	3344.6	-22.1	-0.66
2	B	719.8	729.3	-9.5	-1.32
	C	698.0	706.1	-8.1	-1.16
	A	3071.1	3099.5	-28.4	-0.93
3	B	1285.0	1300.1	-15.1	-1.18
	C	1248.7	1284.1	-35.4	-2.84

	A	2755.9	2790.3	-34.4	-1.25
4	B	2675.6	2707.5	-31.9	-1.19
	C	2653.3	2672.9	-19.6	-0.74
5	A	2336.9	2381.7	-44.8	-1.92
	A	1464.2	1470.2	-6.0	-0.41
6	B	768.2	796.5	-28.3	-3.68
	C	580.6	598.6	-18.0	-3.10
	A	1165.7	1171.0	-5.3	-0.46
7	B	661.2	679.8	-18.6	-2.81
	C	454.0	461.5	-7.5	-1.66
	A	1166.3	1217.9	-51.6	-4.42
8	B	767.6	769.5	-1.9	-0.25
	C	513.0	522.9	-9.9	-1.92
	A	862.5	875.7	-13.2	-1.53
9	B	754.2	766.4	-12.2	-1.61
	C	513.7	522.7	-9.0	-1.75

HF-3c

	A	4293.9	4217.7	76.2	1.77
1	B	1395.9	1380.6	15.3	1.10
	C	1130.2	1116.0	14.2	1.25
	A	3322.5	3170.5	152.0	4.58
2	B	719.8	713.0	6.8	0.94
	C	698.0	688.0	10.0	1.44
	A	3071.1	2992.5	78.6	2.56
3	B	1285.0	1259.6	25.4	1.98
	C	1248.7	1209.1	39.6	3.17
	A	2755.9	2710.5	45.4	1.65
4	B	2675.6	2648.6	27.0	1.01
	C	2653.3	2647.6	5.7	0.21
5	A	2336.9	2295.4	41.5	1.77
	A	1464.2	1427.9	36.3	2.48
6	B	768.2	756.6	11.6	1.51
	C	580.6	572.0	8.6	1.49
	A	1165.7	1160.9	4.8	0.41
7	B	661.2	657.7	3.5	0.53
	C	454.0	454.9	-0.9	-0.20
	A	1166.3	1164.1	2.2	0.19
8	B	767.6	749.9	17.7	2.31
	C	513.0	503.9	9.1	1.78
	A	862.5	863.2	-0.7	-0.08
9	B	754.2	737.6	16.6	2.20

	C	513.7	508.3	5.4	1.06

DFTB3-D3

	A	4293.9	4248.3	45.6	1.06
1	B	1395.9	1380.8	15.1	1.08
	C	1130.2	1116.6	13.6	1.20
	A	3322.5	3181.3	141.2	4.25
2	B	719.8	712.4	7.4	1.03
	C	698.0	687.5	10.5	1.50
	A	3071.1	3005.6	65.5	2.13
3	B	1285.0	1247.3	37.7	2.94
	C	1248.7	1222.0	26.7	2.14
	A	2755.9	2722.0	33.9	1.23
4	B	2675.6	2653.2	22.4	0.84
	C	2653.3	2634.0	19.3	0.73
5	A	2336.9	2295.0	41.9	1.79
	A	1464.2	1431.6	32.6	2.22
6	B	768.2	759.2	9.0	1.17
	C	580.6	573.8	6.8	1.17
	A	1165.7	1166.1	-0.4	-0.03
7	B	661.2	638.8	22.4	3.39
	C	454.0	448.0	6.0	1.33
	A	1166.3	1199.2	-32.9	-2.82
8	B	767.6	747.6	20.0	2.60
	C	513.0	511.6	1.4	0.28
	A	862.5	858.7	3.8	0.44
9	B	754.2	732.7	21.5	2.84
	C	513.7	504.7	9.0	1.76

PM7

	A	4293.9	4222.9	71.0	1.65
1	B	1395.9	1406.7	-10.8	-0.77
	C	1130.2	1136.3	-6.1	-0.54
	A	3322.5	3057.7	264.8	7.97
2	B	719.8	743.0	-23.2	-3.23
	C	698.0	695.2	2.8	0.41
	A	3071.1	3063.8	7.3	0.24
3	B	1285.0	1294.3	-9.3	-0.72
	C	1248.7	1243.8	4.9	0.39
	A	2755.9	2760.6	-4.7	-0.17
4	B	2675.6	2663.6	12.0	0.45

	C	2653.3	2621.3	32.0	1.21
5	A	2336.9	2315.9	21.0	0.90
	A	1464.2	1435.4	28.8	1.96
6	B	768.2	791.9	-23.7	-3.09
	C	580.6	592.7	-12.1	-2.08
	A	1165.7	1176.7	-11.0	-0.95
7	B	661.2	645.4	15.8	2.38
	C	454.0	452.9	1.1	0.24
	A	1166.3	1222.4	-56.1	-4.81
8	B	767.6	761.2	6.4	0.84
	C	513.0	516.6	-3.6	-0.71
	A	862.5	895.0	-32.5	-3.77
9	B	754.2	741.1	13.1	1.73
	C	513.7	520.4	-6.7	-1.31

PM6

	A	4293.9	4207.1	86.8	2.02
1	B	1395.9	1395.2	0.7	0.05
	C	1130.2	1125.3	4.9	0.43
	A	3322.5	2752.6	569.9	17.15
2	B	719.8	849.4	-129.6	-18.00
	C	698.0	816.1	-118.1	-16.92
	A	3071.1	3018.6	52.5	1.71
3	B	1285.0	1287.8	-2.8	-0.22
	C	1248.7	1230.4	18.3	1.46
	A	2755.9	2736.3	19.6	0.71
4	B	2675.6	2649.5	26.1	0.98
	C	2653.3	2608.0	45.3	1.71
5	A	2336.9	2300.7	36.2	1.55
	A	1464.2	1405.8	58.4	3.99
6	B	768.2	778.3	-10.1	-1.32
	C	580.6	580.8	-0.2	-0.03
	A	1165.7	1156.6	9.1	0.78
7	B	661.2	633.9	27.3	4.13
	C	454.0	441.8	12.2	2.68
	A	1166.3	1159.3	7.0	0.60
8	B	767.6	743.1	24.5	3.19
	C	513.0	499.2	13.8	2.68
	A	862.5	903.4	-40.9	-4.74
9	B	754.2	722.3	31.9	4.24
	C	513.7	514.6	-0.9	-0.18

OM2

	A	4293.9	4265.2	28.7	0.67
1	B	1395.9	1419.8	-23.9	-1.71
	C	1130.2	1152.2	-22.0	-1.94
	A	3322.5	2503.3	819.2	24.66
2	B	719.8	981.6	-261.8	-36.38
	C	698.0	943.8	-245.8	-35.22
	A	3071.1	3154.3	-83.2	-2.71
3	B	1285.0	1355.5	-70.5	-5.48
	C	1248.7	1185.7	63.0	5.05
	A	2755.9	2798.3	-42.4	-1.54
4	B	2675.6	2688.9	-13.3	-0.50
	C	2653.3	2654.6	-1.3	-0.05
5	A	2336.9	2372.2	-35.3	-1.51
	A	1464.2	1438.5	25.7	1.76
6	B	768.2	829.7	-61.5	-8.01
	C	580.6	615.5	-34.9	-6.02
	A	1165.7	1196.3	-30.6	-2.62
7	B	661.2	651.1	10.1	1.53
	C	454.0	458.2	-4.2	-0.93
	A	1166.3	1264.1	-97.8	-8.39
8	B	767.6	766.8	0.8	0.11
	C	513.0	526.2	-13.2	-2.58
	A	862.5	900.8	-38.3	-4.44
9	B	754.2	752.6	1.6	0.21
	C	513.7	527.0	-13.3	-2.60