A new set of DFT-D parameters for graphitic materials with small basis sets

Karol Strutyński,[†] Manuel Melle-Franco,[†,‡] Maria J. R. N. Ramos,[†] and José A. N. F. Gomes[*,†]

REQUIMTE, Departamento de Química, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre S/N, 4169-007 Porto, Portugal, and Departamento de Informática, Centro de Ciências e Tecnologias da Computação, Universidade do Minho, 4710-057 Braga, Portugal

E-mail: jfgomes@fc.up.pt

CCSD(T)/CBS interaction energies

Table 1: CCSD(T)/CBS interaction energies

system	E_{int} [kcal/mol]	E_{int} [meV]
PD_a	-2.73	-118.4
TT_b	-2.82	-122.3
TT_a	-2.80	-121.4
PB_b	-2.72	-118.0
T_a	-2.70	-117.1
V_{C_S}	-2.74	-118.8
T_b	-2.40	-104.1
$X_{D_{2d}}$	-1.79	-77.6
$S_{D_{6d}}$	-1.71	-74.2
$S_{D_{6h}}$	-1.71	-74.2

[*]To whom correspondence should be addressed
[†]University of Porto
[‡]University of Minho

DFT-D parameters

Table 2: DFT-D parameter values for various basis sets. Scaling factor s_6, radius scaling r_{rscl} [Å], damping function steepness α, coefficients C_6 [Jnm^{6}mol^{-1}], vdW radius R_A^0 [Å], root mean square geometrical displacements (RMSD [Å]) and the root mean square of the binding energy error ($RMS(\Delta BE)$ [kcal/mol]) are presented.

Basis	s_6	r_{scl}	α	$C_{6,C}$	$C_{6,H}$	R_C^0	R_H^0	RMSD	$RMS(\Delta BE)$
6-31G	1.2100	1.3810	20	1.75	0.14	1.32	0.91	0.1022	0.2156
6-31G*	1.1650	1.3730	20	1.75	0.14	1.32	0.91	0.0938	0.2089
6-31G**	1.1350	1.3610	20	1.75	0.14	1.32	0.91	0.0853	0.2106
6-31+G*	1.4270	1.3560	20	1.75	0.14	1.32	0.91	0.0971	0.1518
6-31++G	1.4410	1.3900	20	1.75	0.14	1.32	0.91	0.1263	0.1899
6-311G	1.4650	1.3810	20	1.75	0.14	1.32	0.91	0.1073	0.1538
6-311G*	1.4140	1.3790	20	1.75	0.14	1.32	0.91	0.1022	0.1428
6-311G**	1.3480	1.3480	20	1.75	0.14	1.32	0.91	0.0765	0.1365
6-311+G*	1.5070	1.3700	20	1.75	0.14	1.32	0.91	0.0914	0.1110
TZV	1.3750	1.3060	20	1.75	0.14	1.32	0.91	0.0603	0.1221
TZVP	1.3790	1.2910	20	1.75	0.14	1.32	0.91	0.0511	0.1185
VTZP	1.4480	1.3130	20	1.75	0.14	1.32	0.91	0.0637	0.1282
6-31G	1.2530	1.3830	15	1.75	0.14	1.32	0.91	0.0982	0.2121
6-31G*	1.2050	1.3730	15	1.75	0.14	1.32	0.91	0.0905	0.2050
6-31G**	1.1720	1.3600	15	1.75	0.14	1.32	0.91	0.0814	0.2065
6-311G	1.5040	1.3770	15	1.75	0.14	1.32	0.91	0.1064	0.1480
6-311G*	1.4790	1.3800	15	1.75	0.14	1.32	0.91	0.1013	0.1276
6-311G**	1.3820	1.3410	15	1.75	0.14	1.32	0.91	0.0734	0.1272
6-31G	1.6190	1.4890	6	1.75	0.14	1.32	0.91	0.0858	0.2149
6-31G*	1.5190	1.4580	6	1.75	0.14	1.32	0.91	0.0768	0.2084
6-31G**	1.4500	1.4300	6	1.75	0.14	1.32	0.91	0.0640	0.2059
6-311G	1.8110	1.4320	6	1.75	0.14	1.32	0.91	0.1245	0.1562
6-311G*	1.8160	1.4520	6	1.75	0.14	1.32	0.91	0.1150	0.1331
6-311G**	1.6890	1.4010	6	1.75	0.14	1.32	0.91	0.0841	0.1254
TZV	1.5320	1.2500	6	1.75	0.14	1.32	0.91	0.0367	0.1028
TZVP	1.5130	1.2190	6	1.75	0.14	1.32	0.91	0.0334	0.0896

Performance

Single point calculations without symmetry executed parallelly (three threads). The workstation was an Intel(r) Quad core Q8400 with 2.66GHz CPU and 4Gb of memory.

Table 3: Number of functions and computation time of different systems and basis sets (run time is normalized by number of cycles).

basis set	n. fun. benz	time [s] benz	n. fun. dim	time [s] dim	n. fun. pyr	time [s] pyr	n. fun. c60	time [s] c60
6-31G	66	3.63333	132	7.35000	164	11.21111	540	585.55000
6-31G*	96	2.40000	192	8.80000	244	14.38889	840	1524.62222
6-31G**	114	2.80000	228	10.68750	274	17.31111	840	1758.05556
6-311G	96	3.33333	192	12.54286	238	19.64444	780	1184.18750
6-311G*	126	3.47143	252	14.76250	318	39.67778	1080	3020.86667
6-311G**	144	4.27143	288	19.90000	348	56.23333	1080	3012.16667
TZV	102	3.70000	204	17.13750	254	25.93429	840	3035.96727
TZVP	150	7.40000	300	82.54444	364	125.74000	1140	5598.45714