1 List of functionals and coefficients for BJ-damping[1]

Functional	s6	a1	s8	a2	Gaussian keywords[a]
B1B95	1.000	0.2092	1.4507	5.5545	`B1B95 IOp(3/174=1000000,175=1450700,177=209200,178=5554500)`
B2GPPLYP	0.560	0.0000	0.2597	6.3332	n.a.[b]
B3PW91	1.000	0.4312	2.8524	4.4693	`B3PW91 IOp(3/174=1000000,175=2852400,177=431200,178=4469300)`
BHLYP	1.000	0.2793	1.0354	4.9615	For backward compatibility only[c]
BMK	1.000	0.1940	2.0860	5.9197	`BMK EmpiricalDispersion=GD3BJ`
BOP	1.000	0.4870	3.295	3.5043	n.a.[b]
BPBE	1.000	0.4567	4.0728	4.3908	`BPBE EmpiricalDispersion=GD3BJ`
CAMB3LYP	1.000	0.3708	2.0674	5.4743	`CAM-B3LYP EmpiricalDispersion=GD3BJ`
LCωPBE	1.000	0.3919	1.8541	5.0897	`LC-wPBE EmpiricalDispersion=GD3BJ`
MPW1B95	1.000	0.1955	1.0508	6.4177	n.a.[b]
MPWB1K	1.000	0.1474	0.9499	6.6223	n.a.[b]
mPWLYP	1.000	0.4831	2.0077	4.5323	`mPW1LYP IOp(3/174=1000000,175=2007700,177=483100,178=4532300)`
OLYP	1.000	0.5299	2.6205	2.8065	`OLYP IOp(3/174=1000000,175=2620500,177=529900,178=2806500)`
OPBE	1.000	0.5512	3.3816	2.9444	`OPBE IOp(3/174=1000000,175=3381600,177=551200,178=2944400)`
oTPSS	1.000	0.4634	2.7495	4.3153	n.a.[b]
PBE38	1.000	0.3995	1.4623	5.1405	n.a.[b]
PBEsol	1.000	0.4466	2.9491	6.1742	n.a.[b]
PTPSS	0.750	0.000	0.2804	6.5745	n.a.[b]
PWB6K	1.000	0.1805	0.9383	7.7627	n.a.[b]
revSSB	1.000	0.4720	0.4389	4.0986	n.a.[b]
SSB	1.000	−0.0952	−0.1744	5.2170	n.a.[b]
TPSSh	1.000	0.4529	2.2382	4.6550	`TPSSh IOp(3/174=1000000,175=2238200,177=452900,178=4655000)`
HCTH120	1.000	0.3563	1.0821	4.3359	not implemented[d]
B2PLYP	0.640	0.3065	0.9147	5.0570	`B2PLYP`
B3LYP	1.000	0.3981	1.9889	4.4211	`B3LYP EmpiricalDispersion=GD3BJ`
B97D	1.000	0.5545	2.2609	3.2297	`B97D3`
BLYP	1.000	0.4298	2.6996	4.2359	`BLYP EmpiricalDispersion=GD3BJ`
BP86	1.000	0.3946	3.2822	4.8516	`BP86 EmpiricalDispersion=GD3BJ`
DSDBLYP	0.500	0.000	0.2130	6.0519	n.a.[b]
PBE0	1.000	0.4145	1.2177	4.8593	`PBE1PBE EmpiricalDispersion=GD3BJ`
PBE	1.000	0.4289	0.7875	4.4407	`PBEPBE EmpiricalDispersion=GD3BJ`
PW6B95	1.000	0.2076	0.7257	6.3750	`PW6B95D3`
PWPB95	0.820	0.0000	0.2904	7.3141	n.a.[b]
revPBE0	1.000	0.4679	1.7588	3.7619	`PBEh1PBE IOp(3/174=1000000,175=1758800,177=467900,178=3761900)`
revPBE38	1.000	0.4309	1.4760	3.9446	n.a.[b]
revPBE	1.000	0.5238	2.3550	3.5016	`PBEhPBE IOp(3/174=1000000,175=2355000,177=523800,178=3501600)`
rPW86PBE	1.000	0.4613	1.3845	4.5062	n.a.[b]
TPSS0	1.000	0.3768	1.2576	4.5865	n.a.[b]
TPSS	1.000	0.4535	1.9435	4.4752	`TPSSTPSS EmpiricalDispersion=GD3BJ`

[a] For implemented methods, the corresponding method keyword is given, and other keywords to select the Dispersion correction. The `IOps(3/174-178)` select the values for s6, s8, sr6 (zero-damping), a1, and a2, respectively. [b] It might be implemented, but the current version of this table ignores this. [c] The *half-and-half* implementations are included in Gaussian 16 for backward compatibility.[2] The keywords are `BHandH` or `BHandHLYP`, but they are not further used in this compilation. [d] While other members of the HCTC family are implemented, e.g. HCTH/407 as `HTCH407` and τ-HCTH as `tHCTH`, the HCTH/120 functional is explicitly mentioned in the manual[2] as not being implemented.

References

[1] Stefan Grimme. *List of functionals and coefficients for BJ-damping*. July 12, 2017. URL: `https://www.chemie.uni-bonn.de/pctc/mulliken-center/software/dft-d3/functionalsbj`.

[2] Gaussian, Inc. *List of Gaussian 16 Rev B.01 Keywords*. Mar. 14, 2018. URL: `http://gaussian.com/keywords/`.

[3] Stefan Grimme et al. "A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu". In: *The Journal of Chemical Physics* 132.15 (2010), p. 154104. DOI: `10.1063/1.3382344`.

[4] Stefan Grimme, Stephan Ehrlich, and Lars Goerigk. "Effect of the damping function in dispersion corrected density functional theory". In: *Journal of Computational Chemistry* 32.7 (2011), pp. 1456–1465. DOI: `10.1002/jcc.21759`.

[5] Daniel G. A. Smith et al. "Revised Damping Parameters for the D3 Dispersion Correction to Density Functional Theory". In: *The Journal of Physical Chemistry Letters* 7.12 (2016), pp. 2197–2203. DOI: `10.1021/acs.jpclett.6b00780`.