A Critical Study of Charge Transfer Parameter for the Calculation of Interaction Energy Using Local Hard-Soft Acid-Base Principle

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Table S1:
Values of Second order approximation of ΔN (ΔN_{2nd})

Complex	DFT/6-311G(d,P)/B3LYP		MP2/6-311G(d,P)		CCSD(T)/6-311G(d,P)	
	1st root (Acceptable)	2nd root (Unphysical)	1st root (Acceptable)	2nd root (Unphysical)	1st root (Acceptable)	2nd root (Unphysical)
SUC-BUTL(1)	0.02938	-59.38731	0.01420	-30.4046	0.04161	17.1612
FA-FD(2)	0.03093	87.5111	0.02536	-32.3750	0.03302	-25.4912
AA-FD(3)	0.02571	110.0049	0.01697	-42.1845	0.02486	-34.2743
FRM-FD(4)	0.01396	180.5229	0.00805	-60.8148	0.00342	-27.1833
NFRM-FD(5)	0.00982	-147.3240	0.00224	-27.2529	0.00261	-36.0292
ATM-FD(6)	0.01127	162.5473	0.00385	-29.9199	0.00121	-50.2490

NATM-FD(7)	0.00552	-217.1717	0.00095	-41.6844	0.00449	-115.12174
ACT-HCL(8)	0.05165	104.2306	0.04439	151.7263	0.03647	50.7158
ACT-LICL(9)	0.06417	-125.1701	0.06325	-87.6711	0.06513	120.6395
BUTY-HCL(10)	0.07572	-74.7857	0.06085	-128.2110	0.07441	70.2384
BUTY-LICL(11)	0.09593	-25.6933	0.08612	-31.7158	0.10417	-190.1300