

Article

An Ab Initio Investigation of the 4,4'-Methylene Diphenyl Diamine (MDA) Formation from the Reaction of Aniline with Formaldehyde

R. Zsanett Boros^{1,2}, László Farkas¹, Károly Nehéz³, Béla Viskolcz² and Milán Szóri^{2*}

¹ Wanhua-BorsodChem Zrt, Bolyai tér 1., H-3700, Kazincbarcika, Hungary; boros.zsanett0711@gmail.com (R.Zs.B.); laszlo.farkas@borsodchem.hu (L.F.)

² Institute of Chemistry, University of Miskolc, Miskolc-Egyetemváros A/2, H-3515, Miskolc, Hungary; bela.viskolcz@uni-miskolc.hu (B.V.); milan.szori@uni-miskolc.hu (M.Sz.)

³ Department of Information Engineering, University of Miskolc, Miskolc-Egyetemváros Informatics Building, H-3515 Miskolc, Hungary; aitnehez@uni-miskolc.hu (K.N.)

* Correspondence: milan.szori@uni-miskolc.hu; Tel.: +36-46-565-111/1337 (M.Sz.)

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Supporting Information

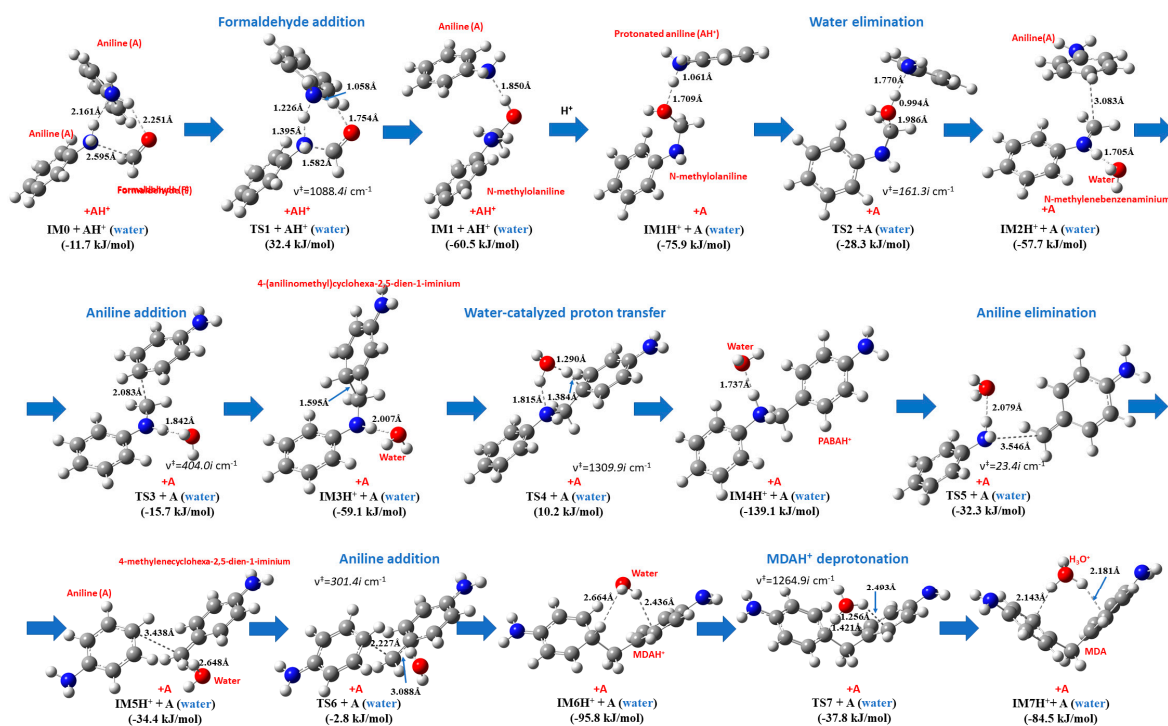


Figure S1. Transition state structures (obtained at B3LYP/6-31G(d) level of theory) for MDA synthesis in aqueous phase. The G3MP2B3 relative energies are also given.

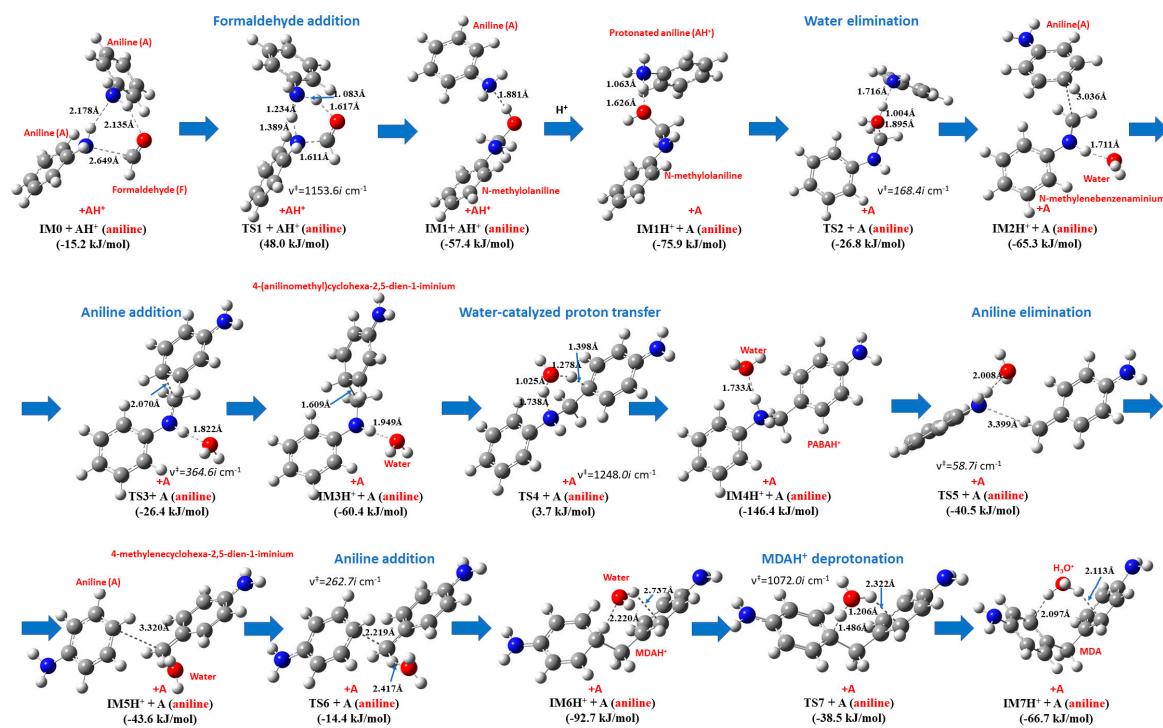


Figure S2. Transition state structures (obtained at B3LYP/6-31G(d) level of theory) for MDA synthesis in aniline. The G3MP2B3 relative energies are also given.