Bulgarian Chemical Communications, Volume 49, Special Edition B, 2017

SUPPLEMENTARY DATA

Stereoselectivity in the Diels–Alder addition of S-hydroxy-N-methylsuccinimide acrylate to cyclopentadiene: origins and DFT computational models

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Table S1. – Total electronic energies with Gibbs free energy corrections at 298 K of transition structures for the [4+2] addition reaction of S-hydroxy-N-methylsuccinimide acrylate (AS) to cyclopentadiene (CPD) by DFT methods at the 6-311G(d,p) basis set level, solvent CH_2Cl_2. **Pos** and **neg** refer to positive and negative dihedral angles between adjacent carbonyl groups, see Scheme 2 and Fig. 1. Also shown are M06-2x[d)] and MN12sx[d)] results at the 6-311++G(d,p) basis set level.

TS	PBE	B97D	M06L	M11L	M06-2x	M06-2x[d]	MN12sx	MN12sx[d]
NC1 pos	-859.059825	-859.478417	-859.937937	-859.828166	-859.693563	-859.706385	-859.351174	-859.367988
NC2 pos	-859.058543	-859.477428	-859.937093	-859.827934	-859.692027	-859.707920	-859.350072	-859.367598
XC1 pos	-859.059838	-859.478171	-859.936866	-859.827344	-859.692413	-859.704417	-859.351195	-859.366418
XC2 pos	-859.057990	-859.476756	-859.935993	-859.826721	-859.691080	-859.705332	-859.348728	-859.365937
NT1 pos	-859.056379	-859.475520	-859.934498	-859.825087	-859.690298	-859.707230	-859.347900	-859.365731
NT2 pos	-859.057793	-859.475800	-859.935360	-859.826342	-859.691620	-859.705125	-859.348955	-859.36574
XT1 pos	-859.055509	-859.474102	-859.93269	-859.823622	-859.687797	-859.704098	-859.345883	-859.363876
XT2 pos	-859.057403	-859.475858	-859.934427	-859.824034	-859.688857	-859.704242	-859.345097	-859.366346
NC1 neg	-859.060405	-859.477888	-859.935824	-859.825716	-859.690367	-859.708192	-859.348267	-859.366498
NC2 neg	-859.061679	-859.479155	-859.936186	-859.827065	-859.692048	-859.707471	-859.350022	-859.367069
XC1 neg	-859.059120	-859.476588	-859.934019	-859.824932	-859.689009	-859.706977	-859.346888	-859.364325
XC2 neg	-859.060039	-859.477383	-859.935288	-859.825951	-859.690199	-859.706353	-859.348388	-859.364993
NT1 neg	-859.058876	-859.476204	-859.934561	-859.825073	-859.690415	-859.705854	-859.348189	-859.366451
NT2 neg	-859.057614	-859.474198	-859.933238	-859.823928	-859.689507	-859.707241	-859.345705	-859.365007
XT1 neg	-859.057941	-859.475756	-859.920734	-859.823803	-859.688704	-859.703243	-859.346153	-859.364277
XT2 neg	-859.056776	-859.474987	-859.918566	-859.822007	-859.687453	-859.704746	-859.345083	-859.362707