

Supporting Information

Role(s) of TMA in Polymerization

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A. Full Gaussian Citation.

Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

B. Tables

B1. Tables with Final Energies, Enthalpy and Entropy corrections in Hartree for R=Me

Structure	TPSSTPSS-E	H_corr	TAS_corr	M06-2X-E	M06-2X-E(PCM)
3_Me+	-2052.573099	0.71161592	0.119763	-2051.931147	-2051.962145
5_Me+	-2414.809299	0.82819891	0.143645	-2414.100397	-2414.13137
2_Me+	-1690.319096	0.59541874	0.101432	-1689.733983	-1689.767485
6_Me+_propene_A	-1808.267039	0.681274	0.112763	-1807.645282	-1807.677207
6_Me+_propene_B	-1808.268601	0.68142808	0.111803	-1807.645006	-1807.677506
6_Me+_propene_C	-1808.269156	0.68118032	0.112787	-1807.647022	-1807.678269
6_Me+_propene_D	-1808.270909	0.68136457	0.112819	-1807.649553	-1807.680663

B2. Tables with Final Energies, Enthalpy and Entropy corrections in Hartree for R=iBu

Structure	TPSSTPSS-E	H_corr	TAS_corr	M06-2X-E	M06-2X-E(PCM)
2alpha_iBu+	-1808.272939	0.68294787	0.111604	-1807.644172	-1807.679176
2beta_iBu+	-1808.279797	0.68318998	0.109509	-1807.653811	-1807.688537
2gamma_iBu+	-1808.279163	0.68382475	0.109654	-1807.653664	-1807.685753
6alpha_iBu+_propene_A	-1926.22491	0.76913874	0.120951	-1925.56025	-1925.591343
6alpha_iBu+_propene_B	-1926.225856	0.7689516	0.121282	-1925.56076	-1925.591558
6alpha_iBu+_propene_C	-1926.218131	0.76885853	0.122435	-1925.551161	-1925.582471
6alpha_iBu+_propene_D	-1926.220729	0.76914686	0.121706	-1925.555219	-1925.586179
6beta_iBu+_propene_A	-1926.221746	0.76961232	0.120222	-1925.560071	-1925.591172
6beta_iBu+_propene_B	-1926.221612	0.76936827	0.119161	-1925.560215	-1925.591534
6beta_iBu+_propene_C	-1926.219302	0.76906938	0.122927	-1925.556346	-1925.588192
6beta_iBu+_propene_D	-1926.218647	0.76929562	0.122232	-1925.557184	-1925.589024
3_iBu+_A	-2170.52354	0.80000689	0.127229	-2169.840337	-2169.870714
3_iBu+_B	-2170.52723	0.79999947	0.127593	-2169.843691	-2169.874183
4beta_iBu+_A	-2170.515369	0.80011454	0.129539		
4beta_iBu+_B	-2170.497578	0.79899064	0.12981		
6alpha_iBu+_propene_InsertionTS_A	-1926.211552	0.76901046	0.116819	-1925.541466	-1925.571422
6alpha_iBu+_propene_InsertionTS_B	-1926.218405	0.76855471	0.117514	-1925.551782	-1925.581546
6beta_iBu+_propene_InsertionTS_A	-1926.2052	0.76885974	0.116436	-1925.539752	-1886.272462
6beta_iBu+_propene_InsertionTS_B	-1926.201968	0.76911844	0.115391	-1925.535869	-1925.569676
4alpha_iBu+_A	-2170.517783	0.79985954	0.12953	-2169.833679	-2169.864574
5alpha_iBu+_A	-2532.764017	0.91623272	0.150563	-2532.016718	-2532.046965
5alpha_iBu+_B	-2532.762821	0.9158978	0.151268	-2532.011241	-2532.041415
5alpha_iBu+_C	-2532.764192	0.9157031	0.15272	-2532.01507	-2532.045556
5alpha_iBu+_D	-2532.763986	0.91617986	0.151841	-2532.017127	-2532.04741
5alpha_iBu+_E	-2532.762762	0.91674499	0.150041	-2532.0156	-2532.046113
5alpha_iBu+_F	-2532.762766	0.91593986	0.150809	-2532.011267	-2532.041571

5alpha_iBu+_G	-2532.763	0.91604436	0.150837	-2532.011842	-2532.042368
5alpha_iBu+_H	-2532.764269	0.91585034	0.15195	-2532.015517	-2532.045887

B3. Tables with Final Energies, Enthalpy and Entropy corrections in Hartree for small molecules

Structure	TPSSTPSS-E	H_corr	TΔS_corr	M06-2X-E	M06-2X-E(PCM)
TMA DIMER	-724.4689441	0.230015129	0.060723	-724.3326661	-724.3340118
AlMe3	-362.221393	0.113661992	0.042166992	-362.148569	-362.1496104
ethene	-78.60514788	0.054247884	0.026216	-78.57115492	-78.5718058
propene	-117.932912	0.083400953	0.030104	-117.8827427	-117.8834133