Electronic Supplementary Material (ESI) for RSC Advances.

Understading the regioselectivity of Michael addition reaction to asymmetric divinylic compounds.

SUPPORTING INFORMATION

Associated content

Reference Cartesian coordinates for all studied non-symmetric crosslinkers and N,N-diethylamine and the relative energy of conformers.

Table 1: Relative energy of conformers of asymmetric crosslinkers.

Conformer	Subunit 1	Subunit 2	Relative Energy (Kcal/mol)
AOEMA			
1	Trans-Acrylate	Trans-Methacrylate	0.29
2	Cis-Acrylate	Trans-Methacrylate	0.00
3	Trans-Acrylate	Cis-Methacrylate	0.65
4	Cis-Acrylate	Cis-Methacrylate	0.37
AAEA			
1	Trans-Acrylate	Trans-Acrylamide	1.55
2	Cis-Acrylate	Trans-Acrylamide	1.07
3	Trans-Acrylate	Cis-Acrylamide	0.39
4	Cis-Acrylate	Cis-Acrylamide	0.00
AAEMA			
1	Trans-Acrylamide	Trans-Methacrylate	1.29
2	Cis-Acrylamide	Trans-Methacrylate	0.00
3	Trans-Acrylamide	Cis-Methacrylate	1.59
4	Cis-Acrylamide	Cis-Methacrylate	0.35
AVP			
1	Trans-acrylate	Trans-VP	0.33
2	Cis-acrylate	Trans-VP	0.00
3	Trans-acrylate	Cis-VP	3.50
4	Cis-acrylate	Cis-VP	3.17

MAEA			
1	Trans-methacrylamide	Trans-acrylate	0.29
2	Cis-methacrylamide	Trans-acrylate	0.92
3	Trans-methacrylamide	Cis-acrylate	0.00
4	Cis-methacrylamide	Cis-acrylate	0.56

AOEMA: 2-(AcryloylOxy)-Ethyl-MethAcrylate

C	-5.70150	-0.23225	-0.00056
C	-4.44959	-0.69367	0.00032
C	-3.29964	0.24416	0.00000
O	-3.36576	1.45609	-0.00104
O	-2.12648	-0.43937	0.00088
C	-0.93933	0.37119	0.00052
C	0.22845	-0.59819	0.00051
O	1.41367	0.21419	0.00032
C	2.58671	-0.46792	-0.00034
C	3.79169	0.41490	-0.00011
O	2.64103	-1.68192	-0.00047
C	5.10649	-0.31802	-0.00064
C	3.67667	1.74882	0.00057
H	-6.55563	-0.90111	-0.00035
H	-5.88990	0.83698	-0.00151
H	-4.21930	-1.75430	0.00128
H	-0.92575	1.01505	0.88479

H	-0.92604	1.01475	-0.88395
H	0.21408	-1.24201	-0.88366
H	0.21424	-1.24183	0.88482
H	5.18994	-0.96941	0.87521
H	5.94350	0.38378	-0.00047
H	5.18966	-0.96866	-0.87706
H	2.70903	2.23576	0.00097
H	4.55684	2.38494	0.00075

B3LYP/6-31G(d,p) Energy: 38.2182 KJ/mol

AAEA: 2-(Acrylamidoethyl)-Acrylate

C	-5.18777	-0.28453	0.33562
C	-4.01542	0.34256	0.44540
C	-2.78145	-0.25512	-0.12467
O	-2.71168	-1.31156	-0.71926
O	-1.71321	0.54747	0.10520
C	-0.44895	0.06335	-0.38589
C	0.56846	1.17765	-0.14798
N	1.89217	0.80787	-0.61771
C	2.77133	0.11714	0.17840
O	2.49528	-0.20206	1.33082
C	4.08160	-0.19684	-0.46801
C	5.02289	-0.86538	0.19856
H	-6.09986	0.13458	0.74736
H	-5.24987	-1.24083	-0.17477
H	-3.91095	1.29792	0.94990
H	-0.53935	-0.18837	-1.44734
H	-0.16275	-0.84174	0.15707
H	0.63723	1.38352	0.92245
H	0.24848	2.09193	-0.65690
H	2.14090	0.99902	-1.57626
H	4.24655	0.13360	-1.49220
H	4.83475	-1.18368	1.21938
H	5.98248	-1.10490	-0.24739

B3LYP/6-31G(d,p) Energy: -63.042 KJ/mol

AAEMA: 2-(Acrylamido)ethyl methacrylate

C	-3.80757	1.51612	0.39071
C	-3.71767	0.19384	0.20229
C	-2.40664	-0.46207	-0.08949
O	-2.27714	-1.66063	-0.24739
O	-1.37045	0.40733	-0.16573
C	-0.08171	-0.17950	-0.42452
C	0.90090	0.97898	-0.58490
N	2.24506	0.51005	-0.87250
C	3.12247	0.18040	0.13036
O	2.82873	0.29071	1.31680
C	4.45404	-0.30554	-0.34285
C	5.39377	-0.66546	0.53165
C	-4.89009	-0.74799	0.26766
H	-5.81372	-0.20638	0.48428
H	-4.73543	-1.50851	1.03973
H	-5.00929	-1.28884	-0.67673
H	-2.93566	2.15699	0.33891
H	-4.76283	1.98615	0.60523
H	0.21072	-0.81961	0.41245
H	-0.13385	-0.79802	-1.32624
H	0.57077	1.64123	-1.39109
H	0.93853	1.55443	0.34265
H	2.50834	0.34279	-1.83170
H	4.63567	-0.35747	-1.41506

H	5.18886	-0.60437	1.59611
H	6.36841	-1.02080	0.21407

B3LYP/6-31G(d,p) Energy: -52.4655 KJ/mol

AVP: 3-(2-(acryloyloxy)ethyl)-N-Vinyl-2-pyrrolidone

C	-2.44512	1.86699	-0.39203
C	-1.43531	0.72170	-0.58966
C	-3.81940	1.17163	-0.37469
N	-3.50681	-0.17515	0.09494
C	-2.15927	-0.48814	0.01019
C	-0.04307	0.97505	0.00352
C	0.98672	-0.06103	-0.42699
O	2.24724	0.33572	0.15706
C	3.33513	-0.34500	-0.26879
C	4.60651	0.08912	0.38989
C	4.61332	1.03982	1.33208
C	5.83904	-0.62995	-0.08912
O	3.28669	-1.22250	-1.10973
C	-4.46105	-1.10574	0.50033
C	-5.78328	-0.90537	0.51674
O	-1.66818	-1.55399	0.34502
H	-2.37973	2.63566	-1.16554
H	-2.26518	2.34979	0.57503
H	-1.33272	0.51054	-1.66556
H	-4.28119	1.13173	-1.37092
H	-4.52925	1.65549	0.30363
H	-0.10682	0.99378	1.09788
H	0.30274	1.96663	-0.31306
H	1.09323	-0.09679	-1.51624

H	0.71832	-1.06081	-0.08003
H	3.70013	1.52873	1.64933
H	5.53916	1.34776	1.80924
H	5.74576	-1.70903	0.06970
H	6.72877	-0.27034	0.43302
H	5.97881	-0.48949	-1.16590
H	-4.00852	-2.04190	0.81056
H	-6.24695	0.02197	0.19913
H	-6.44015	-1.69599	0.85745

B3LYP/6-31G(d,p) Energy: 30.8446 KJ/mol

MAEA: 2-(Methacrylamido)ethyl acrylate

C	-4.92262	-0.54021	-0.49408
C	-3.75828	0.32644	-0.09858
C	-2.42928	-0.38527	-0.07232
C	-3.85460	1.64183	0.13080
O	-2.19120	-1.32326	-0.82764
N	-1.51604	0.07034	0.84311
C	-0.19442	-0.52076	0.96442
C	0.84713	0.26583	0.17171
O	2.11026	-0.39262	0.38212
C	3.19368	0.22746	-0.14711
O	3.13571	1.27741	-0.75437
C	4.42696	-0.55300	0.12596
C	5.61317	-0.12250	-0.30675
H	-5.09866	-1.32626	0.24965
H	-4.69935	-1.04835	-1.43643
H	-5.83697	0.04725	-0.60413
H	-4.80842	2.15736	0.06734
H	-2.98746	2.25809	0.34906
H	-1.81001	0.76471	1.51185
H	-0.25072	-1.54297	0.58357
H	0.09275	-0.55845	2.01997
H	0.91544	1.30594	0.50590
H	0.60427	0.26830	-0.89504
H	4.31049	-1.47653	0.68423
H	5.68698	0.80638	-0.86406

H	6.52537	-0.67899	-0.11889

B3LYP/6-31G(d,p) Energy: -11.8106 KJ/mol

N,N-Diethylamine

N	-0.01657	-0.87409	-0.44798
C	-1.32429	-0.52826	0.11448
C	-1.65618	0.96070	0.00596
C	1.15133	-0.49687	0.36153
C	1.83628	0.78175	-0.13055
H	0.00288	-1.87609	-0.60423
H	-1.41991	-0.83777	1.17363
H	-2.07521	-1.09737	-0.44657
H	-0.99369	1.57036	0.62799
H	-2.68237	1.14687	0.34071
H	-1.55813	1.29946	-1.02966
H	1.87887	-1.31628	0.31349
H	0.88259	-0.38941	1.42743
H	2.14235	0.66881	-1.17479
H	2.72601	0.99966	0.47149
H	1.16980	1.64644	-0.07218

B3LYP/6-31G(d,p) Energy: -10.1493 KJ/mol

Compound Name	E_{HOMO} (eV)	E_{LUMO} (eV)	$\mu=(\varepsilon_H+\varepsilon_L)/2$	$\eta=\varepsilon_L-\varepsilon_H$	$\varpi=\mu^2/2\eta$	ΔN_{max}
Diethylamine	−5.820	2.219	−3.60	8.04	0.80	0.45