

Supporting Information

Thermally Reversible Diels–Alder Based Polymerization: An Experimental and Theoretical Assessment

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Table S1. Influence of different organic solvents and time on the HDA reaction between **1** and **2** ($C_{IPDI-SA}^0 = C_{P-Di-Linker}^0 = 1.8$ M) with 1.1 equivalents of zinc chloride at 50 °C.

Product	Solvent	$M_n^a / \text{g mol}^{-1}$	<i>PDI</i>	$M_n^a / \text{g mol}^{-1}$	<i>PDI</i>
		after 2 h	after 2 h	after 4 h	after 4 h
7	Acetonitrile	3200	2.27	4800	2.50
4	THF	1700	2.56	3100	2.13
8	Toluene	2200	1.96	3000	1.98
9	Dioxane	2300	1.89	2300	2.47
10	Chloroform	2200	2.43	2700	2.95
11	DMSO	1900	2.26	2300	2.30
12	NMP	2500	2.60	2300	2.51
13	DMF	2300	2.38	2200	2.39

^arelative to linear poly(styrene) standards

Table S2. Comparison of the experimental and theoretical m/z values for the structures assigned to the peaks in Figure 3b.

Structure	m/z_{exp}	m/z_{theor}	$\Delta m/z$
A	441.32	441.27	0.05
B	829.16	828.77	0.39
C	971.20	971.30	0.1
D	1109.12	1109.19	0.07
E	1243.36	1243.02	0.34
F	1389.32	1389.58	0.26
G	1569.32	1569.51	0.19
H	1919.28	1919.6	0.32

Table S3. Summary of conditions for the rDA reactions of **7** in acetonitrile ($c = 20 \text{ mg mL}^{-1}$) at 120, 140, 160, 180, and 219 °C and the calculated percentage of debonding.

<i>Temperature /</i> °C	<i>Time /</i> min	$M_n^a /$ g mol ⁻¹	DP_n	<i>Debonding / %</i>
120	0	4800	10.1	9.88
	10	4400	9.28	10.8
	30	3600	7.59	13.2
	60	2800	5.91	16.9
	160	2100	4.43	22.6
140	10	3200	6.75	14.8
	30	3100	6.54	15.3
	60	2400	5.06	19.8
	160	2000	4.22	23.7
160	10	2800	5.91	16.9
	30	2200	4.64	21.5
	60	1900	4.01	24.9
	160	1600	3.38	29.6
180	30	1100	2.31	43.1
219	30	800	1.69	59.3

^arelative to linear poly(styrene) standards.

Table S4. Zero-point-energy (ZPE), thermal correction (TC), entropy (S), electronic energy at 0K (E(0K), at the employed level of theories).

	ZPE ^a	TC ^a	S ^a	E (0 K) /Hartree	
				B3LYP 6- 311+G(3df,2p)	MP2 GTMP2Large
	kJ/mol	kJ/mol	J/mol.K		
1	1167.3	100.3	1046.1	-3430.34758	-
2	1530.8	93.3	954.6	-1348.31321	-
3-13	2714.8	188.4	1711.5	-4778.67224	-
14	523.2	37.2	494.2	-518.05807	-516.81214
15	355.8	38.7	504.1	-1521.55198	-1519.21582
16	893.9	71.7	754.7	-2039.62049	-2036.08524

^aZPE, TC and S are calculated at B3LYP/6-31G(d) level of theory.

Table S5. G3MP2//B3LYP Zero-point-energy (ZPE), thermal correction (TC), entropy (S) and electronic energy (E(0K) for the core system)^a.

	ZPE ^a	TC ^a	S ^a	E (0 K)		
				QCISD(T)/6-31G(d)	MP2/6-31G(d)	MP2/GTMP2Large
				Hartree	Hartree	Hartree
14-core	220.1	14.7	276.3	-155.46711	-155.42260	-155.61408
15-core	144.1	16.3	310.6	-873.63815	-873.57249	-873.83903
16-core	381.3	26.6	395.9	-1029.17415	-1029.05031	-1029.50762

^a The core system is:

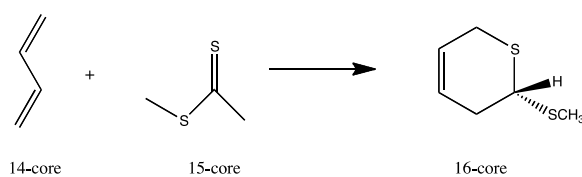


Table S6. B3LYP/6-31G(d) Optimized Geometries As Gaussian Archives.

1

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2

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3-13

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610727524, -6.0064275664, 3.6000235495\N, 0.1176601024, -6.7543851271, 5.29
36104886\H, -0.3760490543, -6.997879431, 3.3126147535\C, -0.5231702538, -7.
9039550739, 5.6590237029\H, 0.8174981299, -6.4076151676, 5.9332483703\O, -0
.1461768807, -8.2578751727, 6.9188183502\O, -1.3216290524, -8.5202776069, 4
.9748676638\C, -0.7768517505, -9.4532676006, 7.4397213863\C, -0.572436019,
-9.4775738574, 8.918560036\H, -1.8385957521, -9.4218400408, 7.1703131583\H
, -0.3377402493, -10.3334023563, 6.9566743547\C, 0.0017816093, -10.49582713
37, 9.5800737308\H, -0.9451651702, -8.6131652849, 9.467911652\C, 0.16344279
57, -10.5576237036, 11.0239107467\H, 0.3759080151, -11.3496176337, 9.012470
9021\C, 0.7321761222, -11.58546379, 11.6761042626\H, -0.2054770079, -9.7041
297313, 11.5947969661\C, 0.9159857796, -11.6708115607, 13.1610444957\H, 1.0
958926802, -12.4343749703, 11.0944798177\H, 0.4067126884, -12.5519746659, 1
3.5752805289\H, 1.9777433842, -11.7731107884, 13.4247431229\H, 0.524436564
9, -10.7826098841, 13.6680673614\Version=EM64L-G03RevE.01\State=1-A\HF=
-4777.5461047\RMSD=2.308e-09\RMSF=7.265e-06\Thermal=0.\Dipole=-0.04145
78, 0.783754, -0.1719529\PG=C01 [X(C42H66N2O10P2S4)]\@

14

1\1\GINC-X130\FOpt\RB3LYP\6-31G(d)\C8H13N1O2\MXN501\18-Apr-2011\0\#b3
lyp/6-31G* OPT Freq=Noraman maxdisk=134217728\title\0,1\C, -0.0215114
437, -0.0620384372, 0.0106818689\C, -0.0126340584, 0.0743950618, 1.50319435
69\C, 1.0701099612, -0.0586795174, 2.2875434043\C, 1.0511596436, 0.07499616
75, 3.7355085303\C, 2.1277901702, -0.04909909, 4.5289640323\C, 2.0990606767
, 0.1432992736, 6.0093204031\O, 2.6158478124, -1.0606311782, 6.6268022319\C
, 2.8800419503, -0.9531866661, 7.9563848247\H, -0.9717469117, 0.3001772417,
1.9727747372\H, 2.0348515532, -0.2825574402, 1.8295979612\H, 0.0838633874,
0.2971538333, 4.1894799677\H, 3.1008376752, -0.2778025919, 4.0942445073\H,
1.0835903954, 0.3306154986, 6.374801329\H, 2.725388716, 0.9846087783, 6.327
4435782\H, -0.7020723194, -0.8623645465, -0.311486171\H, 0.9762558238, -0.2
871659417, -0.3804233811\H, -0.3762198062, 0.8597060816, -0.4709321544\O, 2
.6916898412, 0.0525781157, 8.6189974049\N, 3.405308508, -2.1148153715, 8.44
84052629\H, 3.4905420771, -2.115992208, 9.4541934066\C, 3.4648113512, -3.38
12151739, 7.7368424063\H, 4.1407610811, -4.051922385, 8.2742537561\H, 2.483

2576564,-3.8670606818,7.6490212999\H,3.8596583833,-3.2225886402,6.7315
829422\\Version=EM64L-G03RevE.01\State=1-A\HF=-517.8641665\RMSE=6.790e
-09\RMSE=2.096e-06\Thermal=0.\Dipole=-0.0632223,-0.8719039,-0.7009787\
PG=C01 [X(C8H13N1O2)]\\@

15

1\1\GINC-X8\FOpt\RB3LYP\6-31G(d)\C4H9O3P1S2\MXN501\01-Apr-2011\0\\#b31
yp/6-31G* OPT Freq=Noraman maxdisk=134217728\\title\\0,1\P,-0.14455307
52,0.1925037186,0.1277372157\O,0.4557365844,0.0110934037,1.4668254813\
O,0.8735589069,0.362753873,-1.1098210447\O,-1.0763842563,1.5184074784,
-0.0194127854\C,2.0760350181,1.1410661718,-0.9199124801\H,2.5902054254
,0.8296085916,-0.0077129924\H,2.7027036476,0.9483996547,-1.7916247458\
H,1.829004429,2.2058004768,-0.8667932456\C,-1.8174928206,1.9906153759,
1.1262605624\H,-1.1977980258,1.9550906642,2.0247583704\H,-2.1031884016
,3.0196814839,0.901580553\H,-2.7165108304,1.3826588671,1.2708605547\C,
-1.2107255048,-1.1941335055,-0.4868566394\S,-1.4667360312,-2.472099038
1,0.5147918615\S,-1.9984430911,-1.1749130084,-2.0501372507\C,-1.533206
9011,0.3573320127,-2.9465445562\H,-0.4812736126,0.3402530947,-3.229675
6315\H,-1.7517095539,1.2441976547,-2.3515829611\H,-2.1618531018,0.3454
170715,-3.8411244023\\Version=EM64L-G03RevE.01\State=1-A\HF=-1521.2738
653\RMSE=7.996e-09\RMSE=9.572e-06\Thermal=0.\Dipole=0.0077595,1.750565
2,-1.1632304\PG=C01 [X(C4H9O3P1S2)]\\@

16

N-N= 2.468841553926D+03 E-N=-9.744787489070D+03 KE= 2.026793061114D+03
1\1\GINC-X126\FOpt\RB3LYP\6-31G(d)\C12H22N1O5P1S2\MXN501\18-Apr-2011\0
\\#b31yp/6-31G* OPT Freq=Noraman maxdisk=536870912\\title\\0,1\C,0.641
0208758,1.8162221471,-0.6293877658\C,0.6009676734,0.6779522886,0.37154
34155\C,-0.8251285658,0.1093046322,0.6547546947\S,-1.9798027598,1.5203
297585,0.9859099688\C,-1.7871481149,2.5439739069,-0.5386884486\C,-0.36
20170345,2.6082980906,-1.0073678767\C,1.6492493595,-0.3866353577,-0.00
47844376\O,2.930747402,0.252486225,0.1698361123\C,4.0042755239,-0.5138
175332,-0.1709220409\S,-0.6755251057,-0.8702919563,2.240305176\C,-2.39
86247191,-1.114396163,2.8205076027\O,-1.5567278629,-1.0612577488,-0.59
81524972\O,-0.462554512,-2.2335436814,-0.8416391231\C,-0.644156296,-3.
5594043825,-0.3064745814\C,-2.3527081079,3.9349788518,-0.2147129478\O,
-2.9160066135,-1.5710136973,-0.2730502217\O,-1.4150678125,-0.219500512
3,-1.9699620548\C,-1.889467951,-0.811649017,-3.1947508974\H,-2.4017272
981,2.0882580753,-1.3241686723\H,-2.3120312907,-1.8252169481,3.6476956
21\H,-3.0173542748,-1.5337527626,2.0265485272\H,-2.8272652698,-0.18226
38409,3.1927892656\H,-0.1630453863,3.3823493249,-1.749976339\H,1.62716
60606,1.9895386372,-1.0535969222\H,0.9294931585,1.0835192332,1.3393719
019\H,-1.7848310117,-0.0462769726,-3.9653545073\H,-1.2796334189,-1.682
7117161,-3.4524558493\H,-2.9387107276,-1.1047080178,-3.0973332678\H,-1
.707479124,-3.7929344284,-0.2164362922\H,-0.1626193938,-4.2448753059,-
1.0070635897\H,-0.162960963,-3.6266606644,0.6725831969\H,-2.3210706493
,4.5630399483,-1.1131176661\H,-3.3954541937,3.8734154992,0.1147246497\
H,-1.7672144764,4.4256519868,0.5692183758\H,1.5977450493,-1.2627155461
,0.6445272218\H,1.5499120172,-0.7252413231,-1.0369904466\O,3.928369430
1,-1.6444871357,-0.6172957886\N,5.1743469546,0.1447608934,0.0761458458
\H,5.9875599212,-0.3463417426,-0.2643540693\C,5.3002539553,1.540763064
5,0.4602067023\H,6.3139921756,1.7099746156,0.8330137802\H,5.1146934526
,2.2301183098,-0.3751443532\H,4.5938319242,1.771555965,1.2599905984\\V
ersion=EM64L-G03RevE.01\State=1-A\HF=-2039.1641526\RMSE=9.903e-09\RMSE
=3.971e-06\Thermal=0.\Dipole=0.6367924,0.8117886,-0.6149505\PG=C01 [X(
C12H22N1O5P1S2)]\\@

14-core:

1\1\GINC-X149\FOpt\RB3LYP\6-31G(d)\C5H6\MXN501\17-May-2010\0\\#g3mp2b3
maxdisk=268435456\\title\\0,1\C,0.,0.73493267,0.99130253\C,0.,-0.7349
3267,0.99130253\C,0.,1.18099709,-0.28166353\C,0.,0.,-1.2173806\C,0.,-1.
.18099709,-0.28166353\H,-0.87820124,0.,-1.88159249\H,0.87820124,0.,-1.
88159249\H,0.,2.21380099,-0.61089219\H,0.,1.34726002,1.88744438\H,0.,-

1.34726002,1.88744438\H,0.,-2.21380099,-0.61089219\\Version=EM64L-G03RevE.01\State=1-A1\HF=-194.1010581\RMSD=1.913e-09\RMSF=3.261e-05\Thermal=0.\Dipole=0.,0.,0.1720201\PG=C02V [C2(C1),SGV(C4H4),SGV'(H2)]\\@

15-core

1\1\GINC-X141\FOpt\RB3LYP\6-31G(d)\C2H4S2\MXN501\26-Feb-2010\0\#g3mp2
b3 maxdisk=1342177280\\title\\0,1\C,-0.0194608066,0.,0.0276476607\S,0.0601817878,0.,1.6629641274\H,0.8861332587,0.,-0.5849958384\S,-1.4096810566,0.,-1.0149352678\C,-2.8034539814,0.,0.1564703315\H,-3.7137451066,0.,-0.4473034278\H,-2.7660024325,-0.8910208319,0.7867805217\H,-2.7660024325,0.8910208319,0.7867805217\\Version=EM64L-G03RevE.01\State=1-A'\HF=-874.987138\RMSD=4.590e-09\RMSF=6.179e-05\Thermal=0.\Dipole=0.7171458,-0.5312955,0.\PG=CS [SG(C2H2S2),X(H2)]\\@

16-core:

1\1\GINC-X150\FOpt\RB3LYP\6-31G(d)\C6H10S2\MXN501\25-Mar-2010\0\#g3mp2
b3 maxdisk=5368709120\\title\\0,1\C,-0.0026566346,0.2035157308,-0.0021200229\C,0.0085193102,0.0385570258,1.5193177701\C,1.3964350065,-0.0749178151,2.1034264084\C,2.5385790063,0.2698818824,1.5020765195\C,2.6748168877,0.873376965,0.1300325873\S,1.1094752583,1.5825626224,-0.5250876434\H,3.4783101949,0.107665812,2.0299875867\H,1.4454345522,-0.4857243942,3.1107761084\H,-0.5645512372,-0.8643099095,1.7728941845\H,-0.5231202252,0.880110018,1.986845728\H,3.0791908399,0.1392480884,-0.5808018845\H,3.3851862225,1.7080662458,0.1536676573\S,-1.714752442,0.5062288075,-0.5729954459\H,0.358696573,-0.7185977505,-0.4713359019\C,-1.5474149706,0.1376466129,-2.3556823257\H,-2.5289797184,0.3149451491,-2.8029519358\H,-0.814568619,0.7968200948,-2.8266236846\H,-1.2681917261,-0.9078030706,-2.5177617234\\Version=EM64L-G03RevE.01\State=1-A'\HF=-1031.0156602\RMSD=6.796e-09\RMSF=2.557e-05\Thermal=0.\Dipole=0.5456309,-0.7390349,-0.0428827\PG=C01 [X(C6H10S2)]\\@