Synthesis of Twist-twist Pi Conjugated Di-sec-alkylstilbenes and Stilbene Polymers

James E. Gano*, D.J. Osborn III, Nagendra Kodali, Padmanabhan Sekher, Min Liu,

Eddie D. Luzik, Jr.

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Figure S1. ¹H NMR spectrum of **4e**

Figure S2. ¹H NMR spectrum of **5e**

Figure S3. ¹H NMR spectrum of **5d**

Figure S4. ¹H NMR spectrum of **5c**

Figure S5. ¹H NMR spectrum of **7e**

Figure S7. ¹H NMR spectrum of **7c**

Figure S8. ¹³C NMR spectrum of 4e

Figure S9. ¹³C NMR spectrum of 5e

S10

Figure S10. ¹³C NMR spectrum of **5d**

S11

Figure S11. ¹³C NMR spectrum of **5c**

S12

Figure S12. ^{13}C NMR spectrum of **7e**.

Figure S13. ¹³C NMR spectrum of **7d**

S15

Figure S14. ¹³C NMR spectrum of 7c

S15 Macspartan/MOPAC output for 5a syn,syn trans

MacSPARTAN semi-empirical program: Release 1.0

Geometry Optimization

AM1

Number of basis functions: 104

Number of electrons: 104

Total molecular charge: 0

Multiplicity: 1

Point group: C1

Number of independent degrees of freedom: 126

No useable symmetry or symmetry intentionally disabled

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	0.4818949	-0.4728124	-0.0116328
C	2	0.1661688	-1.9097213	-0.0114380
C	3	-0.4113541	-4.6510899	-0.0110122
C	4	0.0208923	-2.6030494	1.1978388
C	5	0.0228555	-2.6038343	-1.2205020
C	6	-0.2651824	-3.9675467	-1.2178203
C	7	-0.2671475	-3.9667660	1.1955826
H	8	0.1384808	-2.0642301	2.1499014
H	9	0.1419825	-2.0656372	-2.1727242
H	10	-0.3770585	-4.5044746	-2.1711417
H	11	-0.3805796	-4.5030614	2.1490761
H	12	-0.6391423	-5.7267398	-0.0108561
C	13	-0.4818846	0.4728174	-0.0122183
C	14	1.9454904	-0.1299914	-0.0111483
C	15	2.6286807	-0.6584573	-1.2580009
C	16	2.6285155	-0.6608309	1.2347829
H	17	2.0532513	0.9946045	-0.0100417
H	18	2.1538179	-0.2295301	-2.1727128
H	19	2.5514281	-1.7716617	-1.3080420
H	20	3.7085425	-0.3749887	-1.2488937
H	21	2.5511298	-1.7741110	1.2827785
H	22	2.1536212	-0.2335514	2.1502506
H	23	3.7084030	-0.3774505	1.2262956
C	24	-1.9454785	0.1299913	-0.0125780
C	25	-0.1661585	1.9097267	-0.0124131
C	26	0.4113299	4.6511028	-0.0128470
C	27	-0.0216061	2.6035817	1.1966444
C	28	-0.0221189	2.6033146	-1.2216952
C	29	0.2659036	3.9670265	-1.2194455
C	30	0.2664081	3.9673062	1.1939574
H	31	-0.1397286	2.0651827	2.1488777
H	32	-0.1406962	2.0646833	-2.1737410
H	33	0.3783490	4.5035359	-2.1729358
H	34	0.3792531	4.5040220	2.1472852
H	35	0.6390826	5.7267603	-0.0130299
C	36	-2.6287361	0.6610595	-1.2582666
C	37	-2.6284457	0.6582125	1.2344940
H	38	-2.0532272	-0.9945923	-0.0138795
H	39	-2.1535831	0.2344960	-2.1739225
H	40	-2.5519750	1.7744020	-1.3057105
H	41	-3.7084727	0.3770781	-1.2499446
H	42	-2.5504553	1.7713209	1.2851665
H	43	-2.1539592	0.2284555	2.1490001
H	44	-3.7084908	0.3754477	1.2251272

Heat of Formation: 35.341 kcal/mol

S16 Macspartan/MOPAC output for 5a syn, anti trans

MacSPARTAN semi-empirical program: Release 1.0

Geometry Optimization

AM1

Number of basis functions: 104

Number of electrons: 104

Total molecular charge: 0

Multiplicity: 1

Point group: C1

Number of independent degrees of freedom: 126

No useable symmetry or symmetry intentionally disabled

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	-0.0751592	1.7749180	-0.0079416
C	2	-0.9572936	2.9518562	-0.0044443
C	3	-2.5577916	5.2545339	0.0099950
C	4	-1.3215600	3.5718619	-1.2081386
C	5	-1.3938904	3.5064502	1.2070928
C	6	-2.1918366	4.6493721	1.2118055
C	7	-2.1201837	4.7141894	-1.1988323
H	8	-0.9691390	3.1520937	-2.1625121
H	9	-1.1013772	3.0335801	2.1568127
H	10	-2.5312354	5.0746504	2.1676374
H	11	-2.4029607	5.1907909	-2.1488585
H	12	-3.1873837	6.1558755	0.0155128
C	13	-0.5113179	0.4975800	-0.0399203
C	14	1.3946167	2.1089587	0.0262622
C	15	1.7676105	2.7771535	1.3361072
C	16	1.7885282	2.9838689	-1.1481116
H	17	1.9906482	1.1526760	-0.0507591
H	18	1.5294489	2.1045319	2.1951137
H	19	1.2046177	3.7329350	1.4667942
H	20	2.8610906	3.0023404	1.3502025
H	21	1.2640318	3.9689014	-1.1030080
H	22	1.5227127	2.4851865	-2.1108353
H	23	2.8901323	3.1658562	-1.1316139
C	24	-1.9445433	0.0434108	-0.0994999
C	25	0.4306035	-0.6371240	-0.0258359
C	26	2.1542614	-2.8445347	0.0043086
C	27	0.5701682	-1.4424979	-1.1645280
C	28	1.1597481	-0.9500429	1.1289519
C	29	2.0153822	-2.0503508	1.1421978
C	30	1.4317270	-2.5375363	-1.1486615
H	31	-0.0066969	-1.2046368	-2.0709108
H	32	1.0555051	-0.3196152	2.0247860
H	33	2.5822442	-2.2909770	2.0534680
H	34	1.5397490	-3.1616103	-2.0478309
H	35	2.8310696	-3.7109718	0.0161019
C	36	-2.6377914	0.4937079	-1.3696661
C	37	-2.7334392	0.4577637	1.1256994
H	38	-1.9375535	-1.0892381	-0.1164760
H	39	-2.0519064	0.1742576	-2.2649377
H	40	-2.7477889	1.6045747	-1.3926850
H	41	-3.6552444	0.0364765	-1.4267451
H	42	-2.8654907	1.5660166	1.1598069
H	43	-2.2084640	0.1320796	2.0553264
H	44	-3.7439985	-0.0175331	1.1014669

Heat of Formation: 37.176 kcal/mol

S17 Macspartan/MOPAC output for 5a anti,anti trans

MacSPARTAN semi-empirical program: Release 1.0

Geometry Optimization

AM1

Number of basis functions: 104

Number of electrons: 104

Total molecular charge: 0

Multiplicity: 1

Point group: C1

Number of independent degrees of freedom: 126

No useable symmetry or symmetry intentionally disabled

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	0.3105791	1.9057876	0.0007245
C	2	0.5072378	0.4439330	0.0008249
C	3	-0.5072378	-0.4439330	0.0008249
C	4	1.9769194	0.1035689	0.0003069
C	5	-1.9769194	-0.1035689	0.0003069
C	6	-0.3105791	-1.9057876	0.0007245
C	7	0.1015528	4.6998138	0.0006182
C	8	0.2679761	2.6132077	-1.2084403
C	9	0.2647559	2.6130660	1.2098738
C	10	0.1560886	4.0026904	1.2072729
C	11	0.1592080	4.0028435	-1.2059467
H	12	0.3221320	2.0650810	-2.1610047
H	13	0.3160982	2.0647897	2.1624975
H	14	0.1166357	4.5495243	2.1607339
H	15	0.1222335	4.5498006	-2.1594352
H	16	0.0165412	5.7960060	0.0005958
C	17	-0.1015528	-4.6998138	0.0006182
C	18	-0.2679761	-2.6132077	-1.2084403
C	19	-0.2647559	-2.6130660	1.2098738
C	20	-0.1560886	-4.0026904	1.2072729
C	21	-0.1592080	-4.0028435	-1.2059467
H	22	-0.3221320	-2.0650810	-2.1610047
H	23	-0.3160982	-2.0647897	2.1624975
H	24	-0.1166357	-4.5495243	2.1607339
H	25	-0.1222335	-4.5498006	-2.1594352
H	26	-0.0165412	-5.7960060	0.0005958
C	27	-2.3987486	0.6451486	1.2477331
H	28	-2.5469861	-1.0828324	0.0031393
C	29	-2.3982970	0.6380064	-1.2515808
H	30	-1.9658033	1.6670599	-1.2731915
C	31	2.3982970	-0.6380064	-1.2515808
C	32	2.3987486	-0.6451486	1.2477331
H	33	2.0572428	-0.0878383	-2.1613102
H	34	1.9658033	-1.6670599	-1.2731915
H	35	3.5116661	-0.7231906	-1.2818973
H	36	-3.5116661	0.7231906	-1.2818973
H	37	-2.0572428	0.0878383	-2.1613102
H	38	2.5469861	1.0828324	0.0031393
H	39	2.0515583	-0.1042822	2.1606875
H	40	3.5125413	-0.7237783	1.2809257
H	41	1.9727035	-1.6770289	1.2599394
H	42	-2.0515583	0.1042822	2.1606875
H	43	-3.5125413	0.7237783	1.2809257
H	44	-1.9727035	1.6770289	1.2599394

Heat of Formation: 39.579 kcal/mol

S18 Macspartan/MOPAC output for 6a syn, syn cis

MacSPARTAN semi-empirical program: Release 1.0

Geometry Optimization

AM1

Number of basis functions: 104

Number of electrons: 104

Total molecular charge: 0

Multiplicity: 1

Point group: C1

Number of independent degrees of freedom: 126

No useable symmetry or symmetry intentionally disabled

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	0.4833721	-0.4665420	0.0498396
C	2	1.9105960	-0.1129976	0.1070935
C	3	4.6341374	0.5346559	0.2167925
C	4	2.6970468	-0.1587672	-1.0518871
C	5	2.5019854	0.2599019	1.3218222
C	6	3.8568980	0.5821179	1.3738029
C	7	4.0517530	0.1642671	-0.9948387
H	8	2.2396822	-0.4470569	-2.0099865
H	9	1.8902610	0.3005093	2.2351114
H	10	4.3123806	0.8763854	2.3305778
H	11	4.6610826	0.1281782	-1.9096441
H	12	5.7025241	0.7904920	0.2595798
C	13	-0.4754808	0.4772467	-0.0734457
C	14	0.1751118	-1.9352249	0.1340599
C	15	1.1576141	-2.6726517	1.0233809
C	16	0.1539047	-2.5578212	-1.2500398
H	17	-0.8479562	-2.0605517	0.5960756
H	18	1.2216463	-2.1807969	2.0237347
H	19	2.1772734	-2.6784658	0.5681257
H	20	0.8239310	-3.7292112	1.1617316
H	21	1.1527342	-2.4552232	-1.7392109
H	22	-0.6095135	-2.0584397	-1.8933714
H	23	-0.0951787	-3.6436341	-1.1751874
C	24	-1.9391169	0.1458343	-0.1576003
C	25	-0.1446441	1.9099282	-0.1301160
C	26	0.4597466	4.6434535	-0.2382180
C	27	-0.1983807	2.6939201	1.0301931
C	28	0.2142607	2.5088193	-1.3453781
C	29	0.5149466	3.8687053	-1.3965589
C	30	0.1031589	4.0536050	0.9739490
H	31	-0.4758241	2.2307046	1.9886905
H	32	0.2608632	1.8991784	-2.2597701
H	33	0.7983279	4.3301260	-2.3537796
H	34	0.0609898	4.6609816	1.8897904
H	35	0.6986295	5.7157784	-0.2803953
C	36	-2.6918593	1.1158354	-1.0477953
C	37	-2.5612595	0.1161879	1.2265590
H	38	-2.0483906	-0.8794872	-0.6186675
H	39	-2.2008274	1.1870272	-2.0480703
H	40	-2.7140807	2.1355785	-0.5932488
H	41	-3.7429247	0.7652362	-1.1862170
H	42	-2.4725348	1.1164753	1.7154866
H	43	-2.0511835	-0.6400540	1.8699826
H	44	-3.6434912	-0.1480737	1.1518871

Heat of Formation: 36.888 kcal/mol

S19 Macspartan/MOPAC output for 6a syn, anti cis

MacSPARTAN semi-empirical program: Release 1.0

Geometry Optimization

AM1

Number of basis functions: 104

Number of electrons: 104

Total molecular charge: 0

Multiplicity: 1

Point group: C1

Number of independent degrees of freedom: 126

No useable symmetry or symmetry intentionally disabled

		Cartesian Coordinates (Angstroms)		
Atom		X	Y	Z
C	1	0.4763705	-0.5252349	-0.0493613
C	2	1.9041514	-0.1547135	-0.0488259
C	3	4.6253142	0.5133211	-0.0405486
C	4	2.6196993	-0.0805527	-1.2516846
C	5	2.5664776	0.1049141	1.1584490
C	6	3.9198149	0.4388224	1.1599508
C	7	3.9731063	0.2523578	-1.2453028
H	8	2.1065377	-0.2878211	-2.2027528
H	9	2.0117063	0.0449372	2.1065597
H	10	4.4305048	0.6451825	2.1118686
H	11	4.5264217	0.3099736	-2.1939501
H	12	5.6924485	0.7778224	-0.0375059
C	13	-0.4845127	0.4232871	-0.0714336
C	14	0.2230568	-2.0049959	-0.0055484
C	15	0.7715224	-2.6096792	1.2738675
C	16	0.8133321	-2.6993820	-1.2186460
H	17	-0.8873033	-2.1977647	-0.0191019
H	18	0.2772872	-2.1476128	2.1621225
H	19	1.8724833	-2.4386014	1.3516293
H	20	0.5787348	-3.7092963	1.2878581
H	21	1.9234668	-2.5800129	-1.2428067
H	22	0.3884256	-2.2674744	-2.1564867
H	23	0.5733721	-3.7894302	-1.1854451
C	24	-1.9721374	0.2044095	-0.0585931
C	25	-0.1315360	1.8553511	-0.1036314
C	26	0.4600073	4.5927046	-0.1651980
C	27	-0.4408394	2.6725854	0.9928608
C	28	0.4724809	2.4235460	-1.2319549
C	29	0.7646029	3.7863939	-1.2611445
C	30	-0.1412090	4.0327565	0.9621714
H	31	-0.9216370	2.2321186	1.8791415
H	32	0.7263089	1.7855352	-2.0918568
H	33	1.2393771	4.2241647	-2.1513244
H	34	-0.3808186	4.6655514	1.8291030
H	35	0.6937761	5.6667333	-0.1887910
C	36	-2.4533158	-0.4587031	1.2166965
C	37	-2.4653823	-0.5085959	-1.3015571
H	38	-2.4582080	1.2297504	-0.0748536
H	39	-2.1905700	0.1784424	2.0965113
H	40	-1.9969238	-1.4640464	1.3719494
H	41	-3.5636742	-0.5782608	1.1838383
H	42	-1.9785336	-1.5017892	-1.4427502
H	43	-2.2494394	0.1115728	-2.2054098
H	44	-3.5696278	-0.6644038	-1.2339672

Heat of Formation: 38.356 kcal/mol

S20 Macspartan/MOPAC output for 6a anti, anti cis

MacSPARTAN semi-empirical program: Release 1.0

Geometry Optimization

AM1

Number of basis functions: 104

Number of electrons: 104

Total molecular charge: 0

Multiplicity: 1

Point group: C1

Number of independent degrees of freedom: 126

No useable symmetry or symmetry intentionally disabled

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	0.6457085	-0.8056027	0.1314557
C 2	-0.7449030	-0.3300886	0.3364350
C 3	-3.3941651	0.4734805	0.7514431
C 4	-1.1701509	0.0731491	1.6088975
C 5	-1.6591468	-0.3357168	-0.7243036
C 6	-2.9775154	0.0664018	-0.5155312
C 7	-2.4885385	0.4763924	1.8122833
H 8	-0.4572375	0.0733471	2.4463624
H 9	-1.3307388	-0.6544590	-1.7246294
H 10	-3.6892524	0.0628913	-1.3538964
H 11	-2.8143519	0.7969904	2.8125465
H 12	-4.4338803	0.7918200	0.9138538
C 13	1.5556474	0.0599960	-0.3629865
C 14	0.7541548	-2.2502475	0.5320939
C 15	1.9268417	-2.5946444	1.4217620
C 16	0.6662504	-3.1747605	-0.6663260
H 17	-0.1675148	-2.4668636	1.1621757
H 18	2.0585638	-1.8164506	2.2116384
H 19	2.8764272	-2.6912284	0.8460269
H 20	1.7347762	-3.5760561	1.9226363
H 21	1.5655537	-3.0938553	-1.3196345
H 22	-0.2361320	-2.9237455	-1.2756024
H 23	0.5800173	-4.2327436	-0.3181168
C 24	3.0093459	-0.1054207	-0.7073404
C 25	1.1305028	1.4557624	-0.6336150
C 26	0.4231529	4.1104262	-1.1712999
C 27	0.7379761	1.8352262	-1.9237189
C 28	1.1734291	2.4179781	0.3829735
C 29	0.8190380	3.7389443	0.1131330
C 30	0.3830117	3.1566881	-2.1882491
H 31	0.7065409	1.0840356	-2.7264468
H 32	1.4846706	2.1260947	1.3968585
H 33	0.8517556	4.4886640	0.9170178
H 34	0.0705925	3.4466191	-3.2020080
H 35	0.1426766	5.1524083	-1.3818558
C 36	3.3476727	-1.3193951	-1.5423677
C 37	3.8943315	-0.0015871	0.5193078
H 38	3.2761997	0.7859844	-1.3611152
H 39	2.5899088	-1.4604601	-2.3502600
H 40	3.4013440	-2.2488051	-0.9292943
H 41	4.3483461	-1.1721459	-2.0197723
H 42	3.7535474	-0.8669878	1.2072775
H 43	3.6594991	0.9361247	1.0798220
H 44	4.9664652	0.0272860	0.2067614

Heat of Formation: 44.128 kcal/mol

(E)-7,10-Dibutyl-8,9-diphenyl-8-hexadecene, 5d. Yield = 4.6 g (12 %): *mp* 75-88.2 °C; FTIR

(KBr) 3067m, 738m, 702s cm⁻¹; MS (*m/z*) 488 (M⁺), 91 (100 %); ¹H NMR (400 MHz): δ 7.33 (t, *J* = Hz, 4H), 7.26 (t, *J* = Hz, 2H), 7.08 (d, *J* = Hz, 4H), 2.17 - 2.06 (m, 2H), 1.41-0.99 (m, 32H), 0.87 ppm (m, 12H); ¹³C NMR (100 MHz) δ 142.2, 139.8, 130.2, 127.3, 126.0, 42.7, 33.7, 33.7, 33.4, 33.4, 32.0, 32.0, 30.3, 29.6, 29.6, 28.0, 28.0, 22.9, 22.7, 22.7, 14.2, 14.1 ppm; HRMS ESI calcd for C₃₂H₄₈ + Na 455.3654, found 455.3622.

(E)-5,8-Dibutyl-6,7-diphenyl-6-dodecene, 5c. Yield = 4.2 g (61 %): *mp* = 110-112 °C; FTIR

(KBr) 3048m, 741m, 701s cm⁻¹; MS (*m/z*, %) 432 (M⁺, 14), 91 (100); ¹H NMR (400 MHz) δ = 0.80 (t, 12H, *J* = 6.9 Hz), 0.84-0.94 (m, 4H), 1.00-1.13 (m, 16H), 1.25-1.33 (m, 4H), 2.00-2.04 (m, 2H), 7.02 (d, 4H, *J* = 6.9 Hz), 7.19 (t, 2H, *J* = 7.8 Hz), 7.26 (t, 4H, *J* = 7.0 Hz); ¹³C NMR (100 MHz) δ = 14.2, 22.9, 30.3, 33.3, 42.7, 126.0, 127.3, 130.1, 139.8, 142.1; UV (Hexane, nm, ε) 264 (500), 258 (700), 226 (shoulder); ANAL calcd for C₃₂H₄₈: C, 88.81; H, 11.19; found: C, 89.07; H, 10.86.

(E)-4,7-Dipropyl-5,6-diphenyldec-5-ene, 5b. Yield = 80%: *mp* = 108-110 °C; MS (*m/z*, %)

376 (M⁺, 24), 91 (100); ¹H NMR (400 MHz) δ = 0.70 (t, 12H, *J* = 7.2 Hz), 0.80-0.95 (m, 4H), 0.98-1.20 (m, 8H), 1.25-1.40 (m, 4H), 2.05-2.15 (m, 2H), 7.01 (d, 4H, *J* = 8.4 Hz), 7.18 (t, 2H, *J* = 8.4 Hz), 7.26 (t, 4H); ¹³C NMR (100 MHz) δ = 14.4, 21.1, 35.9, 42.4, 126.0, 127.3, 130.1, 139.8, 142.2; UV (Hexane, nm, ε) λ = 264 (600), 258 (800), 224 (shoulder); ANAL calcd for C₂₈H₄₀: C, 89.29; H, 10.71; found C, 88.93; H, 10.44.

(E)-7,10-Dibutyl-8,9-di(4-iodophenyl)-8-hexadecene, 7d. Yield = 401 mg (79 %): *mp* 82 - 84

$^{\circ}\text{C}$, MS (m/z) 740(M^+ , 100 %); ^1H NMR (400 MHz) δ 7.64 (d, J = 8.00 Hz 4H), 6.77 (d, J = 8.40 Hz, 4H), 2.06 (m, 2H), 1.42 - 0.90 (m, 32H), 0.86 ppm (m, 12H); ^{13}C NMR (100 MHz) δ 141.7, 139.0, 136.5, 132.0, 91.9, 42.8, 33.6, 33.6, 33.2, 33.2, 32.0, 30.3, 29.6, 29.6, 28.0, 28.0, 22.9, 22.7, 22.7, 14.1 ppm; HRMS calcd for $\text{C}_{36}\text{H}_{54}\text{I}_2$ 740.2319, found 740.2322.

(E)-5,8-Dibutyl-6,7-di(4-iodophenyl)-6-dodecene, 7c. Yield = 378 mg (80 %): *mp* 145 - 150

$^{\circ}\text{C}$, MS (m/z) 684(M^+ , 100 %); ^1H NMR (400 MHz) δ 7.66 (d, J = 8.40 Hz, 4H), 6.79 (d, J = 8.40 Hz, 4H), 2.06 (m 2H), 1.42-0.94 (m, 24H), 0.84 ppm (t, J = 6.40 Hz, 12H); ^{13}C NMR (100 MHz) δ 141.7, 139.0, 136.5, 132.0, 91.9, 42.8, 33.6, 33.6, 33.2, 33.2, 32.0, 30.3, 29.6, 29.6, 28.0, 28.0, 22.9, 22.7, 22.7, 14.2 ppm; HRMS calcd for $\text{C}_{40}\text{H}_{62}\text{I}_2$ 796.2945, found 796.2923; HRMS calcd for $\text{C}_{32}\text{H}_{46}\text{I}_2$ 684.1693, found 684.1662.