

Electronic Supplementary Material of the Article:

Effect of Length on the Transport and Magnetic Properties of Diradical Substituted Molecular Wires

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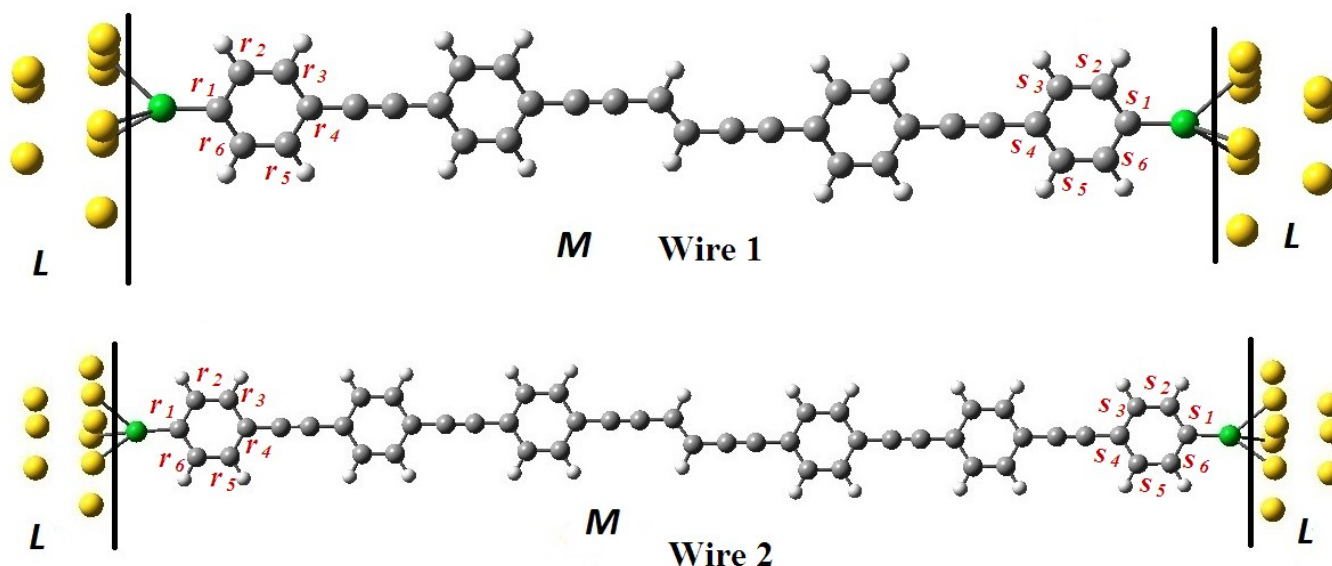


Figure S1. Molecular wire1 and molecular wire 2.

Table S1. Orbital coefficients for molecular wire 1 and wire 2 (B3LYP/6-31G(d,p)).

Atom	Site	Orbital	Molecular wire 1		Molecular wire 2	
			HOMO	LUMO	HOMO	LUMO
1	r_2	2p _z	0.0725	0.0708	-0.0477	-0.0408
2	r_3	2p _z	-0.0205	0.0142	0.0129	-0.0071
3	r_4	2p _z	-0.0863	-0.0823	0.0560	0.0464
4	r_5	2p _z	-0.0205	0.0142	0.0130	-0.0071
5	r_6	2p _z	0.0721	0.0705	-0.0477	-0.0408
6	s_2	2p _z	0.0721	-0.0705	-0.0485	0.0402
7	s_3	2p _z	-0.0205	-0.0142	0.0143	0.0082
8	s_4	2p _z	-0.0863	0.0823	0.0572	-0.0465
9	s_5	2p _z	-0.0205	-0.0142	0.0130	0.0059
10	s_6	2p _z	0.0725	-0.0708	-0.0502	0.0424

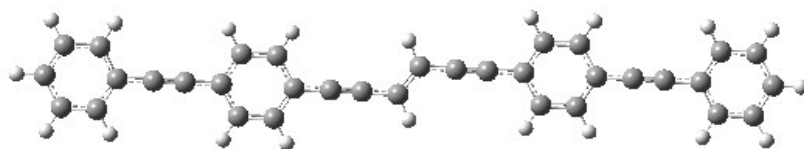
Table S2. The energy (a.u.), $\langle S^2 \rangle$ and magnetic exchange coupling constant (J in cm⁻¹) values of the diradical based molecular wire 1 (B3LYP/6-31G(d,p)).

Diradicals		Triplet	BS	J (cm ⁻¹)
1(a)	Energy (a.u)	-1384.81939	-1384.81859	168.83
	$\langle S^2 \rangle$	2.12	1.08	
1(b)	Energy (a.u)	-1384.81940	-1384.81926	30.42
	$\langle S^2 \rangle$	2.08	1.08	
1(c)	Energy (a.u)	-1384.81786	-1384.81784	4.39
	$\langle S^2 \rangle$	2.08	1.08	
1(l)	Energy (a.u)	-1384.81813	-1384.81843	-67.38
	$\langle S^2 \rangle$	2.084	1.108	
1(m)	Energy (a.u)	-1384.81680	-1384.81685	-10.21
	$\langle S^2 \rangle$	2.084	1.089	
1(n)	Energy (a.u)	-1384.815334	-1384.81534	-1.58
	$\langle S^2 \rangle$	2.076	1.077	

Table S3. The energy (a.u.), $\langle S^2 \rangle$ and magnetic exchange coupling constant (J in cm^{-1}) values of the diradical based molecular wire 2 (B3LYP/6-31G(d,p)).

Diradicals		Triplet	BS	$J(\text{cm}^{-1})$
2(a)	Energy (a.u)	-1999.26030	-1999.25949	169.36
	$\langle S^2 \rangle$	2.123	1.082	
2(b)	Energy (a.u)	-1999.25952	-1999.25938	30.42
	$\langle S^2 \rangle$	2.10	1.09	
2(c)	Energy (a.u)	-1999.25940	-1999.25938	4.39
	$\langle S^2 \rangle$	2.09	1.09	
2(d)	Energy (a.u)	-1999.26018	-1999.26017	2.19
	$\langle S^2 \rangle$	2.08	1.08	
2(e)	Energy (a.u)	-1999.25866	-1999.25866	0.15
	$\langle S^2 \rangle$	2.078	1.078	
2(l)	Energy (a.u)	-1999.25951	-1999.26173	-500.10
	$\langle S^2 \rangle$	2.076	1.100	
2(m)	Energy (a.u)	-1999.25984	-1999.26023	-85.55
	$\langle S^2 \rangle$	2.092	1.107	
2(n)	Energy (a.u)	-1999.25953	-1999.25959	-14.81
	$\langle S^2 \rangle$	2.089	1.093	
2(o)	Energy (a.u)	-1999.26034	-1999.26035	-2.57
	$\langle S^2 \rangle$	2.085	1.086	
2(p)	Energy (a.u)	-1999.26113	-1999.26113	-0.44
	$\langle S^2 \rangle$	2.079	1.079	

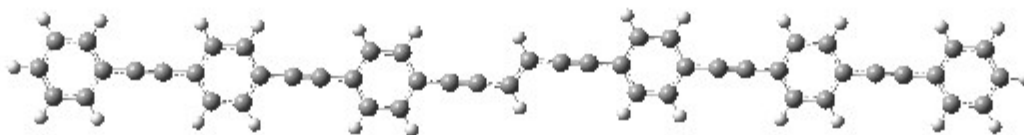
Optimized Cartesian coordinates



Wire 1

C	-0.42327800	-0.53372100	-0.00066800
C	0.42326500	0.53351400	-0.00061400
H	-0.00258700	-1.53748200	-0.00074300
H	0.00259600	1.53728300	-0.00054700

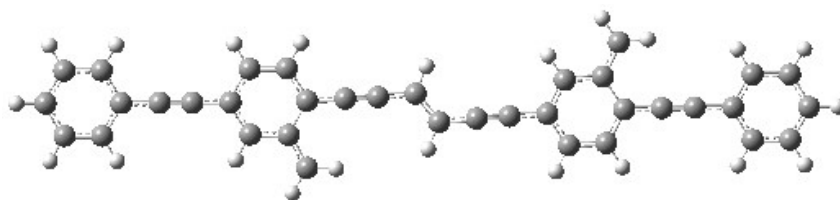
C	1.82639200	0.42554600	-0.00063100
C	3.04519500	0.36890100	-0.00064600
C	-1.82640300	-0.42577700	-0.00062400
C	-3.04520800	-0.36912800	-0.00061500
C	4.46182100	0.29407700	-0.00059800
C	5.11989700	-0.95528000	-0.00048000
C	5.24618200	1.46827100	-0.00063400
C	6.50388700	-1.02684600	-0.00037900
H	4.52709200	-1.86389500	-0.00046000
C	6.63009100	1.39590400	-0.00053300
H	4.75102600	2.43357300	-0.00073200
C	7.28764600	0.14696500	-0.00038900
H	6.99924600	-1.99203300	-0.00027800
H	7.22300100	2.30444400	-0.00055200
C	-4.46182800	-0.29424000	-0.00048400
C	-5.24624500	-1.46840500	-0.00041700
C	-5.11984700	0.95514100	-0.00041300
C	-6.63014600	-1.39597500	-0.00027800
H	-4.75112400	-2.43372500	-0.00047400
C	-6.50383700	1.02677000	-0.00027600
H	-4.52700900	1.86373500	-0.00046900
C	-7.28764700	-0.14700300	-0.00020200
H	-7.22310100	-2.30448600	-0.00022500
H	-6.99915200	1.99198000	-0.00022600
C	8.70700000	0.07322300	-0.00022600
C	9.92256000	0.01040600	0.00006700
C	-8.70699700	-0.07319700	-0.00002600
C	-9.92255400	-0.01031000	0.00015400
C	-11.34485300	0.06082200	0.00040100
C	-12.12081500	-1.11616800	0.00040600
C	-12.00092900	1.30858200	0.00064600
C	-13.51039100	-1.04242700	0.00065500
H	-11.62001600	-2.07872200	0.00021100
C	-13.39109100	1.37183100	0.00089400
H	-11.40782500	2.21719200	0.00064200
C	-14.15055500	0.19929500	0.00090000
H	-14.09660400	-1.95662300	0.00065600
H	-13.88448100	2.33928900	0.00108400
C	11.34486000	-0.06065400	0.00040000
C	12.12079400	1.11633900	0.00056800
C	12.00096400	-1.30841300	0.00058000
C	13.51037700	1.04262000	0.00090800
H	11.61999500	2.07889300	0.00043200
C	13.39112100	-1.37164000	0.00091900
H	11.40786600	-2.21702600	0.00045100
C	14.15056600	-0.19908400	0.00108500
H	14.09657000	1.95682900	0.00103500
H	13.88452900	-2.33908800	0.00105600
H	15.23510000	-0.25271700	0.00134800
H	-15.23508800	0.25295300	0.00109200



Wire 2

C	0.41481500	0.54010100	-0.00006100
C	-0.41482600	-0.54044200	-0.00004800
H	-0.02150600	1.53715200	-0.00006600
H	0.02149400	-1.53749300	-0.00002700
C	-1.81933500	-0.45438000	-0.00004000
C	-3.03891700	-0.41676500	-0.00003400
C	1.81932300	0.45403900	-0.00005000
C	3.03890500	0.41643200	-0.00004200
C	-4.45629200	-0.36384600	-0.00002900
C	-5.13348700	0.87542600	-0.00006200
C	-5.22246900	-1.55017600	0.00000900
C	-6.51822100	0.92583100	-0.00005700
H	-4.55466600	1.79298500	-0.00009100
C	-6.60714200	-1.49923900	0.00001400
H	-4.71243400	-2.50767700	0.00003500
C	-7.28383000	-0.26023600	-0.00001900
H	-7.02837700	1.88326600	-0.00008300
H	-7.18599900	-2.41677700	0.00004400
C	4.45628100	0.36355100	-0.00003300
C	5.13351000	-0.87570400	-0.00003600
C	5.22242700	1.54990100	-0.00002200
C	6.51824500	-0.92607200	-0.00002700
H	4.55471300	-1.79327800	-0.00004500
C	6.60710200	1.49900000	-0.00001200
H	4.71236700	2.50738800	-0.00001900
C	7.28382200	0.26001500	-0.00001600
H	7.02842600	-1.88349400	-0.00002900
H	7.18593500	2.41655300	-0.00000300
C	-8.70328900	-0.20841100	-0.00001500
C	-9.92032900	-0.16439500	-0.00001200
C	8.70328200	0.20822700	-0.00000600
C	9.92032500	0.16425000	0.00000000
C	11.34035500	0.11499500	0.00000900
C	12.01994500	-1.12181700	-0.00000800
C	12.10292100	1.30245800	0.00003500
C	13.40537400	-1.16889700	0.00000100
H	11.44375700	-2.04108500	-0.00002800
C	13.48828600	1.25502800	0.00004400
H	11.59076900	2.25887100	0.00004800
C	14.16803100	0.01837900	0.00002700
H	13.91762500	-2.12522900	-0.00001200
H	14.06461200	2.17417600	0.00006400
C	-11.34035800	-0.11506800	-0.00000800
C	-12.10298300	-1.30249400	0.00004000
C	-12.01988500	1.12177800	-0.00005300
C	-13.48834600	-1.25499300	0.00004300
H	-11.59088000	-2.25893200	0.00007400

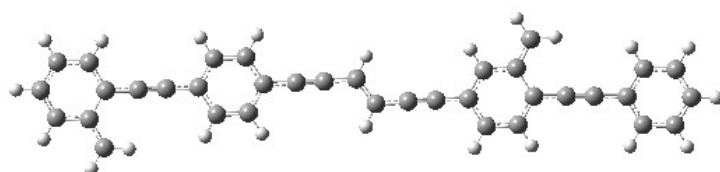
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H	-11.44365100	2.04101700	-0.00009100
C	-14.16802800	-0.01830900	-0.00000300
H	-14.06471800	-2.17411200	0.00008000
H	-13.91751300	2.12528600	-0.00008600
C	-15.58880600	0.03013400	0.00000000
C	-16.80520100	0.07126900	-0.00000100
C	15.58881100	-0.02999300	0.00003700
C	16.80520800	-0.07106100	0.00004600
C	-18.22863100	0.11757800	0.00000000
C	-18.90618600	1.35377700	-0.00005300
C	-18.98416300	-1.07256900	0.00005400
C	-20.29724400	1.39306700	-0.00005200
H	-18.32887800	2.27250400	-0.00009500
C	-20.37484300	-1.02280900	0.00005500
H	-18.46688100	-2.02637400	0.00009500
C	-21.03638500	0.20762700	0.00000200
H	-20.80722800	2.35188300	-0.00009400
H	-20.94516400	-1.94700400	0.00009700
C	18.22864200	-0.11727200	0.00005700
C	18.90628200	-1.35342400	0.00003500
C	18.98409100	1.07292800	0.00009100
C	20.29734300	-1.39261700	0.00004600
H	18.32903800	-2.27219100	0.00001000
C	20.37477400	1.02326400	0.00010200
H	18.46674300	2.02669600	0.00010800
C	21.03640200	-0.20712600	0.00007900
H	20.80739300	-2.35139800	0.00002900
H	20.94503200	1.94749900	0.00012800
H	-22.12168300	0.24253600	0.00000200
H	22.12170200	-0.24196000	0.00008800



Wire 1(a)

C	0.35192300	-0.59224100	-0.00000900
C	-0.51501000	0.46331900	-0.00008300
H	-0.05176000	-1.60297300	0.00006400
H	-0.10868400	1.47311100	-0.00013000
C	-1.91171200	0.33607500	-0.00007900
C	-3.13382100	0.27004200	-0.00007000
C	1.75059800	-0.45983800	0.00000900
C	2.96861000	-0.37706400	0.00001000
C	-4.54002500	0.20013400	-0.00003900
C	-5.23062800	-1.07609100	-0.00006300

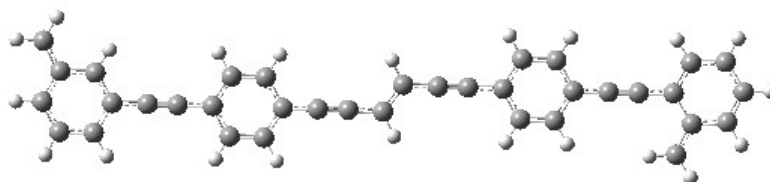
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C	-6.65578700	-1.05346000	-0.00004500
C	-6.68051700	1.37163100	0.00002200
H	-4.76898800	2.33802200	0.00001200
C	-7.38340600	0.13419300	0.00000300
H	-7.18748000	-1.99962300	-0.00006100
H	-7.24212800	2.29921100	0.00005600
C	4.38422800	-0.28294500	0.00001100
C	5.18153900	-1.45998400	0.00009700
C	5.01883200	0.96128900	-0.00006400
C	6.56438400	-1.36722400	0.00010000
H	4.69584700	-2.42943200	0.00015200
C	6.43554700	1.09337500	-0.00005500
H	4.41417400	1.86255200	-0.00013800
C	7.22220400	-0.12343400	0.00003100
H	7.16550200	-2.27056900	0.00015400
C	-8.80637600	0.11875800	0.00001500
C	-10.02318400	0.11743700	0.00001700
C	8.63586800	-0.07953700	0.00003100
C	9.85517200	-0.05714000	0.00003700
C	11.27763100	-0.04673700	0.00003000
C	12.00165200	-1.25735800	0.00012700
C	11.98955800	1.17077000	-0.00007600
C	13.39284900	-1.24503100	0.00011900
H	11.45885700	-2.19685600	0.00020700
C	13.38089400	1.17219000	-0.00008200
H	11.43867300	2.10560700	-0.00014900
C	14.08775500	-0.03291400	0.00001400
H	13.93790700	-2.18433600	0.00019300
H	13.91661400	2.11684800	-0.00016300
C	-11.44766700	0.11007100	0.00001500
C	-12.17080700	1.32001700	0.00020000
C	-12.15816900	-1.10738000	-0.00013000
C	-13.56239700	1.30761900	0.00021600
H	-11.62816600	2.25963800	0.00032600
C	-13.54980600	-1.10938900	-0.00011000
H	-11.60569200	-2.04124200	-0.00025900
C	-14.25680500	0.09547000	0.00005900
H	-14.10767000	2.24681400	0.00035600
H	-14.08531100	-2.05419200	-0.00022600
H	-15.34265300	0.08980800	0.00007700
H	15.17356500	-0.02748300	0.00000700
C	-4.54471600	-2.29216300	-0.00011400
H	-3.46262200	-2.32670200	-0.00025300
H	-5.08705200	-3.23087100	-0.00013400
C	7.02796900	2.36088400	-0.00011800
H	6.41557700	3.25543900	-0.00017000
H	8.10421700	2.47710100	-0.00005400



Wire 1(b)

C	0.53696000	-0.49046100	-0.00026200
C	-0.30443900	0.58108300	-0.00028600
H	0.11148600	-1.49218400	-0.00024100
H	0.12137000	1.58268600	-0.00028200
C	-1.70779700	0.48029700	-0.00029500
C	-2.92711200	0.43024200	-0.00030100
C	1.94066800	-0.38877400	-0.00022800
C	3.15930300	-0.33363600	-0.00019800
C	-4.34338700	0.36272200	-0.00028000
C	-5.00825700	-0.88356200	-0.00017800
C	-5.12244600	1.54105900	-0.00026300
C	-6.39200700	-0.94841900	-0.00009400
C	-6.50609600	1.47589000	-0.00019100
H	-4.62244800	2.50387100	-0.00031300
C	-7.17132400	0.22959900	-0.00012200
H	-6.89096800	-1.91179100	-0.00001200
H	-7.09433300	2.38745000	-0.00018800
C	4.57803500	-0.26985300	-0.00017100
C	5.34969900	-1.46315200	-0.00015500
C	5.23830800	0.96019000	-0.00016500
C	6.73441600	-1.39975700	-0.00013100
H	4.84363600	-2.42213100	-0.00016500
C	6.65755600	1.06239700	-0.00014300
H	4.65286100	1.87405100	-0.00018400
C	7.41816700	-0.17025500	-0.00011900
H	7.31623000	-2.31565000	-0.00012600
C	-8.58865800	0.16578300	-0.00002200
C	-9.80780800	0.12273500	0.00005500
C	8.83271700	-0.15589200	-0.00012000
C	10.05213600	-0.15849600	-0.00007700
C	11.47459400	-0.17593700	0.00012600
C	12.17510500	-1.40027500	0.00018300
C	12.20985900	1.02759500	0.00025400
C	13.56630800	-1.41467400	0.00036700
H	11.61434200	-2.32916600	0.00007900
C	13.60095600	1.00231100	0.00043400
H	11.67703200	1.97284300	0.00020600
C	14.28445200	-0.21619300	0.00049400
H	14.09319900	-2.36429400	0.00040700
H	14.15473500	1.93649900	0.00053000
C	-11.22299900	0.09191300	0.00015500
C	-11.94130100	1.30042100	0.00034600
C	-11.94196200	-1.16612800	0.00012000
C	-13.33235000	1.31451600	0.00049400
H	-11.38595700	2.23277400	0.00037500
C	-13.36996700	-1.10198800	0.00027300
C	-14.04611800	0.10118300	0.00045300
H	-13.86372600	2.26094600	0.00063000
H	-15.13207000	0.11216700	0.00056400
H	15.37016700	-0.23172600	0.00063700
C	7.27641500	2.31762700	-0.00014000
H	6.68271900	3.22469900	-0.00015800
H	8.35484500	2.41135900	-0.00011900

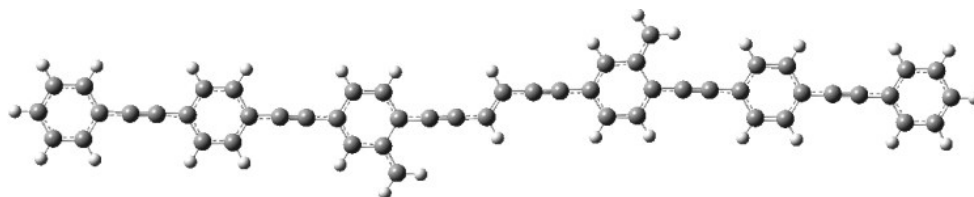
H	-4.42000300	-1.79512900	-0.00015400
H	-13.92238900	-2.03750100	0.00022700
C	-11.28573100	-2.39909100	-0.00005700
H	-11.85121200	-3.32423200	-0.00006400
H	-10.20487900	-2.46165300	-0.00018700



Wire 1(c)

C	-0.32697500	-0.55373800	0.00004700
C	0.49664200	0.53155400	0.00006900
H	0.11521200	-1.54821400	0.00004500
H	0.05463500	1.52610800	0.00009800
C	1.90145600	0.45330600	0.00008300
C	3.12135500	0.42181600	0.00009100
C	-1.73196200	-0.47614700	0.00004700
C	-2.95175600	-0.44631800	0.00004500
C	4.53854200	0.37456300	0.00007500
C	5.22075400	-0.86223100	-0.00009000
C	5.30096700	1.56364900	0.00021900
C	6.60531600	-0.90773400	-0.00013800
C	6.68546700	1.51782100	0.00018900
H	4.78758800	2.51939300	0.00034900
C	7.36802900	0.28103000	0.00000100
H	7.11766200	-1.86405100	-0.00027300
H	7.26085200	2.43754500	0.00029700
C	-4.36962600	-0.40269200	0.00003800
C	-5.12797700	-1.59386900	0.00015500
C	-5.05500600	0.83190400	-0.00008100
C	-6.51316500	-1.55187800	0.00015400
H	-4.61174500	-2.54806300	0.00025200
C	-6.44025500	0.87302400	-0.00009500
H	-4.48234400	1.75333900	-0.00017200
C	-7.19789300	-0.31773000	0.00002300
H	-7.08592600	-2.47325200	0.00025200
C	8.78625900	0.23684200	-0.00003600
C	10.00581000	0.21026100	-0.00005700
C	-8.61873700	-0.27515100	0.00003900
C	-9.83508800	-0.23667600	0.00004800
C	-11.25980100	-0.20023900	0.00004000
C	-12.00232700	-1.40501800	0.00030100
C	-11.93890500	1.02299600	-0.00022800
C	-13.39896900	-1.36323400	0.00029300
H	-11.47599400	-2.35314100	0.00050500
C	-13.35983400	1.08411100	-0.00024200
C	-14.07273200	-0.15142600	0.00003000
H	-13.96100600	-2.29261700	0.00049100

C	11.42147300	0.19788200	-0.00001400
C	12.12405400	1.41545200	0.00024400
C	12.15646700	-1.05076100	-0.00024400
C	13.51492600	1.44741800	0.00027800
H	11.55680300	2.34061100	0.00041500
C	13.58341700	-0.96838100	-0.00021500
C	14.24413400	0.24344300	0.00004200
H	14.03407900	2.40060300	0.00048400
H	15.32985500	0.26831400	0.00006800
H	-15.15880100	-0.12972500	0.00002500
H	4.64533700	-1.78195100	-0.00018400
H	-6.95674500	1.82706900	-0.00019100
H	14.14776500	-1.89674100	-0.00039500
C	11.51598300	-2.29213200	-0.00047400
H	12.09324800	-3.20996200	-0.00061900
H	10.43603100	-2.36852000	-0.00052700
H	-11.36840400	1.94643900	-0.00043000
C	-14.03503200	2.31919200	-0.00051500
H	-13.48986500	3.25637100	-0.00066700
H	-15.11830200	2.36499900	-0.00055700

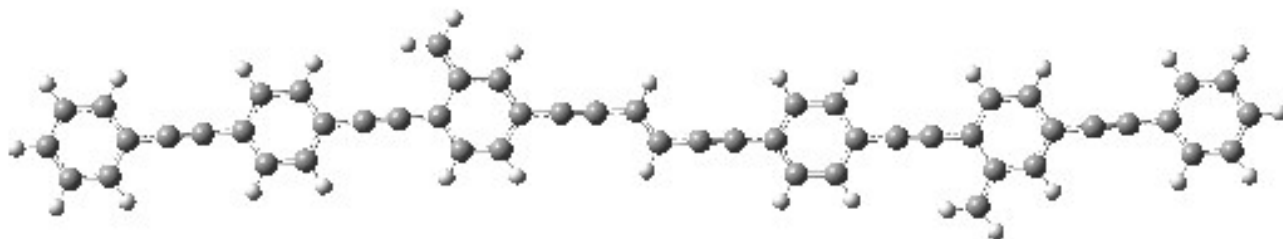


Wire 2(a)

C	0.33879100	0.53345700	0.00001700
C	-0.45797800	-0.57615300	-0.00008300
H	-0.12998500	1.51563600	0.00009600
H	0.01252800	-1.55759700	-0.00016100
C	-1.85986600	-0.53623200	-0.00009100
C	-3.08369900	-0.53122400	-0.00010000
C	1.74302100	0.49168000	0.00002600
C	2.96388700	0.49460800	0.00003600
C	-4.49120100	-0.50368600	-0.00010100
C	-5.16608500	0.73455300	-0.00001000
C	-5.26582400	-1.73076500	-0.00019100
C	-6.54778800	0.80915000	-0.00000500
C	-6.68595500	-1.61294400	-0.00018200
C	-7.33203900	-0.37857000	-0.00009100
H	-7.04594300	1.77226900	0.00006600
H	-7.27996200	-2.52126000	-0.00024900
C	4.38234600	0.47817100	0.00005200
C	5.08708400	-0.75696300	-0.00004500
C	5.11054600	1.66988000	0.00016000
C	6.47254600	-0.77086900	-0.00003500
H	4.52816000	-1.68611000	-0.00012800
C	6.53332900	1.69318100	0.00017400

H	4.57681000	2.61486500	0.00023600
C	7.22444700	0.41911000	0.00007100
H	7.00243500	-1.71773000	-0.00011100
C	-8.75209100	-0.29886500	-0.00008100
C	-9.96693000	-0.21911500	-0.00007000
C	8.63597800	0.35411900	0.00007000
C	9.85422600	0.28277500	0.00006600
C	11.26994800	0.18748400	0.00006100
C	11.90747400	-1.07269800	-0.00006900
C	12.07436600	1.34799500	0.00018100
C	13.28998200	-1.16748900	-0.00008100
H	11.29982700	-1.97146300	-0.00016200
C	13.45682600	1.25245000	0.00016900
H	11.59690100	2.32221900	0.00028300
C	14.09365300	-0.00716900	0.00003700
H	13.76881400	-2.14097600	-0.00018400
H	14.06469700	2.15104300	0.00026200
C	-11.38581900	-0.13462200	-0.00005300
C	-12.17716700	-1.30290700	-0.00013100
C	-12.03461900	1.11839700	0.00004400
C	-13.56102200	-1.22149600	-0.00011200
H	-11.68859200	-2.27156600	-0.00020700
C	-13.41856800	1.19958200	0.00006300
H	-11.43601700	2.02323800	0.00010400
C	-14.21010200	0.03145700	-0.00001400
H	-14.15978200	-2.12619500	-0.00017200
H	-13.90713700	2.16822200	0.00013800
C	-15.62937800	0.11463100	0.00000900
C	-16.84439100	0.18542700	0.00002900
C	15.51151000	-0.10456000	0.00002000
C	16.72590100	-0.18733900	0.00000400
C	-18.26636000	0.26552900	0.00004700
C	-18.91458800	1.51734100	0.00014200
C	-19.04970400	-0.90649500	-0.00002800
C	-20.30434700	1.58935600	0.00016100
H	-18.31578400	2.42220700	0.00020100
C	-20.43881400	-0.82404100	-0.00000800
H	-18.55499000	-1.87219200	-0.00010200
C	-21.07119100	0.42164800	0.00008600
H	-20.79161200	2.55991700	0.00023500
H	-21.03074000	-1.73455400	-0.00006700
C	18.14684800	-0.28164300	-0.00001000
C	18.78250300	-1.53995000	-0.00015400
C	18.94184500	0.88256800	0.00011700
C	20.17144000	-1.62583300	-0.00017000
H	18.17465300	-2.43876000	-0.00025300
C	20.33002600	0.78619400	0.00010000
H	18.45681100	1.85315700	0.00022900
C	20.94987800	-0.46579800	-0.00004300
H	20.64900400	-2.60119400	-0.00028200
H	20.93106600	1.69070900	0.00019900
H	-22.15537000	0.48210900	0.00010200
H	22.03339400	-0.53708300	-0.00005600
C	7.22057400	2.91139300	0.00028400
H	6.67820400	3.85003700	0.00036000
H	8.30255400	2.94541700	0.00029600

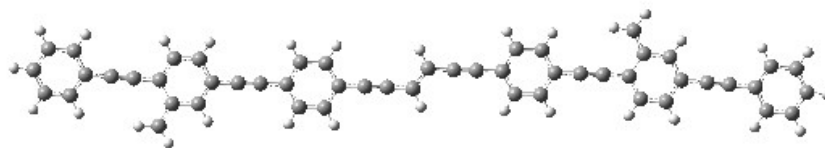
H	-4.57554500	1.64481000	0.00005700
C	-4.66234200	-2.98998200	-0.00028400
H	-5.26608300	-3.89042900	-0.00034800
H	-3.58495000	-3.09714300	-0.00029500



Wire 2(b)

C	-0.48845500	0.62186400	-0.00103700
C	0.31908600	-0.47547600	-0.00111700
H	-0.03198500	1.60984700	-0.00099100
H	-0.13748900	-1.46342500	-0.00119100
C	1.72480400	-0.41814200	-0.00112100
C	2.94510000	-0.40551000	-0.00109600
C	-1.89456600	0.56430200	-0.00099400
C	-3.11445300	0.55488200	-0.00092700
C	4.36259900	-0.38191700	-0.00100300
C	5.06591200	0.84325800	-0.00083500
C	5.10455400	-1.58402700	-0.00108100
C	6.45082300	0.86520900	-0.00072000
C	6.48947200	-1.56197000	-0.00096700
H	4.57482500	-2.53077500	-0.00122500
C	7.19311000	-0.33697300	-0.00076800
H	6.98056100	1.81194300	-0.00058100
H	7.04788600	-2.49212800	-0.00102200
C	-4.53409700	0.52351100	-0.00085300
C	-5.22527800	-0.71859200	-0.00074600
C	-5.27406300	1.70714000	-0.00087000
C	-6.61069200	-0.74700300	-0.00063800
H	-4.65667800	-1.64184700	-0.00074000
C	-6.69711200	1.71574400	-0.00076600
H	-4.75016900	2.65762200	-0.00096000
C	-7.37469900	0.43500900	-0.00063700
H	-7.13069000	-1.69932300	-0.00054800
C	8.61103700	-0.31173500	-0.00061600
C	9.83097700	-0.27830700	-0.00044700
C	-8.78575300	0.35519900	-0.00049500
C	-10.00306600	0.27068400	-0.00034200
C	-11.41771900	0.15959300	-0.00014800
C	-12.04095000	-1.10768400	0.00010300
C	-12.23513700	1.31093800	-0.00019300
C	-13.42230400	-1.21812200	0.00031800
H	-11.42315500	-1.99950600	0.00013200

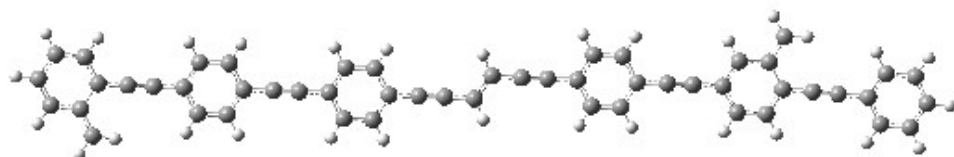
C	-13.61644800	1.19976800	0.00002000
H	-11.76870900	2.29049200	-0.00039500
C	-14.23900100	-0.06695000	0.00028600
H	-13.89009700	-2.19695800	0.00051600
H	-14.23445200	2.09142400	-0.00001400
C	11.24315800	-0.22324400	-0.00023400
C	12.04008500	-1.43303000	-0.00032800
C	11.89098400	1.02602900	0.00008200
C	13.45659100	-1.28819500	-0.00007800
C	13.27311300	1.12905200	0.00032800
H	11.28289200	1.92471500	0.00014400
C	14.07948300	-0.04078600	0.00025800
H	14.06829300	-2.18470100	-0.00014900
H	13.75098500	2.10238400	0.00058300
C	15.49888200	0.06555000	0.00052500
C	16.71141200	0.16669500	0.00077300
C	-15.65568300	-0.18039700	0.00052800
C	-16.86904900	-0.27704000	0.00074700
C	18.13171500	0.27745900	0.00106900
C	18.75269600	1.54284400	0.00162000
C	18.93995100	-0.87738500	0.00082800
C	20.14062400	1.64489000	0.00192600
H	18.13451900	2.43459600	0.00180600
C	20.32700600	-0.76502200	0.00113700
H	18.46610500	-1.85348300	0.00040100
C	20.93239900	0.49398200	0.00168700
H	20.60680800	2.62574700	0.00235400
H	20.93842200	-1.66256900	0.00094800
C	-18.28881500	-0.38781600	0.00100300
C	-18.90976500	-1.65344500	0.00140200
C	-19.09730700	0.76706000	0.00087000
C	-20.29760100	-1.75553900	0.00166500
H	-18.29145100	-2.54509000	0.00150500
C	-20.48427000	0.65448500	0.00113400
H	-18.62362800	1.74323900	0.00056000
C	-21.08949400	-0.60464600	0.00153300
H	-20.76374600	-2.73640700	0.00197400
H	-21.09582800	1.55192500	0.00102900
H	22.01503100	0.57774600	0.00192700
H	-22.17210700	-0.68853200	0.00173800
C	-7.39700200	2.92714400	-0.00078800
H	-6.86430000	3.87129400	-0.00088600
H	-8.47927000	2.94996900	-0.00070900
H	4.50624500	1.77262700	-0.00079200
C	11.45983500	-2.70563700	-0.00064400
H	12.08061400	-3.59436900	-0.00071300
H	10.38477400	-2.83264100	-0.00082800



Wire 2(c)

C	-0.34973300	-0.48815600	0.00707100
C	0.47217000	0.59851100	0.00675800
H	0.09390300	-1.48197800	0.00731600
H	0.02865700	1.59238000	0.00658300
C	1.87700900	0.52245500	0.00656100
C	3.09699100	0.49321100	0.00622400
C	-1.75471000	-0.41245600	0.00702000
C	-2.97457300	-0.38411600	0.00681700
C	4.51412200	0.44991300	0.00567200
C	5.20015300	-0.78496700	0.00513000
C	5.27276300	1.64149100	0.00555400
C	6.58465800	-0.82623400	0.00441000
C	6.65730100	1.60010100	0.00484000
H	4.75631600	2.59554700	0.00599300
C	7.34362700	0.36541000	0.00420700
H	7.10112500	-1.78026800	0.00395200
H	7.22866000	2.52236300	0.00471400
C	-4.39231800	-0.34216000	0.00635800
C	-5.07913600	0.89176100	0.00535600
C	-5.14918300	-1.53442900	0.00677600
C	-6.46429800	0.93130000	0.00469000
H	-4.50752500	1.81382600	0.00506200
C	-6.53425600	-1.49423100	0.00611300
H	-4.63171400	-2.48793300	0.00758100
C	-7.22046300	-0.26061600	0.00500400
H	-6.98187700	1.88474700	0.00387800
C	8.76120500	0.31989400	0.00327700
C	9.98043400	0.26800900	0.00231900
C	-8.64070600	-0.22017200	0.00415000
C	-9.85782500	-0.19081500	0.00324300
C	-11.27981200	-0.14702600	0.00187200
C	-11.95914200	1.10024900	-0.00052800
C	-12.02950400	-1.32342800	0.00275700
C	-13.34507800	1.14085700	-0.00205500
H	-11.38283700	2.01875600	-0.00120400
C	-13.45283700	-1.31948700	0.00126200
H	-11.51422900	-2.27864600	0.00462900
C	-14.11893900	-0.03361700	-0.00127000
H	-13.85647400	2.09783400	-0.00393600
C	11.39173800	0.19051700	0.00112800
C	12.20791200	1.38727100	0.00140700
C	12.01924400	-1.06894800	-0.00048300
C	13.62183000	1.21968000	-0.00009000
C	13.39960900	-1.19430200	-0.00190500
H	11.39670800	-1.95769000	-0.00065100
C	14.22460600	-0.03768100	-0.00175200

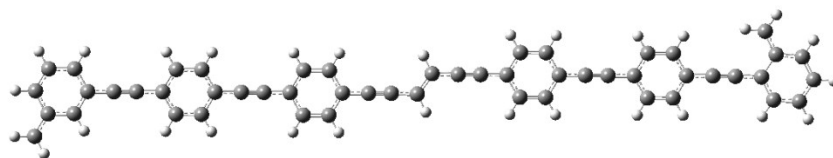
H	14.24795900	2.10617700	0.00005100
H	13.86168400	-2.17522600	-0.00316900
C	15.64210100	-0.16702100	-0.00332400
C	16.85278000	-0.28835800	-0.00474700
C	-15.53089600	0.05809700	-0.00304100
C	-16.74657100	0.15253300	-0.00468500
C	18.27094400	-0.42377800	-0.00644500
C	18.86955200	-1.69990600	-0.00925400
C	19.09937500	0.71665700	-0.00540800
C	20.25544400	-1.82646800	-0.01099800
H	18.23570300	-2.58058700	-0.01005700
C	20.48423700	0.57978900	-0.00716400
H	18.64284800	1.70096900	-0.00323800
C	21.06736100	-0.68968000	-0.00996800
H	20.70422200	-2.81540500	-0.01317400
H	21.11141100	1.46640000	-0.00634600
C	-18.16389900	0.27577300	-0.00675900
C	-18.77160700	1.54868300	-0.01053900
C	-18.98626500	-0.86995500	-0.00516300
C	-20.15792300	1.66619400	-0.01267800
H	-18.14339400	2.43335900	-0.01178100
C	-20.37164400	-0.74163900	-0.00731900
H	-18.52489000	-1.85204200	-0.00223900
C	-20.96289000	0.52421800	-0.01108800
H	-20.61294700	2.65226100	-0.01560700
H	-20.99319300	-1.63217800	-0.00606100
H	22.14835200	-0.79246100	-0.01133400
H	-22.04446800	0.62017500	-0.01276800
H	4.62755300	-1.70642400	0.00524000
C	11.64791600	2.66907000	0.00306200
H	12.28272600	3.54782800	0.00322100
H	10.57500100	2.81306400	0.00420100
H	-7.10600600	-2.41620600	0.00640000
C	-14.16377800	-2.52487400	0.00221300
H	-13.63965900	-3.47384100	0.00412900
H	-15.24619600	-2.53754800	0.00108600



Wire 2(d)

C	-0.33212000	-0.48477700	-0.00602800
C	0.50054800	0.59343000	-0.00563300
H	0.10151100	-1.48300500	-0.00623000
H	0.06714200	1.59174900	-0.00545300
C	1.90480400	0.50301700	-0.00531400
C	3.12422500	0.46100400	-0.00490000
C	-1.73639300	-0.39517100	-0.00609700
C	-2.95590900	-0.35508500	-0.00600300
C	4.54144100	0.40190800	-0.00435700
C	5.21294100	-0.84039800	-0.00403000
C	5.31292700	1.58472200	-0.00407600
C	6.59750400	-0.89701400	-0.00335700
C	6.69744200	1.52745500	-0.00340700
H	4.80726100	2.54453900	-0.00435500
C	7.36831300	0.28546700	-0.00299800
H	7.10329800	-1.85676400	-0.00306600
H	7.28052700	2.44230800	-0.00315800
C	-4.37315700	-0.30015500	-0.00558000
C	-5.04892500	0.93993300	-0.00472400
C	-5.14075100	-1.48562300	-0.00589600
C	-6.43357300	0.99197100	-0.00411800
H	-4.46902800	1.85681200	-0.00449900
C	-6.52530600	-1.43310200	-0.00529500
H	-4.63180600	-2.44370300	-0.00657600
C	-7.20060600	-0.19325100	-0.00435600
H	-6.94260500	1.95000700	-0.00341100
C	8.78797300	0.22695900	-0.00214400
C	10.00455800	0.18079500	-0.00134600
C	-8.61984100	-0.14014500	-0.00353400
C	-9.83700600	-0.09570800	-0.00269500
C	-11.25655900	-0.04704500	-0.00165400
C	-11.93746700	1.18948400	0.00003500
C	-12.01873800	-1.23516000	-0.00218300
C	-13.32241400	1.23578400	0.00123800
H	-11.36194600	2.10917400	0.00043600
C	-13.40367700	-1.18898600	-0.00099200
H	-11.50591400	-2.19120800	-0.00350200
C	-14.08560500	0.04750600	0.00078100
H	-13.83520700	2.19181600	0.00258700
C	11.42578800	0.11621300	-0.00055400
C	12.19291400	1.28131400	-0.00069000
C	12.08641400	-1.14107300	0.00047200
C	13.61605100	1.25611800	0.00021300
C	13.47156000	-1.20235200	0.00139000
H	11.49643300	-2.05085900	0.00056800
C	14.26284100	-0.03954100	0.00132300
H	13.96864500	-2.16684000	0.00220200
C	15.67324900	-0.15276400	0.00235500
C	16.88725600	-0.26668500	0.00334000
C	-15.50412100	0.09769700	0.00216800
C	-16.72261000	0.15219000	0.00349500
C	18.30229100	-0.41396200	0.00474400
C	18.88791700	-1.69719500	0.00709600

C	19.14433500	0.71736800	0.00384500
C	20.27196800	-1.83877100	0.00853700
H	18.24443600	-2.57083100	0.00778200
C	20.52729500	0.56499700	0.00529600
H	18.70007300	1.70731600	0.00201100
C	21.09656900	-0.71089100	0.00765500
H	20.70980100	-2.83259100	0.01036000
H	21.16419800	1.44462800	0.00458800
C	-18.13628100	0.23284700	0.00523500
C	-18.75733300	1.49379000	0.00818000
C	-18.95141300	-0.96492100	0.00410600
C	-20.14318700	1.61703600	0.01008400
H	-18.13048700	2.37967200	0.00900300
C	-20.36983200	-0.78910700	0.00615100
C	-20.94967100	0.46352400	0.00905500
H	-20.59862800	2.60224700	0.01239000
H	-20.99389300	-1.67844300	0.00536900
H	22.17633100	-0.82550400	0.00878400
H	-22.03143600	0.55945700	0.01053500
H	4.62997200	-1.75532700	-0.00427900
H	-7.10523500	-2.34996400	-0.00549500
H	-13.97807000	-2.10937500	-0.00137900
C	-18.39337800	-2.24562700	0.00117800
H	-17.32072300	-2.39234400	-0.00029600
H	-19.02932800	-3.12379700	0.00056700
H	11.69192700	2.24410200	-0.00147400
C	14.34505700	2.45068400	0.00005600
H	15.42755300	2.44703400	0.00053100
H	13.83534100	3.40745800	-0.00093500

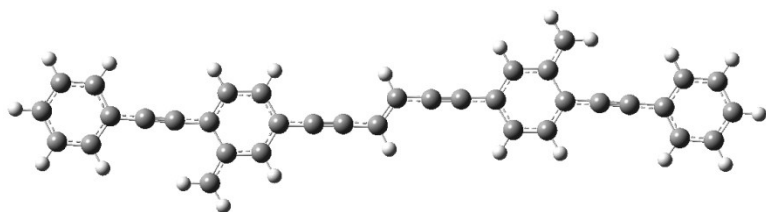


Wire 2(e)

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C	0.36071500	-0.52978600	0.00128600
H	-0.05253700	1.54392800	0.00113000
H	-0.06596700	-1.53099600	0.00137900
C	1.76431200	-0.43009800	0.00123700
C	2.98346500	-0.38045500	0.00116800
C	-1.88287600	0.44325100	0.00121300
C	-3.10206100	0.39407900	0.00118200

C	4.40025100	-0.31359100	0.00105600
C	5.06520000	0.93230000	0.00082000
C	5.17802400	-1.49234900	0.00115400
C	6.44936900	0.99630000	0.00067200
C	6.56212700	-1.42781200	0.00100800
H	4.67740800	-2.45480400	0.00134100
C	7.22655500	-0.18220000	0.00075500
H	6.95010600	1.95869100	0.00048200
H	7.14999500	-2.33960300	0.00107900
C	-4.51884400	0.32819300	0.00111100
C	-5.18480200	-0.91719700	0.00108200
C	-5.29572800	1.50758500	0.00104400
C	-6.56898500	-0.98013300	0.00097200
H	-4.59768300	-1.82946700	0.00114000
C	-6.67983400	1.44416100	0.00093700
H	-4.79434200	2.46963900	0.00107200
C	-7.34532000	0.19902000	0.00088900
H	-7.07046900	-1.94213500	0.00094400
C	8.64545700	-0.11640000	0.00057000
C	9.86199200	-0.06038400	0.00038900
C	-8.76408400	0.13448400	0.00073700
C	-9.98082800	0.07975200	0.00057600
C	-11.39991400	0.01879000	0.00035400
C	-12.06992500	-1.22368000	0.00012700
C	-12.17246600	1.20017800	0.00033400
C	-13.45440400	-1.28211200	-0.00012800
H	-11.48634900	-2.13827900	0.00014700
C	-13.55695200	1.14186600	0.00008100
H	-11.66803700	2.16068000	0.00051300
C	-14.22797800	-0.10057500	-0.00016400
H	-13.95880600	-2.24259200	-0.00030800
C	11.28151300	0.00266700	0.00016200
C	12.05542700	-1.17740700	0.00027200
C	11.94906000	1.24599300	-0.00019700
C	13.44029700	-1.11661300	0.00002500
C	13.33401400	1.30638500	-0.00044500
H	11.36402000	2.15964600	-0.00028500
C	14.10789500	0.12653200	-0.00034100
H	13.83702100	2.26761000	-0.00072800
C	15.52841300	0.18849600	-0.00062000
C	16.74423800	0.23864300	-0.00085600
C	-15.64599700	-0.16343100	-0.00046000
C	-16.86391900	-0.22932100	-0.00074200
C	18.16815000	0.30234800	-0.00103900
C	18.82522600	1.55570700	-0.00145900
C	18.93045700	-0.87077300	-0.00081200
C	20.22146600	1.61065300	-0.00164700
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C	20.35219000	-0.83350500	-0.00099700

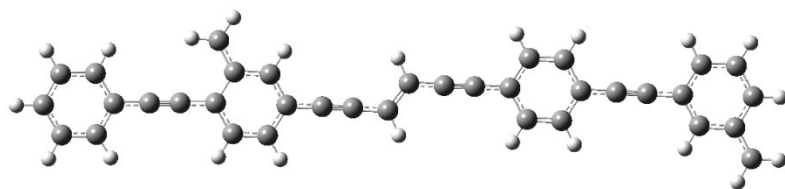
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C	-18.27674600	-0.32362900	-0.00110000
C	-18.88542900	-1.59058800	-0.00158800
C	-19.10353000	0.86610800	-0.00098900
C	-20.27000200	-1.72743600	-0.00198300
H	-18.24991400	-2.47027000	-0.00166100
C	-20.52017100	0.67638400	-0.00140800
C	-21.08772400	-0.58187000	-0.00189300
H	-20.71575000	-2.71707000	-0.00236100
H	-21.15294400	1.55954800	-0.00133700
H	22.06262200	0.50236100	-0.00158300
H	-22.16849800	-0.68836500	-0.00220300
H	4.47737100	1.84411200	0.00074700
H	-7.26697800	2.35641800	0.00087900
H	-14.13941400	2.05716800	0.00006100
C	-18.55798400	2.15219800	-0.00049400
H	-17.48680700	2.30932600	-0.00016900
H	-19.20244400	3.02413600	-0.00042300
H	11.55250300	-2.13869400	0.00054900
H	14.02553000	-2.03010900	0.00010800
H	20.71781200	2.57672000	-0.00198200
C	21.11144900	-2.01873800	-0.00078800
H	20.63279500	-2.99153100	-0.00049900
H	22.19527500	-1.98923600	-0.00099300



1(l)

C	0.41938400	-0.53666700	-0.00050400
C	-0.41938600	0.53670200	-0.00056000
H	-0.00846900	-1.53739300	-0.00043800
H	0.00847300	1.53742600	-0.00063400
C	-1.82344100	0.43878500	-0.00052500
C	-3.04252700	0.39399600	-0.00048000
C	1.82344000	-0.43874600	-0.00053300
C	3.04252600	-0.39395200	-0.00053000
C	-4.46076300	0.32134500	-0.00036700
C	-5.11549000	-0.93996900	-0.00016400
C	-5.23502000	1.48307200	-0.00045000
C	-6.49995700	-1.00831200	-0.00004300
C	-6.65764000	1.45009400	-0.00033300
C	-7.29754900	0.15055100	-0.00011700
H	-6.99213300	-1.97531700	0.00011500
C	4.46076600	-0.32132900	-0.00040100
C	5.23500400	-1.48306600	-0.00033700
C	5.11551000	0.93997600	-0.00032600

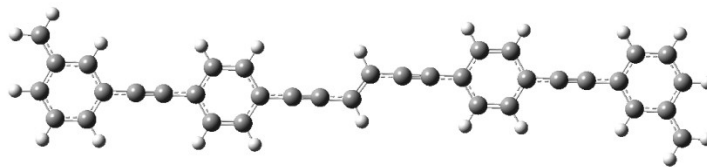
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H	4.52049600	1.84645200	-0.00038100
C	7.29755500	-0.15056600	-0.00012600
C	-8.70700100	0.02974700	0.00002000
C	-9.92046200	-0.09083900	0.00014900
C	8.70700500	-0.02978200	0.00001600
C	9.92047000	0.09078200	0.00014000
C	11.33451900	0.24629100	0.00031500
C	12.18329400	-0.88003900	-0.00001500
C	11.91253100	1.53301900	0.00083300
C	13.56531000	-0.71939500	0.00017200
H	11.74494500	-1.87261700	-0.00041900
C	13.29569400	1.68284200	0.00101800
C	14.12698500	0.55986900	0.00069000
H	14.20745500	-1.59520600	-0.00008700
C	-11.33451500	-0.24632100	0.00033300
C	-12.18326700	0.88002800	0.00028000
C	-11.91255300	-1.53303600	0.00057300
C	-13.56528600	0.71941300	0.00046400
H	-11.74489600	1.87259600	0.00009500
C	-13.29572000	-1.68283000	0.00075600
C	-14.12698700	-0.55984000	0.00070300
H	-14.20741200	1.59523700	0.00042200
H	-15.20605100	-0.68083400	0.00084700
H	15.20604700	0.68088300	0.00083600
H	-4.52046300	-1.84643600	-0.00010200
H	11.26384000	2.40278900	0.00108800
H	-11.26388200	-2.40282200	0.00061300
H	13.72759600	2.67925300	0.00142000
H	-13.72764400	-2.67923200	0.00094100
H	-4.73894800	2.44838600	-0.00061000
C	-7.39325200	2.64051000	-0.00042500
H	-6.88882200	3.60006800	-0.00058700
H	-8.47571200	2.63086800	-0.00033800
H	6.99215900	1.97530400	-0.00013800
C	7.39322300	-2.64053100	-0.00016000
H	8.47568300	-2.63090800	-0.00005100
H	6.88879400	-3.60009100	-0.00024700



1(m)

C	-0.61878300	-0.48135200	-0.00028300
C	0.21630900	0.59451100	-0.00023300
H	-0.18798300	-1.48078700	-0.00030500
H	-0.21500800	1.59375000	-0.00020400
C	1.62078900	0.50187700	-0.00020500
C	2.84007900	0.45968900	-0.00018000
C	-2.02343100	-0.38713400	-0.00029700

C	-3.24215600	-0.33816700	-0.00031200
C	4.25769800	0.40223000	-0.00013900
C	4.93110400	-0.83881600	-0.00012400
C	5.02734100	1.58602200	-0.00011100
C	6.31597100	-0.89321200	-0.00006200
C	6.41212200	1.53079400	-0.00006400
H	4.52026500	2.54511000	-0.00012600
C	7.08491700	0.29018300	-0.00003400
H	6.82328600	-1.85216400	-0.00003800
H	6.99367800	2.44664100	-0.00004100
C	-4.66147100	-0.28084500	-0.00031800
C	-5.42775600	-1.47743500	-0.00040100
C	-5.32702400	0.94619300	-0.00020700
C	-6.81277700	-1.42011300	-0.00040400
H	-4.91751000	-2.43419500	-0.00045000
C	-6.74669500	1.04220800	-0.00020500
H	-4.74557700	1.86260200	-0.00012300
C	-7.50185800	-0.19363300	-0.00035200
H	-7.39057000	-2.33854100	-0.00044400
C	8.50542500	0.23407000	0.00001700
C	9.72131700	0.18423600	0.00006300
C	-8.91651700	-0.18535000	-0.00024500
C	-10.13589100	-0.19304300	-0.00010800
C	-11.55827800	-0.21618900	0.00015800
C	-12.25395200	-1.44326900	0.00019700
C	-12.29826600	0.98444000	0.00037200
C	-13.64509700	-1.46312700	0.00044200
H	-11.68954900	-2.36995000	0.00003100
C	-13.68925100	0.95370400	0.00061700
C	-14.36794800	-0.26748300	0.00065500
H	-14.16825400	-2.41480800	0.00046700
C	11.14574900	0.13496400	0.00014300
C	11.89890000	1.33308400	0.00016500
C	11.81393500	-1.09421200	0.00018400
C	13.29510100	1.27896200	0.00022900
H	11.38096300	2.28581700	0.00013500
C	13.23425400	-1.16789200	0.00026100
C	13.95807900	0.06120500	0.00027200
H	13.86536100	2.20332100	0.00024600
H	15.04391200	0.02989500	0.00032200
H	-15.45359200	-0.28729000	0.00084500
H	4.34964200	-1.75472200	-0.00013900
H	-11.76914600	1.93176600	0.00034000
H	11.23530600	-2.01258100	0.00015600
C	13.89846500	-2.40899100	0.00032000
H	14.98128200	-2.46445600	0.00018700
H	13.34495900	-3.34126900	0.00018900
H	-14.24669400	1.88570800	0.00078000
C	-7.37102100	2.29485500	-0.00009800
H	-8.44984400	2.38390400	-0.00006100
H	-6.78122700	3.20446300	-0.00005800

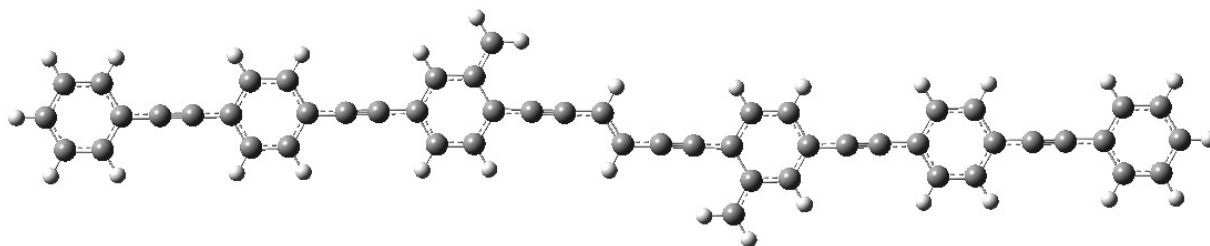


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C	-0.40892900	-0.54468700	-0.00034200
C	0.40891800	0.54465800	-0.00032200
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H	-0.03822700	1.53691300	-0.00024200
C	1.81445200	0.47397700	-0.00032900
C	3.03430500	0.44977700	-0.00033700
C	-1.81446300	-0.47400600	-0.00027000
C	-3.03431600	-0.44983900	-0.00021200
C	4.45244500	0.41197800	-0.00029600
C	5.14266200	-0.81987600	-0.00030700
C	5.20604100	1.60610400	-0.00015600
C	6.52808000	-0.85556000	-0.00022700
C	6.59142500	1.56956400	-0.00006500
H	4.68607200	2.55826700	-0.00011600
C	7.28099400	0.33815800	-0.00010400
H	7.04831900	-1.80756500	-0.00026600
H	7.16053400	2.49319800	0.00003800
C	-4.45245400	-0.41203300	-0.00011600
C	-5.20605300	-1.60615900	-0.00005700
C	-5.14267000	0.81981800	-0.00006400
C	-6.59143400	-1.56961900	0.00003000
H	-4.68608000	-2.55831900	-0.00010100
C	-6.52809000	0.85550000	0.00004900
H	-4.57364500	1.74350100	-0.00009500
C	-7.28100100	-0.33821100	0.00006900
H	-7.16054700	-2.49325000	0.00004800
C	8.70204400	0.30106700	-0.00001800
C	9.91850800	0.26707300	0.00005600
C	-8.70205000	-0.30112300	0.00010400
C	-9.91851300	-0.26711700	0.00013900
C	-11.34338700	-0.23559800	0.00014300
C	-12.08181400	-1.44286500	0.00020200
C	-12.02661400	0.98531800	0.00009500
C	-13.47859200	-1.40579300	0.00021900
H	-11.55228200	-2.38920600	0.00024300
C	-13.44772800	1.04164700	0.00010800
C	-14.15644600	-0.19626700	0.00017000
H	-14.03749700	-2.33706200	0.00026800
C	11.34338300	0.23560900	0.00014600
C	12.08176700	1.44290500	0.00025700
C	12.02665800	-0.98528200	0.00012500
C	13.47854600	1.40588800	0.00034300
H	11.55219600	2.38922400	0.00027400
C	13.44777400	-1.04155300	0.00021000
C	14.15644600	0.19638500	0.00032200
H	14.03741900	2.33717600	0.00042400
H	15.24258200	0.17840800	0.00038400
H	-15.24258100	-0.17824100	0.00018100
H	4.57363400	-1.74355800	-0.00043400

H	-7.04832500	1.80750700	0.00010100
H	-11.45921900	1.91067500	0.00005500
H	11.45929600	-1.91065700	0.00004200
C	14.12720200	-2.27435500	0.00018500
H	15.21062100	-2.31644000	0.00035900
H	13.58524600	-3.21339100	0.00006200
C	-14.12710900	2.27446300	0.00006800
H	-13.58512200	3.21348100	0.00014400
H	-15.21052700	2.31659000	0.00009300

2(l)

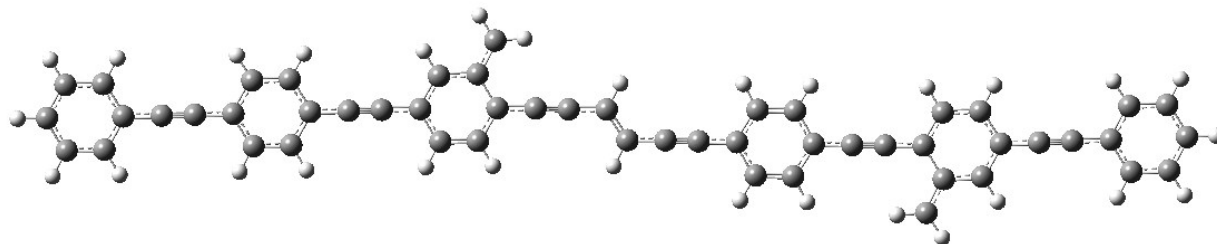


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H	0.07313900	-1.53588500	-0.00048200
C	-1.80194600	-0.51512300	-0.00052200
C	-3.02431300	-0.51106200	-0.00050500
C	1.80195200	0.51530300	-0.00058900
C	3.02431900	0.51123500	-0.00057400
C	-4.43577300	-0.48358400	-0.00047700
C	-5.11027800	0.75156600	-0.00042000
C	-5.20653100	-1.71049000	-0.00049100
C	-6.49456200	0.82471800	-0.00036400
C	-6.62454100	-1.59698000	-0.00043200
C	-7.27478500	-0.36204000	-0.00036500
H	-6.99333100	1.78749500	-0.00031600
H	-7.21706700	-2.50625800	-0.00043700
C	4.43577800	0.48373000	-0.00053900
C	5.11025800	-0.75143700	-0.00046100
C	5.20656200	1.71061500	-0.00055600
C	6.49453800	-0.82461900	-0.00039300
H	4.52152000	-1.66286300	-0.00044800
C	6.62457000	1.59707600	-0.00047100
C	7.27478800	0.36212200	-0.00039600
C	-8.69514900	-0.28751700	-0.00029200
C	-9.91036300	-0.21409600	-0.00021300
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C	9.91036200	0.21411800	-0.00020500
C	11.32958600	0.13575300	-0.00009800
C	11.98371600	-1.11449600	0.00001500

C	12.11592100	1.30741500	-0.00009400
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H	11.38898000	-2.02188100	0.00001100
C	13.50010900	1.23191600	0.00002400
H	11.62322100	2.27398300	-0.00018200
C	14.15452900	-0.01825900	0.00014200
C	-11.32958900	-0.13575800	-0.00009300
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H	-14.09495800	-2.13922500	-0.00005100
H	-13.86074700	2.15624600	0.00034400
C	-15.57413800	0.09530500	0.00030600
C	-16.78944000	0.16096300	0.00043000
C	15.57413100	-0.09540300	0.00027200
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C	-18.21172100	0.23521500	0.00057200
C	-18.86506000	1.48436500	0.00070500
C	-18.99025500	-0.94001100	0.00058500
C	-20.25510200	1.55068900	0.00084900
H	-18.26997300	2.39167900	0.00069600
C	-20.37969100	-0.86324100	0.00073000
C	-21.01715600	0.37985100	0.00086200
H	-20.74633900	2.51924500	0.00095200
H	-20.96788700	-1.77616700	0.00073900
C	18.21171100	-0.23535700	0.00057100
C	18.86503500	-1.48451700	0.00067200
C	18.99025800	0.93985800	0.00065200
C	20.25507600	-1.55085700	0.00084800
H	18.26993600	-2.39182200	0.00061000
C	20.37969400	0.86307200	0.00082900
H	18.49160900	1.90353000	0.00057500
C	21.01714400	-0.38002700	0.00092800
H	20.74630200	-2.51941700	0.00092400
H	-22.10157200	0.43587500	0.00097500
H	22.10155900	-0.43606500	0.00106600
H	-4.52156300	1.66300600	-0.00041400
H	-18.49159300	-1.90367600	0.00048200
H	6.99328700	-1.78740600	-0.00033300
H	13.86070000	-2.15630200	0.00022200
H	20.96790000	1.77599100	0.00089100
H	-11.62317700	-2.27399400	-0.00027900
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H	-3.51898900	-3.07271200	-0.00060700
H	-5.19729400	-3.87289700	-0.00054900
H	14.09499400	2.13916400	0.00002600

H	7.21711500	2.50634100	-0.00046100
C	4.59679800	2.97051400	-0.00065200
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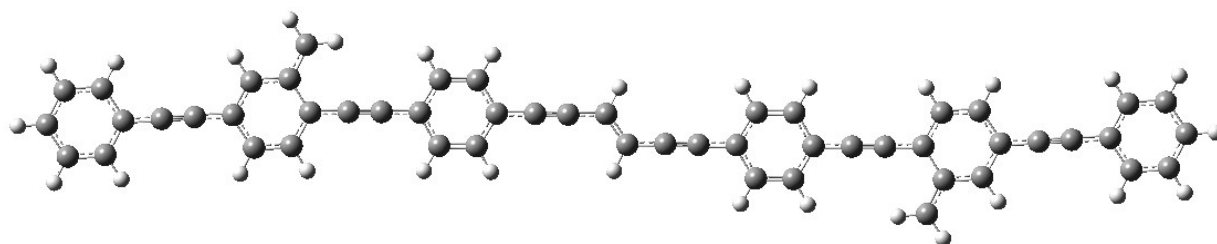
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C	2.88410000	0.40223300	-0.00566500
C	-4.58183700	-0.52786500	-0.00516200
C	-5.24605300	0.71471400	-0.00443600
C	-5.36506500	-1.74830100	-0.00528300
C	-6.62816400	0.80035600	-0.00371800
C	-6.78331500	-1.62035700	-0.00453900
C	-7.42068400	-0.38034900	-0.00371700
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H	-7.38433800	-2.52404300	-0.00456900
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C	5.00654300	-0.84359300	-0.00471100
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C	6.42717300	1.56321500	-0.00513100
H	4.51118900	2.52969800	-0.00619100
C	7.13213700	0.33927500	-0.00433700
C	-8.84017700	-0.29082800	-0.00280600
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C	11.18339600	0.22966900	-0.00156700
C	11.83218200	-1.01849000	0.00055300
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C	13.39483300	1.29724700	-0.00084700
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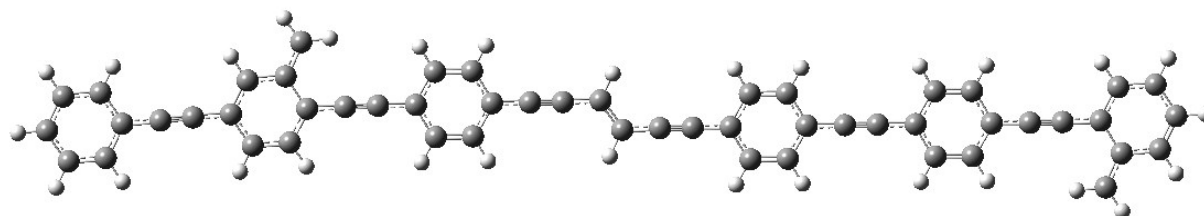
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C	18.69531500	-1.52575100	0.00928200
C	18.87861900	0.89478400	0.00516500
C	20.08340500	-1.62552000	0.01113100
H	18.07859700	-2.41851100	0.01015100
C	20.26585400	0.78469500	0.00703200
H	18.40317600	1.87010300	0.00284800
C	20.87329500	-0.47331800	0.01001900
H	20.55120300	-2.60560600	0.01345500
H	-22.23796100	0.57788800	0.00998100
H	21.95606000	-0.55532200	0.01147000
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H	6.98437500	2.49409500	-0.00527900
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H	-3.69293000	-3.12702900	-0.00677700
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C	11.39609900	2.71234900	-0.00456500
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H	12.01554500	3.60200200	-0.00515300
H	14.00552300	2.19444100	-0.00138100

2(n)



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C	-6.58698300	-1.58327800	0.00799800
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C	12.13757600	1.40730200	0.00285100
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H	11.35054400	-1.94332800	-0.00158800
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H	-14.17222900	-2.14104800	0.00108200
H	-13.81709900	2.14303600	-0.00539500
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C	-16.79448700	0.23378500	-0.00706000
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C	16.79448200	-0.23383300	-0.00706500
C	-18.21369800	0.35774900	-0.00974400
C	-18.82273900	1.62892100	-0.01385100
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C	-21.01219200	0.60064600	-0.01524600
H	-20.66654100	2.72926300	-0.01975000

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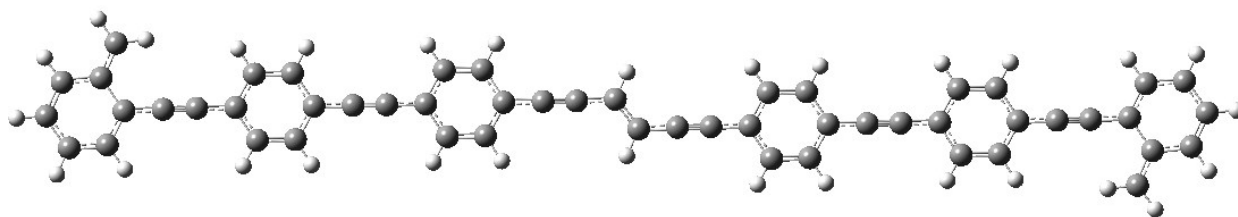
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C	2.89249700	-0.32120000	-0.00266700
C	-4.59993800	0.47643200	-0.00204100
C	-5.27853000	-0.76253100	-0.00195500
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C	-6.66276300	-0.81206700	-0.00167100
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H	-4.85492400	2.62056900	-0.00193600
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H	-7.17352900	-1.76916200	-0.00159200
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C	4.31000400	-0.27441900	-0.00248900

C	4.99288700	0.96177000	-0.00204800
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C	6.45559700	-1.41970400	-0.00244200
H	4.55634000	-2.41943400	-0.00305200
C	7.13801300	-0.18375700	-0.00196100
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H	13.78690800	2.16155400	0.00133100
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H	-18.29554600	-2.65297200	0.00273700
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H	20.55401000	2.52870000	0.00595600
H	-22.22377900	-0.89936600	0.00402500
H	21.97333600	0.47655600	0.00484900
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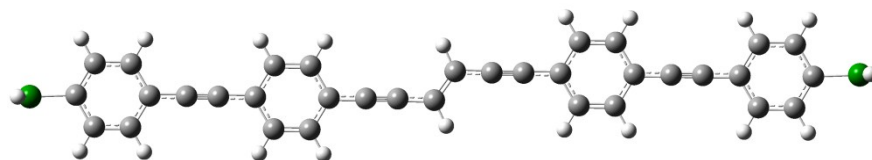
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H	20.92105900	-1.75450500	0.00219900
C	18.31691900	-2.30455700	0.00022900
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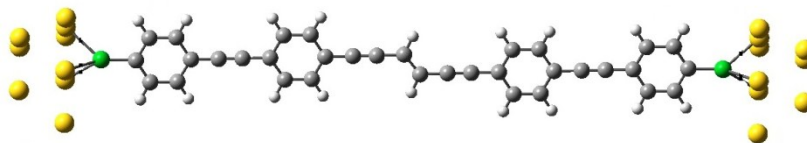
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C	-1.82275500	-0.43949700	-0.02179100
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C	5.23407000	1.51031500	-0.01947700
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C	6.61826800	1.44893900	-0.01728100
H	4.73126400	2.47162600	-0.02128300
C	7.28559600	0.20478800	-0.01473200
H	7.01391200	-1.93677000	-0.01283200
H	7.20405800	2.36206600	-0.01735900
C	-4.45890700	-0.32876900	-0.01931100
C	-5.12681300	0.91557500	-0.01697300
C	-5.23394900	-1.50937200	-0.01959400
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H	-4.54112200	1.82876300	-0.01678700
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H	-4.73106400	-2.47064300	-0.02144100
C	-7.28558400	-0.20401300	-0.01478600
H	-7.01407400	1.93756600	-0.01279600
C	8.70445200	0.14233800	-0.01187100
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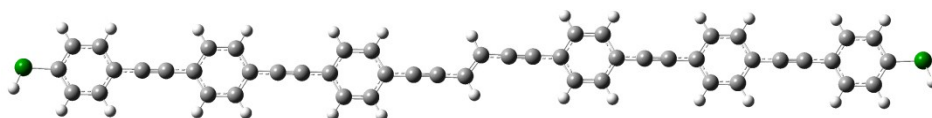
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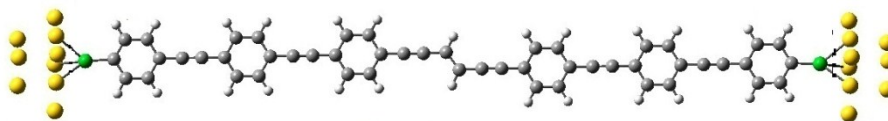
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Au	0.00000000	-1.66276561	-24.66729685
Au	1.44000000	0.83138439	-24.66729685
Au	-1.44000000	0.83138439	-24.66729685
Au	-2.88000000	-1.66276561	-24.66729685
Au	2.88000000	-1.66276561	-24.66729685
Au	0.00000000	3.32554439	-24.66729685