Electronic Supplemental Information of the Article:

Magnetic and Transport Properties of Conjugated and Cumulated Molecules: the π-System Enlightens Part of the Story

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Table S1 The energy (a.u.), $\langle S^2 \rangle$ and magnetic exchange coupling constant (J in (cm^{-1})) of the odd cumulene based diradicals (B3LYP-D /6-311++G(d,p)).

Diradicals		Triplet	BS	J (cm^{-1})
1(a)	Energy (a.u.)	-1183.48377	-1183.48355	48.05
	$\langle S^2 \rangle$	2.136	1.124	
1(b)	Energy (a.u.)	-1259.65614	-1259.65566	101.73
	$\langle S^2 \rangle$	2.208	1.169	
1(c)	Energy (a.u.)	-1335.83327	-1335.83239	176.10
	$\langle S^2 \rangle$	2.320	1.223	

Table S2 The energy (a.u.), $\langle S^2 \rangle$ and magnetic exchange coupling constant (J in (cm^{-1})) of the odd cumulene based diradicals (CAM-B3LYP /6-311++G(d,p)).

Diradicals		Triplet	BS	J (cm^{-1})
1(a)	Energy (a.u.)	-1182.84108	-1182.84058	106.44
	$\langle S^2 \rangle$	2.261	1.235	
1(b)	Energy (a.u.)	-1258.96336	-1258.96194	279.92
	$\langle S^2 \rangle$	2.453	1.340	
1(c)	Energy (a.u.)	-1335.09014	-1335.08668	587.94
	$\langle S^2 \rangle$	2.824	1.529	

Table S3 The energy (a.u.), $\langle S^2 \rangle$ and magnetic exchange coupling constant (J in (cm^{-1})) of the even cumulene based diradicals (B3LYP/6-311++G(d,p)).

Diradicals		**Triplet**	**BS**	***J* (cm^{-1})**
2(a)	**Energy (a.u.)**	-1221.50674	-1221.51048	-1003.86
	$\langle S^2 \rangle$	2.119	1.302	
2(b)	**Energy (a.u.)**	-1297.67951	-1297.68382	-1291.24
	$\langle S^2 \rangle$	2.137	1.404	
2(c)	**Energy (a.u.)**	-1373.85534	-1373.86026	-1679.34
	$\langle S^2 \rangle$	2.156	1.513	

Table S4 The energy (a.u.), $\langle S^2 \rangle$ and magnetic exchange coupling constant (J in (cm^{-1})) of the even cumulene based diradicals (B3LYP-D /6-311++G(d,p)).

Diradicals		**Triplet**	**BS**	***J* (cm^{-1})**
2(a)	**Energy (a.u.)**	-1221.56528	-1221.56946	-1172.14
	$\langle S^2 \rangle$	2.118	1.335	
2(b)	**Energy (a.u.)**	-1297.74438	-1297.74873	-1302.45
	$\langle S^2 \rangle$	2.137	1.406	
2(c)	**Energy (a.u.)**	-1373.92099	-1373.92594	-1695.14
	$\langle S^2 \rangle$	2.156	1.515	

Table S5 The energy (a.u.), $\langle S^2 \rangle$ and magnetic exchange coupling constant (J in (cm^{-1})) of the even cumulene based diradicals (CAM-B3LYP /6-311++G(d,p)).

Diradicals		Triplet	BS	J (cm^{-1})
2(a)	Energy (a.u.)	-1220.89356	-1220.90261	-3256.97
	$\langle S^2 \rangle$	2.226	1.616	
2(b)	Energy (a.u.)	-1297.02294	-1297.03155	-3429.87
	$\langle S^2 \rangle$	2.253	1.703	
2(c)	Energy (a.u.)	-1373.14718	-1373.15792	-6158.36
	$\langle S^2 \rangle$	2.296	1.913	

Table S6 The energy (a.u.), $\langle S^2 \rangle$ and magnetic exchange coupling constant (J in (cm^{-1})) of the diradical based on conjugated systems (B3LYP/6-311++G(d,p)).

Diradicals		**Triplet**	**BS**	***J*** **(cm^{-1})**
3(a)	**Energy (a.u.)**	-1222.77595	-1222.77989	-565.03
	$\langle S^2 \rangle$	2.117	1.225	
3(b)	**Energy (a.u.)**	-1300.20673	-1300.20855	-450.12
	$\langle S^2 \rangle$	2.133	1.245	
3(c)	**Energy (a.u.)**	-1377.63530	-1377.63681	-373.53
	$\langle S^2 \rangle$	2.147	1.264	

Table S7 The energy (a.u.), $\langle S^2 \rangle$ and magnetic exchange coupling constant (J in (cm^{-1})) of the diradical based on conjugated systems (B3LYP-D/6-311++G(d,p)).

Diradicals		Triplet	BS	J (cm^{-1})
3(a)	Energy (a.u.)	-1222.84466	-1222.84684	-536.49
	$\langle S^2 \rangle$	2.117	1.227	
3(b)	Energy (a.u.)	-1300.27678	-1300.27863	-456.71
	$\langle S^2 \rangle$	2.133	1.247	
3(c)	Energy (a.u.)	-1377.70835	-1377.70988	-379.74
	$\langle S^2 \rangle$	2.148	1.266	

Table S8 The energy (a.u.), $\langle S^2 \rangle$ and magnetic exchange coupling constant (J in (cm^{-1})) of the diradical based on conjugated systems (CAM-B3LYP/6-311++G(d,p)).

Diradicals		Triplet	BS	J (cm^{-1})
3(a)	Energy (a.u.)	-1222.17266	-1222.17652	-1029.03
	$\langle S^2 \rangle$	2.217	1.393	
3(b)	Energy (a.u.)	-1299.55258	-1299.55564	-828.31
	$\langle S^2 \rangle$	2.249	1.439	
3(c)	Energy (a.u.)	-1376.93172	-1376.93426	-699.12
	$\langle S^2 \rangle$	2.280	1.483	

Singlet and Triplet weightings[*] Considering a general BS state which is a nearly equal superposition of singlet (S) and triplet (T) states. We can write

$$\psi_{BS} = \mathrm{m}\,\psi_S^{BS} + \mathrm{n}\,\psi_T^{BS}$$

Where $m^2 \approx n^2 \approx 1/2$, $m^2 + n^2 = 1$ and $n^2 = 0.5\,\langle S^2 \rangle_{BS}$

Therefore $m^2 = 1 - 0.5\langle S^2 \rangle_{BS}$. The net weights of singlet and triplet components in the BS solution are given in Table S9, Table S10, Table S11.

Table S9 Percent Net Weight of Triplet and Singlet Components in the Computed BS Solution (B3LYP/6-311++G(d,p)). ** $\langle S^2 \rangle_{BS}$ value is taken from ref 55.

System	singlet % weight ($100m^2$)	triplet % weight ($100n^2$)
1(a)**	43.85	56.15
1(b)**	41.70	58.30
1(c)**	39.15	60.85
2(a)	34.90	65.10
2(b)	29.80	70.20
2(c)	24.35	75.65
3(a)	38.75	61.25
3(b)	37.75	62.25
3(c)	36.80	63.20

Table S10 Percent Net Weight of Triplet and Singlet Components in the Computed BS Solution (B3LYP-D/6-311++G(d,p)).

System	singlet % weight ($100m^2$)	triplet % weight ($100n^2$)
1(a)	43.80	56.20
1(b)	41.55	58.45
1(c)	38.85	61.15
2(a)	33.25	66.75
2(b)	29.70	70.30
2(c)	24.25	75.75
3(a)	38.65	61.35
3(b)	37.65	62.35
3(c)	36.70	63.30

***** I. A. Latif, V. P. Singh, U. Bhattacharjee, A. Panda, S. N. Datta, *J. Phys. Chem. A* ,2010, ***114,*** 6648–6656.

Table S11 Percent Net Weight of Triplet and Singlet Components in the Computed BS Solution (CAM-B3LYP /6-311++G(d,p)).

System	singlet % weight ($100m^2$)	triplet % weight ($100n^2$)
1(a)	38.25	61.75
1(b)	33.00	67.00
1(c)	23.55	76.45
2(a)	19.20	80.80
2(b)	14.85	85.15
2(c)	4.35	95.65
3(a)	30.35	69.65
3(b)	28.05	71.95
3(c)	25.85	74.15

Table S12 Bond angle of the couplers of series 1-3 (B3LYP/6-311++G(d,p)) [*taken from reference 55].

Systems	**Bond angle/ º**					
	∠c1-c2-c3	**∠c2-c3-c4**	**∠c3-c4-c5**	**∠c4-c5-c6**	**∠c5-c6-c7**	**∠c6-c7-c8**
1(a)*	**173.87**	**---------**	**---------**	**----------**	**---------**	
1(b)*	**174.35**	**177.97**	**174.35**	**--------**	**---------**	
1(c)*	**174.33**	**178.42**	**179.80**	**178.41**	**174.33**	
2(a)	**173.60**	**173.59**				
2(b)	**172.97**	**178.34**	**178.34**	**174.67**		
2(c)	**172.93**	**178.22**	**179.97**	**179.97**	**178.22**	**172.93**
3(a)	**121.99**	**121.99**				
3(b)	**122.59**	**123.63**	**123.63**	**122.59**		
3(c)	**122.85**	**123.51**	**124.32**	**124.16**	**123.66**	**122.70**

The calculated bond angles within the coupler are given in Table S12. The bond angle of the cumulene coupler deviates from the exact angle of allene (180º), therefore they have a nonlinear C=C=C framework. This bending is higher in case of short chain cumulene coupler than that of long chain cumulene coupler. This is because, on going from diradical substituted cumulene to its higher homologue in each series, the middle allene counterpart goes nearly 180º (e.g, for 2(a) ∠c1-c2- c3=173.60º, for 2(b) ∠c2-c3-c4=178.34º, and for 2(c) ∠c3-c4-c5=179.97º). For this the π-system of short chain cumulene coupler is significantly disturbed and a relatively strong π-

interaction with increasing chain length of the coupler in each series is expected and the coupling constant increases accordingly. Therefore the bending is not the reason of increase in coupling constant for long chain cumulene in each series, rather than the linearity of long cumulene chain (with strong π-interaction) is the reason of increase in coupling constant.

Table S13 Spin density distribution on each atom of the coupler of diradical based on odd cumulenes in their high spin state (B3LYP/6-311++G(d,p)) (taken from reference 55).

Systems	**Spin density on different atoms of coupler**							**Average spin density on each atom of the coupler**
	C1	C2	C3	C4	C5	C6	C7	
1(a)	0.0768	-0.2655	0.0768	--------	--------	--------	--------	0.1397
1(b)	0.1072	-0.2664	0.1572	-0.2665	0.1071	--------	--------	0.1809
1(c)	0.1501	-0.3004	0.2041	-0.3196	0.2041	-0.3004	0.1501	0.2327

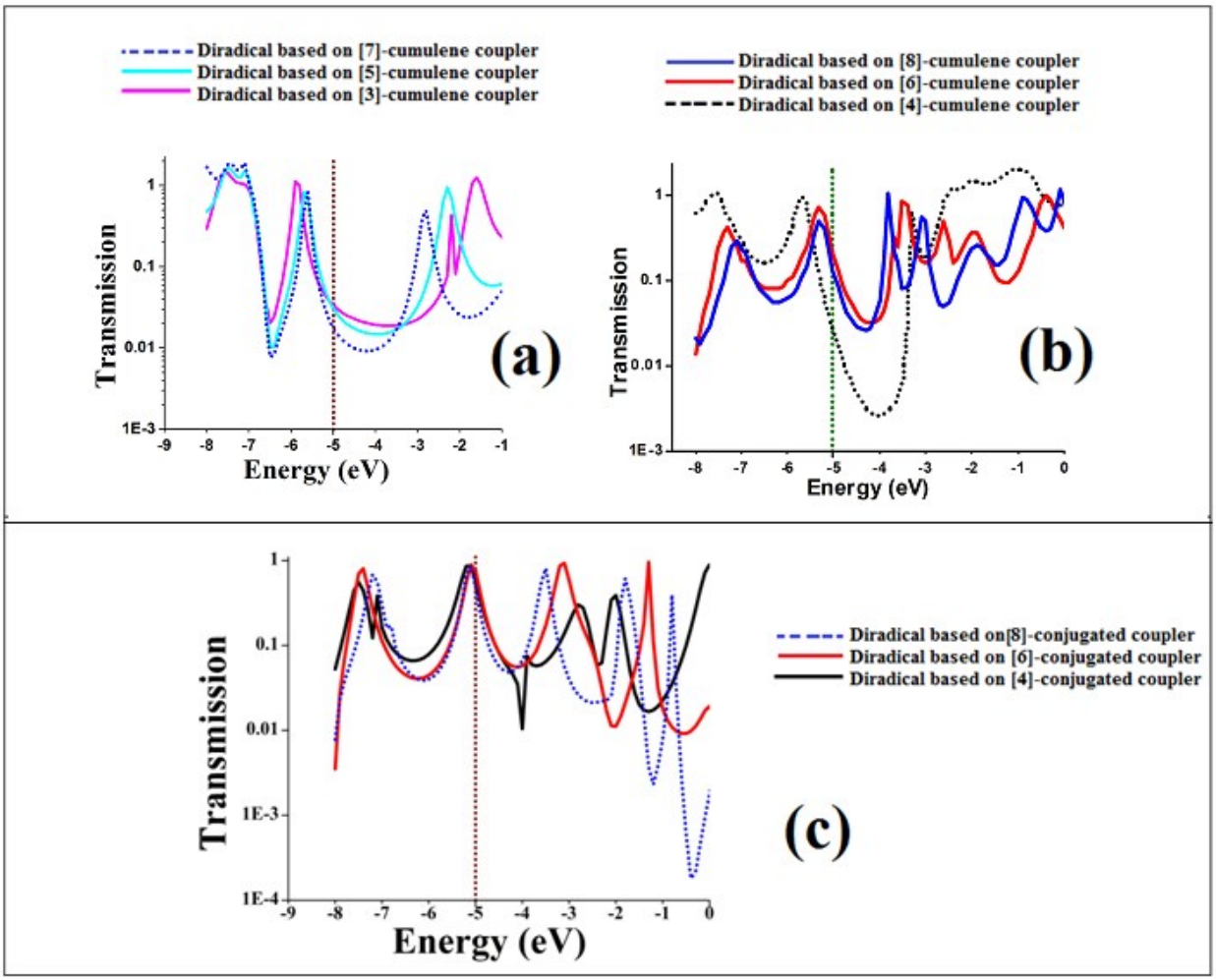


Fig. S1 Transmission spectra of all the designed diradical based molecular wires (for *β* spin). (The transmission is expressed using a log scale). Fig. (a) represents the transmission spectra of

odd cumulene based diradicals, Fig. (b) represents the transmission spectra of even cumulene based diradicals, Fig. (c) represents the transmission spectra of diradicals based on conjugated systems.

Table S14 Energy of $(HOMO-2)_{\alpha}$, $(HOMO-1)_{\alpha}$, $(HOMO)_{\alpha}$ and $(LUMO)_{\alpha}$ for diradical based on odd cumulenes (B3LYP/6-311++G(d,p)) (taken from reference 55).

Systems	$(E_{HOMO-2})_{\alpha}$(eV)	$(E_{HOMO-1})_{\alpha}$(eV)	$(E_{HOMO})_{\alpha}$(eV)	$(E_{LUMO})_{\alpha}$(eV)
1(a)	-6.89275	-5.29989	-5.29309	-1.58143
1(b)	-6.54971	-5.39002	-5.38653	-2.36083
1(c)	-6.29637	-5.47614	-5.47329	-2.83002

Table S15 Energy of $(HOMO-1)_{\alpha}$, $(HOMO)_{\beta}$, $(HOMO)_{\alpha}$ and $(LUMO)_{\alpha}$ for diradical based on conjugated and cumulene couplers (B3LYP/6-311++G(d,p)).

Systems	$(E_{HOMO-1})_{\alpha}$ (eV)	$(E_{HOMO})_{\alpha}$(eV)	$(E_{HOMO})_{\beta}$(eV)	$(E_{LUMO})_{\alpha}$(eV)
2(a)	-5.98562	-5.43414	-5.43414	-2.71938
2(b)	-5.90437	-5.51172	-5.51172	-3.06425
2(c)	-5.85536	-5.57901	-5.57901	-3.29603
3(a)	-5.92453	-5.39471	-5.39471	-2.40915
3(b)	-5.71577	-5.38513	-5.38511	-2.56017
3(c)	-5.54832	-5.36897	-5.37308	-2.66809

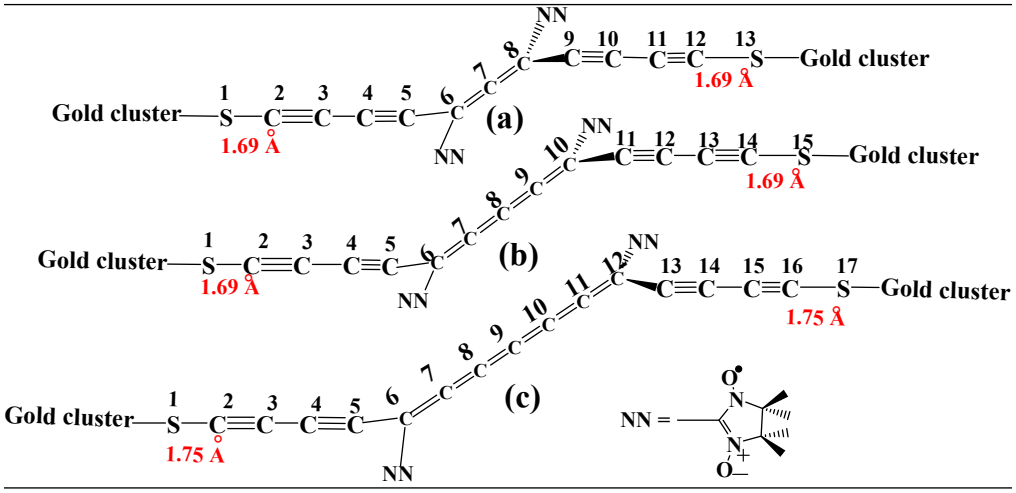


Fig. S2 Odd cumulene based molecular wires used for the transport calculation.

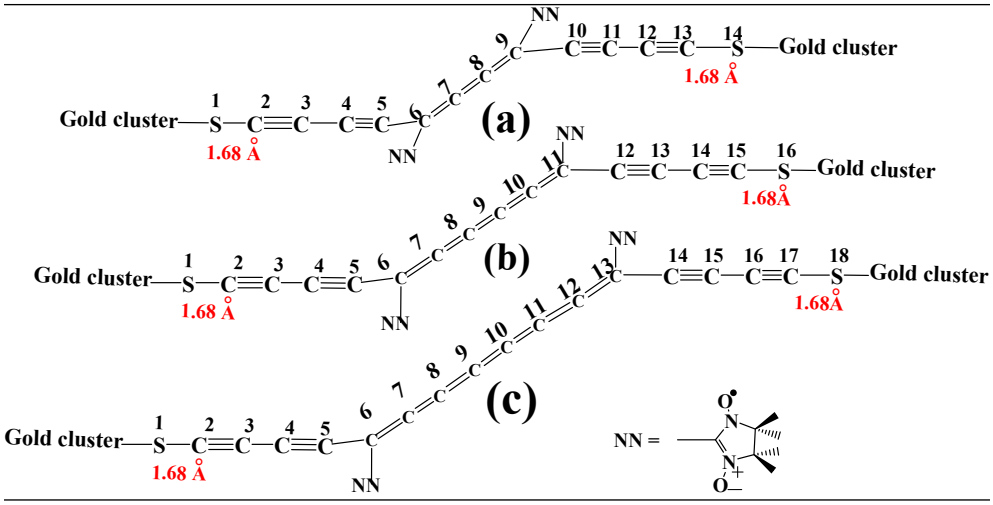


Fig. S3 Designed even cumulene based molecular wires for the transport calculation.

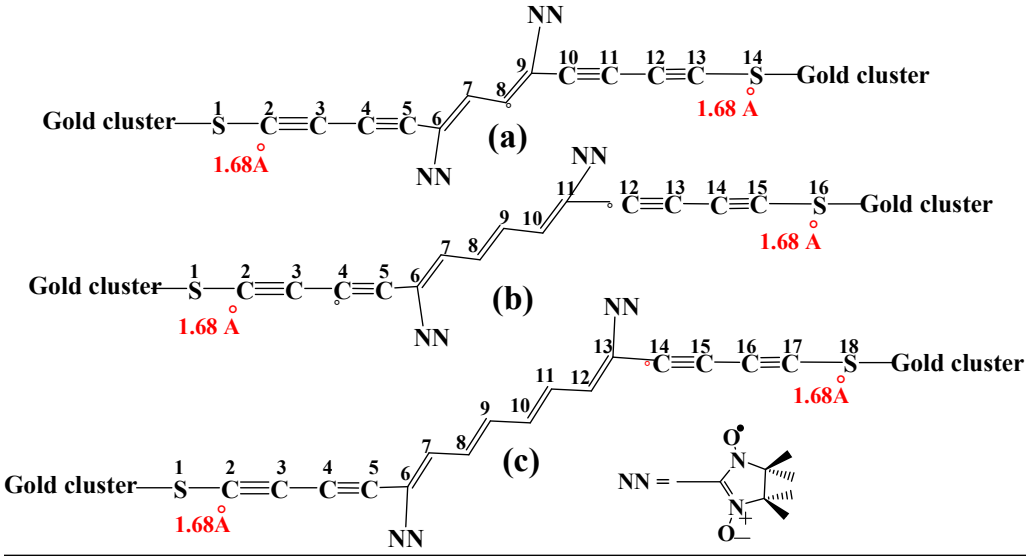


Fig. S4 Designed even conjugated system based molecular wires for the transport calculation.

Table S16 Bond distance between two neighboring atoms of all the molecular wire used for transport calculation (from Supplementary Information Fig. S2, Fig. S3, and Fig. S4). All bonds are in Å unit.

Systems		**S2(a)**	**S2(b)**	**S2(c)**	**S3(a)**	**S3(b)**	**S3(c)**	**S4(a)**	**S4(b)**	**S4(c)**
Distance between atoms (in Å)	Atom (1-2)	1.69	1.68	1.75	1.68	1.68	1.68	1.68	1.68	1.68
	Atom (2-3)	1.22	1.22	1.22	1.22	1.22	1.22	1.22	1.22	1.22
	Atom (3-4)	1.35	1.35	1.36	1.35	1.35	1.35	1.35	1.35	1.35
	Atom (4-5)	1.21	1.22	1.23	1.22	1.22	1.22	1.22	1.22	1.22
	Atom (5-6)	1.42	1.42	1.42	1.41	1.41	1.41	1.41	1.42	1.42
	Atom (6-7)	1.33	1.35	1.37	1.36	1.36	1.38	1.38	1.38	1.39
	Atom (7-8)	1.33	1.27	1.27	1.24	1.25	1.23	1.42	1.42	1.41
	Atom (8-9)	1.42	1.27	1.29	1.36	1.31	1.32	1.38	1.37	1.38
	Atom (9-10)	1.21	1.35	1.29	1.41	1.25	1.24	1.41	1.42	1.42
	Atom (10-11)	1.35	1.42	1.27	1.22	1.36	1.32	1.22	1.38	1.38
	Atom (11-12)	1.22	1.22	1.37	1.35	1.41	1.23	1.35	1.42	1.41
	Atom (12-13)	1.69	1.35	1.42	1.22	1.22	1.38	1.22	1.22	1.39
	Atom (13-14)	------	1.22	1.23	1.68	1.35	1.41	1.68	1.35	1.42
	Atom (14-15)	------	1.69	1.36	-----	1.22	1.22	------	1.22	1.22
	Atom (15-16)	------	------	1.22	-----	1.68	1.35	------	1.68	1.35
	Atom (16-17)	------	------	1.75	-----	------	1.22	------	------	1.22
	Atom (17-18)	------	------	------	-----	------	1.68	------	------	1.68

Full optimized coordinates of all the diradicals at UB3LYP/6-311++G(d,p) Level

2(a)

C	3.01519400	0.47064000	-0.00424500
C	4.89086700	-0.95852800	-0.22035500
C	5.37473200	0.46429900	0.22866900
C	-3.01523000	-0.47073200	-0.00434600
C	-5.37475700	-0.46420300	0.22870300
C	-4.89079900	0.95858500	-0.22035000
N	3.39597600	-0.82900600	-0.02219100
N	4.11669200	1.27006500	0.01687300

N	-3.39591000	0.82894200	-0.02226700
N	-4.11679000	-1.27007000	0.01685600
O	2.62509800	-1.83585000	-0.03986400
O	-2.62494900	1.83572100	-0.04000300
O	4.11334800	2.54064300	0.03339800
O	-4.11354800	-2.54065000	0.03337600
C	5.70281100	0.56934000	1.72842500
H	4.90140500	0.16494400	2.34980000
H	6.62697300	0.03652900	1.96065600
H	5.83584900	1.62185600	1.98398900
C	6.51271000	1.06231300	-0.59569700
H	6.71113000	2.07717200	-0.25041700
H	7.41978100	0.46733800	-0.46384900
H	6.27535900	1.10988100	-1.65773700
C	5.09888000	-1.24442200	-1.71743800
H	6.15849400	-1.38366100	-1.94046900
H	4.56600500	-2.16079800	-1.97646800
H	4.71397700	-0.43642500	-2.34272900
C	5.41695100	-2.12524800	0.61199900
H	4.95302000	-3.04955500	0.26715500
H	6.49905800	-2.21282500	0.48744300
H	5.19362600	-2.01345200	1.67233100
C	-5.41673800	2.12535000	0.61203200
H	-4.95275400	3.04961900	0.26716000
H	-6.49884600	2.21301400	0.48754100
H	-5.19335900	2.01353700	1.67235000
C	-5.09887000	1.24449100	-1.71742100
H	-6.15848500	1.38382200	-1.94039100
H	-4.56592500	2.16081400	-1.97649100
H	-4.71407700	0.43645200	-2.34272700
C	-5.70278000	-0.56921500	1.72847500
H	-6.62689900	-0.03634600	1.96074400
H	-5.83587400	-1.62172200	1.98404800
H	-4.90132300	-0.16486900	2.34981700
C	-6.51282100	-1.06213300	-0.59560700
H	-6.71130900	-2.07697100	-0.25030300
H	-7.41983900	-0.46708400	-0.46373000
H	-6.27552000	-1.10973700	-1.65765700
C	1.68488000	0.99222800	-0.00959900
C	0.56207500	0.27585200	-0.02182200

C	-0.56208900	-0.27615200	-0.02191900
C	-1.68496100	-0.99242200	-0.00977200
H	-1.63325400	-2.07808000	0.00067300
H	1.63308700	2.07788100	0.00073100

2(b)

C	4.23326300	-0.61263900	-0.01597600
C	5.92546400	1.02898100	0.20557800
C	6.58422600	-0.34437900	-0.17363400
C	-4.23322800	0.61258800	-0.01612000
C	-6.58422200	0.34447000	-0.17356000
C	-5.92550900	-1.02893300	0.20558000
N	4.46354900	0.72230500	-0.03581800
N	5.41842300	-1.28164100	0.02622600
N	-4.46359500	-0.72234200	-0.03593300
N	-5.41834400	1.28166100	0.02619700
O	3.58032200	1.63080200	-0.07987400
O	-3.58042500	-1.63089200	-0.08007100
O	5.55724200	-2.54446600	0.05700900
O	-5.55708400	2.54449400	0.05698500
C	6.97786100	-0.45990400	-1.65646800
H	6.15929700	-0.17063500	-2.31837800
H	7.84331000	0.16799700	-1.87640900
H	7.23916300	-1.49781400	-1.86891600
C	7.75064700	-0.77821300	0.71102100
H	8.08037500	-1.77258900	0.40917500
H	8.58621600	-0.08439500	0.59047800
H	7.47889300	-0.82051900	1.76497700
C	6.04150900	1.38938100	1.69661400
H	7.06567900	1.67092100	1.94874900
H	5.38841700	2.23916500	1.90180700
H	5.73801500	0.56155400	2.34043100
C	6.34678400	2.21887600	-0.65353000
H	5.77058500	3.09616100	-0.35876300
H	7.40718000	2.43232100	-0.49810400
H	6.17534400	2.04637500	-1.71536200
C	-6.34697800	-2.21879300	-0.65350600
H	-5.77081600	-3.09611900	-0.35879200
H	-7.40737600	-2.43216600	-0.49800000
H	-6.17560700	-2.04629200	-1.71534900

C	-6.04146100	-1.38933600	1.69662200
H	-7.06563000	-1.67081100	1.94883400
H	-5.38840800	-2.23916400	1.90175600
H	-5.73786300	-0.56153400	2.34042300
C	-6.97799700	0.46003200	-1.65635300
H	-7.84351200	-0.16780600	-1.87621400
H	-7.23924700	1.49796200	-1.86876600
H	-6.15952000	0.17071100	-2.31834800
C	-7.75052900	0.77836100	0.71121600
H	-8.08021500	1.77277000	0.40943000
H	-8.58615700	0.08460500	0.59072900
H	-7.47867300	0.82061600	1.76514800
C	-2.97177600	1.27773400	-0.03041000
C	-1.77388100	0.69143600	-0.04146700
C	-0.59847000	0.24618500	-0.04917400
C	0.59848700	-0.24644400	-0.04912900
C	1.77391700	-0.69164000	-0.04131100
C	2.97184900	-1.27786100	-0.03015200
H	3.04439500	-2.36302300	-0.02632500
H	-3.04425200	2.36290000	-0.02634900

2(c)

C	-5.48671600	0.68534800	-0.00621500
C	-7.05870800	-1.07356800	0.20840600
C	-7.81015000	0.24639000	-0.18811700
C	5.48675700	-0.68541000	-0.00626100
C	7.81016700	-0.24627600	-0.18807200
C	7.05860800	1.07362700	0.20840800
N	-5.61992100	-0.66320200	-0.01860000
N	-6.71810600	1.26699200	0.01966200
N	5.61986000	0.66314900	-0.01865800
N	6.71819100	-1.26696100	0.01966800
O	-4.67141800	-1.50383700	-0.04580400
O	4.67129400	1.50371000	-0.04590000
O	-6.94702800	2.51668500	0.03915800
O	6.94720600	-2.51663600	0.03918900
C	-8.19312300	0.32469000	-1.67631600
H	-7.34856400	0.09148300	-2.32759900
H	-9.00876100	-0.36479000	-1.90219500

H	-8.52573300	1.33993200	-1.89841500
C	-9.01588400	0.60095800	0.67947600
H	-9.41000800	1.56860000	0.36818800
H	-9.79960300	-0.14972600	0.55184300
H	-8.76177000	0.66650100	1.73666600
C	-7.16673200	-1.43264600	1.70034700
H	-8.17181900	-1.78332000	1.94257700
H	-6.45856800	-2.23354200	1.91895100
H	-6.92965600	-0.58210500	2.34250000
C	-7.38186400	-2.29580800	-0.64776000
H	-6.74618300	-3.12687200	-0.34152900
H	-8.42534000	-2.58576200	-0.50245400
H	-7.21170100	-2.11682700	-1.70869000
C	7.38170100	2.29588900	-0.64775200
H	6.74593000	3.12689800	-0.34156000
H	8.42514300	2.58593800	-0.50239400
H	7.21160800	2.11688400	-1.70868900
C	7.16653500	1.43272300	1.70035200
H	8.17158100	1.78348800	1.94262100
H	6.45829200	2.23355600	1.91892300
H	6.92950900	0.58216300	2.34249700
C	8.19321100	-0.32455600	-1.67625500
H	9.00880400	0.36498600	-1.90210400
H	8.52591000	-1.33977400	-1.89833300
H	7.34866200	-0.09141900	-2.32757600
C	9.01589200	-0.60074500	0.67957400
H	9.41009700	-1.56836300	0.36831100
H	9.79956300	0.14999200	0.55196200
H	8.76174200	-0.66629500	1.73675400
C	4.27783300	-1.43785000	-0.01426800
C	3.03953300	-0.93958400	-0.01977500
C	1.83299800	-0.58343700	-0.02644200
C	-1.83292600	0.58323400	-0.02631800
C	-3.03947000	0.93935300	-0.01963900
C	-4.27773700	1.43770300	-0.01417000
H	-4.42724100	2.51523900	-0.01352400
H	4.42740900	-2.51537600	-0.01361200
C	-0.60281300	0.18803200	-0.02964000
C	0.60290300	-0.18818600	-0.02969000

3(a)

C	5.16156900	0.90394600	0.11889800
C	5.45898000	-0.61402300	-0.13993400
N	3.66436400	0.94235700	-0.08759800
C	3.11307800	-0.28737300	0.03951000
N	4.10532700	-1.21697900	0.13864400
C	5.78399600	-0.94725700	-1.60648300
C	6.50266600	-1.24502100	0.77944100
C	5.40515500	1.34955000	1.57087700
C	5.83493000	1.87876600	-0.84468700
O	3.03638000	2.04416600	-0.20317900
O	3.93898800	-2.46910300	0.27551200
H	5.04626200	-0.52625700	-2.29218700
H	6.77066000	-0.56807400	-1.87913600
H	5.78323200	-2.03183500	-1.72654500
H	6.56989000	-2.31223200	0.56701000
H	7.48051900	-0.79244700	0.59749700
H	6.25264000	-1.12790300	1.83317400
H	4.91950800	0.68432000	2.28748500
H	6.47390900	1.37967800	1.79171500
H	4.99512300	2.35213300	1.70313000
H	5.49485400	2.89124200	-0.62658800
H	6.91923900	1.84112100	-0.71417900
H	5.59932000	1.66324500	-1.88620700
C	-1.72605300	0.63931600	-0.07369000
C	-0.68408900	-0.22413100	0.01914000
C	0.68408800	0.22412900	-0.01914800
C	1.72605200	-0.63931800	0.07368400
H	-1.55374800	1.70543400	-0.18106200
H	-0.88140100	-1.28419400	0.12972400
H	0.88140000	1.28419200	-0.12973100
H	1.55374700	-1.70543500	0.18105600
O	-3.93898900	2.46910200	-0.27552600
O	-3.03638200	-2.04416600	0.20318100
C	-5.45897900	0.61402400	0.13994000
N	-4.10532800	1.21697900	-0.13864700
C	-3.11307800	0.28737200	-0.03951500
N	-3.66436500	-0.94235700	0.08759600
C	-5.16157000	-0.90394500	-0.11889800
C	-5.78398000	0.94725200	1.60649300

C	-6.50267300	1.24502300	-0.77942400
C	-5.83493100	-1.87876600	0.84468400
C	-5.40515800	-1.34954300	-1.57087800
H	-5.04624300	0.52624500	2.29218900
H	-5.78321100	2.03183000	1.72656000
H	-6.77064500	0.56807400	1.87915300
H	-7.48052200	0.79244100	-0.59747700
H	-6.56990400	2.31223100	-0.56698500
H	-6.25265300	1.12791400	-1.83315900
H	-5.59931100	-1.66325500	1.88620400
H	-6.91924100	-1.84110800	0.71418500
H	-5.49486900	-2.89124500	0.62657600
H	-4.99512300	-2.35212400	-1.70313700
H	-6.47391200	-1.37967200	-1.79171500
H	-4.91951300	-0.68430900	-2.28748500

3(b)

C	6.34605300	0.92900300	0.11780700
C	6.69869000	-0.57614800	-0.14735000
N	4.84778900	0.91163500	-0.08045100
C	4.34261500	-0.33845400	0.04685500
N	5.37101200	-1.22971500	0.13879800
C	7.02668500	-0.89277400	-1.61701300
C	7.77166500	-1.16995200	0.76312700
C	6.58199200	1.37921300	1.56960700
C	6.97716900	1.93087500	-0.84674400
O	4.17780900	1.99005000	-0.18873000
O	5.25210600	-2.48832600	0.27161900
H	6.27001800	-0.49678400	-2.29696000
H	7.99736200	-0.47743600	-1.89443900
H	7.06424600	-1.97634300	-1.74043200
H	7.87664600	-2.23349900	0.54762000
H	8.73091000	-0.68136500	0.57538300
H	7.52491200	-1.06448800	1.81884700
H	6.12618300	0.69414600	2.28713900
H	7.65026100	1.44883100	1.78376200
H	6.13545500	2.36529600	1.70762100
H	6.60286100	2.92982900	-0.62241400
H	8.06309600	1.93138300	-0.72443000

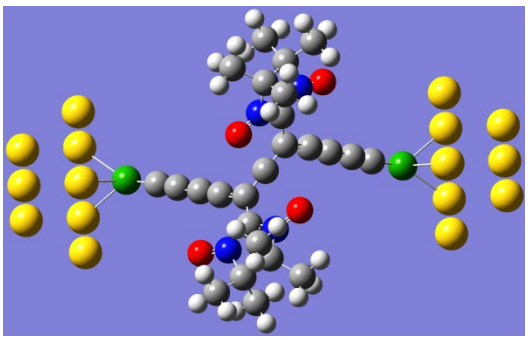
H	6.74160600	1.71078400	-1.88730700
C	-2.97240300	0.74228700	-0.08655600
C	-1.89626200	-0.08271600	-0.00372500
C	-0.54533500	0.40205900	-0.04369000
H	-2.84244400	1.81500000	-0.18836400
H	-2.05795700	-1.14941000	0.10182300
H	-0.39838000	1.47529000	-0.14837400
O	-5.25184600	2.48845100	-0.27032100
O	-4.17803400	-1.99034500	0.18711600
C	-6.69853300	0.57625900	0.14822600
N	-5.37089000	1.22978800	-0.13813300
C	-4.34258800	0.33830200	-0.04708300
N	-4.84790200	-0.91177500	0.07969500
C	-6.34624500	-0.92878700	-0.11801000
C	-7.02579400	0.89206900	1.61823000
C	-7.77183900	1.17073400	-0.76141800
C	-6.97715500	-1.93118000	0.84612800
C	-6.58281200	-1.37799700	-1.57001400
H	-6.26886600	0.49557000	2.29758800
H	-7.06313900	1.97557300	1.74228600
H	-7.99640300	0.47671600	1.89587400
H	-8.73100000	0.68197500	-0.57369800
H	-7.87678200	2.23411900	-0.54509700
H	-7.52545600	1.06605000	-1.81730500
H	-6.74120000	-1.71177200	1.88674300
H	-8.06312500	-1.93146300	0.72419300
H	-6.60306400	-2.93004600	0.62104600
H	-6.13653200	-2.36408200	-1.70884700
H	-7.65117200	-1.44724200	-1.78383800
H	-6.12711400	-0.69255200	-2.28725500
C	0.54534500	-0.40253200	0.04266600
H	0.39840600	-1.47576500	0.14737200
C	1.89626400	0.08229800	0.00279600
H	2.05791700	1.14896800	-0.10304800
C	2.97246000	-0.74259200	0.08607700
H	2.84258900	-1.81528000	0.18819400

3(c)

N	-6.63210700	-1.22496200	0.18866400
C	-5.57562300	-0.37652900	0.03024100
N	-6.04098300	0.88496200	-0.13585800
C	-7.53019500	0.96597700	0.10661000
C	-7.94499100	-0.53504400	-0.07877100
C	-0.67180400	0.22154800	-0.10794000
C	0.67002100	-0.27804200	-0.06283500
C	1.77923400	0.50668600	-0.11777900
C	3.11774400	-0.00454100	-0.06710600
C	4.21337100	0.80036000	-0.09936000
H	4.10738400	1.87851200	-0.16489600
O	-5.33700700	1.93368700	-0.30704500
C	-7.70022000	1.49209500	1.54243800
C	-8.15650400	1.94681600	-0.88255100
C	-9.00384100	-1.04920000	0.89466400
C	-8.33940700	-0.90230300	-1.52025800
O	-6.55352300	-2.48109800	0.36900700
C	5.57252100	0.36709600	-0.04514500
N	6.05104000	-0.89785500	0.03744700
C	7.55228400	-0.93604200	-0.13102600
C	7.92754700	0.54635100	0.21578700
N	6.62104300	1.24000300	-0.07196100
O	5.35787300	-1.96651100	0.08080600
C	7.81033400	-1.31793300	-1.59863900
C	8.14408500	-1.99666700	0.79447700
C	9.03589200	1.16019900	-0.63709600
C	8.22259300	0.78507200	1.70725300
O	6.53030600	2.50580600	-0.14898700
H	8.88128700	-1.39859200	-1.79512700
H	7.34757900	-2.28659900	-1.79435700
H	7.38259200	-0.58885400	-2.28956300
H	9.23233400	-2.01055400	0.69590300
H	7.88889800	-1.82464400	1.83938300
H	7.75800900	-2.97616300	0.51183600
H	9.97870300	0.63933800	-0.45282000
H	8.81290200	1.11541100	-1.70240500
H	9.16013600	2.20837900	-0.36421900
H	9.17800400	0.33851500	1.98949900
H	8.27641400	1.86061200	1.88372000
H	7.44118500	0.37179100	2.34785200

H	3.25685800	-1.07715500	0.00642600
H	1.65587200	1.58502500	-0.20055700
H	-8.75651700	1.62374300	1.78478500
H	-7.20385000	2.46083200	1.61908000
H	-7.25397100	0.82002000	2.27802200
H	-9.23709400	1.99302000	-0.72620900
H	-7.96344800	1.67226400	-1.91891700
H	-7.73943700	2.94006200	-0.71550400
H	-9.95193100	-0.53449200	0.72018500
H	-8.71417400	-0.90835700	1.93519900
H	-9.15387400	-2.11636300	0.72989000
H	-9.30361800	-0.46191600	-1.78118700
H	-8.42218000	-1.98791700	-1.59355700
H	-7.59459000	-0.56673400	-2.24443500
H	-0.79825600	1.29786400	-0.20819700
H	0.79799300	-1.35523900	0.02488300
C	-1.78315800	-0.55778200	-0.02603800
H	-1.66411800	-1.63458200	0.07958100
C	-3.11881400	-0.03787800	-0.06219400
H	-3.25065600	1.03118200	-0.18466100
C	-4.22073300	-0.82658500	0.05129400
H	-4.12459900	-1.90042100	0.17591700

Coordinates of all the molecular wires used for transport calculations



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C	3.64823418	-7.45571458	-0.15482565
C	4.47338306	-6.46246471	-1.04358916
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C	-4.24183349	-6.64817445	1.15222669
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N	2.42744535	-6.61607427	0.13990997
N	3.37325621	-5.55737559	-1.56296818
N	-2.35566247	-6.51271284	-0.27607750
N	-3.09749747	-5.81373172	1.69315984
O	1.58464201	-6.93489607	1.03611396
O	-1.62772390	-6.63454166	-1.31021143
O	3.57016792	-4.76239152	-2.52917656
O	-3.16900948	-5.23419324	2.81736924
C	5.42857521	-5.55664663	-0.24922341
H	4.92771780	-5.07423002	0.59226790
H	6.27605907	-6.13015503	0.13115184
H	5.80661291	-4.77867510	-0.91453745
C	5.20981255	-7.09383326	-2.22205687
H	5.67670006	-6.30841858	-2.81657742
H	5.99195642	-7.76259224	-1.85436842
H	4.54409111	-7.65748246	-2.87452762
C	3.14195136	-8.69771340	-0.90699863
H	3.96765721	-9.37612645	-1.12984337
H	2.42381579	-9.22157813	-0.27408119
H	2.64367049	-8.43306205	-1.84147318
C	4.31093947	-7.87084463	1.15664753
H	3.62120159	-8.49312671	1.72723300
H	5.21238095	-8.45263799	0.94930435
H	4.57986806	-7.01553160	1.77533453
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H	-3.71230817	-8.10285108	-2.02990665
H	-5.19217049	-8.27576173	-1.07129708
H	-4.69854230	-6.68465751	-1.68181126
C	-2.90773169	-8.77199351	0.44746143
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H	-2.26922219	-9.14681381	-0.35404584
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H	-4.91640711	-5.00423402	-0.13341321
C	-4.81693237	-7.50988667	2.27296793
H	-5.22577458	-6.86458948	3.05059685
H	-5.62314591	-8.13541339	1.88153496
H	-4.06548336	-8.15168515	2.73133432
C	-0.80823216	-3.85532232	1.88005362
C	-0.61297229	-2.97032980	2.68838430
C	-0.41235763	-1.99621479	3.60587146
C	-0.22935394	-1.09507876	4.40358382
C	0.93550596	-3.79988677	-1.85379762
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Au	-1.44000000	-0.83137561	9.85280463
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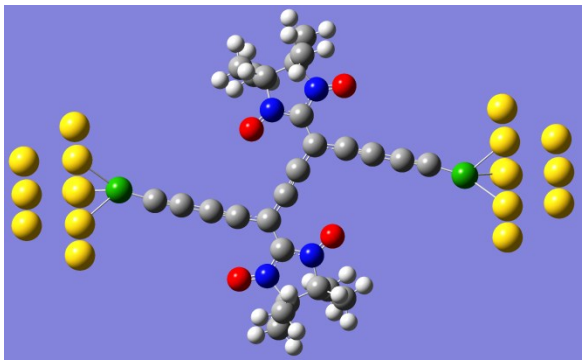

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C	5.34575944	-0.05636431	0.41736964
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C	-4.76063285	-0.32967795	1.00674615
N	3.28847017	-0.08168013	-0.75943347
N	4.13064986	-0.32293596	1.27797027
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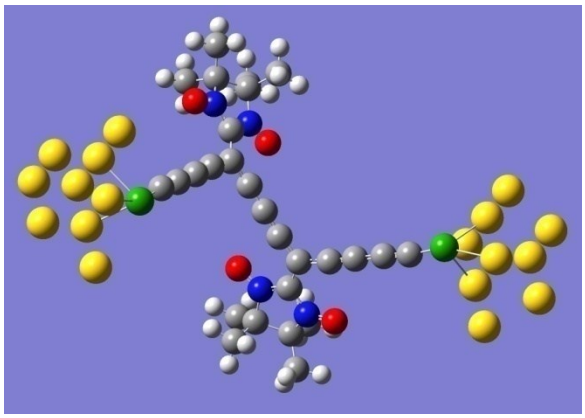

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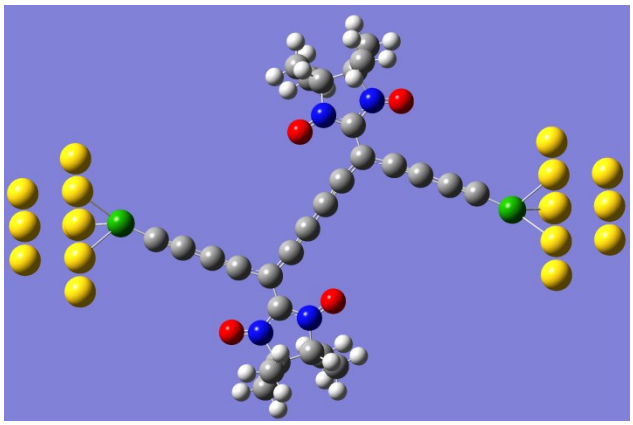

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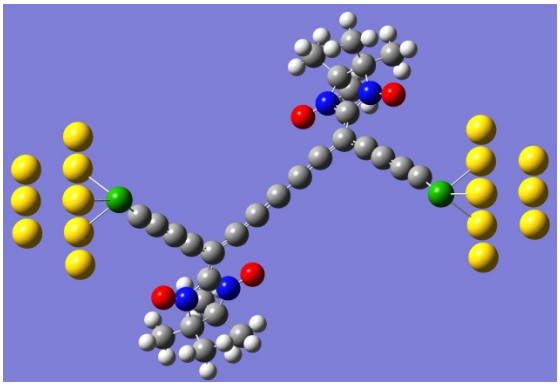

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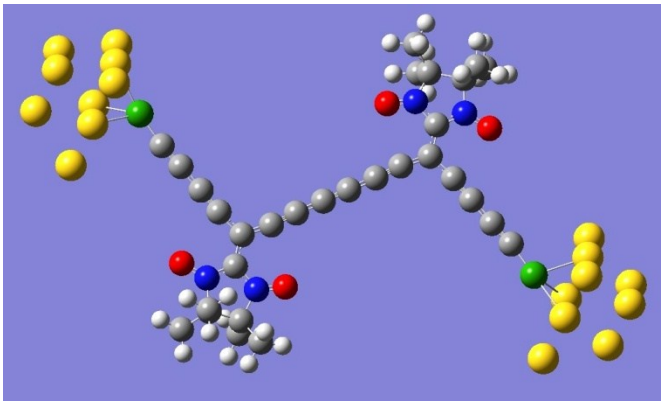

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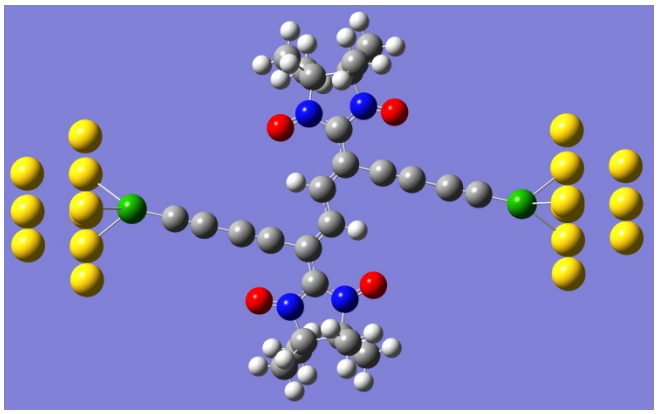

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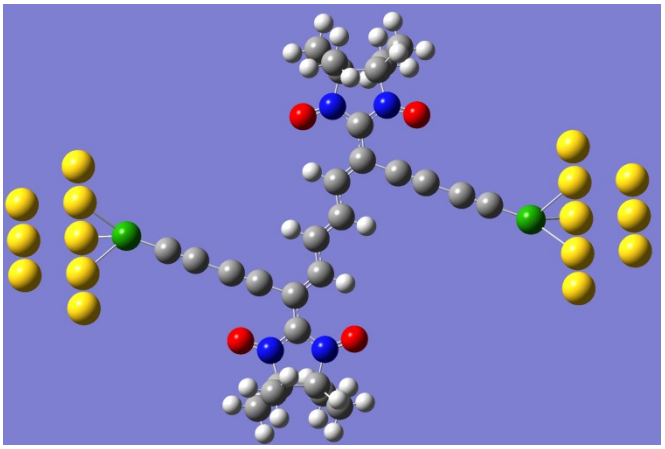

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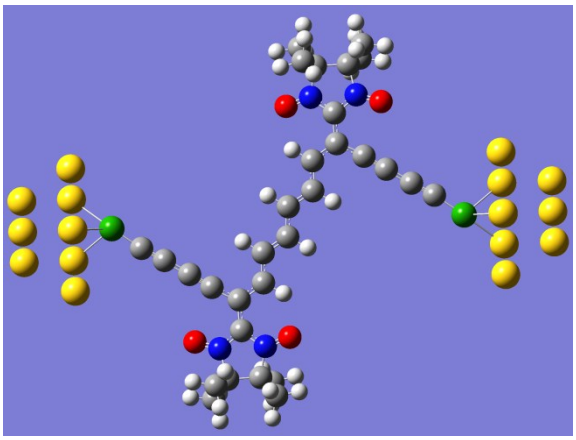

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