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Optical and Electronic Properties of Doubly Ortho-linked *cis*-4,4′-Bis(diarylamino)stilbene/Fluorene Hybrids

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Table S1. Selected Bond Lengths (Å) and Twist Angles (°) for the Molecules 1–6 by DFT//B3LYP/6-31G(d)

Molecule	**1**	**2**	**3**	**4**	**5**	**6**
C(1)-C(2)	1.5648	1.5675	1.5665	1.5660	1.5657	1.5656
C(1)-C(2′)	1.5648	1.5677	1.5651	1.5660	1.5673	1.5662
C(2)-C(3)	1.4209	1.4206	1.4229	1.4209	1.4222	1.4213
C(2′)-C(3′)	1.4209	1.4210	1.4220	1.4220	1.4235	1.4226
C(3)-C(4)	1.4577	1.4526	1.4532	1.4534	1.4529	1.4532
C(3′)-C(4′)	1.4576	1.4526	1.4535	1.4537	1.4524	1.4533
C(4)-C(4′)	1.3453	1.3480	1.3479	1.3477	1.3483	1.3479
C(6)-C(6′)	1.4654	1.4656	1.4649	1.4651	1.4650	1.4650
C(1)-C(5)	1.5535	1.5528	1.5546	1.5540	1.5544	1.5545
C(1)-C(5′)	1.5425	1.5416	1.5420	1.5420	1.5418	1.5415
C(5)-C(6)	1.4092	1.4091	1.4093	1.4093	1.4092	1.4093
C(5′)-C(6′)	1.4034	1.4039	1.4033	1.4034	1.4034	1.4032
C(8)-N(10)		1.3916	1.4190	1.4209	1.4135	1.4157
C(8′)-N(10′)		1.3879	1.4186	1.4235	1.4134	1.4200
N(10)-C(11)		1.4529	1.4219	1.4334	1.4242	1.4234
N(10′)-C(11′)		1.4511	1.4224	1.4281	1.4247	1.4205
N(10)-C(12)		1.4537	1.4216	1.4307	1.4253	1.4311
N(10′)-C(12′)		1.4528	1.4227	1.4289	1.4243	1.4318

C(2)-C(3)-C(4)-C(4′)	20.5	18.4	18.8	19.2	19.2	18.9
C(2′)-C(3′)-C(4′)-C(4)	20.5	18.4	19.4	19.8	18.6	19.2
C(5)-C(1)-C(2)-C(3)	79.5	79.0	77.2	77.4	78.9	77.7
C(5′)-C(1)-C(2′)-C(3′)	171.7	172.2	172.3	172.1	174.1	173.0
C(5)-C(1)-C(2)-C(7)	93.5	93.3	94.7	94.9	94.5	94.5
C(5)-C(1)-C(2′)-C(7′)	93.5	93.5	94.6	94.5	95.1	95.0
C(9)-C(8)-N(10)-C(11)		12.9	41.3	46.8	33.5	38.5
C(9′)-C(8′)-N(10′)-C(11′)		7.0	39.0	41.6	33.1	31.5
C(7)-C(8)-N(10)-C(12)		9.6	43.1	23.4	35.0	27.1
C(7′)-C(8′)-N(10′)-C(12′)		9.6	40.4	41.7	38.4	43.5

Table S2. Selected Bond Lengths (Å) and Twist Angles (º) for the molecules 1–6 in the Cationic States Obtained by DFT//UB3LYP/6-31G(d).

Cation	**1**	**2**	**3**	**4**	**5**	**6**
C(1)-C(2)	1.5505	1.5608	1.5619	1.5611	1.5631	1.5615
C(1)-C(2′)	1.5503	1.5609	1.5611	1.5626	1.5629	1.5612
C(2)-C(3)	1.4374	1.4372	1.4359	1.4326	1.4318	1.4346
C(2′)-C(3′)	1.4407	1.4372	1.4344	1.4339	1.4317	1.4358
C(3)-C(4)	1.4186	1.4176	1.4236	1.4252	1.4305	1.4237
C(3′)-C(4′)	1.4172	1.4176	1.4244	1.4256	1.4306	1.4229
C(4)-C(4′)	1.3859	1.3779	1.3716	1.3700	1.3654	1.3723
C(6)-C(6′)	1.4650	1.4663	1.4659	1.4659	1.4661	1.4659
C(1)-C(5)	1.5622	1.5564	1.5563	1.5562	1.5550	1.5561
C(1)-C(5′)	1.5414	1.5415	1.5411	1.5410	1.5414	1.5411
C(5)-C(6)	1.4096	1.4088	1.4089	1.4089	1.4091	1.4090
C(5′)-C(6′)	1.4055	1.4045	1.4042	1.4041	1.4037	1.4042
C(8)-N(10)		1.3598	1.3855	1.3877	1.3919	1.3855
C(8′)-N(10′)		1.3598	1.3857	1.3931	1.3920	1.3826
C(9)-C(8)-N(10)-C(11)		2.1	25.3	31.1	28.6	27.5
C(9′)-C(8′)-N(10′)-C(11′)		1.9	24.6	28.7	28.5	23.2
C(7)-C(8)-N(10)-C(12)		0.7	27.6	17.5	29.3	22.8
C(7′)-C(8′)-N(10′)-C(12′)		0.6	25.6	30.2	29.4	19.4

1. Cartesian coordinates for the molecules **1- 6** optimized by DFT, HF, and CIS methods.

DFT:

Molecule **1**:

C	-0.00846000	-0.02224400	0.00026800
C	-0.00820600	-0.02167300	1.34560400
H	0.97057900	-0.04087400	-0.47579800
H	0.97101300	-0.03990300	1.82131500
C	-1.11772000	0.08578100	-0.93920200
C	-2.48573500	-0.18248000	-0.66461300
C	-0.74244100	0.49962100	-2.23625800
C	-3.38866400	-0.01621100	-1.73022100
C	-1.65910900	0.67039700	-3.26216700
H	0.31040600	0.69770800	-2.42183000
C	-2.99961400	0.40401200	-3.00084100
H	-4.43526800	-0.23979800	-1.57987300
H	-1.33166200	0.99513600	-4.24594100
C	-1.11711200	0.08715300	2.28539400
C	-2.48523600	-0.18130100	2.01152700
C	-0.74134900	0.50206000	3.58196700
C	-3.38778100	-0.01405300	3.07730800
C	-1.65764100	0.67374000	4.60806100
H	0.31157500	0.70025500	3.76699500
C	-2.99825900	0.40723500	4.34743000
H	-4.43445300	-0.23769300	2.92751000
H	-1.32982600	0.99928700	5.59144500
C	-3.02243100	-0.79006800	0.67383500
C	-4.56406500	-0.73817200	0.67409900
C	-2.80025700	-2.32756300	0.67446000
C	-5.39230900	0.38212200	0.67379000
C	-5.12071500	-2.02642200	0.67472000
C	-1.61181700	-3.05270800	0.67458200
C	-4.03363800	-3.00911400	0.67494000
C	-6.77923100	0.20701000	0.67410100
H	-4.96629100	1.38192100	0.67331300
C	-6.50785800	-2.20394400	0.67502800
C	-1.66415900	-4.45140600	0.67518100
H	-0.65258700	-2.54906400	0.67421600
C	-4.08482100	-4.40389900	0.67554200
C	-7.33309200	-1.07938000	0.67471400
H	-7.43165000	1.07604500	0.67386400
H	-6.93904100	-3.20166700	0.67551100
C	-2.88948500	-5.12383600	0.67565800
H	-0.73751500	-5.01939200	0.67527700
H	-5.03973000	-4.92362500	0.67592200

H	-8.41293300	-1.20187100	0.67495000
H	-2.91195400	-6.21038200	0.67612200
H	-3.74733800	0.50957300	5.12798200
H	-3.74897700	0.50564300	-3.78121300

Molecule **2**:

C	-0.22787500	-0.97992300	0.10054000
C	-0.24654300	-0.88031700	1.44473100
H	0.70719600	-1.32448700	-0.33910600
H	0.67551200	-1.15440500	1.95551800
C	-1.23929400	-0.61919000	-0.87769000
C	-2.62451200	-0.40705900	-0.64444400
C	-0.76724400	-0.47063100	-2.19879100
C	-3.42327500	-0.05400100	-1.74026100
C	-1.56451200	-0.10599000	-3.26713600
H	0.29074700	-0.64560500	-2.38051400
C	-2.93593000	0.12945100	-3.05180400
H	-4.48253000	0.05701100	-1.58344300
H	-1.12179000	-0.01274400	-4.25142100
C	-1.28380000	-0.38308100	2.33179900
C	-2.66219200	-0.21144800	2.03218900
C	-0.84510800	-0.03075900	3.62561700
C	-3.48944100	0.30013100	3.04064100
C	-1.66972700	0.48684500	4.60650500
H	0.21042000	-0.15965300	3.85427100
C	-3.03947800	0.66005200	4.32931200
H	-4.54225500	0.40104900	2.83736200
H	-1.24994300	0.74667100	5.57100300
C	-3.34894400	-0.70699200	0.71286500
C	-4.79471200	-0.17508800	0.65397400
C	-3.62469400	-2.23114600	0.82257600
C	-5.22742200	1.14536500	0.54556000
C	-5.73075400	-1.21921900	0.72119500
C	-2.72393000	-3.28880000	0.90974300
C	-5.00965800	-2.49084400	0.82586800
C	-6.59880200	1.41622300	0.50545000
H	-4.50574300	1.95595600	0.49166200
C	-7.10312500	-0.95045500	0.68242400
C	-3.21409200	-4.59676700	1.00068900
H	-1.65572300	-3.10768400	0.90783000
C	-5.49751000	-3.79543300	0.91698300
C	-7.53108700	0.37284000	0.57392300
H	-6.94295600	2.44378900	0.42125900
H	-7.82798700	-1.75890500	0.73461700
C	-4.58875200	-4.85087900	1.00477000

H	-2.51329600	-5.42487000	1.06898500
H	-6.56751700	-3.98887000	0.91947800
H	-8.59444200	0.59586000	0.54212500
H	-4.95132200	-5.87303400	1.07621600
N	-3.78118700	0.52264200	-4.08504600
N	-3.92289700	1.14160700	5.28532000
C	-3.40595700	1.61964500	6.55415800
H	-4.23979100	1.92401300	7.18978600
H	-2.85948100	0.82776600	7.08202900
H	-2.72719100	2.48072300	6.44195800
C	-5.28496700	1.47839000	4.90865900
H	-5.32751900	2.23333100	4.10848500
H	-5.83611100	0.59428600	4.56348000
H	-5.80849700	1.87476000	5.78086900
C	-5.21828600	0.54590900	-3.86725100
H	-5.64022400	-0.44986500	-3.65362100
H	-5.47560900	1.20640800	-3.03207500
H	-5.70588200	0.94032300	-4.76162600
C	-3.30788000	0.42102500	-5.45495800
H	-2.42192900	1.04759900	-5.61130200
H	-3.05001300	-0.61063400	-5.74573700
H	-4.08711400	0.78205900	-6.12952500

Molecule **3**:

C	-0.25145200	1.19941700	-0.02307400
C	-0.32313600	1.16563600	1.32245400
H	0.73876100	1.37249400	-0.44168700
H	0.61562800	1.31667800	1.85293800
C	-1.27760300	0.95689800	-1.02350400
C	-2.68589800	0.99509100	-0.83000500
C	-0.78499900	0.65433200	-2.31214600
C	-3.49579400	0.71703500	-1.94084700
C	-1.60135500	0.38738800	-3.39517400
H	0.29292100	0.63664800	-2.45340600
C	-2.98947800	0.41843800	-3.21472100
H	-4.57026000	0.74850100	-1.83912600
H	-1.17622600	0.16786000	-4.36882400
C	-1.44936400	0.86657800	2.19081000
C	-2.82787700	0.89534700	1.83920100
C	-1.09840300	0.50257000	3.50938400
C	-3.74969700	0.54065300	2.83323800
C	-2.02425800	0.13322400	4.46821500
H	-0.04252700	0.48441900	3.76768100
C	-3.38117500	0.14517600	4.12819300
H	-4.80813800	0.58984700	2.62544800

H	-1.70699400	-0.16027200	5.46342800
C	-3.38449800	1.46381300	0.48973300
C	-3.39187700	3.01752300	0.54140900
C	-4.89881900	1.18752100	0.39865600
C	-2.32694700	3.90984100	0.63245100
C	-4.71079400	3.51026900	0.48075000
C	-5.55337400	-0.04063600	0.33181700
C	-5.63861200	2.37994100	0.39413400
C	-2.58715200	5.28513100	0.66167700
H	-1.30548100	3.55287300	0.68074300
C	-4.96927200	4.88153200	0.51022000
C	-6.94906300	-0.06930800	0.26289700
H	-4.98779600	-0.96844100	0.33970200
C	-7.03444800	2.35385800	0.32031900
C	-3.89667200	5.76959600	0.60106700
H	-1.75681100	5.98290500	0.73280600
H	-5.98975600	5.25356700	0.46397200
C	-7.68450400	1.12183200	0.25570600
H	-7.46552900	-1.02404100	0.22083700
H	-7.60693600	3.27776800	0.31531100
H	-4.08068600	6.84050500	0.62535200
H	-8.76921000	1.08566400	0.20115000
N	-3.87014600	0.16653000	-4.29800500
C	-3.54933500	-0.84260900	-5.24774600
C	-5.04907900	0.94477300	-4.46673500
C	-3.05845100	-2.08819200	-4.82358000
C	-3.71836000	-0.61093000	-6.62248100
C	-5.02951600	2.33132200	-4.24643400
C	-6.25028100	0.33559700	-4.86414000
C	-2.73751200	-3.07258100	-5.75624500
H	-2.93176700	-2.27688900	-3.76221300
C	-3.41175300	-1.60798600	-7.54655300
H	-4.09087500	0.35141800	-6.95855300
C	-6.18935000	3.08543600	-4.41325300
H	-4.10466700	2.81075000	-3.94214500
C	-7.39987200	1.10131200	-5.04717300
H	-6.27476500	-0.73697700	-5.02825000
C	-2.91582900	-2.84257900	-7.12217500
H	-2.35927900	-4.03082700	-5.40949100
H	-3.54887300	-1.41080200	-8.60665800
C	-7.37963900	2.47898300	-4.81984000
H	-6.15543200	4.15727700	-4.23647600
H	-8.32063000	0.61285900	-5.35568900
H	-2.67162900	-3.61495400	-7.84593600

H	-8.27978100	3.07167300	-4.95615100
N	-4.37673200	-0.21231400	5.07397200
C	-4.26946700	0.23569000	6.41914500
C	-5.47077600	-1.03039800	4.68050300
C	-3.86569800	1.55113800	6.70003300
C	-4.56333400	-0.62859300	7.48645600
C	-5.26758600	-2.13288400	3.83441900
C	-6.77006100	-0.75155700	5.13422200
C	-3.75089900	1.98450100	8.01943400
H	-3.64571100	2.22715800	5.87994500
C	-4.46289700	-0.18004400	8.80203700
H	-4.86946200	-1.64872100	7.27758400
C	-6.34351400	-2.92906300	3.44657500
H	-4.26451400	-2.36022900	3.48772100
C	-7.83665300	-1.56416700	4.75515100
H	-6.93585300	0.10326200	5.78209200
C	-4.05216000	1.12570600	9.07872700
H	-3.43779700	3.00628400	8.21794700
H	-4.69414900	-0.86277100	9.61563700
C	-7.63330600	-2.65446200	3.90647000
H	-6.16719800	-3.78058100	2.79417800
H	-8.83560100	-1.33272100	5.11567200
H	-3.96844300	1.46944900	10.10579300
H	-8.46823700	-3.28264500	3.60906900

Molecule **4**:

C	0.17031100	0.18842400	0.02416800
C	0.17043100	0.12384700	1.37033500
H	1.14878600	0.25149100	-0.44951900
H	1.14880600	0.14320800	1.84797600
C	-0.93426100	0.10196500	-0.91689100
C	-2.31249400	0.31272100	-0.63741100
C	-0.55904800	-0.22760800	-2.23830100
C	-3.21283200	0.17312200	-1.70403500
C	-1.46385000	-0.36120800	-3.27492900
H	0.49789500	-0.37845000	-2.44399100
C	-2.82258800	-0.15484100	-3.01027000
H	-4.26649100	0.34179200	-1.53976200
H	-1.12873900	-0.61064900	-4.27626300
C	-0.93415000	-0.06147400	2.29658100
C	-2.31385400	0.15175400	2.03245800
C	-0.55832800	-0.51347600	3.58186100
C	-3.21841500	-0.12031300	3.07058000
C	-1.46706900	-0.79937500	4.58231900
H	0.49984800	-0.66961300	3.77663100

C	-2.83098800	-0.60848200	4.32597600
H	-4.27089600	0.06973700	2.92381400
H	-1.13432700	-1.16744800	5.54748100
C	-2.87093200	0.82507200	0.73301900
C	-2.68326600	2.36533800	0.81774100
C	-4.41047900	0.73850900	0.72237300
C	-1.51215000	3.11646800	0.87228500
C	-3.93220400	3.01809300	0.83329800
C	-5.21343600	-0.39875600	0.66533700
C	-4.99622600	2.01278200	0.77262100
C	-1.59675600	4.51209700	0.94197800
H	-0.54181300	2.63509000	0.86110700
C	-4.01536300	4.40964600	0.90272100
C	-6.60343200	-0.25362400	0.65615100
H	-4.76845700	-1.38957700	0.63713200
C	-6.38646600	2.15996700	0.76122000
C	-2.83722200	5.15578000	0.95686100
H	-0.68341600	5.09981400	0.98515100
H	-4.98230700	4.90654700	0.91528300
C	-7.18574400	1.01879300	0.70160300
H	-7.23372000	-1.13728500	0.61905500
H	-6.83974100	3.14722900	0.79726000
H	-2.88517400	6.24028000	1.01143000
H	-8.26787800	1.11731900	0.69135200
N	-3.79272100	-0.26086500	-4.04652500
N	-3.79100600	-0.91243800	5.32839900
C	-4.83890200	0.71025400	-4.11034700
C	-6.21974300	0.33493100	-4.24242800
C	-4.50113200	2.05244200	-4.01668900
C	-6.67357300	-1.01307800	-4.24590200
C	-7.20285000	1.38002800	-4.34183500
C	-5.47971200	3.06434900	-4.08022900
H	-3.45601800	2.32261700	-3.90206500
C	-8.01115200	-1.31475000	-4.37412900
H	-5.95526900	-1.81571200	-4.14210400
C	-8.57264600	1.02881900	-4.48787900
C	-6.80428600	2.73901500	-4.25975800
H	-5.17250600	4.10386000	-4.00567600
C	-8.97276200	-0.28634400	-4.50853900
H	-8.33031700	-2.35356100	-4.36938900
H	-9.30371900	1.82943700	-4.57394300
H	-7.56372800	3.51394600	-4.32671500
H	-10.02431900	-0.53798600	-4.61800000
C	-5.14132400	-1.21019400	4.96126300

C	-5.43180300	-2.36635000	4.15676000
C	-6.17659200	-0.41548300	5.41833700
C	-4.43224600	-3.27005200	3.70476800
C	-6.79944200	-2.63587800	3.81562200
C	-7.52075400	-0.70835700	5.09742600
H	-5.94692900	0.44934500	6.03209500
C	-4.75957200	-4.36453700	2.93331100
H	-3.39786900	-3.09332000	3.97512800
C	-7.09826500	-3.76814900	3.01030100
C	-7.82869800	-1.78663800	4.30329600
H	-8.30763700	-0.06064100	5.47399400
C	-6.10418000	-4.61314300	2.57222200
H	-3.97818400	-5.04343000	2.60262900
H	-8.13742400	-3.95992500	2.75256300
H	-8.86063000	-2.01050400	4.04473600
H	-6.34965900	-5.47594700	1.95884500
C	-3.54907500	-0.43743400	6.65897000
C	-3.72260300	-1.32097000	7.77588900
C	-3.14251600	0.86857000	6.86727800
C	-4.07604700	-2.68956100	7.63223300
C	-3.50809400	-0.80270500	9.09699100
C	-2.90837900	1.35931400	8.17090600
H	-3.00691700	1.52212800	6.01097200
C	-4.23499100	-3.49861200	8.73553500
H	-4.21251200	-3.09782900	6.63774500
C	-3.69001600	-1.66515500	10.21194300
C	-3.09985600	0.54745600	9.26462300
H	-2.59275000	2.39089700	8.30069800
C	-4.04965500	-2.98186100	10.03965600
H	-4.50177400	-4.54374500	8.60360600
H	-3.53271900	-1.26224400	11.20979500
H	-2.93375300	0.92414500	10.27086300
H	-4.18385000	-3.62955600	10.90188400
C	-3.66412300	-1.32819900	-4.98662300
C	-3.71941500	-1.10980400	-6.40659700
C	-3.45106600	-2.61055500	-4.50109200
C	-3.83586900	0.17609300	-7.00394600
C	-3.61704500	-2.25179800	-7.27551300
C	-3.31567300	-3.71424100	-5.36659700
H	-3.40109000	-2.76021600	-3.42702600
C	-3.88491700	0.32527600	-8.37213900
H	-3.88472900	1.05336900	-6.37256100
C	-3.68598000	-2.05876900	-8.68233100
C	-3.41598700	-3.54513800	-6.72822600

H	-3.15334600	-4.70238400	-4.94468300
C	-3.82154900	-0.80224400	-9.22347400
H	-3.97075300	1.32011200	-8.80087000
H	-3.61965200	-2.93261600	-9.32637300
H	-3.32997600	-4.39328200	-7.40268500
H	-3.86992400	-0.67156300	-10.30122300

Molecule **5**:

C	-0.41249000	-4.21425800	-0.86908000
C	0.93302700	-4.13988400	-0.91353300
H	-0.84145900	-5.19355200	-1.07632000
H	1.45348100	-5.06673100	-1.14991600
C	-1.40281700	-3.17025400	-0.66840300
C	-1.18864300	-1.88306400	-0.10273600
C	-2.70861200	-3.50495200	-1.09038200
C	-2.29446500	-1.02559000	-0.01218500
C	-3.78667800	-2.64632100	-0.99068100
H	-2.86756800	-4.49454000	-1.51223600
C	-3.58680200	-1.37348200	-0.43846900
H	-2.17351100	-0.04498700	0.42255100
H	-4.77225800	-2.95571400	-1.32146800
C	1.80916700	-2.98849300	-0.78629500
C	1.48008800	-1.72170200	-0.22666500
C	3.11287100	-3.17608200	-1.29458200
C	2.47437400	-0.73558100	-0.23974800
C	4.07419700	-2.18218800	-1.31704100
H	3.35758900	-4.14714900	-1.71822900
C	3.75493700	-0.92577300	-0.78696200
H	2.28046900	0.22664900	0.20922500
H	5.05459500	-2.37069100	-1.74116500
C	0.15502800	-1.41978700	0.55408500
C	0.07908100	0.08478700	0.88204200
C	0.25045200	-2.00769800	1.98983500
C	-0.01923400	1.16020200	0.00195600
C	0.12155700	0.31187300	2.26633100
C	0.34485300	-3.33399200	2.40288200
C	0.22693000	-0.97838600	2.95204600
C	-0.07228500	2.46005100	0.51252900
H	-0.04962400	0.99249300	-1.07116600
C	0.06482000	1.61103300	2.77974600
C	0.41527900	-3.62128300	3.77120700
H	0.36379200	-4.14065900	1.68042100
C	0.29761800	-1.26560200	4.31608800
C	-0.03148600	2.68369400	1.89384100
H	-0.13960900	3.30308200	-0.16953100

H	0.09573100	1.78526000	3.85214200
C	0.39232200	-2.59732200	4.72216100
H	0.48897500	-4.65632100	4.09492000
H	0.27903100	-0.46564400	5.05209000
H	-0.07283200	3.69960100	2.27751400
H	0.44819000	-2.83814400	5.78059400
N	-4.65887100	-0.46300800	-0.29851100
N	4.69731800	0.12748900	-0.77376800
C	4.28725000	1.47150100	-1.00622300
C	4.79564000	2.51879500	-0.21751300
C	3.38807300	1.78636900	-2.03077000
C	4.42141200	3.83323900	-0.45609600
H	5.49163200	2.29164100	0.58384800
C	2.99014000	3.10504900	-2.26340800
H	2.98945200	0.99025700	-2.65146700
C	3.51128200	4.13930100	-1.47864000
H	4.81254800	4.64420600	0.15047600
H	2.29143200	3.30962700	-3.06683000
C	-4.72764900	0.41485100	0.82230000
C	-5.04523900	1.76621200	0.65171000
C	-4.49867200	-0.05986600	2.12605400
C	-5.14607400	2.62859800	1.74560800
H	-5.22254600	2.14874300	-0.34875000
C	-4.57430200	0.79590700	3.21546900
H	-4.25353200	-1.10639400	2.27788400
C	-4.90380400	2.14749200	3.03669700
H	-5.39832100	3.66895400	1.57400500
H	-4.39421300	0.43372900	4.22283800
C	6.08476800	-0.15341600	-0.61347400
C	6.52844200	-1.01030700	0.40999800
C	7.03889800	0.42595900	-1.45652200
C	7.87903600	-1.28452000	0.56986700
H	5.80207500	-1.46199300	1.07856000
C	8.40218700	0.17267300	-1.28714400
H	6.71426800	1.08911400	-2.25231500
C	8.83033100	-0.69196200	-0.27430000
H	8.22497000	-1.94591400	1.35822400
H	9.11181900	0.64385900	-1.95778500
C	-5.71196800	-0.44241000	-1.25703100
C	-5.43017300	-0.43276300	-2.63514200
C	-7.05125500	-0.41569600	-0.85300400
C	-6.45544900	-0.41126600	-3.56997600
H	-4.39681700	-0.44637900	-2.96760500
C	-8.08803400	-0.37112700	-1.78782400

H	-7.28761000	-0.42311100	0.20648400
C	-7.79519500	-0.37558500	-3.15592100
H	-6.24071700	-0.40575600	-4.63419500
H	-9.11296000	-0.34792100	-1.43498900
O	3.20206700	5.46413600	-1.62465500
O	-4.96411700	2.90159200	4.17637500
O	-8.72780800	-0.34441500	-4.15593500
O	10.13440400	-1.01929700	-0.02493600
C	2.30371700	5.82888200	-2.65763100
H	2.68908900	5.54978900	-3.64771100
H	1.31512600	5.37025000	-2.51704600
H	2.20658800	6.91493500	-2.60254000
C	-5.28871500	4.27493100	4.05067400
H	-6.28468800	4.41785500	3.60955000
H	-5.28379800	4.67921500	5.06483900
H	-4.54801400	4.81271900	3.44329100
C	11.13430300	-0.44989300	-0.85229500
H	12.08586300	-0.83927100	-0.48522300
H	11.00489300	-0.74209500	-1.90326100
H	11.14130600	0.64646800	-0.78366300
C	-10.09673400	-0.31983900	-3.79021200
H	-10.34293000	0.57430100	-3.20136900
H	-10.65778900	-0.29946500	-4.72652100
H	-10.37943000	-1.21412400	-3.21841200

Molecule **6**:

C	-0.28664200	1.00971700	0.18997900
C	-0.37776200	1.03346000	1.53453800
H	0.71231600	1.14550100	-0.22157800
H	0.55671300	1.18729000	2.07197600
C	-1.30445700	0.74175100	-0.81217200
C	-2.71469600	0.80686400	-0.63687200
C	-0.80289700	0.37659700	-2.08017900
C	-3.51482500	0.47976800	-1.74039900
C	-1.61040900	0.06466100	-3.15880600
H	0.27618800	0.34460900	-2.21022600
C	-2.99955000	0.10907200	-2.99196800
H	-4.59004000	0.52770900	-1.65421700
H	-1.17473400	-0.20035800	-4.11600500
C	-1.52224900	0.79906500	2.39874700
C	-2.89445300	0.84887300	2.03160700
C	-1.19820400	0.48222000	3.73691100
C	-3.83930000	0.57073200	3.03018100
C	-2.14347300	0.18491600	4.69999800
H	-0.14637000	0.44391400	4.00954800

C	-3.49938200	0.22761200	4.34720000
H	-4.89201500	0.64143800	2.80232200
H	-1.84189100	-0.07689600	5.70865400
C	-3.42085200	1.35796700	0.64784100
C	-3.39534900	2.91196300	0.61716600
C	-4.93862700	1.10880500	0.54554800
C	-2.31328800	3.78532800	0.68610500
C	-4.70147800	3.42787000	0.49891000
C	-5.61714100	-0.10819300	0.53433400
C	-5.65179900	2.31380600	0.45470100
C	-2.54329000	5.16527900	0.63430800
H	-1.30158500	3.40975900	0.77831500
C	-4.92974300	4.80380500	0.44691000
C	-7.01070900	-0.11243300	0.42850900
H	-5.07225100	-1.04497500	0.61288800
C	-7.04574800	2.31151800	0.34638700
C	-3.83996500	5.67285800	0.51497500
H	-1.69955200	5.84842400	0.68820700
H	-5.94034400	5.19421300	0.35599100
C	-7.72000900	1.09092600	0.33354700
H	-7.54530600	-1.05783700	0.42408000
H	-7.59769700	3.24503600	0.27271700
H	-4.00070500	6.74713700	0.47644300
H	-8.80326300	1.07314800	0.24895700
N	-3.89084700	-0.18075000	-4.05877900
C	-3.53642100	-1.11444100	-5.06889000
C	-2.90812800	-2.32633200	-4.72887600
C	-3.83476400	-0.86302200	-6.41734800
C	-2.57744900	-3.24953500	-5.71745200
H	-2.68407900	-2.53770900	-3.68812200
C	-3.51470000	-1.80253000	-7.39695500
H	-4.31718800	0.06878500	-6.69311000
C	-2.88014700	-2.99796800	-7.05826100
H	-2.09173300	-4.17966800	-5.43345400
H	-3.75588000	-1.58836100	-8.43501000
H	-2.62737900	-3.72444900	-7.82521000
N	-4.50690100	-0.08375500	5.29170200
C	-4.38789900	0.32577300	6.64969700
C	-3.81998500	1.56366600	6.99135200
C	-4.85937100	-0.51224200	7.67321100
C	-3.71634000	1.94316700	8.32885800
H	-3.46401800	2.22384300	6.20706400
C	-4.76669000	-0.11648300	9.00558600
H	-5.29545900	-1.47228100	7.41499800

C	-4.19049200	1.11016500	9.34397000
H	-3.27507300	2.90563700	8.57488900
H	-5.13651000	-0.77858100	9.78425900
H	-4.11308600	1.41275900	10.38438500
C	-5.01531900	0.68061300	-4.26784200
C	-6.34029500	0.13477100	-4.33178100
C	-4.82078400	2.04375800	-4.39558600
C	-6.61822200	-1.24670900	-4.14951400
C	-7.43634100	1.03022800	-4.56998300
C	-5.90984000	2.91818400	-4.60382600
H	-3.81178700	2.43956100	-4.33325700
C	-7.90815500	-1.72372000	-4.22135300
H	-5.79810600	-1.92631000	-3.94879700
C	-8.75280400	0.50024200	-4.64613900
C	-7.18917300	2.42255700	-4.70292600
H	-5.72419300	3.98431300	-4.69996100
C	-8.98695300	-0.84522700	-4.48008400
H	-8.10020900	-2.78345700	-4.07629300
H	-9.57693300	1.18455900	-4.83432800
H	-8.03008000	3.08985400	-4.87538800
H	-9.99935700	-1.23566400	-4.54053200
C	-5.76188700	-0.61424300	4.85410900
C	-5.82806200	-1.91007900	4.24122900
C	-6.91869900	0.11675800	5.05251700
C	-4.68878000	-2.73954100	4.05783600
C	-7.10865600	-2.39894100	3.81523200
C	-8.17608700	-0.38507200	4.65104300
H	-6.84916300	1.09274200	5.52297100
C	-4.80284000	-3.97685600	3.46312000
H	-3.72048300	-2.38730800	4.39418600
C	-7.18629600	-3.67763500	3.19921300
C	-8.27006600	-1.61164600	4.03569100
H	-9.06595700	0.21513200	4.81905000
C	-6.06138900	-4.44979800	3.02165200
H	-3.91971200	-4.59676000	3.33437600
H	-8.15971700	-4.03886400	2.87523000
H	-9.23426800	-1.99906200	3.71576700
H	-6.13680000	-5.42611700	2.55043600

HF:

Molecule **1**:

C	-0.00411500	0.02544600	0.01120500
C	-0.00411800	0.02545300	1.33413400
H	0.96145100	0.00281600	-0.46402000
H	0.96144600	0.00282800	1.80936300

C	-1.12641500	0.11357400	-0.93017500
C	-2.46226900	-0.23160400	-0.66566300
C	-0.76755500	0.56688600	-2.20430900
C	-3.35761500	-0.12233100	-1.73478300
C	-1.67708000	0.69205300	-3.22920400
H	0.26115900	0.82659000	-2.38039300
C	-2.98762000	0.33107700	-2.98680300
H	-4.37811300	-0.41075800	-1.60612700
H	-1.36703700	1.04885500	-4.19487500
C	-1.12642100	0.11359300	2.27551000
C	-2.46227700	-0.23158800	2.01100200
C	-0.76755600	0.56690800	3.54964300
C	-3.35761100	-0.12233400	3.08013600
C	-1.67707200	0.69206700	4.57454400
H	0.26115900	0.82661400	3.72572000
C	-2.98760900	0.33107400	4.33215400
H	-4.37810500	-0.41077900	2.95149700
H	-1.36702400	1.04886900	5.54021300
C	-2.98528100	-0.84812100	0.67266900
C	-4.52501700	-0.81135500	0.67264200
C	-2.75489800	-2.37866900	0.67268200
C	-5.35497900	0.29745000	0.67259300
C	-5.06646300	-2.08724400	0.67265600
C	-1.56825000	-3.08895400	0.67269800
C	-3.96829200	-3.06471500	0.67268300
C	-6.72764600	0.11480300	0.67257500
H	-4.94123900	1.29010100	0.67257400
C	-6.44305800	-2.27582400	0.67263900
C	-1.60805500	-4.47699900	0.67271600
H	-0.62188900	-2.58603700	0.67269900
C	-4.01009900	-4.44887700	0.67270100
C	-7.26931600	-1.16715000	0.67260100
H	-7.38004700	0.96968700	0.67254000
H	-6.86414900	-3.26538000	0.67265300
C	-2.81825100	-5.15438000	0.67271700
H	-0.68673500	-5.03194500	0.67272800
H	-4.95001500	-4.97195000	0.67270000
H	-8.33715600	-1.29488200	0.67258500
H	-2.83100600	-6.22976900	0.67273100
H	-3.72700700	0.38900300	5.11079000
H	-3.72702500	0.38902000	-3.76543000

Molecule **2**:

C	0.66201700	-3.34786100	0.01687200
C	-0.66187000	-3.34789600	0.01669700

H	1.13856200	-4.29060500	0.22611800
H	-1.13842100	-4.29066800	0.22580800
C	1.59912800	-2.26375100	-0.28201900
C	1.34332700	-0.88374600	-0.24190500
C	2.88618300	-2.68006500	-0.62489900
C	2.40379100	-0.02412300	-0.52620400
C	3.91439700	-1.82167500	-0.92836400
H	3.08291200	-3.73725300	-0.66210300
C	3.69162300	-0.44669400	-0.86691400
H	2.23646200	1.02364900	-0.46019400
H	4.86898600	-2.22891800	-1.19424600
C	-1.59896300	-2.26380600	-0.28232200
C	-1.34326700	-0.88382800	-0.24201100
C	-2.88597100	-2.68015200	-0.62546000
C	-2.40377500	-0.02418400	-0.52621800
C	-3.91418300	-1.82178900	-0.92887700
H	-3.08261200	-3.73734900	-0.66286900
C	-3.69153200	-0.44676500	-0.86707500
H	-2.23646700	1.02358100	-0.46001200
H	-4.86869100	-2.22903400	-1.19503800
C	-0.00000500	-0.23400000	0.23379500
C	-0.00008200	-0.12809800	1.77728500
C	-0.00005500	1.26161800	-0.13407600
C	-0.00020500	-1.13579300	2.72415700
C	-0.00002200	1.20400300	2.18670700
C	-0.00003000	1.83432000	-1.39550700
C	-0.00001900	2.06566700	0.99539300
C	-0.00021700	-0.79898000	4.07129600
H	-0.00026900	-2.16728200	2.43302800
C	-0.00002200	1.54173800	3.52967600
C	-0.00000500	3.21431300	-1.51300800
H	0.00000000	1.21560800	-2.27494100
C	0.00001000	3.45095700	0.88284100
C	-0.00011400	0.52836500	4.47385400
H	-0.00030100	-1.57983100	4.81099000
H	0.00002500	2.57190500	3.83956500
C	0.00001300	4.01957900	-0.37762400
H	0.00000700	3.66744000	-2.48849300
H	0.00004900	4.07505000	1.75873600
H	-0.00012600	0.77101900	5.52165100
H	0.00002100	5.09002800	-0.48258300
N	4.70819900	0.47313100	-1.10624600
N	-4.70817300	0.47300100	-1.10626000
C	-5.92842500	-0.00199800	-1.71952100

H	-6.61743300	0.82437100	-1.82133300
H	-5.76913400	-0.43744900	-2.70651000
H	-6.41015800	-0.74402000	-1.09485000
C	-4.35311900	1.85350400	-1.35959700
H	-3.88719800	2.30230900	-0.49129900
H	-3.67676500	1.96848900	-2.20600500
H	-5.25336200	2.41505800	-1.56520800
C	4.35297200	1.85349700	-1.36013100
H	3.67663800	1.96807200	-2.20661100
H	3.88696200	2.30257500	-0.49202300
H	5.25315000	2.41509200	-1.56591400
C	5.92845300	-0.00196500	-1.71945400
H	6.41028200	-0.74376100	-1.09458400
H	5.76911100	-0.43774500	-2.70628700
H	6.61739700	0.82441700	-1.82157800

Molecule **3**:

C	-0.02236600	0.04267100	0.00548200
C	-0.01939300	0.02876600	1.32908000
H	0.94080600	0.10282700	-0.47171200
H	0.94534000	0.07957900	1.80401800
C	-1.14254900	-0.07094400	-0.93273700
C	-2.49283800	0.21438700	-0.66756500
C	-0.77956900	-0.48484400	-2.21727600
C	-3.38906200	0.07569700	-1.72872600
C	-1.68013000	-0.61902400	-3.24662400
H	0.25716300	-0.69672900	-2.40968700
C	-3.01265100	-0.32651600	-3.00336400
H	-4.42266600	0.30158500	-1.58859700
H	-1.35625300	-0.93324500	-4.22102400
C	-1.13696900	-0.11252800	2.26635600
C	-2.49035300	0.16435700	2.00538700
C	-0.76999600	-0.55673400	3.53962000
C	-3.38397400	-0.00951500	3.06287000
C	-1.67553500	-0.76176700	4.55362100
H	0.26828700	-0.76631200	3.72570700
C	-3.00990400	-0.47861400	4.31475200
H	-4.41564500	0.23402900	2.93859000
H	-1.35453200	-1.12324700	5.51268600
C	-3.03909800	0.78916300	0.68037800
C	-2.85139300	2.32629600	0.70194300
C	-4.57715900	0.70904900	0.68069200
C	-1.68612100	3.07118500	0.71548500
C	-4.08433500	2.97686600	0.70383400
C	-5.37672000	-0.42194300	0.67648000

C	-5.15394300	1.96891900	0.69182800
C	-1.76620900	4.45767400	0.73096600
H	-0.72542700	2.59680100	0.71419400
C	-4.16622400	4.35905300	0.71870100
C	-6.75339000	-0.27719300	0.68407100
H	-4.93735500	-1.40331100	0.67446000
C	-6.53487900	2.11980500	0.69520200
C	-2.99550400	5.09924600	0.73235500
H	-0.86122300	5.03888600	0.74205200
H	-5.12119900	4.85397600	0.71974600
C	-7.32993700	0.98911400	0.69149300
H	-7.38112300	-1.14985800	0.69056300
H	-6.98274000	3.09743700	0.70157900
H	-3.03987400	6.17381900	0.74443500
H	-8.40080200	1.08719800	0.69644900
N	-3.98014500	-0.42490400	-4.03120200
C	-3.96430300	-1.53909800	-4.90524500
C	-4.90167200	0.62955700	-4.24714400
C	-3.87260300	-2.83023800	-4.39400000
C	-4.03892300	-1.36386000	-6.28349500
C	-4.48166500	1.95553900	-4.23030400
C	-6.24429500	0.34974900	-4.48236800
C	-3.84587400	-3.92031400	-5.24637700
H	-3.82047800	-2.97399600	-3.33057700
C	-4.03147800	-2.46010700	-7.12918200
H	-4.10639500	-0.37096800	-6.68788600
C	-5.39090000	2.97913600	-4.43635900
H	-3.44733000	2.18223200	-4.04985100
C	-7.14343200	1.37714600	-4.70789200
H	-6.57758400	-0.67149800	-4.48950800
C	-3.93000200	-3.74361500	-6.61812400
H	-3.77231000	-4.91104400	-4.83406400
H	-4.09254400	-2.30652400	-8.19202200
C	-6.72454000	2.69769200	-4.68220500
H	-5.04964100	3.99885200	-4.41515600
H	-8.17725800	1.14293600	-4.89041400
H	-3.91712200	-4.59244900	-7.27779700
H	-7.42684100	3.49443000	-4.84936700
N	-3.98653000	-0.64968600	5.32500000
C	-3.74194800	-0.16409100	6.63212300
C	-5.18120300	-1.35489700	5.03947300
C	-3.23496200	1.11806400	6.82206800
C	-4.00174700	-0.95803800	7.74503100
C	-5.14308400	-2.55805400	4.34180400

C	-6.41146100	-0.85401000	5.45343700
C	-2.98473300	1.58882100	8.09936900
H	-3.03785300	1.74030000	5.96877700
C	-3.76727900	-0.47273000	9.02023200
H	-4.38915500	-1.95065400	7.60859600
C	-6.31449300	-3.23908000	4.05722700
H	-4.19686500	-2.95500400	4.02346300
C	-7.57675400	-1.54948900	5.18166800
H	-6.44973800	0.07754300	5.98709700
C	-3.25314600	0.80004400	9.20642800
H	-2.59113300	2.58158400	8.22750600
H	-3.97618500	-1.09916000	9.86931800
C	-7.53729900	-2.74290800	4.47866200
H	-6.26685500	-4.16807200	3.51692200
H	-8.51916000	-1.14852600	5.51026500
H	-3.06523600	1.17140900	10.19770500
H	-8.44485200	-3.27795100	4.26391400

Molecule **4**:

C	0.66145400	-0.01430700	4.07789900
C	-0.66145400	0.01430700	4.07789900
H	1.12200800	-0.02495300	5.05052600
H	-1.12200800	0.02495300	5.05052600
C	1.62974100	-0.02708500	2.98096200
C	1.37301200	-0.00364400	1.60811200
C	2.97091300	-0.05799500	3.39827000
C	2.47359300	-0.00504300	0.74206400
C	4.03638800	-0.05445900	2.53917600
H	3.17084000	-0.07675600	4.45470100
C	3.78981100	-0.02486400	1.16713000
H	2.30075600	0.00355300	-0.31277700
H	5.03970800	-0.07180100	2.91936200
C	-1.62974100	0.02708500	2.98096200
C	-1.37301200	0.00364400	1.60811200
C	-2.97091300	0.05799500	3.39827000
C	-2.47359300	0.00504300	0.74206400
C	-4.03638800	0.05445900	2.53917600
H	-3.17084000	0.07675600	4.45470100
C	-3.78981100	0.02486400	1.16713000
H	-2.30075600	-0.00355300	-0.31277700
H	-5.03970800	0.07180100	2.91936200
C	0.00000000	0.00000000	0.86349200
C	0.00000100	1.18074600	-0.12544100
C	-0.00000100	-1.18074600	-0.12544100
C	0.00017300	2.53066400	0.16303100

C	-0.00047700	0.73739600	-1.44495600
C	-0.00017300	-2.53066400	0.16303100
C	0.00047700	-0.73739600	-1.44495600
C	0.00000000	3.43969600	-0.88526200
H	0.00310900	2.87438400	1.18220700
C	-0.00149700	1.64486400	-2.49243300
C	0.00000000	-3.43969600	-0.88526200
H	-0.00310900	-2.87438400	1.18220700
C	0.00149700	-1.64486400	-2.49243300
C	-0.00098800	2.99980200	-2.20258900
H	0.00566500	4.49464000	-0.67643900
H	0.00026400	1.30928100	-3.51427000
C	0.00098800	-2.99980200	-2.20258900
H	-0.00566500	-4.49464000	-0.67643900
H	-0.00026400	-1.30928100	-3.51427000
H	0.00272900	3.71732000	-3.00365400
H	-0.00272900	-3.71732000	-3.00365400
N	-4.84856800	0.01810000	0.24282300
C	-6.11931800	0.56791900	0.58308300
C	-4.68520200	-0.51797900	-1.06885200
C	-6.27027800	1.97865100	0.78599000
C	-7.20233600	-0.25030300	0.68660100
C	-4.53271000	-1.92980500	-1.25953600
C	-4.71075200	0.31229900	-2.14678100
C	-5.19119700	2.89578600	0.65709800
C	-7.54744000	2.48290600	1.11247600
C	-8.48246400	0.26545500	0.99520300
H	-7.08036000	-1.30539300	0.52592100
C	-4.52813800	-2.85645300	-0.18169700
C	-4.39836300	-2.42507400	-2.57377600
C	-4.58924400	-0.19339400	-3.46201700
H	-4.82906400	1.36886400	-1.99387700
C	-5.38150400	4.22728000	0.85313400
H	-4.21588700	2.52925100	0.40403800
C	-7.71026900	3.87892500	1.31650300
C	-8.64985800	1.59336400	1.21198500
H	-9.31681400	-0.40901400	1.06522100
C	-4.39342200	-4.18967900	-0.40876900
H	-4.62972000	-2.49346300	0.82203500
C	-4.25447400	-3.82314600	-2.77615800
C	-4.43002300	-1.52352600	-3.67042200
H	-4.61714300	0.49043900	-4.29120200
C	-6.65936300	4.72940300	1.19257900
H	-4.55466800	4.90697400	0.75028500

H	-8.68736100	4.25250200	1.56842500
H	-9.61919900	1.99153400	1.45518600
C	-4.25144100	-4.68373800	-1.72619700
H	-4.39332500	-4.87709800	0.41822300
H	-4.15196400	-4.19039000	-3.78238800
H	-4.33214100	-1.91449500	-4.66795300
H	-6.79313600	5.78506000	1.34783100
H	-4.14445000	-5.74121500	-1.89011000
N	4.84856800	-0.01810000	0.24282300
C	6.11931800	-0.56791900	0.58308300
C	4.68520200	0.51797900	-1.06885200
C	6.27027800	-1.97865100	0.78599000
C	7.20233600	0.25030300	0.68660100
C	4.53271000	1.92980500	-1.25953600
C	4.71075200	-0.31229900	-2.14678100
C	5.19119700	-2.89578600	0.65709800
C	7.54744000	-2.48290600	1.11247600
C	8.48246400	-0.26545500	0.99520300
H	7.08036000	1.30539300	0.52592100
C	4.52813800	2.85645300	-0.18169700
C	4.39836300	2.42507400	-2.57377600
C	4.58924400	0.19339400	-3.46201700
H	4.82906400	-1.36886400	-1.99387700
C	5.38150400	-4.22728000	0.85313400
H	4.21588700	-2.52925100	0.40403800
C	7.71026900	-3.87892500	1.31650300
C	8.64985800	-1.59336400	1.21198500
H	9.31681400	0.40901400	1.06522100
C	4.39342200	4.18967900	-0.40876900
H	4.62972000	2.49346300	0.82203500
C	4.25447400	3.82314600	-2.77615800
C	4.43002300	1.52352600	-3.67042200
H	4.61714300	-0.49043900	-4.29120200
C	6.65936300	-4.72940300	1.19257900
H	4.55466800	-4.90697400	0.75028500
H	8.68736100	-4.25250200	1.56842500
H	9.61919900	-1.99153400	1.45518600
C	4.25144100	4.68373800	-1.72619700
H	4.39332500	4.87709800	0.41822300
H	4.15196400	4.19039000	-3.78238800
H	4.33214100	1.91449500	-4.66795300
H	6.79313600	-5.78506000	1.34783100
H	4.14445000	5.74121500	-1.89011000

Molecule **5**:

C	-0.40753800	-3.86352000	-1.76279700
C	0.91443700	-3.79254900	-1.77469300
H	-0.83775500	-4.77576700	-2.13979900
H	1.43459000	-4.65327000	-2.15898700
C	-1.39947800	-2.86230100	-1.36343200
C	-1.19377700	-1.76422600	-0.51038000
C	-2.67783200	-3.07157600	-1.88582200
C	-2.29800400	-0.95922400	-0.23080200
C	-3.75310900	-2.26397200	-1.60330900
H	-2.82954800	-3.91632000	-2.53436600
C	-3.56919600	-1.18511100	-0.74983900
H	-2.19443800	-0.12724200	0.42843700
H	-4.71710500	-2.47552500	-2.02485900
C	1.79534700	-2.68292300	-1.40223300
C	1.47674700	-1.60192700	-0.55927500
C	3.07637500	-2.75037800	-1.95286400
C	2.48401800	-0.66880200	-0.32134200
C	4.04375900	-1.79636400	-1.73530900
H	3.31037800	-3.58079100	-2.59519900
C	3.74714900	-0.73165700	-0.90051900
H	2.31425600	0.14273700	0.35030100
H	5.00932500	-1.88295400	-2.19664200
C	0.14158100	-1.45568200	0.24365000
C	0.06773000	-0.04369400	0.85420200
C	0.20916400	-2.30290500	1.53830300
C	-0.00284800	1.17278100	0.19566100
C	0.08343300	-0.08453400	2.23919900
C	0.29435600	-3.67509200	1.68902300
C	0.16943600	-1.48756000	2.66828900
C	-0.05495600	2.34111900	0.93611400
H	-0.01045400	1.21331300	-0.87876400
C	0.02693100	1.08476000	2.98718800
C	0.33902900	-4.21652500	2.96723600
H	0.32617000	-4.32454100	0.83748000
C	0.21297400	-2.02549600	3.94348900
C	-0.04141800	2.29698400	2.32673600
H	-0.09993900	3.29017700	0.43294300
H	0.03713700	1.05262000	4.06202100
C	0.29845600	-3.40046200	4.08761500
H	0.40588900	-5.28341500	3.08673500
H	0.18080300	-1.38988200	4.81062800
H	-0.08136800	3.21251000	2.88954400
H	0.33361600	-3.83609500	5.07039800
N	-4.63691900	-0.33524100	-0.40475100

N	4.69596400	0.27291800	-0.61192000
C	4.32336500	1.64162900	-0.68491800
C	4.66228900	2.51689100	0.34734600
C	3.62948600	2.14581900	-1.76916100
C	4.32260800	3.84879200	0.28471800
H	5.19873700	2.14078700	1.19912400
C	3.26226500	3.48617500	-1.83280200
H	3.35964700	1.48955700	-2.57641200
C	3.61324900	4.34538100	-0.80659900
H	4.58444900	4.52393500	1.07809000
H	2.71971000	3.83422400	-2.69039000
C	-4.74737900	0.19435400	0.90955500
C	-4.93804600	1.54848000	1.11043600
C	-4.68609900	-0.63786400	2.02753400
C	-5.07956900	2.07675100	2.38837700
H	-4.98587500	2.20532200	0.26119800
C	-4.80250800	-0.12219900	3.29854600
H	-4.53571400	-1.69341200	1.89307300
C	-5.00571500	1.24201000	3.49008600
H	-5.23180400	3.13283200	2.49859900
H	-4.74895700	-0.76087900	4.16045500
C	6.07062700	-0.06246500	-0.49657600
C	6.47859600	-1.03505800	0.41864500
C	7.03790700	0.56101500	-1.26192000
C	7.80575200	-1.37337800	0.54594300
H	5.74115900	-1.52553800	1.02740300
C	8.38553100	0.24216400	-1.12421300
H	6.74886100	1.31474100	-1.97101200
C	8.77494800	-0.73221100	-0.22325300
H	8.11974100	-2.12310200	1.24823500
H	9.10330300	0.75704900	-1.73289300
C	-5.68773600	-0.09502800	-1.32955100
C	-5.41101300	0.42393300	-2.59501900
C	-7.00609300	-0.35075800	-1.00185700
C	-6.42175300	0.66379000	-3.49785700
H	-4.39201600	0.63243700	-2.86586700
C	-8.03740400	-0.09135800	-1.89817400
H	-7.24173000	-0.74840100	-0.03173500
C	-7.74816000	0.41214900	-3.15444500
H	-6.20948100	1.06012300	-4.47344200
H	-9.04685400	-0.29788700	-1.59975900
O	3.31728000	5.66361500	-0.76900400
O	-5.11933600	1.64831000	4.77366100
O	-8.66742100	0.69192000	-4.10370700

O	10.05048800	-1.12616900	-0.01480600
C	2.62853200	6.24640900	-1.83603900
H	3.18379800	6.15719900	-2.76418600
H	1.64550300	5.80443100	-1.96435800
H	2.51645700	7.29185600	-1.58985200
C	-5.31072500	3.00395100	5.05372700
H	-6.23499300	3.37306100	4.62087500
H	-5.36654100	3.08626800	6.12903100
H	-4.48212700	3.60512500	4.69349100
C	11.08361800	-0.53161800	-0.74434900
H	11.99807800	-0.99920000	-0.41087800
H	10.96619500	-0.70050800	-1.80997300
H	11.14056200	0.53557300	-0.55554200
C	-10.02126200	0.46136500	-3.84288200
H	-10.37231300	1.05824100	-3.00730600
H	-10.55533500	0.75280500	-4.73495800
H	-10.21387400	-0.58708300	-3.63967400

Molecule **6**:

C	0.66158600	0.00373400	4.22370300
C	-0.66158600	-0.00373400	4.22370300
H	1.12171700	0.00668000	5.19647200
H	-1.12171700	-0.00668000	5.19647200
C	1.63039800	0.00620300	3.12648100
C	1.37184700	-0.00232700	1.75663000
C	2.97380600	0.01144100	3.54906800
C	2.47588700	-0.00056100	0.88882600
C	4.03513100	-0.00243500	2.68889200
H	3.17133500	0.01219100	4.60602400
C	3.78662300	-0.00605600	1.31564600
H	2.30368700	0.00233900	-0.16598900
H	5.04239200	-0.01152000	3.06134800
C	-1.63039800	-0.00620300	3.12648100
C	-1.37184700	0.00232700	1.75663000
C	-2.97380600	-0.01144100	3.54906800
C	-2.47588700	0.00056100	0.88882600
C	-4.03513100	0.00243500	2.68889200
H	-3.17133500	-0.01219100	4.60602400
C	-3.78662300	0.00605600	1.31564600
H	-2.30368700	-0.00233900	-0.16598900
H	-5.04239200	0.01152000	3.06134800
C	0.00000000	0.00000000	1.01184900
C	0.00000000	1.18087500	0.02300300
C	0.00000000	-1.18087500	0.02300300
C	-0.00420900	2.53074600	0.31154000

C	-0.00030200	0.73733300	-1.29655600
C	0.00420900	-2.53074600	0.31154000
C	0.00030200	-0.73733300	-1.29655600
C	-0.00814300	3.43986100	-0.73656300
H	-0.00788700	2.87473800	1.33060600
C	-0.00320300	1.64488000	-2.34393200
C	0.00814300	-3.43986100	-0.73656300
H	0.00788700	-2.87473800	1.33060600
C	0.00320300	-1.64488000	-2.34393200
C	-0.00730000	2.99979700	-2.05379600
H	-0.01657100	4.49467600	-0.52769400
H	-0.00641000	1.30944900	-3.36581600
C	0.00730000	-2.99979700	-2.05379600
H	0.01657100	-4.49467600	-0.52769400
H	0.00641000	-1.30944900	-3.36581600
H	-0.01383800	3.71741100	-2.85478600
H	0.01383800	-3.71741100	-2.85478600
N	4.86672200	-0.04612600	0.40374300
C	5.97264100	0.82730400	0.57954800
C	4.68349200	-0.63679000	-0.88147200
C	5.80382600	2.13783500	1.01168900
C	7.25704700	0.36682500	0.30456400
C	4.61531300	-2.06147000	-1.00044500
C	4.59421600	0.14280000	-1.99378200
C	6.90282700	2.96624900	1.17555100
H	4.81670000	2.50627200	1.22068900
C	8.34726600	1.20461500	0.45261700
H	7.39268800	-0.64657800	-0.02604300
C	4.74421600	-2.93070400	0.11639100
C	4.43199600	-2.62672700	-2.27984400
C	4.42836700	-0.43209200	-3.27498700
H	4.65254300	1.21109500	-1.89421000
C	8.17825900	2.50821600	0.89415000
H	6.75506300	3.97692400	1.51278100
H	9.33271500	0.83325800	0.23380800
C	4.68006500	-4.27900400	-0.04059900
H	4.89652800	-2.50908800	1.09021500
C	4.36391800	-4.03932900	-2.40843800
C	4.34007500	-1.77821900	-3.41456400
H	4.36350200	0.21163100	-4.13375500
H	9.02810600	3.15529900	1.01649900
C	4.48216700	-4.84476900	-1.32198200
H	4.78179800	-4.92440900	0.81356500
H	4.22064800	-4.46189900	-3.38761200

H	4.20719600	-2.22111600	-4.38598800
H	4.43137600	-5.91361100	-1.42988900
N	-4.86672200	0.04612600	0.40374300
C	-5.97264100	-0.82730400	0.57954800
C	-4.68349200	0.63679000	-0.88147200
C	-5.80382600	-2.13783500	1.01168900
C	-7.25704700	-0.36682500	0.30456400
C	-4.61531300	2.06147000	-1.00044500
C	-4.59421600	-0.14280000	-1.99378200
C	-6.90282700	-2.96624900	1.17555100
H	-4.81670000	-2.50627200	1.22068900
C	-8.34726600	-1.20461500	0.45261700
H	-7.39268800	0.64657800	-0.02604300
C	-4.74421600	2.93070400	0.11639100
C	-4.43199600	2.62672700	-2.27984400
C	-4.42836700	0.43209200	-3.27498700
H	-4.65254300	-1.21109500	-1.89421000
C	-8.17825900	-2.50821600	0.89415000
H	-6.75506300	-3.97692400	1.51278100
H	-9.33271500	-0.83325800	0.23380800
C	-4.68006500	4.27900400	-0.04059900
H	-4.89652800	2.50908800	1.09021500
C	-4.36391800	4.03932900	-2.40843800
C	-4.34007500	1.77821900	-3.41456400
H	-4.36350200	-0.21163100	-4.13375500
H	-9.02810600	-3.15529900	1.01649900
C	-4.48216700	4.84476900	-1.32198200
H	-4.78179800	4.92440900	0.81356500
H	-4.22064800	4.46189900	-3.38761200
H	-4.20719600	2.22111600	-4.38598800
H	-4.43137600	5.91361100	-1.42988900

CIS:

Molecule **1**:

C	-0.09411800	0.28645400	-0.03906500
C	-0.09414200	0.28647800	1.36198900
H	0.86622200	0.51626700	-0.46575200
H	0.86618300	0.51630400	1.78870100
C	-1.11759400	0.11069400	-0.97060900
C	-2.48135000	-0.27028600	-0.69355300
C	-0.74336900	0.35426200	-2.33887800
C	-3.34351100	-0.35375900	-1.79471100
C	-1.62295800	0.27473200	-3.36350600
H	0.28022200	0.62064900	-2.53190700
C	-2.95712900	-0.07964600	-3.08505800

H	-4.36033700	-0.64817600	-1.64488800
H	-1.30993700	0.47568600	-4.37221100
C	-1.11764800	0.11074000	2.29350600
C	-2.48138500	-0.27028500	2.01642300
C	-0.74344700	0.35426000	3.66179100
C	-3.34353200	-0.35392800	3.11757800
C	-1.62303400	0.27461100	4.68641200
H	0.28013200	0.62067500	3.85484300
C	-2.95717700	-0.07985900	4.40794200
H	-4.36032800	-0.64844200	2.96773100
H	-1.31002700	0.47551500	5.69513000
C	-2.99280500	-0.80719300	0.66143300
C	-4.52738800	-0.82353300	0.66144200
C	-2.70575500	-2.33892000	0.66143900
C	-5.38422900	0.26155100	0.66132400
C	-5.02757300	-2.11854600	0.66154000
C	-1.49134600	-2.99970500	0.66139700
C	-3.89909400	-3.06148600	0.66154900
C	-6.75239600	0.03842900	0.66135900
H	-4.99637000	1.26468900	0.66122900
C	-6.39727300	-2.34483000	0.66157500
C	-1.48375600	-4.38775000	0.66145800
H	-0.56497100	-2.45800300	0.66132400
C	-3.88706300	-4.44575900	0.66160700
C	-7.25499500	-1.25820800	0.66149200
H	-7.43018600	0.87328000	0.66128500
H	-6.79148200	-3.34543000	0.66165100
C	-2.66971600	-5.10831700	0.66156100
H	-0.54360400	-4.91021100	0.66142500
H	-4.80705800	-5.00344800	0.66167800
H	-8.31863300	-1.41718300	0.66151400
H	-2.64384500	-6.18330500	0.66160300
H	-3.67902800	-0.14509200	5.20191700
H	-3.67899000	-0.14475200	-3.87903500

Molecule **2**:

C	3.31791100	-0.15383800	-0.79288700
C	3.35586100	-0.18753200	0.60324800
H	4.28791600	-0.07017200	-1.25159900
H	4.34944800	-0.12480800	1.01211900
C	2.25714300	-0.27695500	-1.69053600
C	0.85091500	-0.33777000	-1.38906800
C	2.62614000	-0.36820900	-3.07419200
C	-0.02828400	-0.51531600	-2.45503900
C	1.74477000	-0.54545600	-4.08096000

H	3.67301700	-0.30022100	-3.31110200
C	0.35486400	-0.63371800	-3.79005200
H	-1.07014300	-0.55847800	-2.24250500
H	2.10533200	-0.61027000	-5.08804900
C	2.34523200	-0.35516000	1.55018700
C	0.92463200	-0.40320100	1.32293400
C	2.78868900	-0.51253300	2.90575700
C	0.10437000	-0.63306300	2.42526800
C	1.96304600	-0.73926200	3.94917500
H	3.84697300	-0.45469200	3.08847800
C	0.55928100	-0.81519500	3.73024700
H	-0.94754400	-0.66729300	2.26777400
H	2.37766800	-0.85209200	4.93090500
C	0.23856300	0.00960100	-0.00625100
C	0.08711900	1.55268300	0.03508800
C	-1.23950300	-0.40464800	0.02393000
C	1.06784900	2.52992200	0.03200100
C	-1.25925100	1.91771900	0.08050900
C	-1.76398900	-1.68490500	0.00729300
C	-2.08095900	0.69881100	0.07343800
C	0.68757300	3.86346200	0.07451800
H	2.10764300	2.26916600	-0.00256100
C	-1.63506300	3.24972100	0.12286500
C	-3.13977700	-1.85234600	0.04065600
H	-1.11248200	-2.53971000	-0.03104500
C	-3.45998400	0.53446800	0.10696400
C	-0.65202800	4.22588600	0.11968800
H	1.44481100	4.62758900	0.07236800
H	-2.67412800	3.52736300	0.15781700
C	-3.98291600	-0.74699800	0.09025400
H	-3.55862200	-2.84300300	0.02813700
H	-4.11596900	1.38604500	0.14534700
H	-0.92620300	5.26529300	0.15222300
H	-5.04875000	-0.89004100	0.11577800
N	-0.56847900	-0.80503600	-4.80280800
N	-0.30791600	-1.03635000	4.78222200
C	0.20115400	-1.62765500	6.00238100
H	-0.61926900	-1.78324000	6.68773100
H	0.68750100	-2.58705700	5.83078200
H	0.90891300	-0.97064100	6.49387700
C	-1.72062700	-1.18960600	4.51446300
H	-2.11065500	-0.31550400	4.00799400
H	-1.94271600	-2.06416200	3.90306900
H	-2.24921600	-1.28536000	5.45214300

C	-1.96474900	-0.97291400	-4.46638700
H	-2.15441000	-1.87623100	-3.88671400
H	-2.32555200	-0.12477500	-3.89790600
H	-2.54363300	-1.02404500	-5.37748300
C	-0.12722100	-1.33609600	-6.07593400
H	0.55362600	-0.65518500	-6.57289000
H	0.36649900	-2.30200800	-5.97751000
H	-0.98387200	-1.45953200	-6.72239900

Molecule **3**:

C	-0.08950700	-0.48074200	-0.00875800
C	-0.09202500	-0.43234300	1.38403400
H	0.87550800	-0.69930900	-0.43178000
H	0.87323400	-0.60908100	1.82563100
C	-1.11861100	-0.35778100	-0.94490900
C	-2.48783600	0.01564300	-0.69538300
C	-0.74827800	-0.63962200	-2.30325100
C	-3.34629500	0.05113900	-1.78503300
C	-1.61632600	-0.59978200	-3.33788900
H	0.27987400	-0.88924200	-2.49448700
C	-2.96488100	-0.25054600	-3.09012300
H	-4.36724000	0.32917300	-1.64246600
H	-1.28916100	-0.81423400	-4.33753500
C	-1.13324000	-0.28062000	2.30148900
C	-2.51171900	0.02826200	2.01023800
C	-0.77659500	-0.48935200	3.67631600
C	-3.39694900	0.03463200	3.07986200
C	-1.67273600	-0.48362300	4.68807300
H	0.25601600	-0.69501900	3.89436500
C	-3.03465200	-0.23909500	4.39462800
H	-4.42367700	0.27778600	2.91610900
H	-1.36336900	-0.67807100	5.69752900
C	-3.01174700	0.58501400	0.65250600
C	-2.71480000	2.10909500	0.64073800
C	-4.54666600	0.61178500	0.63821400
C	-1.49666900	2.76438400	0.64139200
C	-3.90139300	2.84322200	0.62424100
C	-5.41528600	-0.46499100	0.63998300
C	-5.03712900	1.90962100	0.62329600
C	-1.47892300	4.15295200	0.62827500
H	-0.57391100	2.21789000	0.65138600
C	-3.88110700	4.22714100	0.61073300
C	-6.78055400	-0.22998700	0.62920800
H	-5.03756800	-1.47176000	0.65473800
C	-6.40469200	2.14873100	0.60901700

C	-2.65916100	4.88176900	0.61333400
H	-0.53477000	4.66849700	0.62938400
H	-4.79771800	4.79036300	0.59852100
C	-7.27191500	1.07091600	0.61273400
H	-7.46532900	-1.05883600	0.63788100
H	-6.78913300	3.15301100	0.59472100
H	-2.62585400	5.95675800	0.60347000
H	-8.33408500	1.23906900	0.60346500
N	-3.88534600	-0.19468400	-4.14124500
C	-3.85071500	-1.16991700	-5.16816200
C	-4.87680400	0.81878300	-4.17983500
C	-3.72698500	-2.52015300	-4.85399800
C	-3.93555800	-0.79023900	-6.50507500
C	-4.53006500	2.14968700	-3.96448400
C	-6.20531400	0.49655900	-4.43706500
C	-3.68117100	-3.46930300	-5.86051300
H	-3.66881400	-2.81935000	-3.82392400
C	-3.90520100	-1.74648400	-7.50425200
H	-4.02578000	0.25064200	-6.75461200
C	-5.49879000	3.13613900	-4.00154300
H	-3.50591700	2.40388000	-3.76416600
C	-7.16614700	1.49173100	-4.48885100
H	-6.48042000	-0.52953700	-4.59607600
C	-3.77348900	-3.09028500	-7.18992300
H	-3.58543900	-4.50881000	-5.60159200
H	-3.97263700	-1.43785900	-8.53233200
C	-6.82079200	2.81490400	-4.26838100
H	-5.21560300	4.15946500	-3.83102100
H	-8.18919000	1.22766600	-4.68989100
H	-3.74347800	-3.83009600	-7.96938800
H	-7.57048900	3.58481900	-4.30252300
N	-3.99796200	-0.27167400	5.41060500
C	-3.71971500	0.30937400	6.67186300
C	-5.26991100	-0.85003900	5.17378600
C	-3.11589700	1.56080500	6.75322300
C	-4.04224000	-0.36544000	7.84634200
C	-5.36956200	-2.10963900	4.58847100
C	-6.43266000	-0.17278200	5.52655000
C	-2.83409600	2.11989600	7.98781400
H	-2.87266100	2.08983700	5.85048400
C	-3.77220100	0.20792800	9.07598600
H	-4.50325200	-1.33408700	7.79056000
C	-6.61058000	-2.67458200	4.35729100
H	-4.47392900	-2.63815400	4.31920700

C	-7.67074200	-0.75121900	5.30485500
H	-6.36292400	0.80222800	5.97190000
C	-3.16289900	1.45062000	9.15547900
H	-2.36760700	3.08787300	8.03413500
H	-4.02827200	-0.32498000	9.97445400
C	-7.76841700	-2.00152700	4.71671100
H	-6.67151400	-3.64968100	3.90728600
H	-8.56081000	-0.21537600	5.58301400
H	-2.94828700	1.89017400	10.11284700
H	-8.73168700	-2.44591500	4.54167400

Molecule **4**:

C	-0.05191800	-0.05869100	-0.03332000
C	-0.05200000	0.05857100	1.35654100
H	0.93247000	-0.11580100	-0.46391500
H	0.93230800	0.11704300	1.78713600
C	-1.09378900	-0.07280100	-0.95985700
C	-2.50385900	0.02491900	-0.70536600
C	-0.68629000	-0.15072100	-2.33883300
C	-3.35237500	0.09709700	-1.80700800
C	-1.54055500	-0.09080000	-3.38084900
H	0.36672700	-0.24163100	-2.53587500
C	-2.92964100	0.05381200	-3.12555400
H	-4.40630000	0.17486600	-1.64100400
H	-1.17622000	-0.13841500	-4.38915700
C	-1.09389000	0.07124200	2.28307700
C	-2.50382300	-0.02843900	2.02858600
C	-0.68649900	0.14973500	3.66205200
C	-3.35223600	-0.10179900	3.13022900
C	-1.54067900	0.08862500	4.70406900
H	0.36639100	0.24211000	3.85909300
C	-2.92956200	-0.05792500	4.44877400
H	-4.40605200	-0.18103900	2.96422700
H	-1.17641000	0.13674700	5.71237700
C	-3.23168000	-0.00227600	0.66160900
C	-4.22542400	1.17927000	0.70073100
C	-4.22374000	-1.18523800	0.62248500
C	-3.94056800	2.52985200	0.74684200
C	-5.54380600	0.73325100	0.68875400
C	-3.93696100	-2.53541200	0.57637000
C	-5.54275600	-0.74109600	0.63446100
C	-4.99097000	3.43509200	0.78116200
H	-2.92232300	2.87585500	0.75209800
C	-6.59315200	1.63822600	0.72369500
C	-4.98607400	-3.44214700	0.54204800

H	-2.91822500	-2.87996500	0.57111100
C	-6.59081200	-1.64756400	0.59951900
C	-6.30801600	2.99317800	0.77007500
H	-4.78383400	4.49005100	0.81055600
H	-7.61407500	1.29963100	0.71204700
C	-6.30374800	-3.00210900	0.55313700
H	-4.77743600	-4.49681000	0.51265000
H	-7.61221700	-1.31042400	0.61116800
H	-7.11088800	3.70831700	0.79372600
H	-7.10560100	-3.71839100	0.52948400
N	-3.83541000	-0.15654500	5.50632100
C	-3.56478400	0.45919600	6.76326300
C	-5.08516900	-0.82260300	5.34540100
C	-3.46760100	1.88493100	6.87580700
C	-3.42375100	-0.32108200	7.87118400
C	-5.12885900	-2.24165500	5.14765200
C	-6.24342300	-0.10931200	5.41287700
C	-3.65399800	2.76324700	5.77284100
C	-3.19956500	2.44419400	8.14424400
C	-3.17441500	0.24947400	9.13939700
H	-3.50500700	-1.38798100	7.77456300
C	-3.96267900	-3.05321800	5.11258600
C	-6.38703400	-2.86436500	5.00650500
C	-7.49945600	-0.74469300	5.28519700
H	-6.19897600	0.95308100	5.56527600
C	-3.56264900	4.11011500	5.93194600
H	-3.86731200	2.35698100	4.80389600
C	-3.10248100	3.85536200	8.27312500
C	-3.05424500	1.59419400	9.27200500
H	-3.07012800	-0.39523800	9.99342200
C	-4.05395100	-4.39806800	4.93755600
H	-3.00011400	-2.59447300	5.22410100
C	-6.44680000	-4.27050300	4.81776200
C	-7.57068900	-2.08304400	5.07811900
H	-8.39472900	-0.15229400	5.34434300
C	-3.27686100	4.66788700	7.19970700
H	-3.70853600	4.75895300	5.08704700
H	-2.89217400	4.27067700	9.24317000
H	-2.85556000	2.03479000	10.23305400
C	-5.31482300	-5.01914200	4.78286000
H	-3.16124700	-4.99724500	4.91526700
H	-7.41121100	-4.73479100	4.70747800
H	-8.52330400	-2.57176500	4.97310600
H	-3.20314500	5.73523200	7.30810400

H	-5.37088100	-6.08384700	4.64207800
N	-3.83562600	0.15116200	-4.18310100
C	-3.56413600	-0.46419600	-5.44004300
C	-5.08632000	0.81546400	-4.02218100
C	-3.46495100	-1.88979400	-5.55259100
C	-3.42420000	0.31628000	-6.54796300
C	-5.13200300	2.23445300	-3.82443000
C	-6.24357000	0.10054800	-4.08966000
C	-3.65011200	-2.76837300	-4.44962700
C	-3.19612900	-2.44867700	-6.82102900
C	-3.17406400	-0.25392200	-7.81617700
H	-3.50695400	1.38306400	-6.45134000
C	-3.96696300	3.04765300	-3.78935800
C	-6.39105100	2.85539600	-3.68328600
C	-7.50049500	0.73416400	-3.96198300
H	-6.19763200	-0.96178200	-4.24205900
C	-3.55687100	-4.11511100	-4.60873500
H	-3.86399700	-2.36240900	-3.48068100
C	-3.09706300	-3.85970700	-6.94991300
C	-3.05200500	-1.59847100	-7.94878900
H	-3.07068200	0.39093800	-8.67020100
C	-4.06012400	4.39237300	-3.61432700
H	-3.00375500	2.59026000	-3.90087100
C	-6.45279200	4.26144800	-3.49454200
C	-7.57360700	2.07241400	-3.75490500
H	-8.39493500	0.14050900	-4.02113100
C	-3.27030100	-4.67247900	-5.87649700
H	-3.70184700	-4.76415500	-3.76383700
H	-2.88617300	-4.27472400	-7.91995800
H	-2.85270200	-2.03878500	-8.90983800
C	-5.32186700	5.01167600	-3.45963600
H	-3.16826200	4.99280300	-3.59203400
H	-7.41785300	4.72438200	-3.38426100
H	-8.52690800	2.55979700	-3.64989300
H	-3.19508600	-5.73971900	-5.98489500
H	-5.37942000	6.07630100	-3.31885400

Molecule **5**:

C	-0.05461700	0.49831300	-0.04450500
C	-0.05984100	0.49612700	1.34893200
H	0.91437200	0.68650500	-0.47330000
H	0.90751000	0.67165300	1.78671000
C	-1.08479100	0.36035300	-0.97752700
C	-2.46076900	0.02042800	-0.71872500
C	-0.70953000	0.58670000	-2.34472400

C	-3.31931500	-0.03567300	-1.80723700
C	-1.57618100	0.52563800	-3.37937700
H	0.32319600	0.81074100	-2.54351900
C	-2.93293300	0.21155000	-3.12351500
H	-4.34504700	-0.28866900	-1.65486500
H	-1.24164800	0.69714000	-4.38473400
C	-1.10447200	0.38962100	2.26908300
C	-2.48775000	0.09345300	1.98710200
C	-0.74726200	0.63407200	3.63753500
C	-3.37392600	0.13395500	3.05442200
C	-1.64371000	0.67297900	4.64847500
H	0.28839500	0.82915600	3.85140900
C	-3.01031900	0.44196300	4.36283800
H	-4.40369900	-0.09894300	2.89593400
H	-1.32988900	0.89246000	5.65129800
C	-2.99469600	-0.49837800	0.64628200
C	-4.52985700	-0.50305800	0.62997500
C	-2.72071400	-2.02571700	0.68208100
C	-5.38294200	0.58560200	0.59742500
C	-5.03956900	-1.79340600	0.65218700
C	-1.51233500	-2.69880800	0.70655900
C	-3.91770300	-2.74301600	0.68349200
C	-6.75144200	0.37027100	0.59097100
H	-4.99000200	1.58655600	0.58219500
C	-6.41052200	-2.01303600	0.64207700
C	-1.51530600	-4.08715800	0.73452100
H	-0.58180000	-2.16569000	0.70375300
C	-3.91813100	-4.12693000	0.71034100
C	-7.26198300	-0.92314300	0.61263600
H	-7.42448300	1.20873600	0.57302500
H	-6.80937200	-3.01166100	0.65631000
C	-2.70607200	-4.79902000	0.73645800
H	-0.57884500	-4.61627200	0.75438400
H	-4.84295900	-4.67668600	0.71057700
H	-8.32656900	-1.07587400	0.60836700
H	-2.68857400	-5.87422600	0.75783900
N	-3.85009200	0.13464300	-4.17143200
N	-3.97167500	0.51768800	5.37386700
C	-5.25528000	1.06240400	5.11192600
C	-6.41254700	0.36151600	5.45280600
C	-5.39077200	2.30608000	4.51900900
C	-7.65738200	0.89755300	5.21272300
H	-6.32775700	-0.60704800	5.90996500
C	-6.64274500	2.84733300	4.25734500

H	-4.51034200	2.86128000	4.25210400
C	-7.78444700	2.14522200	4.60768400
H	-8.54957600	0.35980500	5.47456700
H	-6.70265700	3.81368400	3.79537200
C	-4.91727000	-0.80129600	-4.13429100
C	-6.22432000	-0.40312600	-4.34716000
C	-4.66617700	-2.15317500	-3.89017000
C	-7.26836000	-1.32081900	-4.33311800
H	-6.43860600	0.63331900	-4.53231700
C	-5.69494200	-3.06487700	-3.85602600
H	-3.65712700	-2.48011000	-3.71944400
C	-7.00843300	-2.65661100	-4.08091500
H	-8.26729700	-0.97061500	-4.50654100
H	-5.50419300	-4.10443000	-3.66499100
C	-3.67913700	0.03732100	6.67552700
C	-3.10910900	-1.22462700	6.85606000
C	-3.95566700	0.79936500	7.79728200
C	-2.82102100	-1.69380700	8.11711600
H	-2.89391200	-1.83355600	5.99730700
C	-3.68621500	0.32496300	9.07519800
H	-4.39265200	1.77391100	7.68012100
C	-3.11095100	-0.92373500	9.24121200
H	-2.38242300	-2.66421300	8.25760600
H	-3.92126700	0.94603900	9.91763000
C	-3.75593000	1.02525200	-5.27162800
C	-3.62141300	2.39952600	-5.06749900
C	-3.79992200	0.55616300	-6.57322800
C	-3.52616900	3.26502800	-6.13351900
H	-3.59025300	2.78257300	-4.06405900
C	-3.72353000	1.42418000	-7.65497900
H	-3.90083600	-0.49861600	-6.75133700
C	-3.58021700	2.78515200	-7.43983700
H	-3.42165400	4.32274600	-5.97807000
H	-3.76580200	1.01902600	-8.64730600
O	-9.04769800	2.57978200	4.40721500
O	-7.94473600	-3.62865400	-4.03517800
O	-3.48797600	3.71393700	-8.41534600
O	-2.79973600	-1.47675800	10.43302200
C	-9.26310700	3.82863000	3.81800300
H	-8.83717300	4.62880300	4.41464300
H	-8.85007500	3.87199400	2.81522900
H	-10.33386200	3.95815500	3.76530500
C	-9.28908900	-3.30211600	-4.23405200
H	-9.45429100	-2.88122900	-5.22064700

H	-9.84130200	-4.22599000	-4.14687400
H	-9.64336600	-2.60340500	-3.48307300
C	-3.05821300	-0.77030400	11.61128100
H	-2.73149800	-1.40420600	12.42204000
H	-2.50521800	0.16285600	11.64451300
H	-4.11727200	-0.56327200	11.72621000
C	-3.52348600	3.31546600	-9.75500500
H	-4.46103600	2.82667000	-9.99942200
H	-3.43127200	4.21739900	-10.34141000
H	-2.69992000	2.65034100	-9.99352400

Molecule **6**:

C	-0.07261100	0.03952000	-0.03401900
C	-0.07263800	-0.03923300	1.35716500
H	0.91231100	0.07204700	-0.46567800
H	0.91226200	-0.07236700	1.78882800
C	-1.11426700	0.06498500	-0.96145200
C	-2.52587100	0.01794400	-0.70602500
C	-0.70075700	0.12206900	-2.34064200
C	-3.37832900	0.01334600	-1.80930500
C	-1.55763300	0.11622300	-3.38065600
H	0.35594800	0.15234100	-2.53647500
C	-2.95433500	0.05628100	-3.12470200
H	-4.43431200	-0.01842800	-1.64347400
H	-1.19531400	0.14265600	-4.39096400
C	-1.11431300	-0.06408300	2.28459300
C	-2.52588700	-0.01613400	2.02916800
C	-0.70084200	-0.12148400	3.66378300
C	-3.37834100	-0.01100000	3.13244800
C	-1.55771500	-0.11513300	4.70379600
H	0.35584300	-0.15243000	3.85961600
C	-2.95437700	-0.05426800	4.44784500
H	-4.43430100	0.02149300	2.96661800
H	-1.19541200	-0.14183600	5.71410300
C	-3.25228700	0.00126500	0.66157000
C	-4.24511100	1.18500100	0.67301800
C	-4.24635300	-1.18142300	0.65013200
C	-3.95870200	2.53577300	0.68913900
C	-5.56390300	0.74006800	0.66775800
C	-3.96136200	-2.53249400	0.63399900
C	-5.56467800	-0.73510800	0.65542000
C	-5.00785100	3.44278700	0.69956300
H	-2.94015500	2.88084500	0.69734400
C	-6.61209500	1.64690800	0.67719600
C	-5.01146100	-3.43840900	0.62359700

H	-2.94317700	-2.87863300	0.62576700
C	-6.61382100	-1.64084800	0.64601200
C	-6.32526400	3.00222200	0.69316500
H	-4.79945000	4.49766400	0.71746900
H	-7.63339300	1.30924000	0.67614100
C	-6.32841100	-2.99646200	0.63003200
H	-4.80416700	-4.49350400	0.60567500
H	-7.63476500	-1.30211000	0.64709900
H	-7.12724400	3.71867400	0.70446900
H	-7.13114200	-3.71207200	0.61874800
N	-3.85667100	-0.00129600	-4.19431700
C	-3.67925900	0.82968600	-5.32935900
C	-5.11227600	-0.65506700	-4.02944000
C	-3.23018300	2.13995300	-5.19945900
C	-3.96140200	0.33306400	-6.59979600
C	-5.16641200	-2.08310700	-3.93810500
C	-6.26041700	0.07603500	-3.97779600
C	-3.05726900	2.93234300	-6.32264300
H	-3.02156300	2.53511800	-4.22271600
C	-3.80181800	1.13599500	-7.71366900
H	-4.30446800	-0.67947500	-6.70641400
C	-4.01112100	-2.90484200	-4.03269700
C	-6.42372400	-2.70105400	-3.77211800
C	-7.51671300	-0.55302300	-3.82665200
H	-6.20582600	1.14657300	-4.05138900
C	-3.34385600	2.43891300	-7.58397800
H	-2.70957600	3.94342800	-6.20532500
H	-4.02520100	0.73805400	-8.68761000
C	-4.11128200	-4.25780800	-3.95181400
H	-3.05237400	-2.44562500	-4.17149000
C	-6.49243200	-4.11674700	-3.68449800
C	-7.59682500	-1.90286700	-3.71704000
H	-8.40477100	0.05187000	-3.78897900
H	-3.21384800	3.05834100	-8.45302000
C	-5.37028200	-4.87610000	-3.76966700
H	-3.22792600	-4.86638500	-4.02749000
H	-7.45518400	-4.57903400	-3.55331800
H	-8.54971100	-2.38700300	-3.59462200
H	-5.43282900	-5.94773300	-3.70437600
N	-3.85667400	0.00384000	5.51746000
C	-3.67976600	-0.82727400	6.65248400
C	-5.11187700	0.65839200	5.35261300
C	-3.23151200	-2.13781800	6.52255000
C	-3.96157300	-0.33050000	7.92293600

C	-5.16513800	2.08647200	5.26138100
C	-6.26046200	-0.07200500	5.30089300
C	-3.05906900	-2.93033800	7.64571600
H	-3.02315400	-2.53309200	5.54579500
C	-3.80246900	-1.13355100	9.03679100
H	-4.30400300	0.68225200	8.02958000
C	-4.00934600	2.90749300	5.35604800
C	-6.42207100	2.70520000	5.09542700
C	-7.51637200	0.55783200	5.14977300
H	-6.20652500	-1.14258200	5.37440300
C	-3.34532400	-2.43675200	8.90706500
H	-2.71200900	-3.94163700	7.52837200
H	-4.02558400	-0.73549000	10.01074400
C	-4.10868000	4.26052600	5.27526900
H	-3.05088100	2.44767900	5.49481300
C	-6.48991300	4.12094200	5.00791700
C	-7.59565700	1.90773300	5.04026700
H	-8.40479700	-0.04651700	5.11203500
H	-3.21568400	-3.05627700	9.77609300
C	-5.36730000	4.87960100	5.09315700
H	-3.22495300	4.86855800	5.35099900
H	-7.45238000	4.58382700	4.87676100
H	-8.54824600	2.39246000	4.91787400
H	-5.42919100	5.95127700	5.02794800

2. Energies for the molecules **1- 6** by DFT, HF, and CIS methods.

DFT:

Molecule **1**: E(RHF) = -1039.7096601 a.u.

Molecule **2**: E(RHF) = -1307.6454665 a.u.

Molecule **3**: E(RHF) = -2074.6081485 a.u.

Molecule **4**: E(RHF) = -2689.1680126 a.u.

Molecule **5**: E(RHF) = -2532.6942157 a.u.

Molecule **6**: E(RHF) = -2381.8902688 a.u.

HF:

Molecule **1**: E(RHF) = -1032.9267277 a.u.

Molecule **2**: E(RHF) = -1299.0821140 a.u.

Molecule **3**: E(RHF) = -2061.1414247 a.u.

Molecule **4**: E(RHF) = -2671.7336295 a.u.

Molecule **5**: E(RHF) = -2516.6573926 a.u.

Molecule **6**: E(RHF) = 2366.43659880 a.u.

CIS:

Molecule **1**: E(RHF) = -1032.9052694 a.u.

Molecule **2**: E(RHF) = -1299.0626239 a.u.

Molecule **3**: E(RHF) = -2061.1222617 a.u.

Molecule **4**: E(RHF) = -2671.7160436 a.u.
Molecule **5**: E(RHF) = -2516.6385605 a.u.
Molecule **6**: E(RHF) = -2366.4196095 a.u.

3. HOMO and LUMO energies for the molecules **1- 6** by DFT method.
Molecule **1**: HOMO: -0.20269 a.u.; LUMO: -0.04865 a.u.
Molecule **2**: HOMO: -0.15868 a.u.; LUMO: -0.02665 a.u.
Molecule **3**: HOMO: -0.16948 a.u.; LUMO: -0.04786 a.u.
Molecule **4**: HOMO: -0.16871 a.u.; LUMO: -0.04835 a.u.
Molecule **5**: HOMO: -0.15714 a.u.; LUMO: -0.03882 a.u.
Molecule **6**: HOMO: -0.16870 a.u.; LUMO: -0.04652 a.u.

4. Absorption Data for the Molecules **1–6** by TDDFT at the DFT//B3LYP/6-31G(d) Optimized Geometry.
Molecule **1**:
Excitation energies and oscillator strengths:
Excited state symmetry could not be determined.

Excited State	1:	Singlet-?Sym	3.7396 eV	331.54 nm	f=0.2210
90 -> 91		0.63224			
90 -> 92		0.12556			
Excited State	2:	Singlet-?Sym	3.8367 eV	323.16 nm	f=0.0137
89 -> 91		0.69703			
Excited State	3:	Singlet-?Sym	4.0780 eV	304.03 nm	f=0.0209
87 -> 91		0.11451			
90 -> 91		-0.10132			
90 -> 92		0.68623			
Excited State	4:	Singlet-?Sym	4.3399 eV	285.68 nm	f=0.0143
88 -> 91		0.60934			
89 -> 92		-0.16845			
90 -> 94		0.27380			
Excited State	5:	Singlet-?Sym	4.4420 eV	279.12 nm	f=0.1360
85 -> 91		-0.10430			
88 -> 91		0.12053			
88 -> 92		-0.21254			
89 -> 92		0.56189			
89 -> 93		0.11861			
90 -> 94		0.16829			
Excited State	6:	Singlet-?Sym	4.5296 eV	273.72 nm	f=0.0525
84 -> 94		0.10324			
87 -> 91		0.60530			
90 -> 95		0.28751			
90 -> 97		0.11604			
Excited State	7:	Singlet-?Sym	4.6546 eV	266.37 nm	f=0.0115
85 -> 91		0.14802			

86 -> 91		0.49089			
86 -> 92		0.12274			
88 -> 91		0.19617			
88 -> 92		-0.12744			
89 -> 93		0.27480			
90 -> 94		-0.26013			
Excited State	8:	Singlet-?Sym	4.6720 eV	265.38 nm	f=0.0169
90 -> 93		0.69633			
Excited State	9:	Singlet-?Sym	4.7096 eV	263.26 nm	f=0.0567
85 -> 92		-0.12409			
86 -> 91		-0.25133			
86 -> 92		0.11107			
88 -> 92		-0.21018			
89 -> 92		-0.23991			
89 -> 93		0.49496			
90 -> 94		0.11543			
Excited State	10:	Singlet-?Sym	4.7929 eV	258.68 nm	f=0.0189
85 -> 91		-0.36265			
86 -> 91		0.41083			
88 -> 91		-0.19984			
90 -> 94		0.36555			

Molecule **2**:

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	3.0277 eV	409.50 nm	f=0.0251
114 ->115		0.64769			
114 ->116		0.26329			
Excited State	2:	Singlet-A	3.2548 eV	380.93 nm	f=0.3875
114 ->115		-0.21516			
114 ->116		0.62005			
Excited State	3:	Singlet-A	3.6225 eV	342.26 nm	f=0.0525
114 ->117		0.69641			
Excited State	4:	Singlet-A	3.9383 eV	314.82 nm	f=0.0051
113 ->115		0.61184			
113 ->116		0.23316			
114 ->118		-0.24257			
Excited State	5:	Singlet-A	3.9532 eV	313.63 nm	f=0.0253
111 ->116		0.10271			
112 ->115		0.10434			
113 ->115		0.14657			
113 ->116		0.26084			
114 ->118		0.58658			
Excited State	6:	Singlet-A	4.0943 eV	302.82 nm	f=0.0418
113 ->115		-0.25289			
113 ->116		0.57973			

114 ->118 -0.16125
114 ->121 -0.20532
Excited State 7: Singlet-A 4.1269 eV 300.43 nm f=0.1778
114 ->119 0.67060
Excited State 8: Singlet-A 4.2841 eV 289.40 nm f=0.0189
112 ->115 0.54158
112 ->116 -0.39834
114 ->118 -0.10426
Excited State 9: Singlet-A 4.3899 eV 282.43 nm f=0.1107
111 ->115 -0.27927
112 ->115 0.36936
112 ->116 0.44792
112 ->117 0.13438
Excited State 10: Singlet-A 4.4939 eV 275.89 nm f=0.0109
113 ->117 0.68834
114 ->121 0.12030

Molecule **3**:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.
Excited State 1: Singlet-?Sym 2.8545 eV 434.35 nm f=0.6178
178 ->179 0.66847

Excited state symmetry could not be determined.
Excited State 2: Singlet-?Sym 3.3154 eV 373.97 nm f=0.0226
178 ->180 0.70061
Excited State 3: Singlet-?Sym 3.3292 eV 372.41 nm f=0.0882
177 ->179 0.68135
Excited State 4: Singlet-?Sym 3.6781 eV 337.08 nm f=0.0046
174 ->179 -0.10093
176 ->179 0.15749
177 ->180 0.27334
177 ->183 0.12213
178 ->181 0.58563
Excited State 5: Singlet-?Sym 3.7947 eV 326.73 nm f=0.0052
176 ->179 -0.43011
177 ->180 0.53589
178 ->181 -0.12369
Excited State 6: Singlet-?Sym 3.8024 eV 326.07 nm f=0.0165
176 ->179 -0.11871
177 ->180 -0.12871
177 ->181 0.24639
178 ->181 0.12144
178 ->182 0.27890
178 ->183 0.51397
178 ->184 -0.15723

Excited State	7:	Singlet-?Sym	3.8055 eV	325.80 nm	f=0.0074
176 ->179		0.51054			
177 ->180		0.34002			
178 ->181		-0.25251			
178 ->183		0.16492			
Excited State	8:	Singlet-?Sym	3.9024 eV	317.72 nm	f=0.1616
178 ->182		0.50952			
178 ->183		-0.23062			
178 ->185		0.37869			
Excited State	9:	Singlet-?Sym	3.9225 eV	316.09 nm	f=0.1212
177 ->184		-0.16680			
178 ->183		0.16100			
178 ->184		0.63160			
Excited State	10:	Singlet-?Sym	3.9431 eV	314.43 nm	f=0.0341
177 ->182		-0.11490			
178 ->182		-0.29385			
178 ->183		0.19497			
178 ->185		0.57236			

Molecule **4**:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State	1:	Singlet-?Sym	2.7924 eV	444.01 nm	f=0.6022
230 -> 231		0.66996			
Excited State	2:	Singlet-?Sym	3.0466 eV	406.95 nm	f=0.0793
229 -> 232		0.19544			
230 -> 232		0.65387			
Excited State	3:	Singlet-?Sym	3.0743 eV	403.30 nm	f=0.0636
229 -> 233		-0.13380			
230 -> 233		0.65980			
Excited State	4:	Singlet-?Sym	3.2099 eV	386.26 nm	f=0.0496
229 -> 231		-0.21252			
230 -> 234		0.62519			
Excited State	5:	Singlet-?Sym	3.3069 eV	374.92 nm	f=0.0037
230 -> 235		0.63879			
230 -> 236		0.24613			
Excited State	6:	Singlet-?Sym	3.3161 eV	373.89 nm	f=0.0599
229 -> 231		0.64431			
230 -> 234		0.23022			
Excited State	7:	Singlet-?Sym	3.4435 eV	360.05 nm	f=0.0371
229 -> 234		-0.11886			
230 -> 235		-0.19935			
230 -> 236		0.63611			
Excited State	8:	Singlet-?Sym	3.4948 eV	354.77 nm	f=0.0473
229 -> 232		0.64211			

230 -> 232 -0.22192

Excited State 9: Singlet-?Sym 3.6484 eV 339.83 nm f=0.0211

229 -> 233 0.66192

230 -> 233 0.15995

Excited State 10: Singlet-?Sym 3.6833 eV 336.61 nm f=0.0233

228 -> 231 -0.20567

229 -> 233 -0.10017

229 -> 236 0.10833

229 -> 238 0.13532

230 -> 237 0.53064

230 -> 238 -0.28734

Molecule **5**:

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7769 eV 446.48 nm f=0.6661

210 -> 211 0.66889

Excited State 2: Singlet-A 3.1205 eV 397.33 nm f=0.0274

210 -> 212 0.70057

Excited State 3: Singlet-A 3.2425 eV 382.37 nm f=0.0985

209 -> 211 0.68134

Excited State 4: Singlet-A 3.4658 eV 357.74 nm f=0.0095

209 -> 212 0.28004

209 -> 214 -0.15520

210 -> 213 0.60578

Excited State 5: Singlet-A 3.5532 eV 348.94 nm f=0.0170

209 -> 213 -0.23901

210 -> 214 0.64388

Excited State 6: Singlet-A 3.5766 eV 346.66 nm f=0.0013

209 -> 212 0.64494

210 -> 213 -0.26907

Excited State 7: Singlet-A 3.7207 eV 333.23 nm f=0.0742

210 -> 215 0.69504

Excited State 8: Singlet-A 3.8925 eV 318.52 nm f=0.0179

208 -> 211 0.61985

210 -> 217 0.16711

210 -> 218 -0.11831

210 -> 221 0.15301

Excited State 9: Singlet-A 3.9282 eV 315.63 nm f=0.0621

208 -> 211 -0.21082

209 -> 214 0.13116

209 -> 216 0.11092

209 -> 217 -0.12788

210 -> 216 0.47079

210 -> 217 0.34607

210 -> 221 0.14951

Excited State	10:	Singlet-A	3.9320 eV	315.32 nm	f=0.1235
208 -> 211		-0.11215			
209 -> 216		-0.13781			
209 -> 217		-0.10881			
210 -> 216		-0.40369			
210 -> 217		0.48593			

Molecule **6**:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State	1:	Singlet-?Sym	2.8356 eV	437.25 nm	f=0.4200
203 ->206		0.10604			
204 ->205		0.66694			
Excited State	2:	Singlet-?Sym	3.0432 eV	407.41 nm	f=0.1115
203 ->205		0.10315			
203 ->207		-0.11303			
204 ->206		0.66828			
Excited State	3:	Singlet-?Sym	3.1422 eV	394.57 nm	f=0.1674
204 ->207		0.66263			
Excited State	4:	Singlet-?Sym	3.3723 eV	367.65 nm	f=0.0707
203 ->205		0.10463			
204 ->208		0.68493			
Excited State	5:	Singlet-?Sym	3.3890 eV	365.84 nm	f=0.0851
203 ->205		0.66469			
204 ->206		-0.13058			
204 ->208		-0.10974			
Excited State	6:	Singlet-?Sym	3.5774 eV	346.57 nm	f=0.0138
203 ->206		0.66760			
204 ->207		0.11683			
Excited State	7:	Singlet-?Sym	3.6724 eV	337.61 nm	f=0.0083
202 ->205		-0.11897			
203 ->207		0.44954			
203 ->208		0.10797			
203 ->210		0.10342			
204 ->209		0.45418			
Excited State	8:	Singlet-?Sym	3.7007 eV	335.03 nm	f=0.0118
202 ->205		0.10645			
203 ->207		0.49711			
204 ->209		-0.44012			
Excited State	9:	Singlet-?Sym	3.7809 eV	327.92 nm	f=0.0178
202 ->205		0.12817			
203 ->209		0.20417			
204 ->210		0.63182			
Excited State	10:	Singlet-?Sym	3.7966 eV	326.56 nm	f=0.0092
202 ->205		0.65623			

204 ->209 0.14128
204 ->210 -0.14175

5. Emission Data for the Molecules **1–6** by TDDFT at the CIS/6-31G(d) Optimized Geometry.

Molecule **1**:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State	1:	Singlet-?Sym	3.0482 eV	406.75 nm	f=0.2358
87 -> 91		-0.10240			
90 -> 91		0.61794			
Excited State	2:	Singlet-?Sym	3.4977 eV	354.47 nm	f=0.0225
89 -> 91		0.69664			
Excited State	3:	Singlet-?Sym	3.7028 eV	334.84 nm	f=0.0146
87 -> 91		0.11032			
90 -> 92		0.69382			
Excited State	4:	Singlet-?Sym	4.0174 eV	308.62 nm	f=0.0108
88 -> 91		0.64838			
90 -> 94		0.25545			
Excited State	5:	Singlet-?Sym	4.2047 eV	294.87 nm	f=0.0574
87 -> 91		0.59845			
90 -> 95		0.31600			
90 -> 97		0.11856			
Excited State	6:	Singlet-?Sym	4.3043 eV	288.05 nm	f=0.0277
90 -> 93		0.69632			

Molecule **2**:

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	2.6567 eV	466.69 nm	f=0.2445
114 ->115		0.57557			
114 ->116		0.31184			
Excited State	2:	Singlet-A	2.9038 eV	426.97 nm	f=0.2069
114 ->115		-0.25281			
114 ->116		0.62907			
Excited State	3:	Singlet-A	3.3947 eV	365.23 nm	f=0.0382
114 ->117		0.69899			
Excited State	4:	Singlet-A	3.7755 eV	328.39 nm	f=0.0047
111 ->115		-0.13252			
112 ->115		-0.18506			
113 ->115		0.25221			
114 ->118		0.59721			
Excited State	5:	Singlet-A	3.8714 eV	320.26 nm	f=0.0530
112 ->115		0.16430			
113 ->115		0.58090			
113 ->116		0.10444			
114 ->118		-0.19424			
114 ->121		-0.23543			

Excited State 6: Singlet-A 3.9077 eV 317.28 nm f=0.1740
109 ->115 -0.11931
110 ->115 0.11841
114 ->119 0.67039

Molecule **3**:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.
Excited State 1: Singlet-?Sym 2.4790 eV 500.14 nm f=0.7153
178 ->179 0.64166
Excited State 2: Singlet-?Sym 3.1160 eV 397.90 nm f=0.0444
178 ->180 0.70084
Excited State 3: Singlet-?Sym 3.2168 eV 385.42 nm f=0.0767
177 ->179 0.67147
178 ->186 -0.12847
Excited State 4: Singlet-?Sym 3.5408 eV 350.16 nm f=0.0008
176 ->179 0.34670
178 ->181 0.56925
Excited State 5: Singlet-?Sym 3.6188 eV 342.61 nm f=0.0091
176 ->179 0.59437
178 ->181 -0.34485
Excited State 6: Singlet-?Sym 3.6311 eV 341.45 nm f=0.0232
177 ->181 -0.12485
178 ->182 0.58756
178 ->183 -0.16032
178 ->184 -0.28065

Molecule **4**:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.
Excited State 1: Singlet-?Sym 2.5796 eV 480.64 nm f=0.6589
230 -> 231 0.64373
Excited State 2: Singlet-?Sym 2.7394 eV 452.60 nm f=0.0336
230 -> 232 0.69480
Excited State 3: Singlet-?Sym 2.7419 eV 452.19 nm f=0.0095
230 -> 233 0.69435
Excited State 4: Singlet-?Sym 2.9532 eV 419.84 nm f=0.0099
230 -> 234 0.69398
Excited State 5: Singlet-?Sym 3.0815 eV 402.35 nm f=0.0566
230 -> 235 0.68214
Excited State 6: Singlet-?Sym 3.0834 eV 402.10 nm f=0.0004
230 -> 236 0.70510

Molecule **5**:

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.4261 eV 511.05 nm f=0.7594
210 -> 211 0.64340

Excited State	2:	Singlet-A	2.9604 eV	418.82 nm	f=0.0526
210 -> 212		0.70035			
Excited State	3:	Singlet-A	3.1120 eV	398.41 nm	f=0.0855
209 -> 211		0.67366			
Excited State	4:	Singlet-A	3.3719 eV	367.70 nm	f=0.0051
209 -> 214		-0.10970			
210 -> 213		0.67366			
Excited State	5:	Singlet-A	3.4318 eV	361.28 nm	f=0.0216
209 -> 213		-0.13096			
210 -> 214		0.67784			
Excited State	6:	Singlet-A	3.5474 eV	349.50 nm	f=0.0697
208 -> 211		-0.12073			
210 -> 215		0.68669			

Molecule **6**:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State	1:	Singlet-?Sym	2.5557 eV	485.13 nm	f=0.6485
204 ->205		0.64232			
Excited State	2:	Singlet-?Sym	2.9270 eV	423.59 nm	f=0.0264
204 ->206		0.69145			
Excited State	3:	Singlet-?Sym	2.9718 eV	417.20 nm	f=0.1029
204 ->207		0.68526			
Excited State	4:	Singlet-?Sym	3.1678 eV	391.39 nm	f=0.0000
204 ->208		0.70556			
Excited State	5:	Singlet-?Sym	3.2965 eV	376.10 nm	f=0.0393
202 ->205		-0.10331			
203 ->205		0.66825			
Excited State	6:	Singlet-?Sym	3.5261 eV	351.62 nm	f=0.0001
202 ->205		0.30621			
204 ->209		0.59095			
204 ->212		0.11567			