

Supporting Information

Theoretical Investigation of One- and Two-Photon Absorption Properties of Platinum Acetylide Chromophores

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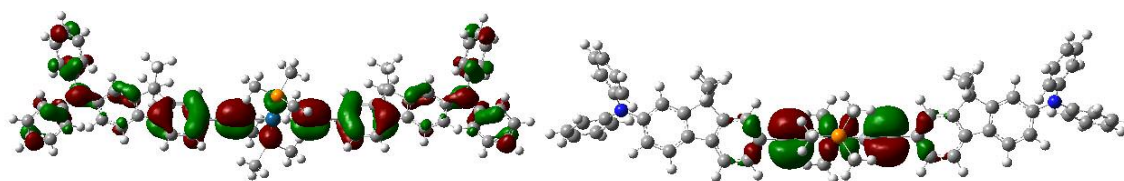
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1. Table 1. Geometric parameters of studied molecules 1-trans and 2-trans

1-trans		
Bond lengths(Å)		
Pt-C1=2.0218 (2.0238)	C1-C2=1.2297 (1.1441)	C2-C3=1.4284 (1.4871)
C3-C4=1.4142 (1.4041)	C4-C5=1.3926 (1.4031)	C5-C6=1.3979 (1.3931)
C6-C15=1.4641 (1.4751)	C7-C9=1.5302 (1.5121)	C9-C10=1.5296 (1.5291)
C10-C11=1.3869 (1.3951)	C11-C12=1.4087 (1.3941)	C12-C13=1.4069 (1.4111)
C13-C14=1.3938 (1.4111)	C14-C15=1.3974 (1.3901)	C12-N=1.4231 (1.4199)
C23-N=1.4209 (1.4421)	C24-N=1.4209 (1.4191)	
Bond angles		
Pt-C1-C2=178.98 (176.88)	C1-C2-C3=179.43 (176.58)	C3-C4-C5=120.71 (121.38)
C4-C5-C6=121.42 (118.57)	C5-C6-C15=131.41 (131.27)	C7-C9-C10=101.19 (100.96)
C9-C10-C11=128.36 (127.57)	C6-C15-C14=131.60 (132.07)	C11-C12-C13=119.45(119.57)
C13-C14-C15=119.48(119.27)	C12-C13-C14=120.91(120.57)	C10-C11-C12=119.53(119.68)
C12-N-C23=119.87 (119.17)	C12-N-C24=119.96 (121.27)	C23-N-C24=120.16 (118.77)
Dihedral angels		
P-Pt-C3-C4=84		
2-trans		
Bond lengths(Å)		
Pt-C1=2.0211 (2.0003)	C1-C2=1.2298 (1.2084)	C2-C3=1.4273 (1.4424)
C3-C4=1.4153 (1.4064)	C4-C5=1.3914 (1.3914)	C5-C6=1.3985 (1.3954)
C6-C7=1.4109 (1.4014)	C7-C9=1.5295 (1.5254)	C9-C10=1.5292 (1.5254)
C10-C11=1.3835 (1.3744)	C11-C12=1.4123 (1.4114)	C12-C13=1.4073 (1.3994)
C13-C14=1.3928 (1.3874)	C14-C15=1.3978 (1.3964)	C12-C16=1.4656 (1.4724)
C16-N=1.3004 (1.3165)	C16-S=1.7936 (1.7753)	S-C17=1.7505 (1.7343)
C17-C18=1.3965 (1.3955)	C17-C22=1.4176 (1.3964)	C18-C19=1.3935 (1.3936)
C19-C20=1.4061 (1.3936)	C20-C21=1.3897 (1.3675)	C21-C22=1.4039 (1.3835)
Bond angles		
Pt-C1-C2=179.06 (176.63)	C1-C2-C3=179.28 (174.43)	C3-C4-C5=121.37 (121.13)
C5-C6-C7=120.14 (120.43)	C6-C7-C9=110.88 (111.12)	C7-C9-C10=101.16 (101.02)
C9-C10-C11=128.60(128.43)	C9-C10-C15=110.76(110.93)	C11-C12-C13=119.30(119.63)
C13-C14-C15=119.15(118.73)	C11-C12-C16=118.66(119.03)	C13-C12-C16=122.03(121.33)
N-C16-S=114.61 (116.52)	S-C17-C22=109.17 (110.92)	S-C17-C18=129.35 (127.83)
Dihedral angels		
P-Pt-C3-C4=80		

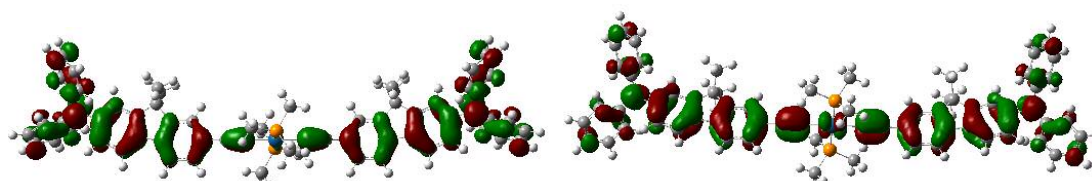
Note: the values in parentheses are the experimental observations of X-ray diffraction in reference [14]

2.
1-cis



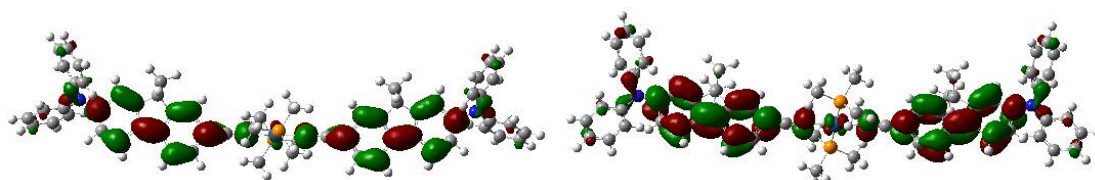
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HOMO-3



HOMO-1

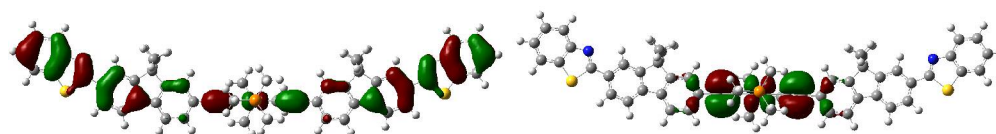
HOMO



LUMO

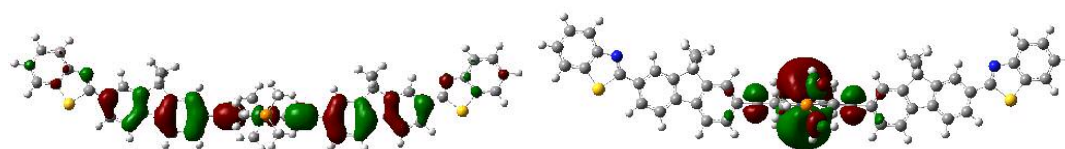
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2-cis



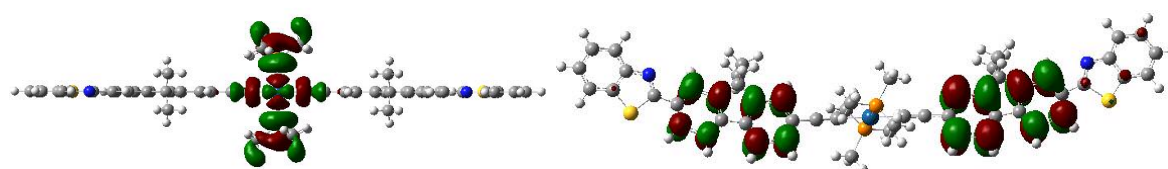
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HOMO-2



LUMO

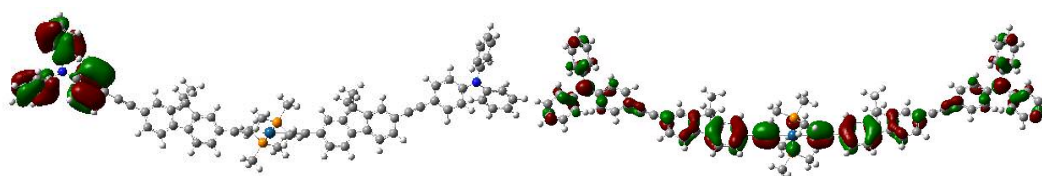
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LUMO+10

LUMO+11

3-cis



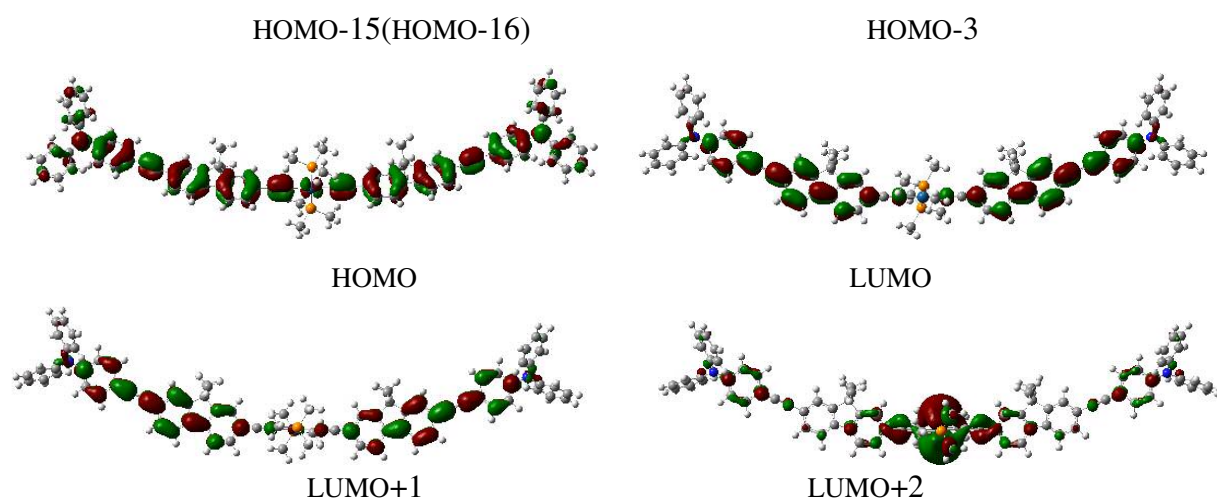
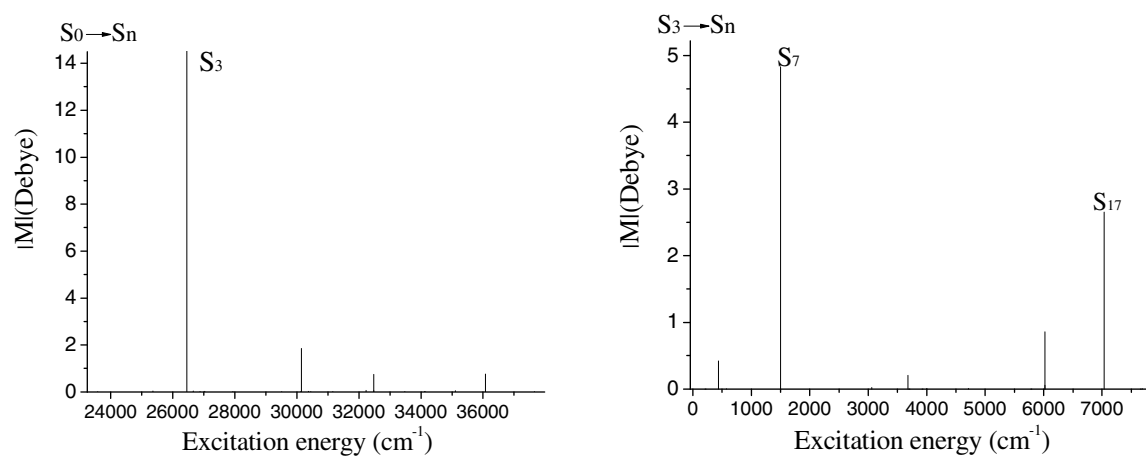
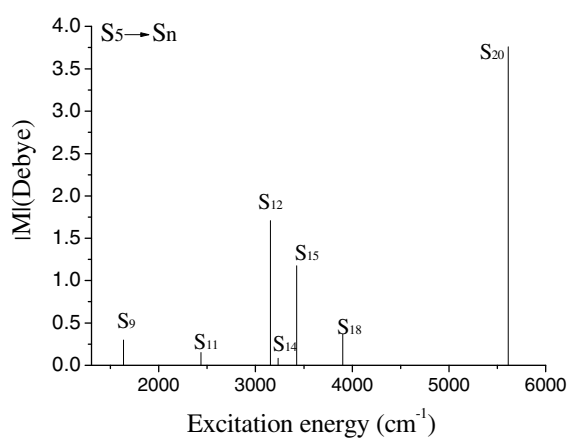
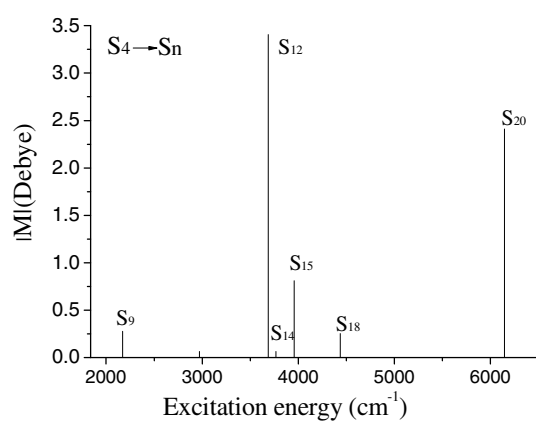
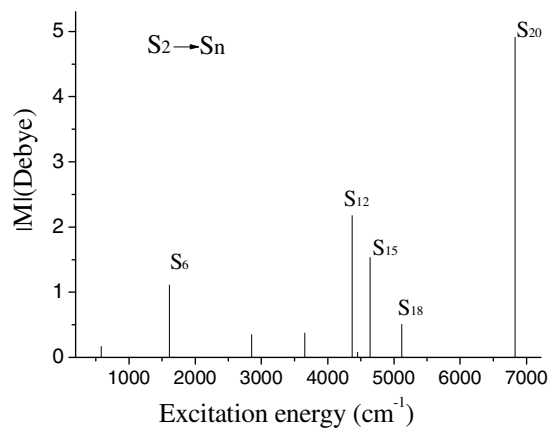
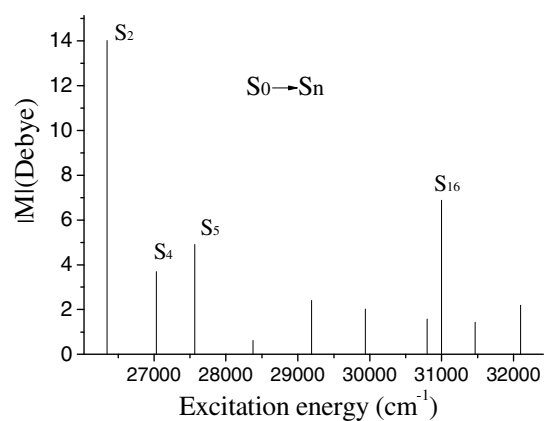


Figure 1 Contour surfaces of the frontier orbitals relevant to the maximum two-photon absorptions for 1-cis, 2-cis and 3-cis

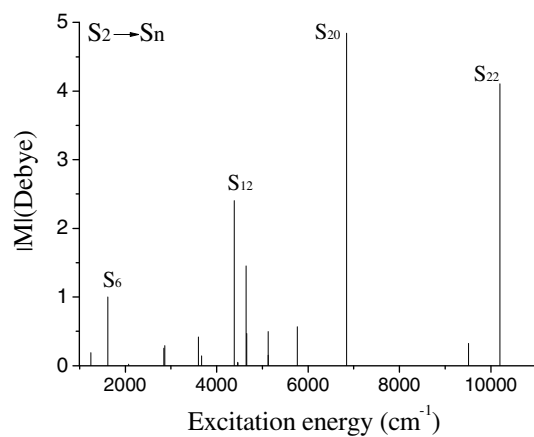
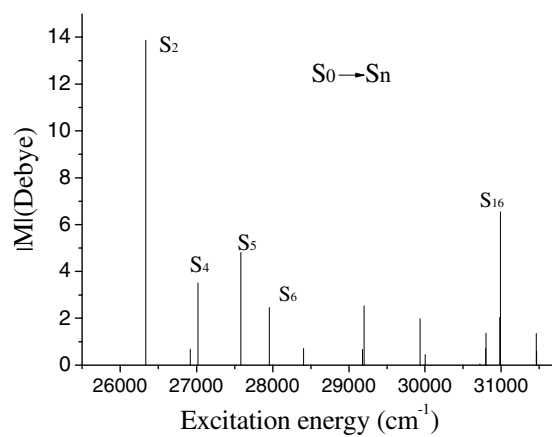
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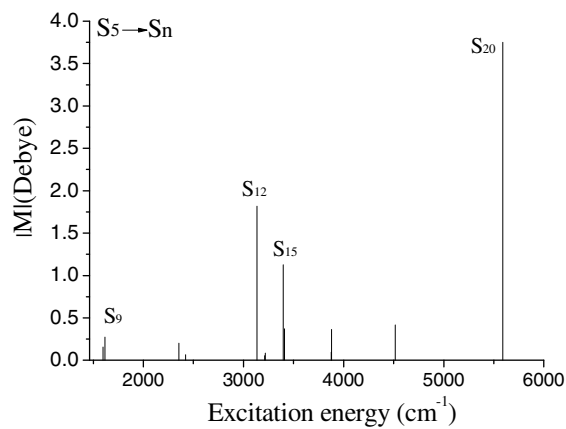
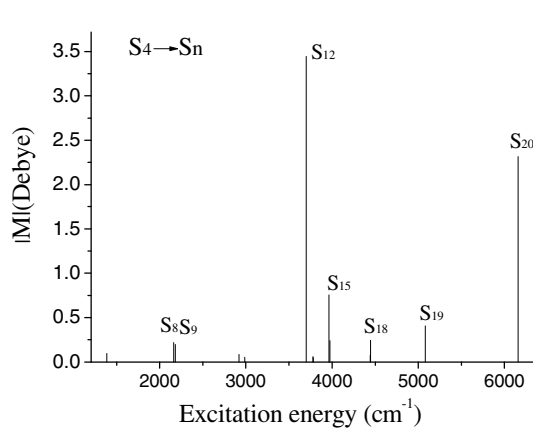


PE2

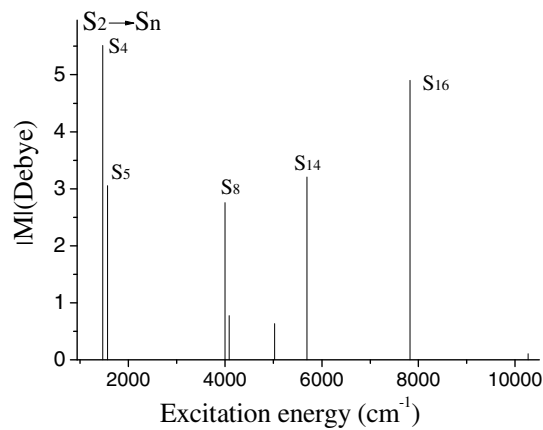
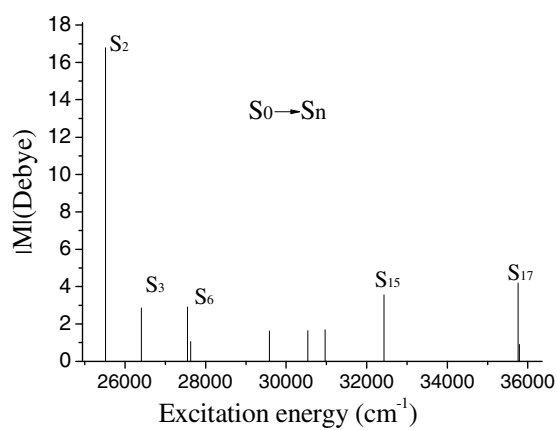


1-trans

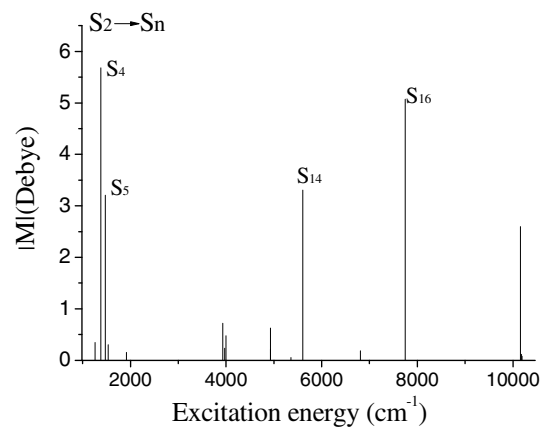
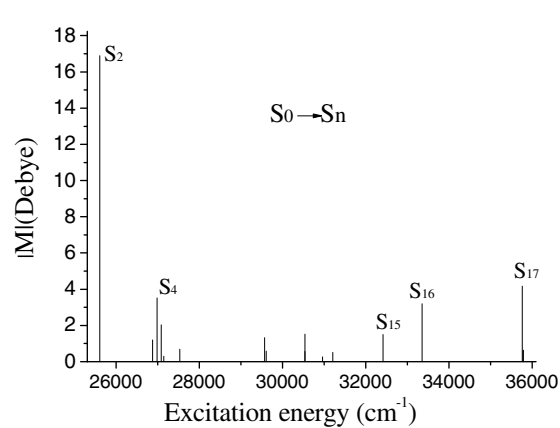




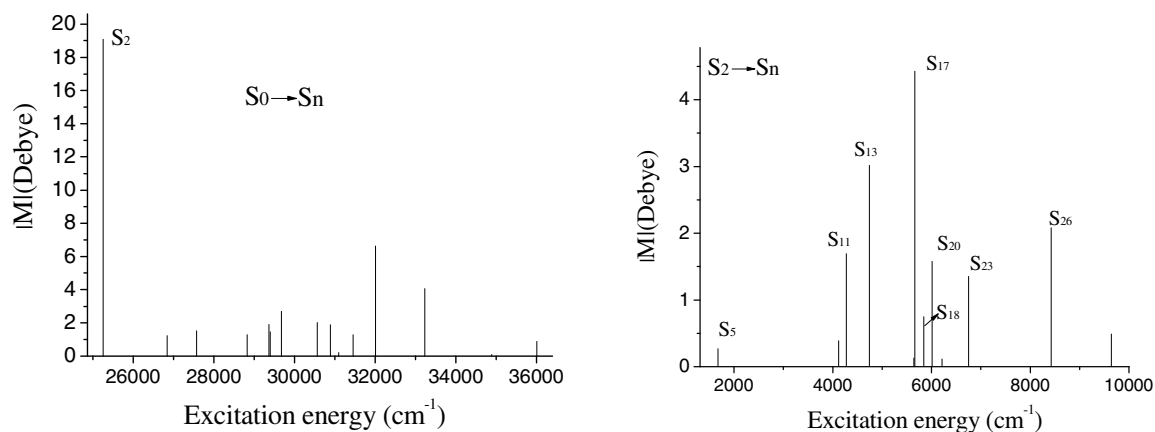
1-cis



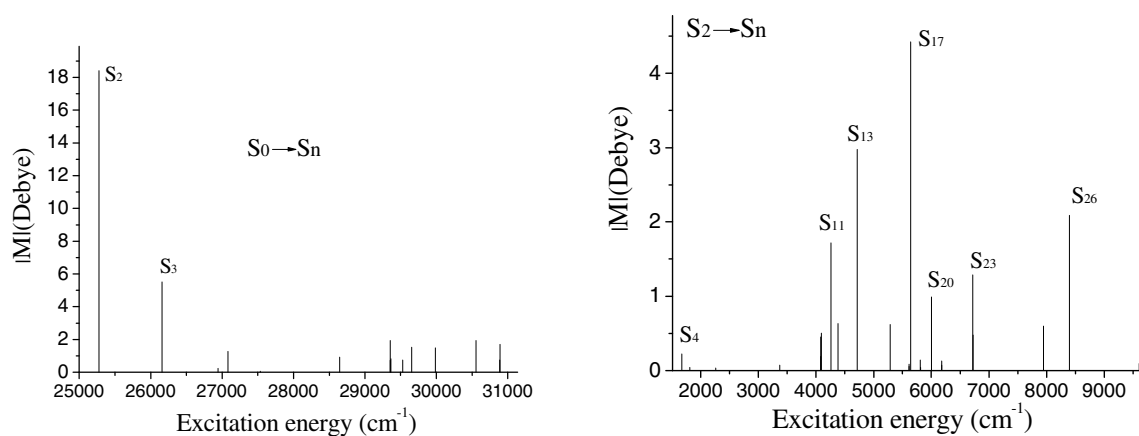
2-trans



2-cis



3-trans



3-cis

Figure 2 ZINDO predicted transition dipole moments between main electronic states

4. Cartesian coordinates of all studied molecules

PE2

Coordinates (Angstroms)		
X	Y	Z
1.444828	3.272341	-.000941
2.030034	3.000216	-.883092
1.255768	4.351546	-.000625
2.030694	2.999730	.880603
-1.051177	3.002793	-1.451563
-2.043447	2.545212	-1.479254

-1.145138	4.092881	-1.392392
-.520712	2.734809	-2.370264
-1.051587	3.003769	1.449390
-1.146079	4.093757	1.389083
-2.043636	2.545735	1.477484
-.521010	2.737068	2.368398
1.049983	-3.002840	1.451293
1.144390	-4.092870	1.391758
2.042072	-2.544929	1.480145
.518508	-2.735445	2.369583
1.052777	-3.003278	-1.449675
2.044881	-2.545313	-1.476811
1.147125	-4.093288	-1.389575
.523004	-2.736280	-2.369063
-1.444817	-3.272140	-.001517
-1.255749	-4.351343	-.000805
-2.031347	-2.999349	.879540
-2.029357	-3.000206	-.884155
4.676357	.024748	.000665
5.406509	.025444	-1.208912
5.406337	.026463	1.210339
6.794099	.026416	-1.209975
4.863209	.025598	-2.149252
6.793942	.027455	1.211590
4.862913	.027420	2.150620
7.518624	.026911	.000861
7.337755	.026721	-2.150052
7.337458	.028574	2.151734
-4.676356	-.024676	-.000609
-5.406334	-.025017	1.209074
-5.406512	-.026825	-1.210178
-6.793924	-.026079	1.210337
-4.862899	-.024838	2.149335
-6.794116	-.027883	-1.211228
-4.863222	-.028050	-2.150536
-7.518624	-.026999	-.000395
-7.337445	-.026115	2.150491
-7.337769	-.029331	-2.151293
8.940981	.026187	.000857
10.158339	.024590	.000413
-8.940981	-.026357	-.000188
-10.158340	-.024830	.000434
11.582474	.021215	.000317
12.301499	.019390	1.213699

12.301381	.019243	-1.213118
13.693792	.015552	1.208715
11.753963	.020887	2.151245
13.693680	.015392	-1.208269
11.753767	.020629	-2.150605
14.395753	.013523	.000188
14.233958	.014101	2.151768
14.233750	.013815	-2.151394
15.482316	.010537	.000126
-11.582474	-.021536	.000730
-12.301671	-.020170	-1.212551
-12.301211	-.019187	1.214266
-13.693963	-.016405	-1.207374
-11.754265	-.021958	-2.150173
-13.693511	-.015420	1.209610
-11.753466	-.020218	2.151676
-14.395754	-.014003	.001251
-14.234261	-.015309	-2.150352
-14.233450	-.013550	2.152810
-15.482317	-.011080	.001465
.000000	.000105	-.000335
2.020460	.027717	.000320
3.250187	.020756	.000452
-2.020461	-.027516	-.000767
-3.250187	-.020607	-.000613
-.136950	2.333454	-.000749
.136953	-2.333240	-.000158

1-trans

1-cis

Coordinates (Angstroms)			Coordinates (Angstroms)		
X	Y	Z	X	Y	Z
0.000000	0.000000	0.000000	-0.000462	-0.845584	0.701602
-0.060213	2.231980	0.684812	-0.138315	-2.491927	-0.950216
0.060213	-2.231980	-0.684812	0.137344	0.797889	2.355827
1.993784	-0.137258	0.306081	2.021432	-0.862382	0.682861
3.205257	-0.242286	0.488969	3.251118	-0.860673	0.689076
-1.993784	0.137258	-0.306081	-2.022410	-0.832478	0.720489
-3.205257	0.242286	-0.488969	-3.252038	-0.845299	0.714822
4.613045	-0.350405	0.704871	4.679420	-0.870422	0.687029
5.119518	-0.883168	1.913031	5.395461	-1.836812	1.431005
5.531800	0.074632	-0.284712	5.409249	0.086055	-0.059012

6.489014	-0.994346	2.139790	6.787801	-1.860824	1.439931
4.414365	-1.207231	2.672852	4.834955	-2.570549	2.002859
6.894646	-0.034094	-0.058030	6.794854	0.062814	-0.048985
5.145381	0.484332	-1.214339	4.861667	0.828918	-0.633297
7.382851	-0.568849	1.152878	7.493386	-0.908891	0.698330
6.850883	-1.408218	3.078016	7.312873	-2.615991	2.020050
8.048776	0.364253	-0.980343	7.768887	0.993958	-0.773956
8.846265	-0.560913	1.110115	8.929985	-0.692096	0.518349
9.257891	-0.017611	-0.124816	9.115161	0.414137	-0.336844
9.803654	-0.979767	2.037895	10.041300	-1.368781	1.028055
10.604193	0.099462	-0.436452	10.388726	0.835730	-0.688504
11.157459	-0.845588	1.734664	11.322470	-0.934979	0.691700
9.506431	-1.394029	2.998088	9.919698	-2.219016	1.694557
11.572168	-0.312664	0.500382	11.511541	0.161957	-0.169003
10.927705	0.504093	-1.391127	10.537101	1.677848	-1.358397
11.908657	-1.153729	2.454844	12.191530	-1.444707	1.095193
-4.613045	0.350405	-0.704871	-4.680364	-0.852236	0.715042
-5.119518	0.883168	-1.913031	-5.397576	-1.813021	1.465101
-5.531800	-0.074632	0.284712	-5.409034	0.100837	-0.036505
-6.489014	0.994346	-2.139790	-6.789914	-1.836000	1.473388
-4.414365	1.207231	-2.672852	-4.838140	-2.542471	2.043461
-6.894646	0.034094	0.058030	-6.794689	0.078676	-0.027053
-5.145381	-0.484332	1.214339	-4.860392	0.841043	-0.613204
-7.382851	0.568849	-1.152878	-7.494342	-0.888463	0.725113
-6.850883	1.408218	-3.078016	-7.315847	-2.586776	2.058405
-8.048776	-0.364253	0.980343	-7.767723	1.006600	-0.757519
-8.846265	0.560913	-1.110115	-8.930662	-0.672494	0.542159
-9.257891	0.017611	0.124816	-9.114644	0.429070	-0.319295
-9.803654	0.979767	-2.037895	-10.042617	-1.346603	1.053858
-10.604193	-0.099462	0.436452	-10.387754	0.848574	-0.675131
-11.157459	0.845588	-1.734664	-11.323326	-0.914915	0.713102
-9.506431	1.394029	-2.998088	-9.921879	-2.193188	1.725143
-11.572168	0.312664	-0.500382	-11.511229	0.177295	-0.153827
-10.927705	-0.504093	1.391127	-10.535296	1.687081	-1.349718
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13.850445	-1.246924	0.521711	13.823498	-0.371708	-0.828426
15.118948	-0.974032	1.060952	15.139634	-0.216380	-0.361328
13.477315	-2.584677	0.308404	13.509856	-1.494851	-1.612393
15.992476	-2.015852	1.367998	16.116162	-1.157962	-0.681386
15.412761	0.055766	1.237260	15.389649	0.643842	0.251361
14.351100	-3.620078	0.635470	14.489426	-2.439854	-1.912061
12.501644	-2.804148	-0.113228	12.497188	-1.620265	-1.981968

15.615246	-3.344973	1.162406	15.799065	-2.277595	-1.454042
16.969455	-1.784679	1.784743	17.128594	-1.020566	-0.310320
14.044430	-4.648573	0.462998	14.227605	-3.301917	-2.520259
16.296116	-4.154484	1.409574	16.561174	-3.013053	-1.695464
13.446701	0.997081	-0.410132	13.135863	1.974865	-0.533466
14.415450	0.931823	-1.425953	13.937641	2.512472	-1.554535
12.966280	2.255679	-0.010665	12.642490	2.832766	0.464040
14.896085	2.099249	-2.016489	14.242698	3.872449	-1.568058
14.786553	-0.036346	-1.746637	14.317655	1.859160	-2.333433
13.440394	3.416213	-0.619699	12.938309	4.194383	0.431584
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14.410696	3.348416	-1.622339	13.742906	4.724069	-0.580007
15.645349	2.028382	-2.800837	14.864235	4.269513	-2.366586
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14.782863	4.255551	-2.089874	13.977130	5.784635	-0.598054
-13.850445	1.246924	-0.521711	-13.821477	-0.361014	-0.815031
-15.118948	0.974032	-1.060952	-15.138389	-0.205060	-0.350342
-13.477315	2.584677	-0.308404	-13.505649	-1.487138	-1.593825
-15.992476	2.015852	-1.367998	-16.113518	-1.149012	-0.667697
-15.412761	-0.055766	-1.237260	-15.390085	0.657488	0.258379
-14.351100	3.620078	-0.635470	-14.483838	-2.434417	-1.890802
-12.501644	2.804148	0.113228	-12.492356	-1.613037	-1.961521
-15.615246	3.344973	-1.162406	-15.794249	-2.271567	-1.435205
-16.969455	1.784679	-1.784743	-17.126578	-1.011111	-0.298540
-14.044430	4.648573	-0.462998	-14.220330	-3.298773	-2.495007
-16.296116	4.154484	-1.409574	-16.555285	-3.008824	-1.674520
-13.446701	-0.997081	0.410132	-13.136129	1.987442	-0.529495
-14.415450	-0.931823	1.425953	-13.937239	2.519797	-1.553845
-12.966280	-2.255679	0.010665	-12.644419	2.850249	0.464602
-14.896085	-2.099249	2.016489	-14.243297	3.879469	-1.573854
-14.786553	0.036346	1.746637	-14.315954	1.862657	-2.330153
-13.440394	-3.416213	0.619699	-12.941215	4.211480	0.425643
-12.222468	-2.315693	-0.777332	-12.031038	2.446745	1.263877
-14.410696	-3.348416	1.622339	-13.745158	4.735953	-0.589173
-15.645349	-2.028382	2.800837	-14.864311	4.272430	-2.374817
-13.057206	-4.380653	0.296212	-12.551792	4.862639	1.204074
-14.782863	-4.255551	2.089874	-13.980156	5.796248	-0.612290
-0.745885	3.366007	-0.593213	-1.051117	-3.992464	-0.398512
-0.817664	4.392183	-0.215489	-1.159498	-4.714016	-1.216066
-0.100338	3.349950	-1.476604	-0.510870	-4.461821	0.429224
-1.736075	3.003835	-0.881458	-2.036448	-3.684941	-0.039015
1.535335	3.012691	1.162052	1.443425	-3.151867	-1.617215
2.227184	2.970353	0.316895	2.030321	-3.580429	-0.800793
1.384617	4.054702	1.465320	1.258054	-3.914928	-2.381331

1.984679	2.448574	1.983298	2.025964	-2.332402	-2.045991
-1.146138	2.504094	2.146519	-1.057517	-1.938639	-2.446257
-1.203551	3.566874	2.407360	-1.166489	-2.754739	-3.169361
-2.144065	2.124207	1.912292	-2.042612	-1.581975	-2.134582
-0.753351	1.942755	2.999710	-0.520621	-1.108684	-2.915544
1.146138	-2.504094	-2.146519	1.054171	0.240500	3.851701
2.144065	-2.124207	-1.912292	2.039345	-0.116517	3.540645
1.203551	-3.566874	-2.407360	1.162919	1.054897	4.576756
0.753351	-1.942755	-2.999710	0.515925	-0.590016	4.318423
0.745885	-3.366007	0.593213	1.052552	2.298725	1.808552
0.100338	-3.349950	1.476604	0.513715	2.770842	0.981462
0.817664	-4.392183	0.215489	1.161371	3.018214	2.627878
1.736075	-3.003835	0.881458	2.037742	1.990549	1.449184
-1.535335	-3.012691	-1.162052	-1.444564	1.458151	3.022171
-1.384617	-4.054702	-1.465320	-1.259587	2.219060	3.788526
-2.227184	-2.970353	-0.316895	-2.029691	1.889462	2.205897
-1.984679	-2.448574	-1.983298	-2.028666	0.638210	3.447903
-8.031989	-1.879791	1.281092	-7.608167	2.470533	-0.289322
-8.052081	-2.464004	0.355363	-7.727797	2.551534	0.795925
-7.128202	-2.153331	1.838000	-6.615544	2.853844	-0.553297
-8.900779	-2.165793	1.885555	-8.356876	3.114378	-0.765720
-8.017762	0.436705	2.301041	-7.587751	0.920893	-2.289543
-7.113125	0.202790	2.874471	-6.592936	1.276485	-2.582085
-8.029904	1.514177	2.107298	-7.699332	-0.109777	-2.641473
-8.885267	0.190797	2.924852	-8.331719	1.541113	-2.803336
8.031989	1.879791	-1.281092	7.609075	2.455779	-0.299327
7.128202	2.153331	-1.838000	6.616888	2.840527	-0.562905
8.052081	2.464004	-0.355363	7.727395	2.531901	0.786435
8.900779	2.165793	-1.885555	8.358459	3.101686	-0.771844
8.017762	-0.436705	-2.301041	7.590674	0.915246	-2.306573
8.029904	-1.514177	-2.107298	7.702163	-0.113878	-2.662964
7.113125	-0.202790	-2.874471	6.596344	1.272536	-2.598660
8.885267	-0.190797	-2.924852	8.335564	1.537445	-2.816622

2-trans

Coordinates (Angstroms)		
X	Y	Z
0.000000	0.000000	0.000000
0.021045	-0.034842	2.020713
0.031396	-0.076132	3.249733

2-cis

Coordinates (Angstroms)		
X	Y	Z
-0.003323	-0.996734	0.040193
0.115480	-0.828755	2.367744
-0.121195	-1.165866	-2.287499

0.035349	-0.108015	4.676679	-1.113757	0.174023	-3.067398
-1.172585	0.012290	5.404643	-1.205157	0.021287	-4.148623
1.246784	-0.258871	5.392744	-2.105007	0.184496	-2.606981
-1.152448	-0.017625	6.790139	-0.633948	1.139088	-2.877982
-2.103753	0.128150	4.856362	1.466147	-1.139858	-3.216563
1.267091	-0.289797	6.783696	2.106209	-1.954025	-2.867430
2.172702	-0.348751	4.832510	1.289177	-1.240757	-4.293090
-2.327146	0.098687	7.762664	1.988279	-0.200699	-3.015766
0.064697	-0.168713	7.487556	-0.943786	-2.713415	-2.851095
2.211560	-0.405961	7.309767	-1.932902	-2.769935	-2.389080
-1.608679	-0.006062	9.108459	-1.040926	-2.736127	-3.942319
-3.335276	-1.056918	7.572708	-0.357541	-3.576762	-2.522193
-3.048326	1.457297	7.614494	1.071469	-2.196001	3.145977
-0.216734	-0.162700	8.922353	2.061607	-2.233832	2.684465
-2.149603	0.035493	10.381157	1.168443	-2.046628	4.227209
-4.134416	-0.998811	8.320577	0.564546	-3.147089	2.956564
-3.796891	-1.006763	6.579679	-1.472840	-0.813169	3.295405
-2.843327	-2.029829	7.672508	-1.293507	-0.729283	4.373021
-3.500363	1.547199	6.619840	-2.084947	0.026153	2.955518
-3.847383	1.554987	8.358440	-2.026358	-1.731627	3.083765
-2.351090	2.290433	7.749727	0.977354	0.695654	2.935473
0.630035	-0.279065	10.028373	1.071802	0.714144	4.026990
-1.301434	-0.080122	11.504458	1.968777	0.726892	2.476178
-3.215051	0.155265	10.549837	0.415148	1.574740	2.606255
0.083276	-0.237078	11.308639	2.017831	-0.990006	0.026739
1.702392	-0.400155	9.900781	3.247420	-1.005977	0.037887
-1.896727	-0.031648	12.842820	4.674307	-1.041214	0.035886
0.744567	-0.327019	12.166390	5.431113	0.154341	0.003780
-3.168880	0.117165	13.067692	5.360987	-2.278716	0.064940
-0.889327	-0.177910	14.319590	6.816160	0.097291	0.000678
-3.458291	0.129609	14.417527	4.905648	1.105441	-0.020114
-2.343649	-0.018725	15.280740	6.750979	-2.336118	0.062362
-4.741893	0.276159	14.966890	4.777909	-3.194510	0.088885
-2.492143	-0.022735	16.669303	7.817914	1.252518	-0.033511
-4.889416	0.272505	16.348698	7.483656	-1.145421	0.030058
-5.592694	0.389627	14.302446	7.254072	-3.299797	0.084876
-3.774980	0.124380	17.193272	9.145749	0.494059	-0.019086
-1.634525	-0.136704	17.325424	7.676136	2.160532	1.208833
-5.878357	0.385539	16.783945	7.665031	2.093074	-1.321255
-3.913379	0.124268	18.270831	8.925010	-0.901068	0.018078
-0.021045	0.034842	-2.020713	10.431701	1.004131	-0.037955
-0.031396	0.076132	-3.249733	8.443414	2.943204	1.204831
-0.035349	0.108015	-4.676679	6.694769	2.648933	1.219756
1.172585	-0.012290	-5.404643	7.781290	1.583469	2.133241

-1.246784	0.258871	-5.392744	6.682783	2.578913	-1.350475
1.152448	0.017625	-6.790139	8.430816	2.876005	-1.365556
2.103753	-0.128150	-4.856362	7.763600	1.467498	-2.214268
-1.267091	0.289797	-6.783696	10.009445	-1.782773	0.036403
-2.172702	0.348751	-4.832510	11.533431	0.120684	-0.019954
2.327146	-0.098687	-7.762664	10.626934	2.071355	-0.066538
-0.064697	0.168713	-7.487556	11.303006	-1.267108	0.017275
-2.211560	0.405961	-7.309767	9.854941	-2.858030	0.064962
1.608679	0.006062	-9.108459	12.886479	0.683452	-0.040992
3.048326	-1.457297	-7.614494	12.144116	-1.955210	0.031538
3.335276	1.056918	-7.572708	13.143567	1.957760	-0.073926
0.216734	0.162700	-8.922353	14.337290	-0.371029	-0.022859
2.149603	-0.035493	-10.381157	14.500485	2.212157	-0.087764
3.847383	-1.554987	-8.358440	15.335070	1.066518	-0.064105
3.500363	-1.547199	-6.619840	15.082555	3.489241	-0.122922
2.351090	-2.290433	-7.749727	16.727037	1.177843	-0.075091
3.796891	1.006763	-6.579679	16.467783	3.599823	-0.133909
4.134416	0.998811	-8.320577	14.440073	4.363956	-0.140938
2.843327	2.029829	-7.672508	17.283679	2.454864	-0.110251
-0.630035	0.279065	-10.028373	17.361034	0.296525	-0.056945
1.301434	0.080122	-11.504458	16.928194	4.583436	-0.161193
3.215051	-0.155265	-10.549837	18.364487	2.564675	-0.119414
-0.083276	0.237078	-11.308639	-2.024187	-1.024199	0.054518
-1.702392	0.400155	-9.900781	-3.253588	-1.051056	0.044089
1.896727	0.031648	-12.842820	-4.680538	-1.082360	0.045949
-0.744567	0.327019	-12.166390	-5.431018	0.116942	0.002779
3.168880	-0.117165	-13.067692	-5.373805	-2.315513	0.091284
0.889327	0.177910	-14.319590	-6.816214	0.067673	0.004675
3.458291	-0.129609	-14.417527	-4.900279	1.064793	-0.031302
2.343649	0.018725	-15.280740	-6.764252	-2.365105	0.093433
4.741893	-0.276159	-14.966890	-4.795837	-3.234201	0.126106
2.492143	0.022735	-16.669303	-7.811130	1.228377	-0.038259
4.889416	-0.272505	-16.348698	-7.490614	-1.170850	0.049783
5.592694	-0.389627	-14.302446	-7.272568	-3.325642	0.129183
3.774980	-0.124380	-17.193272	-9.143211	0.477952	-0.011150
1.634525	0.136704	-17.325424	-7.657716	2.054248	-1.335395
5.878357	-0.385539	-16.783945	-7.659548	2.148692	1.193830
3.913379	-0.124268	-18.270831	-8.930654	-0.918045	0.040125
-0.123183	3.221949	1.545794	-10.426032	0.995702	-0.030507
-0.205337	4.303802	1.393410	-8.418553	2.841653	-1.385377
-0.950976	2.870866	2.167110	-6.672500	2.533467	-1.373251
0.805700	2.993729	2.074933	-7.763582	1.419879	-2.221360
-1.675379	2.931277	-0.888916	-6.675210	2.631175	1.196179
-1.685489	4.024593	-0.961641	-8.422131	2.935886	1.184047

-1.725891	2.491933	-1.888654	-7.764878	1.582180	2.124707
-2.548547	2.598486	-0.319642	-10.020492	-1.792721	0.071907
1.216415	3.117992	-1.023542	-11.533097	0.119394	0.001195
1.233496	2.679094	-2.024509	-10.614821	2.063758	-0.069456
1.076686	4.202617	-1.093046	-11.310997	-1.269308	0.052235
2.173672	2.907412	-0.536965	-9.872540	-2.868555	0.111393
-1.216415	-3.117992	1.023542	-12.882550	0.690738	-0.020002
-1.076686	-4.202617	1.093046	-12.156231	-1.952041	0.077095
-1.233496	-2.679094	2.024509	-13.131208	1.966349	-0.065379
-2.173672	-2.907412	0.536965	-14.340340	-0.353566	0.016212
1.675379	-2.931277	0.888916	-14.486386	2.229840	-0.075597
1.685489	-4.024593	0.961641	-15.328604	1.090255	-0.035791
2.548547	-2.598486	0.319642	-15.059875	3.510457	-0.121655
1.725891	-2.491933	1.888654	-16.719821	1.211065	-0.041414
0.123183	-3.221949	-1.545794	-16.444340	3.630466	-0.127316
0.950976	-2.870866	-2.167110	-14.411509	4.380480	-0.151984
0.205337	-4.303802	-1.393410	-17.267892	2.491446	-0.087599
-0.805700	-2.993729	-2.074933	-17.359754	0.334394	-0.010837
-0.143093	2.331348	-0.063403	-16.898138	4.616884	-0.162915
0.143093	-2.331348	0.063403	-18.347957	2.608574	-0.092818

2-para

Coordinates (Angstroms)		
X	Y	Z

.000004	.000263	-.001300
.527328	-2.268826	.163945
-.527288	2.269363	-.166573
-1.465135	2.890405	1.290928
-1.760544	3.937181	1.157386
-2.352594	2.266676	1.426042
-.842400	2.802103	2.186353
.868402	3.456598	-.330546
1.447815	3.214364	-1.225345
.498439	4.485742	-.397105
1.531190	3.356653	.532720
-1.611150	2.664677	-1.601179
-2.495818	2.024735	-1.554219
-1.909051	3.719240	-1.595755
-1.076246	2.445559	-2.530326
1.465637	-2.889702	-1.293328
2.353105	-2.265921	-1.428125

1.761053	-3.936482	-1.159793
.843165	-2.801353	-2.188934
-.868319	-3.456164	.327468
-.498297	-4.485276	.394171
-1.448085	-3.213959	1.222041
-1.530804	-3.356308	-.536045
1.610823	-2.664134	1.598843
1.908872	-3.718654	1.593419
2.495412	-2.024055	1.552183
1.075616	-2.445163	2.527850
1.988138	.364574	-.019059
3.202501	.561868	-.017349
4.607051	.811300	-.006002
5.535469	-.255094	-.075954
5.104142	2.133871	.082081
6.896340	.005304	-.054081
5.159930	-1.272663	-.145290
6.469832	2.397135	.103883
4.393194	2.952757	.135118
8.058184	-.987777	-.114156
7.371943	1.330488	.036911
6.823892	3.422795	.173891
9.258636	-.043417	-.040211
8.051743	-1.784484	-1.438079
8.032492	-1.959097	1.087270
8.833521	1.301388	.045241
10.606016	-.357675	-.048234
8.925895	-2.443113	-1.497029
7.152895	-2.408149	-1.508514
8.070002	-1.113070	-2.302534
7.132325	-2.584266	1.058919
8.904643	-2.622753	1.067760
8.039166	-1.412906	2.035978
9.775298	2.331454	.121620
11.564551	.676567	.029698
10.957448	-1.382574	-.112791
11.130956	2.012777	.113429
9.463020	3.370187	.187738
12.986282	.320731	.021458
11.860624	2.815854	.174134
13.430177	-.899752	-.045259
14.263800	1.576826	.104437
14.809782	-.950179	-.035984
15.464603	.304697	.042196

15.575303	-2.125446	-.096424
16.857713	.400375	.060682
16.961546	-2.030041	-.077948
15.070087	-3.084295	-.156307
17.598045	-.778610	-.000117
17.353579	1.364488	.120876
17.563153	-2.933444	-.124224
18.683164	-.727350	.012987
-1.988121	-.364076	.016426
-3.202476	-.561414	.014578
-4.607009	-.810912	.002925
-5.535500	.255136	.076997
-5.104001	-2.133219	-.089645
-6.896358	-.005327	.054679
-5.160036	1.272490	.149810
-6.469664	-2.396545	-.111882
-4.392981	-2.951833	-.145857
-8.058278	.987409	.118595
-7.371851	-1.330221	-.040825
-6.823662	-3.421981	-.185396
-9.258668	.043201	.041711
-8.033016	1.962910	-1.079452
-8.051536	1.779495	1.445286
-8.833433	-1.301259	-.048572
-10.606069	.357295	.051272
-8.905162	2.626497	-1.057361
-7.132842	2.587977	-1.049266
-8.040025	1.420020	-2.030056
-7.152724	2.402998	1.517660
-8.925737	2.437826	1.506784
-8.069486	1.105073	2.307401
-9.775132	-2.331149	-.128226
-11.564530	-.676776	-.029944
-10.957598	1.381922	.119530
-11.130815	-2.012625	-.118472
-9.462798	-3.369621	-.198066
-12.986299	-.321113	-.019960
-11.860421	-2.815565	-.181779
-13.430297	.899106	.050647
-14.263700	-1.577114	-.105915
-14.809923	.949398	.042218
-15.464618	-.305333	-.039393
-15.575560	2.124379	.106503
-16.857726	-.401117	-.057509

-16.961800	2.028860	.088390
-15.070435	3.083113	.168991
-17.598179	.777591	.007141
-17.353519	-1.365103	-.120325
-17.563491	2.932053	.137629
-18.683296	.726208	-.005600

3-trans

3-cis

Coordinates (Angstroms)			Coordinates (Angstroms)		
X	Y	Z	X	Y	Z
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-0.001166	-1.777449	-1.515737	-0.122415	-3.236061	-1.813867
0.001166	1.777449	1.515737	0.119598	-1.441067	2.493345
1.159093	1.523866	2.924551	1.046967	-2.511982	3.668997
1.180118	2.399358	3.583292	1.139652	-2.034681	4.651028
0.844730	0.647017	3.498725	0.525932	-3.467842	3.779285
2.158639	1.335571	2.524000	2.039296	-2.704720	3.253202
0.555019	3.365446	0.766722	1.015253	0.166270	2.559591
-0.144226	3.658211	-0.022410	0.473075	0.909431	1.967098
0.607940	4.161940	1.517478	1.112094	0.525236	3.590410
1.539420	3.211218	0.317324	2.006378	0.028514	2.119627
-1.595659	2.199092	2.325181	-1.469425	-1.104461	3.356152
-1.969012	1.326697	2.867538	-2.041987	-2.032066	3.436051
-1.471896	3.040735	3.015668	-1.292088	-0.691533	4.355370
-2.335206	2.453266	1.561587	-2.062459	-0.402086	2.764964
-1.159093	-1.523866	-2.924551	-1.041136	-2.165029	-2.996312
-0.844730	-0.647017	-3.498725	-0.513720	-1.213122	-3.110523
-1.180118	-2.399358	-3.583292	-1.135727	-2.646382	-3.976184
-2.158639	-1.335571	-2.524000	-2.032787	-1.963718	-2.582829
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-0.607940	-4.161940	-1.517478	-1.121919	-5.201908	-2.905243
0.144226	-3.658211	0.022410	-0.490142	-5.582170	-1.278204
-1.539420	-3.211218	-0.317324	-2.018234	-4.694248	-1.439470
1.595659	-2.199092	-2.325181	1.467740	-3.584001	-2.670047
1.471896	-3.040735	-3.015668	1.292413	-3.997930	-3.669205
1.969012	-1.326697	-2.867538	2.046214	-2.659969	-2.748988
2.335206	-2.453266	-1.561587	2.053928	-4.288940	-2.074960
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-4.268351	-2.491582	1.925631	-4.892507	-4.346850	0.947564
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-7.309720	-1.307032	0.990665	-7.491821	-2.227964	0.415258
-6.681282	-2.938892	2.270366	-7.369904	-4.312142	0.995835
-8.084426	0.500488	-0.422567	-7.702307	0.097300	-0.227922
-8.772189	-1.328602	1.008381	-8.919088	-1.910021	0.369094
-9.248000	-0.280286	0.190614	-9.066672	-0.555520	-0.001957
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5.011498	1.870427	-1.434384	5.422999	-3.419914	0.713471
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4.268351	2.491582	-1.925631	4.886521	-4.330461	0.963451
6.884662	0.247608	-0.161510	6.759405	-1.062331	0.066694
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22.061493	0.065626	-1.092104	21.510278	2.542177	0.653679
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19.326518	1.945052	1.639568	19.044390	1.013577	-2.518074
22.322194	3.079620	0.476635	22.326398	0.382283	-1.852516
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