Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

The Mechanism of Different Sensitivity of Meso-Substituted and Unsubstituted Cyanine Dyes in Rotation-Restricted Environments for Biomedical Imaging Applications

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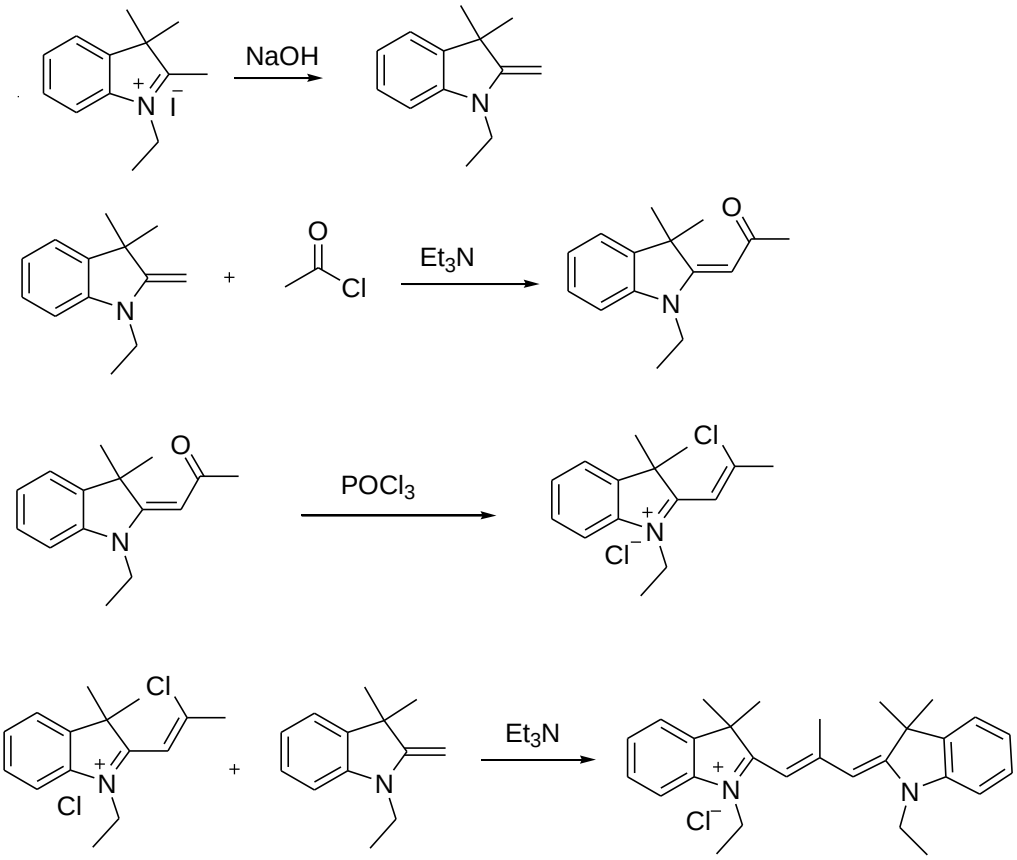
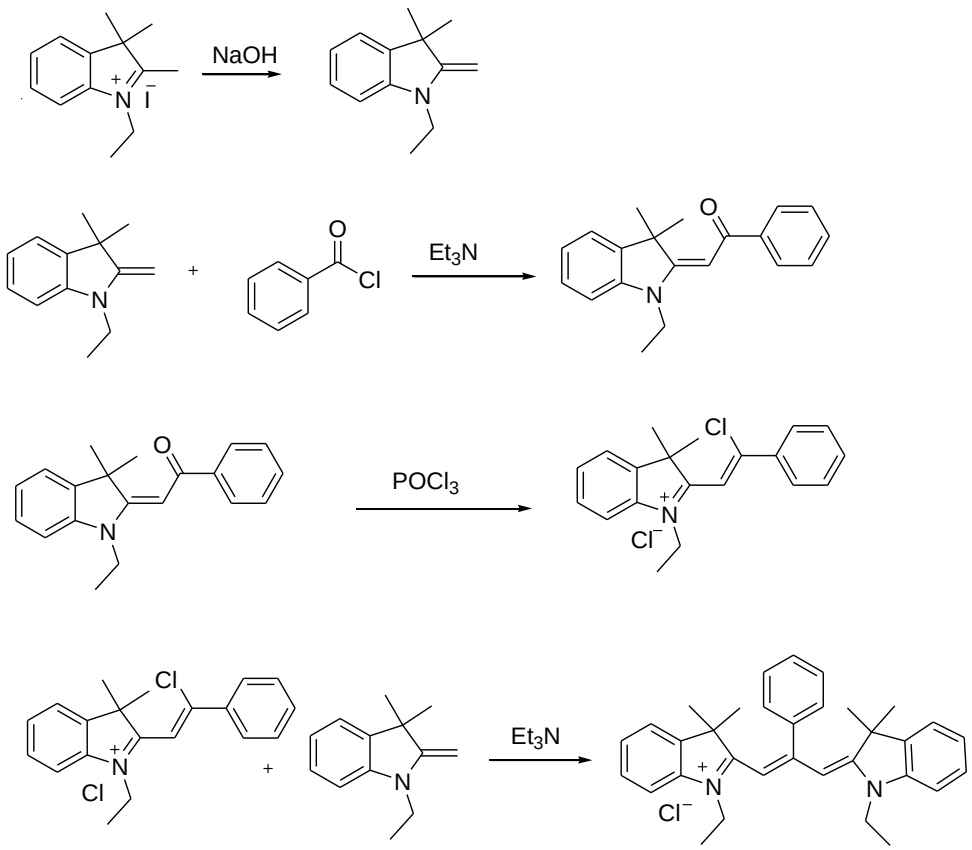
1. Dye synthesis

The synthetic routes for Cy3-CH_3 and Cy3-Ph are outlined in Scheme S1





Scheme S1. Synthetic routes of Cy3-CH_3 and **Cy3-Ph.**

2. Tests of functionals

It is worth recalling that a test with a large number of functionals was performed for photochemical properties for the TO-1 in our previous work, for example, CAM-B3LYP (a range-separated hybrid GGA), M06, M06HF and M062X (hybrid meta-GGAs). As a result, only one parameter Becke's 1998 functional (HFB), which includes the Slater exchange along with corrections involving the gradient of the density, is the more reasonable choice to be in good accordance with the experimental results, and used in both the DFT and TD-DFT methods in the sequential work. The conclusions should help to make an adequate choice of the functional when studying thiazole orange and indole cyanine dyes.

Table S1. A test with a large number of functionals was performed for photochemical properties for the TO-1. The results obtained with B97D, HFS, and HFB functionals are consisting with experimental data (502 nm). B97D, HFS, and HFB functionals were performed for photochemical properties for the Cy. The results obtained with HFB functional are nearly actual experiment. Therefore, we selected the HFB functional for our study.

Functional	**Calcd λ (nm)**	**Functional**	**calcd λ (nm)**	**Functional**	**calcd λ (nm)**
B3LYP	449.25	BHandH	398.93	X3LYP	446.05

B3P86	444.86	BHandHLYP	400.82	LC-wPBE	402.16
B3PW91	445.99	BMK	424.44	CAM-B3LYP	416.50
B1B95	439.35	M06	440.43	VSXC	484.67
mPW1PW91	437.06	M06HF	415.23	HCTH	484.74
mPW1LYP	441.05	M062X	427.67	HCTH93	485.59
mPW1PBE	437.06	tHCTHhyb	456.55	HCTH147	485.73
mPW3PBE	446.10	HSEh1PBE	442.06	HCTH407	484.74
B98	446.04	HSE2PBE	440.80	tHCTH	481.93
B971	448.14	PBEh1PBE	437.39	M06L	455.40
B972	443.01	wB97XD	416.03	**B97D**	**490.42**
PBE1PBE	437.51	wB97	402.03	**HFS**	**501.07**
B1LYP	440.91	wB97X	406.04	XAlpha	488.19
O3LYP	462.65	TPSSh	454.71	**HFB**	**513.09**

Table S2. The initial configuration, basis set and solvation model for mpwpw91 and CAM-B3LYP are the same as that for HFB functional.

	mpwpw91 λ_{abs}(nm)	CAM-B3LYP λ_{abs}(nm)	HFB λ_{abs}(nm)	Exp λ_{abs}(nm)
Cyan 46	446	459	535	553
Cyan 2	442	455	532	541
Cy5	489	502	591	637
Cy5-CH_3	490	504	590	635
Cy5-CHO	450	457	580	600
Cy3	428	436	534	541
Cy3-CH_3	453	463	538	535
Cy3-Ph	459	470	579	580

Comparison of the mpwpw91/tzvp (GGA) with HFB/TZVP showed the excellent performance of HFB functional for predicting absolute absorption energies.

3. XYZ coordinates (angstrom) and SCF Energies (a.u.)

Note: upper case letters before the atomic coordinates indicate the atomic symbol of the atoms involved in the calculations.

Cyan 46 in the S_0 state

Energy = -1633.7413

C	7.25455700	-0.31238500	0.00680900
C	6.27110400	0.71146400	-0.01282000
C	4.89742000	0.33173400	-0.00362300
C	4.54206600	-1.05077300	0.02318600
C	5.52042500	-2.07364600	0.04268600
C	6.88900200	-1.68998500	0.03435200
N	3.76171200	1.20492000	-0.01877500
C	2.52341200	0.56752200	-0.00939700
S	2.74085100	-1.24398400	0.02918200
C	1.24640400	1.19838900	-0.02427100
C	-0.00055700	0.52295700	-0.02178300
C	-1.25619700	1.18520000	-0.01965300
C	-2.52675400	0.54384800	-0.01713700
N	-3.75317800	1.20277100	0.01666600
C	-4.90566600	0.34971100	0.01300400
C	-4.56510100	-1.03869400	-0.02186800
S	-2.76642100	-1.26062200	-0.05748600
C	-6.27843100	0.73431700	0.03980400
C	-7.26953100	-0.28167900	0.03239400
C	-6.91683600	-1.66231000	-0.00070200
C	-5.55167500	-2.05405200	-0.02838200
C	3.96306900	2.70448400	-0.04850500
C	-3.83721100	2.71265400	0.06876700
H	8.31858200	-0.02991800	0.00018900
H	6.57248400	1.76719800	-0.03449200
H	5.22809000	-3.13391600	0.06358200
H	7.66896700	-2.46659400	0.04945900
H	1.22422800	2.29691500	-0.03553700
H	0.00378900	-0.58046100	-0.01808100
H	-1.25269400	2.28472400	-0.01362400
H	-6.58057900	1.78950100	0.06591000
H	-8.33064600	0.01087700	0.05285900
H	-7.70290200	-2.43281000	-0.00528600
H	-5.26600000	-3.11608200	-0.05443000
H	2.99262700	3.22061400	-0.03723900
H	4.51257700	2.97540600	-0.97133800
H	4.54730300	3.00522700	0.84298200
H	-4.89459300	3.01343900	0.10732700
H	-3.36882100	3.14255500	-0.83789300

H	-3.32002900	3.08064700	0.97607800

Cyan 46 in the S1 state

Energy = -1633.7388

C	-7.28514900	-0.25217000	0.00015100
C	-6.29215300	0.75695700	0.00996800
C	-4.91382700	0.36081400	-0.00410600
C	-4.58155600	-1.04356800	-0.02034200
C	-5.57865300	-2.04663300	-0.02820200
C	-6.94183000	-1.64092800	-0.01900400
N	-3.78758200	1.20599000	-0.00211300
C	-2.53549800	0.53625600	-0.00151900
S	-2.79155100	-1.27723000	-0.02264500
C	-1.24667100	1.12550900	0.00867800
C	0.00180800	0.42491100	0.03872400
C	1.25926100	1.11813400	0.01119600
C	2.54069500	0.51981900	0.01390500
N	3.78208000	1.20646200	-0.00802200
C	4.92255500	0.37868800	-0.00832300
C	4.60155500	-1.03133100	0.01553600
S	2.81448500	-1.28821100	0.03836500
C	6.30132900	0.77581400	-0.02936700
C	7.29889100	-0.22941900	-0.02485600
C	6.96282600	-1.62070600	-0.00223200
C	5.60240800	-2.02899400	0.01729600
C	-3.95042000	2.70721800	0.04152900
C	3.83514100	2.71403200	-0.04398000
H	-8.34573300	0.04372600	0.01198200
H	-6.57858400	1.81687800	0.02716900
H	-5.30411700	-3.11185600	-0.04161100
H	-7.73559500	-2.40321600	-0.02316800
H	-1.19562800	2.22451800	-0.00712800
H	-0.00066700	-0.67642500	0.07822900
H	1.22328500	2.21822600	-0.01989100
H	6.59104400	1.83451000	-0.04727300
H	8.35730300	0.07372500	-0.03750700
H	7.76077600	-2.37863900	-0.00170200
H	5.33185000	-3.09523300	0.03540300
H	-2.96492800	3.19501500	-0.04424400
H	-4.42722100	2.99720400	1.00326600
H	-4.58943500	3.02536900	-0.80940100
H	4.88505900	3.04411900	-0.02581500
H	3.30905100	3.12274200	0.84334900
H	3.35083400	3.08279900	-0.97250200

Cyan 2 in the S_0 state

Energy = -1672.7726

C	-7.36266100	0.42166200	-0.41433500
C	-6.19302500	1.21241100	-0.27163600
C	-4.93909500	0.55309600	-0.10165700
C	-4.89144500	-0.87506400	-0.09891200
C	-6.05815700	-1.66679000	-0.23423400
C	-7.30339500	-1.00284600	-0.39384200
N	-3.65245200	1.15271900	0.07619800
C	-2.57673400	0.25884600	0.16175100
S	-3.18838400	-1.45803000	0.08886900
C	-1.21778800	0.67588500	0.20331000
C	0.00000700	-0.06459900	0.38523700
C	1.21777100	0.67586500	0.20324600
C	2.57673800	0.25884300	0.16174100
N	3.65244000	1.15271000	0.07613400
C	4.93909200	0.55307900	-0.10167400
C	4.89144800	-0.87507900	-0.09886800
S	3.18838400	-1.45803500	0.08891100
C	6.19301100	1.21240800	-0.27166400
C	7.36265800	0.42166900	-0.41432800
C	7.30340000	-1.00283700	-0.39379100
C	6.05817100	-1.66679500	-0.23416000
C	-3.46260700	2.64966100	0.17082000
C	3.46264400	2.64967500	0.17064500
C	-0.00002300	-1.55334300	0.78847500
H	-8.33237300	0.92586800	-0.54681400
H	-6.26693000	2.30739500	-0.29950400
H	-5.99707300	-2.76517500	-0.22282300
H	-8.22440400	-1.59509400	-0.50629800
H	-1.08065500	1.75094600	0.02063400
H	1.08064100	1.75090800	0.02045600
H	6.26687800	2.30739300	-0.29952500
H	8.33236700	0.92587700	-0.54681900
H	8.22441400	-1.59508200	-0.50623300
H	5.99710700	-2.76518000	-0.22270700
H	-2.75950300	2.87675600	0.99287900
H	-4.43363600	3.11736900	0.39844000
H	-3.07143500	3.04811700	-0.78722700
H	4.43355700	3.11730400	0.39894000
H	2.75901400	2.87681800	0.99223100
H	3.07214800	3.04817000	-0.78766200
H	-0.00018100	-2.21628000	-0.10576600
H	-0.88702700	-1.80571100	1.40024200
H	0.88710500	-1.80584300	1.40000400

Cyan 2 in the S_1 state

Energy = -1672.7700

C	-7.32216700	0.39586300	-0.60729600
C	-6.17716600	1.20049200	-0.39360100
C	-4.91846700	0.55595600	-0.14949000
C	-4.85709500	-0.88617700	-0.15110100
C	-6.00590200	-1.68492500	-0.36136100
C	-7.24844300	-1.03228800	-0.58951600
N	-3.67404900	1.16504900	0.10288000
C	-2.57338000	0.26904600	0.23899400
S	-3.17407900	-1.45938000	0.15901600
C	-1.22026100	0.68501800	0.30395000
C	0.00001200	-0.04994400	0.57180200
C	1.22024600	0.68505600	0.30387300
C	2.57335800	0.26908800	0.23884600
N	3.67404700	1.16507400	0.10277900
C	4.91846200	0.55595700	-0.14952900
C	4.85706500	-0.88617700	-0.15114100
S	3.17402800	-1.45935100	0.15892200
C	6.17718700	1.20047200	-0.39355900
C	7.32218900	0.39582400	-0.60717600
C	7.24843400	-1.03232500	-0.58942500
C	6.00587000	-1.68494400	-0.36133900
C	-3.50517100	2.65937700	0.22358200
C	3.50521000	2.65940600	0.22348300
C	0.00008200	-1.48021800	1.14730200
H	-8.28942700	0.88666800	-0.79682300
H	-6.25956800	2.29466600	-0.42686400
H	-5.93551800	-2.78277500	-0.35145600
H	-8.15576500	-1.63245700	-0.75677100
H	-1.07305000	1.75251300	0.07807300
H	1.07300400	1.75255400	0.07803400
H	6.25960800	2.29464500	-0.42681600
H	8.28947000	0.88661200	-0.79663800
H	8.15575700	-1.63250900	-0.75662400
H	5.93547000	-2.78279200	-0.35143000
H	-2.79865800	2.87977300	1.04478400
H	-4.48109100	3.11176200	0.46552500
H	-3.12322100	3.08284000	-0.72875700
H	4.48111800	3.11174700	0.46556200
H	2.79860300	2.87981900	1.04459700
H	3.12340000	3.08290200	-0.72889800
H	-0.00010200	-2.26657000	0.35834200
H	-0.88846600	-1.64892900	1.78806200
H	0.88888900	-1.64897900	1.78769000

Cy3 in the S_0 state

Energy = -1072.9171

C	-6.95925200	-1.28465900	-0.08188600
C	-7.27312000	0.10035200	0.00247800
C	-6.24612700	1.08507900	0.06823400
C	-4.90093300	0.63136900	0.04642600
C	-4.57061300	-0.74930300	-0.04389400
C	-5.59903200	-1.71644300	-0.10572600
N	-3.67996600	1.40253000	0.10284300
C	-2.55554800	0.59074000	0.03092600
C	-3.02465400	-0.91540400	-0.05686800
C	-1.24413700	1.14109500	0.02671700
C	1.24413400	1.14110300	-0.02665500
C	0.00000300	0.44942400	0.00000500
C	2.55554800	0.59074400	-0.03090500
C	-3.64815300	2.90223800	0.22233200
N	3.67996300	1.40252900	-0.10284600
C	4.90093300	0.63136300	-0.04646000
C	4.57061200	-0.74930400	0.04389700
C	3.02465100	-0.91540300	0.05690600
C	6.24612400	1.08507500	-0.06835300
C	7.27312000	0.10035100	-0.00261400
C	6.95925300	-1.28465800	0.08180200
C	5.59903600	-1.71644300	0.10570400
C	-2.55389000	-1.60029300	-1.41290300
C	-2.54962200	-1.75599600	1.20756400
C	2.54960400	-1.75605000	-1.20747200
C	2.55390500	-1.60023100	1.41298600
C	3.64815500	2.90224200	-0.22229700
H	-7.76967300	-2.02880500	-0.13125400
H	-8.32579000	0.42430900	0.01693200
H	-6.50790500	2.15028100	0.13086000
H	-5.36239900	-2.78968700	-0.17336900
H	-1.17472800	2.23944700	0.04474900
H	1.17473000	2.23945600	-0.04462900
H	0.00001300	-0.64567500	-0.00003300
H	-3.01882600	3.19466600	1.08551000
H	-4.67248900	3.27293900	0.38557700
H	-3.24084000	3.35067600	-0.70662600
H	6.50789200	2.15027600	-0.13104000
H	8.32579000	0.42430500	-0.01712700
H	7.76967600	-2.02880400	0.13115400
H	5.36240500	-2.78968600	0.17337800
H	-1.45254100	-1.70501600	-1.45229800
H	-2.88435500	-1.00593000	-2.28988400
H	-3.00109600	-2.61284100	-1.48642700
H	-1.45004700	-1.88090200	1.22157300
H	-3.01133400	-2.76394400	1.17011000
H	-2.86218400	-1.26103200	2.15027500

H	3.01130200	-2.76400300	-1.16996600
H	2.86216700	-1.26114200	-2.15021200
H	1.45002800	-1.88095000	-1.22147900
H	3.00110800	-2.61277900	1.48654600
H	1.45255400	-1.70494300	1.45239400
H	2.88438600	-1.00582900	2.28993300
H	4.67251800	3.27295000	-0.38535800
H	3.24070400	3.35064500	0.70661600
H	3.01895500	3.19469300	-1.08556100

Cy3 in the S_1 state

Energy = -1072.9129

C	7.04839100	-1.15815600	0.00268000
C	7.30836000	0.24845300	-0.00037000
C	6.25253800	1.19157100	-0.00252700
C	4.90927800	0.68902300	-0.00152700
C	4.63768100	-0.72667600	0.00145000
C	5.70450800	-1.64621100	0.00361000
N	3.69291600	1.40006000	-0.00326400
C	2.56840600	0.51473100	-0.00119800
C	3.10219500	-0.96300800	0.00163500
C	1.24786100	1.01812800	-0.00110700
C	-1.24785800	1.01812300	0.00156700
C	0.00000200	0.30387700	0.00022800
C	-2.56840500	0.51472500	0.00151600
C	3.58541000	2.89564600	-0.00702000
N	-3.69290900	1.40005600	0.00338900
C	-4.90927600	0.68902400	0.00139900
C	-4.63768500	-0.72667400	-0.00151900
C	-3.10219900	-0.96301300	-0.00134300
C	-6.25253300	1.19157900	0.00205900
C	-7.30836000	0.24846600	-0.00040800
C	-7.04839500	-1.15814400	-0.00341900
C	-5.70451500	-1.64620500	-0.00398400
C	2.66271700	-1.75860600	1.31247200
C	2.66332200	-1.76320100	-1.30668800
C	-2.66361500	-1.76314000	1.30712100
C	-2.66244100	-1.75868300	-1.31204000
C	-3.58539400	2.89564300	0.00712900
H	7.88898200	-1.86935300	0.00433900
H	8.34927100	0.60849300	-0.00105200
H	6.47072100	2.26832600	-0.00482900
H	5.51581300	-2.73097100	0.00588600
H	1.14986700	2.11532100	-0.00201700
H	-1.14986800	2.11531600	0.00250900
H	0.00000500	-0.79087700	0.00014200
H	3.04026000	3.23386400	-0.91257500

H	4.59586200	3.33416700	-0.00962300
H	3.04288200	3.23880400	0.89826500
H	-6.47071300	2.26833500	0.00431500
H	-8.34926800	0.60851000	-0.00000600
H	-7.88899000	-1.86933700	-0.00532400
H	-5.51582400	-2.73096600	-0.00622700
H	1.56690700	-1.91567500	1.33681700
H	2.96239400	-1.20594500	2.22692800
H	3.15589800	-2.75256400	1.32400600
H	1.56751400	-1.92036300	-1.33101200
H	3.15655100	-2.75717700	-1.31452400
H	2.96342600	-1.21369800	-2.22290400
H	-3.15685800	-2.75711000	1.31490500
H	-2.96391000	-1.21358400	2.22324100
H	-1.56781500	-1.92031500	1.33169000
H	-3.15561500	-2.75264500	-1.32362200
H	-1.56662600	-1.91574700	-1.33614500
H	-2.96192800	-1.20607600	-2.22659200
H	-4.59584300	3.33417200	0.00947600
H	-3.04265200	3.23876900	-0.89803900
H	-3.04045000	3.23388000	0.91280200

Cy5 in the S_0 state

Energy = -1149.8536

C	8.10661800	-1.49116600	0.00661600
C	8.48760600	-0.12018900	-0.00393900
C	7.50844200	0.91423900	-0.01039200
C	6.14419100	0.52092700	-0.00565800
C	5.74583600	-0.84283200	0.00514100
C	6.72707900	-1.85980200	0.01119700
N	4.97196300	1.36110200	-0.01033300
C	3.80080800	0.60883700	-0.00238400
C	4.19371900	-0.92643000	0.00869000
C	2.50673300	1.19572800	-0.00337500
C	3.68596000	-1.65510500	1.32896100
C	3.68069800	-1.67672800	-1.29734500
C	5.10748800	2.85914700	-0.02177500
C	1.24935400	0.52904500	-0.00048500
C	-0.00288200	1.20427100	-0.00090400
C	-1.24950900	0.52209400	0.00041000
C	-2.51278100	1.18119300	0.00190600
C	-3.80293800	0.58804800	0.00221600
N	-4.96030900	1.35958900	0.01060800
C	-6.14816200	0.53922400	0.00498700
C	-5.76443300	-0.83125900	-0.00513300
C	-4.21275700	-0.93804500	-0.00774400
C	-7.51066200	0.93940100	0.00820200

C	-8.49858900	-0.08645600	0.00149800
C	-8.13111200	-1.46075800	-0.00799700
C	-6.75467700	-1.83926000	-0.01133900
C	-3.70820700	-1.69362900	1.29846200
C	-3.71180800	-1.67474400	-1.32607600
C	-4.98389500	2.86376200	0.02397600
H	8.88046700	-2.27485600	0.01144500
H	9.55494700	0.15206700	-0.00723900
H	7.81245000	1.97025900	-0.01848700
H	6.44062400	-2.92297000	0.01946200
H	2.45510200	2.29483100	-0.00761500
H	2.58100200	-1.71572100	1.36190000
H	4.03749400	-1.11897400	2.23480900
H	4.08991000	-2.68801300	1.35411600
H	2.57575700	-1.74021400	-1.32345500
H	4.08657100	-2.70913400	-1.30818800
H	4.02646900	-1.15424300	-2.21329700
H	4.11826300	3.33979900	-0.03084400
H	5.66969400	3.16555600	-0.92694900
H	5.66090000	3.18082000	0.88362600
H	1.21149500	-0.57025700	0.00151200
H	-0.00611200	2.30957100	-0.00224900
H	-1.20639900	-0.57750300	0.00120300
H	-2.47457700	2.28147000	0.00364200
H	-7.81271500	1.99588500	0.01562700
H	-9.56308900	0.19672500	0.00373200
H	-8.91164800	-2.23773300	-0.01298300
H	-6.47601300	-2.90454700	-0.01882300
H	-4.12218600	-2.72283900	1.30926300
H	-4.04963900	-1.16839100	2.21446600
H	-2.60358300	-1.76555100	1.32433400
H	-4.12307900	-2.70484700	-1.34894900
H	-2.60707000	-1.74305800	-1.35781400
H	-4.05869400	-1.13824600	-2.23348100
H	-6.02973400	3.20847500	0.04617600
H	-4.49153600	3.25834200	-0.88750600
H	-4.45936200	3.24139000	0.92436500

Cy5 in the S_1 state

Energy = -1149.8516

C	-8.30648100	-1.20204300	0.00045800
C	-8.56620400	0.20261300	-0.00042700
C	-7.50843600	1.14640300	-0.00092500
C	-6.16842400	0.64320400	-0.00053600
C	-5.89615600	-0.76833800	0.00040900

C	-6.96281700	-1.68954500	0.00090100
N	-4.94597700	1.35662800	-0.00093600
C	-3.82770700	0.47797700	-0.00027800
C	-4.35994400	-1.00228200	0.00067100
C	-2.50587700	0.97606600	-0.00046300
C	-3.91904100	-1.79759700	-1.30897700
C	-3.91916100	-1.79594200	1.31131800
C	-4.84075600	2.85335400	-0.00204600
C	-1.26498400	0.24894200	0.00010500
C	-0.00001400	0.90621600	0.00010000
C	1.26500200	0.24896800	0.00036500
C	2.50585600	0.97610100	0.00062500
C	3.82771800	0.47801500	0.00055800
N	4.94597000	1.35664500	0.00113000
C	6.16843500	0.64320600	0.00037500
C	5.89614900	-0.76832000	-0.00049500
C	4.35994200	-1.00225400	-0.00031300
C	7.50845000	1.14637700	0.00044500
C	8.56620300	0.20256800	-0.00049200
C	8.30646300	-1.20208400	-0.00139300
C	6.96279000	-1.68955500	-0.00137900
C	3.91882400	-1.79606100	-1.31077800
C	3.91939500	-1.79742500	1.30952800
C	4.84076800	2.85337700	0.00221500
H	-9.14669100	-1.91381100	0.00081700
H	-9.60674800	0.56385500	-0.00072700
H	-7.72675900	2.22320700	-0.00158900
H	-6.77301600	-2.77415800	0.00159700
H	-2.39759300	2.07231700	-0.00102300
H	-2.82280900	-1.95301600	-1.33392300
H	-4.21996400	-1.24646200	-2.22394300
H	-4.41086600	-2.79220100	-1.31933100
H	-2.82292500	-1.95129300	1.33656200
H	-4.41094700	-2.79055200	1.32286100
H	-4.22018800	-1.24369400	2.22558000
H	-4.29751900	3.19487200	0.90317100
H	-5.85206100	3.28978600	-0.00223600
H	-4.29773700	3.19353000	-0.90790000
H	-1.26554100	-0.85099500	0.00052600
H	-0.00002400	2.01251800	-0.00011800
H	1.26557100	-0.85096800	0.00039400
H	2.39756300	2.07235300	0.00085000
H	7.72681500	2.22317300	0.00110800
H	9.60675100	0.56380200	-0.00051300
H	9.14666100	-1.91386400	-0.00212100
H	6.77296200	-2.77416400	-0.00207900
H	4.41063200	-2.79065900	-1.32234900
H	4.21960700	-1.24389300	-2.22516900
H	2.82258800	-1.95143600	-1.33572000

H	4.41124100	-2.79201800	1.31985300
H	2.82317100	-1.95286400	1.33478600
H	4.22055300	-1.24619200	2.22435800
H	5.85207400	3.28980000	0.00318300
H	4.29710200	3.19350400	0.90769200
H	4.29819400	3.19496600	-0.90337900

Cy5-CH_3 in the S_0 state

Energy = -1266.9822

C	7.78890000	-2.20556800	0.23884000
C	8.32734000	-0.89340200	0.12644000
C	7.47757900	0.23965100	-0.02340000
C	6.07635100	0.00884500	-0.05869100
C	5.52301100	-1.29568200	0.05668500
C	6.37690900	-2.41208000	0.20491700
C	-5.52300600	-1.29568500	0.05670200
C	-6.07634800	0.00883800	-0.05869100
C	-7.47757200	0.23965100	-0.02338100
C	-8.32733300	-0.89339600	0.12650100
C	-7.78889400	-2.20556100	0.23892100
C	-6.37690500	-2.41207900	0.20497800
N	5.00635100	0.96790600	-0.20976900
C	3.75771100	0.34987100	-0.18180800
C	3.97268400	-1.20997900	-0.01515700
C	-3.97268100	-1.20998800	-0.01516800
C	-3.75771100	0.34985900	-0.18185300
N	-5.00633900	0.96789400	-0.20980500
C	5.27033900	2.45219200	-0.37021600
C	5.33739000	3.22734200	0.99187200
C	-5.27033500	2.45218200	-0.37028100
C	-5.33740900	3.22734900	0.99179600
C	2.54545500	1.08657100	-0.28793200
C	1.22008800	0.56572100	-0.28845700
C	0.00000200	1.31394100	-0.38369000
C	-1.22008900	0.56570700	-0.28849400
C	-2.54544500	1.08656100	-0.28800100
C	-0.00003400	2.85448100	-0.53704000
C	3.32869100	-1.75694200	1.33316800
C	3.43786700	-2.01808400	-1.27806600
C	-3.43788700	-2.01809700	-1.27808800
C	-3.32866200	-1.75694700	1.33314100
H	8.46448300	-3.06771900	0.35459000
H	9.41825800	-0.74377900	0.15699300
H	7.90801800	1.24741900	-0.10108600
H	5.96669100	-3.43014700	0.29319400
H	-7.90801000	1.24741800	-0.10108300
H	-9.41825000	-0.74377100	0.15707100

H	-8.46447700	-3.06770800	0.35470500
H	-5.96668800	-3.43014500	0.29326600
H	4.48172300	2.86817600	-1.02346000
H	6.22632900	2.54719400	-0.91858100
H	5.55446000	4.29673200	0.78235500
H	6.14292400	2.82852800	1.64215400
H	4.37437200	3.16663600	1.53891600
H	-6.22631300	2.54716400	-0.91866900
H	-4.48170600	2.86815700	-1.02351500
H	-4.37440300	3.16663500	1.53885900
H	-6.14296200	2.82855600	1.64206600
H	-5.55445800	4.29673900	0.78226000
H	2.65009900	2.17616600	-0.36382800
H	1.08894200	-0.52108500	-0.19268500
H	-1.08894400	-0.52110100	-0.19274000
H	-2.65010100	2.17615300	-0.36392100
H	-0.89176200	3.20971200	-1.09058500
H	0.89186800	3.20980300	-1.09024800
H	-0.00022500	3.35867200	0.45654100
H	2.22323100	-1.70351000	1.30824800
H	3.69110600	-1.17588700	2.20647400
H	3.62011200	-2.81825000	1.47282100
H	2.33508000	-1.96356800	-1.35949100
H	3.72499300	-3.08498000	-1.17732900
H	3.88153300	-1.62209700	-2.21507100
H	-2.33510200	-1.96357700	-1.35953000
H	-3.88157200	-1.62211400	-2.21508500
H	-3.72501000	-3.08499300	-1.17733900
H	-2.22320400	-1.70349500	1.30821200
H	-3.62006200	-2.81826100	1.47278800
H	-3.69107800	-1.17590900	2.20645800

Cy5-CH_3 in the S_1 state

Energy = -1266.9795

C	7.91428700	-2.08559500	0.25403100
C	8.40597400	-0.75463000	0.11701000
C	7.52430700	0.34280100	-0.04986500
C	6.11929000	0.07046000	-0.07362800
C	5.61460200	-1.26877900	0.06304900
C	6.50806000	-2.34358900	0.22766500
C	-5.60795800	-1.26756400	0.05574900
C	-6.11973700	0.06807900	-0.07078300
C	-7.52499200	0.33324200	-0.05096900
C	-8.40577700	-0.77076900	0.08386200
C	-7.90700100	-2.10415600	0.19874100
C	-6.50054700	-2.35496500	0.18830200
N	5.03729600	0.97083700	-0.23128500

C	3.78607100	0.29644400	-0.19044300
C	4.06291500	-1.24474800	-0.00515300
C	-4.05626800	-1.23626500	0.00921500
C	-3.78666400	0.30494600	-0.17175500
N	-5.04445400	0.97819100	-0.21111400
C	5.23772600	2.46316900	-0.40320900
C	5.26320700	3.25592000	0.95114700
C	-5.25209000	2.46710000	-0.37626000
C	-5.29361900	3.24984300	0.98590900
C	2.55520400	0.99231800	-0.29575200
C	1.23081400	0.44897800	-0.29207200
C	-0.00065000	1.20182100	-0.36667200
C	-1.23145500	0.46576400	-0.27194400
C	-2.56235500	1.00782800	-0.27699100
C	0.01960500	2.74284300	-0.49786300
C	3.44047900	-1.81176400	1.34874100
C	3.55421400	-2.09605000	-1.25676300
C	-3.52827300	-2.08853300	-1.23220200
C	-3.45196200	-1.79519100	1.37602400
H	8.62043500	-2.91982500	0.38345600
H	9.49211800	-0.56929500	0.13821100
H	7.91824600	1.36337000	-0.14229500
H	6.13916400	-3.37540700	0.33125900
H	-7.92577100	1.35336200	-0.13283200
H	-9.49208700	-0.59234500	0.10135800
H	-8.60948000	-2.94485300	0.29886700
H	-6.12480900	-3.38334400	0.28131700
H	4.43568100	2.83767000	-1.06751300
H	6.19264600	2.59717400	-0.94803400
H	5.43209900	4.33195000	0.72780400
H	6.08046500	2.90152700	1.60806700
H	4.29883700	3.15982300	1.49152900
H	-6.20096600	2.59949400	-0.92755400
H	-4.44716400	2.85329700	-1.02289600
H	-4.33836800	3.14626000	1.53876700
H	-6.12384300	2.88982900	1.63108600
H	-5.46022000	4.32842000	0.76990200
H	2.63209500	2.08388800	-0.38044300
H	1.10924900	-0.63987400	-0.20947800
H	-1.11487900	-0.62293500	-0.17682500
H	-2.64620500	2.09925000	-0.36267500
H	-0.92889800	3.13799300	-0.92728500
H	0.85469500	3.07903000	-1.15960200
H	0.16835800	3.22881100	0.50515500
H	2.33357900	-1.79411100	1.31986600
H	3.78066700	-1.21150400	2.21823000
H	3.76872000	-2.86018100	1.49369300
H	2.44929300	-2.08021300	-1.33483900
H	3.87863800	-3.15102100	-1.13912000

H	3.98295200	-1.69961700	-2.20151000
H	-2.42333800	-2.07179100	-1.29182900
H	-3.93895300	-1.69655200	-2.18358200
H	-3.85181300	-3.14366100	-1.11650500
H	-2.34507400	-1.76755500	1.36863200
H	-3.77331900	-2.84674300	1.51601200
H	-3.81709100	-1.19726800	2.23567300

Cy5-CHO in the S_0 state

Energy = -1340.7854

C	7.70148800	-2.40421800	0.13368300
C	8.29042600	-1.11097500	0.05592300
C	7.48418900	0.05807400	-0.04502700
C	6.07616800	-0.12012600	-0.06641300
C	5.47203300	-1.40291600	0.01338600
C	6.28321500	-2.55647200	0.11329300
C	-5.40755700	-1.45366200	0.05847900
C	-6.02046700	-0.17895100	-0.06942600
C	-7.42962900	-0.00981900	-0.06445900
C	-8.22816900	-1.18051100	0.07085900
C	-7.63056000	-2.46604200	0.19729000
C	-6.21132500	-2.60909700	0.19193200
N	5.03796000	0.88591200	-0.16919200
C	3.77624600	0.31891800	-0.14468300
C	3.92654800	-1.25229200	-0.03269300
C	-3.86336900	-1.29243400	0.01568000
C	-3.72416700	0.27474300	-0.14456100
N	-4.98761500	0.83040300	-0.19797600
C	5.36316700	2.36713300	-0.27512400
C	5.47021800	3.08061200	1.11697900
C	-5.32155500	2.30533700	-0.35906100
C	-5.44989100	3.06470400	1.00663200
C	2.58916900	1.11646600	-0.21575100
C	1.25901800	0.64347900	-0.20490700
C	0.01740500	1.39821600	-0.28231300
C	-1.21064300	0.62423700	-0.19542800
C	-2.54256100	1.08424200	-0.22941100
C	0.05029900	2.87812600	-0.45629600
O	-0.93964700	3.65389500	-0.50714300
C	3.28015400	-1.81634200	1.30835600
C	3.34309100	-1.99489800	-1.31516400
C	-3.26864300	-2.06741800	-1.24276700
C	-3.21704700	-1.80988700	1.37528000
H	8.34455200	-3.29493900	0.21151700
H	9.38653800	-1.00538400	0.07526300
H	7.95196900	1.05047200	-0.09791300
H	5.83523900	-3.56029300	0.17453800
H	-7.90401100	0.97669000	-0.15489700

H	-9.32509100	-1.08247000	0.07884500
H	-8.26808700	-3.35805700	0.30120700
H	-5.75679000	-3.60694400	0.29050400
H	4.58933100	2.83956300	-0.90636000
H	6.31855200	2.44030400	-0.82659200
H	5.72821000	4.14783500	0.94779800
H	6.26360400	2.62403900	1.74330200
H	4.50889500	3.03546800	1.66826000
H	-6.27094600	2.35210500	-0.92361100
H	-4.54247500	2.76018800	-0.99624400
H	-4.49427400	3.04763200	1.56908200
H	-6.24611200	2.62273000	1.63979500
H	-5.71548000	4.12294300	0.79769200
H	2.74906300	2.19892500	-0.27499000
H	1.10910300	-0.44102800	-0.11622800
H	-1.04173300	-0.45610200	-0.08607900
H	-2.69126900	2.16360400	-0.32235000
H	1.07152100	3.32682800	-0.55845700
H	2.17755600	-1.72062500	1.30300900
H	3.67794100	-1.27902700	2.19389600
H	3.53257000	-2.89178700	1.40735500
H	2.24219900	-1.89661600	-1.37858600
H	3.59167000	-3.07407900	-1.25297000
H	3.78957400	-1.58421500	-2.24428500
H	-2.16858700	-1.96079600	-1.30557600
H	-3.71569600	-1.68820400	-2.18488100
H	-3.50805600	-3.14638200	-1.14931400
H	-2.11539700	-1.70422000	1.36979700
H	-3.46047700	-2.88396200	1.50650400
H	-3.62235800	-1.24891800	2.24255800

Cy5-CHO in the S_1 state

Energy = -1340.7819

C	7.79690000	-2.31930200	0.14259800
C	8.35541900	-1.00343400	0.07804000
C	7.52998700	0.14168500	-0.01903500
C	6.11460600	-0.06572900	-0.05463600
C	5.54148800	-1.37988600	0.01109000
C	6.38076700	-2.50888300	0.10978100
C	-5.49015200	-1.42605400	0.07594700
C	-6.06317700	-0.11791100	-0.06325300
C	-7.47776400	0.08354700	-0.04889100
C	-8.30569000	-1.06058100	0.10142200
C	-7.74327700	-2.36606900	0.23788700
C	-6.32683800	-2.54879300	0.22613700
N	5.08297800	0.89744300	-0.15757500
C	3.79773700	0.28411800	-0.15021600

C	3.99422700	-1.27829600	-0.04853200
C	-3.94173500	-1.31632900	0.01924000
C	-3.75001400	0.23405400	-0.15393800
N	-5.02571100	0.84333200	-0.20529800
C	5.35715300	2.38563400	-0.24613800
C	5.41340000	3.09687200	1.15345300
C	-5.30414900	2.32198300	-0.37882800
C	-5.39529000	3.10602000	0.97739400
C	2.61425900	1.05198000	-0.21741600
C	1.26347700	0.55685700	-0.23929300
C	0.02981600	1.30037000	-0.31170500
C	-1.21862600	0.52676000	-0.23795300
C	-2.55058200	1.00828300	-0.24572600
C	0.07546600	2.78915200	-0.47185700
O	-0.91081900	3.56585000	-0.53107400
C	3.34941400	-1.87914700	1.27936500
C	3.44601800	-2.04030200	-1.33971500
C	-3.37857100	-2.13672700	-1.22838400
C	-3.29800000	-1.85002100	1.37828900
H	8.46167300	-3.19248300	0.21955100
H	9.45028200	-0.87767500	0.10551000
H	7.97407800	1.14418700	-0.05504500
H	5.96062300	-3.52389900	0.15897500
H	-7.92647200	1.08241900	-0.14266900
H	-9.39959300	-0.93228900	0.11665100
H	-8.40528300	-3.23814300	0.35797000
H	-5.90283900	-3.56069000	0.33333500
H	4.57888200	2.83686900	-0.88651000
H	6.32132500	2.50074800	-0.77740400
H	5.62627300	4.17583900	0.99173400
H	6.21732400	2.67090000	1.78818100
H	4.44774700	3.00574600	1.69102900
H	-6.25522000	2.40330800	-0.93897600
H	-4.51197700	2.74134100	-1.02249600
H	-4.44104200	3.04353100	1.54099400
H	-6.21368700	2.71428100	1.61573700
H	-5.60456900	4.17363700	0.75522600
H	2.75195100	2.13720800	-0.25325400
H	1.13082500	-0.53260300	-0.17542200
H	-1.05902900	-0.55797300	-0.15740100
H	-2.67449000	2.09321500	-0.32394800
H	1.09859900	3.23245000	-0.55887200
H	2.24444700	-1.82365000	1.25373500
H	3.71202300	-1.33124100	2.17588900
H	3.64040400	-2.94628700	1.37568800
H	2.34372100	-1.96796800	-1.41556600
H	3.71955900	-3.11337400	-1.27194800
H	3.89500000	-1.62108000	-2.26365700
H	-2.27651100	-2.06106100	-1.30082400

H	-3.82444900	-1.75979500	-2.17403800
H	-3.64725000	-3.20556700	-1.11540400
H	-2.19349400	-1.76835000	1.36449400
H	-3.56784000	-2.91807800	1.51864600
H	-3.68292800	-1.27478700	2.24808600

Cy3-CH_3 in the S_0 state

Energy = -1190.0149

C	-7.19002400	-0.88202100	-0.74412400
C	-7.23411000	0.53878200	-0.68246100
C	-6.06806300	1.29656000	-0.37714000
C	-4.86307600	0.58102700	-0.13989600
C	-4.80423100	-0.83634400	-0.19227300
C	-5.97008600	-1.57812800	-0.49079700
N	-3.55752100	1.09742600	0.18564400
C	-2.60911800	0.07761000	0.32956700
C	-3.36544100	-1.31630200	0.15807800
C	-1.22348800	0.42035900	0.38800500
C	2.58590500	0.08293700	0.22182600
N	3.52680500	1.10088000	0.00536700
C	4.82255600	0.57188700	-0.34497400
C	4.75801700	-0.84620600	-0.36479300
C	3.33352900	-1.31424800	0.04833200
C	6.02275100	1.27427600	-0.64121300
C	7.17135200	0.50443300	-0.98024900
C	7.11843500	-0.91675000	-1.01453900
C	5.90644300	-1.60019400	-0.69781500
C	-2.73951800	-2.15052100	-1.03915200
C	-3.44318600	-2.19814600	1.48374400
C	2.66268900	-2.17029900	-1.10887600
C	3.45906200	-2.16819700	1.38839200
C	-3.31061600	2.58314700	0.36028500
C	3.29349800	2.59179700	0.15612000
C	-0.00248800	-0.27428500	0.71693500
C	1.20561600	0.42061800	0.34369200
C	0.01049300	-1.55374200	1.57769200
C	-3.03141600	3.35309900	-0.97897900
C	3.42331100	3.08874200	1.63794900
H	-8.10207400	-1.44957200	-0.98742300
H	-8.18108300	1.06736400	-0.87552000
H	-6.11538200	2.39336900	-0.33804500
H	-5.94627800	-2.67820000	-0.53232500
H	-1.03562400	1.44989100	0.05273800
H	6.08514100	2.37047900	-0.61447100
H	8.11273600	1.02479600	-1.21782700
H	8.01718100	-1.49384000	-1.28345000
H	5.87445100	-2.70062000	-0.71808100
H	-1.69701300	-2.44920900	-0.81729000

H	-2.74605800	-1.55971500	-1.97853100
H	-3.33789800	-3.07111600	-1.19954500
H	-2.48873600	-2.70907500	1.69651200
H	-4.21606500	-2.98072900	1.34317900
H	-3.72863400	-1.58010400	2.36003300
H	3.25087500	-3.09720900	-1.27029700
H	2.63966300	-1.59916800	-2.06009600
H	1.62709500	-2.45882900	-0.84600300
H	4.22474700	-2.95559100	1.23589500
H	2.51237500	-2.67135100	1.64815200
H	3.77859400	-1.53217400	2.23970200
H	-2.46820000	2.69852700	1.06636400
H	-4.21096000	2.99384500	0.85686900
H	2.29759500	2.83875400	-0.25391000
H	4.03343300	3.09830600	-0.48869900
H	1.00342800	1.45624400	0.03367200
H	0.01774500	-2.48580900	0.97508900
H	-0.87358100	-1.57550500	2.23573000
H	0.89838000	-1.55949500	2.23167700
H	-2.87150100	4.42655400	-0.74044300
H	-3.88934600	3.27721100	-1.67752000
H	-2.12458200	2.97101400	-1.49010300
H	3.26330900	4.18805700	1.66057600
H	4.43329600	2.87358300	2.04397200
H	2.66520700	2.61183500	2.29232800

Cy3-CH_3 in the S_1 state

Energy = -1189.9951

C	-6.49013500	-0.76676100	-1.95029600
C	-6.97138600	0.18143300	-0.99369900
C	-6.12438600	0.69765400	0.01018100
C	-4.76951200	0.23228000	0.03054000
C	-4.27547900	-0.71229500	-0.92841500
C	-5.13920600	-1.21608500	-1.92299000
N	-3.74029800	0.57923600	0.93132500
C	-2.51753200	-0.11670100	0.61944200
C	-2.77749600	-1.00850000	-0.65820300
C	-1.37498100	0.06191600	1.37726800
C	2.38141800	-0.05140800	0.25747500
N	3.03442500	0.93248900	-0.56362600
C	4.43254200	0.64938700	-0.69487600
C	4.74548300	-0.55546700	-0.00287400
C	3.45882200	-1.14178000	0.65377900
C	5.43253100	1.38649600	-1.38673200
C	6.76565300	0.88583900	-1.37229600
C	7.09411000	-0.31632100	-0.68673400
C	6.07224200	-1.04324400	0.00400300

C	-1.89665200	-0.53234900	-1.89776900
C	-2.55051800	-2.55586300	-0.38272500
C	3.14438100	-2.56076300	0.00091000
C	3.67261300	-1.26250100	2.22324300
C	-3.93421000	1.57220300	2.06210100
C	2.40883000	2.15215200	-1.18717100
C	-0.01455500	-0.62645600	1.25135600
C	0.97723700	0.08569500	0.54619000
C	0.11873200	-1.84172700	2.19951600
C	-3.59416600	3.04970700	1.65143400
C	2.40636400	3.42019600	-0.25998600
H	-7.17726300	-1.15269600	-2.71937700
H	-8.01980400	0.51431500	-1.03774600
H	-6.49938900	1.42506200	0.73962100
H	-4.78717600	-1.94364300	-2.66743500
H	-1.45340400	0.76721000	2.22350800
H	5.20512000	2.32207500	-1.92023300
H	7.55448600	1.44606400	-1.90167100
H	8.12940700	-0.68862100	-0.68184200
H	6.32869500	-1.97317200	0.53414600
H	-0.82555500	-0.72757500	-1.70428200
H	-2.03631600	0.55047100	-2.09632000
H	-2.20338300	-1.09756200	-2.79965100
H	-1.47639900	-2.76680200	-0.20653300
H	-2.87311900	-3.13490300	-1.27086500
H	-3.13350500	-2.89954300	0.49367300
H	3.97411700	-3.26547500	0.21849200
H	3.04647900	-2.46745400	-1.10071400
H	2.20961900	-3.00233500	0.39299800
H	4.51991700	-1.94538200	2.43388400
H	2.77868300	-1.66456100	2.73447800
H	3.90863400	-0.26986700	2.66299000
H	-3.30984500	1.23958600	2.91021100
H	-4.98989400	1.49113700	2.37894900
H	1.37885200	1.89704700	-1.49584200
H	2.97102000	2.36600000	-2.11539500
H	0.56122800	0.99208100	0.08126000
H	0.87383100	-2.57297900	1.85916200
H	-0.85052100	-2.38007000	2.28682400
H	0.39724700	-1.51787600	3.23238600
H	-3.79386100	3.70180500	2.52563400
H	-4.22656200	3.38818400	0.80921700
H	-2.52651700	3.15515700	1.36888400
H	1.93745400	4.26962000	-0.80770700
H	3.43884300	3.71603600	0.02175500
H	1.82553600	3.24615900	0.66762200

Cy3-Ph in the S_0 state

Energy = -1380.6408

C	7.29041800	-0.51048200	-0.85567200
C	7.20495300	-1.58024100	0.07838900
C	5.96118800	-1.94141500	0.66953100
C	4.81081400	-1.19909600	0.28753300
C	4.88176200	-0.12426700	-0.63725100
C	6.12377700	0.22939200	-1.21310300
N	3.44229000	-1.36580400	0.71678000
C	2.58827900	-0.43323600	0.11565900
C	3.47292600	0.50621300	-0.81713300
C	1.17595300	-0.59336000	0.23540700
C	-2.60565800	-0.35619000	-0.24017300
N	-3.47292500	-1.22386900	-0.90628900
C	-4.84129300	-1.05546500	-0.47949900
C	-4.90019500	-0.02741900	0.49776700
C	-3.47862700	0.56051300	0.72597900
C	-6.00035400	-1.75107600	-0.91687000
C	-7.24582000	-1.38632100	-0.33126500
C	-7.32151400	-0.36061500	0.65212200
C	-6.14404400	0.33072100	1.06711800
C	2.98992600	0.39014100	-2.32655500
C	3.52947100	2.02590200	-0.35892200
C	-3.49424000	2.10206900	0.34266000
C	-3.01543900	0.36130200	2.23246200
C	3.05374200	-2.42233300	1.73377200
C	-3.08644000	-2.22744900	-1.97590700
C	-0.00191700	0.20076100	-0.04860500
C	-1.19453600	-0.56499700	-0.34155300
C	0.00913900	1.72222100	-0.03828800
C	3.00586600	-1.87724100	3.20333300
C	-2.87727100	-3.68880400	-1.44181500
C	-0.34239300	2.46287900	-1.21151400
C	-0.31584000	3.88209400	-1.20626800
C	0.02726100	4.58717400	-0.02023100
C	0.36056600	3.86279000	1.15698300
C	0.36881800	2.44336900	1.14446000
H	8.26186500	-0.24919200	-1.30412000
H	8.11155300	-2.14191900	0.35412900
H	5.91495500	-2.76650600	1.39310500
H	6.19869100	1.06102000	-1.93082800
H	0.90327400	-1.60380300	0.57406400
H	-5.95581800	-2.54784200	-1.67184600
H	-8.16076500	-1.91216700	-0.64709700
H	-8.29433400	-0.09716700	1.09636500
H	-6.21264500	1.12866600	1.82271200
H	1.96736400	0.79594300	-2.44865300
H	2.99490800	-0.66730600	-2.66343100
H	3.67617500	0.96959400	-2.97813800

H	2.57120900	2.53680800	-0.54391700
H	4.31685600	2.54453400	-0.94331300
H	3.78205600	2.10900600	0.71803200
H	-2.52568100	2.57934300	0.56108900
H	-4.27414400	2.61030800	0.94598100
H	-3.73504900	2.24430700	-0.73068500
H	-3.69698400	0.92214300	2.90494700
H	-1.98598800	0.74028400	2.38261800
H	-3.04464200	-0.71081600	2.51753600
H	3.79441600	-3.23715900	1.64526400
H	2.07695400	-2.85002200	1.44366500
H	-2.17052600	-1.84996700	-2.46572900
H	-3.89551000	-2.20739300	-2.73180100
H	-0.95084500	-1.58302800	-0.67691400
H	2.74531700	-2.71509400	3.88501900
H	2.23893900	-1.08405700	3.31646800
H	3.99092200	-1.46948700	3.51107800
H	-2.61241700	-4.34212700	-2.30073500
H	-3.80082100	-4.08724200	-0.97512000
H	-2.05548500	-3.74060900	-0.69890800
H	-0.61783100	1.92599700	-2.13198300
H	-0.57076600	4.43548900	-2.12448200
H	0.03450600	5.68896200	-0.01335800
H	0.62222800	4.40134300	2.08208100
H	0.63684600	1.89166000	2.05816500

Cy3-Ph in the S_1 state

Energy = -1380.6222

C	6.60526500	-1.88583700	-1.23421300
C	6.88045600	-1.86534800	0.17033100
C	5.91837200	-1.40170700	1.09202200
C	4.66305200	-0.95491100	0.56576000
C	4.37721800	-0.96845700	-0.84085500
C	5.35388200	-1.43726600	-1.74508600
N	3.54754900	-0.45772200	1.27146100
C	2.46995700	-0.11525300	0.37379000
C	2.95280500	-0.42194600	-1.09729000
C	1.28284300	0.39637500	0.86159800
C	-2.41525600	-0.33556700	-0.06805700
N	-3.03647900	-1.57444600	-0.41437000
C	-4.43592700	-1.55685700	-0.11516100
C	-4.79529100	-0.28551100	0.41612000
C	-3.55067200	0.65539000	0.42991000
C	-5.39911100	-2.59093600	-0.29028100
C	-6.74442400	-2.31993600	0.09193900
C	-7.11514500	-1.05636000	0.62994800
C	-6.13489100	-0.02905000	0.78666300

C	2.05568100	-1.51441100	-1.82269600
C	3.02848900	0.90537500	-1.97247900
C	-3.83719200	1.88176700	-0.54286100
C	-3.24564900	1.18514700	1.89544100
C	3.53340400	-0.31318000	2.78481300
C	-2.36209700	-2.75893800	-1.05863100
C	-0.02334100	0.76388900	0.13903800
C	-0.98190800	-0.27407600	0.04152300
C	-0.15334400	2.21703400	-0.25625800
C	4.04981100	1.08554500	3.27342100
C	-1.93853800	-3.89695200	-0.06140500
C	-0.58999600	2.57722800	-1.57581000
C	-0.62085000	3.93059900	-2.00058700
C	-0.20951300	4.97079000	-1.12103800
C	0.23730500	4.63685300	0.18644500
C	0.27150000	3.28242400	0.61216600
H	7.37375900	-2.25608900	-1.92919900
H	7.85653800	-2.21721300	0.53859300
H	6.13628300	-1.38597800	2.16700200
H	5.16076800	-1.46034100	-2.82724800
H	1.23950300	0.56250300	1.94983500
H	-5.12848900	-3.57511100	-0.69729900
H	-7.50464300	-3.10910600	-0.02989900
H	-8.15964900	-0.86811100	0.92710700
H	-6.42995700	0.95009200	1.19603500
H	1.04211700	-1.11762100	-2.01495200
H	1.97282300	-2.43416500	-1.20738800
H	2.51872400	-1.77954700	-2.79455300
H	2.01670400	1.31523900	-2.14411900
H	3.48400100	0.66777400	-2.95542600
H	3.64966300	1.67576700	-1.47185200
H	-3.01405600	2.61534500	-0.51900700
H	-4.76722200	2.39506700	-0.22085200
H	-3.97538200	1.53540400	-1.58874100
H	-4.09721200	1.79799000	2.25947100
H	-2.33508400	1.81533900	1.90946800
H	-3.09863600	0.33903600	2.59910000
H	4.16631600	-1.12528700	3.18430500
H	2.50264700	-0.50237800	3.12912300
H	-1.48204600	-2.37880200	-1.60935900
H	-3.06863100	-3.16350100	-1.81265000
H	-0.53100200	-1.27437700	0.15651100
H	4.02029100	1.09414400	4.38335200
H	3.40821200	1.90868500	2.89844500
H	5.09419300	1.26407000	2.94776600
H	-1.47692600	-4.72611800	-0.63890000
H	-2.81332300	-4.30273600	0.48688800
H	-1.19658300	-3.53541100	0.68055000
H	-0.89227400	1.78472100	-2.27832600

H	-0.95719100	4.17163900	-3.02253800
H	-0.22952200	6.02200300	-1.45294600
H	0.55969600	5.43125300	0.87995200
H	0.61672700	3.05548400	1.63279400