

Supporting Information

Influence of Donor Groups of Organic D- π -A Dyes on Open-circuit Voltage in Solid-state Dye- sensitized Solar Cells

Amalie Dualeh,^a Filippo De Angelis,^{,b} Simona Fantacci,^b Thomas Moehl,^a Chenyi Yi,^a Florian Kessler,^a Etienne Baranoff,^a Mohammad K. Nazeeruddin,^{*,a} Michael Grätzel^{*,a}*

Device fabrication. Fluorine-doped tin oxide glass substrates were etched using HCl and Zinc powder to give the correct electrode configuration. Compact TiO₂ layers were deposited by spray pyrolysis of titanium bis(acetylacetonate)diisopropoxide solution at 450°C using oxygen as a carrier gas after cleaning the substrates by ultrasonication in water and ozone treatment. Mesoporous TiO₂ layers of 2.4-2.7 μ m were prepared via screen-printing. Before and after the deposition of the nanocrystalline TiO₂ layer, the substrates were treated with 20 mM titanium tetrachloride solution at 70 °C for 30 min and sintered at 500 °C for 30min. After cooling to approx. 80°C the films were immersed in a 0.1 mM dye solution for 1 hour. The Y123 sensitizer was synthesized in our lab as reported previously.¹ The sensitizers C220 and C218 were provided by Prof. Peng Wang and JK2 by Prof. Jaejung Ko.

A 0.15 M solution of the hole transport material used, 2,2',7,7'-tetrakis(N,N-di-p-methoxyphenyl-amine)-9,9'-spirobifluorene (spiro-MeOTAD), was prepared in chlorobenzene. The Co(III) complex, tris(2-(1*H*-pyrazol-1-yl)pyridine)cobalt(III) tris(hexafluorophosphate), was added to give a solution which contained 1.3 % of the p-type dopant. This complex was synthesized according to a recently reported procedure.² Additionally 4-*tert*-butylpyridine (0.12 M) and lithium bis(trifluoromethylsulfonyl)-imide salt predissolved in acetonitrile (22.2 mM) were added to the HTM solution. 40 µl of the HTM solution was deposited onto the sensitized substrates and allowed to percolate for 30 s prior to spin coating for 30 s at 2000 rpm. A 200 nm thick silver electrode was deposited by thermal evaporation. The devices were fabricated and sealed under a dry atmosphere.

Device characterization. J-V characteristics of the cells were measured using a Keithley model 2400 digital source meter to record the generated photocurrent upon the application of an external potential bias. The irradiation source was a 450 W xenon lamp (Oriel), equipped with a Schott K113 Tempax sunlight filter to reduce the mismatch between the emission spectrum of the lamp and AM1.5G standard. The measurement of the IPCE spectra was recorded using a Keithley 2400 sourcemeter as a function of the wavelength using a constant white light bias. A 300 W xenon lamp (ILC technology) was used to provide an excitation beam, which was focused through a Gemini-180 double monochromator (Jobin Yvon Ltd.).

Electrochemical Impedance spectroscopy measurements. An Autolab PG30 was used to make the EIS measurements of the ssDSCs at various potentials. A sinusoidal potential perturbation of 10 mV was applied over a frequency range from 1 MHz to 0.1 Hz at 20 °C in the dark to record the impedance spectra.

UV-vis spectroscopy. The UV-vis absorption spectra were recorded in a 10 mm path length quartz cell using a Varian Cary 5 spectrophotometer.

Transient Photovoltage and Photocurrent decay measurements. An array of diodes (Lumiled model LXHL-NWE8 white star) was used to generate a white light bias and a perturbation excitation was produced using a red light pulsed diode (LXHLND98 redstar, 0.2 s square pulse width, 100 ns rise and fall time) controlled by a fast solid-state switch. The voltage and current dynamics were monitored via a Keithley sourcemeter. The voltage decay measurements were conducted at fixed current intervals along the photocurrent-voltage curve measuring the small perturbation transients. Similarly the photocurrent transient decay measurements were performed at fixed potential values.

Computational Details. To gain insight into the electronic and optical properties of the investigated dyes and their interaction with the TiO₂ semiconductor and the spiro-MeOTAD hole conductor, we performed DFT/TDDFT calculations on the C220 and Y123 dyes. The alkyl chains in the CPDT moiety of the two dyes were replaced by methyl groups for simplicity. We calculated the ground and excited states of the two dyes in solution along with the interaction of Y123 with TiO₂, in order to evaluate the dye adsorption geometry and orientation with respect to the semiconductor surface, therefore the dipole component normal to the surface. Furthermore, we evaluate the interaction of the two dyes with the spiro-MeOTAD by means of MP2 single point calculations at the geometry optimized by DFT. The inclusion of dispersion forces by the MP2 method, which are usually poorly described by DFT, is indeed mandatory to provide an accurate interaction energy for the expectedly weak dye/spiro interaction. Geometry optimizations for the dyes in their ground state have been carried out in vacuo using the B3LYP functional,³ while TDDFT excited state calculations were carried out in chloroform solution by the MPW1K functional,⁴ which has shown to provide accurate excitation energies for this class of push-pull dyes.^{5,6} All these calculations, as well as MP2 single point energy evaluations, have been carried out with a 6-31G* basis set as implemented in the Gaussian 03 program package⁷.

Geometry optimization of Y123 on TiO_2 and of the adducts formed by C220 and Y123 with spiro-MeOTAD were performed by the ADF program package,⁸ using the PBE/PBE functional⁹ and a DZ basis set for all atoms. To model the TiO_2 semiconductor we considered a neutral stoichiometric anatase $(\text{TiO}_2)_{38}$ cluster exposing the majority (101) surfaces.^{10,11} Since we are interested here only in the dye orientation with respect to the surface, the use of a reduced TiO_2 model seems fully justified.

Dye adsorption measurements. TiO_2 films of 2.5 μm thickness were sensitized with 0.1 mM dye solution for 1 hour. The dye was then desorbed from the sample by treatment with 0.01 M solution of tetrabutylammonium hydroxide (TBAOH) in dimethylformamide (DMF). The UV-vis spectrum of the resulting dye solution was recorded as described above. Making use of the linear relationship between the absorbance and concentration of the dye, the extent of dye loading on the TiO_2 surface was determined.

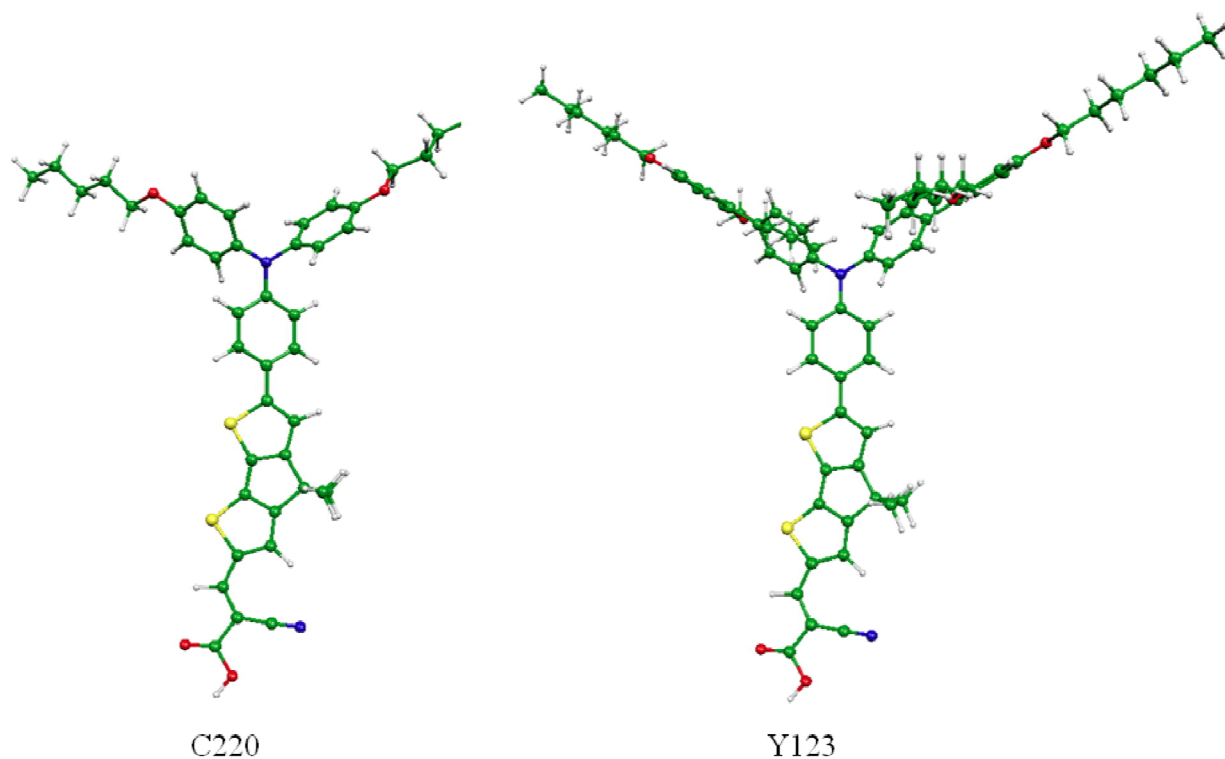


Figure S1. Optimized geometries of the C220 and Y123 dyes.

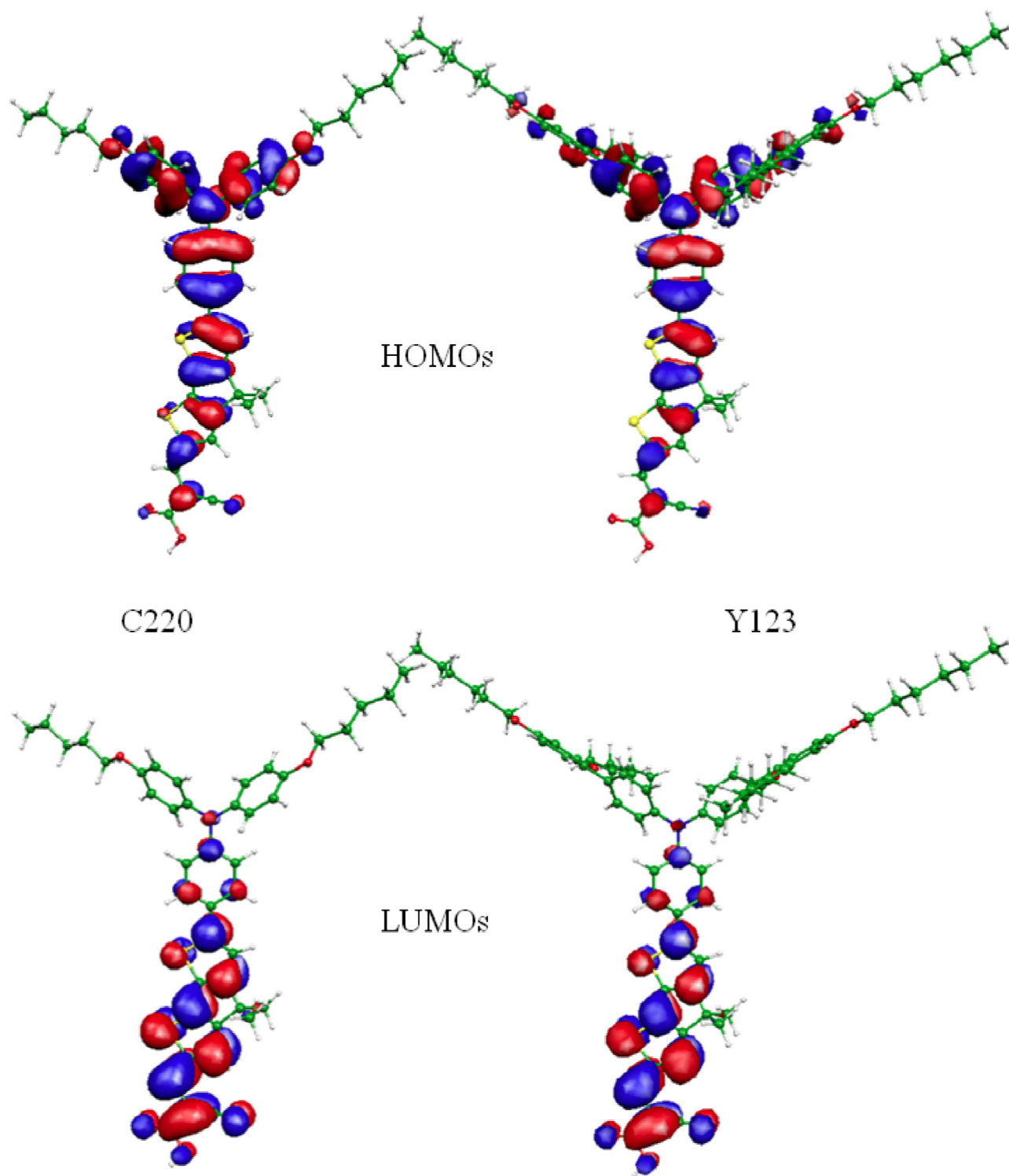


Figure S2. Isodensity plots of the HOMOs and LUMOs for the C220 and Y123 dyes.

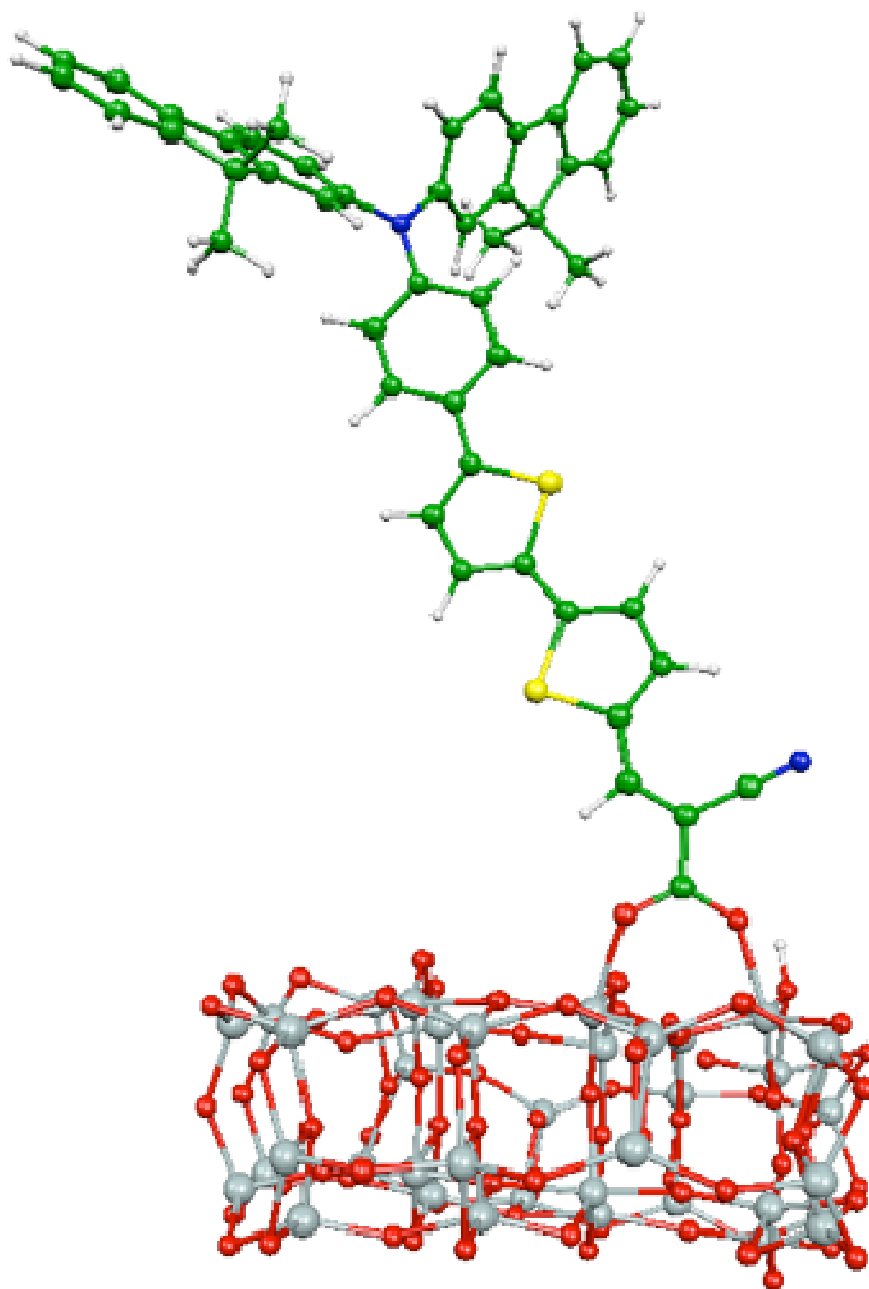


Figure S3. Adsorption geometry of JK2 on TiO₂.

Calculated TDDFT excitation energies, oscillator strengths and composition in terms of Molecular Orbital (MO) contributions for the C220 and Y123 dyes:

Protonated C220 dye (HOMO=190, LUMO=191)

Excited State 1: Singlet-?Sym 2.3803 eV 520.88 nm f=1.7967

189 ->191 0.21370

190 ->191 0.62484

190 ->192 0.10169

Excited State 2: Singlet-?Sym 3.2040 eV 386.97 nm f=0.1307

187 ->191 -0.11669

189 ->191 0.61604

190 ->191 -0.25452

Excited State 3: Singlet-?Sym 3.8375 eV 323.08 nm f=0.2216

189 ->192 0.13101

190 ->191 -0.10857

190 ->192 0.63514

190 ->194 -0.12488

Excited State 4: Singlet-?Sym 4.2129 eV 294.30 nm f=0.0306

189 ->193 -0.13522

190 ->193 0.64360

Excited State 5: Singlet-?Sym 4.3014 eV 288.24 nm f=0.0319

181 ->191 -0.18068

186 ->191 -0.10363

187 ->191 0.61363

189 ->191 0.13403

Deprotonated C220 dye (HOMO=190, LUMO=191)

Excited State 1: Singlet-A 2.7194 eV 455.92 nm f=1.8143

189 ->191 0.24149

190 ->191 0.60999

190 ->192 0.11497

Excited State 2: Singlet-A 3.5002 eV 354.22 nm f=0.0238

189 ->191 0.60053

190 ->191 -0.24385

190 ->192 -0.14827

Excited State 3: Singlet-A 3.9354 eV 315.05 nm f=0.1468

189 ->191 0.12334

189 ->192 0.17496

190 ->191 -0.16634

190 ->192 0.61388

Excited State 4: Singlet-A 4.1465 eV 299.01 nm f=0.0316

189 ->193 -0.19204

190 ->193 0.64145

Excited State 5: Singlet-A 4.2030 eV 294.99 nm f=0.0003

186 ->191 0.63371

186 ->192 -0.23957

Protonated JK2 dye (HOMO=193, LUMO=194)

Excited State 1: Singlet-A 2.4464 eV 506.80 nm f=1.5546

192 ->194 -0.25737

193 ->194 0.61331

193 ->195 0.12503

Excited State 2: Singlet-A 3.1832 eV 389.49 nm f=0.3106

190 ->194 0.14790

192 ->194 0.58946

193 ->194 0.29813

Excited State 3: Singlet-A 3.6775 eV 337.14 nm f=0.3466

192 ->195 -0.11721

193 ->194 -0.12876

193 ->195 0.62220

193 ->197 -0.16192

Excited State 4: Singlet-A 3.8060 eV 325.76 nm f=1.0000

191 ->197 0.10087

192 ->196 0.14133

193 ->196 0.65268

Excited State 5: Singlet-A 4.0731 eV 304.40 nm f=0.0087

191 ->194 0.69770

Deprotonated JK dye (HOMO=193, LUMO=194)

Excited State 1: Singlet-A 2.8137 eV 440.65 nm f=1.7146

192 ->194 0.30825

193 ->194 0.57786

193 ->195 0.14863

Excited State 2: Singlet-A 3.4765 eV 356.64 nm f=0.1259

190 ->194 -0.10761

192 ->194 0.56703

193 ->194 -0.29961

193 ->195 -0.16667

Excited State 3: Singlet-A 3.7690 eV 328.96 nm f=1.1730

191 ->197 0.10334

192 ->196 -0.17281

193 ->196 0.64501

Excited State 4: Singlet-A 3.8794 eV 319.59 nm f=0.2346

192 ->194 0.10837

192 ->195 0.14651

192 ->197 -0.11040

193 ->194 -0.22470

193 ->195 0.59263

193 ->197 0.13749

Excited State 5: Singlet-A 4.1457 eV 299.07 nm f=0.0003

187 ->194 0.62638

187 ->195 -0.24666

Protonated Y123 dye (HOMO=294, LUMO=295)

Excited State 1: Singlet-?Sym 2.3886 eV 519.07 nm f=1.8730

293 -> 295 0.25272

294 -> 295 0.60904

294 -> 296 0.10994

Excited State 2: Singlet-?Sym 3.1409 eV 394.74 nm f=0.1380

291 -> 295 -0.17364

293 -> 295 0.58259

294 -> 295 -0.29514

Excited State 3: Singlet-?Sym 3.7715 eV 328.74 nm f=0.2980

293 -> 296 0.13394

294 -> 295 -0.12202

294 -> 296 0.61329

294 -> 298 0.14035

Excited State 4: Singlet-?Sym 3.8142 eV 325.06 nm f=0.0631

292 -> 295 0.69714

Excited State 5: Singlet-?Sym 4.0075 eV 309.38 nm f=1.0185

292 -> 298 0.10528

293 -> 297 -0.17773

294 -> 297 0.63645

Deprotonated Y123 dye (HOMO=294, LUMO=295)

Excited State 1: Singlet-A 2.7482 eV 451.14 nm f=1.8846

293 -> 295 0.27615

294 -> 295 0.59346

294 -> 296 0.11615

Excited State 2: Singlet-A 3.4958 eV 354.66 nm f=0.0090

291 -> 295 -0.12910

293 -> 295 0.57520

294 -> 295 -0.27213

294 -> 296 -0.16776

Excited State 3: Singlet-A 3.9357 eV 315.03 nm f=0.1880

293 -> 295 0.13584

293 -> 296 0.18043

293 -> 299 0.10652

294 -> 295 -0.18259

294 -> 296 0.60174

Excited State 4: Singlet-A 4.0286 eV 307.76 nm f=1.2240

292 -> 299 0.10458

293 -> 297 -0.25488

294 -> 297 0.61000

Excited State 5: Singlet-A 4.1978 eV 295.36 nm f=0.0003

288 -> 295 0.63243

288 -> 296 -0.23742

The X, Y, Z coordinates of the optimized geometries of C220, JK2 and Y123 (protonated and deprotonated structures):

95

Protonated C220 dye

C	5.655894	1.939724	1.216699
C	4.685968	1.547287	0.277934
C	4.238799	2.489197	-0.655418
C	4.725774	3.796596	-0.643360
C	5.692653	4.180674	0.291002
C	6.156049	3.232457	1.216699
N	4.189436	0.201057	0.270308
C	5.138103	-0.874138	0.357454
C	4.973778	-1.901985	1.302643
C	5.892928	-2.936552	1.385899
C	7.015537	-2.966927	0.542921
C	7.191665	-1.937693	-0.387376
C	6.255544	-0.907612	-0.482075
O	7.873010	-4.039510	0.710949
C	9.052610	-4.145362	-0.155549
C	9.765633	-5.431536	0.263023
C	11.030591	-5.687374	-0.582539
C	11.759522	-6.986403	-0.172839
O	6.247488	5.445058	0.385652
C	5.795012	6.488632	-0.541174
C	6.579824	7.746883	-0.168642
C	6.202997	8.945608	-1.064081
C	6.993415	10.222398	-0.701246
C	2.811077	-0.068174	0.162905
C	1.846714	0.863321	0.601030
C	0.492171	0.591886	0.489295
C	0.025584	-0.620141	-0.059480
C	0.994073	-1.548501	-0.494487
C	2.349896	-1.282702	-0.387749
C	-1.397455	-0.915790	-0.176849
C	-2.012631	-2.161214	-0.240792
C	-3.415831	-2.071805	-0.351637
C	-3.877283	-0.754340	-0.369061
S	-2.587774	0.388419	-0.265652
C	-5.305453	-0.755299	-0.468812
C	-5.763638	-2.085286	-0.516231
C	-7.152286	-2.184849	-0.616911
C	-7.784466	-0.931082	-0.648208
S	-6.585620	0.379751	-0.547913
C	-9.154735	-0.586688	-0.741305
C	-10.251885	-1.403214	-0.829020
C	-11.560441	-0.731275	-0.912296
O	-11.745740	0.486217	-0.910307
C	-10.201036	-2.812665	-0.843840
N	-10.114034	-3.977943	-0.853527

O	-12.584753	-1.649626	-0.995370
H	4.117189	-1.882344	1.964502
H	5.777362	-3.735111	2.106629
H	8.047042	-1.931287	-1.048992
H	6.394177	-0.117253	-1.208921
H	6.013392	1.218133	1.939899
H	6.902633	3.546028	1.934183
H	4.354488	4.501119	-1.374911
H	3.499517	2.198708	-1.391228
H	2.175111	1.795457	1.040226
H	-0.221399	1.316311	0.867285
H	0.673529	-2.474176	-0.957936
H	3.070471	-2.005784	-0.744863
H	-9.407046	0.472345	-0.746208
H	8.746250	-4.193852	-1.208933
H	9.705281	-3.273077	-0.018171
H	6.000747	6.192489	-1.578426
H	4.714967	6.653255	-0.429597
H	-13.447012	-1.154654	-1.049802
H	10.028302	-5.352873	1.323978
H	9.063034	-6.265519	0.154557
H	10.755468	-5.751444	-1.644615
H	11.722377	-4.840064	-0.476077
C	13.019115	-7.239083	-1.028049
H	12.039181	-6.922046	0.886799
H	11.068051	-7.832985	-0.275220
H	6.377245	7.981298	0.882485
H	7.649419	7.526824	-0.260844
H	6.394544	8.693470	-2.116477
H	5.127626	9.151363	-0.969124
C	6.608364	11.417581	-1.598647
H	6.804523	10.474301	0.350443
H	8.067829	10.018764	-0.798386
C	-4.583372	-3.061689	-0.441257
C	-4.488803	-3.922708	-1.724984
C	-4.668207	-3.941721	0.830476
H	-4.733905	-3.312929	1.722504
H	-5.552921	-4.585885	0.782901
H	-3.778204	-4.576159	0.907632
H	-3.595080	-4.555482	-1.687262
H	-5.369853	-4.568104	-1.809593
H	-4.432643	-3.281048	-2.608497
H	-7.707171	-3.110162	-0.666392
H	-1.457628	-3.086242	-0.174862
H	7.178454	12.312927	-1.327848
H	6.809561	11.188820	-2.651805
H	5.541186	11.647199	-1.497084
H	13.522420	-8.163270	-0.723905
H	12.753464	-7.326570	-2.088085
H	13.729791	-6.411084	-0.921598

94

Deprotonated C220 dye

C	5.244401	2.139823	1.367850
C	4.385128	1.589701	0.229168
C	4.409813	2.454827	-0.856494
C	5.236754	3.587508	-0.552351

C	5.739947	3.440673	0.735274
S	3.450016	1.870852	-2.173621
C	3.006218	0.417851	-1.254136
C	3.595106	0.443815	0.001338
C	6.567994	4.504984	1.140760
C	6.709171	5.484383	0.161753
S	5.778839	5.050157	-1.294279
C	2.129208	-0.596413	-1.828341
C	1.918330	-0.711555	-3.217902
C	1.086742	-1.687308	-3.753084
C	0.415478	-2.596212	-2.919449
C	0.612116	-2.491426	-1.532103
C	1.448085	-1.516719	-1.003608
N	-0.441417	-3.590922	-3.463001
C	-0.428023	-4.906711	-2.926704
C	0.789468	-5.544793	-2.624221
C	0.808318	-6.827060	-2.094916
C	-0.387985	-7.524257	-1.871149
C	-1.604604	-6.905632	-2.177147
C	-1.617700	-5.605424	-2.688141
O	-0.256662	-8.787968	-1.360207
C	-1.433615	-9.545684	-1.104374
C	-1.003739	-10.897696	-0.550088
C	-2.192786	-11.814261	-0.235999
C	-1.769450	-13.178371	0.324248
C	-2.955763	-14.095381	0.638467
C	7.445020	6.723486	0.136656
C	8.221509	7.294746	1.093071
C	8.438289	6.699070	2.368639
N	8.595271	6.182793	3.404936
C	4.402427	2.416279	2.632947
C	6.418839	1.194964	1.704217
C	-1.341815	-3.260779	-4.511808
C	-1.552247	-4.145247	-5.585945
C	-2.435385	-3.826461	-6.607935
C	-3.120444	-2.602759	-6.603534
C	-2.911062	-1.709553	-5.547529
C	-2.039760	-2.046756	-4.509351
O	-3.958565	-2.381922	-7.663700
C	-4.656874	-1.142968	-7.732119
C	-5.492729	-1.149978	-9.005294
C	-6.281215	0.150787	-9.202070
C	-7.137009	0.149961	-10.475476
C	-7.915640	1.453410	-10.679104
C	8.923809	8.683558	0.795939
O	9.609133	9.109629	1.746945
O	8.685078	9.139179	-0.341660
H	1.723095	-5.021455	-2.804437
H	1.747438	-7.318755	-1.859969
H	-2.547778	-7.413621	-2.010229
H	-2.568106	-5.129926	-2.909307
H	-1.016691	-5.089019	-5.611770
H	-2.597605	-4.508744	-7.436974
H	-3.426438	-0.756524	-5.510285
H	-1.893237	-1.350442	-3.689895
H	0.958799	-1.755864	-4.829018
H	2.441237	-0.042473	-3.896143

H	1.550250	-1.443342	0.075095
H	0.090896	-3.173160	-0.866939
H	7.401596	7.331148	-0.768653
H	-2.074854	-9.016088	-0.383232
H	-2.011155	-9.672714	-2.032990
H	-5.299855	-1.022045	-6.846975
H	-3.941037	-0.307091	-7.740945
H	-0.339115	-11.378713	-1.279409
H	-0.406838	-10.730576	0.355745
H	-2.859217	-11.319114	0.485920
H	-2.790641	-11.967946	-1.146719
H	-1.103454	-13.673609	-0.396274
H	-1.172571	-13.025041	1.234221
H	-4.825231	-1.319095	-9.860185
H	-6.179211	-2.005966	-8.968945
H	-6.930824	0.324079	-8.331162
H	-5.584541	1.001374	-9.235978
H	-6.489680	-0.030439	-11.345203
H	-7.838928	-0.695109	-10.438250
H	7.021736	0.987980	0.814582
H	7.069702	1.647405	2.460831
H	6.047814	0.241300	2.099646
H	4.000129	1.481565	3.042844
H	5.017320	2.890528	3.406157
H	3.563736	3.082293	2.407357
H	7.059748	4.587251	2.102467
H	3.470256	-0.364131	0.715180
H	-8.518255	1.420295	-11.594009
H	-8.595141	1.645234	-9.839446
H	-7.237849	2.312259	-10.757743
H	-2.620862	-15.060028	1.036604
H	-3.621962	-13.641245	1.382392
H	-3.551896	-14.294901	-0.260584

90

Protonated JK2 dye

C	8.075332	-4.503955	-1.026909
C	6.854492	-4.202568	-0.419159
C	6.202445	-5.153949	0.391730
C	6.769902	-6.406637	0.595177
C	7.993181	-6.709658	-0.015218
C	8.639137	-5.764738	-0.819208
C	4.889430	-4.595404	0.941280
C	4.885023	-3.193958	0.329509
C	6.036725	-2.985944	-0.455901
C	3.936981	-2.192189	0.477381
C	4.121898	-0.962407	-0.182155
C	5.268516	-0.761287	-0.970363
C	6.228163	-1.762897	-1.102371
N	3.162423	0.081881	-0.042301
C	3.617829	1.414125	0.186882
C	3.082689	2.483747	-0.554676
C	3.540419	3.771937	-0.319045
C	4.545720	4.013981	0.638904
C	5.084887	2.953036	1.369739
C	4.613821	1.660561	1.147371
C	4.836587	5.451211	0.659116

C	4.009641	6.086884	-0.289278
C	3.108832	5.073501	-0.995918
C	4.087705	7.462396	-0.475405
C	4.994965	8.204864	0.290376
C	5.814562	7.572788	1.231262
C	5.742078	6.191319	1.422655
C	1.614636	5.371093	-0.736845
C	3.382693	5.038383	-2.516171
C	4.902790	-4.538196	2.485441
C	3.677612	-5.421873	0.455418
C	1.782913	-0.194022	-0.122814
C	0.853081	0.530862	0.646696
C	-0.504303	0.256367	0.563777
C	-1.003339	-0.753821	-0.280915
C	-0.065583	-1.471326	-1.050582
C	1.292505	-1.200564	-0.977840
C	-2.427609	-1.062651	-0.364292
S	-3.646424	0.115222	0.085736
C	-4.957757	-0.998684	-0.272845
C	-4.444536	-2.198415	-0.732034
C	-3.034026	-2.233298	-0.782647
C	-6.331044	-0.615402	-0.079938
S	-7.642522	-1.675807	-0.528002
C	-8.856499	-0.515281	0.012966
C	-8.231479	0.627956	0.505541
C	-6.831056	0.570279	0.452952
C	-10.230469	-0.868806	-0.113487
C	-11.354381	-0.158976	0.224657
C	-11.317812	1.143136	0.800236
N	-11.252974	2.207606	1.270048
C	-12.667635	-0.801461	-0.030946
O	-13.704405	-0.014834	0.338910
O	-12.817713	-1.906254	-0.516060
H	5.399918	0.189071	-1.477629
H	7.107610	-1.587303	-1.716623
H	3.054824	-2.338045	1.094325
H	1.204758	1.301801	1.323702
H	-1.188000	0.814930	1.197748
H	-0.411305	-2.230349	-1.746239
H	1.985532	-1.757943	-1.598839
H	5.015271	0.828060	1.716367
H	5.856251	3.124118	2.116201
H	2.320403	2.283833	-1.302420
H	6.276018	-7.148591	1.218557
H	8.444024	-7.686642	0.137090
H	9.588353	-6.013688	-1.286249
H	3.455195	7.963785	-1.204476
H	5.062535	9.280657	0.152448
H	6.514213	8.161757	1.818359
H	6.382244	5.705242	2.154680
H	-2.472387	-3.109543	-1.085802
H	-5.071757	-3.040209	-1.007330
H	5.753795	-3.954854	2.851326
H	3.982997	-4.077993	2.864763
H	4.972913	-5.546781	2.908826
H	3.652804	-5.479965	-0.637529
H	3.723093	-6.443269	0.850585

H	2.738787	-4.970459	0.796877
H	4.437023	4.827972	-2.722146
H	2.776716	4.264898	-3.002241
H	3.129559	6.000641	-2.975831
H	1.399139	5.403102	0.335980
H	1.332948	6.337370	-1.170784
H	0.981141	4.600781	-1.191789
H	8.582046	-3.773121	-1.652235
H	-6.188806	1.371972	0.800988
H	-8.780828	1.476270	0.893911
H	-10.448697	-1.845958	-0.540677
H	-14.512391	-0.520220	0.132717

89

Deprotonated JK2 dye

C	7.896126	-4.505035	-1.264702
C	6.843169	-4.101988	-0.459836
S	6.440208	-5.379494	0.672022
C	7.696489	-6.442284	0.038972
C	8.373457	-5.803692	-0.990433
C	6.125668	-2.853105	-0.468268
S	6.641121	-1.517620	-1.491293
C	5.325598	-0.486122	-0.940588
C	4.564891	-1.162722	-0.009921
C	5.006937	-2.480606	0.255423
C	5.155392	0.872183	-1.448189
C	5.710561	1.288715	-2.674713
C	5.536521	2.582660	-3.151056
C	4.804285	3.524158	-2.412707
C	4.249277	3.125994	-1.185903
C	4.420588	1.829708	-0.718110
N	4.634274	4.855463	-2.891871
C	5.749012	5.561159	-3.414376
C	7.015839	5.433983	-2.810883
C	8.098618	6.117396	-3.343193
C	7.945919	6.951654	-4.468380
C	6.691107	7.085205	-5.067117
C	5.604700	6.385784	-4.547172
C	9.246500	7.545897	-4.791347
C	10.195972	7.074257	-3.860763
C	9.548609	6.119271	-2.857288
C	11.520331	7.488041	-3.940283
C	11.900178	8.376327	-4.954474
C	10.958306	8.843383	-5.876777
C	9.625208	8.432462	-5.802281
C	10.168673	4.706331	-2.943106
C	9.660322	6.656586	-1.413094
C	7.844648	-7.747818	0.635391
C	8.719625	-8.742630	0.341420
C	8.663146	-10.094855	1.167001
O	7.777776	-10.113036	2.046920
C	3.355185	5.464830	-2.832707
C	2.197580	4.713422	-3.118111
C	0.952606	5.319142	-3.041502
C	0.829922	6.680469	-2.699366
C	1.974398	7.431105	-2.420885
C	3.225505	6.822280	-2.478572

C	-0.590621	7.041446	-2.713144
C	-1.338333	5.898547	-3.066140
C	-0.420468	4.698485	-3.303246
C	-2.723490	5.967918	-3.156011
C	-3.366896	7.183609	-2.890974
C	-2.624881	8.316085	-2.540757
C	-1.232262	8.253948	-2.449552
C	-0.537915	4.174539	-4.751821
C	-0.717267	3.556955	-2.304718
C	9.700321	-8.631268	-0.686452
N	10.494042	-8.512110	-1.535015
O	9.513831	-10.933117	0.808902
H	4.117859	7.394280	-2.246395
H	1.900668	8.479939	-2.143730
H	2.297747	3.668076	-3.394582
H	5.964623	2.869785	-4.106542
H	6.263010	0.576465	-3.281388
H	4.008794	1.560897	0.250081
H	3.693518	3.846600	-0.593630
H	4.630376	6.470139	-5.017214
H	6.554442	7.714116	-5.943517
H	7.127137	4.799150	-1.936890
H	-3.308663	5.091937	-3.427185
H	-4.449937	7.246562	-2.957480
H	-3.136203	9.253625	-2.337378
H	12.259735	7.129064	-3.227742
H	12.934142	8.703758	-5.025455
H	11.266238	9.532051	-6.659525
H	8.897575	8.798914	-6.522383
H	3.682747	-0.732415	0.452885
H	4.510098	-3.151981	0.947516
H	-0.328954	4.968382	-5.476184
H	0.170209	3.356305	-4.926281
H	-1.547146	3.792196	-4.944611
H	-0.642799	3.909233	-1.270938
H	-1.727655	3.160369	-2.458959
H	-0.007602	2.732292	-2.437013
H	9.227639	7.658933	-1.330601
H	9.134076	5.997404	-0.713172
H	10.709648	6.709480	-1.100088
H	10.102838	4.308650	-3.960820
H	11.225483	4.729281	-2.652895
H	9.649627	4.013595	-2.271051
H	-0.660993	9.138215	-2.177560
H	8.310724	-3.874047	-2.045397
H	9.188283	-6.274135	-1.526136
H	7.173753	-8.022349	1.450704

159

Protonated Y123 dye

C	-4.731552	-2.905278	-0.430928
C	-3.555439	-1.926275	-0.333690
C	-4.003685	-0.604363	-0.364475
C	-5.430659	-0.592152	-0.479833
C	-5.901281	-1.917971	-0.523518
S	-2.704602	0.526417	-0.251722
C	-1.528508	-0.788633	-0.140301

C	-2.154806	-2.028539	-0.205172
C	-7.289844	-2.004699	-0.636028
C	-7.909514	-0.745040	-0.680385
S	-6.698868	0.554709	-0.577680
C	-0.104443	-0.506981	-0.001362
C	0.364717	0.704360	0.546390
C	1.720287	0.958579	0.686239
C	2.680095	0.010527	0.277930
C	2.217290	-1.200574	-0.276765
C	0.860781	-1.450778	-0.410459
N	4.061662	0.265942	0.417192
C	4.986683	-0.810334	0.617664
C	4.703593	-1.846915	1.520685
C	5.604332	-2.887996	1.713981
C	6.830383	-2.929541	1.022635
C	7.113154	-1.870931	0.139152
C	6.208447	-0.834950	-0.069339
C	7.789134	-4.055270	1.163786
C	-9.275548	-0.388071	-0.786448
C	-10.380144	-1.194419	-0.875906
C	-10.343281	-2.604376	-0.878761
N	-10.267808	-3.770502	-0.877656
C	-4.631406	-3.773294	-1.709662
C	-4.838775	-3.778637	0.843723
C	4.565266	1.606932	0.356982
C	5.533078	2.044559	1.271554
C	6.035302	3.339953	1.199054
C	5.582193	4.252148	0.227872
C	4.617322	3.797492	-0.691049
C	4.122834	2.499541	-0.631720
C	6.090492	5.647725	0.227093
C	-11.681264	-0.510350	-0.973788
O	-12.714216	-1.419198	-1.056444
O	-11.854728	0.708864	-0.982807
H	3.769373	-1.831747	2.067875
H	5.379961	-3.665373	2.427871
H	8.062724	-1.854009	-0.382598
H	6.448494	-0.030983	-0.753208
H	5.898258	1.359462	2.025916
H	6.802684	3.648078	1.899307
H	4.281854	4.464054	-1.470625
H	3.385865	2.168409	-1.352662
H	2.052248	1.890293	1.123835
H	-0.347436	1.441033	0.902555
H	0.538259	-2.375259	-0.874796
H	2.936938	-1.934999	-0.612162
H	-9.517328	0.673323	-0.801067
H	-13.570912	-0.915847	-1.120940
H	-4.908439	-3.145194	1.732156
H	-5.729030	-4.414557	0.789106
H	-3.955783	-4.421126	0.933631
H	-3.744280	-4.414403	-1.659313
H	-5.517754	-4.410464	-1.800979
H	-4.559310	-3.136354	-2.595432
H	-7.853194	-2.924924	-0.684605
H	-1.609669	-2.958430	-0.126886
C	8.502200	-4.516662	0.043577

C	9.431772	-5.543493	0.123032
C	9.679634	-6.156994	1.355860
C	8.979122	-5.728613	2.485700
C	8.040807	-4.695786	2.398417
H	8.298166	-4.063551	-0.919013
H	9.968076	-5.894849	-0.747397
O	10.617612	-7.174923	1.360574
H	9.161051	-6.199396	3.438806
O	7.321424	-4.251202	3.497943
C	6.333558	6.308945	1.443261
C	6.839917	7.599249	1.500433
C	7.121710	8.283978	0.313168
C	6.879500	7.658139	-0.911857
C	6.366167	6.358642	-0.962694
H	6.095614	5.793522	2.365960
H	7.016244	8.100997	2.441620
O	7.623726	9.566603	0.447829
H	7.087740	8.181839	-1.831562
O	6.107345	5.707082	-2.159415
C	10.898853	-7.876563	2.616555
C	11.951810	-8.934376	2.283954
H	11.278352	-7.172966	3.369773
H	9.983848	-8.345859	3.002435
C	7.644276	-4.765362	4.833591
C	6.744779	-4.001058	5.805923
H	7.445559	-5.843959	4.886696
H	8.703923	-4.588614	5.059233
C	7.939223	10.340748	-0.756309
C	8.473767	11.685202	-0.261070
H	8.695503	9.818874	-1.357892
H	7.037194	10.480286	-1.367195
C	6.516355	6.325093	-3.425616
C	6.212913	5.293691	-4.513184
H	5.952996	7.251715	-3.597820
H	7.588061	6.561399	-3.401105
C	12.333935	-9.767705	3.525049
H	11.550904	-9.585554	1.499112
H	12.835810	-8.429053	1.879123
C	13.401068	-10.839490	3.212331
H	12.715761	-9.100949	4.311025
H	11.436470	-10.260893	3.924063
C	13.776892	-11.680170	4.452039
H	13.024843	-11.505963	2.423942
H	14.303069	-10.349526	2.820619
C	14.846012	-12.746801	4.132214
H	14.148767	-11.011873	5.240151
H	12.873937	-12.169154	4.841276
H	15.097258	-13.332891	5.023050
H	14.483825	-13.435498	3.359855
H	15.763559	-12.273502	3.763462
C	6.985654	-4.431551	7.268113
H	6.940815	-2.929799	5.687535
H	5.700110	-4.181588	5.527925
C	6.074170	-3.675722	8.259914
H	6.805942	-5.511245	7.367762
H	8.035933	-4.249504	7.535650
C	6.310975	-4.100036	9.725712

H	6.251035	-2.595783	8.162705
H	5.023237	-3.857857	7.995978
C	5.392790	-3.341202	10.707721
H	6.137236	-5.180292	9.820029
H	7.361512	-3.916562	9.987802
H	5.577345	-3.653413	11.741474
H	5.566154	-2.260863	10.639801
H	4.338720	-3.532527	10.474798
C	8.856455	12.616845	-1.430102
H	7.704100	12.154984	0.361476
H	9.346729	11.496333	0.373722
C	9.402713	13.976947	-0.942928
H	9.617346	12.128004	-2.054551
H	7.975838	12.790123	-2.064428
C	9.789865	14.913413	-2.108444
H	8.643548	14.469604	-0.319986
H	10.283439	13.806711	-0.308422
C	10.336758	16.268242	-1.609829
H	10.546605	14.418016	-2.731237
H	8.908710	15.082564	-2.741496
H	10.605685	16.918572	-2.449432
H	9.585564	16.785986	-1.001958
H	11.230274	16.118286	-0.992427
C	6.613696	5.803590	-5.913597
H	6.756480	4.373054	-4.274195
H	5.141566	5.064434	-4.487959
C	6.326837	4.765152	-7.020435
H	6.065728	6.729256	-6.138881
H	7.685033	6.048483	-5.921469
C	6.727068	5.268263	-8.424637
H	6.875228	3.839508	-6.797828
H	5.256434	4.517601	-7.016320
C	6.442659	4.220277	-9.521944
H	6.176043	6.191909	-8.646469
H	7.795914	5.520357	-8.424921
H	6.731588	4.595224	-10.509934
H	7.003122	3.298329	-9.327686
H	5.375410	3.971116	-9.548469

158

Deprotonated Y123 dye

C	-4.771687	-2.934930	-0.538252
C	-3.681886	-2.036345	-0.471100
C	-3.990983	-0.666744	-0.490564
C	-5.292193	-0.186199	-0.569302
C	-6.351926	-1.095079	-0.628820
C	-6.092658	-2.470909	-0.615149
C	-2.264841	-2.477219	-0.400350
C	-1.281355	-1.820686	-1.160302
C	0.064675	-2.161435	-1.071162
C	0.482742	-3.199527	-0.223372
C	-0.492682	-3.871919	0.532268
C	-1.832664	-3.511615	0.448645
N	1.852015	-3.557414	-0.123797
C	2.680689	-3.565513	-1.274963
C	4.006685	-3.104836	-1.210017
C	4.823118	-3.122356	-2.334947

C	4.354137	-3.584779	-3.577335
C	3.023695	-4.035205	-3.631647
C	2.203137	-4.037965	-2.508008
C	5.217172	-3.654762	-4.784676
C	5.183486	-4.790460	-5.609584
C	5.951540	-4.911712	-6.761271
C	6.802960	-3.865411	-7.125889
C	6.868385	-2.711538	-6.335356
C	6.082449	-2.608130	-5.178956
O	7.536516	-4.053831	-8.264601
C	8.452051	-3.042446	-8.671734
C	9.150353	-3.523637	-9.937091
C	10.172122	-2.508094	-10.463469
C	10.890055	-2.975268	-11.736384
C	11.916450	-1.964576	-12.263371
C	12.630755	-2.435801	-13.534269
O	6.095841	-1.495166	-4.385180
C	6.878710	-0.367042	-4.762376
C	6.654544	0.723012	-3.722269
C	7.439913	2.002971	-4.035450
C	7.230444	3.108297	-2.992283
C	8.007568	4.394493	-3.300444
C	7.794759	5.492808	-2.253685
O	-7.605628	-0.553466	-0.694725
C	-8.735687	-1.419223	-0.713413
C	-9.986160	-0.549775	-0.738786
C	-11.278885	-1.375215	-0.756322
C	-12.545344	-0.509426	-0.773119
C	-13.844374	-1.325175	-0.788679
C	-15.103751	-0.452721	-0.802558
O	-4.465270	-4.267386	-0.541209
C	-5.504930	-5.231371	-0.673842
C	-4.861085	-6.611840	-0.680338
C	-5.891680	-7.738809	-0.825567
C	-5.259420	-9.136669	-0.824752
C	-6.283288	-10.270219	-0.966023
C	-5.645043	-11.663044	-0.962877
C	2.403134	-3.896728	1.144585
C	2.109563	-3.135025	2.285934
C	2.644882	-3.473463	3.522831
C	3.504231	-4.580106	3.679942
C	3.789082	-5.336624	2.522992
C	3.252416	-5.006294	1.285791
C	4.082481	-4.941126	4.969425
S	3.337625	-4.405268	6.489613
C	4.557323	-5.214593	7.413622
C	5.479558	-5.863540	6.603364
C	5.209062	-5.707579	5.228135
C	4.900936	-5.416023	8.792341
C	6.049184	-6.197126	8.857303
C	6.540744	-6.559850	7.455692
C	6.476299	-6.461772	10.172651
C	5.654762	-5.882334	11.135451
S	4.321205	-4.988946	10.362511
C	6.536381	-8.088435	7.235153
C	7.950160	-5.986429	7.190266
C	5.706036	-5.888041	12.575878

C	6.595627	-6.481379	13.412952
C	6.412668	-6.324041	14.979034
O	5.422039	-5.638849	15.307308
C	7.700813	-7.249181	12.946094
N	8.596996	-7.872542	12.529734
O	7.289037	-6.910611	15.645026
H	4.396518	-2.737628	-0.266055
H	5.842609	-2.763577	-2.250223
H	2.619900	-4.387854	-4.577190
H	1.182232	-4.398524	-2.583790
H	0.798362	-1.626674	-1.665900
H	-1.576793	-1.025557	-1.839890
H	-2.559315	-4.046446	1.049492
H	-0.190926	-4.676325	1.195452
H	1.462756	-2.267649	2.196722
H	2.417034	-2.846349	4.380615
H	4.414842	-6.220326	2.605136
H	3.478723	-5.617848	0.417612
H	4.931998	-5.346436	13.121877
H	7.965862	-4.902242	7.338729
H	8.680852	-6.435877	7.872107
H	8.267812	-6.198892	6.161860
H	6.831367	-8.331826	6.206928
H	7.242847	-8.575882	7.916433
H	5.541887	-8.507553	7.417017
H	7.345157	-7.048433	10.445145
H	5.826303	-6.114408	4.433439
H	4.541558	-5.616711	-5.317291
H	5.916627	-5.804664	-7.376452
H	7.519539	-1.896669	-6.617025
H	-3.172675	0.043975	-0.417956
H	-5.506462	0.877321	-0.570034
H	-6.908177	-3.177557	-0.669639
H	7.915103	-2.100390	-8.861079
H	9.185470	-2.854787	-7.872925
H	7.943017	-0.643306	-4.810072
H	6.577242	-0.018513	-5.761727
H	-8.698650	-2.070966	-1.599745
H	-8.730837	-2.064994	0.177657
H	-6.214905	-5.140077	0.162139
H	-6.061183	-5.057164	-1.607317
H	9.644088	-4.480032	-9.722117
H	8.390209	-3.727274	-10.702321
H	9.669054	-1.550355	-10.663600
H	10.919382	-2.302071	-9.682825
H	11.392317	-3.933734	-11.538789
H	10.145311	-3.178828	-12.519992
H	11.413708	-1.006768	-12.459630
H	12.659989	-1.762004	-11.479377
H	13.357509	-1.693534	-13.883756
H	13.170873	-3.374614	-13.360221
H	11.916801	-2.612035	-14.348351
H	5.580425	0.940841	-3.669938
H	6.944017	0.334694	-2.737478
H	8.512920	1.769301	-4.103591
H	7.146503	2.380433	-5.026457
H	6.157789	3.340442	-2.919899

H	7.527039	2.733562	-2.001784
H	9.079438	4.161042	-3.373725
H	7.709687	4.769031	-4.290394
H	8.360916	6.397894	-2.502014
H	6.736197	5.771121	-2.180960
H	8.117102	5.160609	-1.259308
H	-9.971040	0.108739	0.139158
H	-9.942195	0.102118	-1.620841
H	-11.281268	-2.037082	-1.635109
H	-11.304699	-2.035961	0.122830
H	-12.543300	0.152848	0.105123
H	-12.521493	0.152053	-1.651765
H	-13.846494	-1.986072	-1.667249
H	-13.866715	-1.986802	0.088959
H	-16.014004	-1.063107	-0.814188
H	-15.147302	0.193785	0.082586
H	-15.126306	0.196493	-1.686598
H	-4.133393	-6.655286	-1.500437
H	-4.293162	-6.738883	0.250075
H	-6.625061	-7.673939	-0.007981
H	-6.460310	-7.599429	-1.757191
H	-4.526848	-9.204408	-1.642386
H	-4.689570	-9.276345	0.105428
H	-7.014669	-10.200906	-0.148100
H	-6.852997	-10.130062	-1.895947
H	-6.401129	-12.450404	-1.061888
H	-4.935581	-11.776022	-1.791874
H	-5.095028	-11.844468	-0.031397

256

C220 - spiro MeOTAD adduct

C	-2.641609	1.711923	1.177007
C	-3.653713	1.351648	0.264624
C	-4.065594	2.271098	-0.713315
C	-3.499415	3.557501	-0.764410
C	-2.489875	3.905339	0.149363
C	-2.050685	2.974402	1.112088
N	-4.245985	0.047718	0.333895
C	-3.383912	-1.097673	0.423243
C	-3.559046	-2.036196	1.461387
C	-2.730950	-3.157849	1.538237
C	-1.701949	-3.336126	0.589883
C	-1.509695	-2.394054	-0.432640
C	-2.363821	-1.284023	-0.518288
O	-0.929087	-4.492643	0.752231
C	0.213783	-4.696587	-0.182018
C	0.824930	-6.047732	0.169171
C	2.004996	-6.393555	-0.762269
C	2.500625	-7.840327	-0.566844
O	-1.859303	5.155889	0.195268
C	-2.232495	6.169340	-0.827883
C	-1.361895	7.387414	-0.544342
C	-1.683466	8.566783	-1.486981
C	-0.798307	9.795663	-1.202131
C	-5.643135	-0.117483	0.295759
C	-6.499826	0.916274	0.745447
C	-7.881492	0.758953	0.688942

C	-8.469391	-0.432925	0.190239
C	-7.599740	-1.465476	-0.245964
C	-6.216832	-1.314907	-0.196132
C	-9.904359	-0.598783	0.129876
C	-10.653348	-1.773729	0.157898
C	-12.047415	-1.557969	0.092919
C	-12.414852	-0.211905	0.018005
S	-10.995604	0.899265	-0.007597
C	-13.829466	-0.105318	-0.010624
C	-14.394597	-1.394614	0.040680
C	-15.791880	-1.413669	0.014382
C	-16.374511	-0.130926	-0.058169
S	-15.053241	1.196263	-0.094721
C	-17.717084	0.294215	-0.111140
C	-18.874737	-0.474484	-0.115226
C	-20.151508	0.246798	-0.189863
O	-20.292821	1.488522	-0.244257
C	-18.870723	-1.890362	-0.056599
N	-18.827279	-3.068977	-0.007799
O	-21.251494	-0.638455	-0.196925
H	-4.347080	-1.883018	2.194180
H	-2.846317	-3.896344	2.325820
H	-0.721130	-2.519542	-1.167941
H	-2.250647	-0.559714	-1.323495
H	-2.331615	0.999187	1.936950
H	-1.262551	3.267082	1.798621
H	-3.839623	4.253527	-1.522715
H	-4.835164	1.988865	-1.427106
H	-6.072234	1.825952	1.155781
H	-8.516252	1.549562	1.077424
H	-8.015345	-2.370752	-0.681676
H	-5.567879	-2.108256	-0.560296
H	-17.904778	1.366678	-0.159921
H	-0.170402	-4.692946	-1.210858
H	0.925586	-3.871998	-0.045753
H	-2.033153	5.754697	-1.824929
H	-3.301410	6.401143	-0.721227
H	-22.079345	-0.103162	-0.248823
H	1.162851	-6.023775	1.215246
H	0.039213	-6.814088	0.094727
H	1.705944	-6.256010	-1.815033
H	2.836791	-5.696264	-0.573505
C	3.751303	-8.165447	-1.411123
H	2.721353	-7.997085	0.497120
H	1.688626	-8.540508	-0.816946
H	-1.513232	7.687001	0.502796
H	-0.309710	7.088511	-0.648595
H	-1.544316	8.253444	-2.534027
H	-2.742967	8.849967	-1.375403
C	-1.136090	10.996335	-2.111596
H	-0.912684	10.087581	-0.146561
H	0.258452	9.518171	-1.337078
C	-13.289469	-2.455214	0.106262
C	-13.322482	-3.369346	-1.146044
C	-13.373092	-3.280778	1.414758
H	-13.344862	-2.615460	2.288149
H	-14.305771	-3.861772	1.438522

H	-12.527451	-3.980913	1.473750
H	-12.475608	-4.070052	-1.124798
H	-14.254882	-3.950944	-1.167252
H	-13.260159	-2.763484	-2.060046
H	-16.392650	-2.317006	0.047846
H	-10.185722	-2.746763	0.285377
H	-0.479390	11.851079	-1.899968
H	-1.016045	10.730764	-3.171900
H	-2.175774	11.321539	-1.961148
H	4.135191	-9.169957	-1.183131
H	3.524161	-8.123258	-2.486888
H	4.559304	-7.443476	-1.218195
C	4.492920	0.017760	0.024295
C	5.377899	1.246447	-0.218712
C	5.535693	-1.070163	0.286144
C	3.556525	-0.274894	-1.154485
C	3.498546	0.207817	1.175503
C	6.844250	-0.533105	0.193129
C	6.745788	0.896291	-0.113876
C	7.951291	-1.371130	0.399503
C	7.737464	-2.719646	0.716216
C	6.430577	-3.246981	0.802125
C	5.311724	-2.410996	0.571205
H	8.966039	-0.984858	0.340991
N	6.246068	-4.625680	1.121509
H	4.302034	-2.811830	0.627101
C	7.727717	1.884356	-0.290737
C	7.329700	3.198406	-0.580547
C	5.959246	3.537189	-0.671848
C	4.968200	2.545947	-0.480990
H	8.785772	1.645868	-0.226991
H	8.073732	3.974242	-0.734934
H	3.911351	2.805120	-0.539275
N	5.579168	4.879590	-0.954438
C	2.205764	-0.203598	-0.733113
C	2.170071	0.080227	0.701296
C	1.176780	-0.389474	-1.668552
C	1.505890	-0.669854	-3.001821
C	2.855869	-0.771517	-3.405258
C	3.898321	-0.564971	-2.469328
H	0.139721	-0.266547	-1.375545
H	0.725415	-0.801194	-3.747797
N	3.165784	-1.053060	-4.767109
H	4.938942	-0.625936	-2.785004
C	1.096927	0.210108	1.596731
C	1.365464	0.463686	2.948290
C	2.694116	0.614429	3.409754
C	3.778547	0.487762	2.507198
H	0.071714	0.081581	1.259543
H	0.551344	0.540742	3.664128
N	2.934924	0.890588	4.785124
H	4.803144	0.606136	2.856552
H	8.582942	-3.379767	0.898363
C	4.185975	-0.311395	-5.435813
C	2.404356	-2.018926	-5.494373
C	2.052753	1.751970	5.509310
C	4.045804	0.299541	5.461991

C	4.485198	5.154592	-1.826441
C	6.309873	5.966537	-0.374583
C	5.227749	-5.032473	2.038234
C	7.112220	-5.603548	0.540659
C	1.951692	-1.731043	-6.800594
C	1.234546	-2.684037	-7.525299
C	0.937765	-3.930214	-6.941159
C	1.363479	-4.221624	-5.635834
C	2.110183	-3.267840	-4.921924
H	2.180182	-0.765360	-7.244789
H	0.883972	-2.484943	-8.534157
O	0.207939	-4.815707	-7.758347
H	1.150129	-5.179489	-5.172843
H	2.466732	-3.493184	-3.919998
C	5.065171	-0.959534	-6.330410
C	6.046339	-0.232244	-7.005293
C	6.178482	1.149915	-6.772142
C	5.323101	1.802970	-5.871070
C	4.317920	1.070467	-5.217087
H	4.968349	-2.030224	-6.491830
H	6.733625	-0.711763	-7.696602
O	7.207399	1.786253	-7.493131
H	5.414060	2.867615	-5.683671
H	3.642228	1.563140	-4.522841
C	1.627990	1.405346	6.810100
C	0.784805	2.256832	7.526857
C	0.331431	3.452197	6.937179
C	0.731364	3.798416	5.637020
C	1.607478	2.953852	4.935018
H	1.972388	0.475677	7.256070
H	0.452393	2.012973	8.531985
O	-0.520594	4.233792	7.741920
H	0.396459	4.716810	5.165890
H	1.940469	3.224407	3.936109
C	4.824758	1.067189	6.354746
C	5.893316	0.484712	7.037751
C	6.215729	-0.867177	6.813693
C	5.459046	-1.638149	5.917491
C	4.364873	-1.053175	5.257182
H	4.580739	2.114779	6.512052
H	6.503702	1.056339	7.731258
O	7.321111	-1.348343	7.540995
H	5.694708	-2.682131	5.738858
H	3.761020	-1.636141	4.567099
C	4.594057	-6.285265	1.885462
C	3.615985	-6.700290	2.786252
C	3.219781	-5.854595	3.836915
C	3.838389	-4.606090	4.003844
C	4.853915	-4.207664	3.116136
H	4.890102	-6.938829	1.068546
H	3.137042	-7.672103	2.699991
O	2.191079	-6.358527	4.658272
H	3.556263	-3.949807	4.819778
H	5.347712	-3.249014	3.250550
C	7.655728	-6.638043	1.334327
C	8.484888	-7.605516	0.762086
C	8.812422	-7.527446	-0.605420

C	8.294894	-6.494400	-1.401466
C	7.429423	-5.544211	-0.827178
H	7.413234	-6.683972	2.392130
H	8.904457	-8.413528	1.353590
O	9.672284	-8.539976	-1.071672
H	8.535561	-6.414635	-2.456134
H	7.017338	-4.747092	-1.439357
C	6.684930	7.070981	-1.168198
C	7.386753	8.136116	-0.605620
C	7.748814	8.095675	0.754526
C	7.390810	6.997742	1.552250
C	6.656355	5.942858	0.985861
H	6.413179	7.088956	-2.221678
H	7.683970	8.998303	-1.197304
O	8.473530	9.213718	1.214560
H	7.657090	6.950099	2.603691
H	6.359023	5.095203	1.599447
C	3.589322	6.207009	-1.531293
C	2.526542	6.490155	-2.392285
C	2.325105	5.706553	-3.543813
C	3.204309	4.655183	-3.845277
C	4.290779	4.392643	-2.991996
H	3.738379	6.799188	-0.633592
H	1.838604	7.303709	-2.189267
O	1.206050	6.058538	-4.323801
H	3.066429	4.047660	-4.733143
H	4.980810	3.584110	-3.217424
C	-1.022054	5.499389	7.171663
H	-1.646787	5.927349	7.957724
H	-0.184908	6.168962	6.941369
H	-1.619067	5.301402	6.273472
C	7.730282	-2.748225	7.313957
H	8.608733	-2.884527	7.947447
H	6.929612	-3.432314	7.618964
H	7.990593	-2.901263	6.259999
C	-0.121991	-6.142711	-7.204677
H	-0.679164	-6.642157	-7.999487
H	0.795802	-6.697236	-6.975580
H	-0.746160	-6.037114	-6.309212
C	7.444615	3.216158	-7.215319
H	8.308007	3.478241	-7.829496
H	6.571636	3.810266	-7.510098
H	7.672728	3.362197	-6.152724
C	1.728142	-5.509662	5.771490
H	0.919092	-6.079636	6.233284
H	2.541557	-5.349372	6.490577
H	1.351784	-4.552402	5.390180
C	10.088712	-8.485101	-2.487938
H	10.753644	-9.341490	-2.613019
H	9.216159	-8.579317	-3.144726
H	10.626772	-7.551168	-2.687676
C	8.881943	9.227947	2.630785
H	9.411965	10.174374	2.754970
H	7.999609	9.196060	3.281203
H	9.550731	8.384822	2.842425
C	0.994494	5.313143	-5.581793
H	0.100779	5.759456	-6.021587

H	1.854290	5.446580	-6.248835
H	0.827521	4.250751	-5.371018

320

Y123 - spiro MeOTAD adduct

C	-15.184121	-2.448212	-0.559944
C	-13.917737	-1.611855	-0.349906
C	-14.247321	-0.318060	0.067529
C	-15.654026	-0.194649	0.174132
C	-16.259938	-1.415458	-0.186210
S	-12.805929	0.729116	0.326986
C	-11.748471	-0.727790	-0.135366
C	-12.526496	-1.841283	-0.459280
C	-17.658473	-1.402499	-0.122389
C	-18.192040	-0.165050	0.295883
S	-16.826824	1.069477	0.632478
C	-10.309600	-0.589795	-0.120833
C	-9.667472	0.366475	0.703631
C	-8.281980	0.489047	0.723889
C	-7.477998	-0.337432	-0.093396
C	-8.108246	-1.290455	-0.927453
C	-9.495210	-1.415942	-0.935112
N	-6.074184	-0.208273	-0.078029
C	-5.236409	-1.339784	-0.336077
C	-5.521391	-2.582805	0.257261
C	-4.710446	-3.690257	-0.004972
C	-3.578990	-3.577995	-0.844326
C	-3.282869	-2.311141	-1.397796
C	-4.108566	-1.206252	-1.164079
C	-2.731120	-4.740109	-1.185124
C	-19.513607	0.281297	0.492727
C	-20.705197	-0.408029	0.310330
C	-20.765325	-1.754334	-0.126438
N	-20.770312	-2.876445	-0.491967
C	-15.321353	-2.886048	-2.039697
C	-15.220776	-3.666448	0.395872
C	-5.462990	1.057608	0.198810
C	-4.358502	1.130589	1.065024
C	-3.748998	2.365204	1.313270
C	-4.242600	3.556345	0.732556
C	-5.349863	3.462648	-0.140433
C	-5.945689	2.227904	-0.414259
C	-3.614614	4.850689	1.075390
C	-21.945516	0.325639	0.590781
O	-23.087787	-0.471695	0.365482
O	-22.024622	1.511500	0.980288
H	-6.379270	-2.676448	0.919629
H	-4.937815	-4.644811	0.453899
H	-2.387585	-2.184790	-2.000326
H	-3.873736	-0.237706	-1.599955
H	-3.970994	0.221595	1.519451
H	-2.866785	2.402388	1.946345
H	-5.727590	4.359556	-0.616198
H	-6.787215	2.165787	-1.100526
H	-7.808273	1.211999	1.386170
H	-10.259010	0.989198	1.370734
H	-9.956820	-2.120015	-1.623080

H	-7.500559	-1.912643	-1.582902
H	-19.651577	1.307112	0.835101
H	-23.887377	0.067848	0.575956
H	-15.123702	-3.339604	1.439185
H	-16.166751	-4.213390	0.279090
H	-14.393696	-4.354313	0.160155
H	-14.494914	-3.562283	-2.309268
H	-16.268702	-3.421890	-2.191887
H	-15.294635	-2.011858	-2.702749
H	-18.291161	-2.248091	-0.367275
H	-12.076542	-2.797044	-0.707905
C	-2.201939	-4.864862	-2.489265
C	-1.367475	-5.919919	-2.861239
C	-1.043980	-6.898232	-1.907608
C	-1.555844	-6.824941	-0.603101
C	-2.396931	-5.754851	-0.252501
H	-2.484249	-4.127142	-3.233716
H	-0.970583	-6.012475	-3.866370
O	-0.205183	-7.928157	-2.357339
H	-1.303046	-7.578019	0.130015
O	-2.946416	-5.625217	1.030709
C	-3.158183	5.083125	2.392114
C	-2.517620	6.265839	2.765073
C	-2.323324	7.266453	1.798935
C	-2.774152	7.088525	0.481833
C	-3.419328	5.889854	0.130470
H	-3.345447	4.323869	3.144798
H	-2.179950	6.441852	3.781060
O	-1.675979	8.425719	2.251002
H	-2.628249	7.862457	-0.259152
O	-3.894277	5.648728	-1.166320
C	0.174477	-8.990017	-1.394718
C	1.073941	-9.951047	-2.165975
H	0.704311	-8.532824	-0.548627
H	-0.737377	-9.490635	-1.041552
C	-2.494303	-6.542415	2.100465
C	-3.197872	-6.073257	3.373316
H	-2.783950	-7.569496	1.841052
H	-1.402558	-6.471932	2.193004
C	-1.440339	9.522229	1.281422
C	-0.734752	10.624954	2.066412
H	-0.813410	9.145131	0.462597
H	-2.406815	9.864453	0.887591
C	-3.552410	6.603259	-2.244474
C	-4.084683	5.981568	-3.535401
H	-4.035916	7.567894	-2.037220
H	-2.462761	6.729210	-2.277263
C	1.519836	-11.142624	-1.297386
H	0.524205	-10.306169	-3.048635
H	1.947809	-9.393015	-2.529927
C	2.431169	-12.117199	-2.065856
H	2.051556	-10.774236	-0.405068
H	0.631976	-11.687455	-0.934805
C	2.869584	-13.318899	-1.207001
H	1.903192	-12.480824	-2.963163
H	3.323701	-11.576936	-2.423758
C	3.788634	-14.294348	-1.973868

H	3.388468	-12.949933	-0.309143
H	1.974124	-13.854492	-0.854921
H	4.086323	-15.140678	-1.341242
H	3.278759	-14.695442	-2.861547
H	4.702381	-13.784628	-2.312276
C	-2.828967	-6.942012	4.592097
H	-2.926473	-5.024242	3.552631
H	-4.282999	-6.104250	3.204986
C	-3.541171	-6.478976	5.875201
H	-3.092363	-7.994140	4.390206
H	-1.738087	-6.913382	4.750794
C	-3.184764	-7.343214	7.099673
H	-3.278746	-5.427069	6.079522
H	-4.632972	-6.503251	5.716123
C	-3.905346	-6.879225	8.385811
H	-3.444538	-8.392017	6.889442
H	-2.095580	-7.313687	7.256687
H	-3.630304	-7.505917	9.243665
H	-3.642630	-5.838907	8.625431
H	-4.996425	-6.930436	8.261627
C	-0.411782	11.848911	1.187650
H	-1.378851	10.917969	2.907039
H	0.187319	10.208070	2.493866
C	0.307373	12.957000	1.978693
H	0.221400	11.539334	0.339437
H	-1.342718	12.253900	0.757651
C	0.643197	14.186492	1.113524
H	-0.323794	13.267575	2.828524
H	1.236795	12.549793	2.411569
C	1.374498	15.290388	1.908995
H	1.267359	13.869368	0.263774
H	-0.286637	14.592873	0.686830
H	1.602233	16.155208	1.272405
H	0.757887	15.638775	2.750115
H	2.321342	14.911929	2.320633
C	-3.804193	6.870811	-4.763117
H	-3.616328	4.995010	-3.661444
H	-5.164343	5.816912	-3.427599
C	-4.315708	6.242731	-6.071624
H	-4.280945	7.856454	-4.622736
H	-2.720745	7.053180	-4.848579
C	-4.037019	7.125866	-7.303101
H	-3.839258	5.256735	-6.212980
H	-5.399581	6.057210	-5.990872
C	-4.539722	6.490829	-8.619391
H	-4.518557	8.106039	-7.159871
H	-2.955494	7.314573	-7.375111
H	-4.332094	7.141241	-9.478560
H	-4.048819	5.523150	-8.797510
H	-5.623961	6.315388	-8.578688
C	6.071635	0.153255	0.033725
C	6.915456	1.428987	0.126632
C	7.152063	-0.927180	-0.082557
C	5.083878	0.165134	-1.138251
C	5.134663	-0.053497	1.229197
C	8.440696	-0.338872	-0.061413
C	8.295137	1.111624	0.073223

C	9.577179	-1.155938	-0.164707
C	9.412507	-2.544091	-0.271209
C	8.122065	-3.120000	-0.299791
C	6.973223	-2.297900	-0.211672
H	10.578025	-0.732012	-0.143004
N	7.980188	-4.531932	-0.419819
H	5.977453	-2.737772	-0.243043
C	9.246332	2.140591	0.153117
C	8.808517	3.467044	0.270124
C	7.429855	3.772181	0.329672
C	6.467802	2.735883	0.264197
H	10.311180	1.927602	0.104168
H	9.529161	4.279502	0.317368
H	5.404837	2.966550	0.318475
N	7.010684	5.126930	0.455447
C	3.760326	-0.015210	-0.667116
C	3.790848	-0.143127	0.790524
C	2.696626	-0.045896	-1.581763
C	2.966155	0.120039	-2.947144
C	4.291008	0.291834	-3.408065
C	5.368167	0.306920	-2.489702
H	1.671143	-0.176567	-1.245678
H	2.154180	0.114770	-3.669965
N	4.540628	0.449828	-4.800803
H	6.390890	0.430029	-2.843008
C	2.764934	-0.324625	1.730771
C	3.094977	-0.429424	3.088988
C	4.438322	-0.331994	3.517383
C	5.474087	-0.132749	2.573101
H	1.726177	-0.404213	1.420119
H	2.315842	-0.585695	3.830776
N	4.747808	-0.434125	4.903471
H	6.509074	-0.047944	2.901096
H	10.280626	-3.195254	-0.336051
C	5.524291	1.378432	-5.258509
C	3.787592	-0.302601	-5.754851
C	3.882813	0.155595	5.876946
C	5.907979	-1.146078	5.335636
C	5.872431	5.602171	-0.263875
C	7.746272	6.031814	1.282558
C	6.976557	-5.225326	0.322042
C	8.863995	-5.270831	-1.266413
C	3.264731	0.329927	-6.903354
C	2.542071	-0.404164	-7.845344
C	2.311287	-1.777050	-7.635141
C	2.812516	-2.414450	-6.489420
C	3.563967	-1.675536	-5.559102
H	3.438164	1.392143	-7.053646
H	2.133902	0.062116	-8.737615
O	1.562321	-2.420465	-8.641326
H	2.647245	-3.471751	-6.310070
H	3.967163	-2.163179	-4.675529
C	6.389777	1.029053	-6.317865
C	7.335388	1.941904	-6.787017
C	7.446038	3.209118	-6.183740
C	6.605425	3.561622	-5.116016
C	5.635522	2.648522	-4.667038

H	6.309796	0.043527	-6.768564
H	8.010790	1.691916	-7.600308
O	8.437151	4.049716	-6.728901
H	6.681340	4.534121	-4.641486
H	4.973216	2.910219	-3.846244
C	3.521258	-0.566703	7.034583
C	2.689910	0.011493	7.995259
C	2.187874	1.311822	7.795018
C	2.528043	2.034975	6.641271
C	3.389129	1.457618	5.691743
H	3.904549	-1.573548	7.177491
H	2.403331	-0.525168	8.895253
O	1.349225	1.794695	8.819744
H	2.153828	3.038799	6.469352
H	3.669003	2.014612	4.801511
C	6.711881	-0.627748	6.374224
C	7.832826	-1.331311	6.816826
C	8.180690	-2.551583	6.206967
C	7.399812	-3.069885	5.162028
C	6.255686	-2.370719	4.740019
H	6.446811	0.322099	6.830811
H	8.464639	-0.949564	7.613791
O	9.335336	-3.172651	6.722219
H	7.656999	-4.009299	4.684436
H	5.638671	-2.762142	3.935836
C	6.232600	-6.259115	-0.286976
C	5.266977	-6.956184	0.440547
C	5.012146	-6.610281	1.780676
C	5.732550	-5.572720	2.393254
C	6.724539	-4.893798	1.664529
H	6.420352	-6.510191	-1.327305
H	4.683421	-7.752326	-0.011795
O	4.004858	-7.366587	2.417445
H	5.546865	-5.293904	3.424960
H	7.293524	-4.092319	2.127809
C	9.441602	-6.474742	-0.809156
C	10.299184	-7.203019	-1.635283
C	10.610444	-6.719844	-2.920591
C	10.048825	-5.519854	-3.383850
C	9.164443	-4.805343	-2.557144
H	9.205632	-6.834384	0.188916
H	10.753055	-8.132851	-1.304093
O	11.501567	-7.520681	-3.662529
H	10.270119	-5.135065	-4.373817
H	8.715311	-3.881089	-2.910699
C	8.058708	7.326265	0.814633
C	8.766699	8.216280	1.623562
C	9.194770	7.811419	2.902135
C	8.899999	6.523231	3.375026
C	8.161906	5.641519	2.566205
H	7.734858	7.628213	-0.177922
H	9.015711	9.217589	1.283715
O	9.915897	8.781654	3.627182
H	9.215487	6.193831	4.359469
H	7.915960	4.646962	2.928608
C	4.949002	6.466154	0.363308
C	3.847639	6.953587	-0.341631

C	3.641174	6.562026	-1.677654
C	4.541405	5.688546	-2.307382
C	5.663796	5.222646	-1.600971
H	5.103505	6.749838	1.400909
H	3.121930	7.611713	0.126930
O	2.493826	7.103062	-2.293934
H	4.392710	5.377014	-3.335668
H	6.371536	4.549918	-2.077544
C	0.792477	3.151441	8.662268
H	0.180668	3.303893	9.553515
H	1.600904	3.891270	8.623275
H	0.172906	3.206171	7.759072
C	9.766136	-4.436625	6.095914
H	10.674648	-4.715374	6.633180
H	8.995570	-5.206057	6.225141
H	9.983558	-4.278981	5.032717
C	1.295830	-3.861421	-8.472716
H	0.706666	-4.138213	-9.349094
H	2.238254	-4.421888	-8.453323
H	0.721836	-4.037201	-7.555069
C	8.622787	5.373368	-6.104324
H	9.443390	5.829226	-6.661583
H	7.711053	5.973691	-6.208762
H	8.893714	5.260289	-5.047689
C	3.686300	-7.019869	3.815911
H	2.884463	-7.705528	4.096143
H	4.562768	-7.177277	4.455885
H	3.341351	-5.980965	3.880890
C	11.835584	-7.080587	-5.030172
H	12.515600	-7.846393	-5.408307
H	10.929598	-7.036517	-5.646631
H	12.334908	-6.104688	-5.004343
C	10.374464	8.417264	4.981000
H	10.893766	9.305714	5.345468
H	9.516025	8.187024	5.623374
H	11.062522	7.564709	4.932958
C	2.210168	6.686412	-3.679967
H	1.281237	7.198279	-3.937904
H	3.019331	7.007207	-4.347045
H	2.073472	5.599584	-3.729699

118

JK2 dye on TiO2 (only first and closest TiO2 layers)

C	4.199726	18.636205	7.764542
C	4.180365	17.806554	6.634810
C	5.309639	17.019826	6.298581
C	6.459659	17.058419	7.086440
C	6.480122	17.889739	8.223414
C	5.359339	18.671411	8.557664
C	5.052158	16.203720	5.029446
C	3.622575	16.632057	4.686970
C	3.132131	17.565155	5.633704
C	2.839167	16.227136	3.613323
C	1.525713	16.735992	3.496627
C	1.030732	17.662181	4.435212
C	1.837013	18.088649	5.500750
N	0.697498	16.298432	2.412922

C	-0.064604	17.244693	1.654809
C	-1.390726	16.923206	1.287223
C	-2.097352	17.811712	0.488309
C	-1.516938	19.037572	0.075578
C	-0.213825	19.371358	0.474506
C	0.515918	18.464504	1.256948
C	-2.489574	19.754113	-0.759736
C	-3.663875	18.968627	-0.854995
C	-3.517429	17.665283	-0.065923
C	-4.753713	19.413189	-1.603635
C	-4.665841	20.654065	-2.264767
C	-3.498793	21.433290	-2.170942
C	-2.400106	20.988767	-1.415926
C	-3.610069	16.436458	-1.004795
C	-4.558087	17.588517	1.077890
C	6.038226	16.601788	3.905218
C	5.108890	14.683353	5.325350
C	0.691041	14.932594	2.039770
C	0.596884	14.551030	0.684125
C	0.617924	13.205605	0.327400
C	0.756712	12.185174	1.305606
C	0.844256	12.587317	2.662762
C	0.798506	13.929036	3.029038
C	0.828613	10.780521	0.964150
S	1.082829	10.209303	-0.765277
C	1.091651	8.466024	-0.170054
C	0.914523	8.430162	1.207820
C	0.768764	9.686682	1.821154
C	1.274429	7.378204	-1.070793
C	1.345904	7.375528	-2.463601
C	1.537903	6.113093	-3.052459
C	1.624743	5.050527	-2.135041
S	1.462069	5.683942	-0.411108
C	1.787678	3.658790	-2.301790
C	1.865714	2.918076	-3.460432
C	1.964200	1.446312	-3.337553
O	1.828193	0.751708	-4.450535
Ti	1.737293	-1.219796	-4.899909
O	2.495980	-1.519681	-3.194740
Ti	4.536224	-1.574965	-2.790302
O	4.765505	-0.939409	-4.607344
Ti	4.560667	-1.808702	-6.120862
O	2.787460	-1.394265	-6.425167
C	1.797123	3.466592	-4.768761
N	1.746634	3.936649	-5.848759
O	2.144903	0.927883	-2.173526
Ti	1.633267	-1.014914	-1.410309
O	2.160952	-0.730111	0.462670
Ti	1.643169	-0.725110	2.310058
O	0.069628	0.189780	2.369387
Ti	-1.230139	-1.192364	2.268180
O	-1.296812	-1.475514	4.327158
Ti	-1.381848	-0.950677	5.992978
O	0.284674	-0.203146	6.458728
Ti	1.877209	-1.039619	6.064024
O	2.058861	-1.007013	4.259611
Ti	4.196182	-1.220902	4.301482

O	3.757636	-0.682094	6.022397
O	4.067376	-0.876370	-1.171781
Ti	4.223996	-1.310139	0.680089
O	3.833677	-0.630534	2.483963
O	-0.044521	-0.395860	-1.757637
Ti	-1.315784	-1.737065	-1.306586
O	-1.855823	-2.065600	-3.437297
Ti	-1.113801	-2.383785	-4.999157
O	-0.124831	-0.650120	-5.313382
O	-1.321685	-1.429645	0.497201
O	0.792776	-2.260374	2.339552
H	1.251164	8.288817	-3.054480
H	1.611244	5.963806	-4.124490
H	1.840078	3.053630	-1.391089
H	-0.388339	0.292785	-5.199295
H	0.012375	18.037736	4.324404
H	1.443633	18.804223	6.223700
H	3.209901	15.527999	2.860675
H	0.517225	15.319438	-0.085896
H	0.538244	12.941366	-0.725984
H	0.954735	11.842133	3.447907
H	0.853639	14.212844	4.078455
H	1.540745	18.687959	1.556855
H	0.246023	20.311129	0.166537
H	-1.824824	15.981265	1.629121
H	7.335212	16.457099	6.835484
H	7.372766	17.928596	8.849141
H	5.390051	19.308000	9.442000
H	-5.663066	18.815344	-1.685413
H	-5.509136	21.012692	-2.856580
H	-3.444081	22.389960	-2.690742
H	-1.497112	21.596563	-1.349121
H	5.977712	17.686499	3.718468
H	5.798841	16.066310	2.972302
H	7.070879	16.349808	4.194789
H	4.404995	14.431308	6.134667
H	6.123602	14.389610	5.637731
H	4.841677	14.106463	4.425656
H	-4.469733	18.474057	1.727677
H	-4.399129	16.683233	1.685498
H	-5.578414	17.553937	0.663929
H	-2.868635	16.525598	-1.815280
H	-4.614229	16.369877	-1.453348
H	-3.417635	15.507833	-0.444369
H	3.334835	19.244669	8.031011
H	0.870506	7.497119	1.769507
H	0.597378	9.791826	2.892061

191

Y123 dye on TiO₂ (only first and closest TiO₂ layers)

C	-2.529670	-14.095056	-9.279695
C	-1.238906	-14.339709	-8.746284
C	-0.190020	-14.542152	-9.670010
C	-0.394390	-14.547055	-11.049093
C	-1.689083	-14.327131	-11.544021
C	-2.758523	-14.093038	-10.667127
C	-0.955479	-14.394462	-7.293444

C	-0.039190	-15.349684	-6.795386
C	0.329462	-15.370141	-5.446207
C	-0.238242	-14.444958	-4.555166
C	-1.190158	-13.521181	-5.022856
C	-1.536102	-13.490081	-6.376091
N	0.141879	-14.445063	-3.171399
C	0.246195	-15.691411	-2.471100
C	1.327994	-15.933468	-1.603928
C	1.433203	-17.154702	-0.931228
C	0.476149	-18.177353	-1.122678
C	-0.587999	-17.926313	-2.019505
C	-0.714091	-16.697807	-2.676317
C	0.536915	-19.471877	-0.401718
C	-0.652216	-20.069983	0.070398
C	-0.667973	-21.310453	0.708538
C	0.543660	-21.992245	0.901008
C	1.753478	-21.431061	0.465231
C	1.745592	-20.179167	-0.175047
O	0.440583	-23.235669	1.545302
C	1.684214	-24.010782	1.792414
C	1.250311	-25.287038	2.507071
C	2.453319	-26.182869	2.862923
C	2.039406	-27.468255	3.608309
C	3.247803	-28.347901	3.986904
C	2.840459	-29.634194	4.732027
O	2.921462	-19.557478	-0.620507
C	4.194097	-20.321685	-0.595484
C	5.240452	-19.407302	-1.226841
C	6.634744	-20.063938	-1.261556
C	7.706940	-19.144784	-1.882174
C	9.107653	-19.789214	-1.890472
C	10.184060	-18.871018	-2.502112
O	-1.808125	-14.349255	-12.941614
C	-3.151933	-14.161572	-13.547331
C	-2.940355	-14.290741	-15.052235
C	-4.250035	-14.133087	-15.848128
C	-4.026808	-14.279117	-17.367393
C	-5.325583	-14.131903	-18.183776
C	-5.091033	-14.282421	-19.699997
O	-3.553192	-13.853303	-8.350085
C	-4.953764	-13.782991	-8.837907
C	-5.835553	-13.626503	-7.602283
C	-7.327861	-13.570938	-7.987399
C	-8.266097	-13.442072	-6.770357
C	-9.752019	-13.405387	-7.182139
C	-10.707870	-13.281951	-5.979649
C	0.418535	-13.220523	-2.523225
C	0.985885	-12.142840	-3.243206
C	1.233804	-10.925882	-2.614713
C	0.940036	-10.734881	-1.241639
C	0.372583	-11.825235	-0.529526
C	0.115785	-13.042593	-1.153367
C	1.224609	-9.492200	-0.554915
S	1.238217	-7.870237	-1.466726
C	1.647929	-7.060289	0.098061
C	1.734746	-7.970527	1.158623
C	1.507113	-9.312655	0.797607

C	1.894561	-5.746089	0.586120
C	2.142543	-5.810672	1.974213
C	2.071331	-7.255950	2.466949
C	2.359001	-4.578347	2.586719
C	2.303995	-3.481092	1.704682
S	1.938976	-4.066373	-0.043178
C	2.398722	-2.097703	1.951608
C	2.458368	-1.459815	3.188216
C	2.443736	-2.137960	4.435119
N	2.466593	-2.655027	5.500798
C	0.930746	-7.431666	3.499786
C	3.438098	-7.723649	3.024148
C	2.422750	0.005423	3.244693
O	2.557489	0.703662	2.164877
Ti	1.915316	2.704017	1.782507
O	2.803021	2.995765	3.605389
Ti	4.817198	3.270224	3.188057
O	4.355674	2.792646	1.491298
Ti	4.430532	3.508827	-0.265980
O	4.028572	3.040119	-2.143874
Ti	4.321084	3.917784	-3.854097
O	3.866498	3.590884	-5.627918
Ti	1.970263	3.856984	-5.587286
Ti	-1.281810	3.526335	-5.489238
O	-1.193349	3.832067	-3.766843
Ti	-1.015192	3.245622	-1.784576
O	0.359439	1.973613	-2.114000
Ti	1.866413	2.974747	-1.924416
O	2.192444	3.604713	-3.808066
O	2.228532	0.539351	4.443711
Ti	2.020027	2.381402	5.218782
O	0.210688	1.621300	5.605389
Ti	-0.897825	3.301482	5.578636
O	0.979432	3.916765	5.552462
O	3.155284	2.352020	6.670067
Ti	4.897229	2.940293	6.470815
O	5.232209	2.351674	4.853076
O	2.408880	2.752313	-0.102796
O	0.424214	2.980009	-6.068297
O	-2.814660	2.455709	-5.343009
O	-2.635785	2.316321	-2.240736
O	-1.132295	3.155224	0.008114
Ti	-1.138490	3.168756	1.830911
O	0.284291	1.946740	2.101741
O	-2.798970	2.255705	1.916052
O	-1.658038	3.158864	4.004202
O	-2.173087	2.810797	6.937749
H	0.005396	0.692056	5.327524
H	2.088204	-15.163152	-1.464437
H	2.273548	-17.331731	-0.264671
H	-1.310814	-18.715219	-2.229897
H	-1.540446	-16.521995	-3.366900
H	1.048744	-16.103398	-5.077786
H	0.376324	-16.098504	-7.470420
H	-2.263522	-12.764431	-6.731284
H	-1.647769	-12.821065	-4.321933
H	1.242646	-12.277203	-4.294216

H	1.705881	-10.124010	-3.183255
H	0.074211	-11.692241	0.509917
H	-0.352179	-13.856046	-0.597682
H	2.350215	-1.417068	1.097808
H	4.223495	-7.585270	2.264822
H	3.702762	-7.142535	3.921264
H	3.392470	-8.789290	3.299352
H	0.834750	-8.491845	3.782982
H	1.143206	-6.845210	4.407304
H	-0.023815	-7.089321	3.070473
H	2.560370	-4.454802	3.648445
H	1.592895	-10.153976	1.482943
H	-1.588684	-19.523766	-0.043946
H	-1.590132	-21.757591	1.075799
H	2.690827	-21.954071	0.621402
H	0.821383	-14.673767	-9.285419
H	0.422836	-14.696614	-11.752595
H	-3.754283	-13.905540	-11.053955
H	2.163815	-24.235949	0.826167
H	2.358318	-23.410771	2.425014
H	4.453957	-20.558302	0.448842
H	4.064132	-21.247777	-1.178447
H	-3.827753	-14.945244	-13.168056
H	-3.531590	-13.162825	-13.277756
H	-5.059163	-12.915727	-9.509193
H	-5.186719	-14.715648	-9.376498
H	0.705901	-25.001373	3.422119
H	0.547073	-25.831069	1.855615
H	2.993971	-26.461715	1.939978
H	3.159342	-25.615619	3.497056
H	1.487152	-27.194466	4.526014
H	1.346865	-28.051673	2.974293
H	3.802006	-28.614520	3.068935
H	3.935929	-27.759949	4.621008
H	3.725555	-30.236911	4.992678
H	2.305025	-29.391577	5.665335
H	2.175744	-30.254586	4.107724
H	4.909777	-19.153359	-2.246903
H	5.281159	-18.471442	-0.645838
H	6.943659	-20.327991	-0.233335
H	6.587923	-21.003960	-1.841213
H	7.414976	-18.890912	-2.917571
H	7.746583	-18.197282	-1.314061
H	9.391755	-20.045844	-0.853862
H	9.066203	-20.736022	-2.458660
H	11.171438	-19.360668	-2.493743
H	9.936213	-18.619344	-3.547001
H	10.264379	-17.929422	-1.933452
H	-2.210680	-13.526005	-15.364875
H	-2.493150	-15.278533	-15.251193
H	-4.979519	-14.895162	-15.517497
H	-4.694417	-13.142062	-15.642307
H	-3.298824	-13.517189	-17.701446
H	-3.578123	-15.268210	-17.573696
H	-6.052445	-14.893216	-17.847442
H	-5.772788	-13.142856	-17.976996
H	-6.033121	-14.168447	-20.260198

H	-4.382713	-13.518713	-20.063124
H	-4.671476	-15.275419	-19.933643
H	-5.644353	-14.476775	-6.927755
H	-5.545214	-12.704704	-7.072354
H	-7.502098	-12.714186	-8.663883
H	-7.595446	-14.487181	-8.545332
H	-8.097365	-14.294033	-6.086621
H	-8.018379	-12.521283	-6.211222
H	-9.914080	-12.554152	-7.867894
H	-9.990798	-14.325045	-7.746371
H	-11.757983	-13.253975	-6.313148
H	-10.589041	-14.138311	-5.294926
H	-10.505311	-12.358436	-5.411704

REFERENCES

- (1) Tsao□, H. N.; Yi□, C.; Moehl, T.; Yum, J.-H.; Zakeeruddin, S. M.; Nazeeruddin, M. K.; Grätzel, M. *ChemSusChem* **2011**, *4*, 591-594.
- (2) Burschka, J.; Dualeh, A.; Kessler, F.; Baranoff, E.; Cevey, L.; Yi, C.; Nazeeruddin, M. K.; Grätzel, M. *J. Amer. Chem. Soc.* **2011**, *133*, 18042-18045.
- (3) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 1372-1377.
- (4) Lynch, B. J.; Fast, P. L.; Harris, M.; Truhlar, D. G. *J. Phys. Chem. A* **2000**, *104*, 4811-4815.
- (5) Pastore, M.; Mosconi, E.; De Angelis, F.; Grätzel, M. *J. Phys. Chem. C* **2010**, *114*, 7205-7212.
- (6) Pastore, M.; Fantacci, S.; De Angelis, F. *J. Phys. Chem. C* **2010**, *114*, 22742-22750.
- (7) Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr., T. V.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.;

Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. ; *Gaussian 03*, Revision B05; Gaussian Inc.: Pittsburgh PA, 2003.

(8) te Velde, G.; Bickelhaupt, F. M.; Baerends, E. J.; Fonseca Guerra, C.; van Gisbergen, S. J. A.; Snijders, J. G.; Ziegler, T. *J. Comp. Chem.* **2001**, 22, 931-967.

(9) Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett.* **1996**, 77, 3865-3868.

(10) De Angelis, F.; Tilocca, A.; Selloni, A. *J. Am. Chem. Soc.* **2004**, 126, 15024-15025.

(11) Persson, P.; Bergstrom, R.; Lunell, S. *J. Phys. Chem. B* **2000**, 104, 10348-10351.