

Table 1. Main Configurations, Excitation Energies (nm) and Oscillator Strengths (f) of α 84 Chromophore in PCB Calculated at Various Levels

Table 2. Main Configurations, Excitation Energies (nm) and Oscillator Strengths (f) of β S4 Chromophore in PCB Calculated at Various Levels

Table 3. Main Configurations, Excitation Energies (nm) and Oscillator Strengths (f) of β 155 Chromophore in PCB Calculated at Various Levels

Table 4. Optimized Bond Lengths (Å) for α 84 Chromophores in PCB

Bond (Å)	PCB+ASP87/ Crystal	PCB+ASP87/ Opt sol	PCB+ASP87/ Opt gas	PCBH ⁺ / Opt gas	PCB/ Opt gas
C38-C35	1.6041	1.3434	1.3430	1.3442	1.3424
C34-C35	1.5517	1.5219	1.5221	1.5218	1.5224
C35-C36	1.5139	1.4805	1.4823	1.4794	1.4820
C36-N32	1.4184	1.3924	1.3921	1.3777	1.3968
N32-C33	1.3249	1.3820	1.3864	1.4016	1.3830
C33-C34	1.5327	1.5280	1.5307	1.5286	1.5334
C36-C11	1.4041	1.3638	1.3627	1.3724	1.3573
C11-C42	1.4251	1.4377	1.4379	1.4306	1.4482
C42-N41	1.4075	1.3599	1.3595	1.3763	1.3629
N41-C45	1.4079	1.3859	1.3839	1.3996	1.3785
C45-C44	1.4059	1.4391	1.4392	1.4259	1.4155
C44-C43	1.4262	1.3894	1.3893	1.4005	1.4098
C43-C42	1.4408	1.4363	1.4374	1.4263	1.4203
C45-C9	1.4097	1.3905	1.3916	1.3897	1.4114
C9-C13	1.4076	1.4036	1.4031	1.3995	1.3844
C13-N12	1.4148	1.3843	1.3835	1.3956	1.3865
N12-C16	1.3797	1.3628	1.3608	1.3753	1.3341
C16-C15	1.4296	1.4251	1.4276	1.4193	1.4655
C15-C14	1.4356	1.3986	1.3973	1.4065	1.3777
C14-C13	1.4110	1.4301	1.4312	1.4207	1.4542
C16-C10	1.4054	1.4455	1.4452	1.4384	1.4504
C10-C24	1.4063	1.3608	1.3615	1.3657	1.3593
C24-C25	1.4363	1.4766	1.4779	1.4805	1.4761
C25-C26	1.4238	1.3594	1.3586	1.3562	1.3579
C26-C27	1.4941	1.4871	1.4891	1.4954	1.4902
C27-N23	1.3507	1.3914	1.3980	1.4055	1.3933
N23-C24	1.3811	1.3929	1.3909	1.3793	1.3925
τ N32-C36-C11-C42	32.7525	-6.1396	-4.0567	-7.5434	-5.7637
τ C36-C11-C42-N41	126.5504	150.7658	151.8728	149.1748	142.4253
τ N41-C45-C9-C13	-6.9110	8.0385	8.5629	12.1160	0.8309
τ C45-C9-C13-N12	24.8833	14.4499	15.1464	11.7417	-0.4088
τ N12-C16-C10-C24	135.3097	146.3349	146.1179	147.5057	151.3681
τ C16-C10-C24-N23	8.8698	-7.7717	-7.5261	-4.4504	-2.4086

Table 5. Optimized Bond Lengths (Å) for β 84 Chromophores in PCB

Bond (Å)	PCB+ASP87/ Crystal	PCB+ASP87/ Opt_sol	PCB+ASP87/ Opt_gas	PCBH ⁺ / Opt_gas	PCB/ Opt_gas
C38-C35	1.5742	1.3449	1.3452	1.3444	1.3422
C34-C35	1.5329	1.5219	1.5224	1.5226	1.5233
C35-C36	1.4869	1.4805	1.4809	1.4811	1.4841
C36-N32	1.4338	1.3907	1.3888	1.3760	1.3950
N32-C33	1.3014	1.3837	1.3899	1.4029	1.3837
C33-C34	1.5170	1.5265	1.5290	1.5268	1.5321
C36-C11	1.4239	1.3655	1.3665	1.3736	1.3577
C11-C42	1.4368	1.4343	1.4319	1.4289	1.4478
C42-N41	1.3793	1.3571	1.3566	1.3758	1.3635
N41-C45	1.3657	1.3854	1.3846	1.3951	1.3781
C45-C44	1.4135	1.4453	1.4467	1.4292	1.4162
C44-C43	1.4068	1.3854	1.3837	1.3954	1.4069
C43-C42	1.4455	1.4415	1.4445	1.4326	1.4225
C45-C9	1.3865	1.3884	1.3875	1.3879	1.4070
C9-C13	1.4094	1.4093	1.4110	1.3997	1.3838
C13-N12	1.3931	1.3810	1.3795	1.3898	1.3848
N12-C16	1.3914	1.3623	1.3613	1.3721	1.3336
C16-C15	1.4031	1.4217	1.4219	1.4229	1.4657
C15-C14	1.3979	1.4003	1.4010	1.4029	1.3779
C14-C13	1.4064	1.4302	1.4291	1.4226	1.4530
C16-C10	1.3977	1.4461	1.4464	1.4390	1.4514
C10-C24	1.3870	1.3603	1.3604	1.3653	1.3586
C24-C25	1.4214	1.4774	1.4786	1.4809	1.4761
C25-C26	1.4337	1.3588	1.3581	1.3562	1.3578
C26-C27	1.5042	1.4875	1.4893	1.4950	1.4907
C27-N23	1.3549	1.3920	1.3989	1.4067	1.3946
N23-C24	1.3812	1.3914	1.3898	1.3795	1.3929
τ N32-C36-C11-C42	5.0329	3.6467	3.5132	7.8845	4.7567
τ C36-C11-C42-N41	158.3220	-153.0204	-154.3351	-151.1293	-142.5157
τ N41-C45-C9-C13	21.5192	4.0234	3.7551	14.7803	5.8968
τ C45-C9-C13-N12	0.5108	-1.4873	-1.5392	9.8397	-0.3060
τ N12-C16-C10-C24	143.1456	-146.8467	-146.7987	-148.3740	-148.6650
τ C16-C10-C24-N23	-10.2385	3.9264	4.1184	5.5284	3.1988

Table 6. Optimized Bond Lengths (Å) for β 155 Chromophores in PCB

Bond (Å)	PCB+ASP39/ Crystal	PCB+ASP39/ Opt_sol	PCB+ASP39/ Opt_gas	PCBH ⁺ / Opt_gas	PCB/ Opt_gas
C38-C35	1.5611	1.3460	1.3456	1.3471	1.3454
C34-C35	1.5418	1.5246	1.5246	1.5260	1.5265
C35-C36	1.4876	1.4767	1.4775	1.4752	1.4777
C36-N32	1.4253	1.3973	1.3964	1.3808	1.3993
N32-C33	1.3393	1.3831	1.3893	1.4021	1.3834
C33-C34	1.5293	1.5275	1.5303	1.5256	1.5301
C36-C11	1.4122	1.3625	1.3621	1.3754	1.3611
C11-C42	1.4267	1.4481	1.4486	1.4317	1.4495
C42-N41	1.4071	1.3581	1.3582	1.3766	1.3648
N41-C45	1.3760	1.3863	1.3843	1.3988	1.3767
C45-C44	1.4045	1.4346	1.4325	1.4248	1.4137
C44-C43	1.4100	1.3951	1.3966	1.3988	1.4095
C43-C42	1.4374	1.4254	1.4244	1.4256	1.4194
C45-C9	1.3816	1.3994	1.4028	1.3893	1.4094
C9-C13	1.3969	1.3957	1.3931	1.3989	1.3804
C13-N12	1.3919	1.3832	1.3829	1.3887	1.3849
N12-C16	1.3967	1.3590	1.3570	1.3708	1.3335
C16-C15	1.4296	1.4344	1.4390	1.4235	1.4692
C15-C14	1.4100	1.3902	1.3875	1.4031	1.3759
C14-C13	1.3868	1.4392	1.4415	1.4224	1.4532
C16-C10	1.4214	1.4397	1.4373	1.4397	1.4505
C10-C24	1.4052	1.3626	1.3636	1.3648	1.3590
C24-C25	1.4520	1.4780	1.4796	1.4807	1.4764
C25-C26	1.4482	1.3587	1.3583	1.3561	1.3575
C26-C27	1.5005	1.4866	1.4882	1.4950	1.4904
C27-N23	1.3249	1.3948	1.4020	1.4064	1.3949
N23-C24	1.4056	1.3910	1.3888	1.3803	1.3926
τ N32-C36-C11-C42	-0.6479	-10.7774	-10.0313	-8.9033	-6.2284
τ C36-C11-C42-N41	128.3295	139.5581	139.7820	147.0157	140.6981
τ N41-C45-C9-C13	25.4281	-7.5073	-7.2943	12.1212	-1.2473
τ C45-C9-C13-N12	-21.1685	-6.4177	-6.3845	13.0471	-1.3667
τ N12-C16-C10-C24	-145.1176	-150.3872	-150.7981	-147.1537	-150.7630
τ C16-C10-C24-N23	-14.9061	4.5796	3.6753	5.1990	3.0091