

ELECTRONIC SUPPLEMENTARY INFORMATION

Molecular Engineering of Antiaromatic Orangarin-Based Sensitizers for High-Performance Dye-Sensitized Solar cell Application.

Swati Singh Rajput,^{a,#} Samarth Razdan,^{a,#} Tejendra Banana,^a Neelam Chandravanshi,^a and Md Mehboob Alam^{a,*}

^a Department of Chemistry, Indian Institute of Technology Bhilai, Durg, Chhattisgarh – 491001, India, E-mail: mehboob@iitbhilai.ac.in

[#]These authors have equal contributions

*E-mail: mehboob@iitbhilai.ac.in

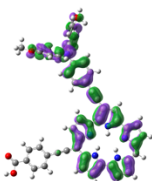
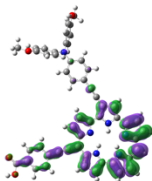
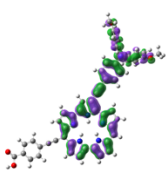
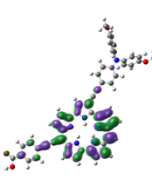
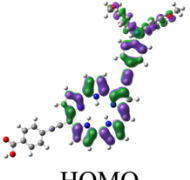
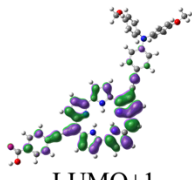
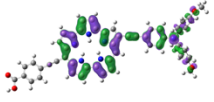
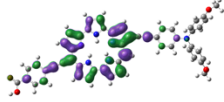
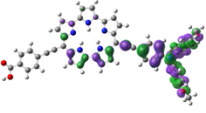
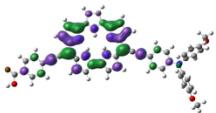
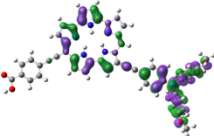
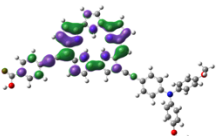
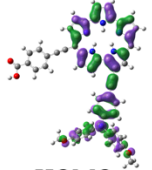
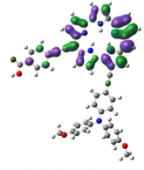
Table of contents

1. HOMO, LUMO, oscillator strength, wavelength, major orbital contribution, and dihedral angles of all triarylamine based dyes considered in this work, calculated at B3LYP/6-311+G(d,p) level of theory using the Gaussian 16 program.
2. HOMO and LUMO orbital diagram for orangarin-triarylamine derivative, calculated at TD-CAM-B3LYP/6-311+G(d,p) level of theory using Gaussian 16 program.
3. Energy levels and HOMO, LUMO, and energy gap of dyes@TiO₂ calculated at TD-CAM-B3LYP/6-311+G(d,p)/LANL2DZ/C-PCM level of theory in acetonitrile, using the Gaussian 16 program.
4. This includes the optimized cartesian coordinates of all dye and dye@TiO₂ considered in this work, that are optimized using GGA/PBE/DNP level of theory, in acetonitrile solvent in Material Studio software.
5. Table showing the values of electron transfer distance for recombination (r_{rec}) and injection (r_{inj}).
6. HOMO and LUMO orbitals showing charge transfer for SM315 adsorbed on (TiO₂)₃₈ surface, at TD-CAM-B3LYP/6-311+G(d,p)/LANL2DZ/C-PCM level of theory.
7. The transition dipole moment integral values, oscillator strengths and excitation energies (in eV) computed for the studied dyes.

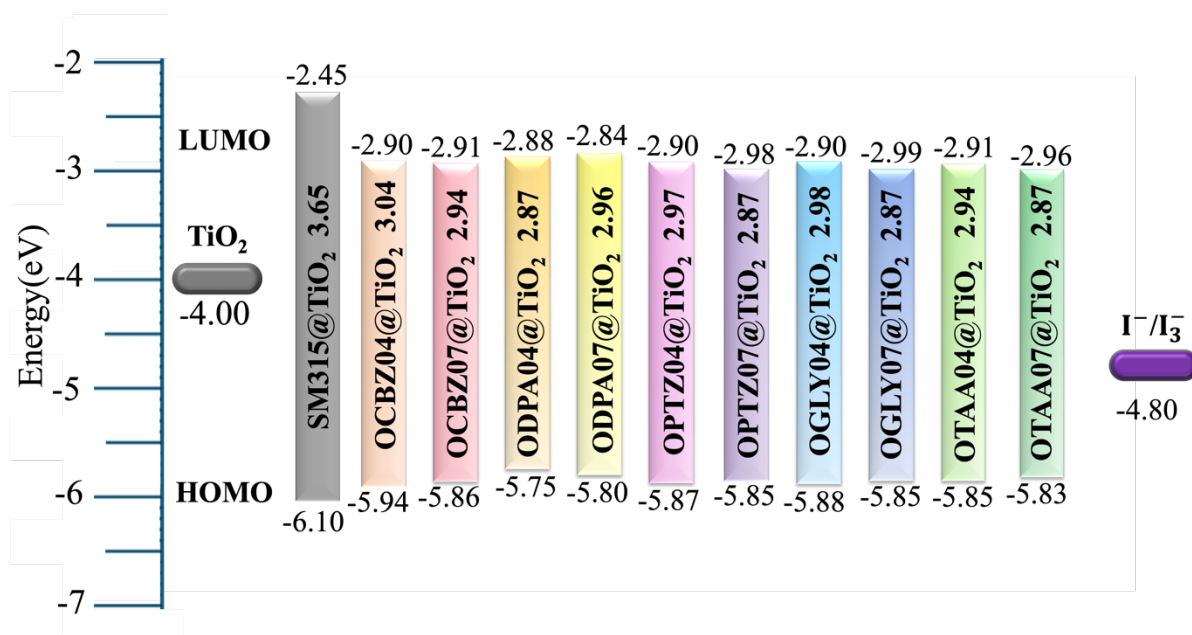
S1: HOMO, LUMO, oscillator strength, wavelength, major orbital contribution, and dihedral angles of all triarylamine based dyes considered in this work, calculated at B3LYP/6-311+G(d,p) level of theory using the Gaussian 16 program.

System	HOMO(eV)	LUMO(eV)	<i>f</i>	Wavelength(nm)	Contribution	Dihedral angle
OTAAD3	-5.981	-3.142	0.8659	392.16(S ₀ →S ₃)	H – L+1 (55.26%)	174.15
OTAAD4	-5.984	-3.124	1.5023	399.82(S ₀ →S ₃)	H – L+1 (59.61%)	165.81
OTAAD5	-5.997	-3.125	1.2082	397.69(S ₀ →S ₃)	H – L+1 (56.73%)	1.710
OTAAD6	-6.025	-3.134	0.7151	401.03(S ₀ →S ₃)	H – L+1 (54.47%)	176.27
OTAAD7	-6.007	-3.171	1.855	447.72(S ₀ →S ₂)	H-1 – L (56.80%)	1.3829
OTAAD8	-6.001	-3.118	0.9232	418.22(S ₀ →S ₂)	H-1 – L (51.10%)	1.6840
OTAAD9	-5.996	-3.106	1.2147	393.33(S ₀ →S ₃)	H – L+1 (58.58%)	23.19

S2: HOMO and LUMO orbital diagram for orangarin-triarylamine derivative, calculated at TD-CAM-B3LYP/6-311+G(d,p) level of theory using Gaussian 16 program.

SYSTEM		
OTAA03	 HOMO	 LUMO+1
OTAA04	 HOMO	 LUMO+1
OTAA05	 HOMO	 LUMO+1
OTAA06	 HOMO	 LUMO+1
OTAA07	 HOMO-1	 LUMO
OTAA08	 HOMO-1	 LUMO
OTAA09	 HOMO	 LUMO+1

S3: Energy levels and HOMO, LUMO, and energy gap of dyes@TiO₂ calculated at TD-CAM-B3LYP/6-311+G(d,p)/LANL2DZ/C-PCM level of theory in acetonitrile, using the Gaussian 16 program.



S4: This includes the optimized cartesian coordinates of all dye and dye@TiO₂ considered in this work, that are optimized using GGA/PBE/DNP level of theory, in acetonitrile solvent in Material Studio software.

OCBZ04

C	-3.12361400	3.47261600	-0.31841100
C	-4.51951800	3.71462200	-0.31186500
C	-5.16837700	2.48091100	-0.20881800
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OCBZ07

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H	9.686397	7.371699	-0.981115
H	8.589249	7.799535	-2.293653
C	10.449342	6.904783	-2.954455
H	10.972320	7.862994	-3.089817
H	11.190620	6.162752	-2.616841
H	10.083393	6.579709	-3.941205
C	8.989444	-2.818725	0.117976
H	9.194096	-3.903425	0.106810
H	8.971891	-2.498980	-0.938995
C	10.125223	-2.096465	0.846741

H	10.135139	-2.409036	1.906067
H	9.923847	-1.010931	0.850869
C	11.505950	-2.348864	0.234433
H	11.705626	-3.433723	0.231109
H	11.494925	-2.037607	-0.824244
C	12.630859	-1.621124	0.971921
H	12.681889	-1.940011	2.024690
H	13.611053	-1.815830	0.512969
H	12.467281	-0.532574	0.964018
C	5.437773	4.622783	0.410222
H	5.837676	4.929324	1.390680
H	4.756829	5.422971	0.078773
C	6.477962	-3.293045	-0.001582
H	6.462312	-2.942732	-1.047577
H	6.690145	-4.372989	-0.030781

ODPA07

C	5.758728	1.306176	0.098818
C	6.630582	2.418747	-0.015331
C	7.943065	1.936972	-0.031266
C	7.882237	0.526099	0.071938
N	6.546855	0.184657	0.149097
H	6.323781	-0.824262	0.239123
H	6.322072	3.458552	-0.073642
H	8.854404	2.522308	-0.118240
C	4.323001	1.289240	0.147280
C	3.421856	2.383556	0.113002
N	3.564793	0.150244	0.239257
C	2.121663	1.872096	0.188139
C	2.220495	0.463277	0.272519
H	3.817810	-0.853190	0.302017
H	1.194496	2.438306	0.182703
C	1.198902	-0.547258	0.402419
C	8.927179	-0.463331	0.093633
C	8.666161	-1.856174	0.211112
C	9.608333	-2.953267	0.227233
N	7.383325	-2.339918	0.312131
C	8.861916	-4.110155	0.339290
H	10.690383	-2.867500	0.160083
C	7.481374	-3.691412	0.385330
H	9.227863	-5.133930	0.374768
C	1.497011	-1.942194	0.477166
C	0.588831	-3.053267	0.577797
N	2.795271	-2.397172	0.450504
C	1.369774	-4.198263	0.609242
H	-0.495870	-2.995050	0.620533
C	2.733063	-3.750323	0.533366
C	6.256590	-4.433552	0.474766
C	5.843108	-5.788225	0.512751

N	5.109468	-3.689027	0.499310
C	4.433345	-5.804691	0.552461
C	3.986174	-4.460817	0.539485
H	5.095703	-2.676156	0.477377
C	10.252662	-0.010589	-0.023405
C	11.400489	0.416323	-0.126527
C	12.725861	0.882647	-0.259970
C	13.810764	-0.028854	-0.248945
C	12.994328	2.265213	-0.410538
C	15.113531	0.431630	-0.390137
H	13.614555	-1.094485	-0.132546
C	14.302162	2.717164	-0.549968
H	12.168589	2.975742	-0.417754
C	15.375304	1.806506	-0.541110
H	15.944527	-0.272543	-0.381408
H	14.490707	3.783601	-0.662458
C	16.784908	2.246545	-0.680536
O	17.750925	1.488142	-0.683886
O	16.915381	3.593234	-0.803088
H	17.874418	3.779718	-0.891891
H	1.029728	-5.229291	0.676624
H	3.706292	3.429298	0.041509
H	6.501543	-6.651940	0.502950
H	3.795795	-6.683464	0.585965
C	-0.125608	-0.113555	0.454263
C	-1.288573	0.282865	0.522617
N	-2.545778	0.691248	0.596694
C	-3.603622	-0.289689	0.605398
C	-4.702367	-0.125719	1.458429
C	-3.509312	-1.418773	-0.216065
C	-5.712420	-1.088117	1.464681
H	-4.766908	0.741813	2.114825
C	-4.525999	-2.375946	-0.189851
H	-2.648908	-1.543085	-0.873920
C	-5.646424	-2.229079	0.643693
H	-6.566308	-0.956400	2.131765
H	-4.442608	-3.252936	-0.834573
C	-2.837118	2.101599	0.652768
C	-3.952414	2.595931	-0.032320
C	-1.993271	2.963759	1.365467
C	-4.252047	3.965716	-0.009161
H	-4.580807	1.915141	-0.607320
C	-2.283276	4.330731	1.379936
H	-1.131730	2.568117	1.904223
C	-3.405827	4.827933	0.708721
H	-1.634906	5.007538	1.938313
H	-3.625369	5.896587	0.734725
C	-6.765478	-3.241903	0.632431
H	-6.363045	-4.232865	0.368156
H	-7.192440	-3.324724	1.644702

C	-5.484519	4.479444	-0.714838
H	-5.376359	5.559503	-0.900701
H	-5.578679	3.990472	-1.697889
C	-7.891287	-2.879392	-0.355964
H	-8.288024	-1.882596	-0.097729
H	-7.467405	-2.795689	-1.371118
C	-9.030995	-3.903030	-0.357499
H	-9.444775	-3.984419	0.663153
H	-8.624960	-4.899029	-0.608531
C	-10.158867	-3.556894	-1.335340
H	-10.560591	-2.557967	-1.087932
H	-9.745679	-3.480357	-2.356864
C	-11.303808	-4.576215	-1.331735
H	-10.899340	-5.574147	-1.574411
H	-11.715786	-4.649605	-0.310545
C	-12.425363	-4.227936	-2.314318
H	-13.230686	-4.977031	-2.288855
H	-12.869824	-3.248548	-2.077706
H	-12.045832	-4.182537	-3.347120
C	-6.770285	4.226554	0.094834
H	-6.675512	4.714626	1.079537
H	-6.864219	3.144765	0.291202
C	-8.036388	4.727063	-0.606120
H	-7.943377	5.810778	-0.797161
H	-8.120654	4.243809	-1.595344
C	-9.310636	4.459476	0.201188
H	-9.217243	4.933398	1.194365
H	-9.402858	3.374164	0.385786
C	-10.590248	4.962883	-0.474777
H	-10.496271	6.046447	-0.662398
H	-10.687964	4.485796	-1.465001
C	-11.849965	4.692480	0.351802
H	-11.783597	5.174943	1.339463
H	-12.752806	5.074366	-0.147797
H	-11.988841	3.612547	0.518711

OPTZ04

C	-4.291764	3.375770	-0.070021
C	-5.707497	3.404941	-0.099680
C	-6.163921	2.084071	-0.088089
C	-5.027604	1.237546	-0.047657
N	-3.917993	2.055392	-0.043412
H	-2.988315	1.601602	-0.008464
H	-6.317661	4.302605	-0.125784
H	-7.196412	1.748618	-0.105879
C	-3.362987	4.466536	-0.062141
C	-3.621733	5.864500	-0.075073
N	-2.006257	4.310422	-0.030119
C	-2.393843	6.526033	-0.050432

C	-1.369119	5.541813	-0.020113
H	-1.410661	3.466083	-0.004522
H	-2.229359	7.599385	-0.049877
C	0.038359	5.662481	0.019722
C	-4.924692	-0.197637	0.011513
C	-3.679004	-0.881647	0.066628
C	-3.437979	-2.303000	0.152586
N	-2.480813	-0.201914	0.048104
C	-2.065273	-2.466769	0.186833
H	-4.198342	-3.079952	0.182444
C	-1.506203	-1.141175	0.123037
H	-1.510069	-3.398957	0.258956
C	0.926580	4.579814	0.057396
C	2.372313	4.590934	0.100409
N	0.473969	3.272781	0.060608
C	2.778378	3.271133	0.126052
H	3.004869	5.475930	0.110078
C	1.568687	2.482013	0.102464
C	-0.142117	-0.677071	0.137747
C	1.145663	-1.229906	0.197507
N	0.021522	0.682898	0.093191
C	2.084050	-0.149456	0.190351
C	1.325550	1.062963	0.123357
H	-0.747420	1.341637	0.046247
C	-6.123395	-0.930820	0.022216
C	-7.179777	-1.561441	0.027266
C	-8.399517	-2.271396	0.028060
C	-8.415699	-3.679134	0.190699
C	-9.628863	-1.585648	-0.131301
C	-9.621603	-4.368160	0.190757
H	-7.476610	-4.216558	0.319357
C	-10.830972	-2.283942	-0.132143
H	-9.625726	-0.503330	-0.257971
C	-10.839788	-3.682740	0.029098
H	-9.633404	-5.450155	0.318846
H	-11.766337	-1.740989	-0.258491
C	-12.095628	-4.472463	0.042366
O	-12.148227	-5.691135	0.185793
O	-13.207229	-3.710900	-0.120041
H	-13.977522	-4.317763	-0.086667
H	3.796484	2.890605	0.154830
H	0.446321	6.674236	0.021710
H	-4.607868	6.317556	-0.098000
H	1.398389	-2.284078	0.245161
C	3.482858	-0.253921	0.235133
C	4.708869	-0.351742	0.251543
C	6.921561	0.720215	0.328683
C	8.307090	0.627526	0.360560
C	8.949022	-0.624066	0.389835
C	8.153032	-1.794638	0.395387

C	6.764847	-1.706209	0.330796
C	6.118450	-0.446896	0.302014
C	10.519796	-3.084397	-0.087255
C	11.069898	-1.787405	-0.064354
C	12.380293	-1.595249	-0.532014
H	12.799820	-0.587200	-0.526871
C	13.135475	-2.673927	-0.997911
C	12.582529	-3.959631	-1.026227
C	11.269236	-4.156624	-0.583391
H	10.815131	0.199324	0.361118
H	6.447823	1.700640	0.309997
H	8.915407	1.533823	0.354158
H	6.166495	-2.617484	0.318571
H	14.153878	-2.503708	-1.348365
H	13.162063	-4.805277	-1.397016
H	10.826491	-5.153236	-0.607548
N	10.334931	-0.697632	0.416542
S	8.909077	-3.394450	0.611101

OPTZ07

C	2.182530	-1.505777	0.110697
C	3.070668	-2.612232	0.106880
C	4.375314	-2.114821	0.047169
C	4.295104	-0.700821	0.006916
N	2.954463	-0.374007	0.047148
H	2.711758	0.633277	0.020235
H	2.771822	-3.655288	0.144493
H	5.294566	-2.692176	0.025113
C	0.749652	-1.507669	0.176194
C	-0.131735	-2.618305	0.237801
N	-0.027918	-0.379034	0.189673
C	-1.438528	-2.125642	0.279786
C	-1.366773	-0.711476	0.252474
H	0.207476	0.630424	0.164916
H	-2.353766	-2.706934	0.337665
C	-2.405609	0.285909	0.289143
C	5.326889	0.301171	-0.062613
C	5.040702	1.695474	-0.096715
C	5.965182	2.805510	-0.146610
N	3.748785	2.163440	-0.067649
C	5.199919	3.955294	-0.138465
H	7.049319	2.732746	-0.182790
C	3.825781	3.518471	-0.089864
H	5.549637	4.984787	-0.163122
C	-2.125714	1.685306	0.257076
C	-3.050818	2.790679	0.315832
N	-0.837659	2.156850	0.166272
C	-2.288684	3.944437	0.258661
H	-4.132764	2.717087	0.392985
C	-0.919301	3.512153	0.164746

C	2.587139	4.241659	-0.041314
C	2.158802	5.590428	0.033722
N	1.450833	3.482935	-0.018301
C	0.751006	5.589521	0.103892
C	0.318558	4.239373	0.079205
H	1.448207	2.471413	-0.070935
C	6.662890	-0.136296	-0.072028
C	7.826403	-0.534700	-0.088559
C	9.167653	-0.976991	-0.091034
C	10.234758	-0.045265	-0.137571
C	9.469935	-2.360649	-0.043616
C	11.550836	-0.488712	-0.129843
H	10.014760	1.020991	-0.176838
C	10.790428	-2.795483	-0.037368
H	8.657593	-3.086018	-0.011065
C	11.845653	-1.864366	-0.076889
H	12.368730	0.230478	-0.159434
H	11.003989	-3.862120	0.003077
C	13.269339	-2.278189	-0.053823
O	14.220166	-1.501120	-0.061289
O	13.433704	-3.625821	-0.018677
H	14.400014	-3.794563	0.003278
H	-2.641951	4.972981	0.276559
H	0.173737	-3.659993	0.243924
H	2.808488	6.460547	0.044741
C	-6.522854	-2.396198	0.477907
C	-7.835506	-2.843200	0.462980
C	-8.909697	-1.931143	0.401306
C	-8.624497	-0.543066	0.377559
C	-7.310514	-0.093182	0.364350
C	-6.229476	-1.009883	0.420535
C	-11.284436	-0.276859	-0.210253
C	-11.300202	-1.684198	-0.148849
C	-12.428336	-2.376103	-0.616958
H	-12.437330	-3.466463	-0.567555
C	-13.525305	-1.680742	-1.131678
C	-13.498387	-0.283017	-1.208146
C	-12.371962	0.413268	-0.755711
H	-10.313216	-3.410040	0.365471
H	-5.707577	-3.117274	0.522688
H	-8.049343	-3.912410	0.488873
H	-7.105909	0.976371	0.328008
H	-14.394920	-2.236544	-1.483579
H	-14.344097	0.264719	-1.624730
H	-12.337920	1.501785	-0.816895
N	-10.210417	-2.396276	0.368029
S	-9.942165	0.648578	0.506422
H	0.106355	6.460264	0.182511
C	-3.733934	-0.157001	0.354480
C	-4.900321	-0.550257	0.399376

OGLY04			
C	11.351036	2.112913	1.255510
C	12.746687	1.869922	1.281244
C	12.965878	0.581757	0.784717
C	11.706569	0.030856	0.445961
N	10.756749	0.985933	0.743369
H	9.768158	0.755702	0.540325
H	13.498504	2.572056	1.628494
H	13.921366	0.081546	0.663174
C	10.626740	3.283915	1.656981
C	11.120603	4.504138	2.198674
N	9.269681	3.407817	1.563239
C	10.029731	5.345213	2.418061
C	8.855305	4.650076	2.016821
H	8.543192	2.759695	1.217184
H	10.049901	6.354308	2.820571
C	7.495632	5.037770	2.020420
C	11.362157	-1.250847	-0.113380
C	10.024364	-1.622604	-0.427683
C	9.536122	-2.878927	-0.948856
N	8.971279	-0.759610	-0.218340
C	8.162850	-2.755584	-1.042828
H	10.140497	-3.746815	-1.200025
C	7.850146	-1.428852	-0.583433
H	7.452105	-3.500941	-1.391777
C	6.441980	4.235853	1.561574
C	5.023817	4.520822	1.547614
N	6.665717	2.970827	1.051913
C	4.401861	3.404944	1.019525
H	4.555076	5.439194	1.893319
C	5.456344	2.464805	0.723806
C	6.595379	-0.735750	-0.445492
C	5.233222	-1.009855	-0.633588
N	6.671864	0.549078	0.026001
C	4.497800	0.157201	-0.247693
C	5.454519	1.132344	0.179096
H	7.542247	1.021071	0.242972
C	12.411946	-2.156438	-0.342817
C	13.337801	-2.943876	-0.528982
C	14.422929	-3.823594	-0.727162
C	14.243598	-5.067493	-1.383390
C	15.718079	-3.470638	-0.274739
C	15.324907	-5.916842	-1.581860
H	13.250641	-5.353602	-1.730227
C	16.793584	-4.327963	-0.475190
H	15.866444	-2.518696	0.233542
C	16.609999	-5.559583	-1.132575
H	15.184913	-6.869202	-2.091885

H	17.783414	-4.036512	-0.126707
C	17.731665	-6.497732	-1.379254
O	17.623339	-7.573524	-1.961425
O	18.918933	-6.049685	-0.893164
H	19.590880	-6.732351	-1.103826
H	3.337597	3.252989	0.857228
H	7.264002	6.029837	2.410259
H	12.165228	4.723127	2.397246
H	4.803350	-1.937369	-0.997028
C	3.105681	0.321272	-0.275117
C	1.887226	0.472015	-0.328069
C	-0.130107	1.862500	-0.024004
C	-1.514126	1.996496	-0.035169
C	-2.355698	0.920039	-0.390139
C	-1.734636	-0.296028	-0.766389
C	-0.351912	-0.443223	-0.724118
C	0.485128	0.635742	-0.355872
C	-4.220399	-1.354686	-0.615833
C	-4.627353	-0.050830	-0.255107
C	-5.940450	0.105739	0.225550
H	-6.293983	1.095144	0.509271
C	-6.797945	-0.986015	0.361645
C	-6.380451	-2.291642	0.043942
C	-5.070103	-2.447036	-0.443804
H	0.485189	2.718506	0.250994
H	-1.952519	2.953320	0.239044
H	0.093137	-1.398247	-1.002657
H	-7.798464	-0.813039	0.758118
H	-4.715120	-3.433754	-0.744037
N	-3.754670	1.056718	-0.371429
S	-2.680055	-1.631278	-1.449540
C	-4.300693	2.378597	-0.157219
C	-4.658474	3.154388	-1.261353
C	-4.457820	2.892466	1.139258
C	-5.170218	4.446468	-1.089931
H	-4.535957	2.748828	-2.266171
C	-4.967115	4.174173	1.320810
H	-4.179541	2.288608	2.003453
C	-5.326466	4.958942	0.207478
H	-5.435179	5.033338	-1.967151
H	-5.089986	4.589060	2.321498
O	-5.812413	6.202529	0.497790
C	-6.189868	7.053785	-0.602294
H	-5.316414	7.254845	-1.240726
H	-6.976555	6.571786	-1.201896
C	-6.708064	8.341407	0.015346
H	-5.924121	8.806668	0.638830
H	-7.582318	8.129962	0.655725
O	-7.074449	9.205053	-1.060839
C	-7.613018	10.443064	-0.585660

H	-6.867001	10.975890	0.030440
H	-8.508108	10.258733	0.034587
C	-7.984476	11.273520	-1.802495
H	-8.714702	10.723358	-2.423942
H	-7.086682	11.466548	-2.417571
O	-8.547200	12.501370	-1.340757
C	-8.934963	13.338253	-2.433840
H	-9.702289	12.846887	-3.056541
H	-9.349891	14.257764	-2.004679
H	-8.067902	13.588559	-3.068872
C	-7.272865	-3.459355	0.195644
C	-8.659143	-3.349895	-0.012821
C	-6.764725	-4.730929	0.539917
C	-9.514264	-4.448901	0.114780
H	-9.088798	-2.391253	-0.306327
C	-7.601227	-5.834396	0.671013
H	-5.697507	-4.857493	0.729143
C	-8.984012	-5.702269	0.454564
H	-10.579333	-4.317822	-0.069212
H	-7.200093	-6.809965	0.949642
O	-9.722889	-6.846477	0.596099
C	-11.147818	-6.743335	0.420401
H	-11.385909	-6.409728	-0.601477
H	-11.565447	-6.024260	1.141607
C	-11.710868	-8.131622	0.666091
H	-11.250740	-8.857487	-0.028039
H	-11.491600	-8.452171	1.699734
C	-13.762251	-9.300371	0.746792
H	-13.299233	-10.120230	0.169671
H	-13.659366	-9.534836	1.821515
C	-15.229680	-9.164394	0.378588
H	-15.335753	-8.984242	-0.707158
H	-15.678642	-8.306995	0.912697
C	-17.272879	-10.346296	0.415434
H	-17.418291	-10.228850	-0.672738
H	-17.704415	-11.300269	0.739782
H	-17.784558	-9.516760	0.933019
O	-13.119874	-8.056997	0.448027
O	-15.882632	-10.379781	0.747540

OGLY07

C	-8.540424	0.289668	-0.377946
C	-9.463394	1.308682	-0.722229
C	-10.750456	0.770549	-0.633115
C	-10.624720	-0.581251	-0.229684
N	-9.274135	-0.832047	-0.087281
H	-8.993275	-1.786017	0.201184
H	-9.200115	2.323020	-1.005131
H	-11.686747	1.283858	-0.828895
C	-7.108502	0.354768	-0.326353

C	-6.256989	1.455788	-0.602685
N	-6.299774	-0.701035	0.008722
C	-4.937606	1.032208	-0.426240
C	-4.970107	-0.330186	-0.036172
H	-6.512996	-1.678932	0.273483
H	-4.037184	1.623509	-0.563736
C	-3.900888	-1.239932	0.281577
C	-11.625058	-1.590211	0.007444
C	-11.297695	-2.914099	0.416670
C	-12.187917	-4.015327	0.709684
N	-9.993150	-3.305665	0.593912
C	-11.386124	-5.080830	1.069801
H	-13.273516	-3.991958	0.652367
C	-10.027747	-4.605567	0.986352
H	-11.702193	-6.080398	1.358525
C	-4.134301	-2.595560	0.664166
C	-3.175414	-3.601969	1.049582
N	-5.406966	-3.108042	0.734531
C	-3.902821	-4.737993	1.359522
H	-2.096134	-3.476610	1.093657
C	-5.284571	-4.394972	1.152227
C	-8.767985	-5.244452	1.239754
C	-8.295858	-6.495858	1.711832
N	-7.655077	-4.483378	1.014837
C	-6.888817	-6.432504	1.761777
C	-6.499923	-5.143113	1.318708
H	-7.683808	-3.529496	0.676148
C	-12.970347	-1.230708	-0.175640
C	-14.145384	-0.905652	-0.341977
C	-15.493893	-0.535859	-0.530049
C	-16.534359	-1.477160	-0.320330
C	-15.831890	0.779564	-0.934178
C	-17.859839	-1.109121	-0.510882
H	-16.282644	-2.492046	-0.013686
C	-17.161406	1.138492	-1.122671
H	-15.038807	1.509489	-1.093432
C	-18.189770	0.197729	-0.916518
H	-18.658352	-1.834155	-0.356013
H	-17.406535	2.153383	-1.431191
C	-19.618664	0.531931	-1.132503
O	-20.548217	-0.255776	-0.979328
O	-19.811682	1.815211	-1.532876
H	-20.777004	1.933775	-1.661125
H	-3.521123	-5.700797	1.690094
H	-6.588229	2.445606	-0.902313
H	-8.916166	-7.342827	1.989915
C	0.133470	1.537652	-0.146777
C	1.430316	2.029565	-0.184691
C	2.542850	1.200980	0.089794
C	2.285039	-0.146667	0.460233

C	0.989216	-0.651232	0.464699
C	-0.120464	0.179242	0.163268
C	4.973618	-0.489378	0.223385
C	4.980420	0.864220	-0.178033
C	6.158425	1.359512	-0.765787
H	6.207089	2.400007	-1.079668
C	7.273324	0.543184	-0.951703
C	7.267743	-0.811959	-0.568253
C	6.086053	-1.308396	0.015668
H	-0.699713	2.202191	-0.372222
H	1.590688	3.073446	-0.442278
H	0.820263	-1.694580	0.729817
H	8.165739	0.982370	-1.396975
H	6.020823	-2.357699	0.305596
N	3.846417	1.700390	0.000285
S	3.585204	-1.178527	1.089552
H	-6.214464	-7.218719	2.087971
C	-2.589077	-0.749573	0.232388
C	-1.432988	-0.324134	0.190132
C	8.446438	-1.682798	-0.778704
C	9.293913	-1.511853	-1.895088
C	8.764932	-2.715880	0.120599
C	10.394392	-2.337676	-2.104403
H	9.069736	-0.739356	-2.632434
C	9.868850	-3.552378	-0.073244
H	8.154819	-2.869138	1.011866
C	10.695392	-3.363190	-1.190530
H	11.027086	-2.207026	-2.983520
H	10.077753	-4.334705	0.654307
C	4.016371	3.121161	-0.219424
C	4.223499	3.961052	0.875624
C	3.976567	3.657768	-1.514932
C	4.396909	5.338039	0.691552
H	4.250576	3.541488	1.881805
C	4.148507	5.025247	-1.708454
H	3.813610	3.005152	-2.373058
C	4.360576	5.873246	-0.605569
H	4.559351	5.971524	1.560947
H	4.123576	5.453007	-2.711085
C	12.120257	-5.201520	-0.581879
H	11.297992	-5.932795	-0.568104
H	12.281655	-4.820377	0.437783
C	13.391609	-5.849369	-1.106310
H	13.241229	-6.211129	-2.139172
H	14.216491	-5.115431	-1.111936
C	14.881155	-7.628255	-0.616033
H	15.745671	-6.941245	-0.592420
H	14.782584	-8.024581	-1.642606
C	15.087377	-8.769907	0.366111
H	14.215177	-9.448862	0.346563

H	15.190076	-8.374589	1.393646
C	16.524078	-10.585996	0.835210
H	15.687039	-11.305004	0.814304
H	17.430349	-11.076400	0.460394
H	16.688411	-10.261364	1.877359
C	4.770911	8.100189	0.203078
H	3.928187	8.084220	0.910177
H	5.689318	7.803317	0.731638
C	4.933707	9.481838	-0.406899
H	4.001246	9.786261	-0.914563
H	5.745847	9.471809	-1.155113
C	5.403138	11.724331	0.184473
H	6.195287	11.768579	-0.583590
H	4.462094	12.084832	-0.267349
C	5.777834	12.591036	1.374081
H	6.725044	12.236161	1.819677
H	4.991678	12.535305	2.149061
C	6.276580	14.825079	1.962389
H	7.251259	14.551265	2.402243
H	6.342819	15.829834	1.527920
H	5.513194	14.822491	2.759158
O	4.519074	7.199436	-0.895446
O	5.245039	10.381474	0.656644
O	5.918314	13.932700	0.903484
O	11.804225	-4.116758	-1.476700
O	13.688129	-6.937762	-0.230171
O	16.269784	-9.470117	-0.022051

OTAA04

C	-6.619794	3.505105	-0.432874
C	-8.034854	3.572236	-0.473425
C	-8.530516	2.278275	-0.288525
C	-7.423188	1.409579	-0.137464
N	-6.287607	2.187905	-0.224774
H	-5.373427	1.708415	-0.147610
H	-8.615581	4.477199	-0.625960
H	-9.572459	1.974484	-0.266727
C	-5.656080	4.556991	-0.577656
C	-5.868048	5.945505	-0.804101
N	-4.304284	4.362690	-0.523940
C	-4.619172	6.561664	-0.881831
C	-3.625385	5.557275	-0.711396
H	-3.736973	3.509347	-0.391344
H	-4.417841	7.615601	-1.052444
C	-2.214224	5.626253	-0.729882
C	-7.366752	-0.014179	0.073035
C	-6.142140	-0.734642	0.171106
C	-5.945959	-2.149897	0.385382
N	-4.922957	-0.103188	0.062843
C	-4.578092	-2.357468	0.403115

H	-6.729433	-2.895261	0.499149
C	-3.976989	-1.064886	0.201643
H	-4.052133	-3.298081	0.546435
C	-1.361755	4.524027	-0.578998
C	0.083881	4.482952	-0.597094
N	-1.858618	3.246046	-0.397947
C	0.444609	3.159381	-0.428085
H	0.744230	5.338205	-0.722743
C	-0.789941	2.423043	-0.306591
C	-2.598017	-0.649365	0.134318
C	-1.327628	-1.237347	0.220437
N	-2.392136	0.690511	-0.068515
C	-0.353781	-0.196825	0.058712
C	-1.076426	1.025727	-0.115027
H	-3.140264	1.368175	-0.162618
C	3.671907	-0.595529	0.126754
C	4.283681	-1.849265	0.384844
C	4.521497	0.518059	-0.091855
C	5.664831	-1.978856	0.434495
H	3.658493	-2.724244	0.563853
C	5.902427	0.388944	-0.046052
H	4.081395	1.491010	-0.312727
C	6.505965	-0.861851	0.223127
H	6.104749	-2.952229	0.649600
H	6.525897	1.261831	-0.235874
C	2.266570	-0.457685	0.093727
C	1.042069	-0.336895	0.080901
N	7.901889	-0.989104	0.274557
C	8.720630	0.109628	0.676049
C	8.409587	0.852551	1.832231
C	9.862571	0.450624	-0.063900
C	9.215079	1.916676	2.222207
H	7.530192	0.596441	2.423650
C	10.687468	1.508784	0.330595
H	10.109068	-0.114838	-0.963236
C	10.362152	2.254282	1.476682
H	8.979827	2.492617	3.118228
H	11.566712	1.744950	-0.265837
C	8.539739	-2.212532	-0.094693
C	8.189035	-2.877294	-1.278598
C	9.558926	-2.749946	0.712904
C	8.826522	-4.064980	-1.649421
H	7.417567	-2.461419	-1.927380
C	10.206009	-3.924517	0.345259
H	9.838765	-2.242689	1.636741
C	9.846955	-4.591337	-0.841527
H	8.538169	-4.551980	-2.579113
H	10.993530	-4.344514	0.972262
C	12.267808	3.687304	1.206285
H	12.681582	4.555340	1.729168

H	13.007278	2.873771	1.202477
H	12.009745	3.964394	0.174711
C	10.213132	-6.445035	-2.326039
H	10.369453	-5.817686	-3.215143
H	10.894649	-7.300485	-2.357121
H	9.173051	-6.799977	-2.296235
O	11.090746	3.312361	1.946424
O	10.549793	-5.730934	-1.121512
C	-8.587193	-0.700938	0.193346
C	-9.667908	-1.278100	0.296427
C	-10.902377	-1.957553	0.394291
C	-10.940802	-3.360267	0.596806
C	-12.123639	-1.249664	0.270095
C	-12.159484	-4.024974	0.659592
H	-10.007943	-3.913656	0.701785
C	-13.338608	-1.923718	0.331577
H	-12.103927	-0.171266	0.117274
C	-13.369238	-3.318001	0.526496
H	-12.187890	-5.103091	0.813068
H	-14.267615	-1.365294	0.227477
C	-14.641340	-4.075827	0.607386
O	-14.718990	-5.287226	0.794494
O	-15.739856	-3.292159	0.455679
H	-16.522883	-3.879139	0.523443
H	1.449227	2.745681	-0.395075
H	-1.769482	6.610586	-0.879284
H	-6.838538	6.423454	-0.897205
H	-1.108889	-2.288043	0.382253

OTAA07

C	-4.371941	-1.187300	0.080664
C	-5.126716	-2.376600	0.236658
C	-6.482248	-2.031701	0.223643
C	-6.564744	-0.626859	0.057131
N	-5.269258	-0.155601	-0.023610
H	-5.144021	0.865204	-0.150763
H	-4.710858	-3.374162	0.341365
H	-7.328614	-2.705110	0.318092
C	-2.946406	-1.029345	0.038995
C	-1.938839	-2.021314	0.164146
N	-2.304946	0.172216	-0.124958
C	-0.697195	-1.384715	0.073954
C	-0.935172	-0.001591	-0.107271
H	-2.658482	1.139150	-0.247458
H	0.281262	-1.851498	0.130546
C	-0.013991	1.097804	-0.252927
C	-7.704220	0.248471	-0.032566
C	-7.580911	1.654132	-0.224756
C	-8.626086	2.646712	-0.345634

N	-6.349573	2.257801	-0.322646
C	-7.993559	3.862692	-0.516349
H	-9.695919	2.458945	-0.307046
C	-6.579655	3.583637	-0.496845
H	-8.458597	4.837422	-0.641236
C	-0.451403	2.446903	-0.416823
C	0.344271	3.637364	-0.584516
N	-1.787280	2.770282	-0.434949
C	-0.545534	4.691784	-0.708380
C	-1.859875	4.116089	-0.604581
C	-5.433205	4.438408	-0.614484
C	-5.160581	5.817478	-0.787662
N	-4.216475	3.819669	-0.544753
C	-3.759748	5.978158	-0.817208
C	-3.176362	4.694000	-0.663240
H	-4.097916	2.821189	-0.422949
C	3.926583	0.223419	-0.201777
C	4.910190	1.238768	-0.357100
C	4.377975	-1.112866	-0.034719
C	6.261067	0.938037	-0.337305
H	4.592102	2.271156	-0.503555
C	5.728610	-1.416228	-0.016223
H	3.647126	-1.911383	0.095452
C	6.706630	-0.396860	-0.159651
H	6.988572	1.738305	-0.464571
H	6.041771	-2.448384	0.132918
C	2.556772	0.531958	-0.210585
C	1.354531	0.805362	-0.233053
N	8.063976	-0.700704	-0.122506
C	8.537015	-2.021857	-0.414185
C	8.202801	-2.650078	-1.626469
C	9.358512	-2.691268	0.501086
C	8.675718	-3.927533	-1.910686
H	7.576258	-2.129646	-2.351327
C	9.843353	-3.972695	0.220658
H	9.620462	-2.211353	1.444624
C	9.498282	-4.599710	-0.987165
H	8.427187	-4.417035	-2.853140
H	10.475395	-4.471096	0.952724
C	9.036254	0.286474	0.240382
C	8.900524	1.021535	1.425299
C	10.154238	0.508384	-0.582668
C	9.849280	1.983680	1.783348
H	8.042804	0.845501	2.074756
C	11.108790	1.455956	-0.228271
H	10.274570	-0.064325	-1.502904
C	10.959799	2.206553	0.952972
H	9.714923	2.540262	2.708760
H	11.978640	1.635086	-0.860849
C	10.743566	-6.575295	-0.426703

H	10.959605	-7.530017	-0.915523
H	11.681119	-6.035351	-0.233413
H	10.210348	-6.752659	0.517755
C	11.826021	3.910426	2.405226
H	11.879852	3.272900	3.299464
H	12.677221	4.597460	2.388984
H	10.888091	4.484257	2.409124
O	9.913682	-5.849025	-1.355261
O	11.943573	3.122640	1.204746
C	-8.983932	-0.326519	0.067961
C	-10.095312	-0.843746	0.157142
C	-11.372697	-1.439745	0.253676
C	-12.547173	-0.674580	0.043442
C	-11.502654	-2.819202	0.551759
C	-13.797866	-1.273362	0.115412
H	-12.459617	0.387930	-0.182390
C	-12.758454	-3.409245	0.624987
H	-10.606678	-3.415028	0.724739
C	-13.920831	-2.645320	0.406389
H	-14.698411	-0.683164	-0.053474
H	-12.839713	-4.470808	0.853259
C	-15.277918	-3.239023	0.471193
O	-16.321591	-2.614819	0.301045
O	-15.266056	-4.570538	0.740158
H	-16.201271	-4.865610	0.762868
H	-2.117088	-3.083164	0.306671
H	-5.904510	6.604685	-0.872897
H	-3.217199	6.910682	-0.942824
H	-0.309943	5.743151	-0.854016
H	1.429926	3.684961	-0.615356

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C	-4.88050600	8.13928700	1.05466300
C	-5.44834200	6.84174500	0.92869800
C	-4.40043300	5.92775900	0.82342700
C	-3.18535900	6.65795200	0.89077800
N	-3.51971500	7.98723100	1.02910200
H	-2.74818700	8.67197200	1.11451300
H	-6.51104000	6.62274400	0.91455300
H	-4.48003300	4.85077000	0.71334600
C	-5.53366400	9.41080100	1.14710700
C	-6.92713600	9.70992600	1.16789800
N	-4.86690200	10.59989400	1.19430100
C	-7.06472100	11.09362000	1.21529900
C	-5.75727200	11.65907400	1.23072600
H	-3.85765800	10.81948800	1.20550300

H	-7.99170100	11.65911500	1.24745100
C	-5.32986900	13.00501600	1.24895700
C	-1.81715100	6.21456700	0.84431100
C	-0.71681700	7.10094900	0.98389500
C	0.69699200	6.78473300	0.93316600
N	-0.89289800	8.45178700	1.16204900
C	1.36825600	7.97797500	1.07369600
H	1.12594000	5.79445000	0.80910800
C	0.34673400	8.99160100	1.20981100
H	2.44243800	8.14057400	1.07856900
C	-3.99007000	13.41258900	1.29540100
C	-3.44335800	14.75655300	1.24776100
N	-2.96343500	12.49541900	1.37211200
C	-2.07349400	14.62513700	1.29509600
H	-4.01797300	15.67563800	1.16549200
C	-1.81414700	13.20358800	1.37355500
C	0.43481000	10.41990500	1.31876200
C	1.44349200	11.39735700	1.24274400
N	-0.75239100	11.08747900	1.44328800
C	0.81123700	12.67123000	1.29455800
C	-0.60167800	12.43427400	1.40168700
H	-1.65542300	10.63179900	1.52193200
C	-1.55870800	4.84642600	0.64917800
C	-1.28059300	3.66196600	0.47901100
C	-1.04745300	2.27363700	0.36055100
C	0.25295200	1.71999900	0.46110800
C	-2.15076400	1.40629500	0.18451300
C	0.42866000	0.33748400	0.44832700
H	1.11255700	2.37938100	0.57551500
C	-1.96662300	0.03009800	0.18293300
H	-3.14927200	1.82803100	0.07743600
C	-0.68027600	-0.52061200	0.34468400
H	1.42974600	-0.08401900	0.53602700
H	-2.82278400	-0.63226700	0.06688800
C	-0.54130500	-2.00768300	0.45716100
O	0.62779400	-2.52942800	0.42274500
O	-1.63567000	-2.65094600	0.59701400
H	-1.32870700	15.41608000	1.27277000
H	-6.10832300	13.76812800	1.21813600
H	-7.72224200	8.97138000	1.15047800
C	3.71420600	16.65869200	0.49637500
C	2.36417400	17.15515700	2.28659400
C	4.33805500	16.03651400	-0.58460500
C	4.05792800	17.95942900	0.93978300
C	1.42016300	17.09678000	3.30962500
C	3.20783600	18.27125000	2.07569000
C	5.34282300	16.75832900	-1.23988900
H	4.05287300	15.03510900	-0.90804600
C	5.07046200	18.66084200	0.26883600
C	1.32060500	18.21177400	4.14881600

H	0.79501000	16.21539000	3.45638500
C	3.09072700	19.37593500	2.93169000
C	5.70484600	18.05192700	-0.81831900
H	5.85192100	16.30644500	-2.09192500
H	5.35886300	19.66313000	0.58824600
C	2.14702800	19.33582600	3.96310600
H	0.58936500	18.20395000	4.95775700
H	3.72602800	20.25216600	2.79661000
H	6.49601100	18.58471100	-1.34724900
H	2.04758300	20.18884100	4.63482300
N	2.67392100	16.16579400	1.32180900
H	2.50990500	11.22221300	1.14726100
C	1.44773900	13.92131200	1.24702600
C	2.06955700	14.97790500	1.23543400
Ti	-3.92883900	-8.12317700	-6.89247500
Ti	-0.58322000	-8.27399000	-6.97385300
Ti	2.61431500	-8.91842900	-7.40810900
Ti	5.96197100	-8.24758300	-7.24063900
Ti	-4.09596300	-8.60930100	3.00763200
Ti	2.96832300	-7.94785900	3.60011100
Ti	6.20213700	-7.71579500	3.39994000
Ti	-4.21964800	-4.85934900	3.19101500
Ti	-0.68835300	-4.37040600	3.52656500
Ti	2.56695200	-4.11029100	4.00236200
Ti	5.79504100	-4.04544000	3.27040000
Ti	-5.96240100	-9.09653400	-2.34648300
Ti	-2.29887800	-9.82834800	-1.96983200
Ti	1.40537700	-9.44892900	-2.21990400
Ti	4.88099300	-9.27038300	-2.12053200
Ti	-5.60494200	-5.67880400	-2.50688800
Ti	-2.24158900	-6.20427000	-1.67335200
Ti	1.22705000	-5.84516000	-2.64882000
Ti	4.82884300	-5.71191000	-2.58792700
Ti	-4.24798500	-9.76003300	-4.55309300
Ti	-0.68827800	-9.97659400	-4.60990200
Ti	2.79633900	-10.18858100	-4.99088000
Ti	6.07668200	-9.97588000	-4.98158600
Ti	-4.03510900	-5.98489600	-4.94924800
Ti	-0.69090700	-6.12661300	-4.92699200
Ti	5.95528200	-6.36262000	-5.06635900
Ti	-3.74410200	-6.84629600	5.24611500
Ti	-0.58254800	-5.89188400	5.82913700
Ti	2.73161000	-6.22985500	5.92235300
Ti	6.18253500	-5.79352400	5.48986800
Ti	-5.90609800	-8.46884200	0.82281800
Ti	-2.16442800	-8.67729500	0.64863500
Ti	1.42759500	-8.27387600	1.00506300
Ti	4.95999400	-7.93529700	0.45310300
Ti	-5.85242300	-5.08160600	0.79962800
Ti	-2.21811200	-4.69200300	0.72830000

Ti	1.09642400	-4.67098400	0.45979600
Ti	4.87514900	-4.28981900	0.22954100
O	-3.65738300	-7.94135500	-4.98043600
O	-0.65764500	-8.11999600	-4.92994300
O	2.64128000	-8.46846000	-5.62552800
O	5.36324400	-8.22401100	-5.36806800
O	-4.33757600	-8.54203300	4.90176500
O	2.72059300	-8.03877000	5.40814800
O	7.13545800	-7.28657300	5.00817500
O	-4.52788100	-5.16470300	5.00968800
O	-0.97128800	-4.16779300	5.42071300
O	2.55277400	-4.22156300	5.73836500
O	6.69830200	-4.08750800	4.90969600
O	-6.34814200	-9.58833000	-0.61255800
O	-2.41409300	-10.36960400	-0.24610700
O	1.78381200	-9.45831000	-0.44930200
O	5.05822900	-9.68657200	-0.39736200
O	-6.61239600	-6.73081900	0.88249400
O	-1.90602400	-6.46516200	0.26473600
O	1.55446300	-6.47196300	0.65102000
O	4.76102400	-5.96835700	0.55481600
O	-4.16877600	-9.21698100	-2.52115300
O	-0.48009400	-9.98622200	-2.46429100
O	3.24179100	-9.74696200	-2.94528900
O	6.34906600	-9.70987900	-3.16580100
O	-3.87184500	-6.26939500	-2.70482800
O	-0.89920000	-6.19341500	-2.85536700
O	3.00577800	-5.53164600	-2.33192000
O	6.60413800	-6.40385100	-3.43688000
O	-2.31734300	-8.24190600	-7.68883000
O	0.91613500	-8.46634100	-8.02728300
O	4.31709500	-8.41686100	-8.05064800
O	-5.83336100	-9.18702400	2.49241400
O	-2.59805000	-9.38975300	2.44739800
O	1.49622900	-8.67877100	2.88470800
O	4.79105100	-8.65593000	3.81505000
O	-5.88093700	-4.30120700	2.52830300
O	-2.54103800	-4.06218200	2.88399400
O	0.95675900	-3.47621100	3.40277700
O	4.18246300	-3.30692700	3.49392800
O	-6.44768300	-7.31558100	-2.45038600
O	-2.15581800	-8.15948200	-1.36032100
O	1.29918300	-7.71425100	-2.53310500
O	4.85075300	-7.47713000	-1.63815200
O	-5.91834200	-4.61281400	-1.01930000
O	-2.49561800	-4.44437700	-1.06155100
O	0.62508500	-4.70625600	-1.24257900
O	5.39760800	-4.29298400	-1.55747000
O	-4.53378700	-9.80991500	-6.39703000
O	-0.69472000	-10.18792500	-6.36951400

O	2.58085200	-10.63129900	-6.83016800
O	6.87528100	-9.76169600	-6.69536400
O	-4.53716300	-6.37532100	-6.71460000
O	-0.44342600	-6.39638100	-6.71351500
O	6.60208400	-6.58551200	-6.89633900
O	-3.54402100	-6.73708700	3.34160400
O	-0.32062600	-6.10880300	4.02413100
O	2.72531100	-6.01948700	3.90114500
O	5.49300000	-5.91625200	3.60916300
O	-6.02306300	-9.98701000	-4.00202100
O	-2.51067500	-10.45605600	-4.02677200
O	1.14769300	-10.52909000	-4.22026400
O	4.60753400	-10.93697100	-5.05282700
O	-5.53719400	-5.08202300	-4.24838000
O	-2.39487000	-5.24258700	-5.01307100
O	0.91796200	-5.36307500	-4.41787500
O	4.52590100	-5.45495600	-4.50167900
O	-2.17460800	-6.81276300	6.16563000
O	1.04242800	-6.24189500	6.69696100
O	4.60528300	-6.05254700	6.36621400
O	-4.14878400	-8.07829500	0.89143600
O	-0.39883000	-8.62530700	0.94969700
O	3.51610000	-8.16400300	1.48157300
O	6.43385700	-7.96919600	1.57118600
O	-4.07525900	-5.27412600	1.13357700
O	-0.41966600	-4.78385600	1.55431700
O	2.97471600	-3.80711800	0.70387500
O	6.14308300	-3.72051700	1.47926100
H	2.81999100	-2.83754500	0.73676400

OCBZ07@TiO₂

C	8.10208800	1.26210400	1.06721200
C	7.22646600	0.15476500	0.91363700
C	5.92610500	0.61710700	1.09419300
C	5.99960100	2.01010100	1.35726700
N	7.32845100	2.36103700	1.32218500
H	7.57079100	3.34976800	1.49965000
H	7.53113000	-0.86342400	0.69412100
H	5.01156900	0.03571000	1.03853000
C	9.52676400	1.29515700	1.01628200
C	10.43497100	0.22655700	0.79379200
N	10.26821800	2.42684000	1.21378900
C	11.72396600	0.74885700	0.86578800
C	11.61083800	2.13652200	1.13452500
H	9.99979700	3.40860700	1.40869000
H	12.65217000	0.20225200	0.74280100
C	12.62421700	3.13956800	1.31529300
C	4.96059400	2.95528900	1.64153600
C	5.19909000	4.34045600	1.84431500
C	4.23382200	5.39645200	2.08214300

N	6.46827500	4.84739300	1.84895300
C	4.95991700	6.55823000	2.22734900
H	3.15408900	5.27920100	2.12818000
C	6.34841000	6.17748200	2.08935200
H	4.58021400	7.55871900	2.41771900
C	12.31859900	4.50273700	1.61703600
C	13.22786100	5.60930700	1.81392800
N	11.02229100	4.92964500	1.73661300
C	12.44512400	6.72065900	2.04596800
H	14.31264000	5.56053200	1.77981300
C	11.07906700	6.26233800	1.99158700
C	7.56793300	6.91694200	2.18790000
C	7.98153400	8.26672600	2.35543100
N	8.71147000	6.18029300	2.07934500
C	9.38317400	8.28727300	2.33039500
C	9.83198900	6.94944500	2.14672400
H	8.71868400	5.17272900	1.97268800
C	3.66799400	2.43393300	1.76984400
C	2.59660900	1.85960000	1.92530700
C	1.33733200	1.25228700	2.08052600
C	0.24634100	2.03267000	2.52679600
C	1.14616900	-0.11227100	1.75737500
C	-1.01597400	1.46911000	2.59288100
H	0.40653100	3.07745400	2.78762800
C	-0.12626900	-0.66731300	1.82684800
H	1.99359600	-0.71199100	1.42654800
C	-1.21608500	0.12668900	2.22240200
H	-1.86792500	2.07102000	2.90067000
H	-0.29012500	-1.70750800	1.54800500
C	-2.61252400	-0.37490100	2.13706800
O	-3.51582600	0.49473300	2.38780200
O	-2.82979600	-1.58624100	1.78825200
H	12.77428400	7.73764700	2.24205800
H	10.15781000	-0.80587800	0.60765500
C	17.52661300	2.73958700	0.98665800
C	16.74220700	0.65192200	0.40043800
C	17.62584400	4.07202400	1.37416700
C	18.64899600	1.92144100	0.72026700
C	15.92922300	-0.43769600	0.10272300
C	18.15398200	0.60528100	0.34619000
C	18.91596900	4.59787600	1.50571300
H	16.74073600	4.67755200	1.56855300
C	19.93121400	2.47000000	0.85864400
C	16.57045500	-1.62673100	-0.26082300
H	14.84322600	-0.37150900	0.15170300
C	18.77494700	-0.59481700	-0.02346400
C	20.05196800	3.80714400	1.25206100
H	19.03722300	5.63836300	1.80739000
H	20.81930100	1.86795100	0.66433800
C	17.97430700	-1.70263600	-0.32524000

H	15.97078000	-2.50647200	-0.49561400
H	19.86154100	-0.66609300	-0.07950600
H	21.04302100	4.24815600	1.36062700
H	18.44477700	-2.64301500	-0.61314200
N	16.35223400	1.96142200	0.79588800
H	7.32182800	9.12170200	2.46947100
H	10.02008300	9.16213600	2.42098300
C	13.95291600	2.73741600	1.16712200
C	15.11008300	2.37304100	0.97826100
Ti	-6.17164600	3.49587000	-6.35659200
Ti	-5.63089700	0.24202400	-6.95001600
Ti	-5.45256300	-2.86293000	-8.04846400
Ti	-4.25544300	-6.06746100	-8.13135400
Ti	-10.15273800	1.63050900	2.52184200
Ti	-8.39397800	-5.30298300	2.31503400
Ti	-7.48635200	-8.36073100	1.78867800
Ti	-6.82657500	2.21104300	4.15932600
Ti	-5.83350100	-1.27138200	4.09830500
Ti	-5.09352400	-4.48857200	4.18408500
Ti	-4.15529800	-7.46422200	3.08781100
Ti	-9.04047500	4.43199300	-2.28281100
Ti	-9.16386200	0.69727300	-2.73738100
Ti	-8.00966100	-2.79901500	-3.34335000
Ti	-7.19853000	-6.18865400	-3.66598300
Ti	-5.78913700	4.55696000	-1.17292500
Ti	-5.94071300	1.05331500	-1.09520500
Ti	-4.58593800	-2.08079000	-2.35019700
Ti	-3.77888600	-5.57788100	-2.76377000
Ti	-8.54408300	3.12115500	-4.78317000
Ti	-8.03939200	-0.35270500	-5.42126500
Ti	-7.41554100	-3.69714800	-6.33439800
Ti	-6.60356200	-6.85456100	-6.72595600
Ti	-4.90841800	3.49218600	-3.75423000
Ti	-4.40392800	0.22344800	-4.24289500
Ti	-3.28598500	-6.26500800	-5.42814400
Ti	-9.27419100	1.07390900	5.20035900
Ti	-7.99411300	-2.01420400	5.64541000
Ti	-7.67265800	-5.28756000	5.13061900
Ti	-6.45374300	-8.49632300	4.42559800
Ti	-9.60243300	3.85464000	0.83748200
Ti	-8.96947300	0.20453400	0.08374500
Ti	-8.08348100	-3.31388200	0.03983200
Ti	-6.84965200	-6.59654700	-0.81124100
Ti	-6.48337400	4.24131500	2.10716000
Ti	-5.47140500	0.75543200	1.70395000
Ti	-4.66995600	-2.41741500	0.97028700
Ti	-3.44278300	-5.98757700	0.34928800
O	-6.61492800	2.86884300	-4.57236600
O	-6.22390800	-0.07733900	-5.01233900
O	-5.64775800	-3.20216300	-6.25098200

O	-4.99853700	-5.86336100	-6.32308800
O	-10.81869800	1.47814600	4.30739300
O	-9.14968900	-5.42040700	3.97762700
O	-7.46413200	-9.53115800	3.29562500
O	-7.81773900	2.12201500	5.73942900
O	-6.32981100	-1.37329100	5.95858700
O	-5.79840200	-4.82184900	5.73934100
O	-4.58781500	-8.67522600	4.44729300
O	-10.19191800	4.43641300	-0.84524300
O	-10.27317400	0.43054000	-1.33911000
O	-8.57948200	-3.52866000	-1.77920800
O	-8.13786900	-6.76598100	-2.26431200
O	-8.16418700	4.75696900	1.65167500
O	-6.87673200	0.36078200	0.53220800
O	-6.27858900	-3.13791400	0.38168900
O	-5.11656300	-6.14038900	0.02631200
O	-8.75154800	2.70487100	-2.73250100
O	-8.81215500	-1.00309900	-3.50714200
O	-7.66813800	-4.48946900	-4.36492400
O	-6.94742400	-7.45352200	-5.00283000
O	-5.92614100	2.83144500	-1.81434600
O	-5.23569600	-0.00161100	-2.35857700
O	-4.05288100	-3.82764400	-2.22349500
O	-3.78321800	-7.21868600	-4.04333700
O	-5.70520400	2.07377900	-7.35638400
O	-5.14841100	-1.02846200	-8.19336500
O	-4.44493700	-4.32184000	-8.69635300
O	-10.83470200	3.35206300	2.07914400
O	-10.33915900	0.17566300	1.51197300
O	-9.12511200	-3.84703600	1.56835100
O	-8.77994700	-7.20161900	1.99550800
O	-6.37163500	4.02442200	3.98698900
O	-5.71975600	0.70387300	3.93921500
O	-4.63788100	-2.72260500	4.04623200
O	-3.86315500	-5.84896200	3.79265000
O	-7.46693300	5.15658200	-1.62741500
O	-7.79631900	0.61032400	-1.60639100
O	-6.33070200	-2.40492100	-2.95690300
O	-5.72169200	-6.01685900	-2.55367400
O	-5.40646900	4.71381500	0.63745500
O	-4.61506100	1.35121600	0.20612400
O	-4.18409100	-1.64652800	-0.54302700
O	-2.72321500	-6.14996900	-1.36523200
O	-8.00801400	3.76518300	-6.45201100
O	-7.62097800	-0.02418000	-7.11039900
O	-7.23211100	-3.15984700	-8.15454800
O	-5.66292500	-7.25404600	-8.32987300
O	-4.74722800	4.27592300	-5.44845500
O	-3.98015200	0.31362200	-6.01839900
O	-2.72954200	-6.55626800	-7.28375000

O	-8.45889900	1.28724000	3.47754700
O	-7.54044100	-1.93634500	3.86934900
O	-6.78007000	-4.85252300	3.35451800
O	-6.05604100	-7.46590300	2.75385600
O	-9.28090700	4.71389300	-4.12073300
O	-9.03551900	1.24273700	-4.81984100
O	-8.30787400	-2.29082100	-5.52495500
O	-7.73920500	-5.53221600	-6.94542700
O	-4.62354900	4.91913300	-2.55466700
O	-3.89020100	2.00819400	-3.75307800
O	-3.56847800	-1.34243100	-3.72210000
O	-2.91800800	-4.87637400	-4.37320500
O	-9.24149700	-0.62903500	5.83610400
O	-8.29538300	-3.81374200	6.07543100
O	-7.29375200	-7.17009100	5.35463100
O	-8.93657900	2.18934900	0.78895300
O	-8.72909100	-1.57764300	0.12551500
O	-7.69452600	-5.43663700	0.24848600
O	-6.97902100	-8.25396000	0.00215800
O	-6.45571400	2.42295900	2.09825000
O	-5.51889800	-1.17297600	2.10630900
O	-3.53076700	-4.16221200	1.19874800
O	-3.14195000	-7.40343800	1.53473800
H	-2.67082100	-3.87325400	1.57329800

ODPA04@TiO₂

Ti	-1.752806	-11.227008	-5.780004
Ti	1.591170	-11.415676	-5.854919
Ti	4.798742	-12.051669	-6.266403
Ti	8.145116	-11.372802	-6.124867
Ti	-1.962801	-11.487416	4.124455
Ti	5.113720	-10.951629	4.767257
Ti	8.340147	-10.699835	4.590772
Ti	-2.058034	-7.739540	4.241604
Ti	1.495101	-7.358816	4.584413
Ti	4.749359	-7.091691	5.017499
Ti	7.978841	-7.038069	4.364406
Ti	-3.788763	-12.060473	-1.205414
Ti	-0.133160	-12.881941	-0.813506
Ti	3.573170	-12.577711	-1.068482
Ti	7.081547	-12.379106	-0.967805
Ti	-3.399002	-8.653653	-1.446789
Ti	-0.051410	-9.263032	-0.609924
Ti	3.426214	-8.988830	-1.590725
Ti	7.036467	-8.834747	-1.497741
Ti	-2.080178	-12.784998	-3.390970
Ti	1.483360	-13.060681	-3.452041
Ti	4.987110	-13.268982	-3.822612
Ti	8.269096	-13.059400	-3.840994
Ti	-1.838839	-9.032636	-3.894906

Ti	1.492156	-9.216095	-3.859844
Ti	8.175338	-9.456854	-3.974716
Ti	-1.626351	-9.688466	6.342013
Ti	1.550288	-8.769105	6.954663
Ti	4.849129	-9.134440	7.022436
Ti	8.303902	-8.737725	6.629755
Ti	-3.776356	-11.378074	1.939035
Ti	0.004385	-11.640727	1.775341
Ti	3.609341	-11.430052	2.168129
Ti	7.163399	-11.036998	1.619337
Ti	-3.667520	-7.993607	1.838236
Ti	-0.026881	-7.760359	1.814494
Ti	3.291611	-7.864855	1.573414
Ti	7.085787	-7.400520	1.320190
O	-1.470374	-10.990825	-3.872769
O	1.523611	-11.216680	-3.817795
O	4.831416	-11.564706	-4.490857
O	7.558879	-11.313906	-4.252215
O	-2.215794	-11.388473	6.019823
O	4.807052	-10.968116	6.560970
O	9.273600	-10.237788	6.192986
O	-2.406041	-8.006984	6.054760
O	1.212348	-7.057183	6.463270
O	4.707026	-7.141247	6.756176
O	8.859283	-7.059780	6.021066
O	-4.230134	-12.521139	0.523355
O	-0.312733	-13.356876	0.921436
O	3.953425	-12.607024	0.706615
O	7.284257	-12.779844	0.758925
O	-4.460564	-9.622114	1.950498
O	0.221368	-9.550745	1.363732
O	3.772171	-9.639280	1.830682
O	6.981949	-9.074485	1.649158
O	-1.993266	-12.216065	-1.368264
O	1.690144	-13.133303	-1.295308
O	5.429438	-12.856925	-1.779220
O	8.548057	-12.798080	-2.026656
O	-1.671145	-9.282226	-1.629691
O	1.268874	-9.268241	-1.815699
O	5.201774	-8.660680	-1.297797
O	8.807449	-9.514055	-2.335019
O	-0.144287	-11.409714	-6.571271
O	3.097842	-11.628955	-6.895423
O	6.494643	-11.557841	-6.927637
O	-3.713031	-12.049978	3.629188
O	-0.461510	-12.281401	3.589260
O	3.694013	-11.792923	4.048685
O	6.923000	-11.627555	5.041757
O	-3.691985	-7.146912	3.532064
O	-0.343552	-7.021733	3.936324

O	3.135749	-6.478348	4.399001
O	6.367764	-6.276584	4.529075
O	-4.261974	-10.274217	-1.347156
O	0.102267	-11.205291	-0.280874
O	3.451749	-10.842258	-1.397058
O	7.052141	-10.582992	-0.526989
O	-3.702660	-7.546431	0.014127
O	-0.254193	-7.505030	0.021135
O	2.813851	-7.951243	-0.128456
O	7.584474	-7.406363	-0.479531
O	-2.383725	-12.885484	-5.234374
O	1.475753	-13.322347	-5.202385
O	4.766833	-13.752558	-5.653934
O	9.065531	-12.875669	-5.562169
O	-2.344885	-9.466536	-5.646245
O	1.720676	-9.536655	-5.645933
O	8.801403	-9.709769	-5.811719
O	-1.401356	-9.618939	4.437880
O	1.830063	-9.082939	5.173703
O	4.873644	-9.004801	4.982736
O	7.635804	-8.895712	4.749283
O	-3.866881	-12.972738	-2.838456
O	-0.355967	-13.501203	-2.866597
O	3.329999	-13.597165	-3.055387
O	6.801286	-14.019225	-3.896921
O	-3.326709	-8.099350	-3.200112
O	-0.198237	-8.302030	-3.974562
O	3.110103	-8.481579	-3.363727
O	6.748878	-8.549040	-3.422022
O	-0.076190	-9.637646	7.293694
O	3.177513	-9.104541	7.830598
O	6.704983	-8.964925	7.493959
O	-2.016645	-11.030671	1.988196
O	1.771939	-11.697000	2.092175
O	5.728023	-11.267626	2.637637
O	8.607958	-11.034205	2.785138
O	-1.900039	-8.234820	2.204765
O	1.757393	-7.940564	2.654695
O	5.182465	-6.967552	1.781893
O	8.358205	-6.822429	2.562364
C	4.642585	5.269129	0.666300
C	5.346624	4.037320	0.659793
C	4.411757	3.015694	0.809017
C	3.131749	3.619901	0.913286
N	3.313106	4.977846	0.827552
H	2.482402	5.584578	0.876798
H	6.421546	3.926485	0.552424
H	4.602763	1.948119	0.840397
C	5.129194	6.599169	0.506142
C	6.460629	7.063174	0.307288

N	4.312133	7.689241	0.493364
C	6.407400	8.445609	0.164333
C	5.042356	8.842863	0.277964
H	3.287344	7.779633	0.594646
H	7.243623	9.115969	-0.007214
C	4.421081	10.104302	0.178360
C	1.837241	3.019848	1.051640
C	0.624756	3.737926	1.162215
C	-0.722773	3.208441	1.235271
N	0.604706	5.103626	1.137902
C	-1.563083	4.297632	1.234556
H	-1.000915	2.158609	1.269058
C	-0.702764	5.454586	1.167228
H	-2.648999	4.300898	1.278031
C	3.039369	10.320786	0.294276
C	2.311477	11.562508	0.114434
N	2.157112	9.296614	0.562988
C	0.975951	11.261803	0.266703
H	2.754858	12.529389	-0.110732
C	0.918508	9.844400	0.547808
C	-0.979584	6.852568	1.057446
C	-2.098254	7.672163	0.876498
N	0.127269	7.661741	1.020451
C	-1.622777	9.001791	0.695572
C	-0.180479	8.953585	0.765564
H	1.075600	7.309647	1.092318
C	1.789305	1.629170	1.029079
C	1.759491	0.407518	1.004735
C	1.744952	-0.989238	1.045915
C	0.521482	-1.674289	1.214792
C	2.967677	-1.694371	0.976136
C	0.531283	-3.050815	1.362480
H	-0.410917	-1.112038	1.256887
C	2.965242	-3.070083	1.127168
H	3.896571	-1.146092	0.825946
C	1.751840	-3.744186	1.333246
H	-0.396089	-3.599605	1.515160
H	3.896986	-3.631148	1.091930
C	1.753295	-5.207391	1.513762
O	0.625349	-5.767014	1.697363
O	2.886660	-5.800694	1.478832
H	0.129347	11.938421	0.189800
H	5.064222	10.961024	-0.021239
H	7.341722	6.430327	0.264019
H	-3.136534	7.358854	0.860182
C	-2.400513	10.132780	0.485355
C	-3.123968	11.115824	0.348350
N	-3.841113	12.224921	0.225656
C	-5.196641	12.145103	-0.239017
C	-6.164781	13.037032	0.246130

C	-5.557220	11.138493	-1.144702
C	-7.480428	12.929315	-0.205722
H	-5.892213	13.795936	0.979015
C	-6.881375	11.039677	-1.575593
H	-4.805002	10.439892	-1.512631
C	-7.864487	11.938405	-1.126848
H	-8.227681	13.629209	0.173812
H	-7.151979	10.258765	-2.289230
C	-3.194759	13.468894	0.547557
C	-3.435367	14.604191	-0.231907
C	-2.271002	13.502544	1.601345
C	-2.765116	15.805011	0.043547
H	-4.139603	14.553155	-1.062872
C	-1.581914	14.689166	1.857777
H	-2.093427	12.611159	2.202551
C	-1.829542	15.833318	1.091121
H	-0.850207	14.717796	2.666043
H	-1.286006	16.756188	1.301993
C	-9.438465	12.858424	-2.872835
H	-8.752704	12.547490	-3.678992
H	-9.118692	13.868570	-2.566167
C	-4.370104	17.728570	-0.200435
H	-4.197969	18.007810	0.852742
H	-5.196207	16.997166	-0.195763
C	-10.873267	12.921364	-3.402562
H	-11.184860	11.919218	-3.744860
H	-11.551001	13.189721	-2.573209
C	-11.050348	13.931546	-4.540153
H	-10.395400	13.654984	-5.385148
H	-10.707296	14.924117	-4.198158
C	-12.496425	14.048008	-5.034845
H	-13.146416	14.297512	-4.178718
H	-12.834507	13.063132	-5.399500
C	-12.676992	15.096632	-6.134218
H	-13.723761	15.153677	-6.468312
H	-12.381422	16.096719	-5.780469
H	-12.059016	14.861134	-7.014627
C	-4.782615	18.961764	-1.003620
H	-3.950994	19.687589	-1.014371
H	-4.954639	18.671355	-2.054716
C	-6.039467	19.643024	-0.452784
H	-5.867267	19.922126	0.601700
H	-6.871171	18.916359	-0.446066
C	-6.455772	20.885769	-1.243139
H	-5.617384	21.602975	-1.253986
H	-6.632313	20.604051	-2.295150
C	-7.703654	21.570707	-0.678969
H	-7.546494	21.872035	0.368290
H	-7.961561	22.473163	-1.252907
H	-8.571403	20.893663	-0.703981

C	-9.268803	11.902871	-1.673602
H	-9.980528	12.195614	-0.885279
H	-9.528485	10.878374	-1.982562
C	-3.104596	17.040707	-0.747805
H	-3.271364	16.772546	-1.803214
H	-2.262210	17.748612	-0.721036
H	4.987929	-6.005339	1.734479

ODPA07@TiO₂

Ti	-4.560174	-11.906208	-4.608449
Ti	-1.210434	-11.935293	-4.681572
Ti	2.045442	-12.449660	-5.069667
Ti	5.375118	-11.665619	-4.815993
Ti	-4.715938	-12.436708	5.277435
Ti	2.412514	-11.546373	5.759223
Ti	5.586806	-11.177249	5.517747
Ti	-4.967182	-8.696584	5.487082
Ti	-1.418602	-8.131963	5.763333
Ti	1.837587	-7.731070	6.212045
Ti	5.053486	-7.540509	5.458383
Ti	-6.569809	-12.970793	-0.063557
Ti	-2.887182	-13.593399	0.311319
Ti	0.792040	-13.134434	0.041178
Ti	4.263186	-12.986346	0.188506
Ti	-6.335474	-9.543096	-0.206742
Ti	-2.949539	-9.961475	0.613636
Ti	0.529507	-9.520659	-0.361228
Ti	4.138423	-9.218055	-0.131773
Ti	-4.836013	-13.562476	-2.274587
Ti	-1.278081	-13.677607	-2.346696
Ti	2.234316	-13.809698	-2.705172
Ti	5.533380	-13.515431	-2.659821
Ti	-4.749162	-9.785708	-2.652041
Ti	-1.399409	-9.821359	-2.617059
Ti	5.333648	-9.882535	-2.562184
Ti	-4.405214	-10.676628	7.523313
Ti	-1.246010	-9.659868	8.055154
Ti	2.083355	-9.860007	8.107804
Ti	5.509808	-9.305536	7.648506
Ti	-6.545093	-12.361166	3.103779
Ti	-2.786139	-12.394739	2.914811
Ti	0.791389	-11.914906	3.214953
Ti	4.336283	-11.435538	2.586934
Ti	-6.603949	-8.971090	3.100561
Ti	-2.984396	-8.455150	3.026608
Ti	0.334120	-8.315848	2.687202
Ti	4.123706	-7.712102	2.360814
O	-4.300955	-11.724391	-2.692041
O	-1.300722	-11.810477	-2.644211
O	2.063761	-12.073732	-3.268841

O	4.805032	-11.747175	-2.935332
O	-4.946515	-12.388369	7.174163
O	2.171385	-11.655758	7.573233
O	6.520448	-10.749071	7.122397
O	-5.250865	-9.020403	7.305401
O	-1.672383	-7.944478	7.666596
O	1.838756	-7.853225	7.946786
O	5.979196	-7.584979	7.082865
O	-6.954964	-13.487544	1.662800
O	-3.008061	-14.111940	2.036748
O	1.203821	-13.108318	1.824041
O	4.464095	-13.255070	1.957907
O	-7.310488	-10.645125	3.175411
O	-2.648024	-10.243451	2.547388
O	0.800692	-10.101692	2.818837
O	4.194706	-9.443802	2.244585
O	-4.771236	-13.026955	-0.236426
O	-1.061703	-13.744076	-0.178947
O	2.633444	-13.501006	-0.639162
O	5.776240	-13.364681	-0.828264
O	-4.578858	-10.074412	-0.398559
O	-1.591554	-9.908930	-0.551784
O	2.285566	-9.174464	-0.015594
O	5.940685	-9.780107	-0.896893
O	-2.946780	-11.975039	-5.404306
O	0.331742	-12.044204	-5.685227
O	3.742844	-11.857895	-5.651548
O	-6.433058	-13.084438	4.768263
O	-3.182070	-13.135715	4.711324
O	1.007287	-12.409523	5.051753
O	4.233995	-12.224267	5.920906
O	-6.649305	-8.190148	4.828886
O	-3.302566	-7.869766	5.175233
O	0.195680	-7.185528	5.614899
O	3.421574	-6.857578	5.695806
O	-7.121864	-11.207242	-0.156886
O	-2.750037	-11.915492	0.889067
O	0.645542	-11.412400	-0.285589
O	4.136528	-11.197775	0.515791
O	-6.692550	-8.493379	1.282719
O	-3.230022	-8.202941	1.240461
O	-0.107824	-8.309740	0.976575
O	4.485765	-7.495230	0.576814
O	-5.120794	-13.610727	-4.119865
O	-1.274008	-13.861948	-4.106727
O	2.047333	-14.185184	-4.564781
O	6.328061	-13.180718	-4.361692
O	-5.224411	-10.178526	-4.421525
O	-1.161652	-10.056198	-4.409559
O	5.977185	-10.000223	-4.396768

O	-4.233500	-10.548436	5.617649
O	-1.004481	-9.864439	6.246427
O	2.041145	-9.628657	6.094417
O	4.786488	-9.424114	5.776905
O	-6.603618	-13.853112	-1.719949
O	-3.084205	-14.214314	-1.758463
O	0.564321	-14.173637	-1.972768
O	4.077732	-14.486336	-2.797778
O	-6.285237	-8.943980	-1.947741
O	-3.132423	-8.995215	-2.691335
O	0.204355	-9.029407	-2.118316
O	3.847936	-9.056536	-2.075185
O	-2.819356	-10.611377	8.410492
O	0.403401	-9.960643	8.894836
O	3.954104	-9.610761	8.545043
O	-4.805336	-11.905908	3.162449
O	-1.014001	-12.317111	3.222332
O	2.910678	-11.475213	3.654890
O	5.832434	-11.289170	3.684323
O	-4.819676	-9.096580	3.423531
O	-1.186333	-8.520240	3.797904
O	2.211916	-7.420378	2.932286
O	5.385890	-7.252862	3.653105
C	0.151031	4.956326	0.391412
C	1.030704	3.864168	0.627446
C	0.256032	2.766504	0.992775
C	-1.104468	3.177910	0.984803
N	-1.120995	4.506058	0.618423
H	-2.044887	4.969637	0.554619
H	2.111305	3.899518	0.533209
H	0.606283	1.771574	1.248995
C	0.472342	6.292142	-0.006823
C	1.749682	6.859981	-0.266425
N	-0.455065	7.278987	-0.206441
C	1.556633	8.193823	-0.620650
C	0.163782	8.452413	-0.578652
H	-1.488919	7.289887	-0.127842
H	2.321551	8.912955	-0.896546
C	-0.572873	9.662216	-0.842876
C	-2.302207	2.439785	1.271914
C	-3.597599	3.028243	1.212131
C	-4.890455	2.407195	1.438899
N	-3.760972	4.347006	0.884875
C	-5.834524	3.387667	1.234476
H	-5.063278	1.370191	1.712870
C	-5.098015	4.582894	0.887289
H	-6.914719	3.296113	1.310640
C	-2.003825	9.721325	-0.764822
C	-2.875393	10.839660	-1.040246
N	-2.739183	8.625012	-0.412256

C	-4.166010	10.383048	-0.852009
H	-2.567250	11.837942	-1.341011
C	-4.044840	9.004628	-0.455114
C	-5.522616	5.901457	0.540303
C	-6.748663	6.596288	0.341471
N	-4.530222	6.797999	0.265258
C	-6.436547	7.900960	-0.063102
C	-5.016668	8.012131	-0.111569
H	-3.542711	6.582420	0.332511
C	-2.164262	1.082413	1.608869
C	-2.000340	-0.102151	1.891052
C	-1.839702	-1.476309	2.174441
C	-2.972906	-2.291307	2.412204
C	-0.551936	-2.063674	2.205144
C	-2.818931	-3.652926	2.642330
H	-3.967158	-1.846172	2.402565
C	-0.410236	-3.428322	2.436462
H	0.327320	-1.443464	2.033877
C	-1.540188	-4.238726	2.639690
H	-3.695314	-4.277587	2.807731
H	0.582319	-3.876235	2.441190
C	-1.405325	-5.719254	2.794314
O	-2.487866	-6.375493	2.959112
O	-0.230812	-6.229055	2.730203
H	-5.090114	10.942775	-0.973806
H	2.696814	6.333706	-0.195265
H	-7.742088	6.177897	0.469561
H	-7.139583	8.691536	-0.309386
C	0.145212	10.802386	-1.182140
C	0.774605	11.824505	-1.464131
N	1.463942	12.909903	-1.762191
C	0.758011	14.116591	-2.119854
C	1.210125	15.355943	-1.647218
C	-0.405187	14.034258	-2.894400
C	0.488483	16.507831	-1.960229
H	2.103469	15.419374	-1.026432
C	-1.119884	15.198066	-3.188932
H	-0.744956	13.067556	-3.267224
C	-0.690089	16.454238	-2.727835
H	0.837536	17.469635	-1.579630
H	-2.028564	15.121786	-3.789593
C	2.906111	12.871752	-1.696874
C	3.661138	13.573661	-2.644746
C	3.530284	12.107351	-0.703098
C	5.062698	13.538658	-2.602333
H	3.157499	14.143978	-3.425786
C	4.924977	12.057441	-0.670341
H	2.935697	11.573782	0.037340
C	5.686238	12.766674	-1.606119
H	5.420912	11.467156	0.100785

H	6.776411	12.722252	-1.561957
C	-1.441045	17.714998	-3.072383
H	-2.506088	17.482065	-3.226847
H	-1.383697	18.415989	-2.224256
C	5.876726	14.359771	-3.572721
H	6.879068	13.915710	-3.674487
H	5.408539	14.336380	-4.569469
C	-0.888979	18.415409	-4.329828
H	0.188918	18.605185	-4.189794
H	-0.975706	17.731871	-5.191264
C	-1.603618	19.734127	-4.638573
H	-1.514227	20.404621	-3.765765
H	-2.683303	19.544716	-4.772631
C	-1.055176	20.447233	-5.879271
H	0.030511	20.608528	-5.753832
H	-1.168066	19.789947	-6.759517
C	-1.734170	21.791269	-6.161302
H	-2.819142	21.631250	-6.286036
H	-1.620304	22.442118	-5.277501
C	-1.177569	22.504980	-7.396647
H	-1.679362	23.469649	-7.562375
H	-0.098996	22.699214	-7.288252
H	-1.317403	21.896081	-8.303307
C	6.014554	15.825056	-3.114396
H	6.432386	15.843166	-2.093552
H	5.008431	16.272744	-3.044725
C	6.888651	16.674723	-4.040364
H	7.901433	16.237682	-4.088424
H	6.484626	16.634700	-5.067122
C	6.987945	18.136519	-3.592040
H	7.377164	18.173044	-2.559026
H	5.973454	18.571255	-3.552565
C	7.871456	19.004382	-4.493552
H	8.887737	18.575790	-4.526117
H	7.487306	18.963198	-5.527212
C	7.946544	20.462930	-4.033964
H	8.354478	20.532984	-3.013494
H	8.588886	21.064605	-4.693724
H	6.947025	20.924531	-4.024777
H	2.013563	-6.460149	2.999863

OPTZ04@TiO₂

Ti	-4.411833	-7.674100	-4.298342
Ti	-1.061050	-7.887588	-4.354410
Ti	2.182382	-8.517725	-4.671078
Ti	5.543652	-7.887702	-4.424292
Ti	-4.652819	-8.046769	5.614844
Ti	2.522884	-7.486528	6.144370
Ti	5.725999	-7.220329	5.914560
Ti	-4.701248	-4.295284	5.747930

Ti	-1.114755	-3.908488	6.057934
Ti	2.146118	-3.629805	6.422948
Ti	5.376960	-3.553680	5.758302
Ti	-6.499777	-8.581336	0.268612
Ti	-2.857981	-9.425269	0.660343
Ti	0.848002	-9.187987	0.428932
Ti	4.326554	-9.153165	0.578345
Ti	-6.077716	-5.173260	0.068655
Ti	-2.719409	-5.808387	0.911599
Ti	0.760486	-5.574286	-0.040391
Ti	4.359687	-5.394446	0.236453
Ti	-4.792333	-9.278327	-1.939434
Ti	-1.236522	-9.597182	-1.998809
Ti	2.276676	-9.890270	-2.306818
Ti	5.596573	-9.738466	-2.261965
Ti	-4.498369	-5.520160	-2.374251
Ti	-1.162700	-5.744344	-2.316101
Ti	5.557648	-6.104110	-2.175895
Ti	-4.232272	-6.253732	7.827186
Ti	-1.037386	-5.330894	8.419941
Ti	2.264314	-5.680876	8.416404
Ti	5.715878	-5.285604	7.984400
Ti	-6.469181	-7.923277	3.429132
Ti	-2.698149	-8.199563	3.261049
Ti	0.907351	-7.981549	3.599420
Ti	4.496437	-7.598530	2.977451
Ti	-6.325118	-4.530081	3.350988
Ti	-2.664574	-4.314739	3.343961
Ti	0.638758	-4.408084	3.025272
Ti	4.441200	-3.866706	2.699606
O	-4.160353	-7.474525	-2.377491
O	-1.145016	-7.739075	-2.328274
O	2.192961	-8.148390	-2.865126
O	4.953026	-7.941643	-2.551283
O	-4.850274	-7.946755	7.511027
O	2.237675	-7.502635	7.946950
O	6.684772	-6.768394	7.499122
O	-5.013422	-4.570050	7.564974
O	-1.371438	-3.616354	7.946659
O	2.115892	-3.684533	8.161534
O	6.273614	-3.598875	7.403544
O	-6.941884	-9.038759	2.001227
O	-3.019685	-9.905458	2.398814
O	1.246420	-9.212215	2.209543
O	4.559139	-9.419914	2.341804
O	-7.124563	-6.156913	3.443963
O	-2.460484	-6.116926	2.872928
O	1.063301	-6.196977	3.165157
O	4.479405	-5.604135	2.608578
O	-4.710625	-8.756875	0.107200

O	-1.043274	-9.683395	0.172413
O	2.671865	-9.632802	-0.239338
O	5.830913	-9.571717	-0.430904
O	-4.346492	-5.788113	-0.096659
O	-1.379698	-5.863684	-0.274099
O	2.513111	-5.254209	0.343545
O	6.149015	-6.020112	-0.504052
O	-2.802585	-7.847506	-5.078327
O	0.497863	-8.063952	-5.327054
O	3.903070	-7.995927	-5.257048
O	-6.401484	-8.607178	5.121866
O	-3.150126	-8.839454	5.074625
O	1.100978	-8.353571	5.456964
O	4.328412	-8.178569	6.380664
O	-6.348407	-3.711957	5.060930
O	-2.973829	-3.603461	5.443743
O	0.515539	-3.021400	5.840856
O	3.764200	-2.804880	5.930376
O	-6.946811	-6.791377	0.138058
O	-2.625882	-7.755626	1.207770
O	0.813581	-7.455634	0.104069
O	4.253412	-7.362809	0.892927
O	-6.404819	-4.072274	1.526320
O	-2.862867	-4.040804	1.551513
O	0.124766	-4.420307	1.328906
O	4.770247	-3.669468	0.914258
O	-5.062147	-9.339622	-3.787063
O	-1.229960	-9.807559	-3.757374
O	2.105673	-10.251481	-4.174535
O	6.418662	-9.446966	-3.960939
O	-4.971483	-5.901908	-4.141919
O	-0.937169	-6.011646	-4.109495
O	6.216825	-6.249955	-4.000740
O	-4.064085	-6.182158	5.912784
O	-0.770254	-5.632409	6.638462
O	2.261025	-5.537512	6.373106
O	5.019653	-5.413290	6.103287
O	-6.576164	-9.466952	-1.387231
O	-3.078993	-10.023554	-1.417632
O	0.580948	-10.185482	-1.608591
O	4.098289	-10.640163	-2.393853
O	-6.001423	-4.610292	-1.681937
O	-2.841229	-4.812893	-2.398105
O	0.472927	-5.045641	-1.803814
O	4.088904	-5.238689	-1.708060
O	-2.664532	-6.212321	8.746908
O	0.609345	-5.671176	9.257120
O	4.130327	-5.524030	8.864018
O	-4.710424	-7.588139	3.473521
O	-0.920700	-8.246924	3.582775

O	3.077891	-7.617542	4.037648
O	5.983758	-7.489932	4.100497
O	-4.555680	-4.760983	3.699858
O	-0.871424	-4.523933	4.136677
O	2.543604	-3.554565	3.297897
O	5.735993	-3.374751	3.945002
C	-4.959259	7.446983	-1.651815
C	-5.603251	6.269145	-1.190447
C	-4.610915	5.349231	-0.853363
C	-3.355813	5.961246	-1.101828
N	-3.608560	7.225214	-1.580227
H	-2.803869	7.830490	-1.801904
H	-6.677376	6.125936	-1.121616
H	-4.752411	4.346929	-0.462433
C	-5.527019	8.667386	-2.139442
C	-6.893525	9.046961	-2.269238
N	-4.773540	9.712824	-2.585289
C	-6.925397	10.332757	-2.802362
C	-5.580418	10.754276	-3.005670
H	-3.750819	9.835653	-2.665369
H	-7.807869	10.924831	-3.026862
C	-5.047455	11.951504	-3.531250
C	-2.023983	5.463660	-0.916605
C	-0.849695	6.215196	-1.169998
C	0.528550	5.811933	-0.979871
N	-0.909106	7.496671	-1.647388
C	1.301853	6.887484	-1.353619
H	0.869443	4.848364	-0.612514
C	0.373268	7.911162	-1.769567
H	2.386380	6.961428	-1.344125
C	-3.677823	12.220263	-3.660031
C	-3.036271	13.406347	-4.192395
N	-2.719134	11.318039	-3.244894
C	-1.678519	13.200667	-4.084423
H	-3.543390	14.275964	-4.603524
C	-1.521151	11.893523	-3.487457
C	0.565478	9.230311	-2.298600
C	1.630943	10.074459	-2.637993
N	-0.588013	9.904124	-2.602579
C	1.070015	11.278525	-3.162490
C	-0.359937	11.128337	-3.127948
H	-1.512734	9.513501	-2.459656
C	-1.863724	4.159158	-0.443590
C	-1.648909	3.041823	0.007392
C	-1.429594	1.804846	0.632665
C	-0.135360	1.439408	1.075539
C	-2.537349	0.963379	0.878838
C	0.033891	0.261413	1.788991
H	0.714965	2.085823	0.859693
C	-2.361227	-0.197642	1.611269

H	-3.520867	1.244754	0.502599
C	-1.082134	-0.540495	2.080041
H	1.022478	-0.037076	2.137878
H	-3.204577	-0.851739	1.821736
C	-0.935451	-1.802539	2.831189
O	0.235068	-2.305052	2.947441
O	-2.009761	-2.320042	3.287515
H	-0.878771	13.870363	-4.386512
H	-5.761037	12.707168	-3.860476
H	-7.744258	8.430944	-1.994742
H	2.688555	9.859754	-2.526289
C	1.768617	12.394448	-3.624461
C	2.414782	13.361457	-4.022953
C	2.443960	15.625258	-4.965846
C	3.146596	16.713044	-5.454780
C	4.556422	16.706660	-5.485725
C	5.246940	15.572783	-4.988835
C	4.543233	14.471073	-4.516017
C	3.128836	14.477056	-4.493285
C	7.460277	16.791293	-6.053327
C	6.548764	17.789702	-6.456540
C	6.971974	18.793391	-7.344592
H	6.255762	19.552505	-7.662811
C	8.281385	18.801432	-7.822288
C	9.181261	17.801394	-7.430277
C	8.768983	16.797481	-6.549417
H	4.646089	18.554048	-6.345578
H	1.354996	15.643703	-4.956081
H	2.614171	17.583837	-5.839566
H	5.083787	13.598809	-4.148044
H	8.595726	19.580838	-8.515927
H	10.203497	17.799410	-7.809418
H	9.465514	16.018630	-6.237711
N	5.228522	17.786990	-6.011848
S	7.016470	15.566064	-4.849444
H	2.341193	-2.592189	3.310181

OPTZ07@TiO₂

Ti	-3.407865	-8.543844	-6.226496
Ti	-0.065120	-8.732207	-6.283277
Ti	3.175807	-9.373503	-6.629716
Ti	6.537425	-8.738960	-6.365502
Ti	-3.640169	-9.054740	3.667123
Ti	3.502006	-8.476231	4.173093
Ti	6.701023	-8.279076	3.956991
Ti	-3.695485	-5.297265	3.825639
Ti	-0.148858	-4.856995	4.137919
Ti	3.118725	-4.632820	4.597690
Ti	6.348782	-4.614160	3.886278
Ti	-5.501131	-9.539646	-1.697653

Ti	-1.852098	-10.297146	-1.302723
Ti	1.855989	-10.026394	-1.548203
Ti	5.323187	-10.043381	-1.386755
Ti	-5.118824	-6.126864	-1.842453
Ti	-1.740435	-6.664949	-0.995060
Ti	1.759083	-6.406174	-1.952847
Ti	5.367111	-6.272038	-1.683195
Ti	-3.778167	-10.197166	-3.901618
Ti	-0.227497	-10.479175	-3.955258
Ti	3.276405	-10.777588	-4.284117
Ti	6.593926	-10.609974	-4.224940
Ti	-3.510991	-6.426230	-4.261699
Ti	-0.171282	-6.622968	-4.210119
Ti	6.560424	-6.972757	-4.100844
Ti	-3.250262	-7.279447	5.892354
Ti	-0.066506	-6.395128	6.430724
Ti	3.246019	-6.763878	6.505463
Ti	6.694074	-6.390806	6.075947
Ti	-5.437504	-8.917610	1.471742
Ti	-1.711705	-9.150365	1.316703
Ti	1.881184	-8.794484	1.625666
Ti	5.450211	-8.505495	1.017783
Ti	-5.341413	-5.528319	1.447873
Ti	-1.683899	-5.116519	1.370211
Ti	1.624431	-5.181441	1.064082
Ti	5.437389	-4.772701	0.804518
O	-3.154466	-8.380690	-4.306823
O	-0.154960	-8.613045	-4.250357
O	3.196115	-9.028496	-4.820807
O	5.951941	-8.808299	-4.488829
O	-3.878486	-8.966883	5.560434
O	3.240424	-8.563518	5.985745
O	7.647265	-7.876774	5.563929
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C	12.618338	12.951938	-9.336798
H	13.020284	13.513107	-8.479517
H	11.996259	13.620704	-9.949556
C	13.749654	12.378695	-10.176263
H	14.370352	11.692682	-9.573351
H	13.336029	11.816784	-11.032260
C	15.548493	13.098646	-11.545425
H	16.247875	12.391915	-11.063705
H	15.104340	12.600685	-12.425522
C	16.277458	14.362455	-11.971030
H	16.754223	14.841331	-11.096672
H	15.556528	15.081536	-12.402056
C	17.982418	15.151606	-13.395456
H	18.505696	15.648822	-12.560642
H	18.717228	14.802913	-14.130434
H	17.303332	15.880124	-13.871856
O	14.520440	13.491325	-10.630007
O	17.263412	14.002209	-12.938936
H	0.536596	-7.421463	4.840735

OGLY07@TiO₂

Ti	-6.834208	-13.763840	-6.678428
Ti	-3.486787	-13.843732	-6.751919
Ti	-0.242281	-14.394090	-7.152625
Ti	3.093944	-13.648869	-6.882690
Ti	-7.014634	-14.564589	3.185603
Ti	0.115194	-13.829775	3.732647
Ti	3.299825	-13.504532	3.512432
Ti	-7.203733	-10.826456	3.500668
Ti	-3.658717	-10.337295	3.819051
Ti	-0.402282	-10.017291	4.290387
Ti	2.816387	-9.856276	3.553608
Ti	-8.863589	-14.920833	-2.168791
Ti	-5.193376	-15.609193	-1.806807
Ti	-1.501444	-15.207884	-2.060499

Ti	1.972364	-15.095319	-1.913939
Ti	-8.575865	-11.493784	-2.214745
Ti	-5.195439	-11.988404	-1.400389
Ti	-1.712913	-11.583755	-2.361390
Ti	1.894276	-11.340453	-2.121200
Ti	-7.136334	-15.478398	-4.391885
Ti	-3.579432	-15.647686	-4.464704
Ti	-0.071198	-15.817917	-4.825171
Ti	3.230918	-15.552365	-4.778958
Ti	-6.990055	-11.694563	-4.665538
Ti	-3.644985	-11.783435	-4.628806
Ti	3.070546	-11.925410	-4.581634
Ti	-6.692478	-12.876079	5.484083
Ti	-3.523224	-11.937154	6.064488
Ti	-0.198235	-12.203669	6.124492
Ti	3.236651	-11.687226	5.690776
Ti	-8.835304	-14.400489	1.012446
Ti	-5.075025	-14.494468	0.832659
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Ti	-8.836051	-11.011850	1.103809
Ti	-5.202080	-10.550948	1.055243
Ti	-1.887544	-10.505167	0.741064
Ti	1.907631	-9.930743	0.451844
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O	-3.571159	-13.774336	-4.714112
O	-0.224354	-14.065791	-5.342018
O	2.518149	-13.771214	-5.007145
O	-7.261086	-14.566597	5.082276
O	-0.143562	-13.985738	5.539524
O	4.234460	-13.126184	5.129588
O	-7.500092	-11.194148	5.308166
O	-3.927924	-10.205150	5.725378
O	-0.403998	-10.189275	6.021179
O	3.738531	-9.957536	5.179505
O	-9.259238	-15.482202	-0.458332
O	-5.329631	-16.180684	-0.099184
O	-1.099378	-15.260235	-0.277400
O	2.174276	-15.445107	-0.160294
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O	-4.898146	-12.326027	0.528925
O	-1.439109	-12.295200	0.843758
O	1.945288	-11.658053	0.321883
O	-7.065705	-14.998903	-2.341652
O	-3.370016	-15.766574	-2.299595
O	0.335303	-15.567891	-2.754805
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O	-6.825874	-12.042693	-2.414510
O	-3.847288	-11.943752	-2.576529
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O	1.459790	-13.802760	-7.721632
O	-8.743094	-15.169571	2.656230
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O	-2.033209	-9.412027	3.718275
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O	-9.387810	-13.146980	-2.211152
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O	-5.442010	-10.240771	-0.721554
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O	2.289144	-9.673534	-1.328250
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O	4.033220	-15.185053	-6.470133
O	-7.469525	-12.030268	-6.445640
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O	-6.502808	-12.693887	3.583841
O	-3.273992	-12.092435	4.253943
O	-0.227386	-11.914259	4.115924
O	2.525094	-11.745288	3.812452
O	-8.910255	-15.757335	-3.847246
O	-5.395778	-16.171225	-3.892361
O	-1.744997	-16.184608	-4.098676
O	1.766464	-16.507418	-4.937741
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O	-5.363382	-10.924344	-4.683501
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O	-5.113395	-12.874386	6.384209
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O	1.673055	-11.999728	6.574405
O	-7.087633	-13.975189	1.093382
O	-3.304618	-14.463929	1.147162
O	0.636194	-13.748951	1.623395
O	3.550999	-13.585069	1.677460
O	-7.053865	-11.167729	1.426037
O	-3.414246	-10.683508	1.845077
O	0.000336	-9.635951	1.015552
O	3.166712	-9.512971	1.763693

C	-0.438314	2.702926	0.243184
C	0.248369	1.459851	0.158773
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C	-1.982961	1.055779	0.285906
N	-1.775314	2.418058	0.320459
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H	-0.522697	-0.624719	0.141127
C	0.103260	4.025993	0.248230
C	1.462875	4.431003	0.157751
N	-0.650441	5.166355	0.336036
C	1.494779	5.823604	0.197236
C	0.157259	6.281903	0.313544
H	-1.671640	5.317731	0.421706
H	2.373805	6.458816	0.151605
C	-0.371111	7.617902	0.411320
C	-3.295068	0.474113	0.346836
C	-4.481632	1.257709	0.428504
C	-5.861804	0.815329	0.468615
N	-4.424147	2.624603	0.497333
C	-6.632183	1.952745	0.568654
H	-6.205017	-0.215494	0.429801
C	-5.705432	3.060927	0.587562
H	-7.715674	2.018675	0.624096
C	-1.767574	7.878921	0.559906
C	-2.438790	9.155911	0.678790
N	-2.683131	6.861040	0.596447
C	-3.786447	8.880420	0.788158
H	-1.963269	10.132674	0.680884
C	-3.903829	7.443294	0.726911
C	-5.900143	4.475331	0.681241
C	-6.988205	5.384347	0.790141
N	-4.769350	5.236859	0.674830
C	-6.456652	6.681686	0.835967
C	-5.038927	6.570338	0.758010
H	-3.834550	4.853051	0.605968
C	-3.381379	-0.928607	0.341963
C	-3.422936	-2.154893	0.395120
C	-3.462635	-3.562282	0.510414
C	-4.693593	-4.260769	0.536995
C	-2.253495	-4.289219	0.625617
C	-4.708092	-5.644675	0.682876
H	-5.627326	-3.707466	0.439804
C	-2.280283	-5.670680	0.766563
H	-1.302600	-3.757926	0.605817
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H	-5.656690	-6.180029	0.700885
H	-1.347717	-6.225558	0.853742
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H	2.312329	3.760265	0.074428
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C	3.614196	10.493364	0.065057
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C	4.052802	12.893964	0.189440
C	2.654379	13.106906	0.346847
C	1.769865	12.035951	0.405393
C	2.226171	10.704263	0.264599
C	3.337557	15.704338	0.808746
C	4.665882	15.251721	0.648464
C	5.698151	16.153393	0.971779
H	6.735484	15.852837	0.846117
C	5.419725	17.434210	1.442178
C	4.096521	17.885567	1.614629
C	3.065380	16.985958	1.290959
H	3.993924	9.479451	-0.052818
H	5.557709	11.362907	-0.109336
H	0.705398	12.225639	0.543493
H	6.256131	18.098567	1.658094
H	2.024354	17.276277	1.432636
N	4.966061	13.947895	0.187177
S	1.948189	14.726528	0.321199
H	-7.015010	7.608972	0.923708
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C	3.792775	19.243121	2.108105
C	4.619983	19.891721	3.050739
C	2.655263	19.935524	1.653844
C	4.315880	21.164988	3.523269
H	5.498599	19.381868	3.448583
C	2.341346	21.216808	2.111802
H	2.005656	19.481480	0.904968
C	3.173424	21.839504	3.055515
H	4.950426	21.650134	4.265599
H	1.461321	21.718031	1.713924
C	6.350860	13.657492	-0.130813
C	6.798150	13.816567	-1.443521
C	7.239229	13.250573	0.874362
C	8.138629	13.573539	-1.767317
H	6.100744	14.141588	-2.216070
C	8.572444	13.009176	0.561138
H	6.886709	13.132093	1.899352
C	9.029870	13.169380	-0.760783
H	8.469281	13.704321	-2.796023
H	9.278264	12.689914	1.328002
C	1.785985	23.791836	3.114400
H	0.879522	23.205412	3.325776
H	1.858447	23.963739	2.029720

C	1.728983	25.119986	3.850682
H	1.630173	24.956097	4.938452
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C	0.345606	27.050268	3.991431
H	1.213522	27.721662	3.865829
H	0.181240	26.895193	5.073084
C	-0.892835	27.655686	3.349791
H	-1.745608	26.959729	3.452407
H	-0.716310	27.821457	2.270892
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C	10.886274	12.978309	-2.295216
H	10.312697	12.320828	-2.965497
H	10.838632	14.012959	-2.668073
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H	12.879670	13.158654	-1.475247
C	14.277362	12.104671	-3.437764
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C	14.844270	12.168808	-4.846554
H	14.825917	13.208634	-5.220557
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C	16.815767	11.726303	-6.071897
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H	16.272447	11.100295	-6.800670
O	10.354369	12.905268	-0.955339
O	12.921846	12.567054	-3.476730
O	16.187119	11.684241	-4.787866
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O	0.581700	25.799461	3.338261
O	-1.178218	28.892518	4.002420
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C	5.458488	14.706063	-1.119141
H	5.226934	12.580221	-0.933930
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H	6.527542	14.640182	-1.316711
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N	5.562742	17.145958	-1.292757
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H	5.198964	19.537106	-2.445798
C	4.474930	20.743082	0.659079
H	4.475632	19.575795	2.474890
H	4.567075	21.639063	-1.324615
C	6.657786	17.164291	-2.198965
C	6.587813	16.484344	-3.427123
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C	7.658828	16.503266	-4.320381
H	5.680467	15.941874	-3.693620
C	8.891573	17.918615	-2.771418
H	7.900602	18.414118	-0.930926
C	8.822787	17.223339	-3.995929
H	7.566831	15.972765	-5.265904
H	9.801209	18.469918	-2.530110
C	3.949511	23.086782	0.668084
H	3.645880	23.816201	1.424764
H	4.894354	23.401748	0.204123
H	3.164402	22.999816	-0.096185
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H	9.130124	16.958863	-6.705199
H	10.897777	16.762317	-6.484931
H	9.779526	15.506385	-5.860695
O	4.117662	21.843462	1.379647
O	9.926028	17.308863	-4.790266
C	-1.969621	2.798168	1.471309
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C	-0.641659	-0.492793	1.033643
C	-2.849380	-0.608206	2.066892
C	-0.581199	-1.882708	1.024791
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C	-2.781673	-1.995545	2.045603
H	-3.724778	-0.107607	2.480310
C	-1.649842	-2.646647	1.523664
H	0.293676	-2.384703	0.612589
H	-3.606041	-2.588164	2.439122
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Ti	-3.161342	-10.191426	-6.039971
Ti	-0.118257	-10.895923	-7.078956
Ti	3.227726	-10.321992	-7.510547
Ti	-4.851260	-10.714014	4.380235
Ti	2.240329	-10.270774	3.697766
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Ti	-1.282705	-6.626014	4.366922
Ti	2.011397	-6.442232	4.270223
Ti	5.049418	-6.443118	2.959598
Ti	-7.641289	-11.013053	-0.538059
Ti	-3.986242	-11.835746	-0.841927
Ti	-0.383418	-11.528901	-1.761311

Ti	3.072682	-11.440211	-2.293282
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OTAA07@TiO₂

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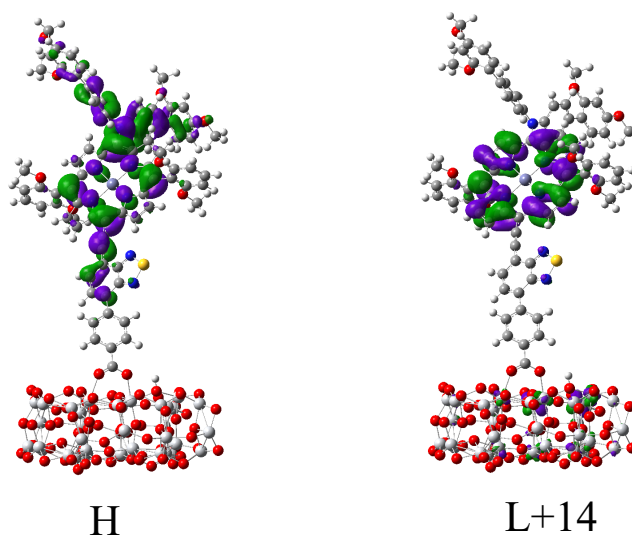
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O	-6.580651	-6.352982	7.137283
O	-11.696332	1.090255	1.705477
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O	-7.390176	-8.658568	2.230711
O	-9.073314	2.086553	2.036512
O	-7.273832	-1.116869	2.425338
O	-5.032849	-3.904444	1.611498
O	-3.761425	-6.810032	2.306714
H	-4.211617	-3.377385	1.720930

S5: Table showing the values of electron transfer distance for recombination (r_{rec}) and injection (r_{inj}).

Dye@TiO₂	r_{rec} (Å)	r_{inj} (Å)
OCBZ04@TiO ₂	19.46	1.29
OCBZ07@TiO ₂	22.53	1.29
ODPA04@TiO ₂	18.18	1.39
ODPA07@TiO ₂	22.53	1.28
OPTZ04@TiO ₂	19.39	1.28
OPTZ07@TiO ₂	22.52	1.29
OGLY04@TiO ₂	18.10	1.28
OGLY07@TiO ₂	22.58	1.35
OTAA04@TiO ₂	18.60	1.28
OTAA07@TiO ₂	22.53	1.29
SM315@TiO ₂	31.02	1.28

S6: HOMO and LUMO orbitals showing charge transfer for SM315 adsorbed on (TiO₂)₃₈ surface, at TD-CAM-B3LYP/6-311+G(d,p)/LANL2DZ/C-PCM level of theory.



S7: The transition dipole moment integral values, oscillator strengths and excitation energies (in eV) computed for the studied dyes.

Dye	μ	f	Excitation Energy (eV)
OCBZ04	5.05	1.60	2.56
OCBZ07	4.97	1.50	2.48
ODPA04	4.81	1.42	2.49
ODPA07	5.57	1.82	2.39
OPTZ04	4.58	1.29	2.50
OPTZ07	5.82	1.87	2.25
OGLY04	4.58	1.29	2.52
OGLY07	4.59	1.09	2.10
OTAA04	5.59	1.91	2.50
OTAA07	6.28	2.10	2.17
SM315	4.08	1.06	2.60