Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary information:

Electronic and Optical Properties of Metalloporphyrins of Zinc on TiO2 Cluster in Dye-sensitized Solar-Cells (DSSC). A Quantum Chemistry Study

Fernando Mendizabal, Raúl Mera-Adasme, Wen-Hua Xu and Dage Sundholm

1.- Tables.

Table S1. Main geometric parameters of the LD13 and YD2-o-C8 ligands with different methods including gas and solvent effect (solv). Distances are given in pm and angles in degrees.

Method	System	Zn-N	N-C	C-C1	ZnNCC1°	C2-C3	NCC1C2°	C5-O1	C5-O2	O2C5O1°
B3LYP	LD13	204.8	137.9	140.8	3.48°	121.6	178.0°	123.4	138.4	121.1°
CAM-B3LYP	LD13	204.5	138.5	140.7	3.05°	121.3	178.2°	123.2	138.3	121.0°
B3LYP (solv)	LD13	205.1	137.8	140.9	3.49°	121.6	177.7°	123.9	137.5	121.4°
CAM-B3LYP (solv)	LD13	204.8	138.4	141.0	3.12°	121.5	178.1°	123.9	136.8	121.1°
B3LYP	YD2-o-C8	204.5	138.5	140.6	3.15°	121.6	178.3°	123.5	138.5	121.1°
CAM-B3LYP	YD2-o-C8	204.3	138.1	140.2	2.75°	120.8	178.1°	122.9	138.2	121.3°
B3LYP (solv)	YD2-o-C8	204.5	138.6	141.0	4.65°	121.7	177.5°	124.0	137.2	121.4°
CAM-B3LYP (solv)	YD2-o-C8	204.4	138.3	141.2	3.55°	121.5	177.2°	123.7	136.9	121.2°

Table S2. Main geometric parameters of the LD13 and YD2-o-C8 on [TiO_2] cluster with different methods including gas and solvent effect (solv). Distances are given in pm and angles in degrees.

Method	System	Zn-N	N-C	ZnNCC2°	NCC1C2°	Ti1-O1	Ti2-O2	C5-O2	C5-O1O2C5O1°	Ti1O1C5
B3LYP	LD13	205.1	136.9	0.04°	179.4°	217.4	214.7	127.4	129.7	128.4°	134.9°
CAM-B3LYP	LD13	205.3	136.6	0.06°	179.6°	217.2	214.5	127.7	129.4	129.1°	134.5°
B3LYP (solv)	LD13	205.1	136.9	0.02°	179.5°	215.7	212.4	130.1	129.9	127.8°	135.1°
CAM-B3LYP (solv)	LD13	205.2	136.8	0.04°	179.3°	215.4	213.0	130.4	129.3	127.5°	135.2°
B3LYP	YD2-o-C8	205.0	137.4	2.10°	177.7°	221.0	214.3	127.9	127.6	129.9°	133.6°
CAM-B3LYP	YD2-o-C8	204.6	137.0	1.80°	178.3°	220.7	214.0	127.5	127.2	129.2°	133.2°
B3LYP (solv)	YD2-o-C8	205.3	137.4	3.05°	177.3°	219.5	215.2	128.2	127.9	129.0°	133.9°
CAM-B3LYP (solv)	YD2-o-C8	204.8	136.9	2.45°	178.1°	219.1	214.8	128.0	127.2	128.6°	133.1°

Table S3. Natural Population Analysis (NPA) charges (au) for the $–CO_2^–$ group in LD13 attached to TiO_2, with both systems solvent phase at the B3LYP-D3 and CAM-B3LYP levels.

System	Method	Zn	C5	O1	O2	Ti1	Ti2
LD13-TiO_2	B3LYP	+1.597	+0.873	-0.676	-0.676	+1.462	+1.459
	CAM-B3LYP	+1.225	+0.905	-0.607	-0.607	+1.061	+1.057
LD13	B3LYP	+1.599	+0.815	-0.638	-0.713		
	CAM-B3LYP	+1.264	+ 0.831	-0.630	-0.713		
TiO_2	B3LYP					+1.659	+1.663
	CAM-B3LYP					+1.350	+1.352

Table S4. Natural Population Analysis (NPA) charges (au) for the $–CO_2^–$ group in YD2-o-C8 attached to TiO_2, with both systems solvent phase at the B3LYP-D3 and CAM-B3LYP levels.

System	Method	Zn	C5	O1	O2	Ti1	Ti2
YD2-o-C8-TiO_2	B3LYP	+1.583	+0.928	-0.706	-0.706	+1.527	+1.524
	CAM-B3LYP	+1.284	+0.894	-0.628	-0.628	+1.031	+1.023
YD2-o-C8	B3LYP	+1.589	+0.818	-0.649	-0.714		
	CAM-B3LYP	+1.278	+0.881	-0.656	-0.730		
TiO_2	B3LYP					+1.659	+1.663
	CAM-B3LYP					+1.350	+1.352

2.- Wavelenghts (λ) and oscillator strenghts (f) for the UV/Vis spectra of the LD13 and YD2-o-C8 dyes calculated with TDDFT and the B3LYP, CAMB3LYP and BHHLYP density functionals. The ADC(2)-calculated spectra for LD13 is also given. All spectra were calculated in gas phase and with the COSMO solvation model (epsilon = 7.5, THF), without and with TiO_2 cluster. Wavelengths (λ) are given in nm and oscillator strength (f).

Table S5. LD13

B3LYP (gas)			**B3LYP (solv)**			**CAM-B3LYP (gas)**			**CAM-B3LYP (solv)**			**BHHLYP (solv)**	
λ\nm	***f***		**λ\nm**	***f***		**λ\nm**	***f***		**λ\nm**	***f***		**λ\nm**	*f*
615	0.771		631.9	0.955		597	0.567		615	0.774		557	0.563
580	0.064		582.2	0.099		562	0.001		565	0.002		538	0.003
430	0.678		438.3	1.115		384	2.222		400	1.731		361	3.661
427	0.953		433.9	0.949		383	1.476		397	2.312		346	0.088
410	0.052		415.7	0.031		343	0.016		353	0.001		341	2.305
406	0.712		412.1	0.447		312	0.055		350	0.015		318	0.076
398	0.477		405.5	0.521		294	0.188		314	0.053		315	0.005
379	0.001		384.0	0.004					305	0.002		311	0.066
378	0.097		379.8	0.001					298	0.001		305	0.012
370	0.001		374.7	0.007					295	0.264		309	0.014
365	0.106		372.1	0.002									
364	0.014		367.6	0.023									
356	0.027		360.0	0.113									
340	0.013		352.1	0.051									
332	0.070		344.4	0.036									
321	0.020		342.9	0.036									
315	0.164		334.8	0.052									
304	0.026		319.7	0.127									
300	0.011		302.9	0.020									
			302.5	0.002									
			301.6	0.055									

ADC(2) (gas)		**ADC(2) (solv)**	
λ\nm	***f***	**λ\nm**	*f*
603	0.248	612	0.318
582	0.004	583	0.007
386	2.992	401	2.955
381	2.045	398	2.135
355	0.001	357	0.000
348	0.004	350	0.002
338	0.025	346	0.021

Table S6. LD13-TiO_2

B3LYP (gas) λ\nm	*f*		B3LYP (solv) λ\nm	*f*		CAM-B3LYP (gas) λ\nm	*f*		CAM-B3LYP (solv) λ\nm	*f*		BHHLYP (solv) λ\nm	*f*
602	0.835		606	0.929		583	0.561		591	0.687		540	0.475
578	0.019		598	0.015		554	0.007		550	0.001		524	0.007
474	0.012		565	0.005		400	0.006		392	2.546		546	0.001
457	0.010		462	0.005		388	2.182		389	1.608		499	0.005
444	0.002		445	0.862		377	1.225		368	0.008		495	0.001
443	0.001		437	0.425		341	0.009		364	0.007		359	3.556
441	0.037		436	0.015		339	0.226		353	0.006			
440	0.005					338	0.009		352	0.006			
439	0.011					337.7	0.011		347	0.009			
438	0.002					337.2	0.008		342	0.013			
437	0.001								340	0.015			
436	0.002								335	0.006			
435	0.002								330	0.005			
434	0.672								325	0.006			
433	0.002								322	0.006			
432	0.009								320	0.011			
431	0.002								319	0.016			
430	0.315								318	0.013			
427	0.004												

Table S7. YD2-o-C8

B3LYP (gas) λ\nm	*f*		B3LYP (solv) λ\nm	*f*		CAM-B3LYP (gas) λ\nm	*f*		CAM-B3LYP (solv) λ\nm	*f*		BHHLYP (solv) λ\nm	*f*
640	0.349		690	0.392		595	0.232		605	0.329		549	0.258
533	0.065		613	0.020		576	0.001		579	0.001		533	0.003
498	0.053		545	0.142		428	0.413		446	0.355		453	0.089
430	0.010		519	0.042		387	1.126		412	1.219		403	0.279
425	0.257		443	0.637		392	1.530		404	1.802		359	3.102
411	0.398		442	0.419		350	0.175		361	0.279		334	1.394
408	0.442		425	0.086		328	0.005		336	0.005		337	0.005
389	0.275		424	0.457		320	0.026		324	0.046		319	0.026
379	0.027		419	0.557		317	0.039		320	0.008		311	0.028
368	0.031		404	0.390		312	0.020		318	0.027		308	0.001
363	0.145		393	0.159		312	0.085		316	0.024			
361	0.112		388	0.048		310	0.013		313	0.068			
359	0.021		370	0.021		305	0.011		311	0.019			
356	0.018		367	0.010		303	0.027		308	0.027			
352	0.035		366	0.027					303	0.043			
337	0.016		364	0.025									
336	0.064		361	0.048									
335	0.105		360	0.092									
322	0.026		356	0.029									
317	0.011		350	0.026									
313	0.095		349	0.051									
310	0.010		348	0.021									
309	0.067		342	0.026									
308	0.049		339	0.016									
			334	0.053									
			331	0.015									
			318	0.129									
			311	0.154									

Table S8. YD2-o-C8-TiO_2

B3LYP (gas) λ\nm	*f*	B3LYP (solv) λ\nm	*f*	CAM-B3LYP (gas) λ\nm	*f*	CAM-B3LYP (solv) λ\nm	*f*	BHHLYP (solv) λ\nm	*f*
610	0.422	621	0.532	595	0.447	611	0.560	557	0.381
588	0.006	603	0.017	567	0.021	565	0.010	537	0.001
510	0.025	529	0.034	402	0.447	439	0.128	536	0.001
481	0.021	489	0.021	400	0.005	404	1.079	404	0.286
468	0.001	484	0.001	394	0.004	393	2.200		
456	0.011	468	0.001	391	1.587	360	0.007		
415	0.648	466	0.001	386	1.116	358	0.006		
400	0.010	456	0.011	384	0.004	356	0.328		
396	0.046	456	0.002	378	0.003	349	0.005		
381	0.002	454	0.774	376	0.002	347	0.005		
376	0.003	447.4	0.009	373	0.004	342	0.005		
370	0.015	447.2	0.446	370	0.002	338.8	0.007		
365	0.322	446.9	0.004	366	0.002	338.8	0.017		
		443.4	0.002	365	0.002	336	0.011		
		443.3	0.021	353	0.005	335	0.011		
		443	0.357	346	0.028	331	0.006		
		441	0.022	344	0.007	330	0.006		
		437	0.063	342	0.004	322	0.003		
		436	0.003	341	0.006	321	0.015		
		435	0.002	341	0.006	320	0.046		
		429	0.001	339	0.004	316.9	0.009		
				338	0.002	316.7	0.004		
						316.1	0.021		

3.- Table S9. The strongest singlet excitation energies calculated for LD13 and YD2-o-C8 in THF are compared to experimental data [14,34]. The excitation energies and oscillator strengths have been calculated at the TDDFT/B3LYP level using COSMO with ε=7.6. All calculated excitation energies are reported as supplementary information. The orbital contributions and the character of the transitions are also given.

System	λ_{calc}	λ_{exp}	f^a	Contribution[b]	Transition type
LD13	632 (Q)	672	0.955	195a → 196a (89%)	MLMLCT (dxz/dyz+π→ π*+dxz)
	438 (B)	458	1.156	194a → 196a (56%)	LMLCT (π→π*+dxz)
				195a → 197a (28%)	MLMLCT (dxz/dyz+π→ π*+dxz)
	434 (B)		0.950	195a → 198a (43%)	MLLCT (dxz/dyz+π→ π*)
				194a → 197a (35%)	LLMCT (π→π*+dxz)
YD2-o-C8	690 (Q)	645	0.392	295a → 296a (93%)	MLLCT (dxz/dyz+π→ π*)
	545 (T)	581	0.149	294a → 296a (78%)	MLLCT (dxz/dyz+π→ π*)
	443 (B)	448	0.637	295a → 298a (41%)	MLLCT (dxz/dyz+π→ π*)
				292a → 296a (19%)	LLCT (π→π*)
				293a → 297a (15%)	LLCT (π→π*)
	419 (B)		0.557	294a → 297a (19%)	MLLCT (dxz/dyz+π→ π*)
				291a → 296a (18%)	LLCT (π→π*)
				292a → 296a (17%)	LLCT (π→π*)
				293a → 296a (17%)	LLCT (π→π*)

[a]Oscillator strength.
[b]The reported values are |coefficient|^2 × 100%.

LD13. The electronic structure of this model is described with the three absorption peaks as mentioned above. The electronic transitions are assigned to individual states as ligand-to-ligand, metal-ligand-to-ligand, metal-ligand-to-metal-ligand and ligand-to-ligand-metal charge transfer (LLCT, MLLCT, MLML and LLMCT). The theoretical calculations given in Table S9 show good agreement with the experimental results [22]. In general, the bands are a mixture of excitations. The Q band is formed by the transition at 632 nm. This transition is mainly composed of 195a → 196a (dxz/dyz+π→π*+dxz) (HOMO-LUMO). This band corresponds to MLMLCT. The frontier MOs are shown in Figure 7. The 195a (HOMO) has a porphyrin π and and *d* orbitals of zinc character, while the arrival orbital 196a (LUMO) shows a main composition centered on the porphyrin, adjacent substituents and same dxz orbital of zinc. Both orbitals have a predominant π character.

The B band is formed by two transitions, the one at 438 nm is composed mainly of 194a → 196a (π→π*+dxz) of the LMLCT type. The 194a (HOMO-1) contains a dominant contribution of the porhyryrinic ring. The second transition at 434 nm has a main

contribution from a 195a → 198a (dxz/dyz+π→ π*) excitation which is associated with MLLCT.

YD2-o-C8. The electronic structure of the model is described with the three absorption peaks which were mentioned above. The electronic transitions are assigned to individual states as ligand-to-ligand and metal-ligand-to-ligand charge transfers (LLCT and MLLCT), respectively. The theoretical results, given in Table 3, show good agreement with the experimental data [14]. Some of the bands are a mixture of excitations. Band Q is formed by a transition at 690 nm is composed mainly of 295a → 296a (dxz/dyz+π→π*), corresponding to a HOMO-LUMO transition. This band corresponds to MLLCT. The frontier MOs are shown in Figure 9. The 295a (HOMO) has a porphyrin π character and Zn atom shows a dxz/dyz contributions, while the arrival orbitals 296a (LUMO) shows a main composition centered on the porphyrin and phenylethynyl carboxylic acid.

The T band is formed by a transition at 545 nm, and it shows a principal component 294a → 296a (dxz/dyz+π→ π*) of the MLLCT type. We point out that the 294a orbital corresponds to a π orbital of the porphyrin ring and *d* orbitals from the Zn atom. Thus, in the transition involved this orbital goes to the 296a orbital, which is centered mainly on the porphyrin and phenylethynyl carboxylic acid. Finally, the B band is formed by multiple transitions, being the two main transitions at 443 nm: 295a → 298a (dxz/dyz+π→ π*) of the MLLCT type. The 235a (HOMO) has mixtures of the MOs of Zn orbitals, diarylamino, and a lower contribution of phenylethynyl carboxylic acid, while the 298a MO (LUMO+2) contains a principal contribution of phenylethynyl carboxylic acid with porhyryrin. The second transition at 419 nm has a principal 294a → 297a (dx2-y2+π→ π*) excitation which is associated with MLLCT. These results are very similar to those reported previously for YD2 [33].

4.- Calculated B3LYP electronic spectra of LD13 in solvent.

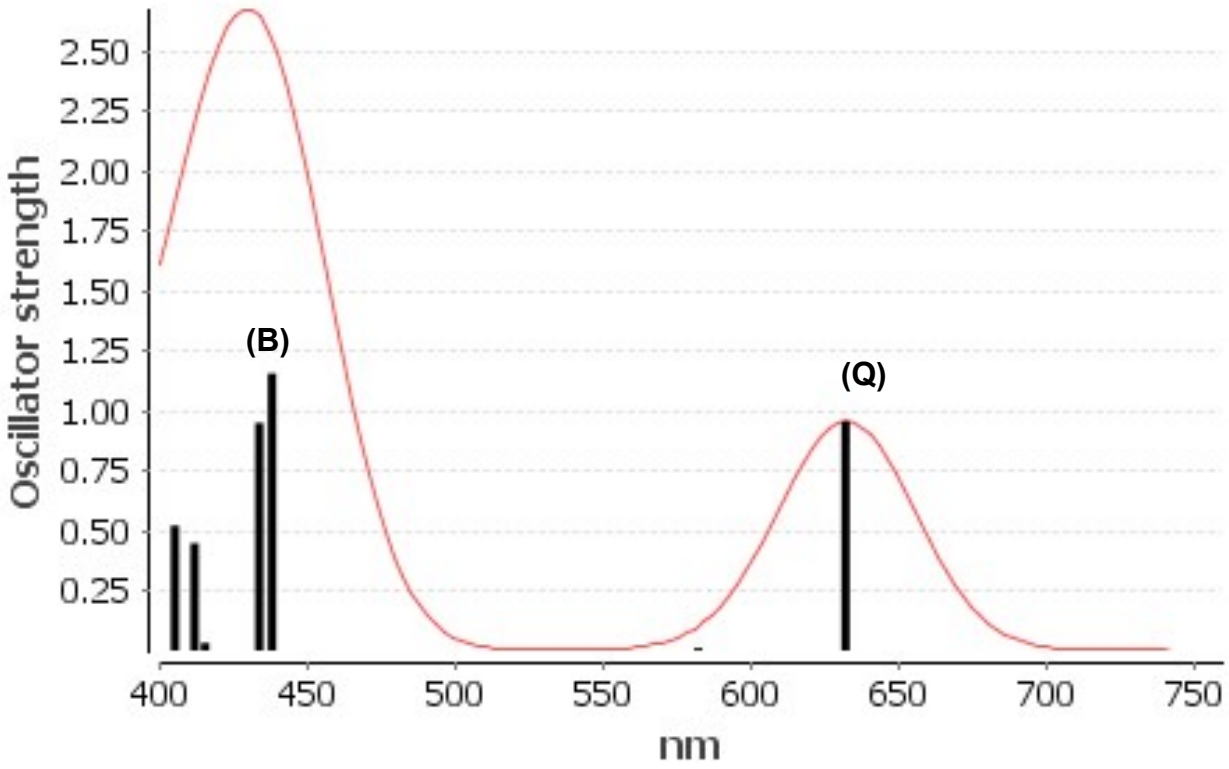

Figure S1.

5.- Calculated B3LYP electronic spectra of YD2-o-C8 in solvent.

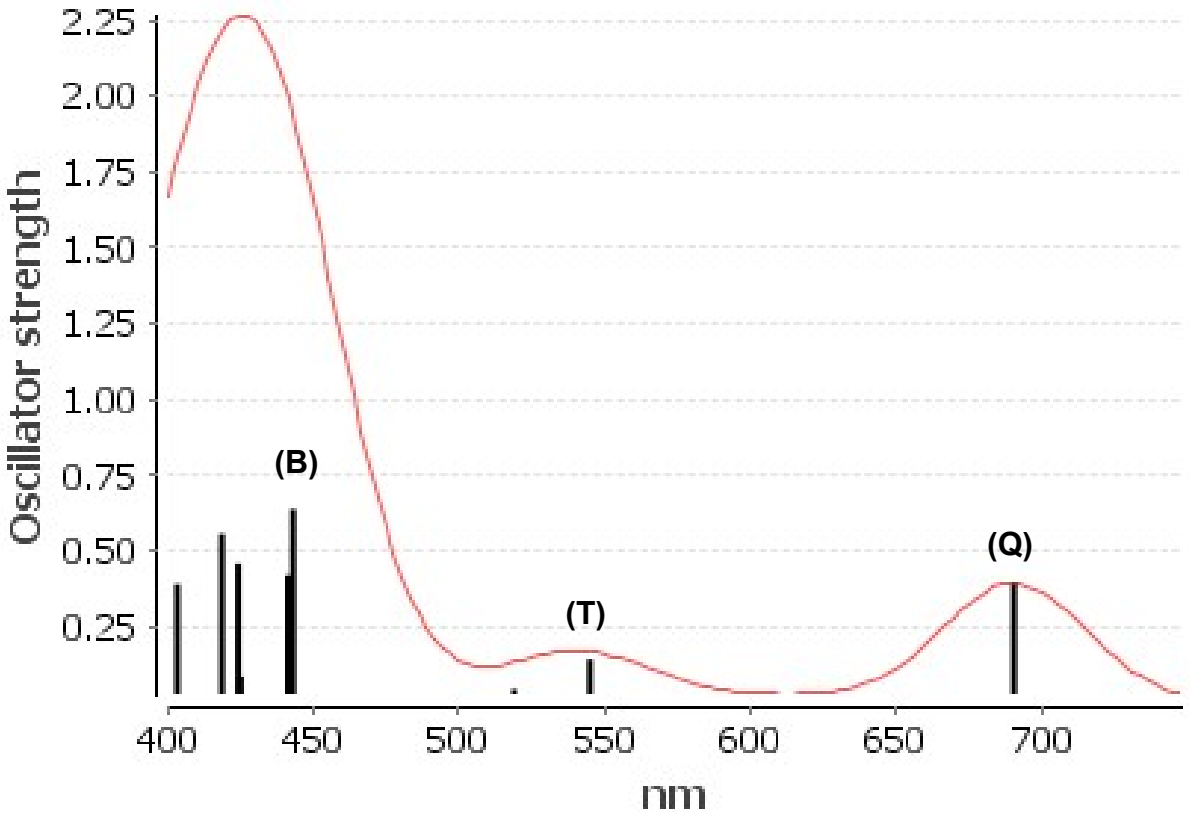

Figure S2.

6.- Most important active molecular orbitals in the electronic transitions of LD13 models at the B3LYP level in solvent.

LD13

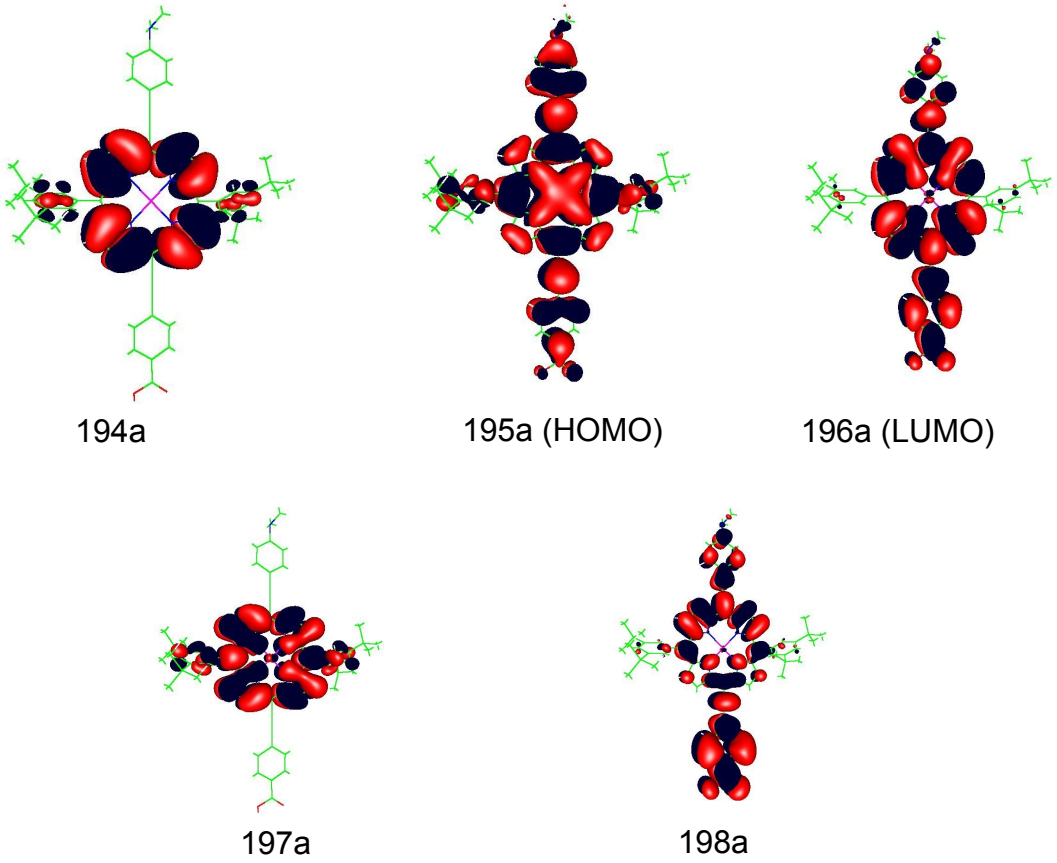

Figure S3.

7.- Most important active molecular orbitals in the electronic transitions of YD2-o-C8 models at the B3LYP level in solvent.

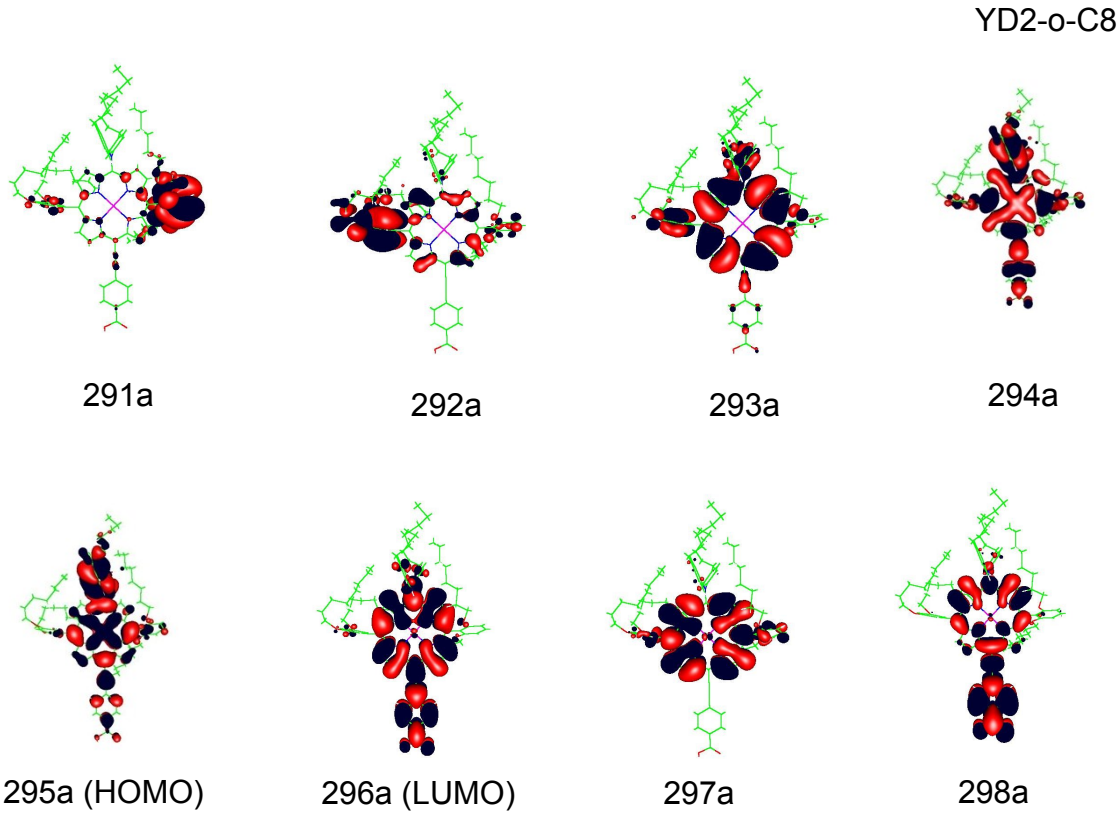

Figure S4.

8- Frontier Orbitals on TiO_2 cluster in system LD13-TiO_2 at the B3LYP level.

LD13-TiO_2

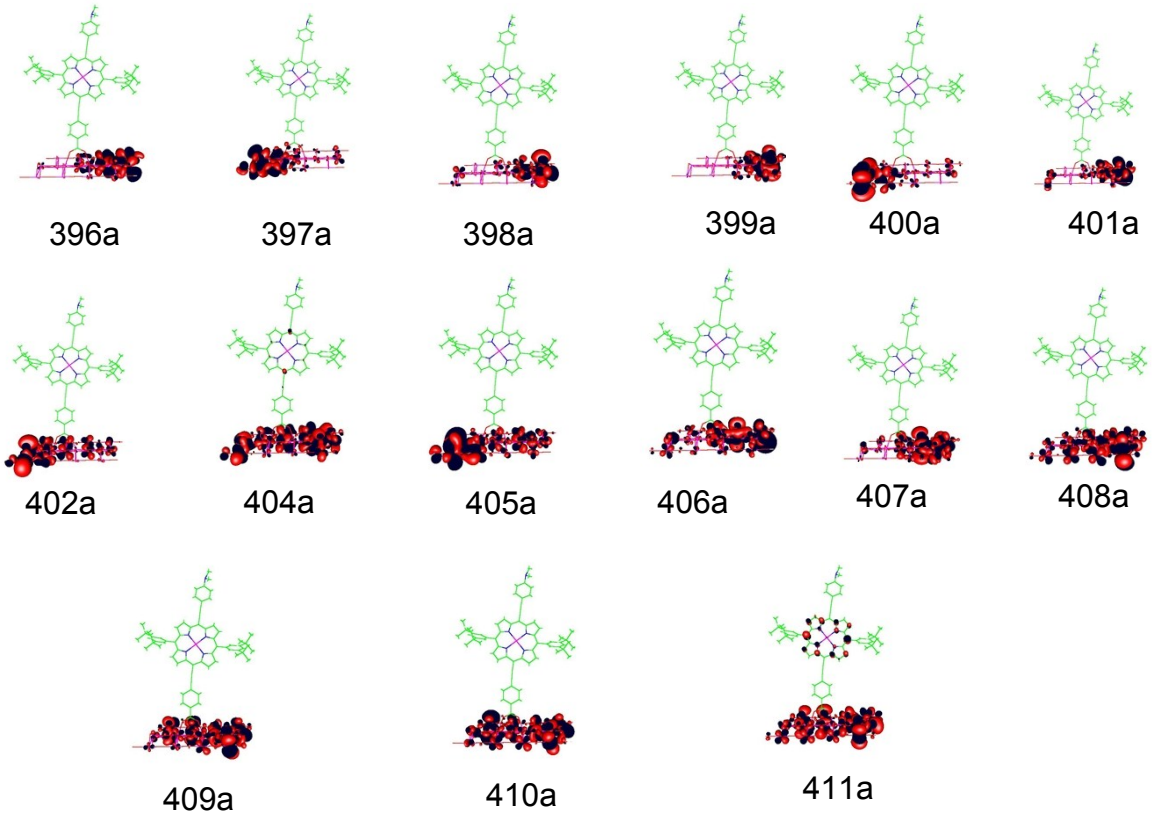

Figure S5.

9.- Frontier Orbitals on TiO_2 cluster in system YD2-o-C8-TiO_2 at the B3LYP level.

YD2-o-C8-TiO_2

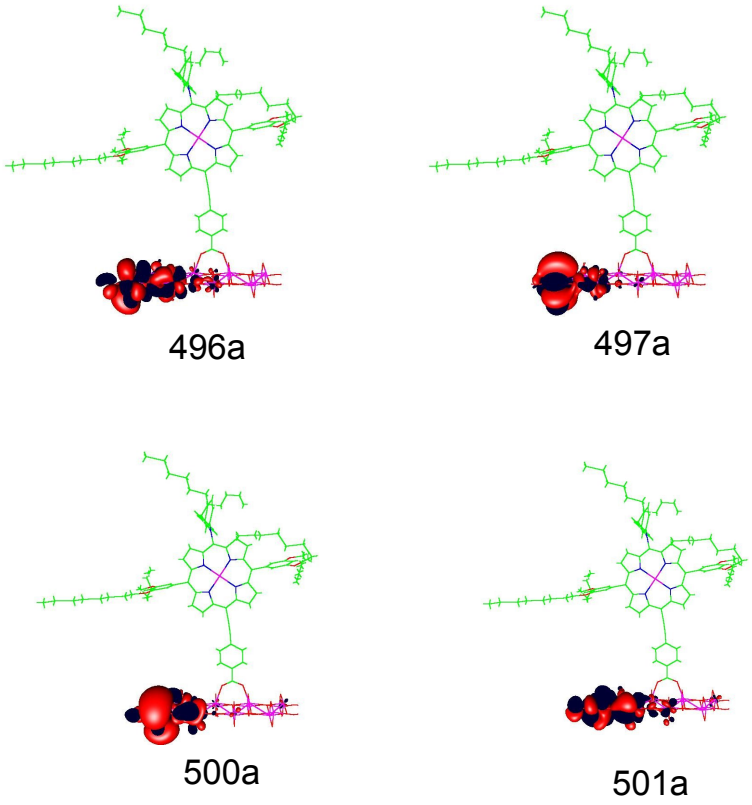

Figure S6.

10.- Cartesian coordinates (in Angstroms) for the optimized geometries of the systems studied in this work at the B3LYP level.

Tables S10. LD13 (Gas)

140

Zn	-0.0462490	-0.3751564	-2.0134178
C	-2.0275466	1.9191687	-2.5393842
C	-2.1838199	3.1278728	-3.3076582
C	-1.0242844	3.3233274	-3.9956108
C	-0.1289060	2.2416834	-3.6514547
N	-0.7750689	1.3871979	-2.7642840
H	-3.0771449	3.7390734	-3.3223863
H	-0.7965223	4.1247426	-4.6860174
C	-2.0964058	-1.7388710	-0.1531081
C	-3.4034597	-1.5253106	0.4255462
C	-3.8880350	-0.3573140	-0.0807690
C	-2.8859450	0.1723265	-0.9701064
N	-1.7988637	-0.6760417	-0.9996920
H	-3.8832140	-2.1825793	1.1386837
H	-4.8376459	0.1165633	0.1323543
C	1.9191167	-2.6923879	-1.5222461
C	2.0266745	-3.9627373	-0.8535369
C	0.8606060	-4.1646084	-0.1770933
C	0.0199748	-3.0134201	-0.4116727
N	0.6885302	-2.1290368	-1.2486510
H	0.5864955	-5.0234790	0.4209903
C	2.0198232	1.0084589	-3.8390792
C	3.3804601	0.8667712	-4.3035991
C	3.8626106	-0.3053784	-3.8024643
C	2.8138599	-0.8977820	-3.0142037
N	1.6999225	-0.0819570	-3.0398564
H	3.9038646	1.5805050	-4.9258203
H	4.8473107	-0.7330843	-3.9414274
C	2.9236496	-2.1237027	-2.3290222
C	1.1715222	2.0825841	-4.1422946
C	-1.2666281	-2.8330075	0.1139798
C	-3.0123919	1.3756044	-1.6919575
C	1.6971353	3.1388778	-5.0566245
C	1.8735524	4.4466247	-4.5985636
C	2.3575611	5.4527074	-5.4397787
C	2.6758024	5.1091763	-6.7596512
C	2.5181864	3.8073091	-7.2510910
C	2.0188287	2.8334792	-6.3811205
H	3.0559817	5.8752053	-7.4225534
C	-1.7911219	-3.8883163	1.0301908
C	-1.1795061	-4.1109521	2.2672743
C	-1.6539150	-5.0958137	3.1376770
C	-2.7640773	-5.8454025	2.7318209
C	-3.4045943	-5.6464080	1.5030930
C	-2.8972581	-4.6569792	0.6568876
C	-4.2228103	2.0928312	-1.5502448
C	-5.2659945	2.7034012	-1.4157380
C	-6.4784082	3.4085342	-1.2492714
C	-7.5014894	2.8928350	-0.4260901
C	-8.6904981	3.5846490	-0.2575624
C	-8.8914273	4.8104176	-0.9065718
C	-7.8812356	5.3304510	-1.7276839
C	-6.6916654	4.6427614	-1.8986672
H	-7.3476280	1.9413101	0.0788186

H	-9.4741458	3.1824148	0.3783455
H	-8.0502082	6.2827509	-2.2255803
H	-5.9096749	5.0505136	-2.5357571
C	-10.1316526	5.5799232	-0.7576648
O	-10.3766983	6.6631228	-1.2963811
O	-11.0529278	4.9686960	0.0751855
H	-11.8624074	5.5309530	0.1361640
H	-0.3271877	-3.4927574	2.5311778
H	-3.3488075	-4.4622380	-0.3109180
H	1.8699731	1.8118212	-6.7239888
H	1.6238170	4.6666333	-3.5627311
C	2.8736798	3.4157723	-8.6955375
C	2.5132994	6.8818204	-4.8925913
C	1.1291641	7.4046592	-4.4381529
H	0.6928976	6.7724151	-3.6501418
H	1.2183384	8.4281440	-4.0386781
H	0.4245769	7.4252078	-5.2848996
C	3.0728450	7.8555417	-5.9458426
H	2.4098876	7.9351355	-6.8207574
H	3.1669393	8.8607193	-5.5066982
H	4.0710997	7.5481464	-6.2929646
C	3.4805167	6.8713539	-3.6850819
H	3.1085705	6.2343848	-2.8689669
H	4.4716236	6.4952453	-3.9838786
H	3.6035572	7.8914783	-3.2859282
C	1.6106207	2.8803890	-9.4110438
H	1.1986981	1.9952204	-8.9041485
H	0.8236635	3.6505826	-9.4402589
H	1.8519968	2.5936233	-10.4476678
C	3.4183563	4.6051171	-9.5082529
H	4.3377857	5.0149769	-9.0631094
H	3.6615801	4.2738781	-10.5296704
H	2.6788859	5.4166141	-9.5890722
C	3.9583037	2.3120627	-8.6721834
H	3.6120770	1.4103794	-8.1449183
H	4.2277127	2.0180978	-9.6998878
H	4.8684647	2.6725366	-8.1669663
C	-1.0014582	-5.3798907	4.5009086
C	-4.6251573	-6.5057432	1.1337330
C	-5.1921704	-6.1470172	-0.2521070
H	-5.5242192	-5.0985143	-0.2975109
H	-4.4516770	-6.3110954	-1.0494265
H	-6.0642462	-6.7825011	-0.4709685
C	-5.7416540	-6.2862489	2.1824632
H	-6.0473586	-5.2284346	2.2092731
H	-6.6258392	-6.8954581	1.9326370
H	-5.4132185	-6.5689371	3.1940105
C	-4.2205102	-7.9988555	1.1177693
H	-3.8527022	-8.3329578	2.0996589
H	-5.0865599	-8.6269167	0.8512997
H	-3.4238722	-8.1778753	0.3786731
H	-3.1452255	-6.6155685	3.3994755
C	-2.0444222	-5.1820227	5.6262208
H	-2.9031401	-5.8609342	5.5126585
H	-1.5870597	-5.3803468	6.6093457
H	-2.4271922	-4.1494882	5.6246075
C	-0.4880399	-6.8394961	4.5257727
H	-0.0148732	-7.0622469	5.4962639
H	-1.3045466	-7.5617469	4.3747642
H	0.2579058	-7.0023518	3.7319271
C	0.1906829	-4.4471758	4.7816986

H	0.9862426	-4.5651093	4.0300059
H	-0.1152706	-3.3901038	4.7994680
H	0.6245930	-4.6858855	5.7651537
H	2.8866175	-4.6181903	-0.9077656
C	4.1373949	-2.8387650	-2.4658116
C	5.1819899	-3.4475515	-2.5937853
C	6.4016784	-4.1482597	-2.7546168
C	7.4042634	-3.6543140	-3.6134336
C	6.6418697	-5.3523468	-2.0645630
H	5.8762656	-5.7445365	-1.3973896
C	7.8414089	-6.0341326	-2.2301815
H	8.0356055	-6.9645541	-1.7012416
C	8.8319869	-5.5405465	-3.0822333
H	7.2307945	-2.7250963	-4.1538917
C	8.5992085	-4.3435567	-3.7713013
H	9.3655953	-3.9508012	-4.4384700
N	10.0622628	-6.2712334	-3.2288607
C	11.2475587	-5.6214380	-2.6660662
H	12.0709892	-6.3504823	-2.6135314
H	11.6017823	-4.7490838	-3.2606710
H	11.0294772	-5.2749157	-1.6465872
C	10.2740586	-6.8867867	-4.5401562
H	11.1100249	-7.6004581	-4.4746291
H	9.3726958	-7.4392060	-4.8393992
H	10.5137239	-6.1533623	-5.3425850

Table S11. LD13 (solv)

140

Zn	-0.0456722	-0.3749025	-2.0140009
C	-2.0272008	1.9221613	-2.5397010
C	-2.1838244	3.1323437	-3.3073782
C	-1.0231773	3.3279127	-3.9954053
C	-0.1275673	2.2453199	-3.6520823
N	-0.7742717	1.3906746	-2.7646454
H	-3.0750911	3.7473889	-3.3237143
H	-0.7974499	4.1323378	-4.6831241
C	-2.0978319	-1.7412661	-0.1533846
C	-3.4060235	-1.5282303	0.4245974
C	-3.8914046	-0.3593199	-0.0816131
C	-2.8879392	0.1710635	-0.9705647
N	-1.8008051	-0.6777077	-1.0001976
H	-3.8896565	-2.1850386	1.1356833
H	-4.8432872	0.1103921	0.1332079
C	1.9217862	-2.6933208	-1.5211820
C	2.0306744	-3.9639536	-0.8513928
C	0.8641493	-4.1657434	-0.1738018
C	0.0222509	-3.0148290	-0.4091603
N	0.6909650	-2.1302596	-1.2466117
H	0.5952317	-5.0250189	0.4264596
C	2.0220288	1.0092672	-3.8429090
C	3.3828716	0.8669486	-4.3086753
C	3.8657404	-0.3059066	-3.8070911
C	2.8165003	-0.8976731	-3.0175490
N	1.7024047	-0.0816234	-3.0435153
H	3.9084587	1.5769667	-4.9335963
H	4.8513536	-0.7311747	-3.9501935
C	2.9255727	-2.1237853	-2.3301751
C	1.1731413	2.0849797	-4.1445304
C	-1.2662766	-2.8350191	0.1151653
C	-3.0125451	1.3760034	-1.6923764
C	1.6986526	3.1413399	-5.0588902

C	1.8735721	4.4493777	-4.5997849
C	2.3585740	5.4554498	-5.4413389
C	2.6775755	5.1113025	-6.7617173
C	2.5202691	3.8087359	-7.2534999
C	2.0212124	2.8342252	-6.3832510
H	3.0580391	5.8773067	-7.4246768
C	-1.7908115	-3.8905700	1.0313179
C	-1.1776169	-4.1135458	2.2680104
C	-1.6534655	-5.0979262	3.1390904
C	-2.7648500	-5.8472062	2.7333524
C	-3.4058004	-5.6476306	1.5040848
C	-2.8984155	-4.6576974	0.6575386
C	-4.2231700	2.0938067	-1.5508008
C	-5.2661053	2.7055362	-1.4169122
C	-6.4793242	3.4109321	-1.2501669
C	-7.5007146	2.8928722	-0.4258281
C	-8.6902568	3.5847886	-0.2571922
C	-8.8924020	4.8112811	-0.9065139
C	-7.8823216	5.3321226	-1.7284393
C	-6.6916926	4.6451518	-1.9004995
H	-7.3491460	1.9419333	0.0805095
H	-9.4693086	3.1765889	0.3802603
H	-8.0444465	6.2836860	-2.2296001
H	-5.9123135	5.0558323	-2.5386828
C	-10.1352486	5.5769589	-0.7545365
O	-10.3766829	6.6640044	-1.2978096
O	-11.0510308	4.9706868	0.0722114
H	-11.8714640	5.5174625	0.1467286
H	-0.3236534	-3.4976805	2.5327281
H	-3.3521137	-4.4629727	-0.3094295
H	1.8743906	1.8125602	-6.7272792
H	1.6228125	4.6713374	-3.5644695
C	2.8759484	3.4171130	-8.6978407
C	2.5141688	6.8846073	-4.8943564
C	1.1297820	7.4069400	-4.4396213
H	0.6952061	6.7753078	-3.6499526
H	1.2207005	8.4306890	-4.0414135
H	0.4249642	7.4273100	-5.2864156
C	3.0741332	7.8575086	-5.9479672
H	2.4111158	7.9366996	-6.8229336
H	3.1677898	8.8622915	-5.5079113
H	4.0723465	7.5494675	-6.2948229
C	3.4806229	6.8731947	-3.6860107
H	3.1066340	6.2367894	-2.8700453
H	4.4724380	6.4981708	-3.9850167
H	3.6025353	7.8937470	-3.2878983
C	1.6125891	2.8805857	-9.4124818
H	1.2028200	1.9941694	-8.9054552
H	0.8256453	3.6512556	-9.4428275
H	1.8554328	2.5944513	-10.4488246
C	3.4199391	4.6069452	-9.5100920
H	4.3394958	5.0166672	-9.0649695
H	3.6623850	4.2747364	-10.5313180
H	2.6801102	5.4182981	-9.5901347
C	3.9602174	2.3129218	-8.6736294
H	3.6121057	1.4109627	-8.1477706
H	4.2290061	2.0205195	-9.7018225
H	4.8704874	2.6732474	-8.1681458
C	-1.0010838	-5.3819197	4.5023482
C	-4.6268700	-6.5062313	1.1347737
C	-5.1938762	-6.1469438	-0.2508934

H	-5.5268437	-5.0985193	-0.2951108
H	-4.4530350	-6.3102545	-1.0483001
H	-6.0653993	-6.7834934	-0.4686312
C	-5.7425002	-6.2866571	2.1845949
H	-6.0487119	-5.2286851	2.2108751
H	-6.6260781	-6.8960368	1.9333826
H	-5.4132211	-6.5717448	3.1952851
C	-4.2224162	-7.9995704	1.1197391
H	-3.8553618	-8.3326897	2.1023204
H	-5.0898726	-8.6258923	0.8541817
H	-3.4270953	-8.1796437	0.3789622
H	-3.1464071	-6.6170952	3.4011247
C	-2.0447782	-5.1845215	5.6273086
H	-2.9027883	-5.8643031	5.5129539
H	-1.5862820	-5.3840295	6.6095764
H	-2.4261151	-4.1510704	5.6272032
C	-0.4889013	-6.8420861	4.5267412
H	-0.0160373	-7.0633250	5.4976192
H	-1.3068995	-7.5631307	4.3773283
H	0.2578359	-7.0048296	3.7332370
C	0.1911249	-4.4492647	4.7828944
H	0.9868620	-4.5683879	4.0313986
H	-0.1148343	-3.3919802	4.8000807
H	0.6235976	-4.6887479	5.7667451
H	2.8896463	-4.6216246	-0.9025178
C	4.1394976	-2.8392888	-2.4668251
C	5.1837929	-3.4497135	-2.5935962
C	6.4024157	-4.1548176	-2.7507980
C	7.4084554	-3.6634974	-3.6083132
C	6.6350367	-5.3593616	-2.0577286
H	5.8678273	-5.7502589	-1.3916841
C	7.8338151	-6.0452879	-2.2198957
H	8.0186942	-6.9754669	-1.6868801
C	8.8281066	-5.5551740	-3.0704171
H	7.2428805	-2.7343208	-4.1513713
C	8.6018865	-4.3574696	-3.7622590
H	9.3690922	-3.9655354	-4.4283575
N	10.0584834	-6.2912637	-3.2132047
C	11.2439773	-5.6129045	-2.6702638
H	12.0829149	-6.3243538	-2.6362663
H	11.5641051	-4.7355770	-3.2739668
H	11.0381304	-5.2706700	-1.6466652
C	10.2713105	-6.8782291	-4.5437075
H	11.1207335	-7.5765581	-4.4975834
H	9.3772028	-7.4396242	-4.8483406
H	10.4927085	-6.1220640	-5.3280262

Table S12. LD13-TiO2 (gas)

193

Ti	7.8633895	5.3962343	14.2455952
Ti	4.3243172	5.1736184	12.9235313
Ti	0.7852422	4.9511021	11.6014578
Ti	-2.7538300	4.7284862	10.2793939
O	7.1643089	5.5481449	16.0914262
O	3.6252339	5.3256285	14.7693527
O	0.0861616	5.1030126	13.4472889
O	-3.4529107	4.8803967	12.1252250
O	6.2348045	5.2542881	13.2125448
O	2.6956360	5.0317658	11.8904364
O	-0.8434362	4.8091499	10.5683725

O	-4.3825112	4.5866335	9.2462990
Ti	3.4678864	9.5992735	19.8878385
Ti	-0.0712793	9.3766517	18.5657397
Ti	-3.6103543	9.1541353	17.2436662
Ti	-7.1494266	8.9315194	15.9216024
Ti	4.3608377	7.5333287	17.8451771
Ti	0.8216692	7.3108063	16.5230686
Ti	-2.7174031	7.0881904	15.2010047
Ti	-6.2564781	6.8656740	13.8789312
Ti	3.4312371	7.2395654	14.9662511
Ti	6.9703121	7.4620818	16.2883246
Ti	-0.1078351	7.0169495	13.6441872
Ti	-3.6469101	6.7944332	12.3221137
O	4.1669317	9.4473711	18.0421007
O	0.6277660	9.2247492	16.7200019
O	-2.9113063	9.0021333	15.3979380
O	-6.4503813	8.7796169	14.0758645
O	5.0964388	9.7411283	20.9209917
O	1.5573638	9.5186119	19.5989182
O	-1.9817085	9.2959961	18.2768544
O	-5.5207834	9.0734797	16.9547808
O	-9.0598557	8.8508638	15.6327170
O	5.0599183	7.3814181	15.9993460
O	1.5207498	7.1588958	14.6772375
O	-2.0183224	6.9362799	13.3551737
O	-5.5573974	6.7137635	12.0331002
O	3.6617897	7.6853306	19.6909053
O	0.1226239	7.4627088	18.3688065
O	-3.4164484	7.2400929	17.0467426
O	-6.9555233	7.0175765	15.7246691
O	2.7321918	7.3914679	16.8119889
O	6.2712668	7.6139843	18.1340624
O	-0.8068804	7.1688520	15.4899251
O	-4.3459554	6.9463356	14.1678515
O	7.6693574	7.3101794	14.4425867
O	4.1302824	7.0876630	13.1205132
O	0.5912102	6.8650471	11.7984493
O	-2.9478621	6.6424312	10.4763855
H	6.0448758	9.7811735	21.0644459
H	-9.8683787	8.7804536	15.1198318
O	9.7737833	5.4768980	14.5345738
H	10.5821775	5.5473103	15.0475172
H	-5.3308901	4.5466024	9.1029730
O	0.6058086	9.0320724	13.4473572
O	2.7916545	9.1907592	14.2535322
C	1.6864830	9.6705838	13.7745370
C	1.6424806	11.1497375	13.5618543
C	0.4883884	11.7359749	13.0244877
C	2.7479539	11.9482592	13.8822885
C	0.4464343	13.1009416	12.7846160
H	-0.3608824	11.0949249	12.7949388
C	2.7138632	13.3168637	13.6447562
H	3.6274411	11.4683506	14.3094688
C	1.5645960	13.9121009	13.0805120
H	-0.4461803	13.5570486	12.3538509
H	3.5781855	13.9385777	13.8821793
C	1.5161113	15.2965616	12.7888537
C	1.4242827	16.4747605	12.4949928
C	1.2698878	17.8285533	12.1163492
C	2.3596761	18.7100122	12.3369979
C	0.0279324	18.1965691	11.5335649

C	-2.0713056	18.0184938	10.7389735
C	3.6251984	20.5126631	12.4010675
C	4.3934773	19.4368106	12.9723077
C	3.6090221	18.3208802	12.9309395
N	2.3852802	20.0419848	12.0213982
C	-1.5893583	19.3680063	10.6038045
N	-0.3045669	19.4503945	11.0973585
C	-2.3245432	20.4270093	10.0484725
C	4.0833116	21.8311648	12.2606468
C	-1.8666696	21.7467358	9.9027872
C	3.3504024	22.8954399	11.7043041
H	-3.0594516	17.6721462	10.4264711
H	3.8453798	17.3100951	13.2717301
H	5.4120254	19.5312043	13.3568097
C	-1.0683882	17.2932697	11.3144668
H	-1.0614507	16.2318865	11.5714819
N	-0.6284050	22.2059916	10.2824096
N	2.0681428	22.8024419	11.2132141
C	1.7170116	24.0442287	10.7656981
C	0.4973306	24.3864108	10.1924237
C	2.8207555	24.9763303	10.9780139
C	3.8300965	24.2378605	11.5648409
Zn	0.8780018	21.1225124	11.1528704
C	-2.6291890	22.8292461	9.3303683
C	-0.5880984	23.5410340	9.9677064
C	-1.8351022	23.9391934	9.3715544
H	-3.6482569	22.7403833	8.9457249
H	-2.0686628	24.9511408	9.0268829
H	4.8145369	24.5970993	11.8704333
C	5.4590528	22.1504882	12.7404421
C	5.6551158	22.6043163	14.0476596
C	6.5494225	22.0422948	11.8727669
C	6.9269239	22.9710543	14.5001489
H	4.7799607	22.6755025	14.7026499
C	7.8371721	22.3999968	12.2861712
H	6.3642150	21.6810130	10.8555122
C	7.9919825	22.8640806	13.5979777
H	8.9939204	23.1618659	13.9340774
C	-3.7085228	20.1405569	9.5707359
C	-3.9309092	19.7731777	8.2408340
C	-4.7917518	20.2755568	10.4435168
C	-5.2267955	19.5562899	7.7601815
H	-3.0605205	19.6693398	7.5838487
C	-6.1027656	20.0672684	10.0022963
H	-4.5844281	20.5601522	11.4807344
C	-6.2875790	19.7176137	8.6594383
H	-7.3117114	19.5646216	8.2949650
C	9.0535587	22.3330399	11.3534837
C	10.1615690	21.4882020	12.0030962
C	8.7091350	21.7080111	9.9993052
C	9.5701495	23.7620510	11.1125737
H	10.4963380	21.9109096	12.9667451
H	9.8135058	20.4566643	12.1922189
H	11.0446071	21.4357769	11.3391721
H	7.9507260	22.2957227	9.4522743
H	9.6134213	21.6668698	9.3657450
H	8.3304771	20.6760361	10.1079746
H	10.4529643	23.7507170	10.4455405
H	8.7910219	24.3881501	10.6407298
H	9.8691137	24.2530139	12.0561259
C	7.1777039	23.5081219	15.9155119

C	5.9181680	23.4559699	16.7840756
C	8.2690554	22.6712048	16.6029048
C	7.6390352	24.9722897	15.8140794
H	5.1046770	24.0799576	16.3726864
H	5.5376163	22.4246217	16.8921074
H	6.1447971	23.8365197	17.7964892
H	9.2266474	22.7052880	16.0537944
H	8.4593505	23.0497338	17.6248854
H	7.9652082	21.6117221	16.6811349
H	7.8318552	25.3903733	16.8202687
H	8.5685995	25.0680130	15.2252391
H	6.8675808	25.5950097	15.3257568
C	-5.5156328	19.1902379	6.2983842
C	-4.2334782	18.9240257	5.5061047
C	-6.3867219	17.9247922	6.2378012
C	-6.2635298	20.3612584	5.6381776
H	-3.5826293	19.8149915	5.4582217
H	-3.6473970	18.0947026	5.9410889
H	-4.4852983	18.6450735	4.4668361
H	-7.3591726	18.0618153	6.7431938
H	-6.5962377	17.6529247	5.1864035
H	-5.8781422	17.0691733	6.7172841
H	-6.4968560	20.1290612	4.5817239
H	-7.2165295	20.5802141	6.1531016
H	-5.6518858	21.2814723	5.6609381
C	-7.3207730	20.2336157	10.9202946
C	-8.1582888	18.9444458	10.9066493
C	-6.9169676	20.5258627	12.3674351
C	-8.1730686	21.4065158	10.4066384
H	-8.5289815	18.7008771	9.8953621
H	-7.5647426	18.0826807	11.2617988
H	-9.0397733	19.0487057	11.5668066
H	-6.3504264	21.4699126	12.4576965
H	-7.8205978	20.6226596	12.9957842
H	-6.3004244	19.7140768	12.7932024
H	-9.0635340	21.5499592	11.0474216
H	-7.5925480	22.3471111	10.4102939
H	-8.5263250	21.2351464	9.3739013
H	2.8431738	26.0169807	10.7301347
C	0.3402323	25.8574206	9.7645800
C	0.2176957	27.0048083	9.4308620
C	0.0326825	28.3483014	9.0199082
C	1.0610111	29.2972288	9.1641544
C	-1.1915109	28.7597960	8.4578888
H	-1.9912995	28.0298294	8.3421591
C	0.8681996	30.6131246	8.7579177
C	-1.3740493	30.0766204	8.0561554
H	-2.3243187	30.3901045	7.6249448
C	-0.3467256	31.0165164	8.1997889
H	2.0078977	28.9844349	9.6021862
H	1.6531280	31.3575095	8.8697824
N	-0.5200666	32.3863353	7.7896281
C	-1.4517322	33.1675149	8.6071511
H	-1.3308095	34.2389883	8.3801166
H	-2.5204129	32.9017479	8.4425647
H	-1.2332630	33.0108311	9.6728766
C	-0.6510813	32.5967239	6.3455605
H	-0.5351614	33.6689334	6.1211713
H	0.1393211	32.0455135	5.8173065
H	-1.6293053	32.2663642	5.9274743

Table S13. LD13-TiO2 (solv)

193

Ti	7.8633895	5.3962343	14.2455952
Ti	4.3243172	5.1736184	12.9235313
Ti	0.7852422	4.9511021	11.6014578
Ti	-2.7538300	4.7284862	10.2793939
O	7.1643089	5.5481449	16.0914262
O	3.6252339	5.3256285	14.7693527
O	0.0861616	5.1030126	13.4472889
O	-3.4529107	4.8803967	12.1252250
O	6.2348045	5.2542881	13.2125448
O	2.6956360	5.0317658	11.8904364
O	-0.8434362	4.8091499	10.5683725
O	-4.3825112	4.5866335	9.2462990
Ti	3.4678864	9.5992735	19.8878385
Ti	-0.0712793	9.3766517	18.5657397
Ti	-3.6103543	9.1541353	17.2436662
Ti	-7.1494266	8.9315194	15.9216024
Ti	4.3608377	7.5333287	17.8451771
Ti	0.8216692	7.3108063	16.5230686
Ti	-2.7174031	7.0881904	15.2010047
Ti	-6.2564781	6.8656740	13.8789312
Ti	3.4312371	7.2395654	14.9662511
Ti	6.9703121	7.4620818	16.2883246
Ti	-0.1078351	7.0169495	13.6441872
Ti	-3.6469101	6.7944332	12.3221137
O	4.1669317	9.4473711	18.0421007
O	0.6277660	9.2247492	16.7200019
O	-2.9113063	9.0021333	15.3979380
O	-6.4503813	8.7796169	14.0758645
O	5.0964388	9.7411283	20.9209917
O	1.5573638	9.5186119	19.5989182
O	-1.9817085	9.2959961	18.2768544
O	-5.5207834	9.0734797	16.9547808
O	-9.0598557	8.8508638	15.6327170
O	5.0599183	7.3814181	15.9993460
O	1.5207498	7.1588958	14.6772375
O	-2.0183224	6.9362799	13.3551737
O	-5.5573974	6.7137635	12.0331002
O	3.6617897	7.6853306	19.6909053
O	0.1226239	7.4627088	18.3688065
O	-3.4164484	7.2400929	17.0467426
O	-6.9555233	7.0175765	15.7246691
O	2.7321918	7.3914679	16.8119889
O	6.2712668	7.6139843	18.1340624
O	-0.8068804	7.1688520	15.4899251
O	-4.3459554	6.9463356	14.1678515
O	7.6693574	7.3101794	14.4425867
O	4.1302824	7.0876630	13.1205132
O	0.5912102	6.8650471	11.7984493
O	-2.9478621	6.6424312	10.4763855
H	6.0448758	9.7811735	21.0644459
H	-9.8683787	8.7804536	15.1198318
O	9.7737833	5.4768980	14.5345738
H	10.5821775	5.5473103	15.0475172
H	-5.3308901	4.5466024	9.1029730
O	0.5977483	9.0117360	13.4633021
O	2.7836052	9.1755487	14.2690726
C	1.6727531	9.6622795	13.8011634

C	1.6264411	11.1348315	13.5882712
C	0.4770231	11.7277971	13.0485356
C	2.7300583	11.9400534	13.8978728
C	0.4362350	13.0924991	12.8029454
H	-0.3793080	11.0992800	12.8178498
C	2.6974152	13.3080645	13.6552231
H	3.6160952	11.4762490	14.3247109
C	1.5516057	13.9087366	13.0920947
H	-0.4583799	13.5402047	12.3737026
H	3.5639933	13.9230045	13.8909153
C	1.5069865	15.2947769	12.7971159
C	1.4224366	16.4723076	12.4974575
C	1.2698878	17.8285533	12.1163492
C	2.3596761	18.7100122	12.3369979
C	0.0279324	18.1965691	11.5335649
C	-2.0713056	18.0184938	10.7389735
C	3.6251984	20.5126631	12.4010675
C	4.3934773	19.4368106	12.9723077
C	3.6090221	18.3208802	12.9309395
N	2.3852802	20.0419848	12.0213982
C	-1.5893583	19.3680063	10.6038045
N	-0.3045669	19.4503945	11.0973585
C	-2.3245432	20.4270093	10.0484725
C	4.0833116	21.8311648	12.2606468
C	-1.8666696	21.7467358	9.9027872
C	3.3504024	22.8954399	11.7043041
H	-3.0594516	17.6721462	10.4264711
H	3.8453798	17.3100951	13.2717301
H	5.4120254	19.5312043	13.3568097
C	-1.0683882	17.2932697	11.3144668
H	-1.0614507	16.2318865	11.5714819
N	-0.6284050	22.2059916	10.2824096
N	2.0681428	22.8024419	11.2132141
C	1.7170116	24.0442287	10.7656981
C	0.4973306	24.3864108	10.1924237
C	2.8207555	24.9763303	10.9780139
C	3.8300965	24.2378605	11.5648409
Zn	0.8780018	21.1225124	11.1528704
C	-2.6291890	22.8292461	9.3303683
C	-0.5880984	23.5410340	9.9677064
C	-1.8351022	23.9391934	9.3715544
H	-3.6482569	22.7403833	8.9457249
H	-2.0686628	24.9511408	9.0268829
H	4.8145369	24.5970993	11.8704333
C	5.4590528	22.1504882	12.7404421
C	5.6551158	22.6043163	14.0476596
C	6.5494225	22.0422948	11.8727669
C	6.9269239	22.9710543	14.5001489
H	4.7799607	22.6755025	14.7026499
C	7.8371721	22.3999968	12.2861712
H	6.3642150	21.6810130	10.8555122
C	7.9919825	22.8640806	13.5979777
H	8.9939204	23.1618659	13.9340774
C	-3.7085228	20.1405569	9.5707359
C	-3.9309092	19.7731777	8.2408340
C	-4.7917518	20.2755568	10.4435168
C	-5.2267955	19.5562899	7.7601815
H	-3.0605205	19.6693398	7.5838487
C	-6.1027656	20.0672684	10.0022963
H	-4.5844281	20.5601522	11.4807344
C	-6.2875790	19.7176137	8.6594383

H	-7.3117114	19.5646216	8.2949650
C	9.0535587	22.3330399	11.3534837
C	10.1615690	21.4882020	12.0030962
C	8.7091350	21.7080111	9.9993052
C	9.5701495	23.7620510	11.1125737
H	10.4963380	21.9109096	12.9667451
H	9.8135058	20.4566643	12.1922189
H	11.0446071	21.4357769	11.3391721
H	7.9507260	22.2957227	9.4522743
H	9.6134213	21.6668698	9.3657450
H	8.3304771	20.6760361	10.1079746
H	10.4529643	23.7507170	10.4455405
H	8.7910219	24.3881501	10.6407298
H	9.8691137	24.2530139	12.0561259
C	7.1777039	23.5081219	15.9155119
C	5.9181680	23.4559699	16.7840756
C	8.2690554	22.6712048	16.6029048
C	7.6390352	24.9722897	15.8140794
H	5.1046770	24.0799576	16.3726864
H	5.5376163	22.4246217	16.8921074
H	6.1447971	23.8365197	17.7964892
H	9.2266474	22.7052880	16.0537944
H	8.4593505	23.0497338	17.6248854
H	7.9652082	21.6117221	16.6811349
H	7.8318552	25.3903733	16.8202687
H	8.5685995	25.0680130	15.2252391
H	6.8675808	25.5950097	15.3257568
C	-5.5156328	19.1902379	6.2983842
C	-4.2334782	18.9240257	5.5061047
C	-6.3867219	17.9247922	6.2378012
C	-6.2635298	20.3612584	5.6381776
H	-3.5826293	19.8149915	5.4582217
H	-3.6473970	18.0947026	5.9410889
H	-4.4852983	18.6450735	4.4668361
H	-7.3591726	18.0618153	6.7431938
H	-6.5962377	17.6529247	5.1864035
H	-5.8781422	17.0691733	6.7172841
H	-6.4968560	20.1290612	4.5817239
H	-7.2165295	20.5802141	6.1531016
H	-5.6518858	21.2814723	5.6609381
C	-7.3207730	20.2336157	10.9202946
C	-8.1582888	18.9444458	10.9066493
C	-6.9169676	20.5258627	12.3674351
C	-8.1730686	21.4065158	10.4066384
H	-8.5289815	18.7008771	9.8953621
H	-7.5647426	18.0826807	11.2617988
H	-9.0397733	19.0487057	11.5668066
H	-6.3504264	21.4699126	12.4576965
H	-7.8205978	20.6226596	12.9957842
H	-6.3004244	19.7140768	12.7932024
H	-9.0635340	21.5499592	11.0474216
H	-7.5925480	22.3471111	10.4102939
H	-8.5263250	21.2351464	9.3739013
H	2.8431738	26.0169807	10.7301347
C	0.3402323	25.8574206	9.7645800
C	0.2176957	27.0048083	9.4308620
C	0.0392693	28.3530966	9.0232162
C	1.0699664	29.3002032	9.1722999
C	-1.1829450	28.7672791	8.4572021
H	-1.9892452	28.0455009	8.3362943
C	0.8800143	30.6176382	8.7669870

C	-1.3618129	30.0851793	8.0558861
H	-2.3125140	30.3901588	7.6207125
C	-0.3328348	31.0242132	8.2060082
H	2.0203313	28.9947029	9.6068957
H	1.6733249	31.3536382	8.8789430
N	-0.4973915	32.3963579	7.7964076
C	-1.4593381	33.1619893	8.6016615
H	-1.3730847	34.2300205	8.3504007
H	-2.5152437	32.8558167	8.4338822
H	-1.2299394	33.0365194	9.6688064
C	-0.6541915	32.5874276	6.3477505
H	-0.5700557	33.6594502	6.1133461
H	0.1449607	32.0521790	5.8167404
H	-1.6321361	32.2286815	5.9586558

Table S14. YD2-o-C8 (gas)

230

Zn	2.7818904	-0.7306277	0.0403006
C	5.1790883	-2.6546089	-0.0909450
C	5.5167203	-4.0538350	0.0096901
C	4.3690380	-4.7284834	0.3004019
C	3.3089898	-3.7524526	0.3968623
N	3.8325426	-2.4873457	0.1468339
H	6.5097188	-4.4608574	-0.1329187
H	4.2434828	-5.7946201	0.4408877
C	4.6154102	1.6401981	-0.6429899
C	6.0057240	1.9571323	-0.8721485
C	6.7069036	0.7922533	-0.8093172
C	5.7611318	-0.2625687	-0.5291069
N	4.4945850	0.2723024	-0.4244938
H	6.3888799	2.9513296	-1.0615503
H	7.7726704	0.6480108	-0.9340958
C	0.3536702	1.1680535	0.0811788
C	-0.0076353	2.5453590	-0.1441111
C	1.1368189	3.2120734	-0.4670415
C	2.2222778	2.2587664	-0.4323488
N	1.7173239	1.0121018	-0.1112836
H	-1.0128336	2.9406658	-0.0733779
H	1.2412971	4.2617315	-0.7107510
C	0.9471981	-3.0876210	0.7755692
C	-0.4280426	-3.3847633	1.1008881
C	-1.1271963	-2.2163282	1.0377014
C	-0.1930455	-1.1812066	0.6811994
N	1.0721311	-1.7275318	0.5455123
H	-0.8165403	-4.3656864	1.3350748
H	-2.1830963	-2.0704829	1.2183513
C	-0.5292649	0.1547702	0.4504913
C	1.9748290	-4.0365771	0.6778607
C	3.5718966	2.5635380	-0.6559430
C	6.0932839	-1.6247268	-0.3945979
C	1.5579080	-5.4608459	0.8389191
C	1.8599151	-6.1880752	1.9900973
C	1.3199425	-7.4642487	2.1621499
C	0.5024123	-8.0385220	1.1831441
C	0.2156656	-7.2977657	0.0340650
C	0.7459550	-6.0248068	-0.1451230
H	2.4699057	-5.7632613	2.7813889
H	0.1157002	-9.0456861	1.2993807

H	0.4791440	-5.4619910	-1.0328031
C	3.9060205	3.9956727	-0.8960703
C	3.7946532	4.9256824	0.1437283
C	4.0366374	6.2846833	-0.0673210
C	4.4154847	6.7129379	-1.3357078
C	4.5532162	5.8093705	-2.3889306
C	4.2950644	4.4548897	-2.1632196
H	4.6136962	7.7695257	-1.5100467
C	7.4452485	-1.9906613	-0.5925512
C	8.6050820	-2.3088090	-0.7746770
C	9.9488635	-2.6804569	-1.0013487
C	10.9169359	-1.7125973	-1.3449000
C	12.2304764	-2.0829962	-1.5785754
C	12.6197547	-3.4258990	-1.4772489
C	11.6676421	-4.3950094	-1.1319067
C	10.3516291	-4.0285252	-0.8966736
H	10.6197971	-0.6692977	-1.4267996
H	12.9793861	-1.3404655	-1.8451202
H	11.9697205	-5.4353912	-1.0513765
H	9.6147306	-4.7829906	-0.6291489
C	14.0217005	-3.7660416	-1.7421614
O	14.2883056	-5.1181176	-1.6080204
O	14.9101735	-2.9685436	-2.0566306
N	-1.9188633	0.5061756	0.5666712
C	-2.6634574	0.6918394	-0.6326305
C	-2.3927882	-0.0966729	-1.7582860
C	-3.1078538	0.0895001	-2.9356726
C	-4.1193553	1.0525924	-3.0330852
C	-4.3733254	1.8404112	-1.9047514
C	-3.6539382	1.6765374	-0.7246293
H	-1.6195406	-0.8573483	-1.7094381
H	-2.8768326	-0.5409370	-3.7949856
H	-5.1430162	2.6112503	-1.9524172
H	-3.8647794	2.3094970	0.1347660
C	-2.5259269	0.5143534	1.8469792
C	-1.7629905	0.8196123	2.9821786
C	-2.3321315	0.7659004	4.2508616
C	-3.6742009	0.4202385	4.4369535
C	-4.4299616	0.1293779	3.2949939
C	-3.8727333	0.1620674	2.0223488
H	-0.7153642	1.0864203	2.8656396
H	-1.7145199	1.0025591	5.1177104
H	-5.4768330	-0.1558503	3.4058154
H	-4.4790339	-0.1051546	1.1609610
C	-4.9247972	1.1967925	-4.3013934
H	-4.2434854	1.3333679	-5.1574201
H	-5.5350065	2.1113648	-4.2471636
C	-5.8311483	-0.0184792	-4.5981199
H	-6.3453944	0.1547833	-5.5585418
H	-5.1939676	-0.9056545	-4.7519576
C	-6.8575372	-0.3416152	-3.5023599
H	-7.4202398	-1.2397441	-3.8077008
H	-6.3212627	-0.6207716	-2.5803668
C	-7.8414750	0.7920702	-3.1648815
H	-7.2945089	1.6194657	-2.6833271
H	-8.5493656	0.4198348	-2.4034299
C	-8.6412486	1.3523594	-4.3516117
H	-9.2926479	2.1617378	-3.9801659
H	-7.9551516	1.8297771	-5.0726896
C	-9.4978708	0.3103363	-5.0772120
H	-10.1797045	-0.2001131	-4.3759301

H	-10.1123022	0.7771797	-5.8631570
H	-8.8793088	-0.4633781	-5.5591460
C	-4.3065633	0.4123518	5.8046150
H	-5.0047381	-0.4378717	5.8881162
H	-3.5320905	0.2557181	6.5725846
C	-5.0679860	1.7140246	6.1150522
H	-5.8238297	1.8744169	5.3288806
H	-4.3675829	2.5621334	6.0400636
C	-5.7310159	1.7087979	7.4950542
H	-6.4710148	0.8901031	7.5390679
H	-4.9704482	1.4641228	8.2566975
C	-6.3958669	3.0397610	7.8807561
H	-6.8249681	2.9386786	8.8931840
H	-5.6169734	3.8188856	7.9537729
C	-7.4947785	3.5341307	6.9254379
H	-7.0555034	3.7655866	5.9410318
H	-7.8798630	4.4931678	7.3104919
C	-8.6596126	2.5559131	6.7491854
H	-8.3383371	1.6216291	6.2611015
H	-9.1029271	2.2859208	7.7227173
H	-9.4567677	2.9939485	6.1277477
H	15.2434449	-5.2827221	-1.7973027
H	3.9476484	6.9899725	0.7543955
H	4.8496890	6.1650392	-3.3707148
O	3.4419042	4.4074732	1.3797130
O	4.3778989	3.4778932	-3.1375666
O	1.6374572	-8.0864349	3.3613914
O	-0.6114466	-7.7412037	-0.9880569
C	2.5125372	5.1448068	2.2360163
H	1.7689307	5.6593042	1.6043121
H	3.0633456	5.9028196	2.8166062
C	1.8555124	4.1198143	3.1390546
H	1.3916972	3.3505167	2.5015466
H	2.6382263	3.6124416	3.7250471
C	0.8055335	4.7340659	4.0676771
H	0.0315639	5.2314010	3.4582232
H	1.2651952	5.5244514	4.6891221
C	0.1575455	3.6885701	4.9820388
H	-0.2745573	2.8876371	4.3585982
H	0.9484022	3.2146936	5.5883439
C	-0.9293784	4.2418763	5.9122606
H	-1.1872229	3.4707665	6.6591443
H	-0.5215168	5.0954507	6.4845343
C	-2.2154339	4.6729776	5.1981626
H	-1.9896338	5.4331726	4.4308754
H	-2.6327587	3.8049135	4.6564844
C	-3.2731042	5.2357195	6.1517794
H	-2.8630975	6.1207501	6.6696590
H	-3.4795920	4.4929631	6.9422544
C	-4.5772618	5.6087587	5.4446902
H	-5.3329030	5.9804907	6.1541851
H	-4.4068473	6.3930495	4.6888272
H	-5.0073346	4.7360143	4.9270147
C	4.7901362	3.8099596	-4.4934507
H	5.7961493	4.2633179	-4.4748873
H	4.0859566	4.5404000	-4.9279828
C	4.7837031	2.5076561	-5.2690101
H	5.4662286	1.8009435	-4.7712053
H	3.7764709	2.0675684	-5.1996127
C	5.1811691	2.6889848	-6.7361971
H	6.1942632	3.1260117	-6.7974624

H	4.5036615	3.4174440	-7.2177429
C	5.1486808	1.3759621	-7.5243390
H	5.8248014	0.6462725	-7.0442504
H	4.1359923	0.9395924	-7.4597318
C	5.5373480	1.5385341	-8.9957867
H	6.5549571	1.9645172	-9.0609229
H	4.8670538	2.2775915	-9.4713097
C	5.4852591	0.2272661	-9.7848693
H	6.1536630	-0.5127320	-9.3080588
H	4.4668728	-0.1974264	-9.7194015
C	5.8730866	0.3832735	-11.2585942
H	6.8922244	0.8041349	-11.3223017
H	5.2072481	1.1268882	-11.7316613
C	5.8097897	-0.9329240	-12.0373479
H	6.0962125	-0.7946007	-13.0918551
H	6.4884656	-1.6847527	-11.6008227
H	4.7915602	-1.3561711	-12.0181905
C	0.7429406	-9.0705572	3.9787324
H	-0.2110061	-9.1151078	3.4302087
H	1.2396099	-10.0491761	3.9042339
C	0.4917990	-8.6884326	5.4311459
H	0.0487984	-9.5738276	5.9195714
H	1.4620041	-8.5098446	5.9223062
C	-0.4422833	-7.4814463	5.6302508
H	-1.3202212	-7.6089812	4.9727649
H	-0.8336853	-7.4997407	6.6622187
C	0.2079226	-6.1137903	5.3791957
H	1.0247937	-5.9764017	6.1086782
H	0.6831224	-6.1049988	4.3901130
C	-0.7578670	-4.9237250	5.4612491
H	-0.1689727	-3.9941729	5.3759815
H	-1.2405307	-4.8912108	6.4553460
C	-1.8354523	-4.9199680	4.3685278
H	-2.5657014	-5.7269734	4.5534642
H	-1.3619523	-5.1547590	3.3981409
C	-2.5842925	-3.5890839	4.2471267
H	-3.0002341	-3.3077429	5.2309035
H	-1.8697652	-2.7931719	3.9785169
C	-3.7072871	-3.6345096	3.2095420
H	-4.4757526	-4.3768125	3.4841698
H	-4.1963384	-2.6544802	3.1065234
H	-3.3147346	-3.9196496	2.2198299
C	-1.7307820	-8.6530360	-0.7286667
H	-1.4160935	-9.6610879	-1.0371237
H	-1.9608735	-8.6696958	0.3499413
C	-2.9295903	-8.1685578	-1.5379072
H	-3.5746456	-9.0398604	-1.7446944
H	-2.5562546	-7.8211959	-2.5108604
C	-3.7902266	-7.0961066	-0.8417769
H	-4.2415003	-7.5711202	0.0480675
H	-4.6354087	-6.8396684	-1.5047830
C	-3.0988848	-5.7949112	-0.3877024
H	-3.6968620	-5.3709831	0.4357359
H	-2.1155914	-6.0253100	0.0494284
C	-2.9350040	-4.6882203	-1.4405492
H	-3.9345579	-4.3312723	-1.7495415
H	-2.4531036	-3.8328143	-0.9397960
C	-2.1320878	-5.0496053	-2.7002281
H	-2.7627194	-5.6561726	-3.3714865
H	-1.2775144	-5.6906103	-2.4308947
C	-1.6256921	-3.8081556	-3.4580041

H	-1.3818151	-4.0856949	-4.4969740
H	-2.4434562	-3.0666368	-3.5227559
C	-0.3905638	-3.1632055	-2.8153708
H	-0.5542828	-2.9209564	-1.7545307
H	0.4758955	-3.8428803	-2.8639369
H	-0.1074276	-2.2305387	-3.3284801

Table S15. YD2-o-C8 (solv)

230

Zn	2.8916315	-0.7327510	0.2366719
C	5.3236141	-2.5874097	-0.1503753
C	5.7023696	-3.9804293	-0.1183369
C	4.5929605	-4.6939851	0.2315103
C	3.5201274	-3.7493472	0.4328249
N	3.9928004	-2.4633196	0.1843350
H	6.6926602	-4.3602671	-0.3380469
H	4.5071698	-5.7668317	0.3558749
C	4.5899656	1.6981473	-0.5911117
C	5.9566425	2.0655841	-0.8816342
C	6.7015703	0.9251600	-0.8637759
C	5.8077271	-0.1652078	-0.5513933
N	4.5296776	0.3246419	-0.3726887
H	6.3001486	3.0713181	-1.0857829
H	7.7643762	0.8242782	-1.0469755
C	0.4028736	1.0762553	0.4162944
C	-0.0283914	2.4302431	0.1700376
C	1.0578075	3.1245742	-0.2736448
C	2.1836743	2.2207084	-0.2758502
N	1.7540467	0.9654652	0.1222527
H	-1.0320522	2.8047257	0.3194357
H	1.0947186	4.1668499	-0.5615750
C	1.1946453	-3.1534672	1.0676309
C	-0.1578491	-3.5113674	1.4210525
C	-0.8951533	-2.3647422	1.4365147
C	-0.0088817	-1.2847996	1.0885495
N	1.2696168	-1.7804966	0.8949330
H	-0.5058401	-4.5191620	1.5984454
H	-1.9520929	-2.2627499	1.6378282
C	-0.4105452	0.0384754	0.8776276
C	2.2273655	-4.0723897	0.8338870
C	3.5071247	2.5790117	-0.5727542
C	6.1888604	-1.5196434	-0.4716875
C	1.8309413	-5.5114181	0.9220374
C	1.6498071	-6.1389654	2.1537584
C	1.0656188	-7.4069927	2.2004391
C	0.6713164	-8.0608631	1.0307746
C	0.8492092	-7.4136958	-0.1942216
C	1.4512946	-6.1592660	-0.2551790
H	1.8929344	-5.6356589	3.0849799
H	0.2343845	-9.0529209	1.0724656
H	1.5412292	-5.6627531	-1.2166902
C	3.7761445	4.0114561	-0.8850906
C	3.6509436	5.0020078	0.0966417
C	3.8863826	6.3475288	-0.1940064
C	4.2651504	6.7071271	-1.4837372
C	4.4026437	5.7450724	-2.4847218
C	4.1517305	4.4050290	-2.1823998
H	4.4573219	7.7530366	-1.7177063
C	7.5386840	-1.8390743	-0.7499279

C	8.6953634	-2.1273605	-0.9933416
C	10.0335088	-2.4810204	-1.2797804
C	10.9829560	-1.4973429	-1.6305846
C	12.2911081	-1.8558890	-1.9138020
C	12.6903135	-3.1992813	-1.8557499
C	11.7529954	-4.1830232	-1.5069616
C	10.4426596	-3.8303612	-1.2225612
H	10.6821983	-0.4530565	-1.6789690
H	13.0205231	-1.0962403	-2.1850335
H	12.0544588	-5.2253681	-1.4593806
H	9.7203982	-4.5980127	-0.9529665
C	14.0858334	-3.5311523	-2.1653715
O	14.3607978	-4.8727375	-2.0751930
O	14.9614861	-2.7114601	-2.4816810
N	-1.7915680	0.3437165	1.1098061
C	-2.6242504	0.5936348	-0.0223407
C	-2.5431375	-0.2296740	-1.1505425
C	-3.3486694	0.0184575	-2.2581152
C	-4.2660359	1.0771654	-2.2698048
C	-4.3286170	1.8981973	-1.1364211
C	-3.5140370	1.6717525	-0.0321433
H	-1.8493007	-1.0665591	-1.1581871
H	-3.2711452	-0.6378991	-3.1260970
H	-5.0213421	2.7398047	-1.1184705
H	-3.5713650	2.3269758	0.8340794
C	-2.3121898	0.3027913	2.4264624
C	-1.4558432	0.4328561	3.5293786
C	-1.9602858	0.3821023	4.8247875
C	-3.3270994	0.2143191	5.0726616
C	-4.1714450	0.0824192	3.9650206
C	-3.6807964	0.1093992	2.6648071
H	-0.3906373	0.5796259	3.3716662
H	-1.2715524	0.4940683	5.6626828
H	-5.2404029	-0.0660992	4.1200123
H	-4.3658539	-0.0262937	1.8335356
C	-5.1855874	1.2881660	-3.4482047
H	-4.5909603	1.3670363	-4.3732276
H	-5.7103282	2.2485893	-3.3345119
C	-6.2142227	0.1507070	-3.6363673
H	-6.8350449	0.3873419	-4.5164685
H	-5.6748507	-0.7782674	-3.8878900
C	-7.1083962	-0.1212282	-2.4173433
H	-7.7822981	-0.9588147	-2.6624602
H	-6.4784944	-0.4731329	-1.5830800
C	-7.9366306	1.0773524	-1.9241708
H	-7.2601469	1.8411078	-1.5064443
H	-8.5651370	0.7390022	-1.0811923
C	-8.8375478	1.7397107	-2.9781201
H	-9.3649401	2.5831503	-2.5011403
H	-8.2159087	2.1866864	-3.7731945
C	-9.8651944	0.7939511	-3.6072330
H	-10.4870104	0.3136930	-2.8322123
H	-10.5383557	1.3362743	-4.2902844
H	-9.3805374	-0.0075625	-4.1877794
C	-3.8825683	0.2447666	6.4726682
H	-4.7685401	-0.4087228	6.5354306
H	-3.1406085	-0.1579422	7.1811478
C	-4.2812090	1.6645282	6.9162979
H	-4.9788499	2.0785646	6.1700978
H	-3.3875458	2.3118638	6.8911586
C	-4.9104749	1.7091346	8.3104065

H	-5.8485510	1.1276480	8.3025395
H	-4.2427119	1.1944097	9.0231340
C	-5.1768721	3.1308696	8.8309678
H	-5.6375430	3.0589686	9.8322996
H	-4.2091133	3.6442183	8.9710723
C	-6.0709741	4.0069877	7.9369504
H	-5.5567345	4.2129520	6.9824508
H	-6.1944949	4.9874605	8.4272844
C	-7.4512369	3.4076936	7.6517680
H	-7.3797720	2.4815042	7.0590814
H	-7.9775910	3.1618379	8.5900314
H	-8.0815362	4.1131690	7.0870781
H	15.3088199	-5.0567751	-2.2892501
H	3.7865419	7.0974573	0.5859795
H	4.6902163	6.0465549	-3.4870461
O	3.2862854	4.5851662	1.3755077
O	4.2207415	3.3826340	-3.1101395
O	0.8794294	-7.9375053	3.4680139
O	0.4280529	-7.9416501	-1.4081314
C	2.2028728	5.3338291	2.0474437
H	1.5042001	5.6925600	1.2763319
H	2.6290827	6.2063266	2.5643279
C	1.5052869	4.3908062	3.0103588
H	1.3970953	3.4128657	2.5172307
H	2.1273169	4.2369516	3.9070637
C	0.1173615	4.9136885	3.3983906
H	-0.4990137	4.9657538	2.4848039
H	0.1930002	5.9477991	3.7797715
C	-0.5825126	4.0408450	4.4450711
H	-0.5163385	2.9828347	4.1407159
H	-0.0348615	4.1234543	5.3994014
C	-2.0604181	4.4004651	4.6628767
H	-2.4087066	3.9439078	5.6045471
H	-2.1562864	5.4941253	4.7962649
C	-2.9850957	3.9330945	3.5320628
H	-2.6427270	4.3435444	2.5651934
H	-2.9107847	2.8369533	3.4460026
C	-4.4512544	4.3223879	3.7437757
H	-4.5356759	5.4227824	3.7915742
H	-4.7833223	3.9454619	4.7265594
C	-5.3768615	3.7786323	2.6525625
H	-6.4247778	4.0734697	2.8233756
H	-5.0804843	4.1552199	1.6586784
H	-5.3344178	2.6779782	2.6175863
C	4.7889495	3.6243936	-4.4376662
H	5.7957111	4.0591737	-4.3290934
H	4.1536106	4.3382448	-4.9861743
C	4.8333987	2.2789939	-5.1320082
H	5.4461409	1.5906718	-4.5282714
H	3.8136552	1.8620692	-5.1526722
C	5.3890467	2.3708859	-6.5559052
H	6.4156799	2.7770358	-6.5277331
H	4.7878977	3.0890120	-7.1416493
C	5.3977711	1.0180562	-7.2740154
H	5.9973176	0.2982677	-6.6882038
H	4.3697075	0.6142876	-7.2978883
C	5.9448455	1.0903960	-8.7017820
H	6.9790458	1.4789334	-8.6779614
H	5.3546202	1.8232658	-9.2814251
C	5.9263678	-0.2586075	-9.4264659
H	6.5150750	-0.9926439	-8.8462392

H	4.8911312	-0.6454826	-9.4490696
C	6.4707253	-0.1925286	-10.8568399
H	7.5064607	0.1901891	-10.8321420
H	5.8847379	0.5456864	-11.4327755
C	6.4392071	-1.5450237	-11.5734364
H	6.8352065	-1.4696195	-12.5988022
H	7.0437447	-2.2929753	-11.0328535
H	5.4089930	-1.9342178	-11.6378132
C	-0.2241187	-8.8815558	3.7357970
H	-0.9461011	-8.8553966	2.9054330
H	0.2122181	-9.8882853	3.7915458
C	-0.8978763	-8.4859501	5.0396476
H	-1.4624070	-9.3657364	5.3912438
H	-0.1179978	-8.2901964	5.7935905
C	-1.8579049	-7.2903269	4.9365529
H	-2.6061592	-7.5111142	4.1553870
H	-2.4196699	-7.2133176	5.8841491
C	-1.1923433	-5.9362803	4.6557543
H	-0.4264856	-5.7554496	5.4292054
H	-0.6501373	-5.9723647	3.6991514
C	-2.1678595	-4.7519332	4.6185457
H	-1.5856144	-3.8140874	4.6025545
H	-2.7643109	-4.7285140	5.5492657
C	-3.1092571	-4.7502879	3.4084179
H	-3.7583422	-5.6427438	3.4228418
H	-2.5059638	-4.8324168	2.4866194
C	-3.9800777	-3.4934688	3.3248949
H	-4.6699558	-3.4681115	4.1867357
H	-3.3448190	-2.5995219	3.4310874
C	-4.7756091	-3.3997442	2.0214353
H	-5.4371297	-4.2729679	1.8923709
H	-5.4000606	-2.4930207	1.9948308
H	-4.1014301	-3.3644247	1.1476545
C	-0.8011466	-8.7606904	-1.5192670
H	-0.4895303	-9.6419862	-2.0927210
H	-1.1327938	-9.0921714	-0.5252322
C	-1.9084353	-8.0047605	-2.2495193
H	-2.5333211	-8.7680582	-2.7437552
H	-1.4474527	-7.4190267	-3.0564462
C	-2.8430138	-7.1435900	-1.3770930
H	-3.2723465	-7.8096226	-0.6073022
H	-3.6945943	-6.8212147	-2.0021776
C	-2.2598434	-5.9045793	-0.6716135
H	-2.9145700	-5.6698785	0.1850143
H	-1.2794552	-6.1440552	-0.2350517
C	-2.1373356	-4.6237545	-1.5108637
H	-3.1441030	-4.3046081	-1.8363550
H	-1.7723129	-3.8298582	-0.8403610
C	-1.2215864	-4.7018848	-2.7429142
H	-1.7354001	-5.2562934	-3.5448751
H	-0.3187690	-5.2868651	-2.4982035
C	-0.7990401	-3.3205069	-3.2736300
H	-0.4183121	-3.4262277	-4.3031455
H	-1.6931171	-2.6731007	-3.3430050
C	0.2700607	-2.6346691	-2.4144855
H	-0.0536192	-2.5190637	-1.3708714
H	1.2018428	-3.2244769	-2.3986098
H	0.5133312	-1.6296593	-2.7952411

Table S16. YD2-o-C8-TiO2 (gas)

283

Ti	7.8633873	5.3962328	14.2455912
Ti	4.3243160	5.1736169	12.9235277
Ti	0.7852420	4.9511007	11.6014545
Ti	-2.7538292	4.7284849	10.2793910
O	7.1643069	5.5481433	16.0914217
O	3.6252329	5.3256270	14.7693486
O	0.0861616	5.1030112	13.4472851
O	-3.4529097	4.8803953	12.1252216
O	6.2348027	5.2542866	13.2125411
O	2.6956352	5.0317644	11.8904331
O	-0.8434360	4.8091485	10.5683695
O	-4.3825100	4.5866322	9.2462964
Ti	3.4678854	9.5992708	19.8878329
Ti	-0.0712793	9.3766491	18.5657345
Ti	-3.6103533	9.1541327	17.2436614
Ti	-7.1494246	8.9315169	15.9215979
Ti	4.3608365	7.5333266	17.8451721
Ti	0.8216690	7.3108042	16.5230640
Ti	-2.7174023	7.0881884	15.2010004
Ti	-6.2564763	6.8656721	13.8789273
Ti	3.4312361	7.2395634	14.9662469
Ti	6.9703101	7.4620797	16.2883200
Ti	-0.1078351	7.0169475	13.6441834
Ti	-3.6469091	6.7944313	12.3221102
O	4.1669305	9.4473684	18.0420956
O	0.6277658	9.2247466	16.7199972
O	-2.9113055	9.0021308	15.3979337
O	-6.4503795	8.7796144	14.0758605
O	5.0964374	9.7411256	20.9209858
O	1.5573634	9.5186092	19.5989127
O	-1.9817079	9.2959935	18.2768493
O	-5.5207818	9.0734772	16.9547760
O	-9.0598532	8.8508613	15.6327126
O	5.0599169	7.3814160	15.9993415
O	1.5207494	7.1588938	14.6772334
O	-2.0183218	6.9362780	13.3551699
O	-5.5573958	6.7137616	12.0330968
O	3.6617887	7.6853284	19.6908998
O	0.1226239	7.4627067	18.3688013
O	-3.4164474	7.2400909	17.0467378
O	-6.9555213	7.0175745	15.7246647
O	2.7321910	7.3914658	16.8119842
O	6.2712650	7.6139822	18.1340573
O	-0.8068802	7.1688500	15.4899208
O	-4.3459542	6.9463336	14.1678475
O	7.6693552	7.3101773	14.4425826
O	4.1302812	7.0876610	13.1205095
O	0.5912100	6.8650452	11.7984460
O	-2.9478613	6.6424293	10.4763826
H	6.0448741	9.7811708	21.0644400
H	-9.8683759	8.7804511	15.1198276
O	9.7737806	5.4768965	14.5345697
H	10.5821745	5.5473087	15.0475130
H	-5.3308886	4.5466011	9.1029704
O	0.5972212	9.0315095	13.4510772
O	2.7623905	9.2201275	14.2478261
C	1.6556330	9.6635185	13.7944453
C	1.5663439	11.1535965	13.6129573
C	0.4094954	11.7141819	13.0553262

C	2.6270911	11.9921001	13.9781109
C	0.3200698	13.0792082	12.8422086
H	-0.4143822	11.0433361	12.7867020
C	2.5466814	13.3624445	13.7716054
H	3.5193604	11.5368506	14.4243983
C	1.3940362	13.9311754	13.1858679
H	-0.5825675	13.5114976	12.3923488
H	3.3826529	14.0165962	14.0494085
C	1.2949321	15.3095232	12.9096535
C	1.1461787	16.4898070	12.6038620
C	0.9320420	17.8184087	12.1928338
C	1.9449876	18.7739525	12.4609753
C	-0.2917496	18.0972662	11.5290255
C	-2.3414825	17.7828544	10.6531688
C	3.0772908	20.6594448	12.5668950
C	3.8637165	19.6567208	13.2373487
C	3.1618269	18.4884174	13.1683074
N	1.9100586	20.0946772	12.1009266
C	-1.9086294	19.1421659	10.4613054
N	-0.6557034	19.3101763	11.0090481
C	-2.6480931	20.1286661	9.7898537
C	3.4623263	21.9999505	12.3996540
C	-2.2155837	21.4392116	9.5330092
C	2.7301638	22.9825764	11.7132095
H	-3.2969885	17.3756148	10.3144907
H	3.4345254	17.5066187	13.5622301
H	4.8375901	19.8302207	13.7012374
C	-1.3354292	17.1343491	11.3080077
H	-1.2949904	16.0889328	11.6207939
N	-1.0112276	21.9764137	9.9263426
N	1.5125359	22.7907909	11.1022004
C	1.1655547	23.9886709	10.5307728
C	-0.0025332	24.2216167	9.7867596
C	2.1848824	24.9707378	10.7911184
C	3.1502910	24.3491094	11.5304344
Zn	0.4408553	21.0403751	11.0323785
C	-2.9887033	22.4401668	8.8433756
C	-1.0148545	23.2857388	9.5176872
C	-2.2437087	23.5830827	8.8295074
H	-3.9852942	22.2815382	8.4246623
H	-2.5041096	24.5507008	8.3951047
H	4.0757068	24.7771975	11.9227793
C	4.7622978	22.4153449	13.0018898
C	4.8328749	22.6913417	14.3693349
C	5.9010860	22.5389120	12.2040661
C	6.0441674	23.1024549	14.9333594
H	3.9481693	22.6065768	15.0102732
C	7.1156109	22.9305760	12.7782753
H	5.8669561	22.3215460	11.1306958
C	7.1974048	23.2232016	14.1464500
H	8.1450392	23.5247075	14.5999289
C	-4.0237563	19.7630812	9.3411303
C	-4.2679278	19.3904914	8.0181315
C	-5.0710193	19.8059996	10.2641146
C	-5.5667814	19.0527841	7.6222565
H	-3.4576285	19.3442355	7.2817133
C	-6.3690274	19.4833148	9.8585068
H	-4.8976973	20.1010641	11.3051923
C	-6.6283106	19.0991386	8.5365610
H	-7.6417869	18.8379984	8.2242720
H	2.1565436	26.0099003	10.4557210

O	8.1718450	22.9977551	11.9214847
O	6.0075563	23.3659991	16.2684303
O	-5.7101218	18.6918576	6.3169220
O	-7.3244551	19.5753110	10.8247460
C	9.4647734	23.3000255	12.4373701
H	9.7136215	22.6037093	13.2669597
H	9.4786711	24.3324083	12.8468825
C	10.4547575	23.1497294	11.3035365
H	11.4421726	23.5014566	11.6618959
H	10.1590300	23.8377556	10.4872958
C	10.5593913	21.7265123	10.7738032
H	10.8942075	21.0559998	11.5923396
H	9.5466823	21.3755231	10.4972268
C	11.4929575	21.5786548	9.5821410
H	12.5039478	21.9514447	9.8498579
H	11.1441581	22.2387747	8.7610110
C	11.6002773	20.1496176	9.0696042
H	11.9733829	19.4952092	9.8845342
H	10.5847594	19.7706393	8.8332253
C	12.4930452	19.9918054	7.8475202
H	12.1092133	20.6349359	7.0279920
H	13.5066474	20.3830207	8.0768518
C	12.6076440	18.5571606	7.3502687
H	13.0017460	17.9203785	8.1680570
H	11.5923813	18.1654156	7.1380324
C	13.4826223	18.4072666	6.1164071
H	13.5466691	17.3558070	5.7831696
H	13.0885195	19.0002464	5.2693237
H	14.5143696	18.7587393	6.3077202
C	7.0417414	24.1524611	16.8579334
H	7.9350323	23.5185711	17.0421725
H	7.3433085	24.9658922	16.1640238
C	6.5087408	24.7288906	18.1546674
H	6.0479332	23.9012103	18.7285513
H	7.3768408	25.0699961	18.7506488
C	5.5209244	25.8847283	18.0002146
H	6.0342631	26.7307533	17.4963980
H	5.2655462	26.2602601	19.0120611
C	4.2353380	25.5655742	17.2471014
H	4.4806122	25.2499824	16.2178919
H	3.7473646	24.6829621	17.7096409
C	3.2506122	26.7250414	17.2025194
H	3.7444040	27.6071263	16.7422948
H	3.0023691	27.0324537	18.2389331
C	1.9595918	26.4242025	16.4459408
H	1.4589050	25.5498174	16.9123504
H	1.2581112	27.2718195	16.5826931
C	2.1226454	26.1651693	14.9513351
H	2.6633188	27.0197437	14.4933568
H	2.7720476	25.2832432	14.7836453
C	0.8010109	25.9564214	14.2330901
H	0.9445244	25.7781090	13.1534902
H	0.2535196	25.0852059	14.6411593
H	0.1402806	26.8377919	14.3351426
C	-6.9787000	18.2173581	5.8735497
H	-7.2996003	17.3602230	6.5048745
H	-7.7424624	19.0172167	5.9775411
C	-6.8392305	17.7955529	4.4284086
H	-7.8457519	17.5068598	4.0658280
H	-6.5420131	18.6804623	3.8370630
C	-5.8615081	16.6428755	4.2242327

H	-4.8530024	16.9615689	4.5516683
H	-6.1507011	15.8305736	4.9213448
C	-5.7888798	16.0591392	2.8120909
H	-5.3699569	15.0383883	2.8938976
H	-6.8186219	15.9209675	2.4193237
C	-4.9512618	16.8106625	1.7769069
H	-4.8441542	16.1474957	0.8962070
H	-3.9221428	16.9431024	2.1703760
C	-5.4824552	18.1632072	1.3118588
H	-6.5548368	18.0621247	1.0403147
H	-5.4538936	18.8823714	2.1517897
C	-4.7224875	18.7717004	0.1335101
H	-5.0636757	19.8161377	-0.0046057
H	-3.6471581	18.8450692	0.3956018
C	-4.8777144	18.0229417	-1.1825150
H	-4.3439826	18.5338875	-2.0043857
H	-4.4778965	16.9938093	-1.1282482
H	-5.9424824	17.9454857	-1.4759510
C	-8.6880177	19.3904928	10.4650795
H	-8.9589818	20.0744760	9.6317349
H	-8.8585085	18.3512908	10.1083356
C	-9.5234520	19.6867744	11.6894153
H	-9.2334822	18.9866252	12.4962992
H	-9.2543660	20.6977955	12.0516916
C	-11.0207388	19.6077651	11.4325837
H	-11.2892429	18.5935813	11.0715750
H	-11.2919502	20.2979837	10.6067608
C	-11.8558029	19.9455325	12.6592962
H	-11.6052239	19.2405715	13.4782385
H	-11.5593526	20.9469441	13.0338991
C	-13.3576987	19.9269079	12.4157436
H	-13.6038332	20.6276929	11.5908781
H	-13.6616708	18.9241647	12.0503582
C	-14.1794745	20.2886867	13.6440132
H	-13.9440297	19.5795017	14.4647431
H	-13.8587254	21.2838734	14.0168749
C	-15.6832295	20.3034981	13.4067339
H	-15.9137535	21.0109642	12.5842262
H	-16.0039104	19.3085062	13.0370391
C	-16.4871781	20.6748058	14.6418014
H	-17.5735542	20.6846015	14.4403594
H	-16.3088054	19.9608028	15.4679558
H	-16.2096820	21.6788350	15.0150718
N	-0.1955262	25.5443602	9.2762229
C	0.0034421	25.7592855	7.8967555
C	-0.8129212	26.6354958	7.1597947
C	1.0035627	25.0510466	7.2127353
C	-0.6086930	26.8090703	5.7965357
H	-1.6232827	27.1744500	7.6650848
C	1.1827741	25.2260774	5.8446799
H	1.6430767	24.3542028	7.7669378
C	0.3921747	26.1128345	5.1039977
H	-1.2668752	27.4956835	5.2442015
H	1.9732998	24.6564761	5.3360801
C	-0.6609164	26.5459822	10.1487421
C	-0.3446587	27.9008834	9.9479131
C	-1.4307783	26.2060832	11.2741033
C	-0.8240645	28.8739916	10.8180705
H	0.2845663	28.1902480	9.0979420
C	-1.8843192	27.1912470	12.1427383
H	-1.6698544	25.1544261	11.4678941

C	-1.6069956	28.5471695	11.9326365
H	-0.5675502	29.9268598	10.6312675
H	-2.4813287	26.8900326	13.0153087
C	0.6288722	26.3521885	3.6384068
H	1.1294710	25.4688508	3.1973791
H	-0.3444447	26.4459400	3.1208253
C	1.4653440	27.6032030	3.3383562
H	1.4856450	27.7636381	2.2413299
H	0.9518456	28.4903018	3.7629686
C	2.8913989	27.5477527	3.8650517
H	2.8737909	27.3890246	4.9623175
H	3.3938950	26.6530949	3.4438956
C	3.7014491	28.7992022	3.5513442
H	3.1533108	29.6823503	3.9372258
H	3.7501368	28.9395141	2.4506595
C	5.1173559	28.8098763	4.1225901
H	5.0613399	28.6987535	5.2244394
H	5.5628769	29.8088886	3.9476426
C	6.0429264	27.7451339	3.5520674
H	5.6910663	26.7223139	3.7803644
H	6.1193795	27.8274921	2.4506455
H	7.0649572	27.8347365	3.9626448
C	-2.1840835	29.6034722	12.8319180
H	-1.5849915	30.5309145	12.7536045
H	-2.1078119	29.2774040	13.8883393
C	-3.6474668	29.9178527	12.5140136
H	-3.7250639	30.2383679	11.4553851
H	-4.2363304	28.9808215	12.5785892
C	-4.2698515	30.9718938	13.4169132
H	-3.6948021	31.9174203	13.3351238
H	-4.1671715	30.6567073	14.4762059
C	-5.7360707	31.2410526	13.1106796
H	-5.8381384	31.5506611	12.0494255
H	-6.3045282	30.2914710	13.1927811
C	-6.3811017	32.2907597	14.0048428
H	-5.8194266	33.2424762	13.9135315
H	-6.2685650	31.9840589	15.0646943
C	-7.8498623	32.5289359	13.6939570
H	-8.2946378	33.2934900	14.3563333
H	-7.9903266	32.8704200	12.6508812
H	-8.4405945	31.6012929	13.8130952

Table S17. YD2-o-C8-TiO2 (solv)

283

Ti	7.8633895	5.3962343	14.2455952
Ti	4.3243172	5.1736184	12.9235313
Ti	0.7852422	4.9511021	11.6014578
Ti	-2.7538300	4.7284862	10.2793939
O	7.1643089	5.5481449	16.0914262
O	3.6252339	5.3256285	14.7693527
O	0.0861616	5.1030126	13.4472889
O	-3.4529107	4.8803967	12.1252250
O	6.2348045	5.2542881	13.2125448
O	2.6956360	5.0317658	11.8904364
O	-0.8434362	4.8091499	10.5683725
O	-4.3825112	4.5866335	9.2462990
Ti	3.4678864	9.5992735	19.8878385
Ti	-0.0712793	9.3766517	18.5657397
Ti	-3.6103543	9.1541353	17.2436662

Ti	-7.1494266	8.9315194	15.9216024
Ti	4.3608377	7.5333287	17.8451771
Ti	0.8216692	7.3108063	16.5230686
Ti	-2.7174031	7.0881904	15.2010047
Ti	-6.2564781	6.8656740	13.8789312
Ti	3.4312371	7.2395654	14.9662511
Ti	6.9703121	7.4620818	16.2883246
Ti	-0.1078351	7.0169495	13.6441872
Ti	-3.6469101	6.7944332	12.3221137
O	4.1669317	9.4473711	18.0421007
O	0.6277660	9.2247492	16.7200019
O	-2.9113063	9.0021333	15.3979380
O	-6.4503813	8.7796169	14.0758645
O	5.0964388	9.7411283	20.9209917
O	1.5573638	9.5186119	19.5989182
O	-1.9817085	9.2959961	18.2768544
O	-5.5207834	9.0734797	16.9547808
O	-9.0598557	8.8508638	15.6327170
O	5.0599183	7.3814181	15.9993460
O	1.5207498	7.1588958	14.6772375
O	-2.0183224	6.9362799	13.3551737
O	-5.5573974	6.7137635	12.0331002
O	3.6617897	7.6853306	19.6909053
O	0.1226239	7.4627088	18.3688065
O	-3.4164484	7.2400929	17.0467426
O	-6.9555233	7.0175765	15.7246691
O	2.7321918	7.3914679	16.8119889
O	6.2712668	7.6139843	18.1340624
O	-0.8068804	7.1688520	15.4899251
O	-4.3459554	6.9463356	14.1678515
O	7.6693574	7.3101794	14.4425867
O	4.1302824	7.0876630	13.1205132
O	0.5912102	6.8650471	11.7984493
O	-2.9478621	6.6424312	10.4763855
H	6.0448758	9.7811735	21.0644459
H	-9.8683787	8.7804536	15.1198318
O	9.7737833	5.4768980	14.5345738
H	10.5821775	5.5473103	15.0475172
H	-5.3308901	4.5466024	9.1029730
O	0.6100006	9.0362886	13.4472635
O	2.7730361	9.2062495	14.2469376
C	1.6555494	9.6711354	13.8318870
C	1.5523011	11.1622679	13.7446448
C	0.3561737	11.7550284	13.3144662
C	2.6442705	11.9807269	14.0651856
C	0.2601258	13.1298171	13.1729054
H	-0.4989009	11.1085383	13.0849544
C	2.5603736	13.3593913	13.9260481
H	3.5703032	11.5105186	14.4175620
C	1.3696363	13.9588898	13.4575763
H	-0.6751800	13.5848755	12.8234421
H	3.4245703	13.9930843	14.1614577
C	1.2762154	15.3471000	13.2312579
C	1.1504224	16.5369280	12.9558690
C	0.9733502	17.8813994	12.5756445
C	2.0297216	18.7903221	12.8379113
C	-0.2506370	18.2110426	11.9347515
C	-2.3079606	17.9669072	11.0513129
C	3.2472036	20.6223033	12.9166722
C	3.9968126	19.5915835	13.5864607
C	3.2442175	18.4534618	13.5316011

N	2.0464848	20.1084240	12.4727825
C	-1.8534186	19.3264082	10.9127203
N	-0.5925382	19.4488065	11.4606471
C	-2.5821642	20.3555259	10.2961970
C	3.6888916	21.9375752	12.7264450
C	-2.1347918	21.6774114	10.1138457
C	2.9834895	22.9491287	12.0489269
H	-3.2699467	17.5857462	10.7003712
H	3.4842079	17.4639936	13.9292216
H	4.9835800	19.7257598	14.0374304
C	-1.3148239	17.2768787	11.6845452
H	-1.2997557	16.2194739	11.9589750
N	-0.8915097	22.1586237	10.4537342
N	1.7201669	22.8329131	11.5189072
C	1.4133157	24.0506309	10.9631189
C	0.1902925	24.3758903	10.3465556
C	2.5200661	24.9554105	11.1256121
C	3.4870764	24.2772783	11.8090521
Zn	0.5836013	21.1283631	11.4510097
C	-2.9357202	22.7464281	9.5745055
C	-0.8912376	23.4959880	10.1450806
C	-2.1673508	23.8750756	9.6003893
H	-3.9688209	22.6483695	9.2322267
H	-2.4456964	24.8809036	9.2780338
H	4.4655341	24.6456265	12.1254585
C	4.9918058	22.3489201	13.3275467
C	4.9835443	22.8810072	14.6196854
C	6.1717773	22.3270660	12.5842370
C	6.1471474	23.4496073	15.1434433
H	4.0602577	22.9146855	15.2086901
C	7.3470861	22.8653665	13.1297920
H	6.1937581	21.9242352	11.5648171
C	7.3397174	23.4443521	14.4067600
H	8.2478966	23.8758468	14.8365590
C	-3.9410747	20.0236438	9.7797011
C	-4.1383188	19.8930506	8.4028527
C	-5.0093603	19.8498987	10.6634477
C	-5.4105156	19.5803575	7.9099279
H	-3.3094743	20.0210185	7.6968072
C	-6.2830021	19.5522839	10.1623438
H	-4.8735531	19.9549660	11.7462004
C	-6.4936591	19.4116187	8.7833534
H	-7.4863420	19.1764144	8.3934206
H	2.5512236	25.9893470	10.7766245
O	8.4471300	22.7967442	12.3343212
O	6.0329105	24.0062313	16.3808928
O	-5.5004963	19.4613839	6.5597231
O	-7.2655416	19.4214431	11.0941523
C	9.6737414	23.3702384	12.8045120
H	9.9714181	22.8851322	13.7574502
H	9.5262165	24.4511245	13.0031019
C	10.7245982	23.1541543	11.7413724
H	11.6314301	23.7074158	12.0547724
H	10.3806914	23.6312138	10.8024013
C	11.0647779	21.6920632	11.4910110
H	11.4185031	21.2335953	12.4377165
H	10.1394825	21.1468053	11.2196430
C	12.1135454	21.4903789	10.4077083
H	13.0298466	22.0591252	10.6722498
H	11.7510930	21.9385584	9.4594579
C	12.4782675	20.0322895	10.1693200

H	12.8422513	19.5863722	11.1182112
H	11.5614999	19.4635187	9.9079844
C	13.5249014	19.8280941	9.0837026
H	13.1576365	20.2685840	8.1331878
H	14.4386928	20.4040849	9.3422668
C	13.8998227	18.3709065	8.8503074
H	14.2674761	17.9344100	9.8012080
H	12.9851749	17.7972489	8.5957095
C	14.9435563	18.1797129	7.7616072
H	15.1961666	17.1137243	7.6161528
H	14.5875376	18.5733274	6.7905257
H	15.8819197	18.7136598	8.0060181
C	6.8485059	25.1472946	16.6992452
H	7.8117661	24.8040225	17.1272946
H	7.0708346	25.7126720	15.7713011
C	6.1028353	26.0199913	17.6871909
H	5.8053556	25.3957314	18.5531483
H	6.8363170	26.7513996	18.0773504
C	4.8889240	26.7715358	17.1380383
H	5.2011756	27.3681021	16.2553206
H	4.5734638	27.5146535	17.8978647
C	3.6872649	25.9082507	16.7688850
H	3.9700301	25.2127992	15.9611795
H	3.4314191	25.2615634	17.6343388
C	2.4503019	26.6961822	16.3559163
H	2.6743801	27.2952994	15.4481924
H	2.2082611	27.4338072	17.1474786
C	1.2212125	25.8264464	16.0953785
H	1.0152539	25.2148908	16.9993911
H	0.3341552	26.4800280	15.9721215
C	1.3196620	24.9114803	14.8808330
H	1.4596312	25.5282199	13.9715547
H	2.2296743	24.2854826	14.9492492
C	0.1097922	24.0083041	14.7038459
H	0.1978435	23.3962076	13.7875695
H	-0.0106045	23.3182088	15.5608208
H	-0.8257304	24.5942527	14.6242580
C	-6.7579539	19.1111787	5.9656746
H	-7.1322896	18.1658394	6.4103840
H	-7.5020327	19.9066674	6.1724306
C	-6.5130686	18.9567901	4.4830153
H	-7.4923915	18.8635018	3.9765516
H	-6.0699596	19.8996843	4.1130433
C	-5.6222222	17.7635903	4.1371807
H	-4.8164643	17.6859195	4.8940911
H	-6.2220807	16.8397961	4.2483222
C	-4.9907203	17.8172438	2.7409846
H	-4.9320226	16.7934236	2.3269440
H	-5.6602694	18.3745785	2.0533177
C	-3.5855629	18.4197287	2.6910914
H	-3.2189255	18.3596940	1.6472964
H	-2.9033899	17.7727694	3.2826947
C	-3.4522305	19.8512302	3.1994320
H	-4.1371381	20.5119713	2.6260645
H	-3.7959035	19.8990118	4.2508200
C	-2.0347188	20.4177146	3.1313963
H	-2.0176372	21.3876409	3.6654931
H	-1.3547748	19.7532032	3.7033583
C	-1.4887072	20.6155813	1.7242808
H	-0.4807051	21.0687604	1.7422876
H	-1.4072802	19.6618398	1.1707230

H	-2.1428459	21.2843710	1.1316695
C	-8.5969349	19.1407092	10.6514571
H	-8.9316664	19.9259243	9.9418207
H	-8.6188157	18.1700312	10.1135153
C	-9.4932217	19.1045093	11.8670409
H	-9.1103297	18.3419058	12.5726533
H	-9.4202844	20.0777266	12.3899747
C	-10.9430707	18.8095417	11.5108649
H	-11.0072326	17.8259045	11.0022350
H	-11.2995514	19.5523815	10.7676535
C	-11.8779602	18.8182483	12.7122264
H	-11.5220087	18.0811890	13.4611173
H	-11.8160927	19.8052254	13.2151466
C	-13.3283115	18.5220985	12.3590210
H	-13.6724963	19.2460241	11.5912803
H	-13.3919791	17.5258026	11.8742664
C	-14.2764531	18.5658657	13.5488207
H	-13.9346409	17.8431726	14.3190236
H	-14.2121760	19.5635324	14.0314806
C	-15.7275127	18.2731445	13.1914611
H	-16.0601104	18.9905085	12.4136178
H	-15.7889334	17.2730653	12.7158710
C	-16.6726153	18.3339516	14.3808524
H	-17.7162113	18.1176270	14.0879775
H	-16.3866262	17.6012148	15.1591936
H	-16.6598367	19.3346161	14.8533416
N	0.0229182	25.7213742	9.9124673
C	-0.0905151	25.9928238	8.5341473
C	-0.8905025	27.0472373	8.0609588
C	0.5657099	25.1790607	7.5980381
C	-1.0166763	27.2734879	6.6954853
H	-1.4300254	27.6826391	8.7739292
C	0.4141554	25.4107160	6.2340543
H	1.1967004	24.3523062	7.9478547
C	-0.3749470	26.4609655	5.7481842
H	-1.6568994	28.0994980	6.3527152
H	0.9355974	24.7547664	5.5227758
C	-0.0279149	26.7398203	10.8908924
C	0.5894725	27.9845755	10.6888873
C	-0.6554162	26.4926493	12.1201934
C	0.5910582	28.9370506	11.7027044
H	1.0929759	28.1939829	9.7369670
C	-0.6332774	27.4508294	13.1269100
H	-1.1423880	25.5254440	12.2917033
C	-0.0026492	28.6886993	12.9489715
H	1.0967409	29.8979661	11.5296963
H	-1.1170426	27.2234376	14.0870612
C	-0.5039055	26.7423725	4.2764174
H	-0.2559111	25.8275850	3.7046899
H	-1.5588026	26.9805113	4.0424178
C	0.3775463	27.8964809	3.7826388
H	0.1224800	28.1082771	2.7249971
H	0.1164288	28.8168410	4.3449181
C	1.8728404	27.6400918	3.8978309
H	2.1327342	27.4281473	4.9552931
H	2.1217933	26.7145383	3.3398152
C	2.7231425	28.7996195	3.3948584
H	2.4260311	29.7190470	3.9387978
H	2.4818991	28.9949400	2.3284411
C	4.2305824	28.6040375	3.5408217
H	4.4696761	28.4325689	4.6103972

H	4.7374722	29.5510840	3.2707152
C	4.8099527	27.4729545	2.7030623
H	4.3992512	26.4882413	2.9931439
H	4.5894831	27.6174800	1.6274865
H	5.9082455	27.4118600	2.8110346
C	-0.0027849	29.7206418	14.0399828
H	0.8739719	30.3855455	13.9204829
H	0.1202691	29.2185886	15.0199082
C	-1.2747704	30.5701962	14.0734148
H	-1.3993203	31.0738247	13.0931413
H	-2.1535111	29.9021998	14.1792354
C	-1.2838221	31.6056086	15.1876546
H	-0.3993755	32.2671128	15.0800467
H	-1.1529201	31.0935471	16.1636734
C	-2.5468479	32.4532402	15.2274684
H	-2.6755275	32.9659934	14.2511894
H	-3.4306947	31.7897903	15.3311461
C	-2.5617352	33.4875536	16.3446671
H	-1.6772315	34.1480887	16.2381375
H	-2.4299972	32.9718008	17.3177300
C	-3.8279352	34.3279874	16.3784151
H	-3.8079892	35.0686961	17.1985936
H	-3.9675196	34.8836072	15.4314769
H	-4.7253777	33.6966417	16.5217937