

Unraveling Ultrafast Dynamics of the Photoswitchable Bridged Dithienylethenes Under Structural Constraints

Ismail Hamdi,^{*a} Guy Buntinx,^a Olivier Poizat,^a Stéphanie Delbaere,^a Aurélie Perrier,^{b,c}
Yamashita Rikiya,^d Muraoka Ken-ichi,^d Michinori Takeshita,^d and Stéphane Aloïse^{*a}

Supporting Information

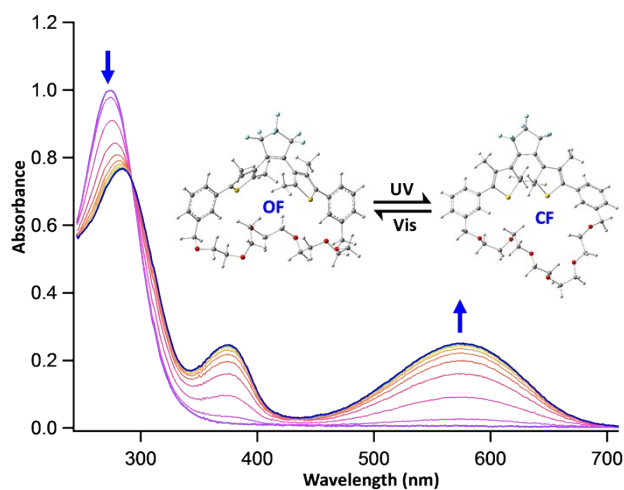


Figure S. 1. Absorption spectral changes of DTE-m₆ in chloroform under UV irradiation @ 340 nm. The blue curve represents the photo-stationary state (PPS).

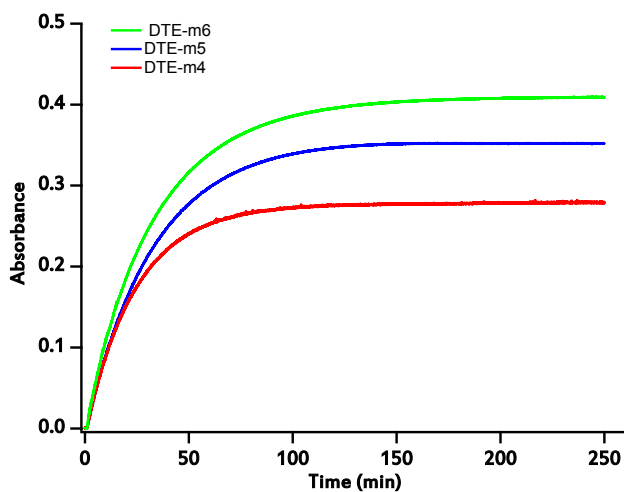


Figure S. 2. Kinetics of appearance of the CF of DTE-m₄, DTE-m₅ and DTE-m₆ recorded @ 580 nm under UV irradiation @ 340 nm in chloroform.

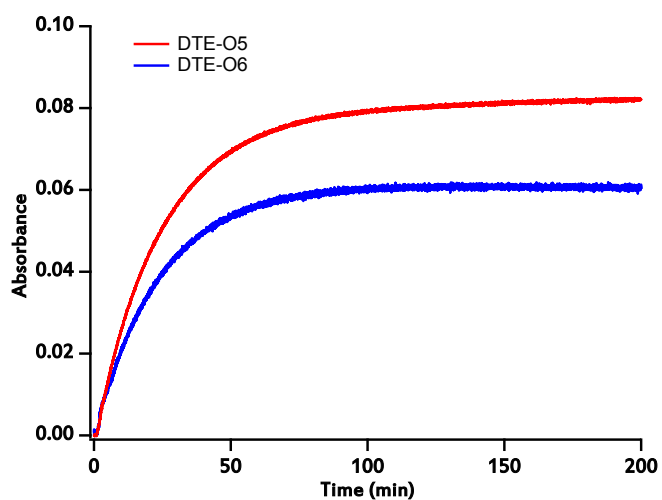


Figure S. 3. Kinetics of appearance of the CF of DTE-O₅ and DTE-O₆ recorded @ 580 nm under UV irradiation @ 340 nm in chloroform.

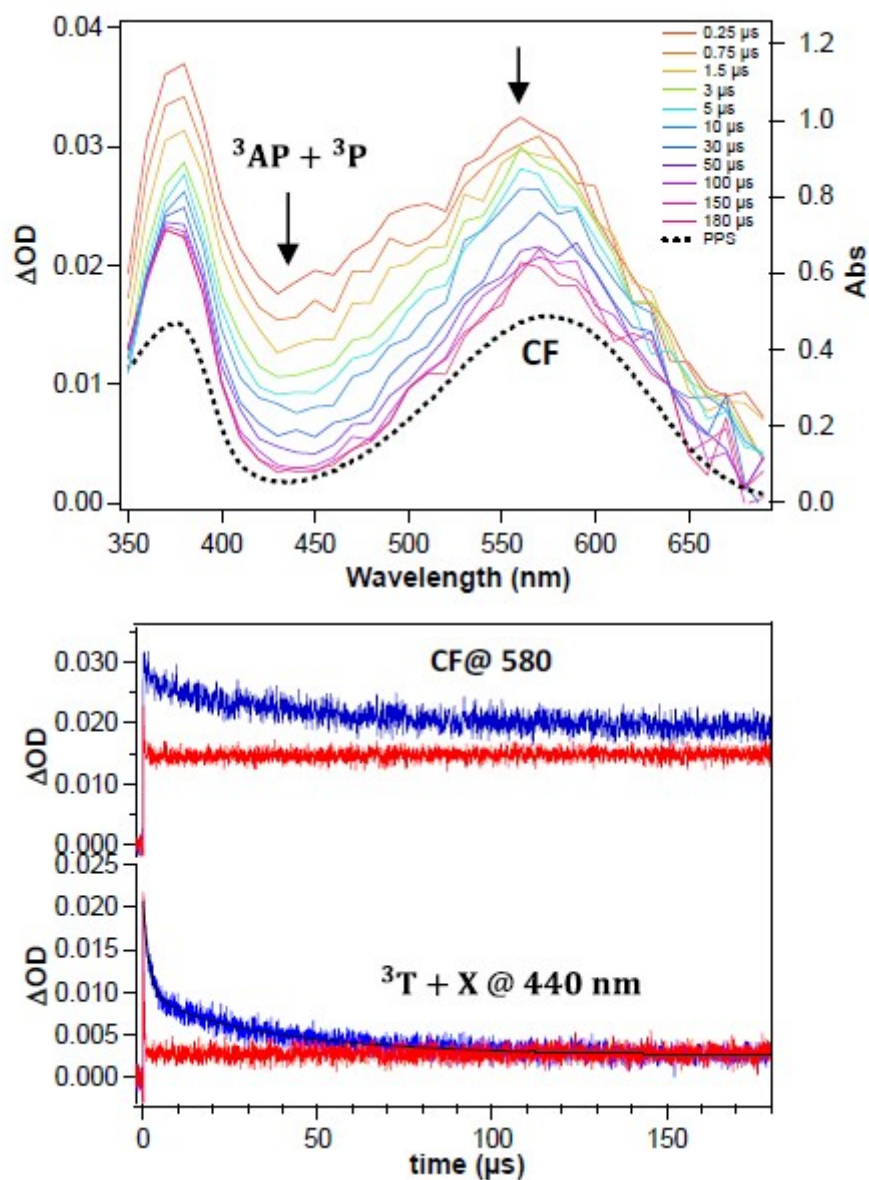


Figure S. 4. (UP) Microsecond time-resolved spectra of DTE- m_6 in chloroform under argon atmosphere after laser excitation @ 355 nm. **(Down)** Kinetics observed for the reaction @ 580 nm and 440 nm under argon atmosphere (bleu curve) and aerated atmosphere (red curve).

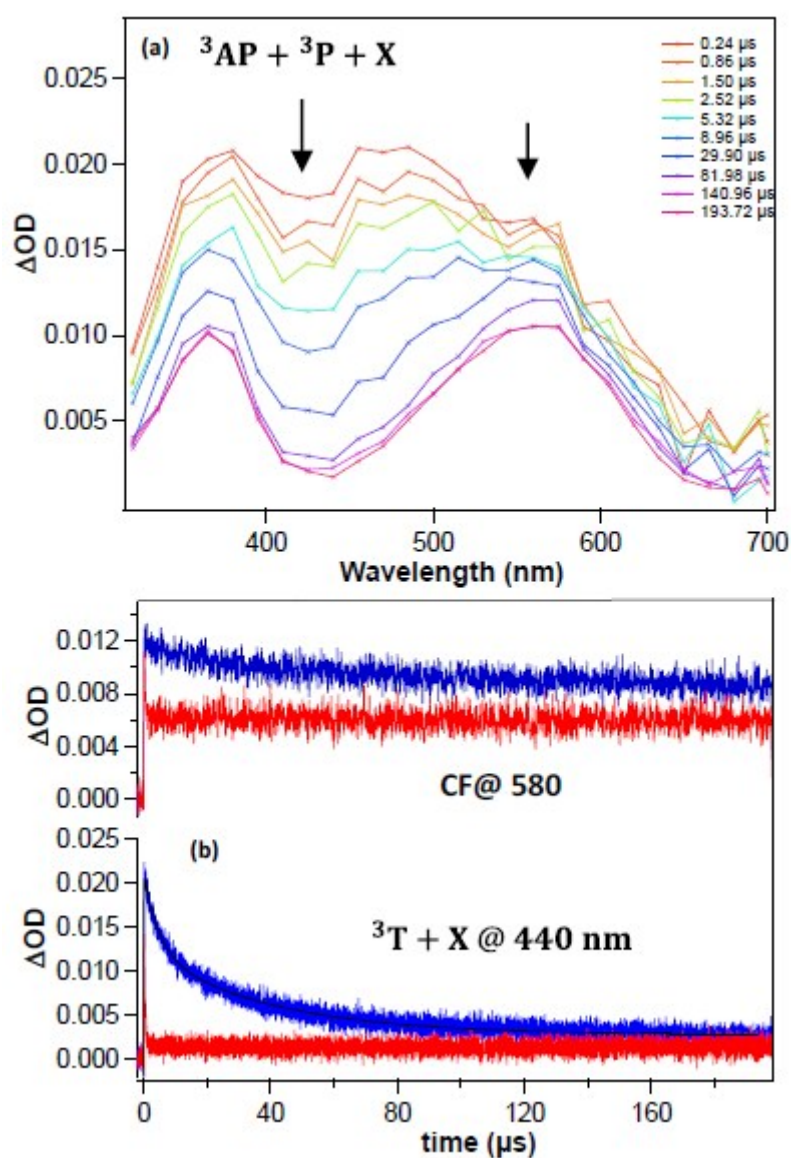


Figure S. 5. (a) Microsecond time-resolved spectra of DTE- O_6 in chloroform under argon atmosphere after laser excitation @ 355 nm. (b) Kinetics observed for the reaction @ 450 nm and 580 nm under argon atmosphere (bleu curve) and aerated atmosphere (red curve).

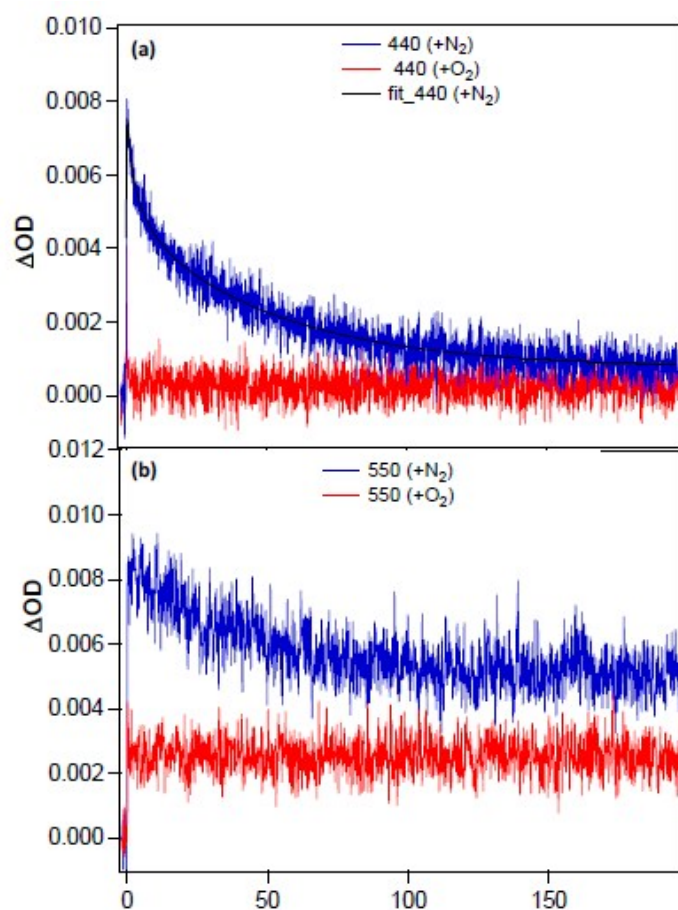


Figure S. 6. Kinetics of DTE- O_5 observed for the reaction @ (a) 440 nm and (b) 550 nm under argon atmosphere (bleu curve) and aerated atmosphere (red curve).

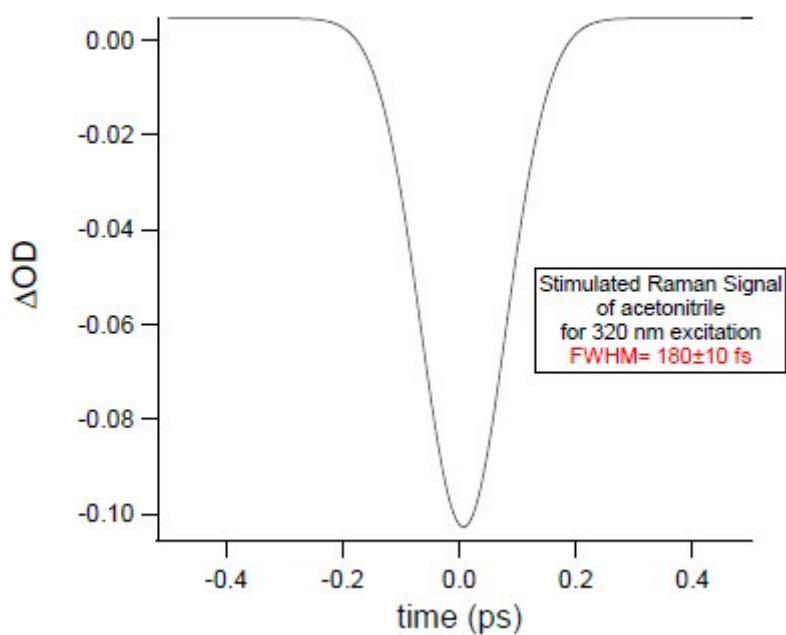


Figure S. 7. Estimation of the temporal resolution of our pump-probe transient absorption setup deduced from the stimulated Raman signal of acetonitrile solvent placed in the same sample cell.

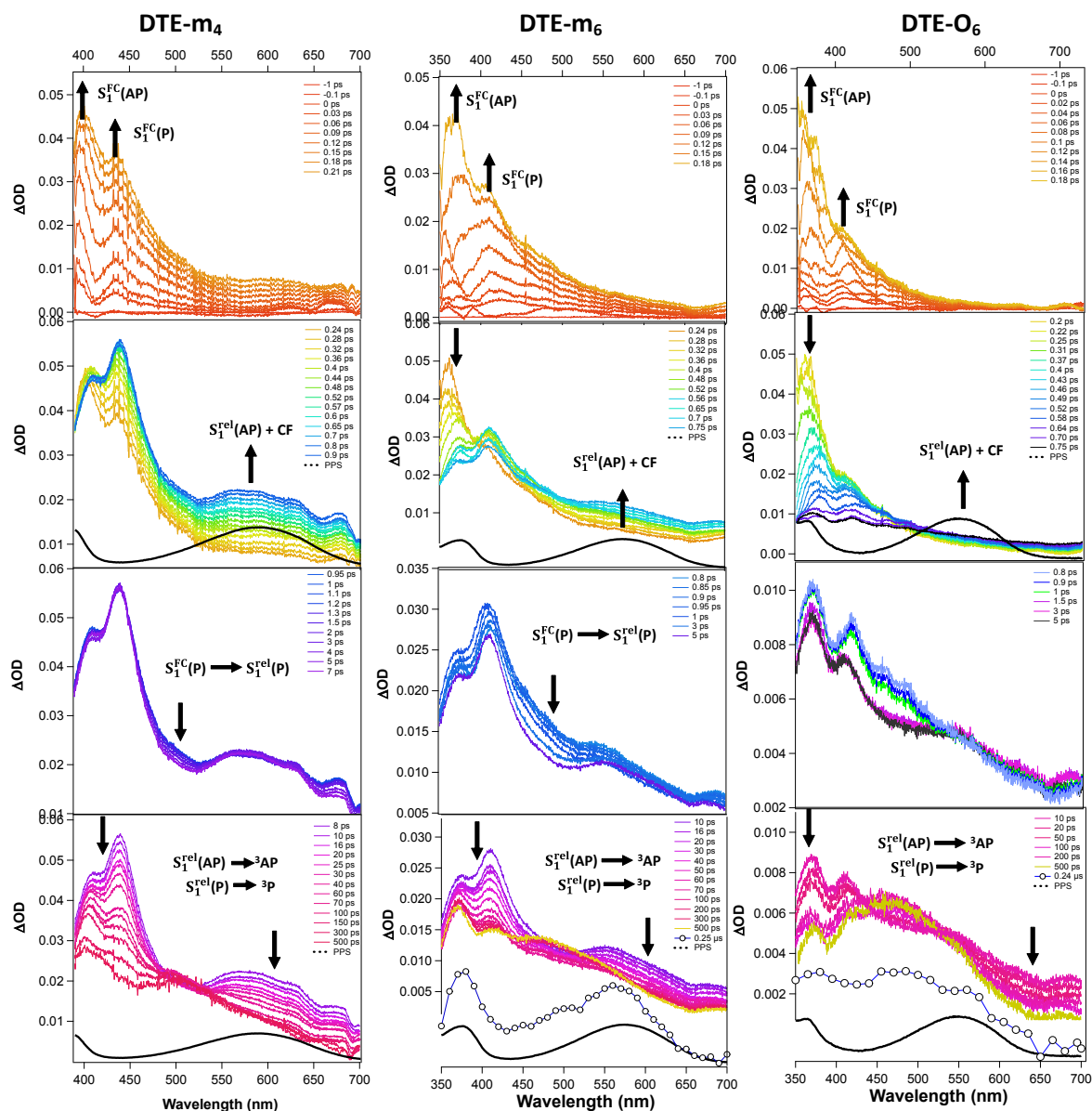


Figure S. 8. Sub-picosecond and picosecond time-resolved absorption spectra of **(left)** DTE-m₄, **(middle)** DTE-m₆ and **(right)** DTE-O₆ in chloroform using 320 nm excitation wavelength. All spectra are corrected from the GVD.

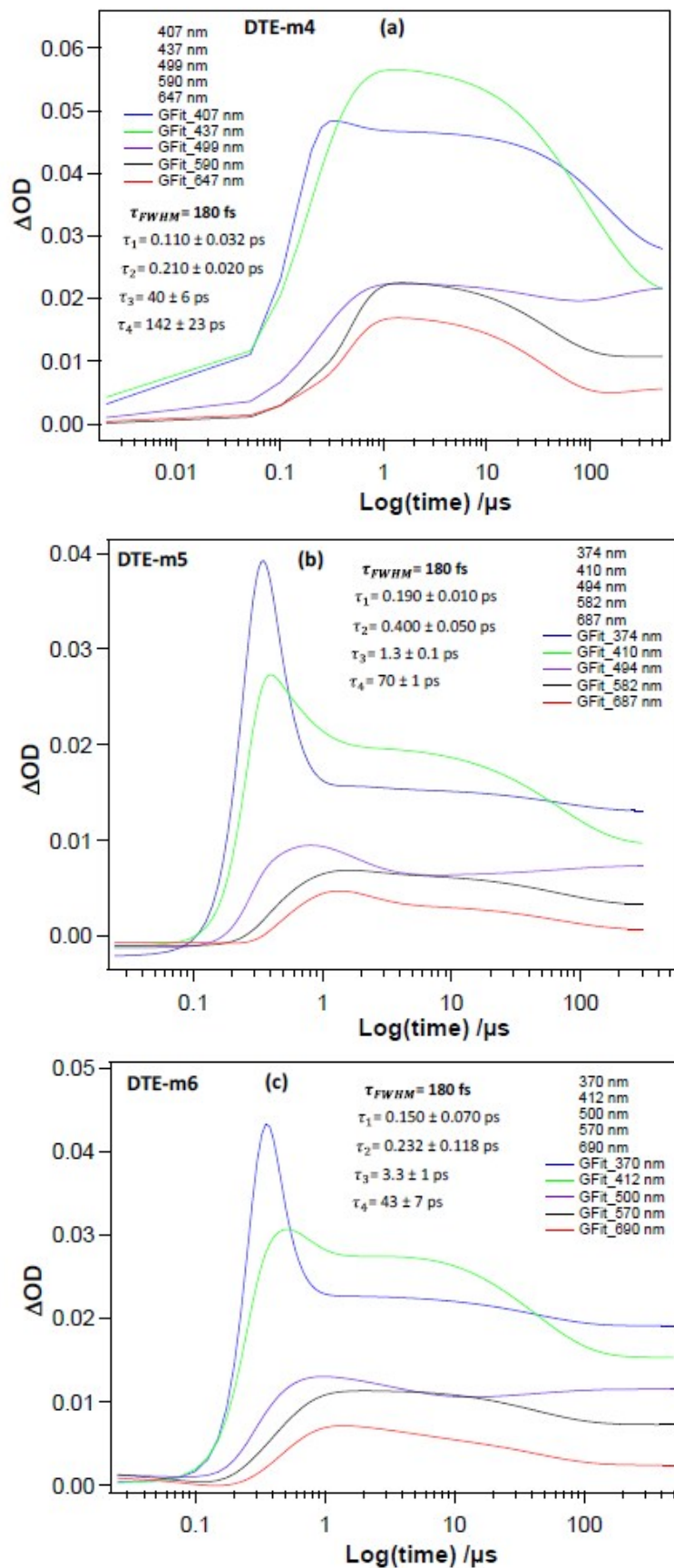


Figure S. 9. Characteristic lifetimes obtained for different species of **(a)** DTE-m₄, **(b)** DTE-m₅ and **(c)** DTE-m₆ by global fitting using four exponential functions convoluted with 180 fs Gaussian function.

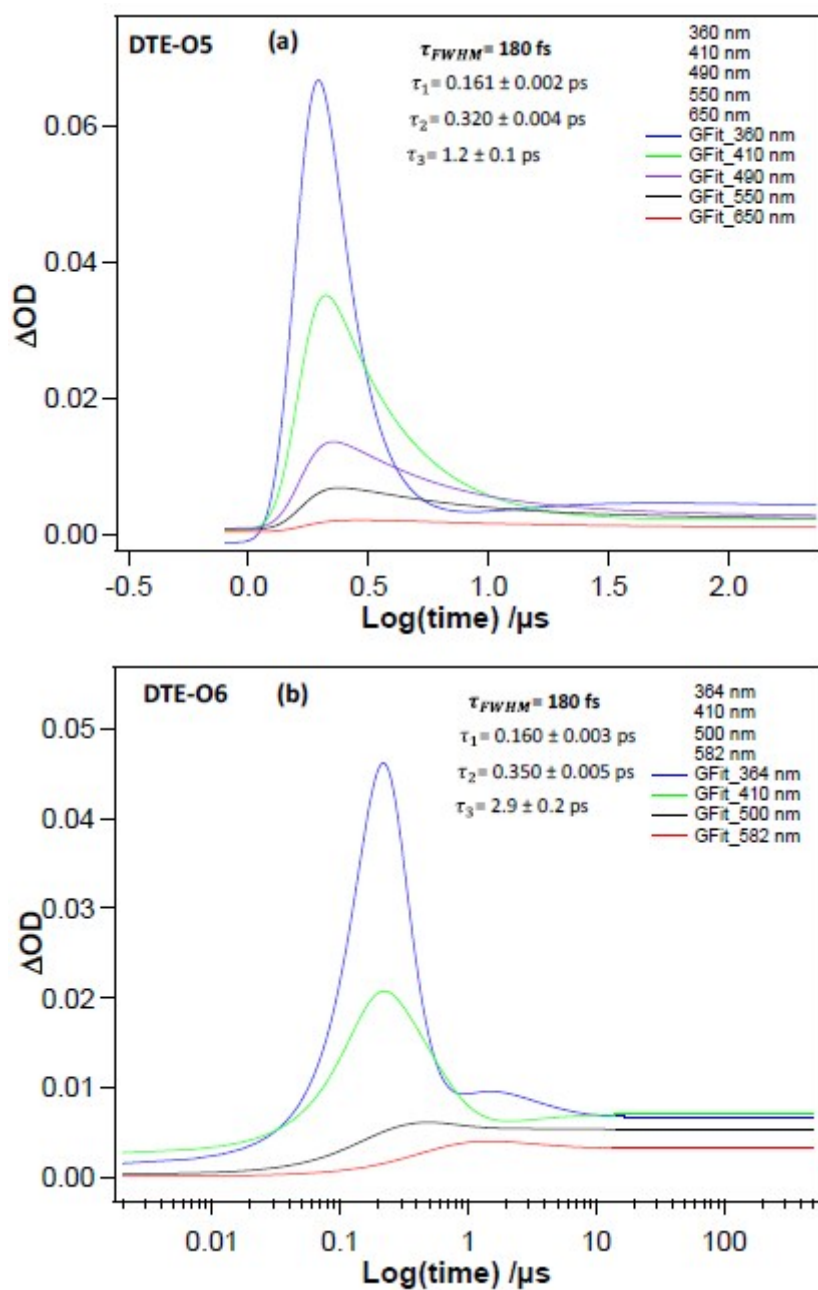


Figure S. 10. Characteristic lifetimes obtained for different species of **(a)** DTE-O₅ and **(b)** DTE-O₆ by global fitting using three exponential functions convoluted with 180 fs Gaussian function.

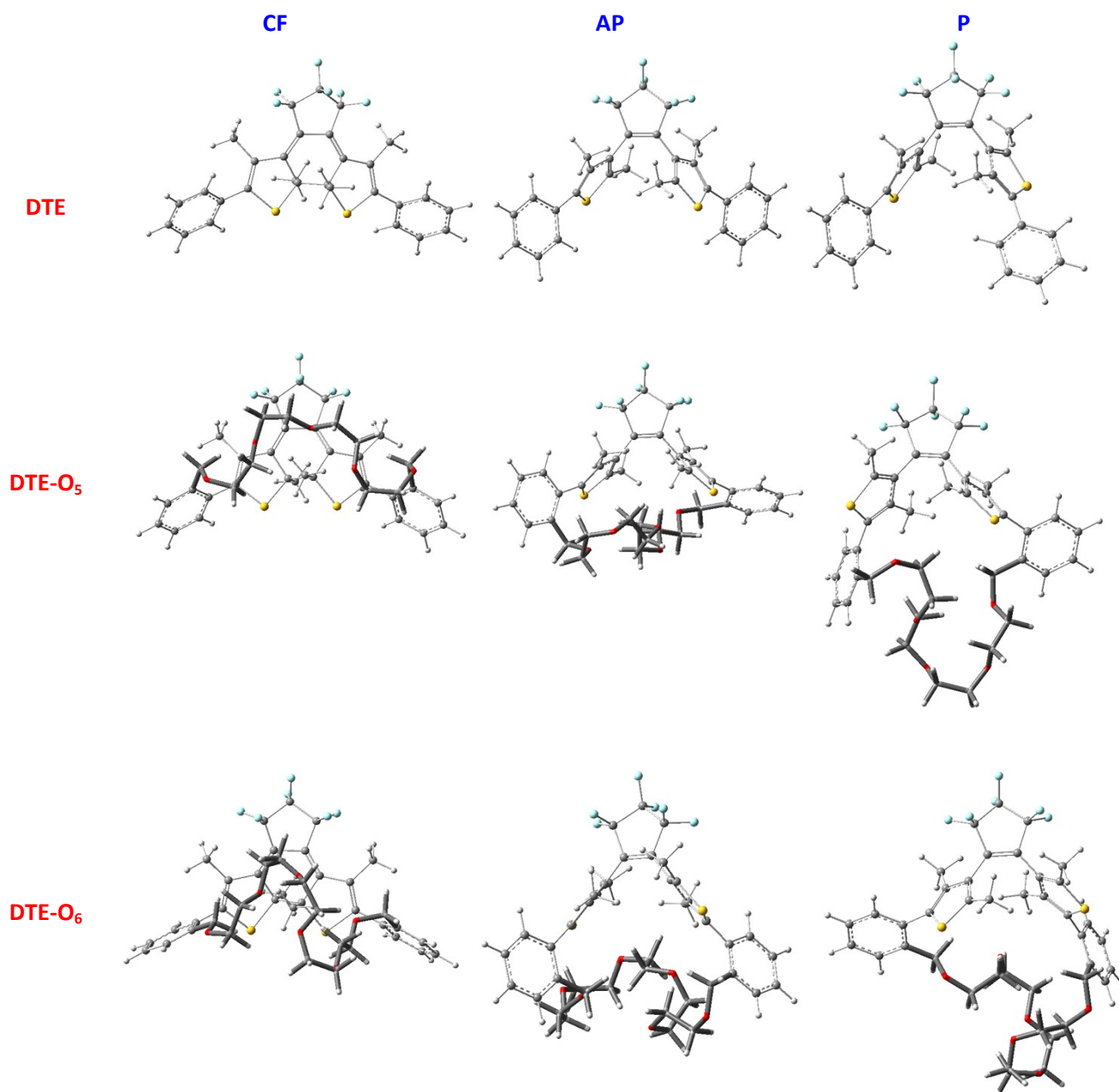


Figure S. 11. Optimized geometries calculated at the ω B97XD/6-31G(d) level for the CF, AP and P of **(top)** DTE, **(middle)** DTE-O₅ and **(down)** DTE-O₆. The DTE is represented by ball and stick model and the polyether chain is represented by tube model.

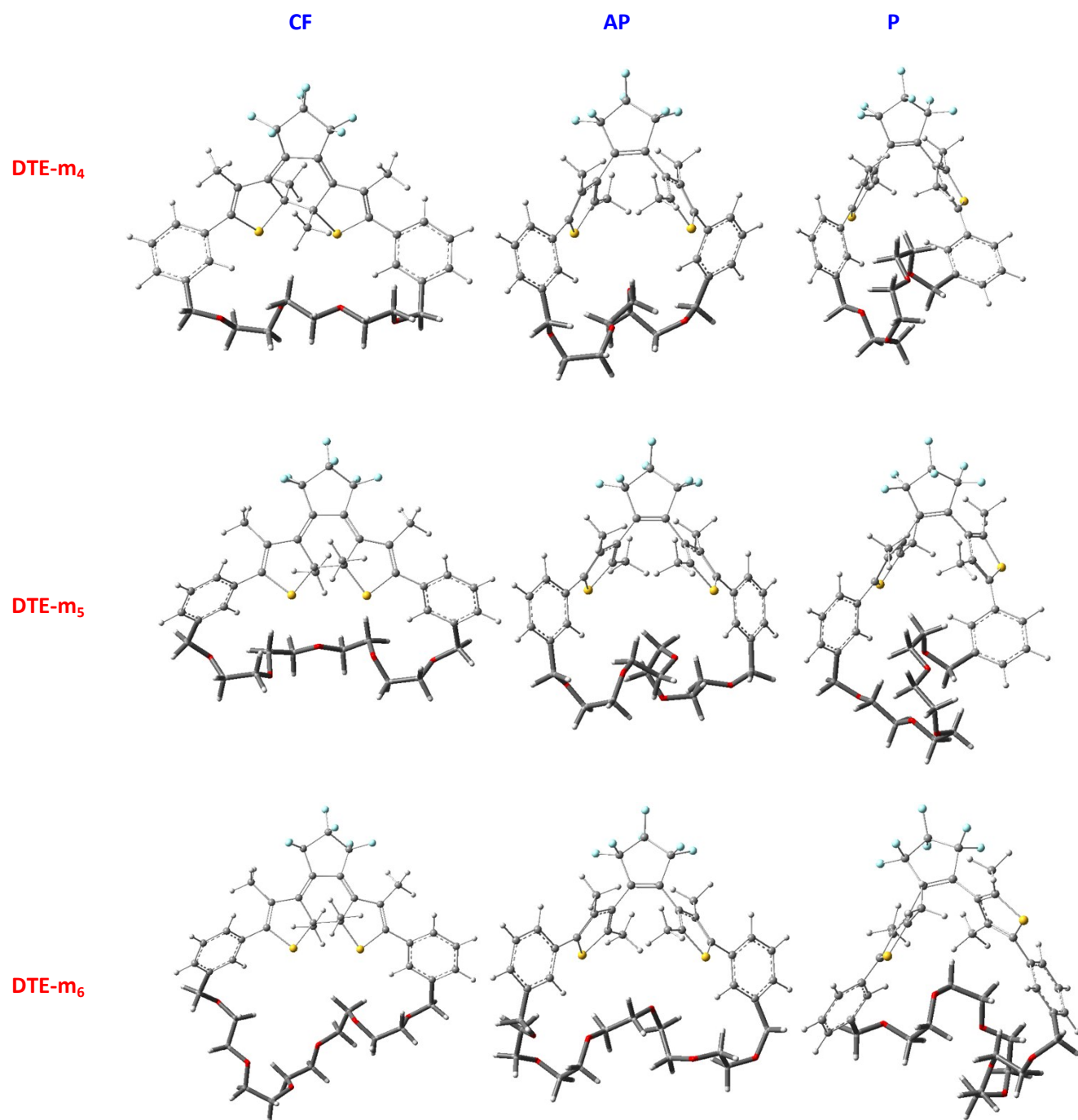


Figure S. 12. Optimized geometries calculated at the ω B97XD/6-31G(d) level for the CF, AP and P of (top) DTE-m₄, (middle) DTE-m₅ and (down) DTE-m₆. The DTE is represented by ball and stick model and the polyether chain is represented by tube model.

Table S. 1. Calculated torsion angles for the CF, AP and P for DTE, DTE-m_x and DTE-O_x.

	torsion angle (°)								
	CF			AP			P		
	ϕ_1	ϕ_2	$\Delta\phi^a$	ϕ_1	ϕ_2	$\Delta\phi$	ϕ_1	ϕ_2	$\Delta\phi$
DTE	134.4	-132.3	2.1	-133.6	-133.3	0.3	45.5	-135.0	-89.5
DTE-m4	126.2	-119.1	7.1	-122.3	-137.3	-15	44.8	-134.0	-89.2
DTE-m5	117.9	-131.3	13.4	-136.5	-145.0	-8.5	45.8	-152.5	-106.7
DTE-m6	124.3	-137.6	13.3	-137.7	-144.6	-6.9	34.8	-128.4	-93.6
DTE-O5	50.6	-56.8	6.2	-61.2	-135.0	-73.8	117.9	-95.2	22.7
DTE-O6	69.4	-81.6	12.2	-138.1	-111.2	26.9	88.6	-136.9	-48.3

^a $\Delta\phi = |\phi_2 - \phi_1|$

S. 13. GEOMETRIES: DTE

CF				AP				P			
C	2.03745	-1.21857	-0.02674	C	0.95767	2.6022	-0.69164	C	0.01095	-2.75968	-0.77805
C	0.62041	-0.72516	0.00636	C	0.63274	1.55369	0.24689	C	-0.09041	-1.71129	0.20945
C	0.60931	0.74429	0.03079	C	1.54286	1.42791	1.26696	C	-1.03288	-1.95095	1.17634
C	2.01598	1.23716	0.19	S	2.81085	2.58716	1.09438	S	-1.81769	-3.46365	0.8909
C	2.88812	0.04945	-0.28797	C	2.11937	3.22611	-0.35044	C	-0.88166	-3.75766	-0.528
C	-0.54156	1.45036	-0.07422	C	-0.53043	0.66027	0.13417	C	0.70547	-0.47461	0.16922
C	-1.78201	0.6401	-0.47513	C	-0.51942	-0.67912	-0.0122	C	0.25489	0.77522	-0.03299
C	-1.8065	-0.65357	0.35318	C	-1.92736	-1.22643	-0.02386	C	1.38961	1.76922	-0.03796
C	-0.51957	-1.4468	0.10619	C	-2.80391	0.02121	-0.26939	C	2.65939	0.88932	-0.11349
S	-3.2322	1.73705	-0.13359	C	-1.94301	1.16101	0.30597	C	2.18604	-0.46308	0.4548
C	-2.16942	3.09683	0.11168	C	0.65696	-1.54118	-0.21372	C	-1.13148	1.19692	-0.30584
C	-0.83966	2.86179	0.11588	C	1.50967	-1.36849	-1.27625	C	-1.88907	1.93574	0.56589
C	-0.76954	-2.88231	0.10012	S	2.80759	-2.50706	-1.20838	S	-3.45311	2.2455	-0.10842
C	-2.0865	-3.15589	-0.01562	C	2.20078	-3.20848	0.24499	C	-3.06805	1.39721	-1.56118
S	-3.1825	-1.79916	-0.11572	C	1.04785	-2.61944	0.6656	C	-1.80764	0.88596	-1.54178
C	-1.71718	0.4101	-2.0005	C	1.42371	-0.37747	-2.39532	C	-1.53022	2.45687	1.9248
C	-1.89494	-0.40913	1.87802	F	-2.23343	1.32859	1.62414	F	2.40925	-0.49547	1.79627
F	2.32323	2.33484	-0.53764	F	-2.20261	2.33515	-0.3058	F	2.8684	-1.49422	-0.08371
F	2.32703	1.51655	1.48792	F	-4.01687	-0.06649	0.29398	F	3.70118	1.40902	0.55013
F	3.08182	0.17448	-1.61778	F	-2.95048	0.20932	-1.59841	F	3.00404	0.7185	-1.40774
F	4.08195	0.0056	0.32078	F	-2.10903	-2.16424	-0.97626	F	1.31348	2.61786	-1.08544
F	2.42156	-1.76227	1.16153	F	-2.29134	-1.77951	1.16408	F	1.4339	2.52553	1.09
F	2.29278	-2.14208	-0.98518	C	1.53531	0.45475	2.40519	C	-1.40969	-1.09352	2.34468
H	-1.04867	0.19633	2.21599	H	1.99942	0.88002	3.29897	H	-1.67957	-1.69839	3.21477
H	-2.82227	0.10133	2.143	H	0.50613	0.18133	2.65552	H	-0.56934	-0.45328	2.62619
H	-1.86121	-1.37047	2.39643	H	2.07526	-0.46248	2.14356	H	-2.26079	-0.44814	2.10071
H	-0.83972	-0.1883	-2.26121	H	1.95627	0.5475	-2.14784	H	-1.31737	3.53055	1.89283
H	-2.61111	-0.10104	-2.36279	H	1.85096	-0.78058	-3.31741	H	-2.34265	2.29576	2.63973
H	-1.63865	1.37739	-2.50318	H	0.37842	-0.12182	-2.59082	H	-0.639	1.95465	2.30503
C	0.16386	3.94489	0.3909	C	0.30037	-3.04668	1.89646	C	-1.1862	0.10448	-2.66164
H	0.84701	3.65296	1.19401	H	0.01223	-2.18705	2.50933	H	-0.16142	0.44064	-2.85337
H	0.76942	4.16806	-0.49069	H	-0.61801	-3.58207	1.63868	H	-1.14564	-0.96294	-2.4195
H	-0.34796	4.86081	0.69652	H	0.9194	-3.70895	2.50696	H	-1.76097	0.21954	-3.58404
C	0.27729	-3.95446	0.19739	C	0.14908	2.96175	-1.90828	C	0.96107	-2.75422	-1.94504
H	0.88674	-3.9982	-0.70865	H	-0.38747	2.09493	-2.30446	H	1.21302	-1.73409	-2.24962
H	0.9535	-3.7697	1.03644	H	-0.59786	3.72611	-1.67638	H	1.89876	-3.25894	-1.69499
H	-0.19384	-4.92981	0.34128	H	0.79767	3.35028	-2.6979	H	0.51997	-3.26598	-2.80455
C	-2.80859	4.48026	0.33344	C	2.947	-4.37706	0.91519	C	-4.1049	1.29164	-2.69493
C	-4.19627	4.61944	0.31037	C	4.12505	-4.8673	0.35181	C	-5.36131	1.87941	-2.54828
C	-1.99932	5.59435	0.55771	C	2.44457	-4.94513	2.08621	C	-3.78716	0.60815	-3.86894
C	-4.77505	5.87317	0.51134	C	4.80091	-5.9262	0.95939	C	-6.30055	1.78352	-3.57582
H	-4.83449	3.74138	0.13434	H	4.52175	-4.41931	-0.57081	H	-5.61186	2.41885	-1.62333
C	-2.57786	6.84762	0.75809	C	3.1199	-6.00391	2.69323	C	-4.7262	0.51188	-4.89582
H	-0.90539	5.48435	0.57605	H	1.51595	-4.55836	2.53028	H	-2.79655	0.14503	-3.98441
C	-3.96585	6.98699	0.73455	C	4.29798	-6.49463	2.1295	C	-5.98309	1.09936	-4.74901
H	-5.8691	5.98283	0.4934	H	5.72982	-6.31252	0.51534	H	-7.29101	2.24714	-3.46028
H	-1.94007	7.72582	0.93453	H	2.72378	-6.45192	3.61601	H	-4.47595	-0.02709	-5.82104
H	-4.42168	7.97504	0.89333	H	4.83057	-7.32886	2.60873	H	-6.72292	1.02394	-5.55908
C	-2.68387	-4.57472	-0.05665	C	2.81461	4.37846	-1.09898	C	-1.10516	-5.04009	-1.35082
C	-4.0625	-4.74797	-0.17881	C	4.00919	4.90745	-0.61042	C	-2.06862	-5.96623	-0.95139

C	-1.84576	-5.68682	0.02815	C	2.24944	4.89307	-2.26611	C	-0.34389	-5.27524	-2.49606
C	-4.6034	-6.03376	-0.21594	C	4.63884	5.95162	-1.28898	C	-2.27083	-7.12815	-1.69722
H	-4.72336	-3.87162	-0.2464	H	4.45533	4.50159	0.30911	H	-2.66935	-5.78088	-0.04913
C	-2.38651	-6.97205	-0.00845	C	2.87859	5.93714	-2.94408	C	-0.54568	-6.43691	-3.24127
H	-0.75894	-5.55	0.12425	H	1.3078	4.47576	-2.65119	H	0.41546	-4.54488	-2.81087
C	-3.76549	-7.14541	-0.13017	C	4.07321	6.46662	-2.4552	C	-1.50903	-7.36355	-2.84154
H	-5.69029	-6.17034	-0.31251	H	5.58078	6.36849	-0.90393	H	-3.0306	-7.85819	-1.38243
H	-1.72602	-7.84862	0.05871	H	2.43303	6.34301	-3.8638	H	0.05452	-6.62248	-4.14375
H	-4.19143	-8.1588	-0.15977	H	4.56937	7.28923	-2.99035	H	-1.6684	-8.27892	-3.42969

S. 14. GEOMETRIES : DTE-m₄

CF				AP				P			
C	2.06853	0.85712	1.47425	C	2.54901	1.87631	-0.43048	C	-1.83614	-0.85738	-1.37218
C	1.29338	-0.0878	0.60491	C	2.46622	0.54065	-0.96752	C	-2.20947	0.05724	-0.31925
C	-0.13397	0.25386	0.66211	C	1.48022	0.37616	-1.9044	C	-3.06127	-0.48498	0.60864
C	-0.33069	1.29993	1.71464	S	0.61284	1.84934	-2.12796	S	-3.42614	-2.12515	0.20565
C	1.05678	1.97868	1.8102	C	1.57761	2.68823	-0.94961	C	-2.44054	-2.06705	-1.20895
C	-1.0452	-0.36685	-0.12962	C	3.23206	-0.58891	-0.41829	C	-1.76114	1.45719	-0.25935
C	-0.45209	-1.15193	-1.30208	C	2.72388	-1.60722	0.30035	C	-2.51948	2.55924	-0.38735
C	0.63957	-2.05019	-0.70428	C	3.81626	-2.53591	0.77039	C	-1.68113	3.81039	-0.30108
C	1.7221	-1.19398	-0.04743	C	5.11919	-1.74716	0.49318	C	-0.22642	3.29585	-0.40752
S	-1.76707	-1.48511	-2.36756	C	4.71164	-0.77205	-0.62924	C	-0.33524	1.83063	0.05863
C	-3.07299	-0.98722	-1.24624	C	1.30592	-1.80243	0.65669	C	-3.96674	2.62666	-0.66161
C	-2.48302	-0.50364	-0.00889	C	0.61824	-0.92163	1.45196	C	-4.8932	3.08164	0.2408
C	3.02081	-1.84626	-0.11894	S	-1.0401	-1.37592	1.56344	S	-6.48152	3.0235	-0.44528
C	3.02646	-2.87017	-1.01089	C	-0.81416	-2.75954	0.53478	C	-5.88429	2.40762	-1.94274
S	1.53954	-3.0784	-1.93788	C	0.49112	-2.87188	0.13262	C	-4.53453	2.23918	-1.93003
C	0.04715	-0.1705	-2.37922	C	1.1146	0.29562	2.16701	C	-4.68681	3.58102	1.63902
C	0.09554	-3.00225	0.38386	F	4.9522	-1.34654	-1.83872	F	-0.11633	1.76287	1.39949
F	-1.27478	2.2249	1.42759	F	5.42895	0.3697	-0.58437	F	0.59307	1.05116	-0.53256
F	-0.63506	0.78194	2.94191	F	6.15116	-2.53614	0.16342	F	0.64257	4.01906	0.31195
F	1.13211	2.93469	0.85924	F	5.44797	-1.0319	1.59069	F	0.15561	3.31115	-1.70245
F	1.28082	2.54192	3.00642	F	3.691	-2.83629	2.08094	F	-1.97064	4.68196	-1.29091
F	2.47135	0.28774	2.64571	F	3.8567	-3.71111	0.09081	F	-1.83862	4.47135	0.87561
F	3.17262	1.38237	0.88875	C	1.10514	-0.8623	-2.65666	C	-3.65183	0.16181	1.82317
H	-0.28099	-2.44123	1.2424	H	0.84313	-0.63612	-3.69426	H	-3.75902	-0.55179	2.64479
H	-0.72095	-3.61367	0.00171	H	1.94444	-1.56247	-2.66712	H	-3.00719	0.97596	2.16514
H	0.88994	-3.66456	0.73333	H	0.24844	-1.36252	-2.19086	H	-4.64019	0.58095	1.60437
H	0.85767	0.45101	-1.99017	H	0.87796	1.20637	1.60602	H	-4.75937	4.67275	1.68355
H	0.41148	-0.70494	-3.25975	H	0.66188	0.38374	3.15886	H	-5.43241	3.16576	2.32368
H	-0.77668	0.48044	-2.68195	H	2.19847	0.2427	2.29461	H	-3.69732	3.30061	2.0042
C	-3.28458	0.13921	1.08778	C	1.00667	-3.9347	-0.79767	C	-3.67654	1.67748	-3.20209
H	-2.75065	0.07065	2.03914	H	1.80413	-3.5454	-1.43562	H	-2.7712	2.26738	-3.38187
H	-3.46823	1.19857	0.88815	H	1.42419	-4.78489	-0.24827	H	-3.36998	0.63719	-3.04884
H	-4.24848	-0.35865	1.20535	H	0.20696	-4.31012	-1.44137	H	-4.29428	1.71793	-4.10274
C	4.17138	-1.52003	0.78831	C	3.52611	2.30464	0.62924	C	-0.9155	-0.52479	-2.51516
H	4.55562	-0.51567	0.59204	H	3.84572	1.45872	1.24405	H	-0.93539	0.54459	-2.74529
H	3.8555	-1.54779	1.83477	H	4.42929	2.73613	0.18637	H	0.12001	-0.78647	-2.27899
H	4.98818	-2.23115	0.65224	H	3.08223	3.05836	1.28563	H	-1.20564	-1.07145	-3.41639
C	4.07083	-3.90866	-1.1469	C	-1.97816	-3.60005	0.20407	C	-2.32094	-3.30264	-2.12033
C	3.75581	-5.19576	-0.70313	C	-3.20541	-3.00348	-0.09434	C	-3.01295	-4.47187	-1.80483
C	5.35151	-3.64082	-1.63253	C	-1.89382	-4.99965	0.2114	C	-1.52042	-3.25217	-3.26183
C	4.71037	-6.20617	-0.70256	H	-3.29464	-1.92118	-0.13231	C	-2.9043	-5.59126	-2.6309
H	2.76411	-5.40625	-0.31265	C	-3.01343	-5.76959	-0.08069	H	-3.6446	-4.51179	-0.90554
C	6.30456	-4.65662	-1.65567	H	-0.95655	-5.48199	0.4702	C	-1.41143	-4.37126	-4.08725
H	5.5994	-2.64354	-1.98323	C	-4.23671	-5.16051	-0.35568	H	-0.97512	-2.33024	-3.51046
C	5.99104	-5.9282	-1.18315	H	-2.93855	-6.85279	-0.06758	C	-2.10321	-5.54096	-3.77148
H	7.30245	-4.44963	-2.03005	H	-5.11461	-5.76901	-0.5571	H	-0.78024	-4.33166	-4.98679
H	6.75008	-6.7069	-1.18404	C	-4.33718	-3.77158	-0.36031	H	-2.01768	-6.4228	-4.42285
C	-4.40151	-1.60529	-1.03782	C	-5.63328	-3.05971	-0.65574	C	-6.85407	2.11772	-3.10338
C	-5.73945	-1.33785	-1.18471	H	-6.48081	-3.76113	-0.64168	C	-8.07352	2.26038	-2.44148
C	-6.81231	-2.22057	-1.1657	H	-5.58344	-2.62395	-1.66285	C	-6.76976	1.7954	-4.45816
H	-5.9124	-0.28071	-1.3621	O	-5.80872	-2.0511	0.31927	C	-9.24383	2.00619	-3.44302
C	-6.58009	-3.5724	-0.94392	C	-6.65626	-0.98985	-0.04807	H	-8.09255	2.51614	-1.37212
H	-7.82027	-1.85037	-1.32412	H	-6.78991	-0.40883	0.86931	C	-7.70275	1.5758	-5.32701

H	-7.40511	-4.27754	-0.92202	H	-7.64974	-1.34849	-0.36156	H	-5.78599	1.69309	-4.93864
C	4.33359	-7.58511	-0.19412	C	-6.08529	-0.09862	-1.1566	C	-9.03817	1.68742	-4.78515
H	5.22488	-8.09035	0.21075	H	-6.18229	-0.57261	-2.13709	H	-10.26669	2.08791	-3.04756
H	3.95838	-8.19455	-1.02291	H	-6.67584	0.8319	-1.18158	H	-9.89882	1.51839	-5.44844
O	3.29651	-7.56621	0.76018	O	-4.71258	0.18155	-1.016	C	-3.66864	-6.88206	-2.28273
C	3.70714	-7.07524	2.01998	C	-4.36123	0.8763	0.16145	H	-3.39438	-7.20496	-1.30017
H	4.08239	-6.04531	1.9413	H	-4.23188	0.18389	1.00525	H	-3.42129	-7.64507	-2.99093
H	4.51959	-7.70382	2.41752	H	-5.15057	1.59632	0.42917	O	-5.07547	-6.62941	-2.3261
C	2.54668	-7.11401	2.98838	C	-3.04803	1.59182	-0.14347	C	-5.99592	-7.72108	-2.40307
H	2.94772	-7.01414	4.01057	H	-2.33326	0.86004	-0.53053	H	-5.95389	-8.20963	-3.3541
H	2.04573	-8.09247	2.92103	H	-3.21074	2.34626	-0.92533	H	-5.82803	-8.43756	-1.6263
O	1.64125	-6.06758	2.7214	O	-2.42308	2.15789	0.98918	C	-7.32356	-6.96581	-2.20672
C	0.59797	-6.02976	3.66871	C	-3.15639	3.12588	1.71229	H	-7.3283	-6.49694	-1.24494
H	-0.00807	-6.94865	3.6118	H	-2.44687	3.51127	2.45125	H	-8.13914	-7.65542	-2.27135
H	1.01259	-5.97694	4.68957	H	-3.98532	2.66191	2.26978	O	-7.46005	-5.9695	-3.22341
C	-0.26326	-4.79948	3.44009	C	-3.73871	4.27448	0.88965	C	-8.77372	-6.03675	-3.78434
H	0.38927	-3.92371	3.36651	H	-4.50989	3.90738	0.20555	H	-9.49902	-5.87629	-3.01422
H	-0.92481	-4.66183	4.30888	H	-4.23003	4.97179	1.58541	H	-8.92569	-7.00121	-4.22207
O	-1.00758	-4.83973	2.2462	O	-2.79957	4.93471	0.07236	C	-8.92581	-4.95199	-4.86682
C	-2.23105	-5.52712	2.33031	C	1.21146	4.05901	-0.54787	H	-8.17044	-5.08435	-5.61301
H	-2.90102	-5.04629	3.06023	C	-0.10283	4.31478	-0.14655	H	-9.8921	-5.0326	-5.31925
H	-2.08012	-6.57049	2.64757	C	2.1461	5.09911	-0.52877	O	-8.78516	-3.66008	-4.27009
C	-2.88377	-5.54496	0.96619	C	-0.4939	5.58589	0.26121	C	-10.09844	-2.89992	-4.48739
H	-2.13371	-5.84056	0.21674	H	-0.82922	3.5084	-0.11958	H	-10.11579	-2.6779	-5.53396
H	-3.67942	-6.30753	0.96548	C	1.75952	6.37155	-0.118	H	-11.0197	-3.36593	-4.20632
O	-3.79699	-4.77806	1.26237	H	3.16686	4.91325	-0.84913	C	-9.91843	-1.5955	-3.68884
C	-4.47855	-5.15515	-0.03565	C	0.44413	6.61842	0.26775	H	-9.83176	-1.87317	-2.65914
H	-5.09674	-6.05886	-0.14767	H	2.48549	7.17901	-0.1128	H	-10.81043	-1.02155	-3.82962
H	-3.68764	-5.21429	-0.79637	H	0.14858	7.61934	0.57364	O	-8.7389	-0.85603	-4.01567
C	-4.95083	-3.91006	-0.70409	C	-1.91137	5.81203	0.73601	C	-8.354	0.37939	-4.62434
C	-4.18853	-2.989	-0.77562	H	-1.95702	5.65999	1.82373	H	-8.10021	1.08789	-3.86375
H	-3.6512	-2.93922	0.14833	H	-2.21435	6.8512	0.54623	H	-9.16713	0.75819	-5.20763

S. 15. GEOMETRIES : DTE-m₅

CF				AP				P			
C	-1.74711	-4.52856	5.26743	C	5.56524	8.56938	4.96482	C	-1.2988	-7.86574	0.29463
C	-1.06685	-3.34304	4.65269	C	6.74655	8.39062	5.77218	C	0.07236	-7.93524	-0.15295
C	0.3691	-3.38519	4.96772	C	7.909	8.31522	5.05106	C	0.7834	-6.78093	0.05296
C	0.61701	-4.51523	5.92166	S	7.57713	8.43361	3.36332	S	-0.21488	-5.58116	0.78481
C	-0.58589	-5.46014	5.68456	C	5.86503	8.57801	3.62977	C	-1.60197	-6.63136	0.80779
C	1.2469	-2.51362	4.41034	C	6.69169	8.11314	7.21582	C	0.64432	-9.08503	-0.87352
C	0.69797	-1.71878	3.22507	C	6.97384	6.93409	7.80054	C	1.06807	-9.09384	-2.15111
C	-0.6648	-1.15252	3.64391	C	6.72622	6.99466	9.28773	C	1.56003	-10.45999	-2.55368
C	-1.61586	-2.29715	3.98653	C	5.93751	8.31289	9.47962	C	1.06456	-11.38128	-1.4135
S	1.92534	-0.39606	2.88766	C	6.34132	9.15018	8.24972	C	0.91579	-10.41591	-0.22032
C	3.05233	-1.06667	4.0604	C	7.41296	5.70312	7.11675	C	0.99783	-7.96517	-3.09669
C	2.61341	-2.15764	4.74964	C	6.62457	5.04368	6.20858	C	2.0913	-7.31616	-3.60757
C	-2.98364	-1.98847	3.60425	S	7.39362	3.89315	5.61161	S	1.59459	-5.95781	-4.55676
C	-3.04713	-0.94202	2.73367	C	8.91577	4.05889	6.43574	C	-0.09092	-6.27707	-4.27601
S	-1.49992	-0.21986	2.30131	C	8.73168	5.13582	7.26307	C	-0.25959	-7.39197	-3.50052
C	0.64977	-2.64773	1.99393	C	5.21577	5.32978	5.79293	C	3.54624	-7.62152	-3.41865
C	-0.59367	-0.24471	4.89358	F	7.43083	9.90614	8.55346	F	2.08209	-10.37444	0.47801
F	1.76905	-5.19225	5.71016	F	5.3611	10.00025	7.88003	F	-0.04227	-10.82711	0.63577
F	0.61322	-4.12609	7.2291	F	6.20206	8.91872	10.64546	F	1.89092	-12.40712	-1.16753
F	-0.28994	-6.27522	4.6493	F	4.61386	8.05301	9.41155	F	-0.1544	-11.8666	-1.73342
F	-0.87771	-6.21151	6.7559	F	6.01976	5.92946	9.72327	F	1.06609	-10.84303	-3.75028
F	-2.45272	-4.20593	6.39072	F	7.86612	7.04922	10.02408	F	2.91446	-10.53457	-2.6338
F	-2.59799	-5.18412	4.44213	C	9.30679	8.12519	5.55148	C	2.21788	-6.49375	-0.26399
H	-0.21331	-0.80578	5.75237	H	10.02039	8.72969	4.98422	H	2.70041	-5.94193	0.54784
H	0.03867	0.62706	4.71773	H	9.37257	8.42436	6.60073	H	2.76378	-7.42969	-0.40689
H	-1.60339	0.10212	5.1292	H	9.61381	7.07587	5.47531	H	2.31083	-5.90144	-1.18075
H	-0.03123	-3.48498	2.16824	H	5.1881	5.88036	4.84621	H	3.93852	-8.20794	-4.25633
H	0.31875	-2.10735	1.10452	H	4.64667	4.40494	5.66151	H	4.13779	-6.70476	-3.3425
H	1.65043	-3.04611	1.80827	H	4.71215	5.93023	6.55431	H	3.70095	-8.20386	-2.50799
C	3.38851	-2.8157	5.85642	C	9.79071	5.70749	8.16444	C	-1.58729	-8.00705	-3.16132
H	2.75209	-2.9641	6.73296	H	9.69392	6.79313	8.2451	H	-1.50798	-9.09873	-3.13806
H	3.76478	-3.79641	5.55438	H	9.71779	5.30452	9.17995	H	-1.9443	-7.67932	-2.18058

H	4.24025	-2.20239	6.15448	H	10.78997	5.48106	7.7836	H	-2.34562	-7.73284	-3.89857
C	-4.18732	-2.69572	4.16226	C	4.1679	8.65244	5.51413	C	-2.2894	-8.98875	0.14316
H	-4.36702	-3.6522	3.66245	H	4.08631	8.1435	6.47851	H	-2.02127	-9.64035	-0.6929
H	-4.04822	-2.90413	5.22519	H	3.86519	9.69183	5.67554	H	-2.33025	-9.61475	1.03966
H	-5.08208	-2.07996	4.0489	H	3.4512	8.19838	4.82409	H	-3.29579	-8.5984	-0.03632
C	-4.24881	-0.3371	2.12802	C	10.19002	3.32301	6.36177	C	-2.88698	-6.12093	1.32107
C	-4.72218	0.95955	1.8895	C	10.69525	2.92863	5.12067	C	-3.34552	-4.85463	0.93648
C	-5.14407	-1.29375	1.6367	C	10.90152	2.97683	7.51934	C	-3.66843	-6.87921	2.19955
C	-5.94963	1.1985	1.88078	H	10.17884	3.20439	4.20521	C	-4.46455	-4.56245	1.49517
H	-4.1464	1.82085	2.21694	C	12.08897	2.26107	7.42294	H	-2.77745	-4.277	0.21322
C	-6.32872	-0.89033	1.02915	H	10.50967	3.24827	8.49447	C	-4.87634	-6.37767	2.67702
H	-4.90511	-2.34953	1.71341	C	12.56981	1.85586	6.17892	H	-3.31972	-7.85382	2.52612
C	-6.62591	0.46264	0.90224	H	12.62971	1.99386	8.32588	C	-5.31196	-5.11336	2.295
H	-7.0206	-1.63629	0.65048	H	13.48516	1.2734	6.11257	H	-5.47184	-6.97431	3.36129
H	-7.55584	0.77048	0.42974	C	11.87063	2.18689	5.02098	H	-6.25628	-4.72486	2.66672
C	4.38077	-0.44034	4.20279	C	12.34681	1.7793	3.64947	C	-1.14756	-5.37977	-4.77416
C	3.91822	0.74852	4.84196	H	13.15386	1.0346	3.71718	C	-1.20011	-4.92703	-6.09487
C	5.65521	-0.9042	4.13006	H	12.75363	2.65941	3.13317	C	-2.15008	-4.98334	-3.88152
C	5.22767	1.90264	4.8739	O	11.24209	1.24979	2.94382	C	-2.25496	-4.1165	-6.5081
H	3.22844	0.47727	5.67331	C	11.34589	1.27712	1.54097	H	-0.43262	-5.22611	-6.80339
C	6.74158	-0.16458	4.69152	H	10.49015	0.69498	1.1862	C	-3.22277	-4.20262	-4.29432
H	5.85669	-1.88677	3.71382	H	12.2597	0.773	1.1878	H	-2.09238	-5.2931	-2.84364
C	6.52694	0.97086	5.4475	C	11.30451	2.68903	0.94603	C	-3.26989	-3.76922	-5.62096
H	7.75051	-0.54135	4.53371	H	12.26263	3.2009	1.07026	H	-2.29675	-3.77159	-7.53689
H	7.35855	1.41193	5.99471	H	11.11984	2.5956	-0.13675	H	-4.1021	-3.15867	-5.96374
O	-5.1622	4.39933	2.31505	O	10.35289	3.53554	1.54639	O	-6.0233	-3.06672	0.23251
C	-5.45046	4.32106	3.69532	C	9.0133	3.10506	1.43373	C	-6.60323	-2.03638	-0.52977
H	-5.87763	3.34236	3.95538	H	8.76223	2.38351	2.22398	H	-7.14271	-1.36805	0.16094
H	-6.18044	5.09763	3.97267	H	8.85084	2.61526	0.46067	H	-5.78679	-1.45323	-0.98779
C	-4.17661	4.53405	4.47779	C	8.15203	4.35808	1.56654	C	-7.54544	-2.37374	-1.66634
H	-4.53513	4.73287	5.50109	H	8.55118	4.83115	2.46826	H	-7.03439	-3.04962	-2.35633
H	-3.76861	5.47487	4.07622	H	8.47468	4.95699	0.7039	H	-7.79491	-1.44332	-2.19637
O	-3.06713	3.68193	4.63616	O	6.78945	4.6939	1.7229	O	-8.74075	-2.95529	-1.17683
C	-2.09593	4.23391	5.49296	C	5.9723	4.51673	0.77039	C	-9.07789	-4.21648	-1.7123
H	-1.67788	5.15795	5.06144	H	5.01123	4.99666	0.98019	H	-9.09307	-4.19169	-2.81255
H	-2.54878	4.50401	6.46201	H	5.86373	3.44982	1.02162	H	-10.09711	-4.41451	-1.36636
C	-1.0028	3.21339	5.75488	C	6.29513	4.6098	-0.72034	C	-8.1767	-5.34947	-1.24987
H	-1.46786	2.27118	6.05794	H	7.2129	4.06059	-0.95178	H	-7.93896	-5.19308	-0.18878
H	-0.38112	3.57367	6.58959	H	5.47841	4.12069	-1.273	H	-8.70764	-6.31098	-1.34957
O	-0.19659	2.90976	4.64199	O	6.44895	5.8214	-1.42335	O	-6.99384	-5.36849	-2.02005
C	0.75976	3.89213	4.31983	C	4.94325	8.56779	2.47882	C	-5.95886	-6.0966	-1.40325
H	1.0783	4.31118	5.2864	C	4.74373	7.73901	1.37102	H	-5.82406	-5.7588	-0.37004
H	0.21076	4.67368	3.77395	C	4.02166	9.6196	2.48864	H	-6.19314	-7.17517	-1.38847
C	2.05374	3.77648	3.54582	C	3.9691	7.96419	0.27509	C	-4.6704	-5.88882	-2.16707
H	1.61118	3.3499	2.63298	H	5.35652	6.85274	1.23832	H	-4.79037	-6.20766	-3.21064
H	2.32712	4.82266	3.33719	C	3.07619	9.7229	1.47241	H	-3.89686	-6.51997	-1.71155
O	3.19413	3.03782	3.927	H	4.05707	10.36065	3.28155	O	-4.23351	-4.54258	-2.09813
C	4.83589	2.63132	3.5044	C	3.04627	8.78861	0.43986	C	-4.31423	-3.82821	-3.30583
H	5.45433	3.52705	3.6562	H	2.36776	10.54578	1.47819	H	-4.22181	-2.77095	-3.03214
H	4.86699	2.37441	2.43404	H	2.31271	8.88601	-0.35712	H	-5.30085	-3.95946	-3.77314
C	-6.30059	4.34834	1.45114	C	5.15557	6.33891	-1.74621	C	-5.00498	-2.38185	0.96657
H	-6.06246	3.7731	0.58092	H	4.91108	6.80401	-0.81412	H	-4.04287	-2.68718	0.61158
H	-6.57147	5.34144	1.15909	H	5.46636	7.08563	-2.44673	H	-5.11655	-1.32631	0.83134
C	-7.47944	3.69205	2.19356	C	3.75722	5.97004	-2.2755	C	-5.13245	-2.72401	2.46266
H	-8.26494	3.47994	1.49864	H	3.73214	5.22296	-3.0411	H	-5.84813	-3.50931	2.58921
H	-7.84126	4.35874	2.94822	C	3.02347	5.7423	-1.53075	H	-5.45524	-1.85719	3.00054
O	-7.0545	2.4873	2.818	O	3.7805	7.32547	-2.73064	O	-3.86297	-3.1507	2.9639
C	-6.75983	1.3335	3.25386	C	3.99454	8.24741	-1.19771	C	-3.64368	-4.51785	2.60652
H	-5.75916	0.9749	3.37629	H	4.14475	9.25925	-1.51158	H	-4.26921	-5.14748	3.20417
H	-7.14007	1.65949	4.1994	H	3.08566	8.17904	-0.63721	H	-2.61777	-4.77054	2.77553

S. 16. GEOMETRIES : DTE-m₆

CF			AP			P		
C	-5.81158	-7.35146 -0.009	C	3.23515	1.34966 -0.12696	C	1.04136	-5.53431 -1.64308
C	-6.03955	-6.37186 -1.12009	C	2.13514	1.9743 0.57046	C	1.97373	-5.97629 -2.65332
C	-5.50923	-6.92418 -2.37574	C	1.68608	1.26618 1.65378	C	2.45793	-4.96532 -3.44319
C	-4.79029	-8.20403 -2.0699	S	2.63708	-0.1817 1.86291	S	1.77114	-3.45473 -2.97621

C	-5.4174	-8.66081	-0.73045	C	3.6201	0.17837	0.47246	C	0.81831	-4.1838	-1.71603
C	-5.71635	-6.31047	-3.56792	C	1.5121	3.23186	0.13102	C	2.29973	-7.38937	-2.90886
C	-6.77891	-5.21113	-3.54845	C	0.2327	3.44089	-0.23304	C	2.0015	-8.08731	-4.02053
C	-6.4788	-4.30399	-2.34836	C	0.03083	4.86924	-0.69185	C	2.46418	-9.51691	-3.90811
C	-6.54869	-5.11652	-1.05724	C	1.46598	5.42454	-0.83279	C	2.80678	-9.67687	-2.40768
S	-6.62069	-4.32263	-5.14701	C	2.27054	4.53874	0.13304	C	3.11226	-8.23313	-1.96044
C	-5.4488	-5.49138	-5.74352	C	-0.86879	2.46521	-0.30687	C	1.24571	-7.58684	-5.18296
C	-5.0893	-6.47215	-4.86787	C	-0.82819	1.36028	-1.1186	C	1.77788	-7.4129	-6.43373
C	-7.07585	-4.3272	0.04337	S	-2.3165	0.4953	-1.03459	S	0.61977	-6.66837	-7.48123
C	-7.70407	-3.19422	-0.39124	C	-2.99572	1.60444	0.1225	C	-0.58837	-6.60723	-6.2329
S	-7.71056	-2.95942	-2.13684	C	-2.10577	2.60172	0.42754	C	-0.12252	-7.15386	-5.06799
C	-8.1704	-5.87695	-3.51046	C	0.28215	0.85694	-1.98632	C	3.15106	-7.74698	-6.93229
C	-5.0702	-3.66814	-2.39753	F	2.24418	5.09102	1.37692	F	4.43953	-7.98092	-2.11655
F	-4.9489	-9.17767	-2.99573	F	3.56637	4.45555	-0.22807	F	2.82577	-8.04543	-0.65562
F	-3.44877	-8.03703	-1.88741	F	1.55334	6.73261	-0.5538	F	3.81807	-10.52752	-2.18537
F	-6.53944	-9.36143	-1.00223	F	1.91065	5.21536	-2.09049	F	1.71282	-10.11338	-1.74702
F	-4.59341	-9.42986	-0.00444	F	-0.63908	4.92353	-1.8633	F	1.509	-10.38941	-4.29403
F	-4.77688	-6.99128	0.80551	F	-0.64569	5.64454	0.19365	F	3.57185	-9.77677	-4.65108
F	-6.88581	-7.56318	0.78854	C	0.55692	1.58161	2.58203	C	3.44324	-5.04328	-4.56736
H	-4.30001	-4.44519	-2.39972	H	0.78163	1.27566	3.60742	H	4.15988	-4.21806	-4.52426
H	-4.95012	-3.03235	-3.27624	H	0.36648	2.65801	2.58464	H	4.00332	-5.97995	-4.50927
H	-4.93527	-3.05264	-1.50406	H	-0.36463	1.07741	2.26857	H	2.9398	-5.00678	-5.53953
H	-8.29261	-6.46449	-2.59667	H	0.84178	0.06375	-1.47675	H	3.16057	-8.71539	-7.44373
H	-8.96638	-5.13059	-3.5551	H	-0.10252	0.44858	-2.92558	H	3.51331	-6.99103	-7.63478
H	-8.26966	-6.54521	-4.36956	H	0.97476	1.66634	-2.22838	H	3.85699	-7.80647	-6.10134
C	-4.03606	-7.50518	-5.1548	C	-2.34775	3.66285	1.46675	C	-0.9453	-7.35803	-3.82803
H	-3.32794	-7.57001	-4.3243	H	-1.41461	3.94321	1.96221	H	-0.66167	-8.29107	-3.33048
H	-4.47396	-8.49733	-5.29076	H	-2.76564	4.57625	1.03286	H	-0.80329	-6.54352	-3.11169
H	-3.4785	-7.2535	-6.05826	H	-3.04309	3.30312	2.22931	H	-2.01011	-7.40613	-4.06822
C	-6.88668	-4.68196	1.49209	C	3.82509	1.87673	-1.40868	C	0.34497	-6.45898	-0.68109
H	-7.60122	-5.44141	1.82317	H	3.09685	2.48189	-1.95652	H	0.26356	-7.46817	-1.09387
H	-5.88441	-5.08233	1.65876	H	4.69465	2.51547	-1.23246	H	0.88801	-6.54052	0.26532
H	-7.01174	-3.79981	2.12358	H	4.13862	1.05317	-2.05578	H	-0.66356	-6.09888	-0.45617
C	-8.35112	-2.1572	0.42173	C	-4.37988	1.3988	0.58451	C	-0.09111	-3.34082	-0.91754
C	-8.34494	-0.75674	0.39161	C	-4.88932	0.10194	0.73395	C	-0.91051	-2.396	-1.54807
C	-9.18101	-2.65986	1.43003	C	-5.23799	2.48331	0.80415	C	-0.1529	-3.45965	0.47509
C	-8.59803	-0.19018	1.61699	H	-4.23944	-0.75845	0.59462	C	-1.61657	-1.73635	-0.70185
H	-7.73739	-0.22804	-0.33774	C	-6.56241	2.2691	1.1746	H	-0.91396	-2.32951	-2.63206
C	-9.86256	-1.78528	2.27018	H	-4.88259	3.49663	0.65269	C	-1.01441	-2.65114	1.21175
H	-9.30688	-3.73167	1.54428	C	-7.06286	0.97685	1.28375	H	0.48991	-4.171	0.98392
C	-9.72732	-0.41026	2.10901	H	-7.21574	3.11977	1.34471	C	-1.81292	-1.70937	0.57174
H	-10.50442	-2.18005	3.05167	H	-8.11092	0.8164	1.52481	H	-1.05035	-2.75035	2.29235
H	-10.26007	0.26737	2.77218	C	-6.22703	-0.11544	1.04506	H	-2.48655	-1.08116	1.14829
C	-4.96011	-5.35849	-7.12946	O	-4.78787	-4.18582	-2.09001	C	-1.89768	-5.96693	-6.44625
C	-4.16736	-4.19496	-6.89795	C	-4.08584	-5.0545	-1.23526	C	-2.70384	-6.23621	-7.55512
C	-4.91957	-6.1937	-8.19972	H	-3.21921	-5.38759	-1.81444	C	-2.35454	-5.06359	-5.47967
C	-3.6758	-3.54633	-8.44239	H	-4.68847	-5.94859	-1.00231	C	-3.95181	-5.62784	-7.66867
H	-3.53767	-4.3504	-5.99249	C	-3.6537	-4.45228	0.1026	H	-2.36781	-6.93662	-8.31472
C	-4.04289	-5.93991	-9.29948	H	-4.5291	-4.26319	0.72669	C	-3.52452	-4.5751	-5.74102
H	-5.49657	-7.11368	-8.19769	H	-3.02432	-5.20124	0.61269	H	-1.71593	-4.81442	-4.63909
C	-3.10828	-4.92425	-9.25761	O	-2.9924	-3.20671	0.03504	C	-4.41264	-4.76796	-6.67571
H	-4.10937	-6.59488	-10.16631	C	-1.7766	-3.17649	-0.68127	H	-4.57904	-5.84414	-8.52827
H	-2.35072	-4.86456	-10.03741	H	-1.87214	-2.53327	-1.56486	H	-5.40036	-4.32119	-6.7631
O	-6.70046	3.64914	-0.0176	H	-1.50817	-4.18003	-1.03439	O	-3.85096	-0.90944	-1.46667
C	-5.47825	3.10256	0.43164	C	-0.69859	-2.65467	0.268	C	-4.92129	-0.34258	-2.18224
H	-5.58177	2.67769	1.43997	H	-0.98466	-1.66257	0.62738	H	-5.14487	0.63914	-1.73387
H	-4.70553	3.88641	0.46827	H	-0.63965	-3.3232	1.13819	H	-4.58174	-0.16669	-3.21674
C	-5.04184	2.01862	-0.52488	O	0.5706	-2.48757	-0.32963	C	-6.22985	-1.09425	-2.30899
H	-4.00376	2.02809	-0.15406	C	1.16304	-3.63137	-0.91422	H	-6.0283	-2.0788	-2.73805
H	-5.09106	2.68241	-1.40227	H	2.2144	-3.35171	-1.03512	H	-6.88549	-0.53437	-2.99127
O	-4.88848	0.83935	-1.2785	H	0.75223	-3.81219	-1.92009	O	-6.87097	-1.20939	-1.0511
C	-3.78619	0.91059	-2.15137	C	1.06967	-4.94479	-0.14089	C	-7.19076	-2.52048	-0.63904
H	-3.93643	1.70328	-2.90231	H	0.03053	-5.19374	0.08753	H	-7.77214	-3.05009	-1.40905
H	-2.86971	1.16311	-1.59157	H	1.43693	-5.73674	-0.80828	H	-7.83007	-2.39929	0.24089
C	-3.57162	-0.4363	-2.81835	O	1.73081	-4.96855	1.10327	C	-5.98568	-3.36284	-0.25453
H	-3.5567	-1.2113	-2.04698	C	4.7568	-0.70045	0.13584	H	-5.27199	-2.72319	0.28249
H	-2.58883	-0.42748	-3.31544	C	4.61695	-2.09447	0.23596	H	-6.3008	-4.17593	0.42068
O	-4.57574	-0.8129	-3.72973	C	5.99414	-0.15296	-0.20323	O	-5.38593	-3.90194	-1.41313
C	-4.5198	-0.15672	-4.97461	C	5.69194	-2.96196	0.03221	C	-4.06575	-4.33515	-1.18675
H	-3.4473	-0.0147	-5.17683	H	3.61565	-2.44264	0.4408	H	-3.4867	-3.5422	-0.70123
H	-4.96937	0.83358	-4.80908	C	7.05807	-0.9988	-0.48479	H	-4.05164	-5.22518	-0.53401

C	-5.07738	-0.56707	-6.31908	H	6.12754	0.92288	-0.22658	C	-3.41692	-4.68882	-2.50609
H	-6.12012	-0.68404	-5.9872	C	6.90501	-2.37353	-0.37654	H	-3.99241	-5.47243	-3.01585
H	-5.0107	0.35288	-6.92075	H	8.02178	-0.58549	-0.76636	H	-2.41667	-5.08988	-2.29899
O	-4.68018	-1.68407	-7.08454	H	7.76685	-3.00146	-0.57851	C	-2.75031	-0.07084	-1.82756
C	-4.90408	-2.53186	-8.5913	C	3.13661	-4.94091	1.06514	H	-2.06884	-0.62142	-2.44185
H	-4.4656	-1.91872	-9.39107	H	3.55839	-3.99688	0.75113	H	-3.11158	0.77871	-2.36853
H	-5.98461	-2.62008	-8.78451	H	3.47088	-5.16619	2.08046	C	-2.02587	0.40198	-0.5535
C	-7.16937	4.78088	0.72008	C	3.87095	-5.83136	0.07607	H	-2.41292	-0.12522	0.29334
H	-8.2332	4.72533	0.82048	H	3.67495	-6.89849	0.21507	H	-2.18357	1.45215	-0.42245
H	-6.90652	5.67883	0.20094	H	3.6209	-5.56731	-0.96271	O	-0.62515	0.14211	-0.67737
C	-6.52154	4.78727	2.11717	O	5.25175	-5.68123	0.30541	C	-0.36755	-1.2343	-0.38746
H	-7.02268	5.54495	2.68258	C	5.99542	-4.46936	0.36897	H	-0.46686	-1.40184	0.66467
H	-5.49712	5.06389	1.97949	H	6.39588	-4.424	1.39041	H	0.62608	-1.48391	-0.69614
O	-6.50117	3.6176	2.92549	H	6.84095	-4.68912	-0.28805	O	-3.26734	-3.54022	-3.34469
C	-6.4083	2.57483	3.89961	C	-6.0287	-3.71543	-1.60001	C	-4.48215	-3.31295	-4.06405
H	-5.55295	1.96683	3.6908	H	-6.68762	-3.62851	-2.46966	H	-4.2605	-2.84019	-4.99801
H	-6.31068	3.00506	4.87443	H	-6.48067	-4.43492	-0.90226	H	-5.12488	-2.68062	-3.48789
C	-7.67986	1.70772	3.84618	C	-5.89268	-2.35852	-0.90632	C	-5.18437	-4.65869	-4.3238
H	-8.40056	2.08841	4.53941	H	-4.92237	-1.93872	-1.19126	H	-5.72132	-4.60828	-5.24794
H	-8.08785	1.73349	2.85735	H	-6.67621	-1.66711	-1.2492	H	-5.86659	-4.86489	-3.5257
O	-7.35216	0.35932	4.19163	O	-5.95545	-2.47214	0.50845	O	-4.20708	-5.70009	-4.39653
C	-8.20584	-0.48776	3.13937	C	-6.79031	-1.52046	1.11322	C	-3.82389	-5.94261	-5.75845
H	-9.05241	-0.35419	3.77997	H	-6.92902	-1.83525	2.15281	H	-4.34984	-6.77917	-6.16886
H	-7.41728	-0.59532	2.42417	H	-7.77389	-1.54968	0.6213	H	-2.77082	-6.1271	-5.80205

S. 17. GEOMETRIES : DTE-O₅

CF				AP				P			
C	0.99538	2.6454	-1.67155	C	3.09356	0.23479	0.0118	C	-1.26673	-2.30871	0.20165
C	0.47271	1.26097	-1.46774	C	1.9396	0.74122	0.70692	C	-2.06499	-1.40749	-0.5945
C	-0.89224	1.20869	-1.6089	C	1.56992	-0.00752	1.79705	C	-1.80939	-1.48325	-1.93849
C	-1.45213	2.58235	-1.83752	S	2.2762	-1.66656	1.47521	S	-0.60004	-2.67079	-2.25246
C	-0.25912	3.54604	-1.60076	C	3.57161	-0.91021	0.59699	C	-0.39892	-3.0501	-0.56645
C	-1.62187	-0.02347	-1.49589	C	1.31105	2.04356	0.43147	C	-3.11951	-0.54092	-0.03326
C	-0.76891	-1.28236	-1.42855	C	0.09827	2.33483	-0.06727	C	-3.19081	0.79936	0.04548
C	0.44557	-1.01911	-0.47403	C	-0.12302	3.83205	-0.08577	C	-4.46829	1.23819	0.7205
C	1.25233	0.0979	-1.10388	C	1.29027	4.42107	0.10503	C	-5.04006	-0.05852	1.33363
S	-1.89678	-2.5832	-0.77824	C	2.02011	3.30469	0.87127	C	-4.40526	-1.1607	0.46499
C	-3.29007	-1.5365	-0.89663	C	-0.91958	1.45521	-0.6719	C	-2.20372	1.81798	-0.36589
C	-2.99902	-0.25128	-1.35346	C	-0.71446	0.87654	-1.89719	C	-2.32988	2.59558	-1.48637
C	2.5944	-0.17541	-1.32122	S	-2.16332	0.12572	-2.45815	S	-0.9918	3.68682	-1.61288
C	2.9783	-1.45863	-0.88643	C	-3.05641	0.58348	-1.03469	C	-0.25852	3.08196	-0.14953
S	1.62252	-2.43009	-0.35502	C	-2.26021	1.2876	-0.16702	C	-1.03909	2.11615	0.42816
C	-0.32935	-1.68379	-2.84817	C	0.52626	0.88922	-2.73637	C	-3.43297	2.62376	-2.5001
C	-0.02691	-0.67786	0.94787	F	1.87064	3.49863	2.20936	F	-5.22617	-1.44296	-0.58233
F	-1.93099	2.74231	-3.09947	F	3.34491	3.3065	0.61729	F	-4.23942	-2.30638	1.15619
F	-2.46117	2.91772	-0.99368	F	1.29235	5.6	0.74151	F	-6.37936	-0.09455	1.34195
F	-0.22972	4.54028	-2.50179	F	1.87298	4.57376	-1.10446	F	-4.58771	-0.18831	2.59881
F	-0.34899	4.09197	-0.37123	F	-0.68839	4.25522	-1.23477	F	-4.2434	2.17614	1.66575
F	1.90889	3.02335	-0.74138	F	-0.91447	4.25546	0.93586	F	-5.36392	1.75879	-0.15789
F	1.58453	2.81543	-2.88928	C	0.45616	0.25635	2.76213	C	-2.43057	-0.69812	-3.05158
H	-0.77865	0.11446	0.93621	H	0.69647	-0.1206	3.75979	H	-2.40185	-1.24631	-3.99667
H	-0.46546	-1.56057	1.42086	H	0.27438	1.33163	2.84051	H	-3.47608	-0.47882	-2.8189
H	0.79881	-0.32818	1.56679	H	-0.46102	-0.2427	2.43589	H	-1.90743	0.25402	-3.19481
H	0.30376	-0.90609	-3.28611	H	1.20812	0.08018	-2.45628	H	-3.99606	3.56082	-2.43892
H	0.23254	-2.62166	-2.82989	H	0.29331	0.7777	-3.79835	H	-3.04277	2.53278	-3.51858
H	-1.20956	-1.81224	-3.48311	H	1.05891	1.83526	-2.60283	H	-4.13396	1.80555	-2.3263
C	-4.10341	0.72176	-1.67448	C	-2.71637	1.82365	1.16212	C	-0.7474	1.39138	1.70614
H	-4.25138	1.46209	-0.88595	H	-1.93176	1.70695	1.91519	H	-1.54941	1.55851	2.4342
H	-3.87918	1.26421	-2.59528	H	-2.95528	2.88963	1.10575	H	-0.68081	0.31403	1.53299
H	-5.04404	0.18388	-1.81413	H	-3.60834	1.29866	1.5118	H	0.19632	1.71954	2.13911
C	3.55937	0.73109	-2.03916	C	3.71715	0.8656	-1.20081	C	-1.34642	-2.36204	1.70494
H	3.1693	0.97726	-3.02985	H	3.33186	1.87156	-1.37812	H	-1.76984	-1.43767	2.10729
H	3.71512	1.67227	-1.50715	H	4.80336	0.93281	-1.08238	H	-1.98958	-3.17601	2.05011
H	4.52674	0.24205	-2.16901	H	3.51956	0.25571	-2.0879	H	-0.3564	-2.51112	2.14513
C	-4.58915	-2.07376	-0.44715	C	-4.52749	0.40489	-0.95457	C	0.541	-4.09041	-0.07654
C	-5.31688	-1.47454	0.59957	C	-5.20619	-0.81925	-1.1255	C	1.91037	-4.18544	-0.40222

C	-5.07506	-3.25298	-1.03439	C	-5.28217	1.56699	-0.73961	C	0.00516	-5.03312	0.81799
C	-6.26272	-3.82978	-0.60793	C	-6.67008	1.53744	-0.67663	C	0.78996	-6.0022	1.4242
H	-4.51087	-3.71067	-1.84204	H	-4.76404	2.51546	-0.63927	H	-1.05837	-5.0029	1.02899
C	-6.98321	-3.23826	0.42789	C	-7.33912	0.33446	-0.8655	C	2.15021	-6.06222	1.13611
H	-6.62528	-4.73656	-1.08196	H	-7.22137	2.45638	-0.50371	H	0.33888	-6.71014	2.11257
H	-7.91143	-3.6831	0.77329	H	-8.42362	0.29454	-0.84106	H	2.78289	-6.8101	1.60374
O	2.65075	0.4713	3.17408	C	-4.50508	-2.15583	-1.26519	C	1.06522	3.57473	0.26308
C	2.70847	1.58476	2.3044	H	-3.59659	-2.07918	-1.8643	C	1.22987	4.05844	1.51753
H	2.47273	1.28973	1.27171	H	-5.1791	-2.86038	-1.77247	C	2.24026	3.59875	-0.64872
H	3.70984	2.03563	2.31423	O	-4.07601	-2.7078	-0.03161	C	2.51748	4.54817	1.99576
C	1.68017	2.59984	2.75051	C	-5.10168	-3.06809	0.88091	H	0.37996	4.08724	2.19377
H	1.90248	3.57549	2.29188	H	-4.8671	-4.0701	1.25842	C	3.46226	4.88884	1.11021
H	1.74207	2.71517	3.84306	H	-6.07239	-3.12345	0.37281	H	2.67117	4.66505	3.06467
O	0.3952	2.16751	2.36148	C	-5.20801	-2.1104	2.06314	H	4.4168	5.2998	1.42782
C	-0.63642	2.82358	3.05448	H	-5.23233	-1.07477	1.69256	O	5.59027	-0.68209	0.17159
H	-0.67328	2.47386	4.09898	H	-6.15098	-2.30831	2.58353	C	6.02369	0.53377	0.74474
H	-0.46645	3.91226	3.08299	O	-4.20081	-2.26656	3.04137	H	6.75847	0.25786	1.50694
C	-1.96469	2.59948	2.35016	C	-2.91367	-1.8087	2.67321	H	6.53131	1.1582	-0.00924
H	-1.92056	3.04294	1.35538	H	-2.47976	-1.31338	3.5494	C	4.91595	1.34718	1.40011
H	-2.74581	3.11551	2.93199	H	-2.98475	-1.06488	1.86938	H	4.1237	1.59133	0.68582
O	-2.32476	1.25296	2.13807	C	-2.00432	-2.96486	2.23901	H	5.34347	2.29931	1.7509
C	-2.43739	0.46272	3.3025	H	-1.71329	-3.55837	3.11041	O	4.40604	0.61857	2.50134
H	-2.95257	1.02381	4.09725	H	-2.54614	-3.62006	1.54811	C	3.00185	0.60349	2.63014
H	-1.44171	0.17393	3.67225	O	-0.80825	-2.48776	1.65525	H	2.59179	1.62465	2.64788
C	-3.23738	-0.79021	2.98363	C	-0.97627	-2.04878	0.31553	H	2.81102	0.14121	3.60325
H	-2.77359	-1.33044	2.14655	H	-0.23201	-1.26394	0.15497	C	2.28324	-0.19973	1.55443
H	-3.21627	-1.44697	3.85958	H	-1.96244	-1.59891	0.17236	H	2.91807	-1.0359	1.23284
O	-4.59689	-0.50685	2.71338	C	-0.81272	-3.16613	-0.70418	H	1.34959	-0.6168	1.9658
C	-4.86448	-0.23251	1.34522	H	-1.35521	-4.05572	-0.37104	O	1.98001	0.64194	0.45645
H	-3.98877	0.22528	0.88908	H	-1.25707	-2.83968	-1.65891	C	1.40149	-0.07053	-0.60772
H	-5.673	0.50642	1.33314	O	0.52598	-3.56826	-0.91282	H	2.05934	-0.89667	-0.8863
C	3.23711	-0.71712	2.69019	C	1.26591	-2.62176	-1.64332	H	0.43559	-0.50077	-0.31028
H	2.9075	-0.91419	1.66276	H	0.77599	-2.40451	-2.60733	C	1.15069	0.83434	-1.79585
H	2.83281	-1.52345	3.3115	H	1.36928	-1.67452	-1.09659	H	0.29601	1.47981	-1.63463
C	4.75627	-0.80622	2.78658	C	2.65898	-3.17306	-1.86593	H	0.93258	0.19838	-2.6594
H	5.03072	-1.85235	2.5789	H	3.07486	-3.47363	-0.89715	O	2.29082	1.5911	-2.17731
H	5.07226	-0.56679	3.80567	H	2.64216	-4.05364	-2.52425	H	4.09135	4.69037	-0.93614
O	5.50148	0.06784	1.95588	O	3.42008	-2.13242	-2.44983	C	4.91333	-0.51099	-1.05041
C	-6.50684	-2.07568	1.01815	C	4.81319	-2.29426	-2.30632	H	4.03737	0.13632	-0.93263
H	-7.05856	-1.61916	1.83558	H	5.1375	-3.2677	-2.70895	H	5.57744	-0.03867	-1.79495
C	4.33215	-2.02106	-0.75274	H	5.27439	-1.51838	-2.93018	C	4.47955	-1.85356	-1.5997
C	5.36541	-1.35073	-0.06139	C	-6.60354	-0.82253	-1.09516	H	5.34987	-2.50495	-1.76325
C	4.58345	-3.30341	-1.26934	H	-7.12741	-1.76189	-1.2531	H	4.00549	-1.66815	-2.57512
C	6.60333	-1.98133	0.08312	C	4.8329	-1.71067	0.22282	O	3.56938	-2.48994	-0.71913
C	5.82067	-3.91143	-1.11767	C	5.47633	-2.48883	1.1851	C	2.64446	-3.31935	-1.40054
H	3.79146	-3.81928	-1.80527	C	5.33171	-1.65754	-1.07902	H	3.18266	-3.97633	-2.10006
C	6.83888	-3.24767	-0.43597	C	6.6192	-3.21399	0.84566	H	1.96382	-2.70221	-1.99829
H	7.38645	-1.46457	0.63163	H	5.08303	-2.53152	2.21115	C	3.16318	4.7754	-0.36341
H	5.99091	-4.89967	-1.53336	C	6.47438	-2.38199	-1.41815	C	2.68679	-5.16651	0.22334
H	7.80995	-3.71604	-0.30907	C	7.1183	-3.15999	-0.45557	H	3.74432	-5.2178	-0.02136
C	5.1933	0.01674	0.57494	H	7.12632	-3.82769	1.60427	C	2.69085	2.74033	-1.59057
H	5.88545	0.72643	0.11115	H	6.86779	-2.33991	-2.44412	H	3.64768	2.50247	-1.17488
H	4.18436	0.39246	0.40488	H	8.0187	-3.73163	-0.72345	H	2.82135	3.34992	-2.46021

S. 18. GEOMETRIES : DTE-O₆

CF				AP				P			
C	4.07455	-2.96633	0.894	C	2.57662	1.44556	-0.15378	C	2.40662	0.43556	0.02419
C	3.04035	-1.98247	0.42945	C	1.40724	1.75802	0.60647	C	3.27893	1.49915	0.45853
C	3.5944	-0.6191	0.48974	C	1.46717	1.35534	1.91602	C	4.19488	1.11897	1.40289
C	4.9406	-0.67393	1.15123	S	3.02928	0.67848	2.25014	S	4.00542	-0.5536	1.78124
C	5.38305	-2.14689	0.97578	C	3.59046	0.94377	0.6182	C	2.68855	-0.74567	0.65656
C	2.92697	0.43727	-0.0449	C	0.40766	2.69741	0.07123	C	3.27156	2.8456	-0.14067
C	1.727	0.05839	-0.91769	C	-0.89016	2.62939	-0.22932	C	2.35788	3.82228	-0.02341
C	0.88934	-0.9828	-0.17044	C	-1.39372	3.97189	-0.7448	C	2.81705	5.05703	-0.76581
C	1.75554	-2.21867	0.06306	C	-0.11568	4.78779	-1.00978	C	3.82584	4.51073	-1.79242
S	0.8321	1.61516	-1.25412	C	0.88947	4.13555	-0.05287	C	4.36479	3.23466	-1.10696
C	2.15284	2.5649	-0.65987	C	-1.85346	1.51639	-0.27444	C	1.11046	3.84477	0.75551

C	3.13993	1.883	-0.01367	C	-1.794	0.55437	-1.24694	C	1.09542	3.84188	2.12879
C	0.998	-3.44875	-0.12253	S	-3.23233	-0.39263	-1.24596	S	-0.5112	4.03016	2.72373
C	-0.19293	-3.23239	-0.74914	C	-3.93129	0.5409	0.04687	C	-1.16669	4.12101	1.11316
S	-0.56661	-1.55475	-1.14775	C	-3.06272	1.48229	0.5005	C	-0.00668	3.96069	0.39092
C	2.27413	-0.42834	-2.28147	C	-0.70338	0.33105	-2.24857	C	2.25787	3.71208	3.06361
C	0.3884	-0.52278	1.21337	F	0.82996	4.75298	1.16106	F	5.54476	3.5135	-0.49593
F	5.88265	0.13148	0.60849	F	2.15676	4.27588	-0.49321	F	4.60187	2.25467	-2.00599
F	4.88807	-0.3849	2.48299	F	-0.27582	6.10353	-0.80082	F	4.78951	5.38607	-2.10888
F	6.03163	-2.25262	-0.20313	F	0.29273	4.59281	-2.28125	F	3.15816	4.16721	-2.91477
F	6.19362	-2.56385	1.95692	F	-2.13277	3.83382	-1.86755	F	1.83138	5.76074	-1.35613
F	3.79559	-3.46279	2.13261	F	-2.15681	4.64071	0.15828	F	3.45469	5.90219	0.08842
F	4.25531	-4.02898	0.07382	C	0.43485	1.53	2.98925	C	5.25375	1.93595	2.07985
H	1.23194	-0.26906	1.86109	H	0.87912	1.49559	3.98773	H	6.25406	1.65257	1.73743
H	-0.25494	0.34637	1.12646	H	-0.06592	2.49635	2.87442	H	5.11724	2.99624	1.8603
H	-0.17834	-1.33212	1.67932	H	-0.32741	0.7456	2.93004	H	5.21795	1.80502	3.16565
H	2.89243	-1.31983	-2.15396	H	0.1455	-0.19361	-1.79552	H	2.05659	4.18934	4.0259
H	1.45919	-0.65617	-2.97241	H	-1.05105	-0.2551	-3.10176	H	2.49481	2.65794	3.24679
H	2.89215	0.3622	-2.71637	H	-0.34173	1.29372	-2.62735	H	3.14198	4.18563	2.62779
C	4.29993	2.53664	0.68821	C	-3.36585	2.39688	1.65495	C	0.01914	3.88042	-1.10913
H	4.51508	2.02096	1.62667	H	-2.444	2.73361	2.13538	H	1.02628	3.6942	-1.48692
H	5.2087	2.51562	0.08189	H	-3.91166	3.29035	1.33862	H	-0.63792	3.07488	-1.45719
H	4.07275	3.57891	0.92128	H	-3.97284	1.88031	2.40473	H	-0.34069	4.8126	-1.55604
C	1.42869	-4.81727	0.33489	C	2.64272	1.71516	-1.63577	C	1.32116	0.63758	-0.99077
H	2.18613	-5.24786	-0.32441	H	1.63745	1.7645	-2.06321	H	1.68467	1.21117	-1.85
H	1.85662	-4.76997	1.33697	H	3.13032	2.66624	-1.86492	H	0.94643	-0.32169	-1.35156
H	0.57311	-5.49435	0.35828	H	3.18959	0.92176	-2.153	H	0.47815	1.18986	-0.55758
C	-1.17723	-4.23344	-1.19121	C	-5.30176	0.28594	0.55003	C	2.16573	-2.10772	0.39133
C	-2.50778	-4.23877	-0.78946	C	-5.68667	-0.87561	1.23149	C	1.62638	-2.92962	1.39583
C	-0.77458	-5.28738	-2.0449	C	-6.16235	1.38422	0.56944	C	2.15944	-2.55762	-0.9377
C	-1.55787	-6.39092	-2.37823	C	-7.43093	1.29793	1.08581	C	1.63196	-3.79553	-1.27636
H	0.24093	-5.23638	-2.42891	H	-5.83612	2.31064	0.10521	H	2.59536	-1.92379	-1.70467
C	-2.85649	-6.50923	-1.82236	C	-7.84953	0.10363	1.65925	C	1.14037	-4.62752	-0.27441
H	-1.1322	-7.16036	-3.0183	H	-8.07389	2.17184	1.07928	H	1.62839	-4.1184	-2.31288
H	-3.51731	-7.34853	-1.98811	H	-8.80736	0.02275	2.16407	H	0.75186	-5.61156	-0.51877
C	2.27547	4.02	-0.88448	O	-3.61679	-4.67257	-1.55716	O	-2.15003	-0.9561	2.18959
C	1.4343	5.1187	-0.54706	C	-2.32384	-5.15652	-1.43398	C	-3.40746	-1.46292	2.58853
C	3.37869	4.42168	-1.64902	H	-1.846	-5.0217	-2.41091	H	-3.30938	-2.20487	3.38844
C	3.7645	5.73786	-1.82347	H	-2.32573	-6.2399	-1.22687	H	-4.04306	-0.64978	2.96899
H	3.97847	3.61505	-2.06213	C	-1.53794	-4.44192	-0.34752	C	-4.05331	-2.13074	1.38465
C	3.01103	6.76376	-1.31182	H	-2.13601	-4.41784	0.57372	H	-4.1433	-1.41258	0.5646
H	4.68858	5.90737	-2.36651	H	-0.61969	-5.00373	-0.12361	H	-5.05747	-2.48439	1.65587
H	3.34398	7.79147	-1.41785	O	-1.26929	-3.08081	-0.65274	O	-3.25321	-3.23746	1.00766
O	-7.03713	1.91288	0.87536	C	-0.03565	-2.87243	-1.30688	C	-2.88172	-3.33143	-0.34673
C	-6.49443	1.20097	1.9636	H	-0.15628	-1.96125	-1.90665	H	-3.76485	-3.35009	-1.0038
H	-6.04627	0.25829	1.63975	H	0.22364	-3.68558	-2.00004	H	-2.37656	-4.29886	-0.42935
H	-7.26236	0.91212	2.70032	C	1.03844	-2.6067	-0.24866	C	-1.9267	-2.2599	-0.85192
C	-5.33487	2.07472	2.3404	H	0.69478	-1.7551	0.34543	H	-1.1371	-2.07171	-0.10986
H	-4.97473	1.73335	3.32115	H	1.14776	-3.46525	0.42706	H	-1.45154	-2.63625	-1.7721
H	-5.53347	3.15476	2.41546	O	2.28198	-2.19283	-0.77444	O	-2.63347	-1.06912	-1.13679
O	-4.37638	1.83494	1.35655	C	2.96916	-3.15962	-1.53657	C	-1.8964	-0.18318	-1.94915
C	-3.08094	2.07536	1.83597	H	3.94789	-2.70539	-1.70399	H	-0.90349	0.00821	-1.52012
H	-3.05118	2.9881	2.4517	H	2.52398	-3.3049	-2.53412	H	-1.75107	-0.62597	-2.94808
H	-2.74398	1.23681	2.46793	C	3.12196	-4.54732	-0.88581	C	-2.63269	1.13864	-2.08327
C	-2.12247	2.16553	0.64603	H	2.21309	-5.12724	-1.06621	H	-3.70712	0.92927	-2.19735
H	-2.00361	1.1585	0.23044	H	3.94931	-5.06988	-1.38556	H	-2.29675	1.64487	-2.9923
H	-1.14001	2.49266	1.00701	O	3.25524	-4.61174	0.51548	C	-1.09473	-1.16968	3.10545
O	-2.58017	2.94391	-0.41117	C	4.95292	0.52658	0.19101	H	-0.25838	-0.57234	2.73085
C	-2.90096	4.30051	-0.17912	C	5.7059	-0.5045	0.76667	H	-1.35902	-0.80197	4.10628
H	-2.93275	4.53544	0.89046	C	5.53812	1.40271	-0.76822	C	-0.72501	-2.65915	3.12214
H	-3.91635	4.44164	-0.57265	C	6.84189	1.28896	-1.23842	H	-0.87101	-3.03262	2.10351
C	-2.03947	5.30169	-0.93753	H	4.90145	2.17478	-1.17129	H	-1.39991	-3.22048	3.77382
H	-1.82881	4.85265	-1.92167	C	7.64672	0.39249	-0.56609	O	0.56388	-2.95067	3.6317
H	-2.70151	6.1581	-1.11015	H	7.21256	1.93862	-2.02547	C	1.66099	-2.50441	2.85332
O	-0.86197	5.85084	-0.39809	H	8.70545	0.25954	-0.76836	H	2.54175	-2.92019	3.35358
C	0.07879	5.01877	0.24165	C	4.18769	-3.81645	1.2283	H	1.75189	-1.41127	2.90342
H	0.19528	5.52213	1.20121	H	3.72379	-2.85096	1.47466	O	-2.38987	2.06187	-1.04336
H	-0.46506	4.09031	0.31187	H	4.36047	-4.35272	2.16871	C	-2.85879	1.21796	0.00072
C	-7.87076	1.24836	-0.08223	C	5.5291	-3.60093	0.53905	H	-2.56491	1.71806	0.92501
H	-7.5842	1.59876	-1.07608	H	6.07492	-4.5393	0.41108	H	-2.38623	0.23145	-0.03578
H	-8.92354	1.48982	0.11698	H	5.39369	-3.1415	-0.44521	C	-4.36628	1.02959	0.01577
C	-7.67796	-0.23969	0.10156	O	6.4325	-2.78138	1.26286	H	-4.72121	0.33015	0.77624

H	-8.40704	-0.89784	-0.38592	C	5.94563	-1.64053	1.87049	H	-4.89458	0.80478	-0.92041
H	-7.80836	-0.23855	1.18987	H	5.01767	-1.80376	2.44369	O	-4.37795	2.36411	0.4988
O	-6.38449	-0.56175	-0.31133	H	6.68267	-1.35579	2.61982	C	1.15554	-4.19757	1.04661
C	-5.85872	-1.74674	0.17329	C	-4.40767	-5.08516	-0.50054	H	0.7524	-4.83801	1.82558
H	-6.24113	-1.96899	1.18705	H	-4.98497	-5.97769	-0.77353	C	-2.68766	4.35023	1.18872
H	-6.15585	-2.59149	-0.46644	H	-3.80662	-5.37322	0.37313	C	-3.32199	4.41946	2.42903
C	-4.32181	-1.61383	0.26815	C	-5.38722	-3.99568	-0.15046	C	-3.43096	4.4889	0.01625
H	-3.91297	-1.96973	-0.70304	H	-6.09284	-3.88945	-0.98637	C	-4.7002	4.62717	2.49707
H	-4.11171	-0.52683	0.26521	H	-5.95509	-4.32576	0.73272	H	-2.73632	4.31092	3.35342
O	-3.62283	-2.47594	1.08128	O	-4.74761	-2.73968	0.00282	C	-4.80865	4.69601	0.08428
C	-3.7451	-3.44768	0.0809	C	-4.88302	-2.1543	1.25767	C	-5.44327	4.76479	1.32484
H	-4.3715	-3.74927	-0.634	H	-3.9903	-2.0667	1.89367	H	-5.20025	4.682	3.47494
H	-3.99336	-4.06215	0.94283	H	-5.46275	-2.83413	1.9254	H	-5.39461	4.80498	-0.8398
C	-3.21273	-5.37388	-1.14273	C	-7.04036	-1.01888	1.51263	H	-6.52931	4.92884	1.37815
H	-3.95594	-5.6171	-0.36902	H	-7.49553	-2.00184	1.40388	C	-4.10345	3.37311	-0.47663
C	1.7996	6.45752	-0.67447	C	6.99194	-0.39005	0.37179	H	-4.73941	3.23114	-1.32533
H	1.03403	7.20894	-0.50712	H	7.7118	-0.83187	1.04545	H	-3.08029	3.30482	-0.78222