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A DFT Mechanistic Study of the Organocatalytic Asymmetric Reaction of Aldehydes and Homophthalic Anhydride

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Supplementary Information

1. Experimental Section

- General procedure for the synthesis of product **19a**.
- ^{1}H, ^{13}C, ^{19}F NMR spectra and HPLC chromatograms of the final compound (**19a**).

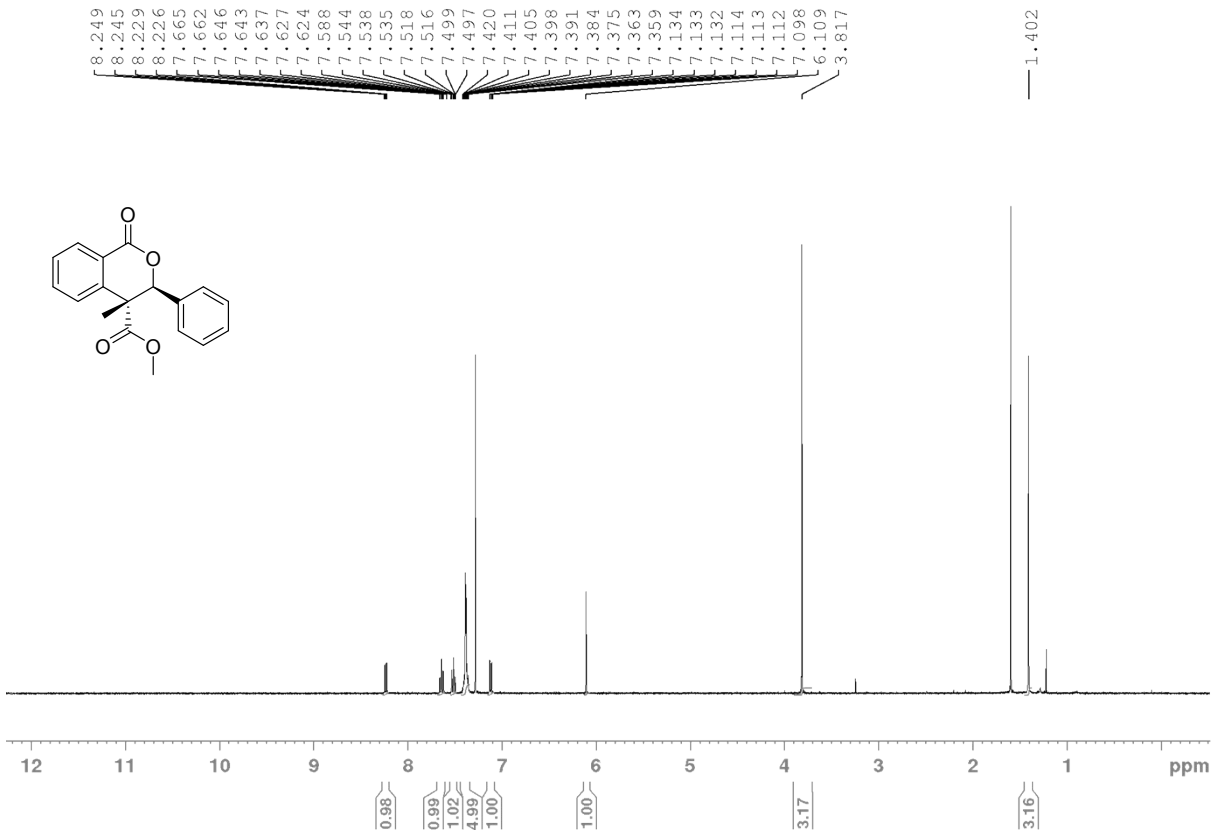
2. Computational study

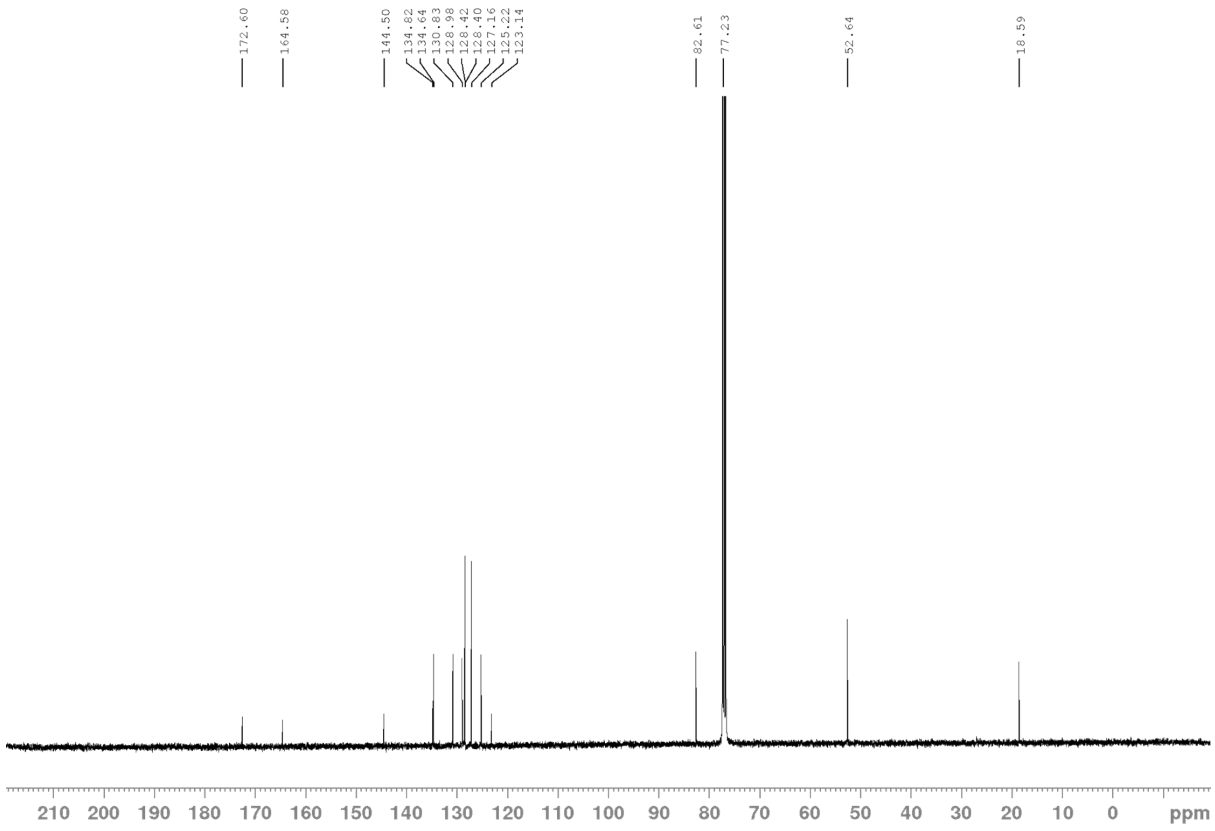
- **Table S1.** G3B3 Optimized Geometries (Cartesian Coordinates in Å) of the Stationary Points in PCM-THF.
- **Fig. S1.** Molecular electrostatic potential (MEP) on the 0.001 a.u. electron density isosurface of the catalyst **3**.
- **Fig. S2.** Molecular graph (QTAIM) for all the complexes in PCM-THF.
- **Table S2.** Electron density [ρ(BCP), a.u.] and Laplacian [$\nabla^2\rho$(BCP), a.u.] in PCM-THF.
- **Fig. S3.** Electron Density Shifts of the structures TS **15a-16a** and complex **16a** for the ***trans*-(*R,R)*** pathway.
- **Fig. S4.** Potential energy surface for all complexes formed (**15**, **16** and **17**) along the two pathways corresponding to the two major products for the reaction with methylhomophthalic anhydride.
- **Table S3.** Relative energies for all TSs and intermediates formed along the four different pathways for the reaction with methylhomophthalic anhydride in PCM-THF.
- **Fig. S5.** Optimised geometries of TS**15-16** for the different pathways corresponding to the reaction with methylhomophthalic anhydride.

Experimental section

Prepared according to the procedure[1] using benzaldehyde (**11**, 25 μl, 0.246 mmol), and anhydride[2] **18** (43.3 mg, 0.246 mmol). Upon esterification, the reaction gave a mixture of esters in a >99 : 1 (*trans* : *cis*) ratio. The major ester (*trans*-**19**) was purified by flash chromatography, eluting in gradient from 100% hexanes to 10% EtOAc in hexanes, to give a white solid (68.5 mg 94%). M.p. 133-135 °C; TLC (hexanes : EtOAc, 9 : 1 v/v): R*f* = 0.26; $[\alpha]^{20} = +36$ (*c* = 0.05, $CHCl_3$); CSP-HPLC analysis: Chiralcel ODH (4.6 mm x 25 cm), hexane/IPA: 85/15, 0.6 mL min^{-1}, RT, UV detection at 254 nm, retention time: 40.92 min (major enantiomer); δ_H (400 MHz, $CDCl_3$): 8.21 (1H, d, $J = 8$), 7.62 (1H, t, $J = 7.7$), 7.49 (1H, t, $J = 7.7$), 7.36 (5H, m), 7.12 (1H, d, $J = 7.8$), 6.08 (1H, s), 3.79 (3H, s), 1.37 (3H, s); δ_c (100 MHz, $CDCl_3$): 172.6, 164.5, 144.5,m 134.8, 134.6, 130.8, 128.9, 128.4, 128.3 2C), 127.1 (2C), 125.2, 123.1, 82.6, 77.2, 52.6, 18.5; υ_{max} (neat)/cm^{-1}): 3292, 3080, 2950, 1719, 1600, 1454, 1383, 1291, 1249, 1125, 1098, 1056, 976, 801, 758, 691; HRMS (m/z – ESI): Found: 319.0941 (M^+ + Na) $C_{18}H_{16}NaO_4$ requires: 319.0940.

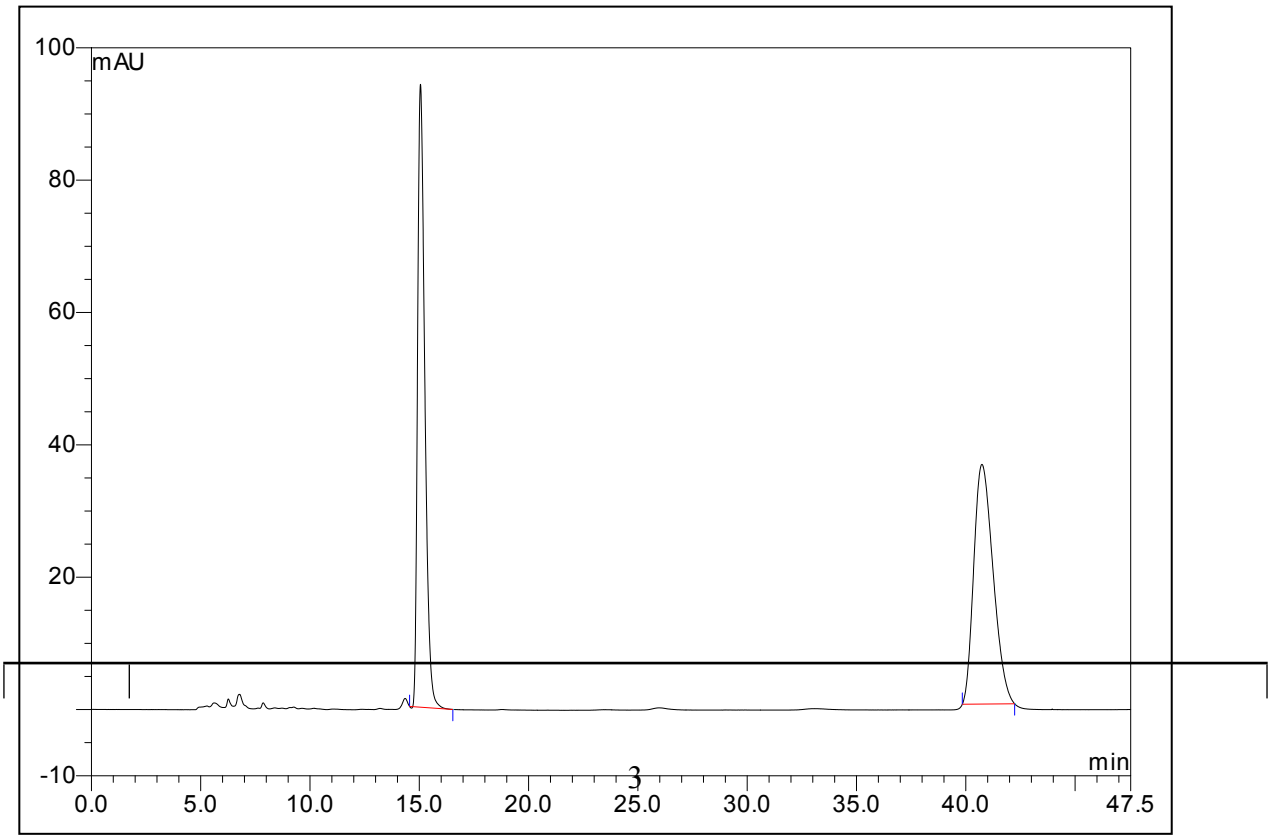
19a





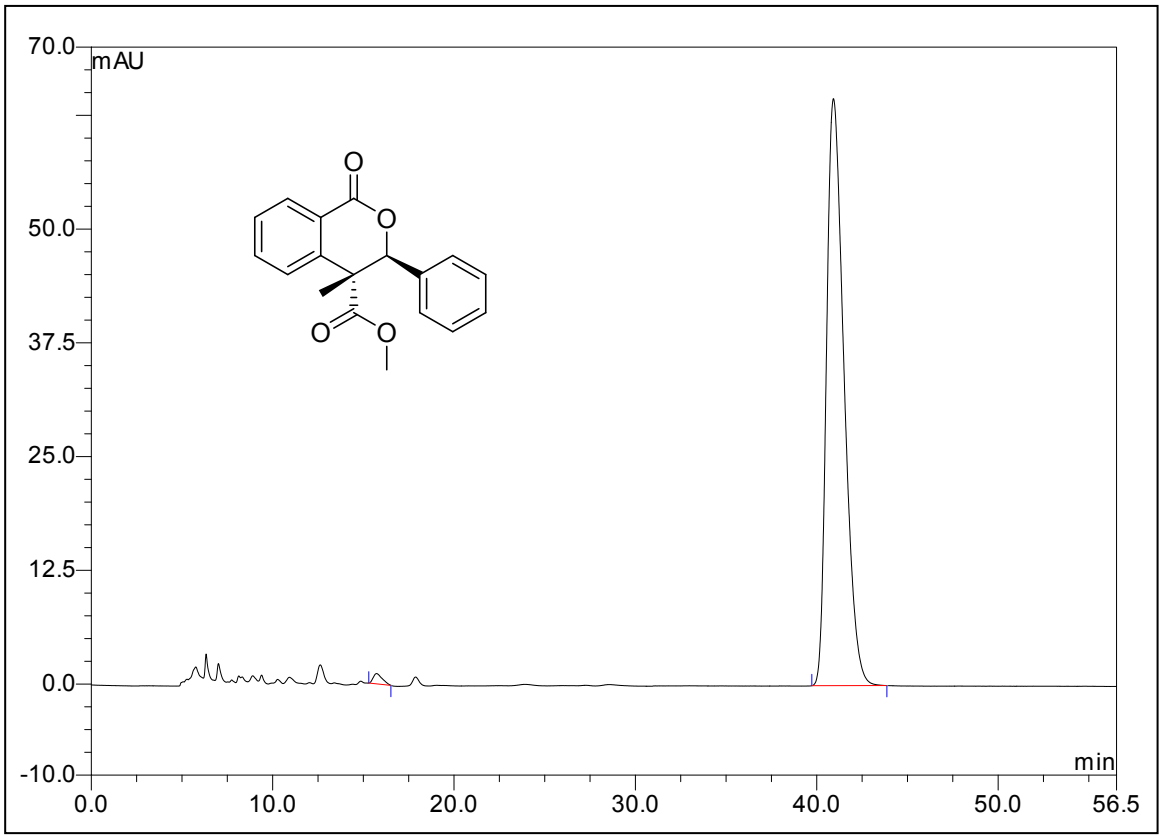
HPLC Data

Racemic			
Control Program:	**85H15IPA06mlmin**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:	**26/09/2016 10:57**	*Sample Weight:*	**1.0000**
Run Time (min):	**47.54**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	15.05	n.a.	94.125	36.098	49.33	n.a.	BMB*
2	40.73	n.a.	36.214	37.083	50.67	n.a.	BMB*
Total:			130.340	73.180	100.00	0.000	

Sample Name:	**19a**	*Injection Volume:*	**20.0**
Vial Number:	**RB5**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**254**
Control Program:	**85H15IPA06mlmin**	*Bandwidth:*	**n.a.**
Quantif. Method:	**fmm**	*Dilution Factor:*	**1.0000**
Recording Time:	**01/04/2017 20:14**	*Sample Weight:*	**1.0000**
Run Time (min):	**56.53**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	15.73	n.a.	1.135	0.659	0.91	n.a.	BMB*
2	40.92	n.a.	64.516	71.972	99.09	n.a.	BMB*
Total:			65.651	72.631	100.00	0.000	

Computational Study

The geometry of the isolated molecules as well as those of the different stationary structures of the Potential Energy Surface (PES) were optimized by using the B3LYP[3] density functional theory (DFT) approach, which combines the Becke's three-parameter nonlocal hybrid exchange potential with the nonlocal correlation functional of Lee, Yang and Parr with standard 6-31G(d)[4] basis sets. Vibrational analyses were performed to confirm that the different optimized structures corresponded to true minima of the PES or to transition states. All these calculations were carried out with the Gaussian09 program.[5] The self-consistent reaction field (SCRF) calculations using the PCM solvation model were carried out re-optimising the gas-phase optimised structures. The dielectric constant in the PCM calculations was set to $\varepsilon = 2.379$ to simulate tetrahydrofuran (THF) similar to the solvent medium used in the experimental studies. Finally, more reliable energies for both local minima and transition states were re-evaluated at the B3LYP/6-31+G(d,p) in PCM-THF conditions.

The characteristics of the intermolecular interactions were analysed by means of the Atoms in Molecules (QTAIM) theory.[6] For this purpose we have located the most relevant bond critical points (BCP), and evaluated the electron density at each of them, by using the QTAIMAll program.[7]

Table S1. G3B3 Optimized Geometries (Cartesian Coordinates in Å) of the Stationary Points in PCM-THF.

***trans*-(*R,R*)**

Complex 15a				TS **15a-16a**				**Complex 16a**			
C	0.4942	3.3402	0.9425	C	0.1632	-2.5800	-2.1817	C	0.0433	-2.7677	-2.0742
C	0.3101	1.9937	0.3782	C	0.1563	-1.6395	-1.0478	C	0.0489	-1.7570	-0.9960
C	1.6641	1.9153	-0.0199	C	1.5368	-1.8242	-0.8136	C	1.4220	-1.9686	-0.7383
C	1.9473	3.2828	0.4957	C	1.6440	-2.8113	-1.9250	C	1.5175	-3.0126	-1.7917
O	2.9068	4.0356	0.5563	O	2.5140	-3.5044	-2.4259	O	2.3759	-3.7524	-2.2467
O	-0.2274	4.1375	1.5355	O	-0.6731	-2.9723	-2.9885	O	-0.7934	-3.1998	-2.8567
N	2.3136	0.9011	-0.6305	N	2.3383	-1.2450	0.1063	N	2.2307	-1.3608	0.1629
N	-0.7206	1.1397	0.3265	N	-0.8008	-0.8725	-0.4987	N	-0.8851	-0.9405	-0.4946
H	1.7350	0.0798	-0.8479	H	1.8860	-0.5502	0.7066	H	1.7902	-0.6379	0.7325
C	3.6749	0.7606	-0.9265	C	3.7072	-1.4288	0.3514	C	3.5910	-1.5679	0.4332
C	4.0765	-0.4639	-1.4824	C	4.2722	-0.6669	1.3867	C	4.1693	-0.7703	1.4340
C	4.6316	1.7565	-0.6809	C	4.5119	-2.3175	-0.3743	C	4.3777	-2.5132	-0.2390
C	5.4208	-0.6977	-1.7597	C	5.6252	-0.7937	1.6868	C	5.5154	-0.9189	1.7541

H	3.3330	-1.2272	-1.6906	H	3.6507	0.0206	1.9515	H	3.5626	-0.0422	1.9632
C	5.9692	1.5034	-0.9825	C	5.8655	-2.4249	-0.0549	C	5.7236	-2.6457	0.1036
H	4.3351	2.7098	-0.2538	H	4.0878	-2.9175	-1.1735	H	3.9466	-3.1310	-1.0212
C	6.3833	0.2810	-1.5145	C	6.4385	-1.6722	0.9699	C	6.3089	-1.8591	1.0953
H	7.4279	0.0961	-1.7305	H	7.4913	-1.7675	1.2050	H	7.3551	-1.9751	1.3488
C	6.9844	2.5989	-0.7831	C	6.7401	-3.3296	-0.8841	C	6.5421	-3.7134	-0.5761
C	5.8313	-2.0564	-2.2591	C	6.2027	-0.0178	2.8409	C	6.1354	-0.0062	2.7786
F	7.1097	3.3672	-1.8917	F	6.0669	-4.4069	-1.3405	F	6.3884	-4.9159	0.0276
F	6.6495	3.4253	0.2306	F	7.2324	-2.6856	-1.9698	F	6.1864	-3.8770	-1.8685
F	8.2132	2.1035	-0.5118	F	7.8038	-3.7828	-0.1839	F	7.8632	-3.4294	-0.5522
F	5.9128	-2.9552	-1.2423	F	5.5569	1.1538	3.0360	F	6.6228	1.1225	2.2079
F	4.9419	-2.5594	-3.1430	F	6.1163	-0.7099	4.0014	F	5.2418	0.3857	3.7140
F	7.0381	-2.0378	-2.8609	F	7.5098	0.2665	2.6518	F	7.1661	-0.5947	3.4218
H	-0.5620	0.2525	-0.1780	H	-0.5735	-0.3992	0.3763	H	-0.6562	-0.4285	0.3552
C	-2.1013	1.5587	0.6184	C	-2.2255	-1.0857	-0.8130	C	-2.3149	-1.0723	-0.8377
C	-2.9376	1.6305	-0.6628	C	-2.9408	-1.7559	0.3647	C	-3.0771	-1.6372	0.3657
C	-3.2546	2.8800	-1.2863	C	-3.3869	-3.1144	0.3150	C	-3.5839	-2.9752	0.3944
C	-3.3683	0.4658	-1.2631	C	-3.1328	-1.0399	1.5287	C	-3.2506	-0.8466	1.4837
C	-2.8664	4.1554	-0.7887	C	-3.2269	-3.9776	-0.8047	C	-3.4482	-3.9112	-0.6687
C	-4.0115	2.8062	-2.5036	C	-4.0283	-3.6140	1.4980	C	-4.2620	-3.3737	1.5948
C	-4.1345	0.4964	-2.4603	C	-3.7890	-1.6201	2.6481	C	-3.9427	-1.3281	2.6279
H	-3.1003	-0.4931	-0.8374	H	-2.7560	-0.0269	1.6103	H	-2.8345	0.1541	1.5081
C	-3.2149	5.3071	-1.4729	C	-3.6896	-5.2809	-0.7522	C	-3.9701	-5.1868	-0.5462
H	-2.2706	4.2323	0.1112	H	-2.7095	-3.6315	-1.6896	H	-2.9045	-3.6409	-1.5638
C	-4.3501	4.0156	-3.1755	C	-4.4966	-4.9593	1.5070	C	-4.7914	-4.6937	1.6767
C	-3.9656	5.2322	-2.6792	C	-4.3354	-5.7718	0.4169	C	-4.6532	-5.5770	0.6395
H	-4.9237	3.9370	-4.0936	H	-4.9829	-5.3167	2.4091	H	-5.3053	-4.9742	2.5907
H	-4.2190	6.1586	-3.1851	H	-4.6865	-6.7989	0.4170	H	-5.0510	-6.5855	0.6953
O	-2.8923	6.5691	-1.0871	O	-3.5782	-6.1861	-1.7586	O	-3.8855	-6.1553	-1.4957
N	-4.4375	1.6419	-3.0569	N	-4.2224	-2.8740	2.6191	N	-4.4339	-2.5602	2.6679
C	-2.1821	6.7449	0.1391	C	-2.9671	-5.7703	-2.9803	C	-3.2479	-5.8362	-2.7328
H	-2.0329	7.8204	0.2424	H	-2.9749	-6.6476	-3.6283	H	-3.2864	-6.7486	-3.3293
H	-1.2126	6.2358	0.1209	H	-1.9365	-5.4355	-2.8208	H	-2.2057	-5.5343	-2.5825
H	-2.7672	6.3714	0.9883	H	-3.5396	-4.9611	-3.4499	H	-3.7828	-5.0330	-3.2540
C	-4.6208	-0.7589	-3.0943	C	-4.0129	-0.8440	3.8982	C	-4.1418	-0.4713	3.8294
C	-4.9840	-0.7578	-4.4525	C	-4.2881	-1.5237	5.0979	C	-4.4807	-1.0665	5.0577
C	-4.7387	-1.9585	-2.3706	C	-3.9662	0.5612	3.9211	C	-4.0087	0.9278	3.7801
C	-5.4389	-1.9202	-5.0703	C	-4.4992	-0.8237	6.2832	C	-4.6714	-0.2919	6.1993
H	-4.9001	0.1672	-5.0125	H	-4.3299	-2.6073	5.0829	H	-4.5893	-2.1447	5.0991
C	-5.1963	-3.1216	-2.9911	C	-4.1807	1.2605	5.1093	C	-4.2028	1.7022	4.9246
H	-4.4958	-1.9925	-1.3129	H	-3.7824	1.1248	3.0114	H	-3.7709	1.4315	2.8482
C	-5.5453	-3.1091	-4.3427	C	-4.4450	0.5731	6.2953	C	-4.5321	1.0978	6.1391
H	-5.7077	-1.9000	-6.1232	H	-4.7034	-1.3690	7.2009	H	-4.9267	-0.7735	7.1396
H	-5.2813	-4.0376	-2.4131	H	-4.1462	2.3466	5.1044	H	-4.1012	2.7823	4.8622
H	-5.8987	-4.0165	-4.8250	H	-4.6095	1.1198	7.2198	H	-4.6812	1.7028	7.0293
C	-1.8787	1.7886	3.7218	C	-1.9846	0.3325	-3.5056	C	-2.0583	0.1780	-3.6080

C	-3.3177	2.1884	4.1207	C	-3.3276	-0.2097	-4.0500	C	-3.4590	-0.2383	-4.1431
H	-1.2428	1.5755	4.5830	H	-1.5208	1.0592	-4.1758	H	-1.5272	0.8072	-4.3291
C	-2.7631	0.6209	1.6514	C	-2.9750	0.2155	-1.2000	C	-2.9666	0.2505	-1.3215
C	-2.4968	-0.6099	3.7740	C	-3.0542	2.3028	-2.4914	C	-2.8901	2.2379	-2.6694
C	-4.3022	1.1245	3.5995	C	-4.4835	0.4013	-3.2333	C	-4.5342	0.4683	-3.2952
H	-3.5664	3.1654	3.6946	H	-3.3518	-1.3025	-3.9800	H	-3.5913	-1.3251	-4.0785
H	-3.3934	2.2783	5.2085	H	-3.4298	0.0468	-5.1090	H	-3.5656	0.0348	-5.1991
H	-2.7781	-0.3984	1.2628	H	-3.0523	0.8636	-0.3259	H	-3.0129	0.9431	-0.4763
C	-4.1910	1.0686	2.0646	C	-4.3864	-0.1033	-1.7795	C	-4.4157	-0.0345	-1.8439
C	-3.9344	-0.2443	4.2391	C	-4.3380	1.9467	-3.2846	C	-4.2696	1.9961	-3.3648
H	-2.4814	-1.5075	3.1524	H	-3.2749	2.7478	-1.5189	H	-3.0167	2.7826	-1.7281
H	-1.8045	-0.7462	4.6063	H	-2.3972	2.9873	-3.0286	H	-2.2352	2.8418	-3.3041
H	-5.3237	1.3910	3.8848	H	-5.4451	0.1056	-3.6624	H	-5.5330	0.2460	-3.6853
H	-4.9261	0.3812	1.6391	H	-5.1603	0.3493	-1.1537	H	-5.1565	0.4451	-1.1966
H	-4.4116	2.0601	1.6546	H	-4.5654	-1.1831	-1.7606	H	-4.6357	-1.1083	-1.8207
H	-3.9259	-0.0988	5.3252	H	-4.1986	2.2293	-4.3350	H	-4.1882	2.2671	-4.4253
H	-2.0344	2.5532	1.0556	H	-2.2375	-1.7492	-1.6750	H	-2.3497	-1.7823	-1.6612
N	-1.9299	0.5069	2.9216	N	-2.2354	1.0600	-2.2142	N	-2.1741	0.9697	-2.3568
C	-4.9145	-1.3468	3.9212	C	-5.5362	2.6965	-2.7619	C	-5.3632	2.8351	-2.7609
C	-5.7602	-1.8723	4.8088	C	-6.2966	3.5072	-3.4993	C	-6.1059	3.7175	-3.4328
H	-4.9040	-1.7265	2.8995	H	-5.7764	2.5564	-1.7073	H	-5.5395	2.7055	-1.6916
H	-6.4580	-2.6583	4.5334	H	-7.1560	4.0218	-3.0782	H	-6.8835	4.2999	-2.9453
H	-5.7876	-1.5374	5.8441	H	-6.0885	3.6874	-4.5523	H	-5.9637	3.8913	-4.4981
C	2.7773	-1.5368	2.8369	C	1.8733	3.4524	-1.7415	C	2.1286	3.1941	-1.8877
C	3.5622	-2.1612	1.8540	C	1.3680	4.5608	-2.4290	C	1.7408	4.2165	-2.7590
C	4.8288	-2.6454	2.1723	C	2.2276	5.4225	-3.1131	C	2.6963	4.8916	-3.5227
C	5.3066	-2.5169	3.4793	C	3.6043	5.1840	-3.1177	C	4.0466	4.5529	-3.4217
C	4.5243	-1.9035	4.4679	C	4.1170	4.0757	-2.4368	C	4.4399	3.5289	-2.5551
C	3.2643	-1.4103	4.1502	C	3.2545	3.2162	-1.7549	C	3.4854	2.8532	-1.7948
H	3.1750	-2.2626	0.8440	H	0.2951	4.7233	-2.4276	H	0.6893	4.4681	-2.8410
H	5.4401	-3.1076	1.4037	H	1.8231	6.2793	-3.6463	H	2.3827	5.6826	-4.1987
H	6.2940	-2.8932	3.7318	H	4.2734	5.8525	-3.6531	H	4.7883	5.0777	-4.0175
H	4.9065	-1.8096	5.4800	H	5.1857	3.8775	-2.4440	H	5.4874	3.2508	-2.4774
H	2.6463	-0.9232	4.8981	H	3.6570	2.3473	-1.2365	H	3.8002	2.0486	-1.1326
C	1.4667	-1.0082	2.4531	C	0.9271	2.5046	-1.0207	C	1.1020	2.4469	-1.0515
O	0.6967	-0.4233	3.2170	O	-0.3458	2.5759	-1.3528	O	-0.2178	2.7119	-1.4448
C	-1.0942	-7.0325	-0.8928	C	0.7905	6.6323	1.1775	C	1.4474	6.6159	0.8879
C	-0.2884	-5.9634	-1.2369	C	1.3749	5.3770	1.0298	C	1.8331	5.2884	0.6961
C	-0.6116	-4.6416	-0.8279	C	0.5750	4.2273	0.9792	C	0.8857	4.2645	0.7692
C	-1.7958	-4.4728	-0.0525	C	-0.8211	4.3743	1.0761	C	-0.4504	4.5974	1.0439
C	-2.6066	-5.5747	0.2886	C	-1.4105	5.6420	1.2057	C	-0.8421	5.9324	1.2208
C	-2.2649	-6.8492	-0.1240	C	-0.6032	6.7703	1.2604	C	0.1107	6.9417	1.1445
H	-0.8215	-8.0327	-1.2207	H	1.4230	7.5143	1.2263	H	2.1950	7.4020	0.8360
H	0.6082	-6.1234	-1.8302	H	2.4538	5.2822	0.9509	H	2.8706	5.0485	0.4861
C	0.1927	-3.5172	-1.1644	C	1.1164	2.8792	0.7219	C	1.2368	2.8280	0.4997
C	-2.1696	-3.1437	0.3857	C	-1.6652	3.1805	1.0881	C	-1.4571	3.5399	1.1828

H	-3.4990	-5.3950	0.8801	H	-2.4907	5.7178	1.2757	H	-1.8832	6.1553	1.4289
H	-2.8866	-7.7001	0.1370	H	-1.0480	7.7543	1.3728	H	-0.1809	7.9771	1.2900
C	-0.1539	-2.2480	-0.7488	C	0.3300	1.7880	1.2895	C	0.3202	1.8662	1.1994
O	0.4151	-1.1384	-0.9416	O	0.7305	0.6541	1.5474	O	0.6171	0.7151	1.4752
O	-1.3287	-2.1154	0.0282	O	-1.0234	1.9669	1.3790	O	-0.9661	2.2338	1.4137
O	-3.1618	-2.8315	1.0435	O	-2.8725	3.1282	0.9847	O	-2.6552	3.6594	1.2000
H	-1.3773	2.5453	3.1166	H	-1.2628	-0.4625	-3.3232	H	-1.4296	-0.6956	-3.4243
H	1.0872	-3.6354	-1.7652	H	2.1758	2.7589	0.9412	H	2.2589	2.5978	0.8097
H	1.1905	-1.1462	1.3943	H	1.3759	1.4906	-1.0112	H	1.3244	1.3734	-1.1070
H	-0.9518	0.2291	2.6986	H	-1.3109	1.4644	-1.7992	H	-0.7040	1.8924	-1.7447

TS **16a-17a**			***trans*-(*R,R*)**	**Complex 15b *trans*-(*S,S*)**				TS **15b-16b**			
C	0.4792	-2.4468	-2.1820	C	-1.46107	-4.01254	0.225477	C	0.858396	-4.03006	-0.02695
C	0.4005	-1.5076	-1.0494	C	-1.19581	-2.56557	0.229154	C	0.750824	-2.56148	0.032708
C	1.8007	-1.5565	-0.8428	C	-2.56327	-2.2448	0.089948	C	2.145541	-2.39571	0.126822
C	1.9725	-2.5416	-1.9525	C	-2.94118	-3.68937	0.070085	C	2.372715	-3.86899	0.080128
O	2.8868	-3.1607	-2.4707	O	-3.96526	-4.34757	-0.02579	O	3.328315	-4.62643	0.099912
O	-0.3259	-2.9172	-2.9800	O	-0.77034	-5.02003	0.312982	O	0.063934	-4.95324	-0.13211
N	2.5885	-0.9126	0.0434	N	-3.15059	-1.03022	0.015093	N	2.86079	-1.25289	0.225984
N	-0.6494	-0.8517	-0.5180	N	-0.07763	-1.8339	0.35477	N	-0.28117	-1.70488	-0.03597
H	2.1270	-0.2551	0.6771	H	-2.49621	-0.23006	0.032614	H	2.303262	-0.39305	0.256184
C	3.9851	-0.9760	0.2125	C	-4.50888	-0.7139	-0.13573	C	4.247657	-1.07111	0.308178
C	4.5575	-0.0731	1.1237	C	-4.85643	0.647258	-0.15387	C	4.711038	0.245492	0.46457
C	4.8058	-1.8850	-0.4676	C	-5.51229	-1.6853	-0.2695	C	5.169198	-2.12473	0.238886
C	5.9305	-0.0918	1.3515	C	-6.18811	1.02225	-0.31545	C	6.076289	0.499971	0.543423
H	3.9270	0.6450	1.6361	H	-4.08919	1.404223	-0.02791	H	4.001748	1.064139	0.524202
C	6.1801	-1.8777	-0.2264	C	-6.83823	-1.28226	-0.42436	C	6.533571	-1.84324	0.319618
H	4.3826	-2.5828	-1.1822	H	-5.26415	-2.7417	-0.24454	H	4.826396	-3.14984	0.135982
C	6.7593	-0.9919	0.6808	C	-7.19448	0.065966	-0.45358	C	7.004931	-0.53972	0.469002
H	7.8273	-1.0007	0.8596	H	-8.22818	0.363752	-0.57861	H	8.067427	-0.33871	0.528085
C	7.0583	-2.8107	-1.0188	C	-7.90209	-2.32668	-0.63597	C	7.518168	-2.97428	0.172024
C	6.5179	0.8351	2.3826	C	-6.55283	2.483268	-0.28111	C	6.559855	1.906327	0.777783
F	7.3962	-2.2766	-2.2175	F	-8.08698	-2.59248	-1.9525	F	8.702438	-2.69413	0.760209
F	8.2142	-3.0879	-0.3753	F	-7.59384	-3.49917	-0.04128	F	7.057721	-4.12136	0.715781
F	6.4460	-3.9869	-1.2756	F	-9.10102	-1.93073	-0.14975	F	7.780821	-3.23685	-1.13097
F	7.8018	1.1512	2.1036	F	-6.79225	2.911445	0.980766	F	5.675732	2.829202	0.338881
F	5.8269	1.9932	2.4756	F	-5.57347	3.263078	-0.78377	F	6.760287	2.150901	2.095034
F	6.5120	0.2764	3.6163	F	-7.67564	2.735842	-0.99495	F	7.73573	2.142895	0.15541
H	-0.5191	-0.2810	0.3152	H	-0.18683	-0.81763	0.244254	H	-0.06191	-0.71287	0.037843
C	-2.0244	-1.3295	-0.7879	C	1.24209	-2.45074	0.259338	C	-1.67196	-2.14085	0.071838
C	-2.5728	-2.1093	0.4124	C	2.023529	-2.01555	-0.98273	C	-2.37965	-1.56053	1.302343
C	-2.7978	-3.5217	0.3723	C	3.029313	-2.87113	-1.54027	C	-3.59352	-2.16016	1.775979
C	-2.8285	-1.4304	1.5864	C	1.789282	-0.79747	-1.58393	C	-1.8747	-0.48351	1.996062
C	-2.5582	-4.3493	-0.7599	C	3.340552	-4.17131	-1.0539	C	-4.1849	-3.32828	1.21879
C	-3.2981	-4.1159	1.5794	C	3.745617	-2.35974	-2.67052	C	-4.22002	-1.53501	2.90171
C	-3.3249	-2.1083	2.7333	C	2.532389	-0.38943	-2.72909	C	-2.56092	0.059268	3.120876

H	-2.6370	-0.3647	1.6426	H	1.026886	-0.13606	-1.19118	H	-0.94433	-0.02751	1.689901
C	-2.8073	-5.7090	-0.6960	C	4.334394	-4.92459	-1.65568	C	-5.3581	-3.84186	1.74684
H	-2.1468	-3.9255	-1.6658	H	2.782866	-4.59069	-0.22688	H	-3.7019	-3.84215	0.398843
C	-3.5476	-5.5184	1.6003	C	4.769166	-3.16041	-3.25424	C	-5.43547	-2.08168	3.404011
C	-3.3120	-6.2957	0.4980	C	5.06156	-4.40415	-2.76214	C	-5.99416	-3.19931	2.844502
H	-3.9287	-5.9483	2.5212	H	5.30242	-2.75317	-4.10733	H	-5.89626	-1.5869	4.252961
H	-3.4966	-7.3654	0.5070	H	5.835075	-5.02366	-3.20482	H	-6.91532	-3.62759	3.226755
O	-2.6025	-6.5850	-1.7140	O	4.700553	-6.17584	-1.27777	O	-5.99145	-4.9586	1.3045
N	-3.5523	-3.4160	2.7136	N	3.493623	-1.15105	-3.23469	N	-3.70973	-0.45094	3.539497
C	-2.1249	-6.0772	-2.9600	C	4.004076	-6.79271	-0.1966	C	-5.41548	-5.69064	0.22539
H	-2.0219	-6.9447	-3.6130	H	4.448088	-7.78214	-0.08301	H	-6.06898	-6.54893	0.06579
H	-1.1551	-5.5804	-2.8470	H	2.935278	-6.89285	-0.41875	H	-4.40642	-6.03936	0.474556
H	-2.8419	-5.3713	-3.3968	H	4.133642	-6.22508	0.733064	H	-5.38025	-5.08561	-0.68905
C	-3.6089	-1.3819	4.0025	C	2.272927	0.918801	-3.39306	C	-2.02862	1.236393	3.863941
C	-3.8414	-2.1124	5.1818	C	3.191149	1.411453	-4.33892	C	-2.86375	1.917313	4.768287
C	-3.6586	0.0223	4.0669	C	1.129732	1.687053	-3.10888	C	-0.7099	1.697673	3.699187
C	-4.1086	-1.4640	6.3847	C	2.978863	2.633452	-4.97239	C	-2.40096	3.022542	5.477869
H	-3.8067	-3.1951	5.1360	H	4.068152	0.816645	-4.56918	H	-3.87993	1.56364	4.901378
C	-3.9281	0.6694	5.2735	C	0.919411	2.910601	-3.74628	C	-0.2472	2.804122	4.413963
H	-3.4992	0.6269	3.1793	H	0.384445	1.337401	-2.40154	H	-0.02664	1.200101	3.019117
C	-4.1528	-0.0678	6.4374	C	1.841384	3.391086	-4.67743	C	-1.08896	3.47292	5.304397
H	-4.2801	-2.0491	7.2844	H	3.701807	2.995361	-5.69873	H	-3.06622	3.534878	6.167798
H	-3.9647	1.7551	5.3004	H	0.028817	3.486952	-3.51217	H	0.777546	3.138428	4.276211
H	-4.3606	0.4393	7.3757	H	1.674761	4.344641	-5.17084	H	-0.72663	4.334198	5.858872
C	-2.0153	0.2131	-3.4313	C	1.531562	-0.07474	2.590106	C	-0.97243	-1.00949	-3.03735
C	-3.2195	-0.5468	-4.0371	C	1.108103	-0.72807	3.924594	C	-1.32036	-2.10564	-4.06804
H	-1.6778	1.0404	-4.0593	H	1.999096	0.90219	2.71712	H	-0.73447	-0.05037	-3.49673
C	-3.0162	-0.1983	-1.1570	C	2.09278	-2.34296	1.55842	C	-2.50475	-1.95377	-1.25259
C	-3.4764	1.8933	-2.3642	C	3.7616	-1.09115	2.868772	C	-3.36889	-0.4712	-2.98996
C	-4.4873	-0.2208	-3.2217	C	1.79128	-2.10163	4.052951	C	-2.63589	-2.77689	-3.63932
H	-3.0279	-1.6248	-4.0224	H	0.021012	-0.8464	3.948061	H	-0.51365	-2.84404	-4.10837
H	-3.3536	-0.2569	-5.0836	H	1.3848	-0.08577	4.766169	H	-1.41969	-1.67695	-5.07079
H	-3.2297	0.3946	-0.2689	H	3.017816	-2.88192	1.339128	H	-3.53077	-1.75621	-0.93735
C	-4.3167	-0.7698	-1.7914	C	1.421287	-2.94041	2.814186	C	-2.48485	-3.20397	-2.16651
C	-4.6571	1.3233	-3.1938	C	3.326591	-1.87482	4.142545	C	-3.77917	-1.73555	-3.80254
H	-3.7810	2.2427	-1.3757	H	4.55201	-1.59779	2.311282	H	-4.15912	-0.12462	-2.3209
H	-2.9660	2.7158	-2.8677	H	4.099548	-0.07898	3.092878	H	-3.08714	0.36316	-3.63344
H	-5.3624	-0.6788	-3.6913	H	1.448656	-2.60685	4.959732	H	-2.84455	-3.64861	-4.2657
H	-5.1796	-0.5173	-1.1693	H	1.731987	-3.98284	2.924453	H	-3.29064	-3.87954	-1.86398
H	-4.2700	-1.8630	-1.8287	H	0.333451	-2.94109	2.696022	H	-1.5482	-3.75823	-2.03648
H	-4.5711	1.6818	-4.2263	H	3.508747	-1.23363	5.011738	H	-3.81773	-1.45883	-4.86201
H	-1.9321	-1.9894	-1.6472	H	1.05222	-3.52592	0.183447	H	-1.62028	-3.22462	0.211097
N	-2.4367	0.8200	-2.1212	N	2.582811	-0.94505	1.923845	N	-2.15971	-0.76281	-2.12928
C	-5.9867	1.7846	-2.6545	C	4.118639	-3.14471	4.332005	C	-5.13949	-2.26152	-3.41649
C	-6.8914	2.4615	-3.3632	C	4.807188	-3.4381	5.435791	C	-6.14354	-2.44566	-4.27509
H	-6.2020	1.5389	-1.6137	H	4.114382	-3.85746	3.506099	H	-5.29664	-2.50116	-2.3638

H	-7.8416	2.7651	-2.9325	H	5.354398	-4.37143	5.534564	H	-7.10575	-2.83411	-3.95284
H	-6.7164	2.7377	-4.4013	H	4.848252	-2.75657	6.283159	H	-6.04122	-2.2134	-5.33345
C	0.6401	4.0839	-1.8561	C	5.205021	2.949009	-0.19386	C	-2.62197	3.610755	-0.25463
C	-0.3969	4.9526	-2.2125	C	5.381966	3.598772	1.041543	C	-3.26005	4.150863	-1.37668
C	-0.1632	6.0097	-3.0953	C	6.112985	4.779138	1.102098	C	-4.11251	5.248458	-1.24679
C	1.1101	6.2092	-3.6331	C	6.669729	5.317023	-0.06629	C	-4.33696	5.81848	0.009162
C	2.1502	5.3426	-3.2853	C	6.496466	4.676766	-1.29645	C	-3.70707	5.281295	1.13581
C	1.9136	4.2862	-2.4044	C	5.765136	3.492684	-1.36145	C	-2.85573	4.183279	1.003342
H	-1.3848	4.7842	-1.7968	H	4.944571	3.163375	1.934492	H	-3.08567	3.688183	-2.34272
H	-0.9778	6.6774	-3.3647	H	6.253883	5.284768	2.052704	H	-4.6048	5.658156	-2.12533
H	1.2908	7.0300	-4.3222	H	7.24005	6.240174	-0.01477	H	-5.00287	6.671382	0.111345
H	3.1427	5.4850	-3.7048	H	6.928417	5.100789	-2.1977	H	-3.8851	5.712075	2.117774
H	2.7253	3.6083	-2.1463	H	5.615714	2.989266	-2.31339	H	-2.37677	3.761917	1.885116
C	0.3970	2.9304	-0.8894	C	4.438905	1.704422	-0.28826	C	-1.72255	2.400922	-0.40035
O	-0.9322	2.5626	-0.7794	H	4.380373	1.254494	-1.29444	H	-1.71518	1.826422	0.542647
C	-0.5300	6.5859	1.9161	O	3.877432	1.159619	0.661941	O	-1.82357	1.710387	-1.51047
C	0.4281	5.6849	1.4436	H	2.935992	-0.42953	1.096955	H	-1.97333	0.185415	-1.61606
C	0.0522	4.3718	1.1614	C	1.10259	6.223768	1.769479	C	0.173472	6.381524	-2.04907
C	-1.2773	3.9745	1.3474	C	1.260125	4.945261	1.26462	C	0.030087	5.461982	-1.01482
C	-2.2411	4.8743	1.8034	C	0.143456	4.085067	1.092915	C	0.225727	4.092376	-1.25115
C	-1.8591	6.1849	2.0932	C	-1.13342	4.593345	1.459617	C	0.567566	3.680451	-2.55274
H	-0.2389	7.6071	2.1458	C	-1.27626	5.896378	1.972588	C	0.69457	4.608777	-3.59956
H	1.4564	6.0026	1.2944	C	-0.17023	6.713887	2.13035	C	0.500947	5.959455	-3.34715
C	0.9346	3.3078	0.5843	H	1.97548	6.861424	1.888739	H	0.027822	7.43921	-1.84755
C	-1.5979	2.5578	1.0330	H	2.248251	4.584399	0.98961	H	-0.2401	5.798386	-0.01846
H	-3.2659	4.5415	1.9348	C	0.260205	2.762499	0.577949	C	-0.00159	3.064305	-0.22487
H	-2.5946	6.8941	2.4619	C	-2.31258	3.754165	1.300492	C	0.841552	2.268048	-2.81113
C	0.7543	2.0186	1.3366	H	-2.27196	6.238625	2.237251	H	0.959375	4.252276	-4.58961
O	1.6524	1.2604	1.6774	H	-0.27827	7.719847	2.524665	H	0.608263	6.685976	-4.14676
O	-0.5250	1.6492	1.5231	C	-0.85331	1.962704	0.420207	C	0.735207	1.826907	-0.41113
O	-2.7148	2.0606	1.0358	O	-0.92772	0.776095	-0.02902	O	0.974244	0.992489	0.47168
H	-1.1641	-0.4409	-3.2488	O	-2.10123	2.484158	0.785474	O	1.062671	1.458168	-1.68225
H	1.9912	3.5745	0.5520	O	-3.46338	4.052356	1.574635	O	0.983166	1.734457	-3.88758
H	1.0324	2.0834	-1.2076	H	1.227393	2.366928	0.291675	H	0.041361	3.411267	0.805104
H	-1.6422	1.3425	-1.6384	H	0.703314	0.042357	1.896704	H	-0.13671	-1.28963	-2.40164

Complex 16b				TS **16b-17b**				**Complex 17b**			
C	0.827863	-4.1422	-0.04513	C	0.858396	-4.03006	-0.02695	C	-1.23881	-3.54549	-1.18521
C	0.724165	-2.66916	-0.09784	C	0.750824	-2.56148	0.032708	C	-0.82139	-2.30991	-0.49965
C	2.117499	-2.50585	0.025645	C	2.145541	-2.39571	0.126822	C	0.460146	-2.82727	-0.22396
C	2.338369	-3.97559	0.097805	C	2.372715	-3.86899	0.080128	C	0.128332	-4.13491	-0.84812
O	3.288605	-4.73385	0.208409	O	3.328315	-4.62643	0.099912	O	0.68782	-5.20479	-1.03272
O	0.035647	-5.06934	-0.10238	O	0.063934	-4.95324	-0.13211	O	-2.23934	-3.89586	-1.80204
N	2.842381	-1.36104	0.060808	N	2.86079	-1.25289	0.225984	N	1.495849	-2.20095	0.376041
N	-0.30162	-1.82469	-0.25843	N	-0.28117	-1.70488	-0.03597	N	-1.38479	-1.12181	-0.26573
H	2.298234	-0.4972	0.032942	H	2.303262	-0.39305	0.256184	H	1.310606	-1.22029	0.627716

C	4.227713	-1.18261	0.166837	C	4.247657	-1.07111	0.308178	C	2.810559	-2.63635	0.569261
C	4.703085	0.137878	0.201139	C	4.711038	0.245492	0.46457	C	3.717391	-1.69748	1.087182
C	5.138804	-2.24664	0.23754	C	5.169198	-2.12473	0.238886	C	3.25241	-3.9308	0.264661
C	6.06868	0.3875	0.301578	C	6.076289	0.499971	0.543423	C	5.049699	-2.04516	1.278217
H	4.003466	0.965664	0.152133	H	4.001748	1.064139	0.524202	H	3.369986	-0.69857	1.327624
C	6.501729	-1.97022	0.340644	C	6.533571	-1.84324	0.319618	C	4.591611	-4.26069	0.481738
H	4.787651	-3.2738	0.214245	H	4.826396	-3.14984	0.135982	H	2.565125	-4.66333	-0.14896
C	6.985031	-0.66182	0.372898	C	7.004931	-0.53972	0.469002	C	5.503455	-3.33303	0.983691
H	8.047073	-0.46541	0.452164	H	8.067427	-0.33871	0.528085	H	6.540724	-3.6033	1.137578
C	7.474277	-3.11163	0.489232	C	7.518168	-2.97428	0.172024	C	5.037433	-5.67451	0.211806
C	6.564561	1.808588	0.268395	C	6.559855	1.906327	0.777783	C	6.033009	-0.99918	1.72887
F	7.695526	-3.40866	1.792567	F	8.702438	-2.69413	0.760209	F	4.733621	-6.49755	1.24395
F	7.030683	-4.2414	-0.10067	F	7.057721	-4.12136	0.715781	F	4.440717	-6.18977	-0.8851
F	8.678614	-2.81779	-0.05159	F	7.780821	-3.23685	-1.13097	F	6.372833	-5.75926	0.022855
F	6.810031	2.223044	-0.99763	F	5.675732	2.829202	0.338881	F	6.992659	-1.51245	2.525875
F	5.664333	2.671309	0.792145	F	6.760287	2.150901	2.095034	F	6.667405	-0.42686	0.672917
F	7.716364	1.956862	0.958144	F	7.73573	2.142895	0.15541	F	5.434318	0.007615	2.407859
H	-0.10221	-0.83018	-0.26427	H	-0.06191	-0.71287	0.037843	H	-0.80345	-0.42074	0.226386
C	-1.70126	-2.24296	-0.1817	C	-1.67196	-2.14085	0.071838	C	-2.77172	-0.82061	-0.62281
C	-2.38443	-1.74516	1.096111	C	-2.37965	-1.56053	1.302343	C	-3.66725	-0.7452	0.61716
C	-3.59879	-2.36152	1.545405	C	-3.59352	-2.16016	1.775979	C	-4.73763	-1.66663	0.841038
C	-1.86678	-0.715	1.849714	C	-1.8747	-0.48351	1.996062	C	-3.42911	0.231359	1.561507
C	-4.20757	-3.48146	0.913464	C	-4.1849	-3.32828	1.21879	C	-5.05128	-2.76268	-0.01061
C	-4.20934	-1.80616	2.715315	C	-4.22002	-1.53501	2.90171	C	-5.53024	-1.44304	2.016838
C	-2.53846	-0.23955	3.012253	C	-2.56092	0.059268	3.120876	C	-4.24065	0.343495	2.722272
H	-0.93672	-0.24588	1.558692	H	-0.94433	-0.02751	1.689901	H	-2.61947	0.939286	1.418195
C	-5.3811	-4.01825	1.41534	C	-5.3581	-3.84186	1.74684	C	-6.12128	-3.5889	0.283991
H	-3.73898	-3.93264	0.049395	H	-3.7019	-3.84215	0.398843	H	-4.42085	-2.98753	-0.86048
C	-5.42409	-2.37647	3.192398	C	-5.43547	-2.08168	3.404011	C	-6.63489	-2.30572	2.271801
C	-5.99847	-3.4485	2.563108	C	-5.99416	-3.19931	2.844502	C	-6.9282	-3.34554	1.431042
H	-5.87326	-1.9369	4.077306	H	-5.89626	-1.5869	4.252961	H	-7.2279	-2.11543	3.160685
H	-6.9203	-3.89323	2.92461	H	-6.91532	-3.62759	3.226755	H	-7.76288	-4.01265	1.622474
O	-6.03279	-5.09197	0.897639	O	-5.99145	-4.9586	1.3045	O	-6.49143	-4.67084	-0.44823
N	-3.68566	-0.76626	3.414994	N	-3.70973	-0.45094	3.539497	N	-5.2777	-0.46094	2.918971
C	-5.47473	-5.74313	-0.24128	C	-5.41548	-5.69064	0.22539	C	-5.73758	-4.98661	-1.61928
H	-6.14476	-6.57325	-0.46768	H	-6.06898	-6.54893	0.06579	H	-6.18754	-5.89343	-2.02506
H	-4.47136	-6.12931	-0.02655	H	-4.40642	-6.03936	0.474556	H	-4.6838	-5.16856	-1.38128
H	-5.42992	-5.06537	-1.10278	H	-5.38025	-5.08561	-0.68905	H	-5.80615	-4.17993	-2.35941
C	-1.99229	0.893178	3.811168	C	-2.02862	1.236393	3.863941	C	-3.97312	1.385433	3.749388
C	-2.84144	1.600551	4.680839	C	-2.86375	1.917313	4.768287	C	-5.00975	1.814064	4.596344
C	-0.64521	1.288455	3.727424	C	-0.7099	1.697673	3.699187	C	-2.69769	1.953344	3.910702
C	-2.36463	2.672753	5.431557	C	-2.40096	3.022542	5.477869	C	-4.78192	2.789409	5.564321
H	-3.87945	1.295325	4.753075	H	-3.87993	1.56364	4.901378	H	-5.99327	1.371654	4.480041
C	-0.16796	2.361369	4.482756	C	-0.2472	2.804122	4.413963	C	-2.47004	2.927441	4.883362
H	0.04804	0.754815	3.085538	H	-0.02664	1.200101	3.019117	H	-1.86595	1.617153	3.298341
C	-1.02486	3.060679	5.334954	C	-1.08896	3.47292	5.304397	C	-3.51096	3.352806	5.711001

H	-3.04029	3.208157	6.093262	H	-3.06622	3.534878	6.167798	H	-5.59812	3.112827	6.204798
H	0.878956	2.643399	4.410097	H	0.777546	3.138428	4.276211	H	-1.47479	3.347929	4.998882
H	-0.65214	3.896002	5.92129	H	-0.72663	4.334198	5.858872	H	-3.33286	4.112991	6.466603
C	-1.06135	-0.71923	-3.10336	C	-0.97243	-1.00949	-3.03735	C	-1.97788	-0.45427	-3.57566
C	-1.39482	-1.67463	-4.28073	C	-1.32036	-2.10564	-4.06804	C	-3.37918	-0.2973	-4.21402
H	-0.83214	0.289614	-3.45758	H	-0.73447	-0.05037	-3.49673	H	-1.16722	-0.29368	-4.28848
C	-2.52126	-1.89792	-1.47541	C	-2.50475	-1.95377	-1.25259	C	-2.87303	0.50106	-1.42567
C	-3.41354	-0.23088	-2.93156	C	-3.36889	-0.4712	-2.98996	C	-1.85413	1.975103	-3.12419
C	-2.69229	-2.41938	-3.92598	C	-2.63589	-2.77689	-3.63932	C	-4.08135	0.932473	-3.60646
H	-0.57758	-2.388	-4.43639	H	-0.51365	-2.84404	-4.10837	H	-3.97866	-1.19567	-4.03602
H	-1.52032	-1.11798	-5.21685	H	-1.41969	-1.67695	-5.07079	H	-3.28357	-0.1826	-5.29781
H	-3.55061	-1.77835	-1.12871	H	-3.53077	-1.75621	-0.93735	H	-2.64028	1.336228	-0.76144
C	-2.4991	-3.03878	-2.5271	C	-2.48485	-3.20397	-2.16651	C	-4.26102	0.701521	-2.093
C	-3.8444	-1.3732	-3.91943	C	-3.77917	-1.73555	-3.80254	C	-3.19772	2.182291	-3.87649
H	-4.21763	0.007838	-2.22797	H	-4.15912	-0.12462	-2.3209	H	-1.71292	2.683872	-2.30603
H	-3.18157	0.685854	-3.48144	H	-3.08714	0.36316	-3.63344	H	-0.98454	2.059616	-3.77697
H	-2.90731	-3.19905	-4.66367	H	-2.84455	-3.64861	-4.2657	H	-5.05973	1.071868	-4.07441
H	-3.28062	-3.77237	-2.29796	H	-3.29064	-3.87954	-1.86398	H	-4.78266	1.539646	-1.62437
H	-1.54466	-3.58014	-2.49751	H	-1.5482	-3.75823	-2.03648	H	-4.88533	-0.1841	-1.93426
H	-3.90669	-0.95405	-4.93132	H	-3.81773	-1.45883	-4.86201	H	-2.99397	2.208888	-4.95286
H	-1.66754	-3.33507	-0.12803	H	-1.62028	-3.22462	0.211097	H	-3.10491	-1.63703	-1.26069
N	-2.20265	-0.59771	-2.14228	N	-2.15971	-0.76281	-2.12928	N	-1.8092	0.593648	-2.50563
C	-5.1923	-1.95844	-3.58689	C	-5.13949	-2.26152	-3.41649	C	-3.85466	3.485714	-3.49862
C	-6.21727	-2.03514	-4.43834	C	-6.14354	-2.44566	-4.27509	C	-4.20324	4.431081	-4.37226
H	-5.32701	-2.33621	-2.57181	H	-5.29664	-2.50116	-2.3638	H	-4.04775	3.646021	-2.43702
H	-7.17123	-2.46815	-4.14883	H	-7.10575	-2.83411	-3.95284	H	-4.68382	5.351842	-4.05339
H	-6.14046	-1.66553	-5.45942	H	-6.04122	-2.2134	-5.33345	H	-4.0191	4.321121	-5.43914
C	-2.60956	3.65637	0.131305	C	-2.62197	3.610755	-0.25463	C	1.807207	4.977649	0.613621
C	-3.34152	4.311249	-0.8647	C	-3.26005	4.150863	-1.37668	C	2.299836	6.049919	-0.13644
C	-4.26842	5.299073	-0.5243	C	-4.11251	5.248458	-1.24679	C	2.940301	7.120275	0.494532
C	-4.47231	5.642348	0.813651	C	-4.33696	5.81848	0.009162	C	3.090827	7.134392	1.881064
C	-3.74771	4.987425	1.813253	C	-3.70707	5.281295	1.13581	C	2.589823	6.072024	2.638645
C	-2.82347	3.998517	1.473943	C	-2.85573	4.183279	1.003342	C	1.950776	5.005105	2.008867
H	-3.18871	4.03308	-1.90172	H	-3.08567	3.688183	-2.34272	H	2.175803	6.064217	-1.21364
H	-4.83328	5.798852	-1.30683	H	-4.6048	5.658156	-2.12533	H	3.318272	7.944953	-0.10362
H	-5.1955	6.409337	1.07725	H	-5.00287	6.671382	0.111345	H	3.587986	7.967699	2.369747
H	-3.90837	5.237019	2.858544	H	-3.8851	5.712075	2.117774	H	2.691627	6.076146	3.720441
H	-2.27624	3.484522	2.260801	H	-2.37677	3.761917	1.885116	H	1.555256	4.188745	2.609466
C	-1.59757	2.58088	-0.22242	C	-1.72255	2.400922	-0.40035	C	1.10553	3.783295	-0.02097
H	-1.68986	1.764037	0.502527	H	-1.71518	1.826422	0.542647	H	0.14221	3.645283	0.480963
O	-1.75919	2.096851	-1.53643	O	-1.82357	1.710387	-1.51047	O	0.735221	4.051373	-1.39408
H	-1.93304	1.117322	-1.51823	H	-1.97333	0.185415	-1.61606	H	-0.86202	0.52656	-2.04482
C	0.161278	6.70452	-1.28762	C	0.173472	6.381524	-2.04907	C	5.340921	1.976046	-1.52285
C	-0.06536	5.607759	-0.45586	C	0.030087	5.461982	-1.01482	C	4.325182	1.960225	-0.56513
C	0.204226	4.312824	-0.90785	C	0.225727	4.092376	-1.25115	C	3.076656	2.513023	-0.85659
C	0.715794	4.144678	-2.20375	C	0.567566	3.680451	-2.55274	C	2.861666	3.096406	-2.11491

C	0.928656	5.245519	-3.04754	C	0.69457	4.608777	-3.59956	C	3.878149	3.106034	-3.07789
C	0.651183	6.526683	-2.5868	C	0.500947	5.959455	-3.34715	C	5.118525	2.545954	-2.78096
H	-0.04647	7.705225	-0.92028	H	0.027822	7.43921	-1.84755	H	6.305004	1.536761	-1.28367
H	-0.45908	5.756889	0.544385	H	-0.2401	5.798386	-0.01846	H	4.5079	1.521668	0.411517
C	-0.09354	3.10052	-0.06885	C	-0.00159	3.064305	-0.22487	C	1.91245	2.465378	0.095115
C	1.081548	2.8091	-2.68581	C	0.841552	2.268048	-2.81113	C	1.546547	3.706656	-2.43251
H	1.323537	5.0782	-4.04389	H	0.959375	4.252276	-4.58961	H	3.683454	3.557399	-4.04539
H	0.822411	7.385069	-3.22875	H	0.608263	6.685976	-4.14676	H	5.910562	2.554101	-3.52393
C	0.756702	1.913221	-0.43747	C	0.735207	1.826907	-0.41113	C	0.974893	1.261835	-0.20719
O	0.965699	0.977143	0.320972	O	0.974244	0.992489	0.47168	O	0.644104	0.535341	0.782355
O	1.232257	1.80576	-1.69836	O	1.062671	1.458168	-1.68225	O	0.594203	1.122363	-1.39718
O	1.340114	2.481249	-3.81356	O	0.983166	1.734457	-3.88758	O	1.162782	3.954614	-3.56028
H	0.072092	3.302463	0.992697	H	0.041361	3.411267	0.805104	H	2.255773	2.365411	1.126876
H	-0.18983	-1.07077	-2.55296	H	-0.13671	-1.28963	-2.40164	H	-1.83257	-1.43284	-3.11833

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Complex 15c				TS **16c-17c**				**Complex 17c**			
C	-0.33674	-3.33474	0.945305	C	0.436502	-2.40741	-1.969	C	0.516557	-2.98287	-1.44665
C	-0.19443	-1.98655	0.374733	C	0.351314	-1.33067	-0.96884	C	0.370188	-1.74686	-0.64901
C	-1.56725	-1.92195	0.043597	C	1.747336	-1.34873	-0.74618	C	1.754428	-1.71446	-0.3636
C	-1.81082	-3.29079	0.573754	C	1.92245	-2.50377	-1.67998	C	1.994008	-2.9843	-1.09466
O	-2.75907	-4.05358	0.68255	O	2.833538	-3.21902	-2.06014	O	2.939082	-3.72426	-1.32513
O	0.422006	-4.12504	1.502116	O	-0.35589	-2.94359	-2.73659	O	-0.23305	-3.67464	-2.12517
N	-2.25261	-0.90907	-0.52611	N	2.525462	-0.56188	0.024847	N	2.470954	-0.79547	0.325856
N	0.820663	-1.1223	0.262273	N	-0.70068	-0.60584	-0.53651	N	-0.67192	-0.96407	-0.3566
H	-1.68798	-0.08015	-0.76501	H	2.083848	0.280384	0.405521	H	1.957739	0.038185	0.603967
C	-3.61894	-0.80277	-0.80975	C	3.906903	-0.64394	0.274848	C	3.848614	-0.74248	0.575119
C	-4.05645	0.415814	-1.35503	C	4.480267	0.391235	1.033288	C	4.348611	0.437452	1.14627
C	-4.54595	-1.82602	-0.57053	C	4.713334	-1.69696	-0.17241	C	4.727788	-1.79415	0.282101
C	-5.40274	0.607491	-1.64379	C	5.836856	0.361891	1.338642	C	5.710579	0.568077	1.400264
H	-3.33753	1.205015	-1.54697	H	3.865418	1.220789	1.363097	H	3.672553	1.256142	1.370725
C	-5.89061	-1.61253	-0.87899	C	6.073599	-1.70042	0.143747	C	6.086592	-1.64464	0.560335
H	-4.22325	-2.77049	-0.14233	H	4.293584	-2.49461	-0.77694	H	4.360118	-2.70385	-0.18249
C	-6.33708	-0.40474	-1.4135	C	6.651781	-0.68399	0.899537	C	6.59675	-0.4713	1.116054
H	-7.38484	-0.25387	-1.64252	H	7.708007	-0.70024	1.13512	H	7.65536	-0.36604	1.316273
C	-6.86612	-2.74283	-0.6782	C	6.909431	-2.84514	-0.36633	C	7.01034	-2.80631	0.300232
C	-5.87328	1.947502	-2.14059	C	6.41906	1.446161	2.205842	C	6.232853	1.888489	1.895857
F	-6.87125	-3.59164	-1.73394	F	6.432282	-4.03698	0.062684	F	7.015383	-3.68012	1.335539
F	-6.56592	-3.48066	0.413064	F	6.911765	-2.89598	-1.71898	F	6.647547	-3.5045	-0.79726
F	-8.13412	-2.29815	-0.52805	F	8.196543	-2.76181	0.032847	F	8.289076	-2.40613	0.120322
F	-6.3354	2.720283	-1.12403	F	7.730779	1.647054	1.95098	F	6.408882	2.763298	0.871269
F	-4.88674	2.646117	-2.7427	F	5.786869	2.628024	2.033445	F	5.379849	2.479171	2.762686
F	-6.88712	1.82932	-3.02567	F	6.319555	1.139384	3.522072	F	7.424593	1.768405	2.516405
H	0.634686	-0.25143	-0.26079	H	-0.55505	0.091555	0.191034	H	-0.52045	-0.18262	0.277235
C	2.210298	-1.49058	0.567713	C	-2.06537	-1.15797	-0.67673	C	-2.06145	-1.37308	-0.63655
C	3.062587	-1.52072	-0.70341	C	-2.49092	-1.93132	0.580951	C	-2.74596	-1.81963	0.662855
C	3.444945	-2.75319	-1.3234	C	-2.72408	-3.34466	0.564719	C	-3.04883	-3.19129	0.94273

C	3.447455	-0.33609	-1.29557	C	-2.63025	-1.25241	1.774564	C	-3.05103	-0.87538	1.622469
C	3.098262	-4.04495	-0.8374	C	-2.60194	-4.17663	-0.5835	C	-2.77577	-4.27455	0.060905
C	4.223783	-2.6433	-2.52359	C	-3.10515	-3.93821	1.814885	C	-3.66367	-3.46389	2.211043
C	4.236781	-0.32981	-2.47799	C	-3.01074	-1.93207	2.96533	C	-3.6708	-1.24157	2.848014
H	3.125029	0.608647	-0.8752	H	-2.43657	-0.18645	1.812412	H	-2.79675	0.165292	1.457199
C	3.510884	-5.17879	-1.51541	C	-2.84892	-5.53537	-0.4936	C	-3.10314	-5.5697	0.422069
H	2.483337	-4.14816	0.0472	H	-2.27179	-3.75991	-1.52435	H	-2.27601	-4.0943	-0.88087
C	4.631548	-3.83549	-3.18791	C	-3.35948	-5.33925	1.862305	C	-3.98913	-4.81063	2.541533
C	4.288098	-5.06864	-2.70215	C	-3.23876	-6.11908	0.743765	C	-3.72027	-5.8366	1.675777
H	5.22264	-3.73058	-4.0922	H	-3.64954	-5.76527	2.81754	H	-4.45708	-4.99305	3.503768
H	4.593226	-5.98206	-3.20314	H	-3.42688	-7.18781	0.772198	H	-3.96366	-6.86587	1.920674
O	3.230033	-6.45423	-1.14083	O	-2.74513	-6.41363	-1.52478	O	-2.87784	-6.6711	-0.34168
N	4.60701	-1.45959	-3.06694	N	-3.24139	-3.23891	2.968864	N	-3.96348	-2.50574	3.124959
C	2.491845	-6.66112	0.063655	C	-2.36029	-5.91435	-2.80604	C	-2.29168	-6.49349	-1.63158
H	2.379038	-7.74176	0.159214	H	-2.31591	-6.78523	-3.46125	H	-2.19581	-7.49511	-2.05283
H	1.505317	-6.1876	0.018635	H	-1.38072	-5.42569	-2.76865	H	-1.30575	-6.02141	-1.56433
H	3.037791	-6.26991	0.93075	H	-3.10363	-5.20464	-3.19011	H	-2.93809	-5.88452	-2.27552
C	4.676704	0.947245	-3.10292	C	-3.16079	-1.21291	4.261224	C	-4.01243	-0.22046	3.875869
C	5.085142	0.958875	-4.44821	C	-3.20661	-1.94768	5.45975	C	-4.19372	-0.6128	5.213747
C	4.707392	2.154963	-2.38359	C	-3.26517	0.187345	4.332256	C	-4.17312	1.137297	3.549246
C	5.499833	2.140285	-5.05808	C	-3.34408	-1.30554	6.687727	C	-4.5145	0.322289	6.195025
H	5.068013	0.027961	-5.00436	H	-3.13113	-3.02818	5.408993	H	-4.07729	-1.66079	5.467866
C	5.125571	3.336999	-2.9959	C	-3.40547	0.828208	5.564057	C	-4.49823	2.071951	4.533279
H	4.42624	2.182275	-1.33508	H	-3.25202	0.789653	3.429942	H	-4.06987	1.474331	2.522287
C	5.520404	3.33647	-4.33498	C	-3.4435	0.087604	6.746699	C	-4.66722	1.670919	5.85982
H	5.804577	2.129066	-6.10125	H	-3.37116	-1.89305	7.601715	H	-4.64351	-0.0011	7.22461
H	5.145592	4.258876	-2.42113	H	-3.48881	1.911315	5.596315	H	-4.62621	3.115474	4.258075
H	5.843026	4.258625	-4.81067	H	-3.55061	0.589617	7.704465	H	-4.91868	2.400523	6.624826
C	1.956265	-1.73909	3.669782	C	-2.45523	0.053966	-3.43318	C	-1.86817	-0.59332	-3.55045
C	3.40325	-2.09768	4.078464	C	-3.70566	-0.79557	-3.76374	C	-3.12598	-1.38704	-4.00989
H	1.308464	-1.54734	4.527225	H	-2.23629	0.797863	-4.20179	H	-1.44214	-0.01872	-4.37976
C	2.828123	-0.53455	1.613092	C	-3.11854	-0.07522	-1.01301	C	-2.9047	-0.28216	-1.34868
C	2.4968	0.676421	3.737937	C	-3.80639	1.839474	-2.39869	C	-3.12764	1.396764	-3.04854
C	4.358974	-0.99869	3.577146	C	-4.86238	-0.37232	-2.83641	C	-4.36722	-0.7447	-3.36104
H	3.686125	-3.06214	3.645013	H	-3.48755	-1.86059	-3.63154	H	-3.0515	-2.43989	-3.71151
H	3.471586	-2.19634	5.166075	H	-3.9843	-0.6523	-4.81214	H	-3.21497	-1.37023	-5.10224
H	2.811617	0.486172	1.228194	H	-3.21475	0.604207	-0.16463	H	-3.10997	0.519297	-0.63494
C	4.265269	-0.93504	2.041502	C	-4.48943	-0.71821	-1.38149	C	-4.25835	-0.90741	-1.83296
C	3.938748	0.352284	4.222009	C	-5.06599	1.158902	-2.99238	C	-4.37568	0.759099	-3.74393
H	2.464368	1.576394	3.120399	H	-3.99638	2.305635	-1.43019	H	-3.43632	2.053668	-2.22882
H	1.791722	0.788492	4.563503	H	-3.3837	2.602984	-3.05193	H	-2.56352	2.010494	-3.75609
H	5.384918	-1.23374	3.873572	H	-5.77941	-0.89838	-3.11663	H	-5.28036	-1.22825	-3.72409
H	4.981864	-0.21966	1.630532	H	-5.2617	-0.37626	-0.68735	H	-5.10308	-0.43115	-1.32529
H	4.525531	-1.91518	1.627645	H	-4.43573	-1.80557	-1.2729	H	-4.31049	-1.9734	-1.58229
H	3.918675	0.197615	5.306666	H	-5.11723	1.378767	-4.06534	H	-4.25041	0.822513	-4.83272
H	2.177561	-2.48936	0.998884	H	-2.00705	-1.8462	-1.51683	H	-1.97495	-2.22156	-1.31171

N	1.975521	-0.45331	2.873795	N	-2.70839	0.823376	-2.16552	N	-2.20047	0.381312	-2.48031
C	4.88683	1.48856	3.927703	C	-6.32855	1.679161	-2.35484	C	-5.64882	1.476608	-3.38717
C	5.697077	2.038484	4.83328	C	-7.32833	2.25357	-3.02537	C	-6.46911	2.058961	-4.26471
H	4.883522	1.872277	2.90738	H	-6.40791	1.570857	-1.2722	H	-5.8964	1.523872	-2.3251
H	6.372713	2.849118	4.574457	H	-8.22388	2.606473	-2.52131	H	-7.37645	2.567825	-3.94951
H	5.716219	1.699669	5.867522	H	-7.28929	2.3925	-4.10406	H	-6.26351	2.048944	-5.33377
C	-1.36548	1.155047	2.433097	C	-0.19642	3.631053	-1.63393	C	0.594384	3.318375	-1.74903
O	-0.77188	0.197888	2.931333	O	-1.20932	2.793919	-1.43625	O	-0.65842	2.896485	-2.2276
C	0.373754	7.066922	-0.30347	C	-1.52083	7.049371	1.110492	C	-0.62924	7.274857	0.080327
C	-0.30514	5.951783	-0.75752	C	-0.47468	6.317463	0.550938	C	0.196647	6.158881	-0.05831
C	0.194097	4.643063	-0.51873	C	-0.50946	4.91827	0.569662	C	-0.33653	4.872243	0.048975
C	1.418043	4.536659	0.204109	C	-1.61514	4.275944	1.14951	C	-1.70906	4.727338	0.299152
C	2.097434	5.685205	0.659496	C	-2.67671	5.011424	1.697075	C	-2.54358	5.848463	0.427039
C	1.58529	6.945258	0.412537	C	-2.625	6.400149	1.681243	C	-2.00046	7.12281	0.31916
H	-0.03234	8.055735	-0.5025	H	-1.47911	8.134953	1.102532	H	-0.20101	8.26978	0.002734
H	-1.23509	6.064798	-1.30889	H	0.371304	6.8289	0.099899	H	1.258067	6.289384	-0.25007
C	-0.47617	3.472812	-0.97387	C	0.492876	4.066358	-0.11657	C	0.510993	3.649348	-0.18131
C	1.970805	3.223963	0.469179	C	-1.63272	2.812475	1.198011	C	-2.28826	3.390431	0.453462
H	3.026894	5.552027	1.204458	H	-3.51724	4.484118	2.136302	H	-3.60102	5.701253	0.618517
H	2.10572	7.831871	0.76156	H	-3.43462	6.980344	2.113306	H	-2.63639	7.995976	0.424113
C	0.049182	2.215949	-0.74165	C	0.715217	2.772955	0.554446	C	-0.02993	2.431352	0.505702
O	-0.36784	1.078294	-1.08493	O	1.752447	2.134284	0.563561	O	0.630571	1.470801	0.84782
O	1.253657	2.145306	0.002862	O	-0.39262	2.166831	1.10685	O	-1.38243	2.328342	0.65117
O	3.010995	2.966061	1.073621	O	-2.59024	2.112882	1.460999	O	-3.45758	3.098666	0.489262
H	1.482757	-2.50904	3.05903	H	-1.56228	-0.55589	-3.29422	H	-1.08509	-1.26667	-3.194
H	-1.39201	3.547858	-1.54902	H	1.444284	4.564084	-0.29934	H	1.526172	3.808902	0.185279
H	0.991471	-0.21197	2.633119	H	-1.86684	1.441902	-1.90348	H	-0.82887	1.93205	-2.10446
C	-2.80985	1.373765	2.52245	C	0.947408	3.173177	-2.53846	C	1.767763	2.415234	-2.11538
C	-3.37356	2.458295	1.829356	C	1.796511	4.11966	-3.12944	C	3.068893	2.743351	-1.70193
C	-3.63184	0.505924	3.263946	C	1.156639	1.820287	-2.82041	C	1.590921	1.301554	-2.94356
C	-4.75009	2.670269	1.869436	C	2.834299	3.723802	-3.97327	C	4.159662	1.965674	-2.08611
H	-2.72997	3.117791	1.251575	H	1.636756	5.178684	-2.93294	H	3.244071	3.619765	-1.08287
C	-5.00263	0.728781	3.311709	C	2.193188	1.417086	-3.66583	C	2.68407	0.520769	-3.33098
H	-3.17994	-0.32898	3.790162	H	0.493745	1.085697	-2.37695	H	0.60279	1.049632	-3.312
C	-5.56073	1.807896	2.61269	C	3.037148	2.367186	-4.24403	C	3.970108	0.846762	-2.90222
H	-5.19168	3.493416	1.317247	H	3.479925	4.472477	-4.42532	H	5.153515	2.230344	-1.73665
H	-5.64263	0.064553	3.884735	H	2.340004	0.360435	-3.8751	H	2.525176	-0.34009	-3.9744
H	-6.63396	1.972941	2.646308	H	3.842122	2.055285	-4.90406	H	4.818307	0.238132	-3.20202
H	-0.80496	1.919283	1.867495	H	-0.50244	4.64243	-1.97855	H	0.762952	4.297314	-2.21237

TS **15c-16c**

C	-0.56331	2.505305	-1.83784	C	0.206755	3.489492	0.969302				
C	-0.45453	1.346551	-0.93543	C	0.188688	2.140219	0.376298				
C	-1.85999	1.253162	-0.79586	C	1.564707	2.199536	0.060527				
C	-2.06607	2.460985	-1.65241	C	1.676318	3.586741	0.588169				
O	-3.00526	3.133713	-2.04321	O	2.550365	4.43318	0.700311				
O	0.230672	3.182946	-2.48344	O	-0.60746	4.187256	1.566016				

Complex 16c

N	-2.62664	0.366579	-0.12855	N	2.345606	1.249838	-0.48996
N	0.628547	0.671565	-0.49515	N	-0.75365	1.197374	0.257174
H	-2.15394	-0.4701	0.234585	H	1.875507	0.34942	-0.69816
C	-4.02001	0.35813	0.065303	C	3.728604	1.247609	-0.70914
C	-4.56675	-0.75943	0.714773	C	4.288679	0.049094	-1.18035
C	-4.8655	1.402237	-0.33751	C	4.559413	2.353691	-0.47572
C	-5.93666	-0.82252	0.962095	C	5.660477	-0.04134	-1.39809
H	-3.92006	-1.57913	1.00849	H	3.640927	-0.80416	-1.35564
C	-6.2328	1.313619	-0.07992	C	5.929777	2.238898	-0.71191
H	-4.46688	2.259454	-0.86926	H	4.142659	3.284464	-0.10226
C	-6.78614	0.211116	0.572869	C	6.499249	1.049627	-1.16987
H	-7.85	0.15508	0.76363	H	7.56556	0.974401	-1.33909
C	-7.11982	2.469555	-0.46277	C	6.800298	3.45211	-0.5145
C	-6.4755	-2.0362	1.671805	C	6.223161	-1.36694	-1.83206
F	-6.6967	3.082988	-1.5891	F	6.774578	4.267624	-1.59645
F	-8.39761	2.079624	-0.67065	F	6.40016	4.195039	0.540991
F	-7.153	3.414691	0.507718	F	8.094474	3.120648	-0.30634
F	-7.82279	-2.03233	1.749219	F	6.179025	-2.28159	-0.82423
F	-6.11075	-3.18002	1.046165	F	5.519986	-1.90188	-2.85548
F	-6.00212	-2.12377	2.937445	F	7.510049	-1.28039	-2.22468
H	0.501636	-0.09663	0.165062	H	-0.51418	0.249718	-0.0675
C	1.93194	1.37438	-0.47117	C	-2.14822	1.442734	0.641849
C	2.204662	1.984068	0.910671	C	-3.04108	1.676433	-0.58429
C	2.257788	3.396703	1.131811	C	-3.72524	2.910432	-0.8152
C	2.376896	1.137445	1.986846	C	-3.18822	0.656578	-1.50207
C	2.075517	4.384391	0.123638	C	-3.61501	4.064411	0.010149
C	2.511305	3.815428	2.48128	C	-4.57454	2.954622	-1.97199
C	2.619731	1.648779	3.291047	C	-4.0238	0.80807	-2.64118
H	2.318768	0.065032	1.836945	H	-2.6684	-0.28287	-1.34614
C	2.145745	5.729176	0.441928	C	-4.33611	5.206376	-0.29096
H	1.841901	4.089412	-0.89	H	-2.92036	4.072451	0.839206
C	2.584017	5.20992	2.764215	C	-5.31255	4.144647	-2.23489
C	2.409079	6.142863	1.777534	C	-5.20415	5.238047	-1.41848
H	2.779928	5.505199	3.790124	H	-5.95608	4.15535	-3.10889
H	2.459	7.207058	1.985974	H	-5.7571	6.151199	-1.61558
O	1.973463	6.746916	-0.44175	O	-4.28817	6.364772	0.416762
N	2.687769	2.955592	3.515637	N	-4.71049	1.925839	-2.84527
C	1.722089	6.422759	-1.80923	C	-3.43391	6.425267	1.559315
H	1.597569	7.377651	-2.3214	H	-3.53369	7.438804	1.94973
H	0.813582	5.820717	-1.91951	H	-2.39034	6.2303	1.289808
H	2.569321	5.879865	-2.24621	H	-3.74938	5.704818	2.324043
C	2.805691	0.74237	4.458847	C	-4.19055	-0.28762	-3.63493
C	2.795934	1.277475	5.759708	C	-5.28983	-0.27002	-4.51184
C	2.994773	-0.64351	4.308615	C	-3.27553	-1.34961	-3.73502
C	2.9645	0.457772	6.872678	C	-5.47248	-1.28325	-5.44962
H	2.652183	2.345423	5.879655	H	-5.99599	0.550034	-4.44295

C	3.165209	-1.46186	5.426209	C	-3.45889	-2.36357	-4.67557
H	3.020266	-1.09972	3.323801	H	-2.39896	-1.38562	-3.09576
C	3.14999	-0.91834	6.711934	C	-4.55827	-2.33731	-5.53537
H	2.948597	0.893119	7.86845	H	-6.33212	-1.25235	-6.11386
H	3.311919	-2.52975	5.287678	H	-2.73691	-3.17323	-4.73469
H	3.281005	-1.55926	7.579637	H	-4.70076	-3.12849	-6.26641
C	2.413287	0.33026	-3.28647	C	-1.22837	0.656837	3.451989
C	3.487936	1.39784	-3.59934	C	-2.44929	1.274561	4.172801
H	2.303037	-0.4114	-4.08009	H	-0.57338	0.101161	4.125682
C	3.134397	0.486553	-0.87557	C	-2.73835	0.266794	1.468241
C	4.080153	-1.24246	-2.3589	C	-2.36903	-1.51668	3.137144
C	4.735354	1.135161	-2.73062	C	-3.71784	0.485621	3.79024
H	3.091142	2.398684	-3.4002	H	-2.56171	2.326845	3.892932
H	3.748063	1.359226	-4.66141	H	-2.29206	1.243377	5.254666
H	3.352384	-0.21256	-0.06969	H	-2.96139	-0.56009	0.794185
C	4.37156	1.352631	-1.24823	C	-3.99291	0.678524	2.28497
C	5.181875	-0.33475	-2.96345	C	-3.46855	-1.01476	4.110918
H	4.375495	-1.70136	-1.41389	H	-2.76315	-2.16949	2.357456
H	3.771961	-2.04016	-3.03577	H	-1.57041	-2.05857	3.644622
H	5.542035	1.815263	-3.0178	H	-4.57144	0.847118	4.369733
H	5.214986	1.104324	-0.59826	H	-4.85753	0.089885	1.967655
H	4.152703	2.411781	-1.08025	H	-4.2401	1.726715	2.089526
H	5.223401	-0.50011	-4.04651	H	-3.08553	-1.07115	5.136417
H	1.836442	2.167331	-1.20921	H	-2.13859	2.335478	1.264987
N	2.839148	-0.42654	-2.05541	N	-1.72791	-0.33757	2.433373
C	6.538492	-0.66448	-2.39543	C	-4.70705	-1.87049	4.032481
C	7.592727	-1.02452	-3.12887	C	-5.24841	-2.5028	5.074273
H	6.641576	-0.59981	-1.31164	H	-5.17392	-1.96355	3.05115
H	8.5547	-1.24377	-2.67381	H	-6.14962	-3.10074	4.971348
H	7.534438	-1.11321	-4.212	H	-4.80998	-2.44868	6.068794
C	0.737528	-3.65517	-1.6706	C	1.149873	-4.03279	1.158493
O	1.742765	-2.79208	-1.16697	O	-0.0651	-4.07437	1.946612
C	1.224407	-6.87068	1.615177	C	-1.33781	-5.36959	-2.77244
C	0.326749	-6.20077	0.776452	C	-0.29121	-4.60865	-2.24971
C	0.566959	-4.86758	0.451798	C	-0.22806	-4.34343	-0.87842
C	1.695437	-4.21473	0.961495	C	-1.23588	-4.84576	-0.04048
C	2.596434	-4.87999	1.789509	C	-2.29284	-5.60045	-0.56805
C	2.354039	-6.21665	2.116961	C	-2.34109	-5.86741	-1.93254
H	1.040252	-7.90879	1.877336	H	-1.36787	-5.58166	-3.83765
H	-0.54689	-6.71319	0.382475	H	0.484599	-4.22352	-2.90599
C	-0.24632	-4.01124	-0.48976	C	0.877995	-3.51534	-0.26902
C	1.859732	-2.77896	0.573274	C	-1.21626	-4.54683	1.412165
H	3.465458	-4.35262	2.17041	H	-3.06056	-5.96984	0.103869
H	3.042915	-6.74788	2.767543	H	-3.15314	-6.45962	-2.34351
C	-0.59877	-2.72962	0.244277	C	0.548986	-1.99852	-0.3131
O	-1.735	-2.26745	0.321138	O	1.323408	-1.27735	-0.98706

O	0.433904	-2.10262	0.787755	O	-0.48571	-1.60243	0.309132
O	2.776698	-2.05003	0.937833	O	-2.17787	-4.68415	2.147652
H	1.433512	0.765157	-3.09554	H	-0.62405	1.397732	2.931332
H	-1.15203	-4.50124	-0.84846	H	1.790808	-3.65549	-0.8519
H	2.127513	-1.13944	-1.76501	H	-0.95853	-0.72035	1.847182
C	0.125058	-3.06399	-2.9335	C	2.186285	-3.2401	1.940928
C	-1.05182	-2.30356	-2.96268	C	3.430636	-2.95742	1.357166
C	0.819633	-3.26662	-4.13717	C	1.949248	-2.81781	3.25498
C	-1.513	-1.75358	-4.16237	C	4.407867	-2.25818	2.065525
H	-1.62856	-2.148	-2.05791	H	3.650905	-3.28014	0.343843
C	0.364501	-2.71338	-5.3347	C	2.929767	-2.1196	3.964908
H	1.723424	-3.87241	-4.13305	H	1.001056	-3.04829	3.725987
C	-0.80651	-1.95082	-5.34962	C	4.160453	-1.83434	3.373161
H	-2.43144	-1.17272	-4.16588	H	5.358543	-2.04445	1.587321
H	0.915446	-2.88769	-6.25512	H	2.728467	-1.80252	4.98485
H	-1.16934	-1.52285	-6.28003	H	4.921604	-1.2899	3.925214
H	1.193678	-4.61559	-1.95777	H	1.495829	-5.07158	1.062206

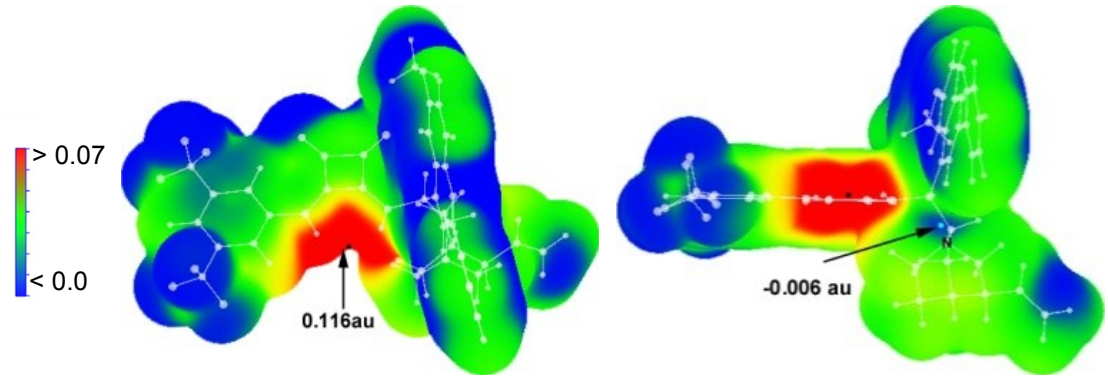
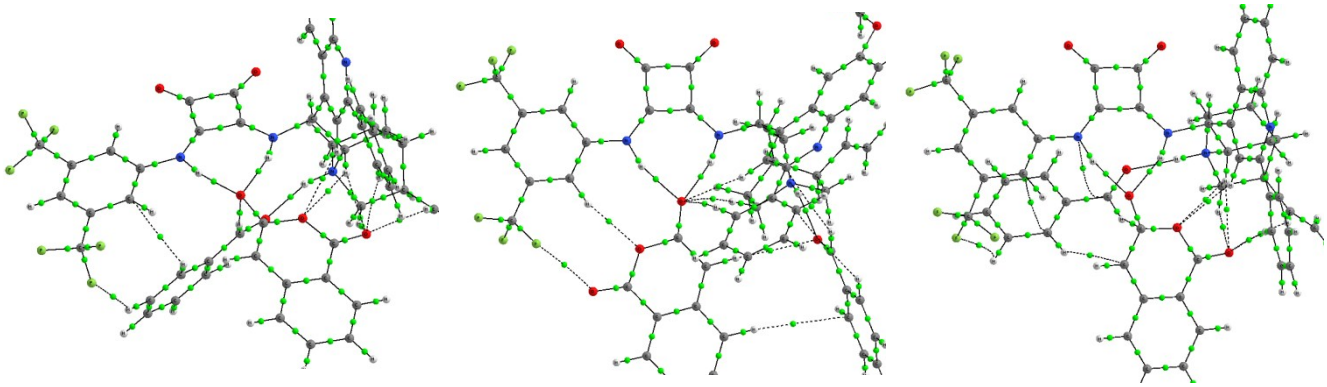


Fig. S1 Molecular electrostatic potential (MEP) on the 0.001 a.u. electron density isosurface of the catalyst **3**



15a **15b** **15c**

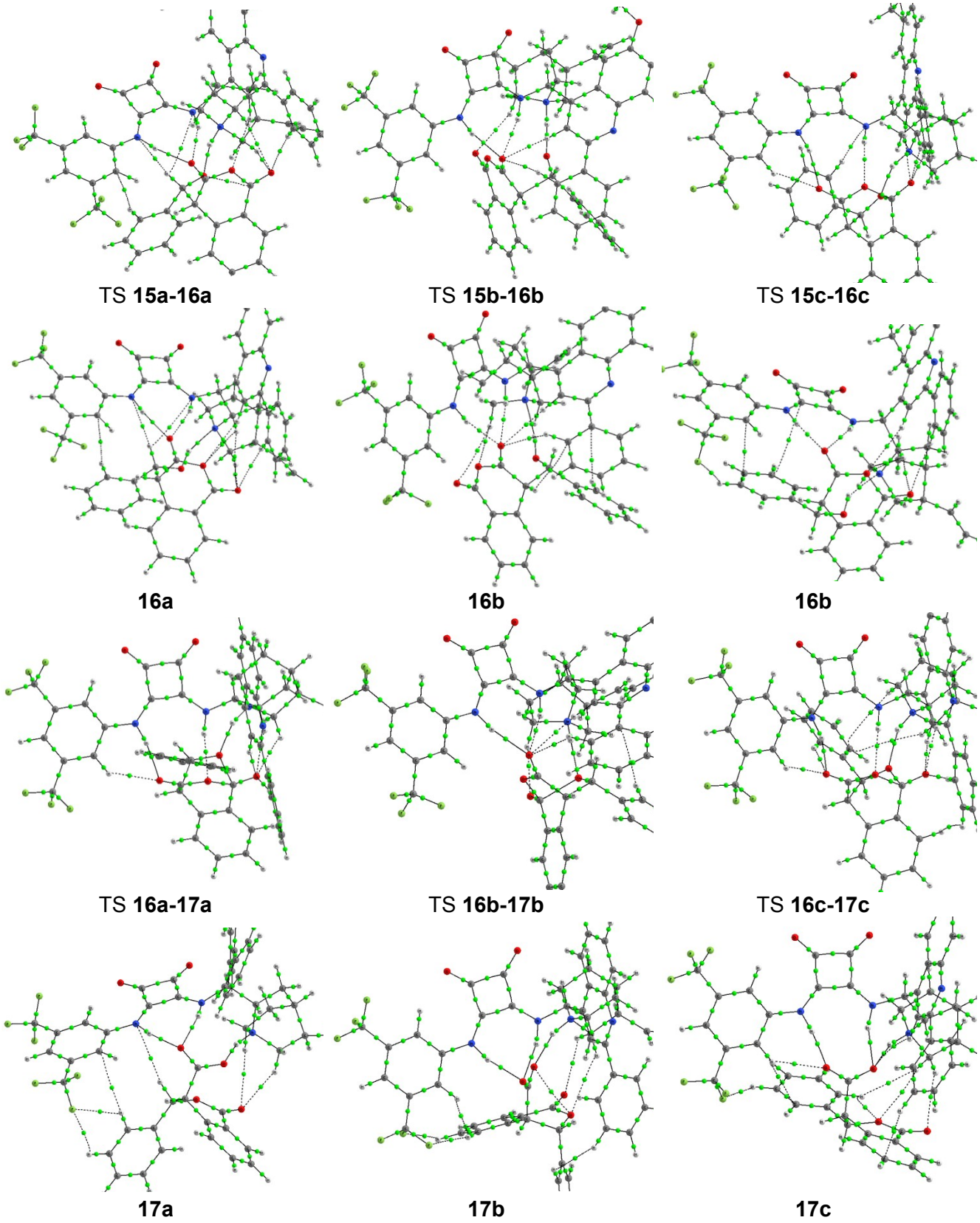


Fig. S2 Molecular graphs corresponding to complexes **7**, **8** and **9**, as well as transition states for all pathways studied, *trans*-(*R,*R), *trans*-(*S,*S) and *Cis*. Green dots correspond to bond critical points.

Table S2. Electron density [ρ(BCP), a.u.] and Laplacian [$\nabla^2\rho$(BCP), a.u.] calculated at B3LYP/6-31+G(d,p) in PCM-THF computational level, using the QTAIM theory.

***trans*-(*R,R*)**	**15a**		**TS 15a_16a**		**16a**		**TS16a_17a**		**17a**	
BCP	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$
$N^2H^{2\cdots}O^1$	0.034	0.099	0.022	0.069	0.021	0.069	-	-	0.033	0.094
$N^3H^{3\cdots}O^1$	0.034	0.121	0.030	0.100	0.026	0.085	0.029	0.097	0.036	0.118
$N^2H^{2\cdots}O^2$	-	-	-	-	-	-	0.013	0.044	-	-
$N^1H\cdots O^4$	0.034	0.105	0.069	0.196	-	-	0.054	0.159	0.044	0.146[a]
$O^4H\cdots N^1$	-	-	-	-	0.042	0.100	-	-	-	-
$N^{2\cdots}HC$	-	-	0.003	0.010	0.003	0.010	-	-	-	-
$N^{3\cdots}HC$	-	-	0.003	0.011	0.003	0.010	-	-	0.004	0.013
$O\cdots C$	-	-	0.013	0.042	-	-	0.082	0.129	-	-
***trans*-(*S,S*)**	**15a**		**TS 15a-16a**		**16a**		**TS16a-17a**		**17a**	
BCP	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$
$N^2H^{2\cdots}O^1$	0.038	0.127	0.022	0.068	0.015	0.052	0.019	0.060	0.038	0.109
$N^3H^{3\cdots}O^1$	0.033	0.098	0.028	0.085	0.023	0.072	0.028	0.085	0.031	0.094
$N^1H\cdots O^4$	0.029	0.098	0.070	0.194	-	-	0.049	0.137	0.046	0.147[a]
$O^4H\cdots N^1$	-	-	-	-	0.041	0.100	-	-	-	-
$O\cdots C$	-	-	-	-	-	-	0.088	0.124	-	-
Cis	**15a**		**TS 15a-16a**		**16a**		**TS16a-17a**		**17a**	
BCP	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$
$N^2H^{2\cdots}O^1$	0.034	0.100	-	-	0.020	0.063	-	-	0.033	0.097
$N^3H^{3\cdots}O^1$	0.037	0.122	0.029	0.096	0.023	0.081	0.033	0.106	0.042	0.134
$N^2H^{2\cdots}O^2$	-	-	0.013	0.043	-	-	0.019	0.060	-	-
$N^1H\cdots O^4$	0.035	0.107	0.060	0.194	-	-	0.039	0.115	0.033	0.111[a]
$O^4H\cdots N^1$	-	-	-	-	0.024	0.061	-	-	-	-
$O\cdots C$	-	-	0.018	0.055	-	-	0.129	0.055	-	-

[a] The HB is formed between N^1H and an oxygen atom belonging to the anhydride.

Since the mechanism of the reaction is governed by proton transfers and the intermediates formed are stabilised by HB interactions, the presence of intermolecular hydrogen bonds (HB) in all complexes was studied and their characteristics analysed by means of the Atoms in Molecules (QTAIM) theory.[6, 8] The main characteristics of the HBs found in these complexes within the QTAIM analysis [i.e. electron density at the bond critical point –ρ(BCP)- and Laplacian of such electron density –$\nabla^2\rho$(BCP)- are summarised in Table S2.

In all structures/complexes considered (15 cases in total), intermolecular HBs were found, characterised by a BCP between the interacting atoms (C, N, O and H, see Fig. S2). The values of the ρ(BCP) found range from 0.003 to 0.088 a.u. and those of the Laplacian (always positive) from 0.010 to 0.194 a.u. (Table S2), all of them indicative of non-covalent closed-shell interactions such as HBs.[9]

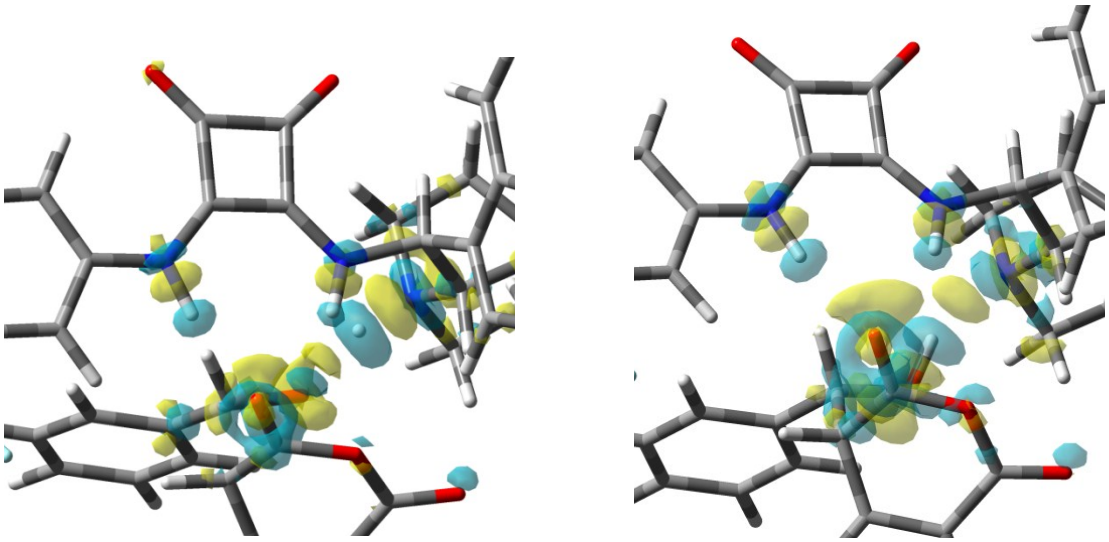
Looking at the first transition state corresponding to the C-C bond formation (TS **15-16**) and that seems to be key in the stereoselectivity of the reaction, it was found that the corresponding ρ(BCP)

value for the $N^1H\cdots O^4$ interaction in the ***trans*-(*R*,R)** pathway, is higher than the corresponding value for the same HB in that TS in the *cis* pathway (0.069 and 0.060 a.u., respectively). It is important to highlight that TS **15a-16a** and complex **16a** present two extra HBs between **N^2** and **N^3** of the squaramide and the H atom of the aldehyde. Those HBs stabilize the complexes and at the same time constrain the position of the reactants and are used as anchors to orientate the molecules towards the C-C bond formation. When complex **16** is formed, a HB is established between the lone pair of the ***N^1*** of the catalyst and the O^4H of the aldehyde, the corresponding ρ(BCP) is 0.042 and 0.024 a.u. for ***trans*-(*R,R*)** and *cis* pathways, respectively. This value is consistent with the distance found for this HB in those pathways, 1.841 and 2.104 Å, respectively. There is an exponential relationship between the ρ(BCP) and HB distances as proved in many works in the literature.[10] Regarding the *cis* pathway, complex **16c** shows π–π interactions betweenni the phenyl ring of aldehyde **2** and the phenyl ring of the catalyst as well as a HB between a F atom of a CF_3 group (in the catalyst) and a H atom from the phenyl ring of the aldehyde. The ρ(BCP) values for those critical points are 0.004 a.u. for the π–π interactions and 0.023 a.u. for the F···H interaction.

For the second transition state, TS **16-17**, which corresponds to the acylation reaction, the ρ(BCP) values for $N^1H\cdots O^4$ are 0.054, 0.049 and 0.039 a.u. for the three different pathways, corresponding to O···H distances of 1.652, 1.711 and 1.799 Å, respectively.

It is worth noting that due to its conformation, all complexes in the ***trans*-(*S,S*)** pathway are able to form HBs between O atoms of the anhydride and the di-CF_3 substituted phenyl ring of the catalyst. Additionally, the ρ(BCP) value of the HB corresponding to $N^1H\cdots O^4$ in complex **16b** is the lowest one in this particular pathway. These characteristics of the electron density of the different complexes and TSs may explain why ***trans*-(*S,S*)** is not thermodynamically favourable.

Additionally, electron density shift maps (EDS) were obtained in order to obtain an insight on the changes of the electron density upon complex formation. Since ***trans*-(*R,R*)** is the most favourable reaction pathway, we only present the EDS maps for the complexes corresponding to that pathway. The EDS maps were obtained following the procedure reported in ref. [11] and they are depicted in Fig. S3.



TS15a-16a Complex **16a**

Fig. S3 Electron Density Shifts maps at 0.003 a.u. of the key structures **TS15a-16a** and complex **16a** for the ***trans*(*R,R*)** pathway at B3LYP/6-31+G(d,p) computational level in PCM-THF. Yellow

and blue areas represent positive (increase) and negative (decrease) electron density regions respectively.

The HB donor and acceptor electron density shift pattern is shown only in the intermolecular region. On the one hand, a blue region is observed surrounding the **(N^{2,3})H^{2,3}** (HB donors), which represents a decrease of the electron density on this area. On the other hand, there is an increase (yellow regions) in the intermolecular electron density on the area located between those H atoms and the nitrogen or oxygen which acts as a HB acceptor.

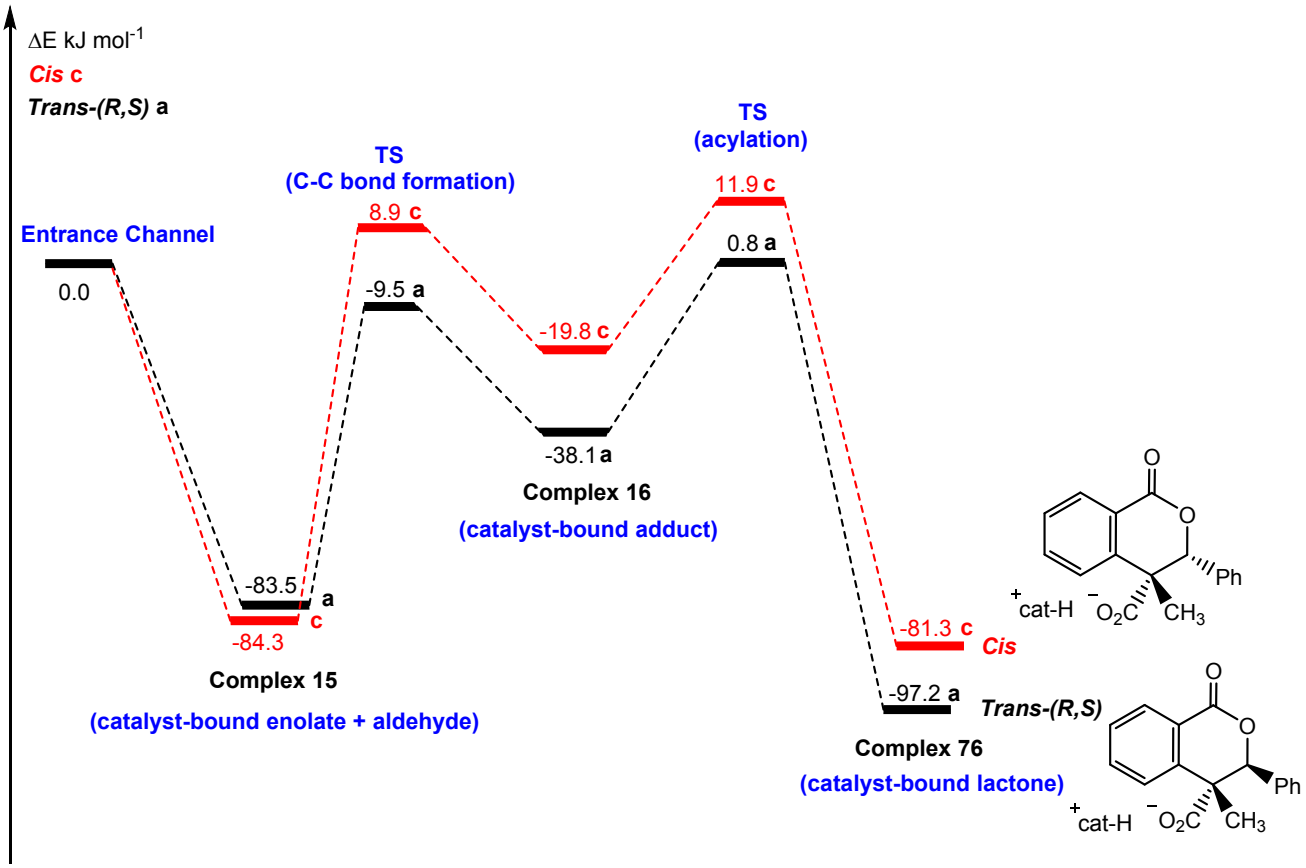


Fig. S4 Potential energy surface for all complexes formed (**15**, **16** and **17**) along the two pathways corresponding to the two major products for the reaction with methylhomophthalic anhydride.

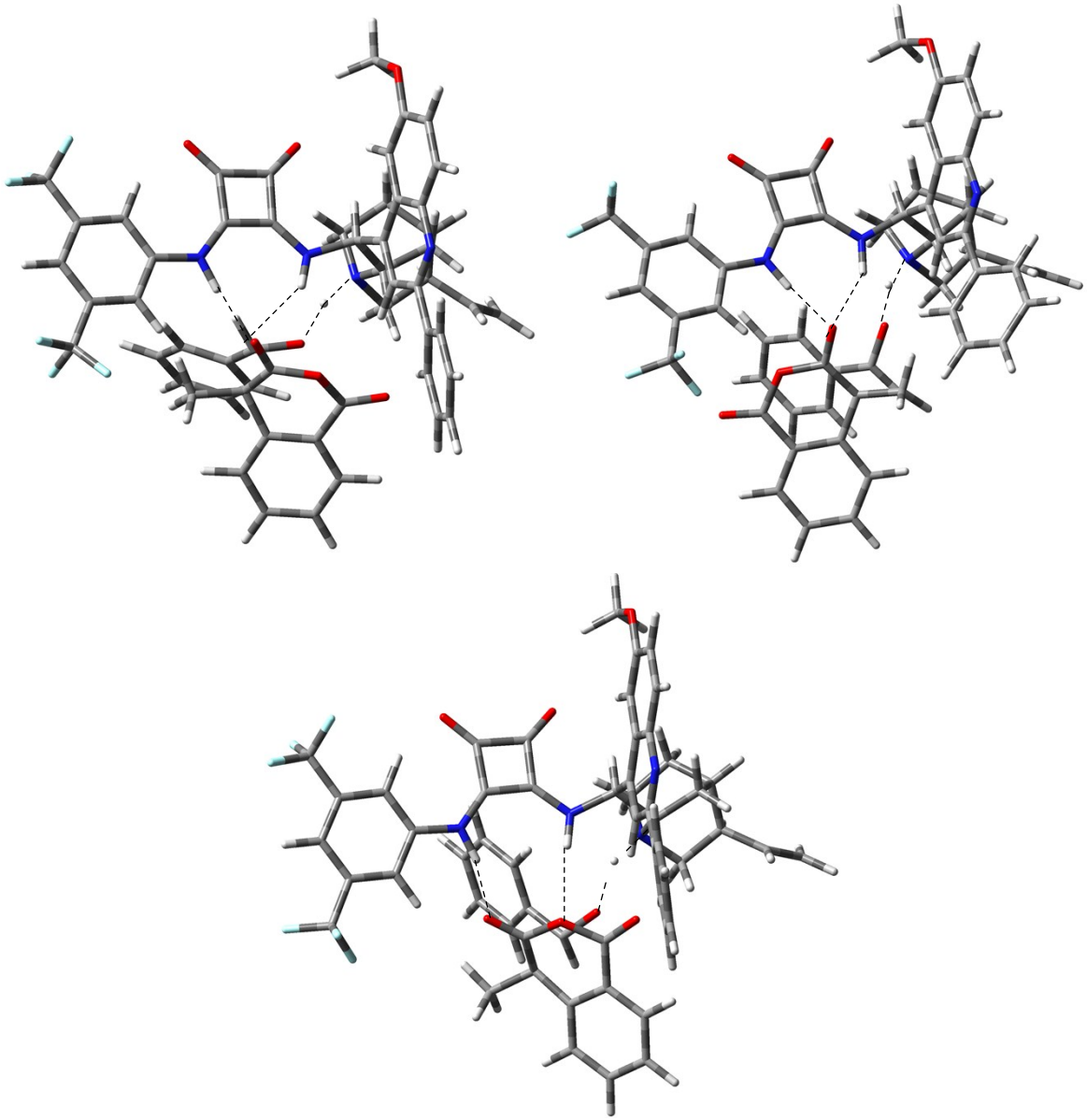


Fig.S5 Optimised geometries of TS**15-16** for ***trans*-(*R,S*)** (*left*), ***trans*-(*S,R*)** (right) and *cis* (*bottom*) pathways corresponding to the reaction with methylhomophthalic anhydride.

Table S3. Relative energies (ΔE) respect to the entrance channel at B3LYP/6-31+G(d,p) in PCM-THF corresponding to the reaction with methylhomophthalic anhydride. All values are in kJ·mol^{-1}.

Complex	*trans*-(*R,S*)	*trans*-(*S,R*)	*Cis*
15	-83.5	-58.6	-84.3
TS 15_16	-9.5	3.9	8.9
16	-38.1	-31.4	-19.8
TS 16_17	0.8	16.5	11.9
17	-97.2	-107.4	-81.3

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