Supporting Information

Insights into the Nature of Self-Extinguishing External Donors for Ziegler-Natta Catalysis: A Combined Experimental and DFT Study

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Section I: Synthesis and NMR studies of donor molecules

Objective:

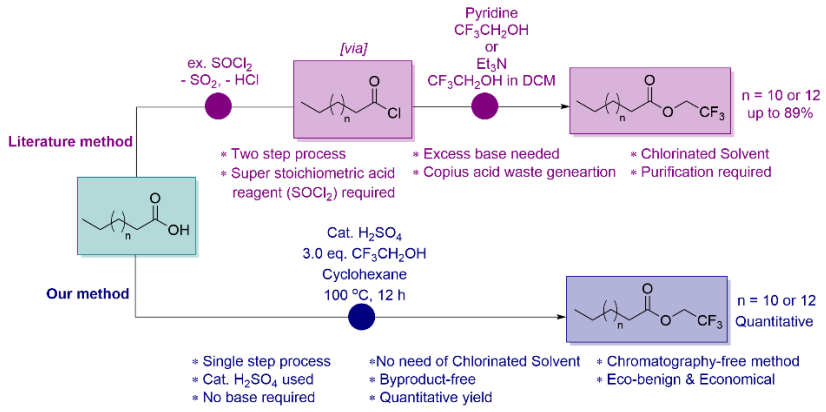
1 A facile synthesis of 2,2,2- trifluoroethyl fatty acid esters

2 Decomposition study with AlR_3 (Multinuclear NMR studies)

(1) General information for synthesis:

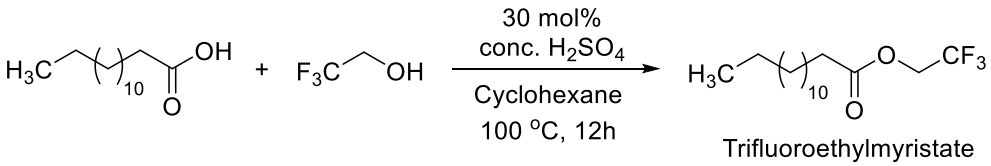
^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded either with JEOL 400 MHz, or BRUKER 500 MHz.1H NMR spectra are reported as follows: chemical shift in ppm (δ) relative to the chemical shift of $CHCl_3$at 7.27 ppm, integration, multiplicities (s = singlet, d = doublet, q = quartet, t =triplet, m = multiplet), and coupling constants (Hz). ^{13}C NMR spectra reported in ppm (δ) relative to the central line of triplet for $CDCl_3$ at 77.0 ppm. CF_3CO_2H used as external standards for ^{19}F NMR. Myristic acid, Palmitic acid and Trifluoroethanol was purchased from Sigma-Aldrich and used without further purification. HPLC grade cyclohexane was purchased from Merck and used as received. Other organic solvents and conc.H_2SO_4 was purchased from local suppliers and used as received.

Comparison of synthetic methodology:



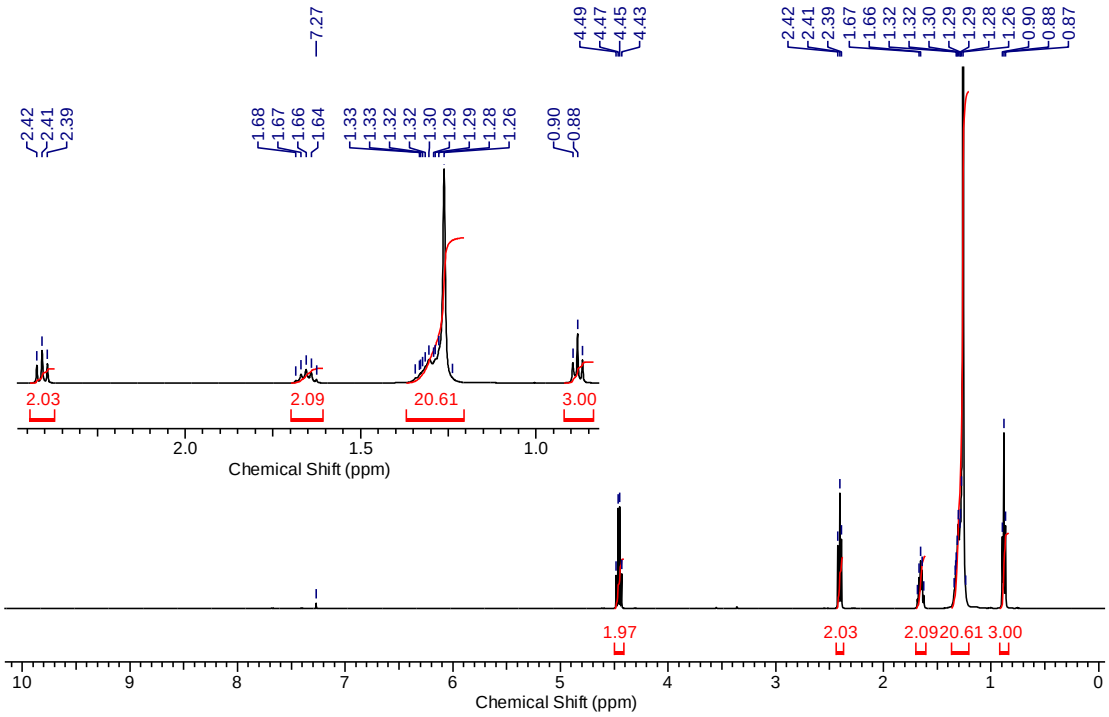
Scheme 1. Synthesis of 2,2,2-trifluoroethyl fatty esters.

(2) Procedure for preparation of Trifluoroethylmyristate (D_1):

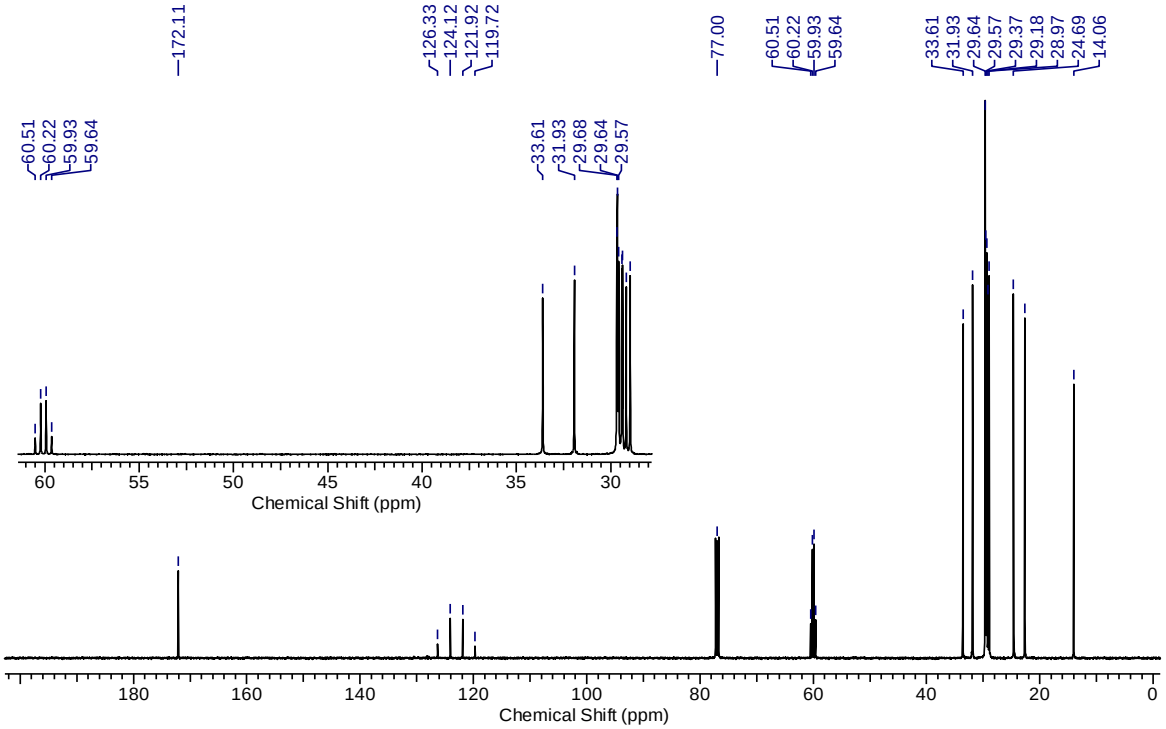


To a solution of myristic acid (50.0 mmol, 1.0 equiv., 11.4 gm,) and 2,2,2-trifluoroethanol (50.0 mmol, 1.0 equiv., 5.0 gm) in 50 mL cyclohexane, was added conc. H_2SO_4 (30 mol %) at ambient temperature and heated to reflux (at 100 ^oC) for 12 h. The mixture was cooled to room temperature, added saturated $NaHCO_3$ solution to neutralize excess H_2SO_4, and then was extracted three times with CH_2Cl_2 (100 mL each time). The combined organic phases were washed with brine solution, dried over anhydrous Na_2SO_4, and concentrated *in vacuu* to give the desired 2,2,2-trifluoroethyl myristate.

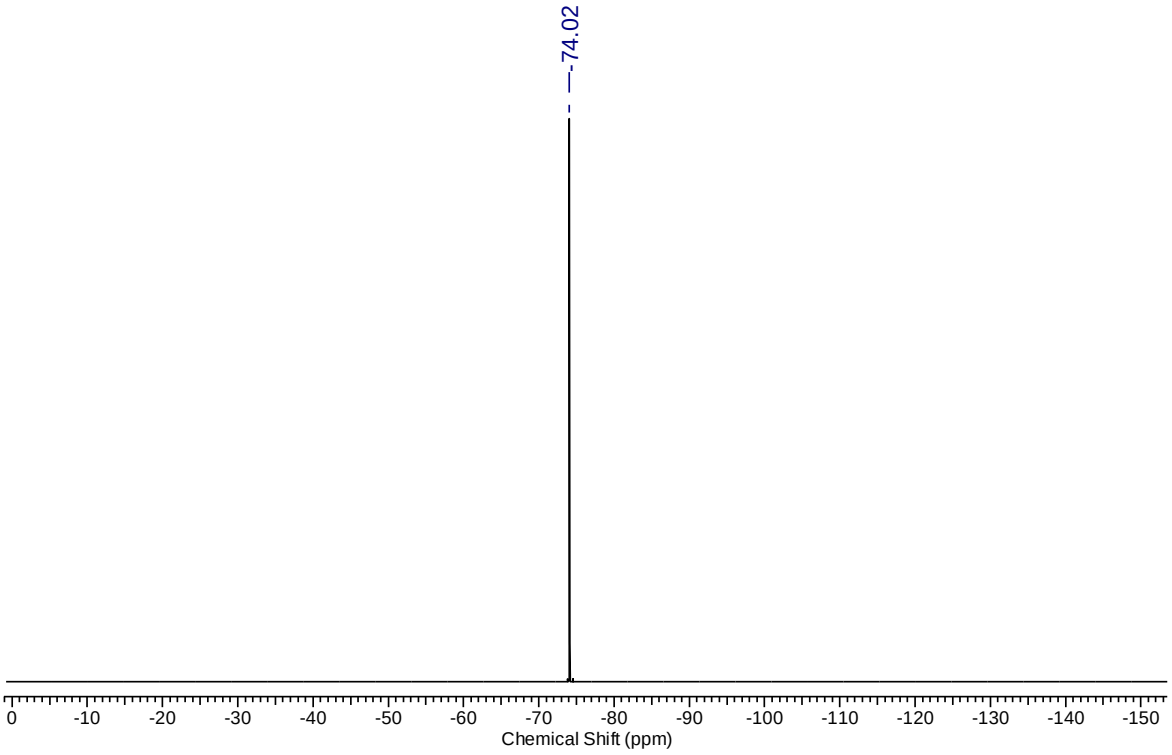
Colourless liquid at 300 K. Isolated Yield: 15.3 gm, 99.0 %. ^1H NMR (500 MHz, $CDCl_3$): δ = 4.46 (q, *J* = 8.5 Hz, 2H), 2.41 (t, *J* = 7.6 Hz, 2H), 1.66 (quin, *J* = 7.4 Hz, 2H), 1.35-1.24 (m, 20H), 0.88 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ = 172.11, 126.33, 124.12, 121.92, 119.72, 60.51, 60.22, 59.93, 59.64, 33.61, 31.93, 29.68, 29.64, 29.57, 29.42, 29.37, 29.18, 28.97, 24.69, 22.69, 14.06. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -74.02. GC data(Rt): 8.356 min (GC Programme: Column HP 5; Method: 80 ^oC hold 1min; 20 ^oC ramp up to 280 ^oC; at 280 ^oC Hold for 10 min; Inlet temp. 300 ^oC, Detector temp. 300 ^oC, H_2 Flow 40 mL, Air Flow 400 mL, N_2 Flow 25 mL per minute, Constant Flow mode).



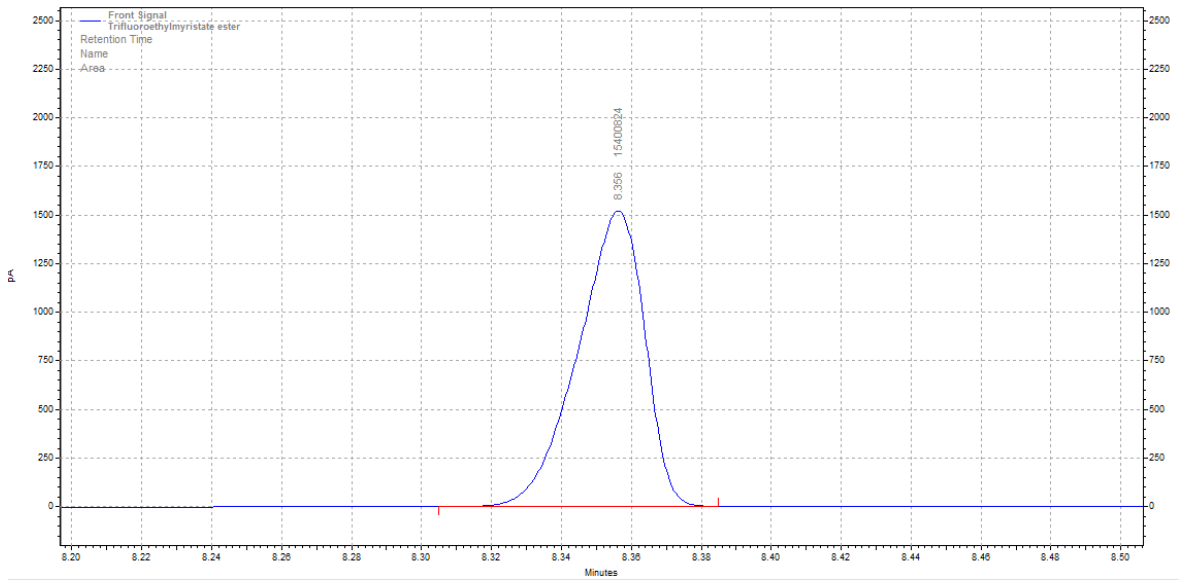
^1H NMR of trifluoroethylmyristate



^{13}C NMR of trifluoroethylmyristate

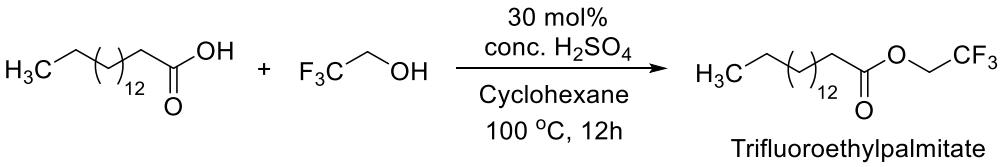


^{19}F NMR of trifluoroethylmyristate



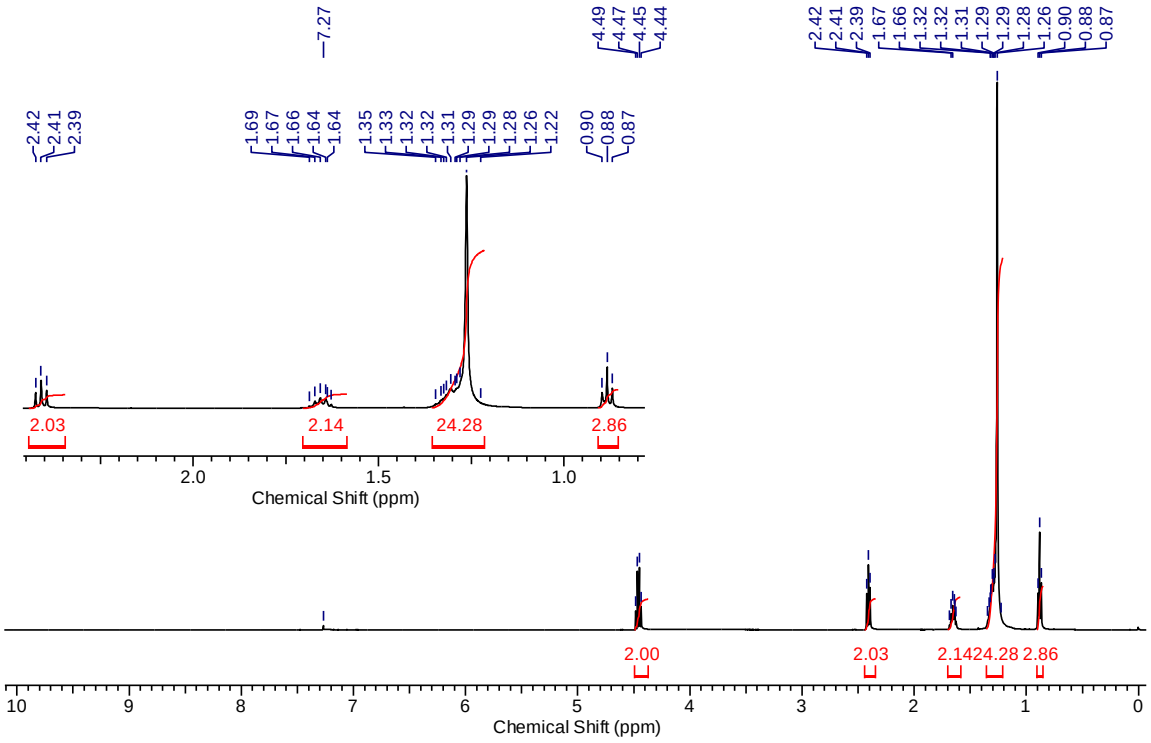
GC Chromatogram of trifluoroethylmyristate

(3) Procedure for preparation of Trifluoroethylpalmitate (D_2):

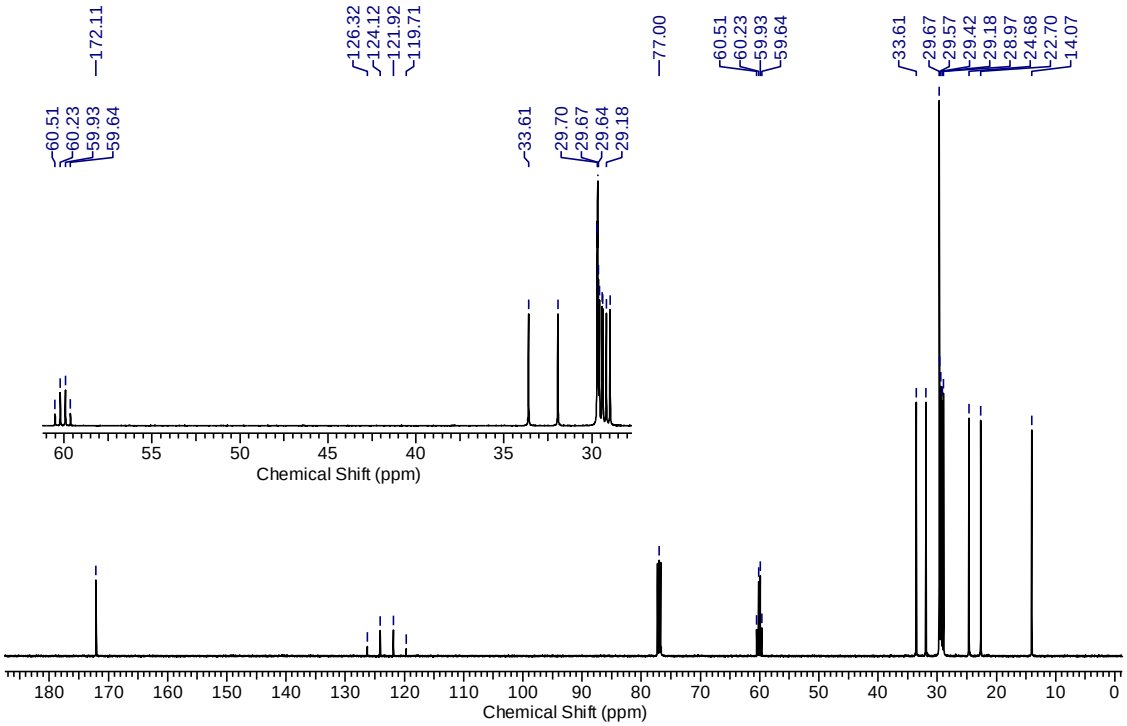


To a solution of palmitic acid (50.0 mmol, 1.0 equiv., 12.82 gm,) and 2,2,2-trifluoroethanol (50.0 mmol, 1.0 equiv., 5.0 gm) in 50 mL cyclohexane was added conc. H_2SO_4 (30 mol %) at ambient temperature and heated to reflux (at 100 ^oC) for 12 h. The mixture was cooled to room temperature, added saturated $NaHCO_3$ solution to neutralize excess H_2SO_4, and then was extracted three times with CH_2Cl_2 (100 mL each time). The combined organic phases were washed with brine solution, dried over anhydrous Na_2SO_4, and concentrated in *vacuum* to give the desired 2,2,2-trifluoroethyl palmitate.

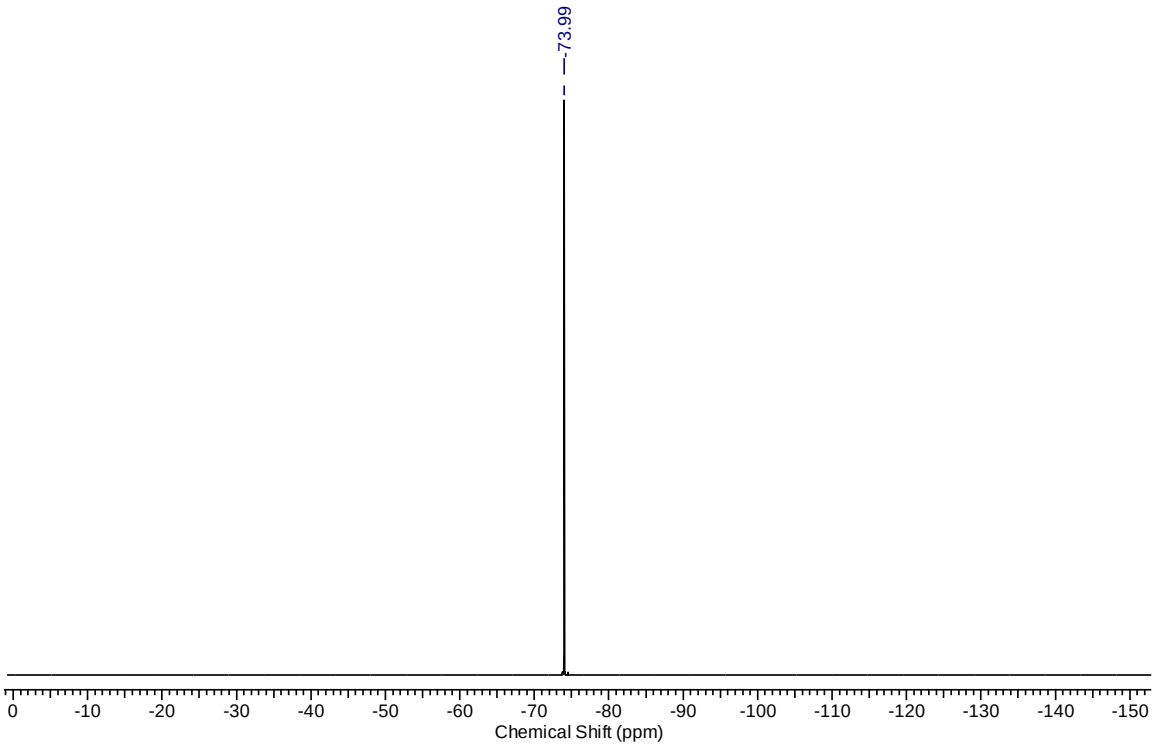
Colourless solid at 300 K. Isolated Yield: 16.5 gm, 98 %. ^1H NMR (500 MHz, $CDCl_3$): δ = 4.46 (q, J = 8.5 Hz, 2H), 2.41 (t, J = 7.8 Hz, 2H), 1.66 (quin, J = 7.4 Hz, 2H), 1.35-1.22 (m, 24H), 0.88 (t, J = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ = 172.11, 126.32, 124.12, 121.92, 119.71, 60.51, 60.23, 59.93, 59.64, 33.61, 31.94, 29.70, 29.67, 29.64, 29.57, 29.42, 29.38, 29.18, 28.97, 24.68, 22.70, 14.07. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -73.99. GC data (Rt): 9.359 min (GC Programme: Column HP 5; Method: 80 ^oC hold 1min; 20 ^oC ramp up to 280 ^oC; at 280 ^oC Hold for 10 min; Inlet temp. 300 ^oC, Detector temp. 300 ^oC, H_2 Flow 40 mL, Air Flow 400 mL, N_2 Flow 25 mL per minute, Constant Flow mode).



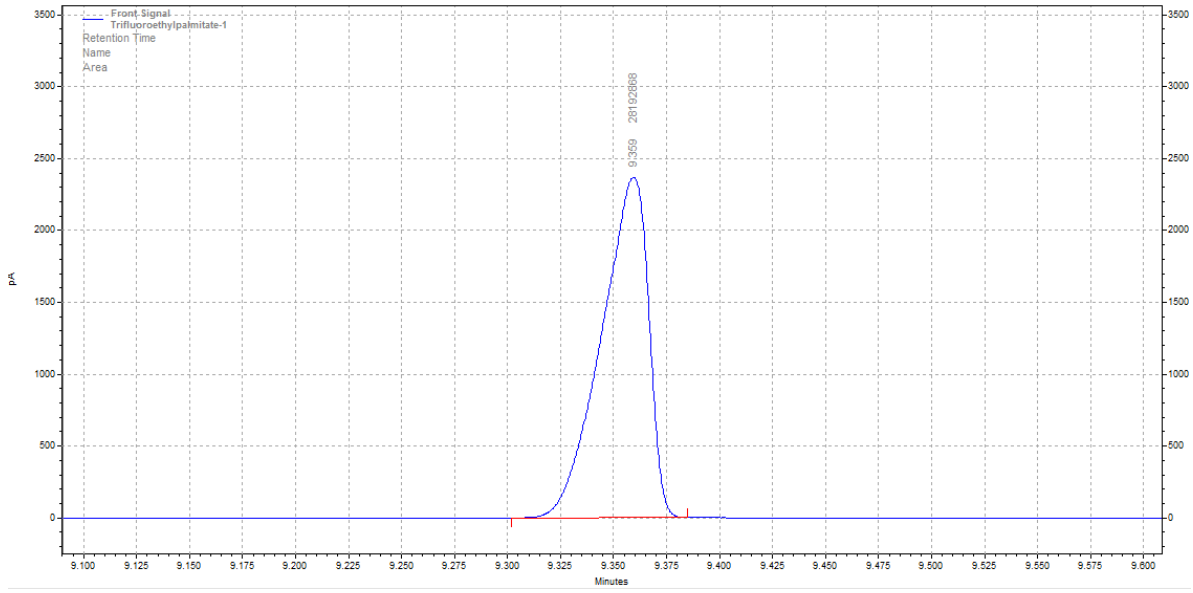
^{1}H NMR of trifluoroethylpalmitate



^{13}C NMR of trifluoroethylpalmitate



^{19}F NMR of trifluoroethylpalmitate



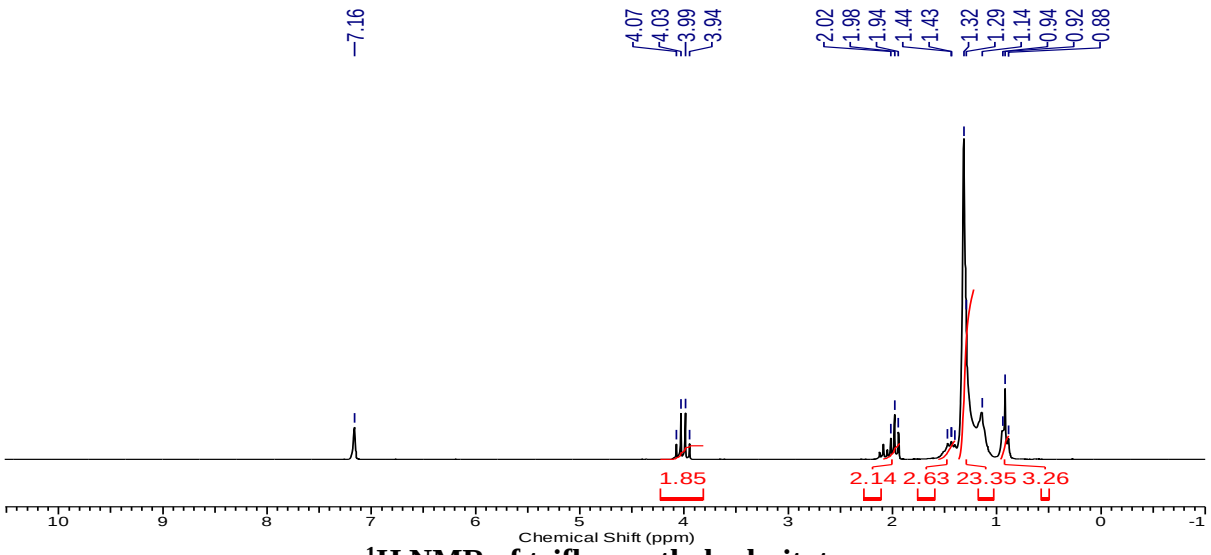
GC Chromatogram of trifluoroethylpalmitate

(4) NMR Studies:

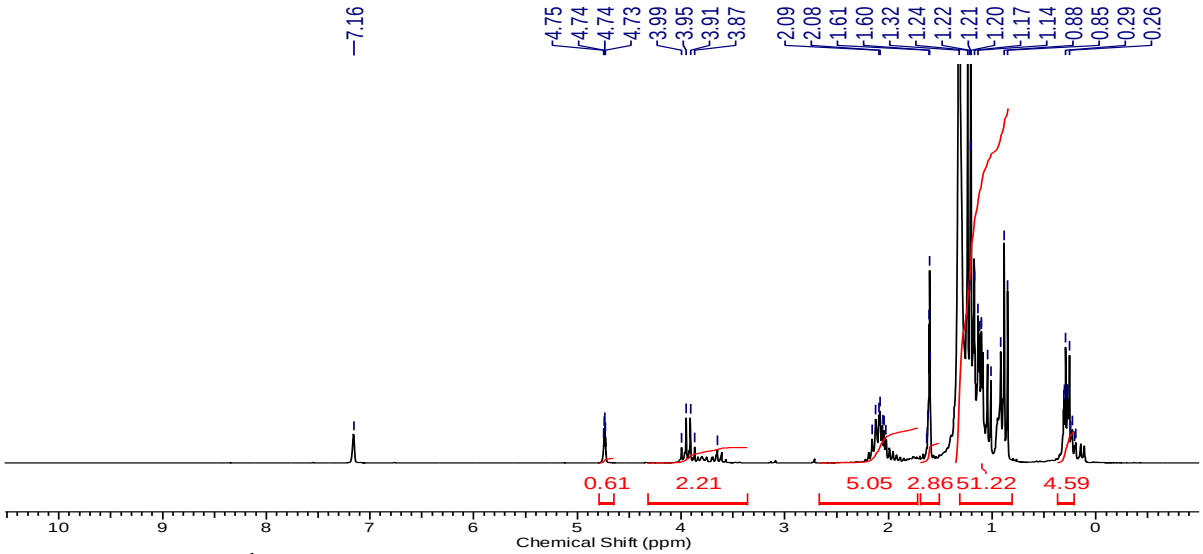
Preparation of the NMR sample

In an oven dried clean NMR tubes were charged with 0.2 mmol of donor molecule and 1:1 ratio of 0.2 mmol triisobutylaluminium and 0.6 mL of deuterated benzene (C_6D_6) under inert atmosphere. Then the NMR tubes were placed on the preheated oil-bath at various temperatures (60 ^oC, 80^oC and 110^oC). After 12 h, the reaction mixture was directly analyzed by NMR.

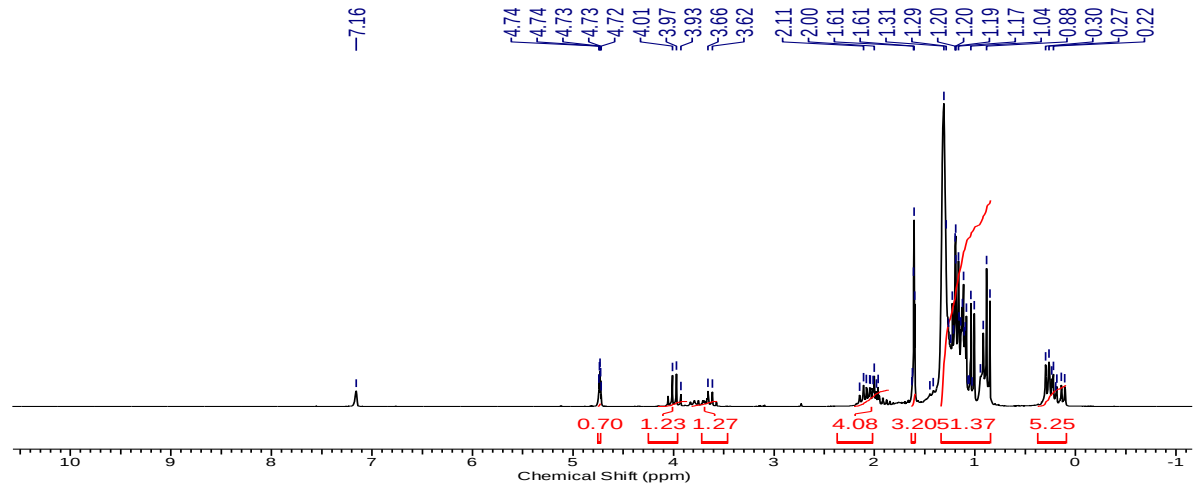
Effect of temperature



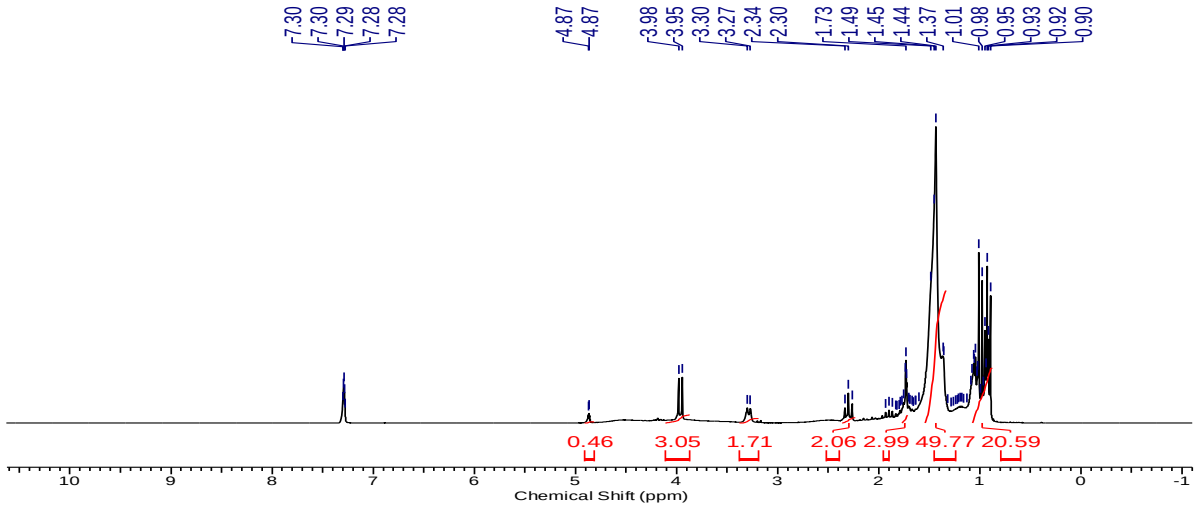
^{1}H NMR of trifluoroethylpalmitate



^{1}H NMR of reaction mixture (Donor + AlR_3) at 60^{o}C

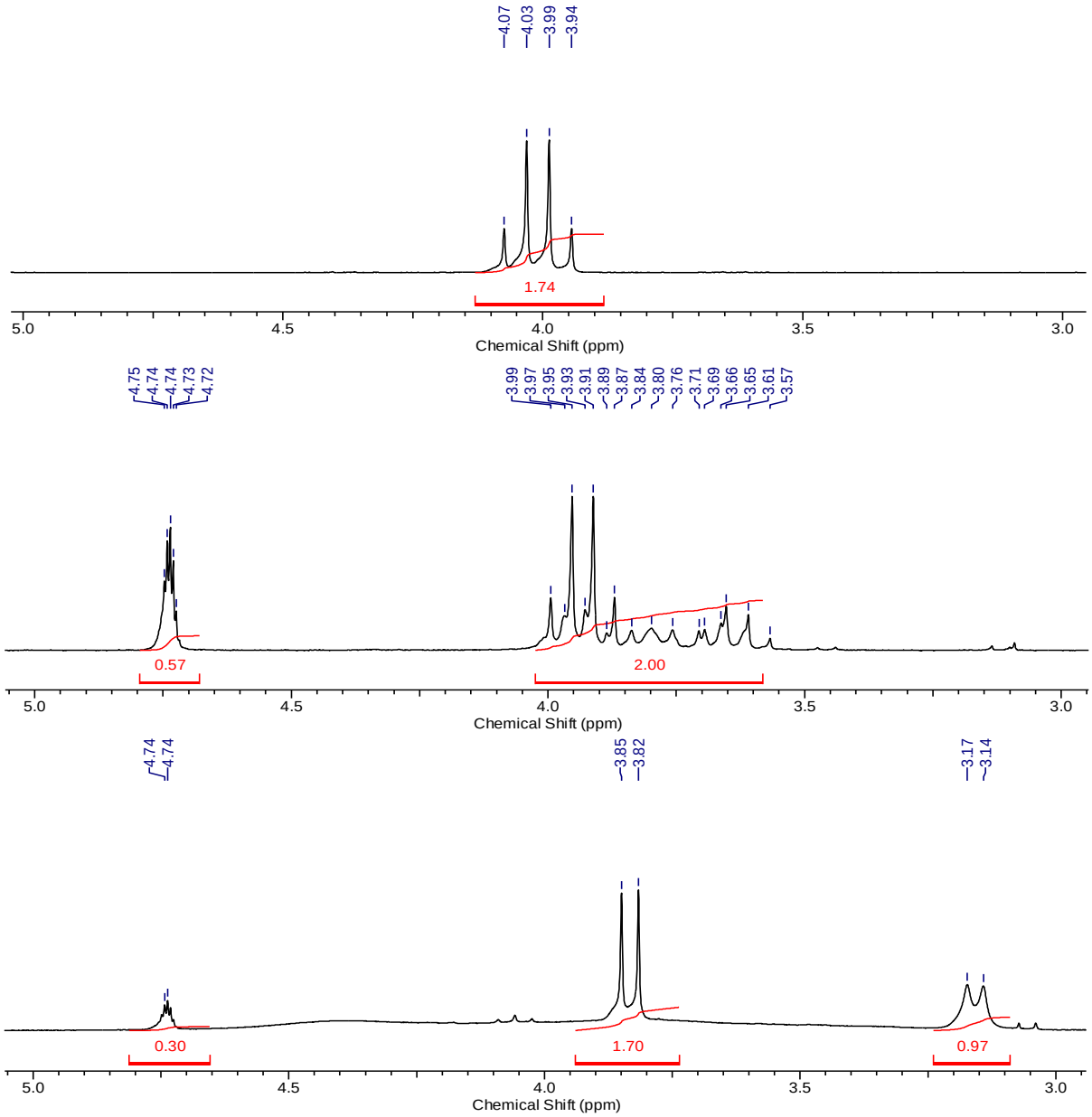


^{1}H NMR of reaction mixture (Donor + AlR_3) at 80^{o}C

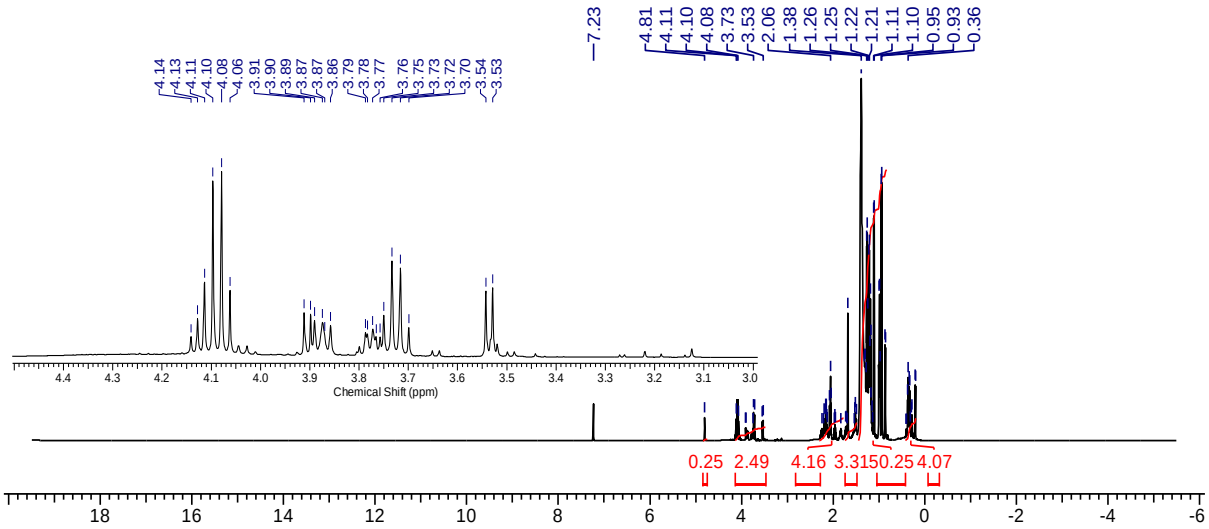


^{1}H NMR of reaction mixture (Donor + AlR_3) at 100^{o}C

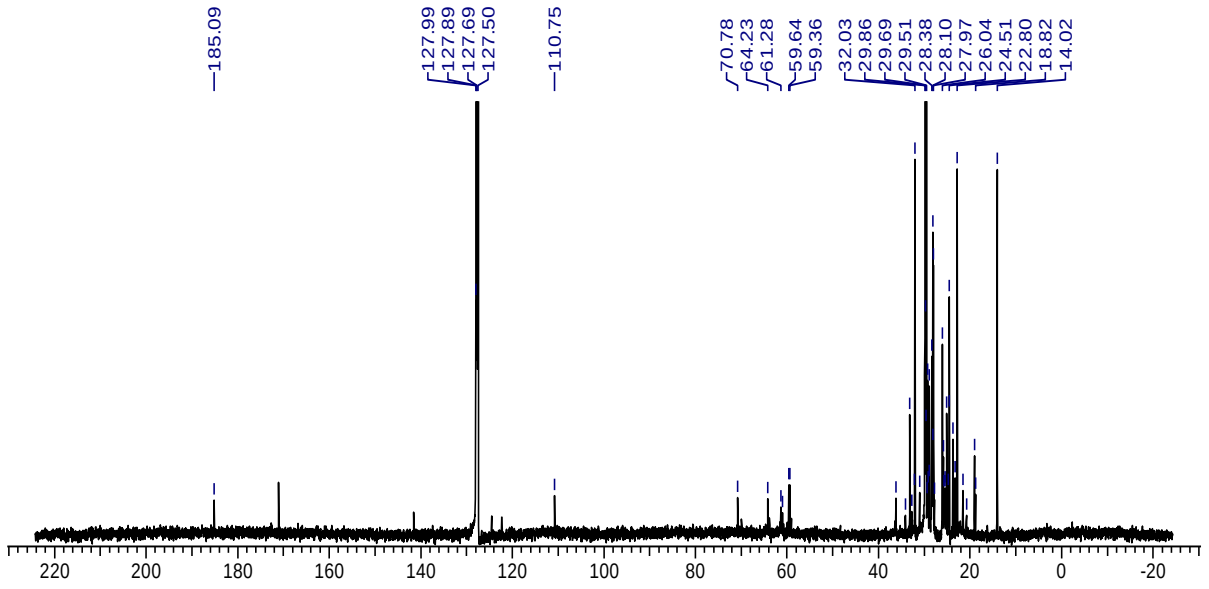
Variable temperature NMR studies illustrate that the donor molecule (palmitic derivative) started compositing at 80 ^{o}C and while increasing the temperature from 80 to 100 ^{o}C the interaction of donor with alkylaluminum reagent is more efficient. The following NMR (expanded) data comparison is clearly indicated the difference. In palmitic acid derivative, the CF_3-CH_2- moiety appeared as a quartet and after the interaction with Al-metal center the quartet disappeared and appeared as two doublets.



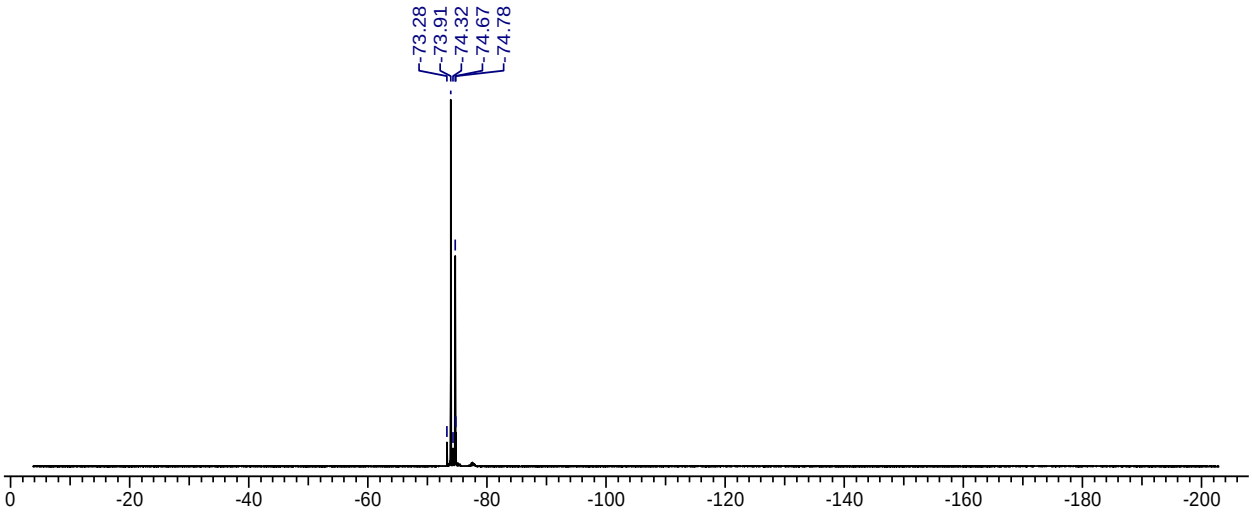
^{1}H NMR comparing of reaction mixtures heated at 80ºC and 100ºC (Reaction of 2,2,2-trifluoroethyl palmitate with AlR_3 in benzene-d6)



^{1}H NMR of reaction mixture at 100 ^{o}C (Reaction of 2,2,2-trifluoroethyl palmitate with AlR_3in benzene-d6)

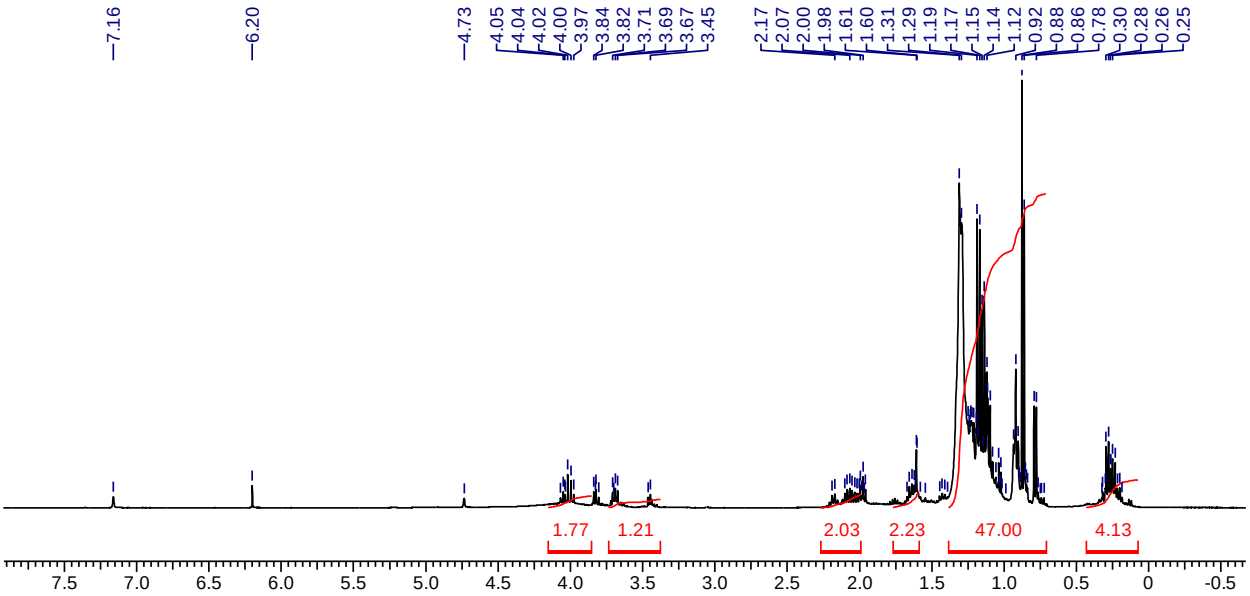


^{13}C NMR of reaction mixture at 100 ^{o}C (Reaction of 2,2,2-trifluoroethyl palmitate with AlR_3 inbenzene-d6)

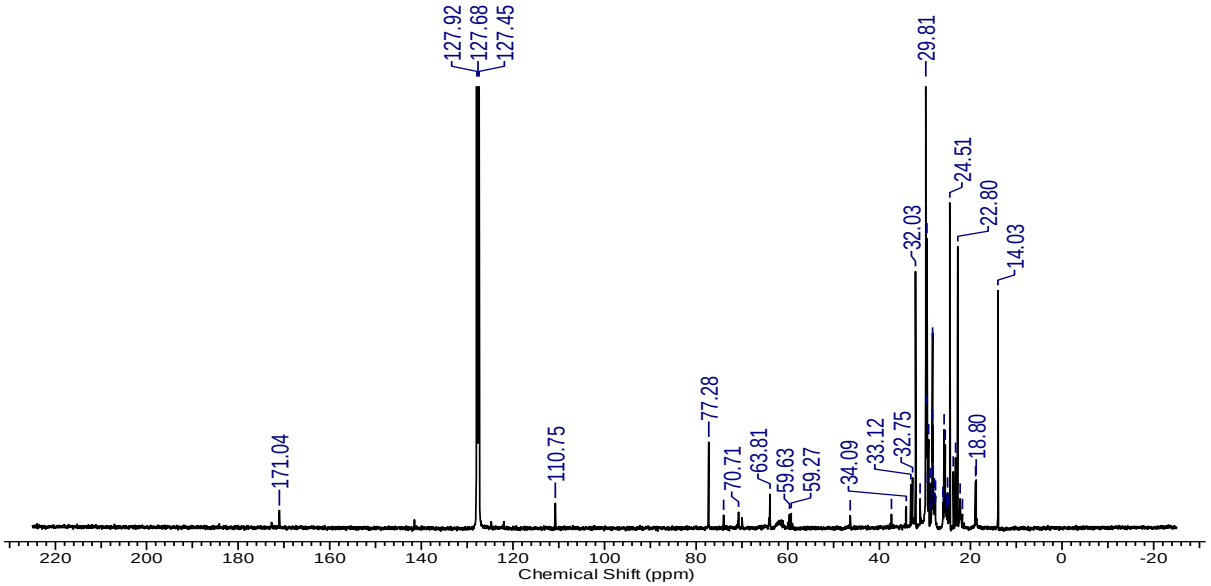


^{19}F NMR of reaction mixture at 100 ^{o}C (Reaction of 2,2,2-trifluoroethyl palmitate with AlR_3in benzene-d6)

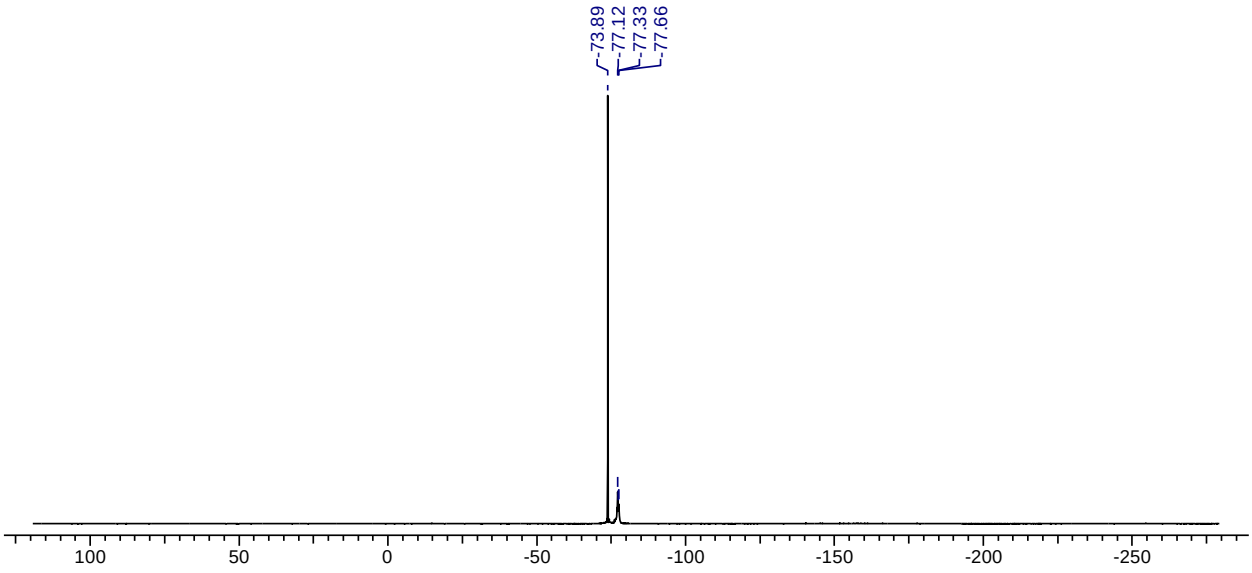
Interaction of 2,2,2-trifluoroethyl myristate with AlR_3 in benzene-d6



^{1}H NMR of reaction mixture at 100 ^{o}C



^{13}C NMR of reaction mixture at 100 ^{o}C



^{19}F NMR of reaction mixture at 100 ^{o}C

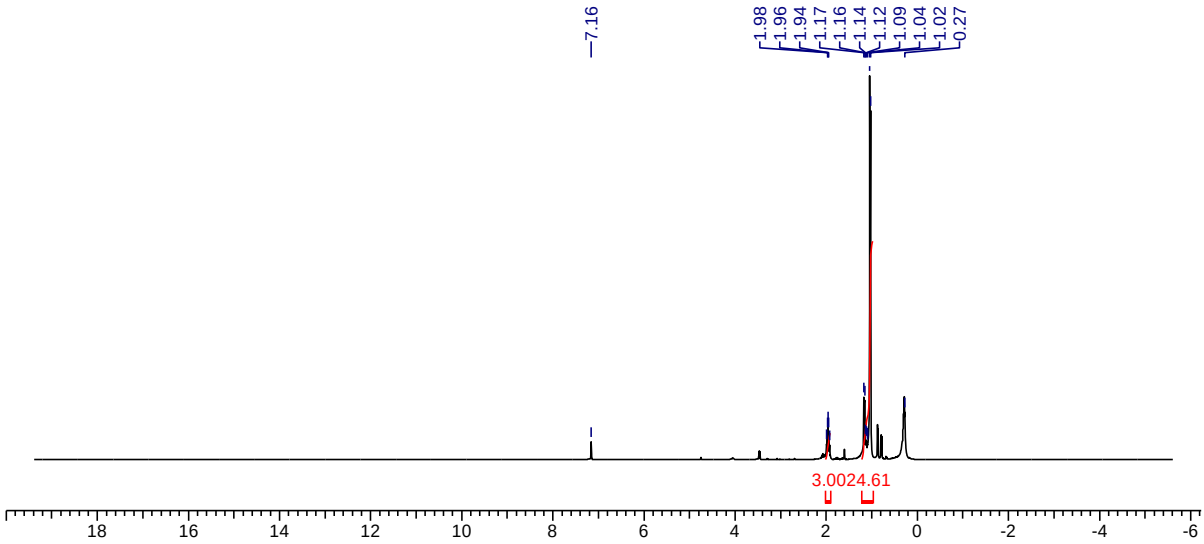
From the above NMR studies, it clearly showed that the decomposition of 2,2,2-trifluoroethyl fatty esters (palmitic and myristate) with AlR_3 reagent follows,

i. Ketonic pathway formation

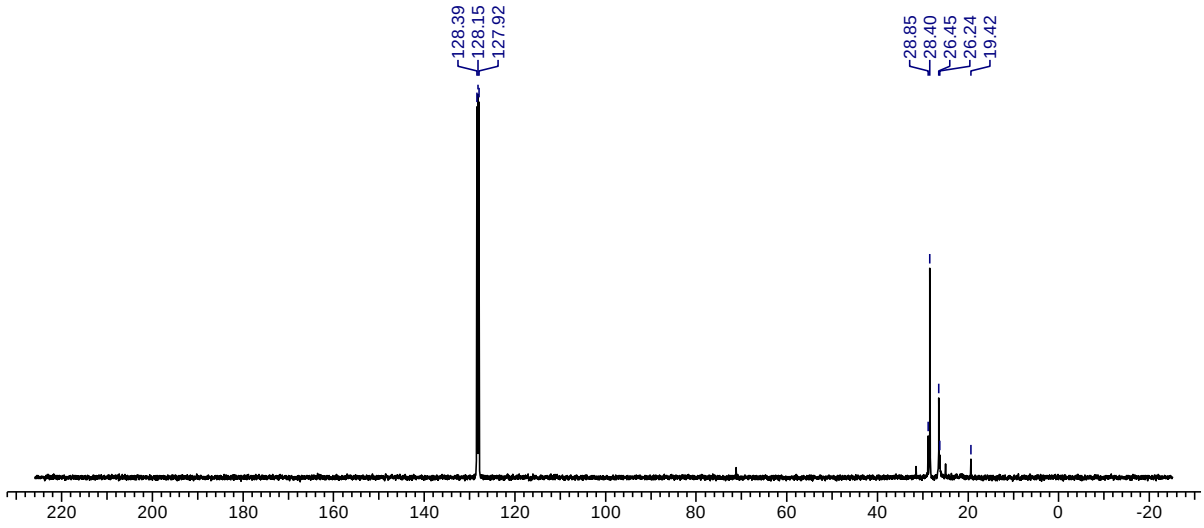
ii. The rate of decomposition for palmitic derivative is better than myristate acid ester

Supporting Data:

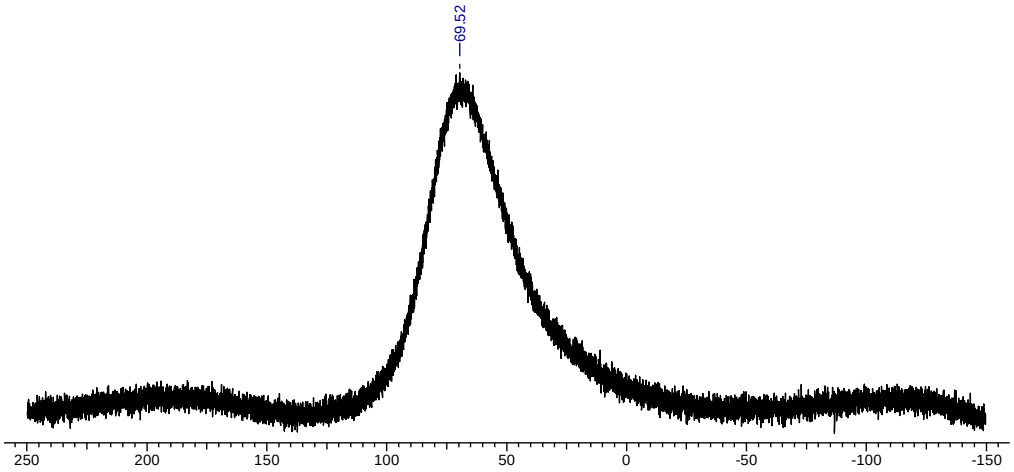
NMR of Starting materials:



^{1}H NMR of Tri *iso*butyl aluminium



^{13}C NMR of Tri *iso*butyl aluminium



^{27}AL NMR of Tri *iso*butyl aluminium

Section II: Optimized geometries at PBE/TZVP level of theory

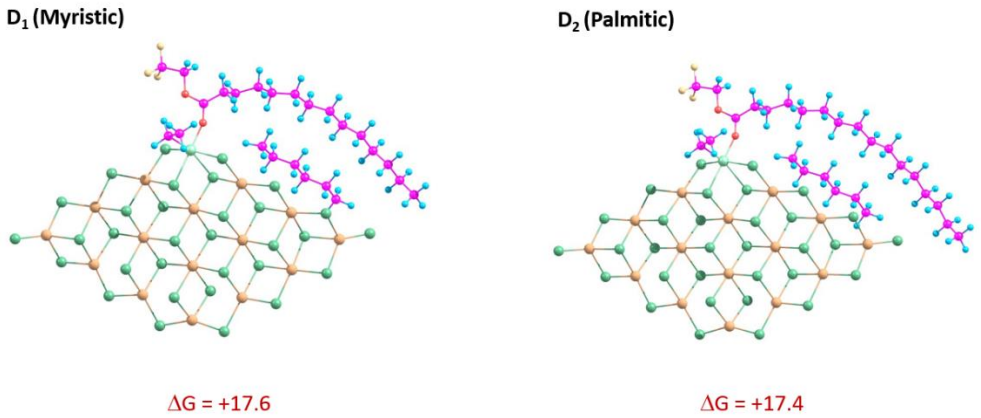


Figure S1. The energy required to displace the alkyl chain of **D₁** and **D₂** by an n-hexane molecule.

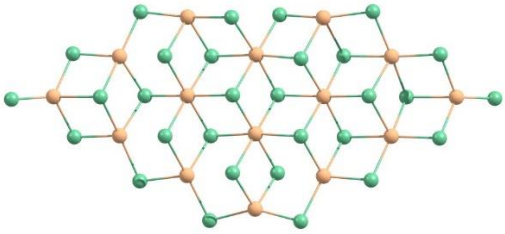


Figure S2. The $MgCl_2$ cluster model employed for this study.

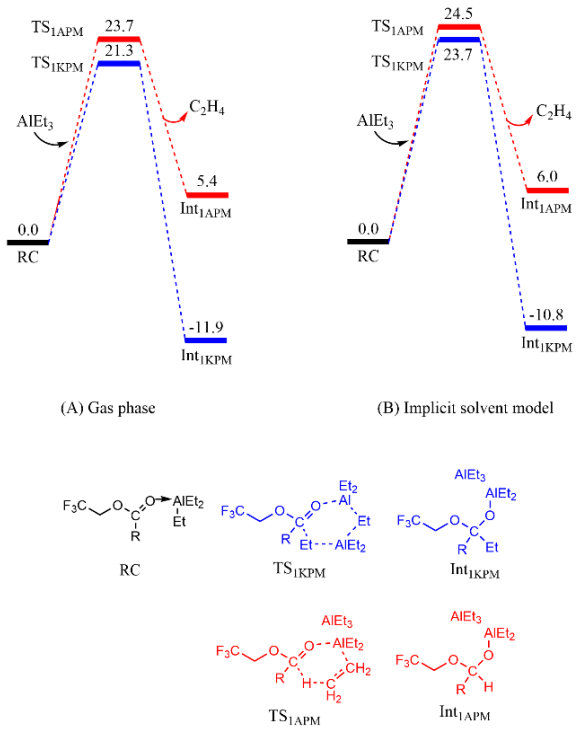


Figure S3. Comparison between the gas phase and implicit solvent model calculations for the rate determining transition states for the reaction between **D₁** and Al_2Et_6.

(A) Optimized geometries and relative energies of various conformations of D_1

(1) **Conformer 1** (most stable conformer)

50

C	1.779725	1.615155	0.251932
O	0.802454	1.357080	1.198654
C	0.915101	0.121016	1.909783
O	2.686764	0.851703	0.000259
H	-0.057350	-0.387214	1.872886
H	1.701840	-0.511020	1.474049
C	1.259906	0.391322	3.369782
F	0.327319	1.161955	3.984564
F	1.331047	-0.790232	4.042280
F	2.457127	1.018293	3.498607
C	1.502565	2.924870	-0.437846
H	2.472518	3.356210	-0.723532
H	0.997771	3.611236	0.256715
C	0.632883	2.713639	-1.693137
H	1.138112	2.001267	-2.365554
H	-0.323311	2.249860	-1.397844
C	0.360136	4.022682	-2.437158
H	1.320534	4.486652	-2.723684
H	-0.133703	4.736025	-1.753592
C	-0.505263	3.834986	-3.685934
H	-0.011813	3.120031	-4.368206
H	-1.465340	3.369853	-3.398814
C	-0.780850	5.140986	-4.435453
H	0.178466	5.606356	-4.724746
H	-1.271399	5.857226	-3.751952
C	-1.649077	4.957588	-5.682501
H	-1.157929	4.244012	-6.368333
H	-2.607342	4.489502	-5.393571
C	-1.929678	6.264630	-6.428131
H	-0.971039	6.732294	-6.717087
H	-2.419566	6.977596	-5.740847
C	-2.800133	6.086182	-7.674342
H	-2.309447	5.375488	-8.363573
H	-3.757888	5.615922	-7.386072
C	-3.083952	7.394701	-8.416044
H	-2.126613	7.865311	-8.704991
H	-3.574579	8.105525	-7.726686
C	-3.955150	7.214513	-9.661581
H	-3.462977	6.503848	-10.349974
H	-4.910939	6.741601	-9.371011
C	-4.243867	8.520191	-10.405997
H	-3.288604	8.994370	-10.696673
H	-4.736923	9.231380	-9.718449
C	-5.114894	8.337605	-11.651893
H	-4.620516	7.627557	-12.337854
H	-6.068165	7.862935	-11.360176
C	-5.397404	9.649387	-12.386207
H	-4.462132	10.128954	-12.715473
H	-5.921989	10.364290	-11.732980
H	-6.022438	9.491182	-13.277212

(2) **Conformer 2** (ΔG = 0.4 kcal/mol w.r.t conformer 1)

50

C	2.077020	1.968218	0.411827
O	1.035362	1.270169	1.003058
C	1.352907	-0.023175	1.521754
O	3.222873	1.574879	0.401013
H	2.441150	-0.167394	1.578177
H	0.895544	-0.116205	2.515010

C	0.765363	-1.099905	0.616300
F	1.251800	-1.015782	-0.647733
F	1.080151	-2.329444	1.108690
F	-0.588031	-1.021224	0.536886
C	1.554496	3.230177	-0.222147
H	2.414227	3.894340	-0.385170
H	0.852350	3.722286	0.468302
C	0.842525	2.936400	-1.557889
H	1.533916	2.394512	-2.224415
H	-0.010643	2.263811	-1.372779
C	0.359804	4.216065	-2.245610
H	1.221657	4.885106	-2.419460
H	-0.319111	4.761496	-1.566005
C	-0.354626	3.956986	-3.574396
H	0.320988	3.403719	-4.250784
H	-1.221803	3.294828	-3.400931
C	-0.824118	5.239692	-4.267074
H	0.045496	5.900281	-4.437048
H	-1.498426	5.794383	-3.590030
C	-1.537111	4.993213	-5.598960
H	-0.866849	4.429636	-6.272560
H	-2.414252	4.342653	-5.429577
C	-1.987124	6.280744	-6.295175
H	-1.108336	6.930302	-6.461009
H	-2.657461	6.844188	-5.621431
C	-2.696710	6.042663	-7.630315
H	-2.028910	5.473232	-8.301512
H	-3.580363	5.399584	-7.465230
C	-3.133481	7.332878	-8.330157
H	-2.249274	7.975648	-8.493846
H	-3.802504	7.902613	-7.660442
C	-3.839146	7.093609	-9.667285
H	-3.170580	6.518578	-10.333061
H	-4.725153	6.453744	-9.502044
C	-4.271336	8.379562	-10.377183
H	-3.386498	9.020938	-10.543845
H	-4.942473	8.955958	-9.714964
C	-4.973689	8.131096	-11.715222
H	-4.301963	7.552323	-12.372862
H	-5.857482	7.491180	-11.545792
C	-5.400497	9.417895	-12.424070
H	-4.532553	10.061935	-12.635946
H	-6.099663	9.999913	-11.803715
H	-5.899865	9.206096	-13.381045

(3) **Conformer 3** (ΔG = 1.3 kcal/mol w.r.t conformer 1)

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C	0.978433	1.659411	-2.902394
O	0.607386	1.887507	-1.588156
C	-0.684069	1.417441	-1.196678
O	0.298465	1.031886	-3.684450
H	-1.092472	0.714563	-1.937134
H	-0.587302	0.938429	-0.214104
C	-1.642985	2.594755	-1.063266
F	-1.845566	3.220304	-2.252546
F	-2.846854	2.151864	-0.613159
F	-1.188645	3.527868	-0.188361
C	2.334664	2.264048	-3.181677
H	2.472222	2.219003	-4.270999
H	3.082794	1.589297	-2.731004
C	2.531463	3.691701	-2.649255
H	2.450726	3.685970	-1.551121
H	3.561376	4.003900	-2.889116
C	1.536289	4.698890	-3.230283
H	0.512479	4.389142	-2.962100

H	1.582625	4.670902	-4.333589
C	1.775765	6.136397	-2.753189
H	1.836470	6.150072	-1.649973
H	2.760492	6.474300	-3.118456
C	0.683909	7.113904	-3.213986
H	0.481458	6.934036	-4.284074
H	1.054433	8.150909	-3.148136
C	-0.615423	6.998359	-2.405299
H	-0.888190	5.937373	-2.286102
H	-0.429401	7.370606	-1.383248
C	-1.808879	7.756909	-3.005661
H	-1.576840	8.835778	-3.043658
H	-2.667953	7.652471	-2.320682
C	-2.234561	7.286414	-4.407423
H	-3.138050	7.844528	-4.708667
H	-1.459889	7.555813	-5.146436
C	-2.507691	5.783636	-4.501704
H	-3.238252	5.490472	-3.725912
H	-1.583535	5.233548	-4.264611
C	-3.020202	5.331445	-5.872403
H	-3.965776	5.856299	-6.094952
H	-2.304323	5.650095	-6.652375
C	-3.241763	3.815767	-5.979032
H	-3.759571	3.589548	-6.927623
H	-3.926762	3.492823	-5.174023
C	-1.957874	2.978983	-5.908202
H	-1.271026	3.309240	-6.707662
H	-1.434475	3.169969	-4.958124
C	-2.213937	1.476533	-6.033818
H	-2.693486	1.231164	-6.994649
H	-2.881819	1.126159	-5.231043
H	-1.279480	0.904372	-5.956186

(4) **Conformer 4** (ΔG = 0.1 kcal/mol w.r.t conformer 1)

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C	1.086491	1.859132	-0.139971
O	0.203710	1.476121	-1.139334
C	-1.188040	1.594557	-0.840216
O	0.727702	2.252422	0.948130
H	-1.685392	0.667285	-1.152867
H	-1.345403	1.778795	0.232113
C	-1.799028	2.749924	-1.622929
F	-1.627324	2.610480	-2.963614
F	-3.136631	2.804657	-1.380127
F	-1.260887	3.944902	-1.266498
C	2.508455	1.687368	-0.616178
H	2.648554	0.623106	-0.865874
H	3.158876	1.926673	0.236242
C	2.860232	2.552960	-1.840498
H	3.860888	2.252761	-2.192977
H	2.157393	2.316894	-2.653498
C	2.857810	4.056049	-1.544662
H	3.537664	4.253181	-0.697988
H	1.856718	4.365957	-1.200101
C	3.292873	4.920531	-2.738349
H	3.370649	5.968671	-2.402585
H	4.312241	4.621020	-3.040031
C	2.369160	4.866906	-3.965540
H	2.303052	3.832296	-4.345241
H	2.832104	5.452087	-4.778685
C	0.958549	5.404017	-3.706828
H	0.483700	4.835270	-2.891606
H	1.028987	6.447036	-3.348183
C	0.044437	5.349399	-4.933279
H	-0.034577	4.303225	-5.279376

H	0.505413	5.912941	-5.764784
C	-1.360324	5.896219	-4.663932
H	-1.811544	5.336428	-3.826338
H	-1.285122	6.944598	-4.323351
C	-2.290500	5.822680	-5.877224
H	-2.345818	4.775323	-6.219745
H	-1.849380	6.395669	-6.713345
C	-3.699167	6.355232	-5.591543
H	-4.160338	5.748366	-4.791385
H	-3.614548	7.378207	-5.185318
C	-4.631528	6.379760	-6.810010
H	-4.170046	6.987821	-7.609630
H	-5.566871	6.898918	-6.535584
C	-4.985375	4.997853	-7.370932
H	-4.067957	4.480806	-7.697250
H	-5.411729	4.380784	-6.560401
C	-5.969689	5.063307	-8.540287
H	-5.553751	5.647787	-9.375991
H	-6.913454	5.544395	-8.238805
H	-6.212830	4.060723	-8.922296

(5) **Conformer 5** (ΔG = 1.3 kcal/mol w.r.t conformer 1)

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C	-15.095053	4.661011	-10.094005
O	-13.729692	4.861945	-9.976412
C	-13.313028	6.169002	-9.572766
O	-15.919762	5.500050	-9.802440
H	-14.181040	6.796965	-9.326052
H	-12.644014	6.076862	-8.707080
C	-12.541073	6.819008	-10.713381
F	-13.288934	6.903621	-11.843385
F	-12.172978	8.078913	-10.356375
F	-11.410603	6.132347	-11.024130
C	-15.383500	3.283692	-10.636134
H	-15.891840	2.721390	-9.836488
H	-14.438198	2.770360	-10.854624
C	-16.296922	3.349463	-11.876229
H	-16.457024	2.316870	-12.226949
H	-17.278751	3.739323	-11.567324
C	-15.750152	4.212043	-13.022374
H	-15.713526	5.267081	-12.699253
H	-16.474863	4.180250	-13.854051
C	-14.368558	3.800027	-13.538830
H	-13.629308	3.905432	-12.728343
H	-14.378076	2.729239	-13.814210
C	-13.914708	4.628418	-14.746120
H	-13.966653	5.700834	-14.485034
H	-14.632631	4.478919	-15.571274
C	-12.498040	4.302975	-15.239549
H	-12.424422	3.221868	-15.457570
H	-12.326156	4.818435	-16.200561
C	-11.388947	4.702580	-14.260239
H	-11.534219	4.179638	-13.301532
H	-11.481144	5.779594	-14.031262
C	-9.978790	4.419850	-14.787201
H	-9.869518	3.336225	-14.976643
H	-9.858754	4.913046	-15.767914
C	-8.854294	4.887191	-13.852387
H	-8.965896	5.970558	-13.665518
H	-7.884749	4.764906	-14.366130
C	-8.796207	4.150427	-12.509155
H	-9.740932	4.297056	-11.959340
H	-8.715776	3.066537	-12.702365
C	-7.635783	4.614699	-11.622383
H	-7.699235	5.710349	-11.504623

H	-6.678793	4.418583	-12.140164
C	-7.598779	3.967044	-10.230946
H	-6.809159	4.453043	-9.633798
H	-8.549076	4.179728	-9.709763
C	-7.351964	2.455877	-10.250893
H	-6.418035	2.217825	-10.784799
H	-8.166981	1.914513	-10.753371
H	-7.266265	2.049790	-9.232035

(6) **Conformer 6** (ΔG = 1.0 kcal/mol w.r.t conformer 1)

50

C	-1.076749	-2.965630	-14.812077
O	0.218601	-2.730541	-14.377114
C	1.117212	-2.157448	-15.328219
O	-1.440968	-2.777015	-15.951774
H	2.058756	-2.720519	-15.294680
H	0.686173	-2.179316	-16.339210
C	1.410024	-0.709156	-14.954361
F	1.972262	-0.598325	-13.723543
F	2.278809	-0.175597	-15.855570
F	0.285107	0.050949	-14.955288
C	-1.915673	-3.476993	-13.666696
H	-1.456818	-4.407806	-13.297767
H	-2.903900	-3.720555	-14.079508
C	-2.033471	-2.465701	-12.510483
H	-2.607038	-2.942664	-11.698800
H	-1.028564	-2.260487	-12.108210
C	-2.709855	-1.152942	-12.913677
H	-3.715006	-1.369005	-13.318218
H	-2.145672	-0.680746	-13.736918
C	-2.827259	-0.161913	-11.752453
H	-3.366220	-0.640948	-10.915136
H	-1.816518	0.070239	-11.371412
C	-3.537022	1.140626	-12.131544
H	-4.552075	0.908329	-12.501573
H	-3.005250	1.610459	-12.977852
C	-3.635983	2.142959	-10.977857
H	-4.163660	1.673164	-10.128324
H	-2.619793	2.376881	-10.611974
C	-4.346960	3.444868	-11.357537
H	-5.370389	3.214438	-11.705268
H	-3.830314	3.902544	-12.220247
C	-4.418046	4.462521	-10.215161
H	-4.934600	4.002815	-9.355412
H	-3.393616	4.692132	-9.868546
C	-5.116882	5.768277	-10.610047
H	-6.160795	5.549708	-10.900270
H	-4.628433	6.168765	-11.515290
C	-5.111338	6.851814	-9.523140
H	-4.067240	7.067856	-9.231359
H	-5.506056	7.789452	-9.951789
C	-5.923663	6.506871	-8.271233
H	-5.512677	5.602095	-7.791279
H	-6.957217	6.250754	-8.569376
C	-5.962201	7.640362	-7.241439
H	-4.929351	7.894279	-6.945298
H	-6.372464	8.547959	-7.717582
C	-6.783316	7.297823	-5.997354
H	-6.376207	6.412577	-5.484150
H	-7.829039	7.074336	-6.261019
H	-6.792148	8.127355	-5.274868

(7) **Conformer 7** (ΔG = 1.7 kcal/mol w.r.t conformer 1)

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C	-4.462460	7.331206	-6.817818
O	-4.659732	8.050361	-7.983887
C	-3.565821	8.864224	-8.417790
O	-3.423311	7.347929	-6.193742
H	-2.715791	8.772674	-7.727031
H	-3.272873	8.556644	-9.430559
C	-4.008785	10.320057	-8.465006
F	-4.457023	10.751582	-7.258059
F	-2.953022	11.099591	-8.824760
F	-5.000975	10.528111	-9.367334
C	-5.695315	6.537762	-6.460849
H	-5.466972	5.484359	-6.694449
H	-6.528566	6.837012	-7.109739
C	-6.040213	6.672976	-4.967671
H	-6.878217	5.991182	-4.747486
H	-5.178073	6.322434	-4.380031
C	-6.409182	8.100021	-4.537334
H	-5.557007	8.775014	-4.731125
H	-6.554634	8.107433	-3.443710
C	-7.663491	8.655278	-5.216919
H	-7.507841	8.688236	-6.305454
H	-8.505740	7.959038	-5.050701
C	-8.065042	10.048803	-4.715896
H	-7.215896	10.743648	-4.847272
H	-8.233879	9.984394	-3.627375
C	-9.319410	10.636995	-5.394901
H	-10.004668	9.813837	-5.661448
H	-9.870444	11.251902	-4.664727
C	-9.049119	11.519785	-6.627095
H	-8.489382	12.411448	-6.294953
H	-10.015176	11.893018	-7.010646
C	-8.273749	10.861306	-7.776778
H	-8.052623	11.625683	-8.541023
H	-7.288559	10.527071	-7.410692
C	-8.992775	9.685534	-8.446366
H	-9.919519	10.046150	-8.927675
H	-9.316642	8.958889	-7.681392
C	-8.119957	8.958617	-9.473386
H	-7.835648	9.659406	-10.279010
H	-7.174288	8.665900	-8.986929
C	-8.792310	7.725994	-10.085201
H	-9.756424	8.027037	-10.531098
H	-9.041016	7.011870	-9.278345
C	-7.950160	7.009065	-11.150315
H	-8.561209	6.217934	-11.616039
H	-7.709920	7.723282	-11.957084
C	-6.654458	6.391247	-10.614634
H	-6.866231	5.671171	-9.807661
H	-5.975529	7.152070	-10.203050
H	-6.112623	5.853321	-11.406554

(8) **Conformer 8** (ΔG = 2.2 kcal/mol w.r.t conformer 1)

50

C	-0.056780	11.176818	-12.477568
O	-1.102059	10.907200	-11.602497
C	-2.220902	11.795152	-11.653711
O	-0.054506	12.122712	-13.233213
H	-2.588315	11.913693	-10.626742
H	-1.938342	12.765515	-12.085867
C	-3.352162	11.210553	-12.496338
F	-3.760686	9.996202	-12.038288
F	-4.423966	12.047682	-12.447931
F	-3.000201	11.052471	-13.795262
C	1.020574	10.131368	-12.347349

H	1.086577	9.804306	-11.300492
H	1.966860	10.616258	-12.622980
C	0.779994	8.914671	-13.273524
H	0.772560	9.267046	-14.317283
H	1.657850	8.255015	-13.171812
C	-0.500375	8.115293	-12.991975
H	-0.565976	7.300432	-13.733128
H	-1.381302	8.753392	-13.172271
C	-0.590556	7.527597	-11.579351
H	0.233421	6.807181	-11.422925
H	-0.443099	8.332591	-10.842814
C	-1.934856	6.849755	-11.298648
H	-2.097683	6.041048	-12.032157
H	-2.740224	7.582555	-11.476658
C	-2.072417	6.267216	-9.883434
H	-3.072137	5.812330	-9.788537
H	-1.354340	5.437848	-9.760139
C	-1.856535	7.269175	-8.734652
H	-0.792388	7.555725	-8.694529
H	-2.061523	6.753039	-7.780584
C	-2.705643	8.547875	-8.804769
H	-2.443137	9.188774	-7.945059
H	-2.431572	9.124520	-9.704866
C	-4.219187	8.314362	-8.805223
H	-4.496455	7.692586	-7.934857
H	-4.506943	7.733965	-9.698678
C	-5.028331	9.615078	-8.777881
H	-4.769204	10.180532	-7.866320
H	-4.724044	10.246479	-9.631193
C	-6.542377	9.391606	-8.847491
H	-6.865372	8.802115	-7.970156
H	-6.764407	8.769957	-9.731765
C	-7.372909	10.680871	-8.926393
H	-7.050281	11.262310	-9.808015
H	-8.427000	10.413317	-9.108647
C	-7.289546	11.558791	-7.674534
H	-6.267236	11.923697	-7.497317
H	-7.600938	10.998034	-6.778882
H	-7.942424	12.439994	-7.759795

(9) **Conformer 9** (ΔG = 1.3 kcal/mol w.r.t conformer 1)

50

C	-6.926192	7.912420	0.122590
O	-6.964539	6.951737	-0.872616
C	-8.173007	6.194869	-0.979944
O	-7.824962	8.084971	0.918232
H	-7.946866	5.130384	-0.829104
H	-8.913830	6.536468	-0.242816
C	-8.746320	6.371243	-2.379093
F	-7.901257	5.925310	-3.342887
F	-9.904449	5.663639	-2.484539
F	-9.024431	7.672621	-2.651697
C	-5.643576	8.701990	0.051324
H	-4.990878	8.278408	-0.722137
H	-5.138825	8.591507	1.023400
C	-5.929377	10.196653	-0.206523
H	-6.473058	10.602197	0.660719
H	-4.959893	10.718984	-0.250698
C	-6.730535	10.477464	-1.484618
H	-6.888930	11.566794	-1.559694
H	-7.738263	10.035806	-1.389968
C	-6.081610	9.971053	-2.776044
H	-5.051975	10.366155	-2.854349
H	-5.989460	8.874165	-2.733904
C	-6.868873	10.363737	-4.030476

H	-6.954845	11.463739	-4.067536
H	-7.899829	9.976690	-3.942156
C	-6.252305	9.860613	-5.342864
H	-6.784145	10.326073	-6.191168
H	-5.207889	10.213422	-5.407076
C	-6.305785	8.337364	-5.514740
H	-7.348190	8.004186	-5.371944
H	-5.722350	7.845406	-4.717932
C	-5.801430	7.840859	-6.876300
H	-6.014590	6.761016	-6.965848
H	-6.383062	8.334407	-7.674059
C	-4.301117	8.062619	-7.107683
H	-3.749971	7.643031	-6.247436
H	-4.077429	9.143349	-7.115978
C	-3.761141	7.434668	-8.399633
H	-2.660183	7.518956	-8.406300
H	-3.983373	6.351877	-8.399183
C	-4.307410	8.059565	-9.687349
H	-4.115827	9.148316	-9.670977
H	-5.404617	7.945205	-9.726369
C	-3.702163	7.458575	-10.959391
H	-2.604614	7.576060	-10.929443
H	-3.890337	6.370592	-10.969607
C	-4.250744	8.086009	-12.242452
H	-4.046341	9.167784	-12.274051
H	-5.341951	7.954384	-12.313187
H	-3.801358	7.635657	-13.139896

(10) **Conformer 10** (ΔG = 2.5 kcal/mol w.r.t conformer 1)

50

C	1.174009	10.383148	-7.058543
O	0.398584	10.581509	-8.190332
C	0.814139	11.628744	-9.070941
O	2.138523	11.063117	-6.784431
H	-0.081158	12.184205	-9.377461
H	1.540102	12.291773	-8.578851
C	1.468182	11.046323	-10.319074
F	0.622205	10.246924	-11.021176
F	1.853521	12.060605	-11.139824
F	2.565861	10.307473	-10.019864
C	0.659483	9.213411	-6.258106
H	-0.343263	8.933359	-6.610342
H	0.586991	9.546594	-5.212252
C	1.617931	8.008461	-6.356213
H	2.607039	8.303213	-5.970266
H	1.237291	7.219291	-5.687093
C	1.747476	7.460757	-7.779192
H	2.214840	8.218789	-8.430540
H	0.735863	7.292134	-8.184456
C	2.554615	6.162512	-7.856356
H	3.539630	6.323230	-7.384032
H	2.047650	5.390198	-7.249751
C	2.769020	5.616847	-9.276884
H	3.389345	4.709345	-9.196353
H	3.367651	6.340375	-9.858416
C	1.478148	5.285257	-10.055121
H	1.649309	4.395182	-10.684724
H	0.690761	4.994570	-9.338057
C	0.974018	6.414481	-10.964194
H	1.779861	6.676304	-11.671032
H	0.796439	7.328813	-10.376140
C	-0.286834	6.066227	-11.768789
H	-0.504481	6.898813	-12.457697
H	-0.072935	5.193993	-12.411014
C	-1.540957	5.756142	-10.932015

H	-1.386230	4.817116	-10.374154
H	-2.379761	5.558124	-11.621459
C	-1.959043	6.853736	-9.941683
H	-2.840661	6.503420	-9.376896
H	-1.162921	6.996115	-9.189839
C	-2.280099	8.206994	-10.581640
H	-3.096961	8.080558	-11.315477
H	-1.407907	8.565558	-11.152904
C	-2.667594	9.281502	-9.560834
H	-3.548924	8.943877	-8.987787
H	-1.846592	9.392800	-8.832835
C	-2.959325	10.640345	-10.200760
H	-3.808931	10.580743	-10.898845
H	-2.090062	10.997323	-10.775207
H	-3.203149	11.401869	-9.444850

(B) Decomposition reaction of D_1 with Al_2Et_6

(1) **RC**

94

C	0.202244	1.721658	2.353067
O	-0.413030	2.287459	3.400077
C	-0.005817	1.818756	4.704397
O	1.103243	0.896435	2.511612
Al	2.494964	-0.539946	2.569479
C	3.452320	0.006236	4.237710
C	4.087524	1.408581	4.190557
C	3.465588	-0.449062	0.823605
C	2.909629	-1.323352	-0.315085
C	1.178338	-2.068440	2.778316
Al	-1.335284	-2.614009	2.866482
C	-1.429616	-3.980535	1.408353
C	-1.083391	-3.460811	0.001662
C	1.840627	-3.432495	3.022841
C	-1.472947	-3.142000	4.793885
C	-1.211968	-2.014625	5.808225
C	-2.055858	-0.798091	2.393181
C	-3.586229	-0.814371	2.209553
H	-0.020620	0.721171	4.746551
H	0.999778	2.184803	4.952314
H	4.239118	-0.741692	4.445133
H	2.764505	-0.067591	5.101291
H	4.608509	1.679462	5.124486
H	3.336416	2.196176	4.005875
H	4.825005	1.490991	3.376286
H	4.518588	-0.725258	1.016562
H	3.516298	0.606548	0.497341
H	2.923571	-2.392311	-0.048692
H	1.863212	-1.076765	-0.554377
H	3.481969	-1.221466	-1.252841
H	-2.465909	-4.368939	1.411633
H	-0.802052	-4.854677	1.653328
H	-0.033564	-3.128552	-0.065436
H	-1.220424	-4.224004	-0.783039
H	-1.707893	-2.596725	-0.279314
H	-0.808776	-3.998942	5.002408
H	-2.496163	-3.535906	4.943003
H	-0.176340	-1.635239	5.740894
H	-1.351963	-2.334502	6.854512
H	-1.882967	-1.155183	5.645151
H	0.596682	-2.047900	1.834688
H	-1.798022	-0.061219	3.173157
H	-1.580860	-0.444316	1.460729
H	-4.100784	-1.132119	3.130893
H	-3.999874	0.173357	1.941523

H	-3.891776	-1.515064	1.415723
H	2.495548	-3.705317	2.181296
H	2.467637	-3.407622	3.926855
H	1.123883	-4.260247	3.151116
H	0.557746	-1.749477	3.640258
C	-0.310370	2.203664	1.029759
H	-1.410823	2.200487	1.085203
H	-0.019834	3.265219	0.933492
C	0.200580	1.378230	-0.149340
H	1.299457	1.434706	-0.190103
H	-0.043457	0.317977	0.025101
C	-0.393717	1.819467	-1.487476
H	-1.495635	1.761487	-1.438768
H	-0.148972	2.880739	-1.672524
C	0.109670	0.968523	-2.657084
H	1.212405	1.020534	-2.696079
H	-0.136112	-0.091561	-2.466649
C	-0.467144	1.388305	-4.011233
H	-1.568971	1.313891	-3.978397
H	-0.239262	2.454614	-4.190130
C	0.062835	0.557064	-5.182898
H	1.164535	0.634757	-5.213812
H	-0.161030	-0.509980	-5.005220
C	-0.511031	0.977148	-6.538897
H	-1.611250	0.877498	-6.516429
H	-0.307028	2.050726	-6.703239
C	0.046512	0.173789	-7.717074
H	1.146707	0.275177	-7.737456
H	-0.156093	-0.900399	-7.556352
C	-0.524245	0.600054	-9.072641
H	-1.622719	0.481641	-9.059675
H	-0.337498	1.678825	-9.222504
C	0.054968	-0.179792	-10.256261
H	1.153696	-0.061779	-10.266440
H	-0.132722	-1.258852	-10.110122
C	-0.511292	0.253402	-11.611271
H	-1.609284	0.127758	-11.605553
H	-0.331258	1.334640	-11.752673
C	0.077383	-0.513801	-12.798949
H	1.174268	-0.388466	-12.801940
H	-0.104254	-1.593588	-12.658214
C	-0.494006	-0.068328	-14.146799
H	-1.584975	-0.214698	-14.183301
H	-0.298136	1.000307	-14.326908
C	-1.011338	2.363158	5.708483
F	-1.066744	3.716985	5.692926
F	-2.259778	1.892492	5.476857
F	-0.634960	1.970155	6.952699
H	-0.053500	-0.633514	-14.981358

(2) **TS_{1APM}**

94

C	3.604456	-0.109786	-2.469637
O	4.519542	-0.600357	-3.426780
C	5.884941	-0.526532	-3.040539
O	3.976680	-0.279580	-1.200667
Al	4.081313	0.827334	0.224445
C	2.456725	0.978094	1.361484
C	2.063061	-0.342487	2.051074
C	4.269992	2.700762	-0.966816
C	3.865959	2.569822	-2.300919
C	5.852443	0.611715	1.142995
C	6.101523	1.695125	2.204700
Al	8.266630	-0.571272	1.108202
C	8.424683	-0.924721	3.071708

C	7.280214	-1.678418	3.770049
C	9.271958	0.994632	0.359143
C	8.865635	1.492229	-1.038220
C	7.865762	-2.100637	-0.121775
C	6.523512	-2.841461	0.022105
H	9.358157	-1.512985	3.172486
H	6.585412	0.665310	0.311348
H	5.853591	-0.404595	1.579913
H	5.335979	2.863901	-0.776082
H	3.585171	3.220852	-0.286204
H	1.608352	1.361941	0.768724
H	9.234735	1.828646	1.082311
H	10.336311	0.690985	0.337722
H	8.691083	-2.820188	0.043303
H	8.006854	-1.765894	-1.165320
H	1.184244	-0.229885	2.707272
H	1.819568	-1.127933	1.317925
H	2.880457	-0.736598	2.676209
H	5.316153	1.676229	2.975851
H	7.065214	1.586644	2.726601
H	6.092967	2.703008	1.760384
H	9.498794	2.319703	-1.400855
H	8.921913	0.691048	-1.792049
H	7.827106	1.870372	-1.051001
H	6.440409	-3.705097	-0.659839
H	6.379750	-3.227794	1.043080
H	5.663446	-2.185781	-0.188972
H	6.162677	0.468148	-2.653961
H	6.135900	-1.277718	-2.277790
H	2.650748	1.751481	2.127073
H	8.634734	0.018962	3.605425
H	7.496130	-1.890016	4.830900
H	6.340248	-1.103055	3.748562
H	7.072217	-2.645698	3.286326
H	3.590052	1.105247	-2.625211
H	4.603777	2.598165	-3.108546
H	2.855336	2.863200	-2.597965
C	2.212666	-0.595768	-2.868835
H	2.056026	-0.345353	-3.929406
H	2.231637	-1.696176	-2.796721
C	1.097102	-0.024700	-1.997071
H	1.291567	-0.285901	-0.945124
H	1.109436	1.079229	-2.046380
C	-0.293897	-0.527138	-2.391675
H	-0.499902	-0.262176	-3.443998
H	-0.307035	-1.630588	-2.346879
C	-1.405364	0.029425	-1.497431
H	-1.187885	-0.227924	-0.445237
H	-1.395554	1.133400	-1.547627
C	-2.800793	-0.481356	-1.866093
H	-3.015725	-0.227357	-2.919685
H	-2.810004	-1.584825	-1.812250
C	-3.913304	0.076729	-0.974169
H	-3.695128	-0.172262	0.079917
H	-3.908735	1.180188	-1.032403
C	-5.306999	-0.443357	-1.337448
H	-5.524355	-0.196416	-2.392261
H	-5.310479	-1.546675	-1.277747
C	-6.422095	0.113308	-0.447842
H	-6.202437	-0.129585	0.607412
H	-6.422913	1.216481	-0.511175
C	-7.813556	-0.415076	-0.807731
H	-8.033150	-0.173003	-1.863209
H	-7.811572	-1.518207	-0.744153
C	-8.930533	0.139295	0.081005
H	-8.708943	-0.099688	1.136799
H	-8.935726	1.242301	0.014586

C	-10.320233	-0.395214	-0.275850
H	-10.542797	-0.156641	-1.331665
H	-10.314976	-1.498362	-0.209754
C	-11.439438	0.156619	0.612342
H	-11.214862	-0.081033	1.666813
H	-11.445009	1.258512	0.544321
C	-12.822095	-0.387645	0.247138
H	-13.085584	-0.135253	-0.791696
H	-12.853556	-1.484741	0.338367
C	6.731145	-0.787542	-4.275702
F	6.541887	0.158833	-5.233450
F	8.049668	-0.761133	-3.928839
F	6.476745	-1.993937	-4.835261
H	-13.606079	0.023889	0.899869

(3) **TS$_{1KPM}$**

94

C	-0.044823	-0.101094	0.353000
O	-0.208834	0.426843	1.611317
C	0.488878	-0.233776	2.662026
O	1.049315	-0.743607	0.116661
Al	2.127479	-2.130483	-0.478245
C	3.375834	-2.521057	1.016924
C	4.391535	-1.387984	1.265649
C	2.750980	-1.868745	-2.350500
C	1.844028	-2.352864	-3.494776
C	0.500168	-3.758731	-0.489417
Al	-1.548776	-3.888007	-0.012572
C	-2.648389	-4.293443	-1.636954
C	-2.432128	-3.325679	-2.813472
C	1.240404	-5.021560	-0.931469
C	-1.797510	-4.852598	1.728735
C	-1.009999	-4.254481	2.907780
C	-1.593445	-1.753186	0.409126
C	-2.898478	-1.153552	0.866851
H	0.395929	-1.329300	2.590262
H	1.556650	0.031138	2.666780
H	3.913212	-3.464229	0.816307
H	2.795748	-2.710008	1.939104
H	5.066416	-1.601496	2.110744
H	3.891142	-0.430946	1.488603
H	5.028094	-1.211724	0.383928
H	3.739372	-2.355137	-2.432404
H	2.959560	-0.789087	-2.470524
H	1.677616	-3.440366	-3.449017
H	0.851525	-1.876646	-3.467978
H	2.269756	-2.136705	-4.488351
H	-3.716871	-4.308202	-1.358047
H	-2.425257	-5.326647	-1.961679
H	-1.376797	-3.292573	-3.132678
H	-3.021936	-3.592178	-3.707365
H	-2.717151	-2.293033	-2.548585
H	-1.503453	-5.908701	1.584954
H	-2.871458	-4.889083	1.982897
H	0.072512	-4.191473	2.694697
H	-1.106053	-4.841355	3.836958
H	-1.352565	-3.233860	3.149880
H	0.346050	-2.995715	-1.274735
H	-0.849532	-1.993831	1.169025
H	-1.276661	-1.624048	-0.625705
H	-3.362694	-1.756102	1.663013
H	-2.779038	-0.134700	1.280099
H	-3.622008	-1.098258	0.040075
H	2.302988	-4.878084	-1.198832
H	1.212843	-5.775870	-0.131635

H	0.748143	-5.464434	-1.809244
H	0.763806	-3.385416	0.517311
C	-0.641573	0.838858	-0.668362
H	-1.697748	1.010574	-0.413010
H	-0.129682	1.808036	-0.519363
C	-0.477915	0.392360	-2.116773
H	0.592864	0.260445	-2.337851
H	-0.948486	-0.595557	-2.265787
C	-1.092211	1.381452	-3.109511
H	-2.164090	1.515055	-2.879264
H	-0.624957	2.373441	-2.974183
C	-0.937621	0.944386	-4.568209
H	0.132966	0.786123	-4.790260
H	-1.426033	-0.036589	-4.709742
C	-1.518208	1.955049	-5.560373
H	-2.589071	2.110828	-5.337653
H	-1.031004	2.934789	-5.404339
C	-1.361983	1.546803	-7.027162
H	-0.293359	1.369493	-7.244647
H	-1.871275	0.580900	-7.195938
C	-1.909969	2.590870	-8.003850
H	-2.978536	2.768510	-7.786132
H	-1.400595	3.555305	-7.824717
C	-1.752140	2.207088	-9.477130
H	-0.685941	2.011015	-9.690734
H	-2.280054	1.255006	-9.666678
C	-2.271457	3.277504	-10.440965
H	-3.337110	3.475438	-10.226343
H	-1.742083	4.227912	-10.245842
C	-2.114096	2.908775	-11.918240
H	-1.050298	2.697736	-12.129853
H	-2.656134	1.967036	-12.119719
C	-2.612957	3.995400	-12.874491
H	-3.676226	4.209019	-12.662068
H	-2.069336	4.936253	-12.671671
C	-2.457847	3.634375	-14.354442
H	-1.396321	3.415382	-14.563822
H	-3.006638	2.698323	-14.558158
C	-2.950550	4.734392	-15.296870
H	-4.017514	4.950900	-15.130766
H	-2.394865	5.671810	-15.137347
C	-0.143666	0.200603	3.975416
F	-0.066882	1.539754	4.167084
F	-1.451067	-0.153737	4.046637
F	0.510048	-0.407813	5.002332
H	-2.828348	4.450220	-16.352414

(4) **Int$_{1APM}$**

88

C	1.607960	-0.578942	-1.801369
O	2.507841	-1.313265	-2.706784
C	3.824767	-1.459156	-2.253846
O	1.880678	-0.891277	-0.484974
Al	1.998016	0.136245	0.958115
C	1.464349	-0.855434	2.590133
C	-0.036446	-1.216329	2.570431
C	1.782084	2.097651	0.703235
C	0.399084	2.622920	1.140727
Al	6.400991	-0.573115	0.426731
C	6.686890	-2.538181	0.327771
C	7.734723	-3.053541	-0.675160
C	4.619753	0.035889	1.181543
C	4.785176	0.771605	2.525402
C	7.805479	0.828647	0.360482
C	9.041962	0.546138	-0.511149

H	6.951465	-2.876676	1.347800
H	1.966024	2.353542	-0.354752
H	2.568772	2.624430	1.271019
H	1.695836	-0.261798	3.490881
H	4.191267	0.698953	0.404710
H	4.019960	-0.890508	1.283969
H	8.121768	1.031481	1.401143
H	7.316936	1.764418	0.031947
H	-0.343966	-1.773093	3.471182
H	-0.675272	-0.319874	2.516517
H	-0.287670	-1.844092	1.700962
H	0.199696	2.406859	2.202335
H	0.307708	3.714197	1.012156
H	-0.417972	2.163156	0.562559
H	3.835946	1.137865	2.950693
H	5.236060	0.116631	3.286529
H	5.443802	1.645735	2.415906
H	9.754238	1.387437	-0.508606
H	9.591377	-0.341814	-0.163373
H	8.767515	0.359306	-1.560795
H	3.866362	-1.633306	-1.166078
H	4.270798	-2.321995	-2.769578
H	2.063625	-1.777948	2.675937
H	5.708328	-3.012671	0.128439
H	7.815339	-4.152818	-0.667201
H	7.492995	-2.754186	-1.706764
H	8.737148	-2.654878	-0.458388
H	1.758619	0.502663	-2.001170
C	0.202741	-1.000134	-2.215338
H	0.098299	-0.848507	-3.301742
H	0.114077	-2.081021	-2.019663
C	-0.879583	-0.229487	-1.458121
H	-0.709697	-0.345065	-0.373699
H	-0.788623	0.850503	-1.673558
C	-2.301788	-0.697691	-1.776384
H	-2.504607	-0.565340	-2.853992
H	-2.374355	-1.783031	-1.583394
C	-3.372779	0.030334	-0.958837
H	-3.140665	-0.077904	0.116372
H	-3.324685	1.113482	-1.171677
C	-4.793007	-0.478628	-1.219064
H	-5.033817	-0.360709	-2.290927
H	-4.830484	-1.564549	-1.017899
C	-5.861960	0.224098	-0.377369
H	-5.609121	0.116568	0.692984
H	-5.838934	1.308776	-0.586529
C	-7.277022	-0.309832	-0.614506
H	-7.538771	-0.190712	-1.681342
H	-7.291842	-1.397319	-0.418831
C	-8.343227	0.370518	0.248786
H	-8.070363	0.262833	1.314212
H	-8.341207	1.456318	0.044223
C	-9.753660	-0.184114	0.033402
H	-10.035165	-0.065531	-1.028467
H	-9.749551	-1.272250	0.225607
C	-10.815047	0.478832	0.915937
H	-10.527027	0.366118	1.976876
H	-10.825934	1.566027	0.719056
C	-12.223054	-0.086151	0.714217
H	-12.515375	0.029579	-0.345293
H	-12.210724	-1.174255	0.907027
C	-13.282720	0.570380	1.604368
H	-12.987220	0.455854	2.661968
H	-13.295601	1.656956	1.409737
C	-14.684808	-0.005445	1.398565
H	-15.018177	0.124561	0.357048
H	-14.707492	-1.084026	1.619941

C	4.711867	-0.254231	-2.566917
F	4.211608	0.921434	-2.124531
F	5.955000	-0.414250	-1.901872
F	5.011024	-0.114790	-3.867566
H	-15.424821	0.484079	2.048942

(5) **Int$_{1KPM}$**

94

C	-0.182711	1.123134	2.387335
O	-0.208834	2.264881	3.311580
C	0.241526	2.026781	4.626585
O	0.951923	0.378963	2.607143
Al	2.143841	-0.878975	2.367215
C	3.311312	-1.045320	3.963562
C	4.352928	0.089048	4.056813
C	2.765220	-1.344084	0.529937
C	1.997712	-2.389319	-0.299113
C	0.377761	-2.768779	2.894809
Al	-1.598734	-2.593286	3.248652
C	-2.845223	-3.023834	1.759619
C	-2.230087	-3.001942	0.349149
C	0.971072	-4.185615	2.945282
C	-2.167066	-2.355339	5.138630
C	-1.022171	-2.069907	6.127044
C	-1.433852	0.241640	2.632502
C	-2.784094	0.931566	2.463972
H	0.657094	1.014907	4.752749
H	1.033626	2.751099	4.878428
H	3.823495	-2.023347	3.951846
H	2.686843	-1.047644	4.874955
H	4.993970	-0.002805	4.949021
H	3.871062	1.078448	4.106555
H	5.023728	0.102987	3.182539
H	3.815600	-1.668731	0.640622
H	2.816939	-0.393558	-0.032185
H	1.988523	-3.374611	0.192132
H	0.945364	-2.103782	-0.459933
H	2.440561	-2.533079	-1.298231
H	-3.713642	-2.343517	1.810224
H	-3.267507	-4.024881	1.967969
H	-1.384221	-3.701847	0.259412
H	-2.957737	-3.274010	-0.432583
H	-1.840927	-2.005107	0.084662
H	-2.717112	-3.263150	5.447857
H	-2.918575	-1.546750	5.186622
H	-0.286327	-2.889515	6.149850
H	-1.383460	-1.929486	7.158144
H	-0.469764	-1.154309	5.861718
H	0.509181	-2.332742	1.882798
H	-1.334850	-0.144117	3.663934
H	-1.354691	-0.603726	1.920024
H	-3.603110	0.273420	2.788060
H	-2.824172	1.847486	3.066727
H	-2.968873	1.200544	1.414046
H	2.056520	-4.203975	2.753936
H	0.813878	-4.647300	3.932264
H	0.500283	-4.842895	2.198753
H	0.837009	-2.130561	3.674729
C	-0.186197	1.806938	1.013124
H	-1.001932	2.546356	0.991937
H	0.756259	2.373511	0.955288
C	-0.298528	0.847933	-0.169416
H	0.462549	0.057408	-0.070098
H	-1.278131	0.338692	-0.157269
C	-0.124337	1.540545	-1.522898

H	-0.917009	2.299490	-1.650542
H	0.830967	2.095117	-1.528161
C	-0.151567	0.569901	-2.706132
H	0.683755	-0.146596	-2.606501
H	-1.076150	-0.034154	-2.663730
C	-0.067819	1.269112	-4.065122
H	-0.926363	1.956812	-4.170843
H	0.835018	1.905741	-4.093187
C	-0.043100	0.308074	-5.255959
H	0.842026	-0.348530	-5.176670
H	-0.922352	-0.359671	-5.205363
C	-0.028603	1.021580	-6.610488
H	-0.927133	1.659574	-6.692636
H	0.835538	1.709496	-6.651417
C	0.026067	0.072344	-7.809941
H	0.939075	-0.546527	-7.744490
H	-0.823314	-0.632975	-7.756648
C	-0.001481	0.794616	-9.159762
H	-0.921865	1.402388	-9.227148
H	0.838644	1.511341	-9.207277
C	0.070520	-0.146702	-10.364717
H	0.999897	-0.741608	-10.307438
H	-0.759456	-0.874676	-10.309067
C	0.016043	0.578817	-11.711886
H	-0.919183	1.164439	-11.772513
H	0.838298	1.316008	-11.763747
C	0.102983	-0.357354	-12.920559
H	1.042271	-0.934580	-12.863714
H	-0.712916	-1.099278	-12.863190
C	0.033197	0.379876	-14.259558
H	-0.912832	0.934954	-14.357582
H	0.854286	1.107566	-14.355728
C	-0.865645	2.226263	5.655878
F	-1.443868	3.449743	5.563917
F	-1.867349	1.303477	5.543837
F	-0.349966	2.104688	6.913756
H	0.102639	-0.314443	-15.109893

(6) **TS_{2APM}**

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C	0.109613	0.918832	2.296938
O	0.209844	1.877425	3.436844
C	-0.849093	1.792594	4.368317
O	1.147766	0.027986	2.339297
Al	2.212677	-0.593685	3.609241
C	3.667031	-1.697050	2.848354
C	3.176763	-3.084623	2.383586
C	1.435468	-0.826855	5.427831
C	0.278297	-1.845163	5.469075
C	3.503461	1.689887	3.974867
Al	2.623974	3.436429	4.463136
C	1.555134	3.629566	6.133185
C	2.204109	4.499127	7.230938
C	5.015435	1.684442	3.700455
C	3.243350	5.005813	3.407947
C	2.930041	6.406269	3.964520
H	-1.267224	0.773937	4.435921
H	-0.471331	2.077123	5.359362
H	4.474411	-1.815604	3.591553
H	4.116487	-1.158176	1.996880
H	3.989771	-3.692852	1.953561
H	2.396022	-2.998526	1.611947
H	2.747113	-3.668605	3.213706
H	1.086549	0.147626	5.812151
H	2.232321	-1.144035	6.123375

H	-0.534063	-1.575990	4.774146
H	0.613038	-2.854408	5.181757
H	-0.171918	-1.930470	6.471799
H	1.332892	2.627706	6.541231
H	0.580567	4.072678	5.859956
H	2.391867	5.524654	6.879809
H	1.561188	4.578861	8.122759
H	3.168953	4.090605	7.570454
H	2.857205	4.911638	2.376404
H	4.338212	4.885155	3.298505
H	1.848178	6.567474	4.086909
H	3.305271	7.209168	3.308769
H	3.389234	6.563415	4.952991
H	3.242380	0.995130	4.800910
H	5.383992	0.697135	3.380568
H	5.270463	2.400001	2.904940
H	5.590591	1.974228	4.592612
H	2.956350	1.421576	3.046958
C	0.104338	1.707315	0.992706
H	-0.712886	2.444961	1.029814
H	1.054252	2.264242	0.925385
C	-0.059454	0.782367	-0.217734
H	0.761792	0.047170	-0.212321
H	-0.992651	0.200908	-0.103960
C	-0.087349	1.515125	-1.561625
H	-0.927681	2.232659	-1.577704
H	0.831749	2.118612	-1.668115
C	-0.205434	0.561639	-2.755053
H	0.629590	-0.161800	-2.720325
H	-1.128026	-0.037631	-2.653261
C	-0.204411	1.261401	-4.117309
H	-1.056649	1.962735	-4.172219
H	0.705821	1.881356	-4.206628
C	-0.267337	0.289127	-5.299113
H	0.576380	-0.421248	-5.226264
H	-1.184492	-0.322115	-5.221791
C	-0.228049	0.973237	-6.668906
H	-1.085362	1.664390	-6.759687
H	0.677761	1.602894	-6.733994
C	-0.241076	-0.009882	-7.842951
H	0.608219	-0.709152	-7.737686
H	-1.153154	-0.631415	-7.789778
C	-0.167372	0.665193	-9.215752
H	-1.025299	1.351269	-9.333860
H	0.736610	1.299386	-9.260303
C	-0.145075	-0.324237	-10.384194
H	0.707019	-1.016117	-10.256515
H	-1.053466	-0.952591	-10.348259
C	-0.047468	0.345625	-11.757774
H	-0.903535	1.031084	-11.893082
H	0.856798	0.980485	-11.790100
C	-0.006733	-0.645928	-12.924298
H	0.846364	-1.332377	-12.784256
H	-0.912010	-1.277273	-12.894770
C	0.100953	0.033621	-14.291138
H	-0.756784	0.699923	-14.472463
H	1.014241	0.645194	-14.359308
C	-2.003820	2.741854	4.049197
F	-1.599064	4.037118	3.997894
F	-2.599268	2.458263	2.856698
F	-2.958766	2.642175	5.016221
H	0.130861	-0.701581	-15.108991
H	-0.863735	0.400055	2.426279

(7) **TS$_{2KPM}$**

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C	-0.180953	1.153740	2.374470
O	-0.094618	2.337025	3.329985
C	-1.168793	3.248852	3.256853
O	1.033728	0.553567	2.435680
Al	2.140619	-0.399952	3.432142
C	3.665882	-0.992621	2.309690
C	3.202217	-1.907022	1.156177
C	1.475200	-1.495698	4.963151
C	1.453318	-3.010685	4.678639
C	3.056891	1.632202	4.592051
Al	2.392664	3.406861	5.280494
C	1.701309	3.364328	7.144081
C	2.408221	2.362821	8.077466
C	4.476701	1.258730	5.053840
C	2.844720	5.017281	4.214783
C	2.636963	6.378569	4.899500
C	-1.325827	0.257811	2.909973
C	-1.353310	-1.177552	2.381662
H	-0.997404	4.052911	2.517362
H	-2.132661	2.766141	3.025213
H	4.418807	-1.520120	2.920357
H	4.180050	-0.107870	1.896413
H	4.035501	-2.216144	0.503154
H	2.460361	-1.403858	0.515966
H	2.730238	-2.830126	1.529436
H	0.472574	-1.151649	5.270994
H	2.128478	-1.304769	5.834595
H	0.767736	-3.266324	3.854919
H	2.448928	-3.383723	4.390538
H	1.130111	-3.597998	5.554228
H	0.627623	3.113397	7.086679
H	1.732638	4.380355	7.573194
H	3.473776	2.605477	8.217052
H	1.953545	2.338422	9.081421
H	2.362875	1.334120	7.684536
H	2.253790	4.962390	3.282203
H	3.894686	4.910699	3.883571
H	1.588264	6.525835	5.198674
H	2.909148	7.222861	4.244875
H	3.244420	6.471887	5.813347
H	2.286552	0.963705	5.033885
H	-2.296660	0.736067	2.703424
H	-1.209321	0.238083	4.005020
H	-2.117311	-1.759939	2.916726
H	-1.580763	-1.230954	1.309923
H	-0.387510	-1.676987	2.540399
H	4.811135	0.274743	4.686941
H	5.210635	1.995080	4.693093
H	4.548331	1.236508	6.151078
H	2.964714	1.712499	3.494820
C	-0.380893	1.739682	0.960248
H	-1.354929	2.250457	0.890117
H	0.401064	2.510373	0.850903
C	-0.251387	0.742483	-0.194320
H	0.620311	0.096056	-0.008983
H	-1.134113	0.083597	-0.232909
C	-0.099267	1.437875	-1.549871
H	-0.947509	2.128080	-1.709816
H	0.807729	2.068917	-1.533375
C	-0.018409	0.461971	-2.726016
H	0.833079	-0.224550	-2.572192
H	-0.923159	-0.172975	-2.734325
C	0.122025	1.154904	-4.083656
H	-0.721843	1.854902	-4.221723
H	1.035136	1.777353	-4.083610
C	0.168425	0.187706	-5.269057

H	1.025136	-0.499338	-5.148796
H	-0.735469	-0.448211	-5.254603
C	0.265534	0.893076	-6.624358
H	-0.585884	1.589685	-6.730570
H	1.174655	1.521019	-6.645319
C	0.282358	-0.061714	-7.820475
H	1.147529	-0.743535	-7.733882
H	-0.615879	-0.704681	-7.785038
C	0.333349	0.657997	-9.170876
H	-0.528116	1.346356	-9.246176
H	1.234779	1.295998	-9.210933
C	0.327805	-0.285253	-10.376221
H	1.199286	-0.962110	-10.315658
H	-0.565064	-0.934636	-10.325798
C	0.344515	0.445326	-11.721563
H	-0.525545	1.125015	-11.776692
H	1.238218	1.093493	-11.774491
C	0.328187	-0.489647	-12.933839
H	1.201468	-1.163352	-12.883701
H	-0.561449	-1.140941	-12.875853
C	0.331064	0.257446	-14.269126
H	-0.549544	0.912758	-14.358699
H	1.225810	0.891941	-14.367169
C	-1.360224	3.923088	4.604466
F	-1.624976	3.041916	5.599234
F	-0.248341	4.631450	4.978269
F	-2.391888	4.806839	4.543457
H	0.318624	-0.435683	-15.123178

(8) **Int_{2APM}**

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C	-0.896649	-0.116695	2.067175
O	-0.364501	0.510245	3.410322
C	-1.341562	1.217892	4.167606
O	-0.778072	-1.449933	2.113381
Al	-0.618743	-2.733192	3.344615
C	-0.198123	-4.475463	2.514544
C	-1.415705	-5.116769	1.816051
C	-1.765054	-2.444103	4.946635
C	-3.257119	-2.309523	4.578194
C	1.665306	-1.751986	3.988515
Al	1.543532	0.270413	4.194223
C	1.236986	0.825139	6.100460
C	2.463954	0.554027	6.996874
C	2.964215	-2.460537	4.406650
C	2.769172	1.367056	3.053499
C	3.494688	2.506280	3.795078
H	-2.336032	0.761280	4.050976
H	-1.055177	1.181313	5.225715
H	0.200255	-5.162738	3.281028
H	0.618812	-4.334400	1.786361
H	-1.166934	-6.083663	1.348357
H	-1.815244	-4.468113	1.020394
H	-2.240495	-5.307451	2.521309
H	-1.432113	-1.543173	5.491866
H	-1.631041	-3.278288	5.656448
H	-3.433936	-1.490709	3.860887
H	-3.645343	-3.224975	4.104561
H	-3.892581	-2.110351	5.456852
H	0.369307	0.285975	6.526871
H	0.984527	1.899367	6.159229
H	3.358805	1.084161	6.635307
H	2.303809	0.873452	8.040273
H	2.718576	-0.517275	7.028909
H	2.188617	1.796172	2.218915

H	3.511558	0.703796	2.573179
H	2.781384	3.198106	4.270340
H	4.131303	3.108935	3.125442
H	4.147000	2.125354	4.596574
H	0.845765	-2.124747	4.656412
H	2.932790	-3.551014	4.250266
H	3.815087	-2.072088	3.826902
H	3.192080	-2.286354	5.468302
H	1.461958	-1.989529	2.926507
C	-0.120119	0.509429	0.921435
H	-0.169988	1.605755	1.001980
H	0.936754	0.212809	1.012984
C	-0.683352	0.041346	-0.425761
H	-0.626116	-1.058342	-0.468529
H	-1.756779	0.297937	-0.481931
C	0.040403	0.642701	-1.633310
H	-0.051236	1.743278	-1.611500
H	1.120612	0.424077	-1.559774
C	-0.496777	0.107827	-2.964138
H	-0.388288	-0.991817	-2.978252
H	-1.582404	0.304909	-3.024077
C	0.188967	0.694440	-4.200954
H	0.045199	1.789755	-4.216805
H	1.279242	0.531122	-4.127389
C	-0.324704	0.092165	-5.512146
H	-0.173033	-1.002287	-5.488599
H	-1.417181	0.244139	-5.579942
C	0.342219	0.662563	-6.766810
H	0.163380	1.751764	-6.815346
H	1.437226	0.537362	-6.686848
C	-0.146595	0.007569	-8.062011
H	0.026658	-1.082235	-8.002555
H	-1.241033	0.135518	-8.145635
C	0.524113	0.552977	-9.325890
H	0.334586	1.638710	-9.402803
H	1.619641	0.441907	-9.232876
C	0.055242	-0.136999	-10.610222
H	0.232942	-1.224228	-10.522532
H	-1.038511	-0.016450	-10.711352
C	0.740669	0.383287	-11.876710
H	0.556277	1.468494	-11.974225
H	1.835004	0.270192	-11.771158
C	0.283500	-0.323440	-13.156496
H	0.461024	-1.408087	-13.052470
H	-0.808619	-0.204008	-13.265664
C	0.985152	0.192114	-14.414818
H	0.797652	1.267221	-14.562208
H	2.075497	0.053766	-14.345493
C	-1.440736	2.691173	3.772305
F	-0.241460	3.316409	3.844803
F	-1.909902	2.855783	2.502797
F	-2.302066	3.324613	4.612372
H	0.638977	-0.333562	-15.316984
H	-1.951980	0.222834	2.069513

(9) **Int$_{2KPM}$**

94

C	-1.483668	-0.902273	1.861103
O	0.609226	1.135989	2.660632
C	1.325006	1.463794	1.511226
O	-0.638167	-1.817677	1.833166
Al	0.342964	-3.020023	3.065030
C	1.537994	-3.950671	1.764691
C	0.842889	-4.542016	0.522986
C	-1.090665	-4.005498	4.057622

C	-1.997845	-4.914180	3.207083
C	1.309087	-1.614809	4.192088
Al	1.340399	0.934097	4.285222
C	0.065050	1.353491	5.748670
C	0.368929	0.700265	7.108241
C	2.236073	-2.181284	5.276677
C	3.292928	1.291874	4.409317
C	3.630896	2.791555	4.538830
C	-2.234429	-0.538205	3.110754
C	-3.620285	-1.215219	3.144968
H	2.423502	1.479615	1.652364
H	1.113005	0.762772	0.681063
H	2.093759	-4.747883	2.291450
H	2.314209	-3.231577	1.441386
H	1.553013	-5.004123	-0.184008
H	0.289607	-3.769676	-0.035674
H	0.111924	-5.319145	0.795726
H	-1.707225	-3.282501	4.624263
H	-0.597216	-4.614370	4.837819
H	-2.496174	-4.358790	2.394826
H	-1.419700	-5.715196	2.721494
H	-2.792648	-5.403222	3.796026
H	-0.965292	1.116320	5.432016
H	0.079819	2.454351	5.854434
H	1.383672	0.945132	7.460071
H	-0.330416	1.022507	7.897224
H	0.308718	-0.398729	7.057514
H	3.822317	0.858472	3.541914
H	3.692028	0.747979	5.283005
H	3.284841	3.369799	3.667789
H	4.714734	2.969708	4.634845
H	3.153359	3.239479	5.424829
H	0.482032	-1.018372	4.633002
H	-2.343174	0.555779	3.144576
H	-1.649261	-0.851545	3.984411
H	-4.136646	-0.942369	4.075039
H	-4.251702	-0.895964	2.303855
H	-3.526495	-2.308700	3.116711
H	3.011006	-2.821326	4.827910
H	2.759349	-1.412839	5.869030
H	1.672372	-2.806307	5.985540
H	1.869439	-1.043793	3.425178
C	-1.803049	-0.161699	0.600077
H	-2.900948	-0.067865	0.520688
H	-1.457051	0.873688	0.778800
C	-1.191382	-0.735698	-0.675288
H	-0.116272	-0.914599	-0.512614
H	-1.627271	-1.728843	-0.875750
C	-1.384266	0.176340	-1.889501
H	-2.459865	0.382577	-2.035129
H	-0.911465	1.154656	-1.690311
C	-0.804929	-0.421790	-3.174366
H	0.259690	-0.668444	-3.012158
H	-1.308549	-1.382258	-3.386711
C	-0.928292	0.495776	-4.393589
H	-1.987553	0.775384	-4.537135
H	-0.388703	1.439474	-4.195894
C	-0.393633	-0.136762	-5.681578
H	0.656435	-0.444096	-5.527681
H	-0.953640	-1.066944	-5.888419
C	-0.474437	0.783297	-6.902522
H	-1.519761	1.111940	-7.044750
H	0.108304	1.701544	-6.706494
C	0.029162	0.128426	-8.191800
H	1.067349	-0.219110	-8.042282
H	-0.567352	-0.779523	-8.395211
C	-0.022003	1.050252	-9.412964

H	-1.056863	1.410292	-9.555896
H	0.587605	1.950657	-9.215624
C	0.463470	0.383239	-10.702946
H	1.492987	0.010059	-10.554825
H	-0.155660	-0.509423	-10.906298
C	0.433308	1.307378	-11.922860
H	-0.594003	1.688274	-12.067742
H	1.059890	2.195733	-11.723241
C	0.908295	0.635810	-13.214787
H	1.931121	0.247911	-13.065800
H	0.275894	-0.246427	-13.417134
C	0.886055	1.571851	-14.424645
H	-0.130209	1.951598	-14.614170
H	1.539234	2.443764	-14.263841
C	0.950213	2.855708	1.004024
F	-0.373931	2.945551	0.672885
F	1.191641	3.821569	1.927663
F	1.663915	3.165511	-0.115699
H	1.227641	1.063196	-15.338199

(10) **TS$_{\text{ЗАРМ}}$**

88

C	-0.762519	-0.403638	1.943001
O	-0.239437	0.896093	3.483834
C	-1.320842	1.594061	4.037628
O	-0.146332	-1.489616	2.176496
Al	-0.264167	-2.730236	3.627338
C	0.619229	-4.391075	2.999186
C	0.046737	-4.918277	1.667264
C	-2.123314	-2.637746	4.344739
C	-3.191097	-3.288101	3.443310
C	1.080224	-1.421718	4.783585
Al	1.396047	0.680023	4.444185
C	1.296163	1.697728	6.162251
C	2.633516	1.712136	6.930188
C	1.781582	-2.097598	5.956786
C	2.910496	0.914658	3.168688
C	4.213089	0.200949	3.577911
H	-2.285126	1.106424	3.796770
H	-1.251494	1.663043	5.137506
H	0.538884	-5.172367	3.774840
H	1.701477	-4.200923	2.888846
H	0.566697	-5.825059	1.316390
H	0.131683	-4.167986	0.865211
H	-1.020947	-5.175272	1.753270
H	-2.392699	-1.581158	4.535601
H	-2.142915	-3.113057	5.342046
H	-3.217459	-2.831064	2.440375
H	-2.993498	-4.360713	3.293300
H	-4.208252	-3.204399	3.860910
H	0.505278	1.282087	6.814792
H	0.987012	2.737184	5.952972
H	3.437554	2.167127	6.330173
H	2.576613	2.282268	7.872693
H	2.969464	0.695648	7.191289
H	3.102288	1.994509	3.037109
H	2.595737	0.555171	2.171940
H	4.586278	0.557244	4.551170
H	5.028530	0.348020	2.849731
H	4.070235	-0.888594	3.674328
H	0.045258	-1.073503	4.912005
H	1.584173	-3.178563	6.050522
H	2.871846	-1.979208	5.876395
H	1.483064	-1.628836	6.905616
H	1.514813	-1.512427	3.778100

C	-0.340591	0.416929	0.769959
H	-0.779502	1.419105	0.838809
H	0.754838	0.514922	0.792420
C	-0.773805	-0.272309	-0.542505
H	-0.344913	-1.286929	-0.574322
H	-1.871258	-0.391322	-0.559875
C	-0.322785	0.521264	-1.771463
H	-0.753255	1.537059	-1.731673
H	0.772915	0.652058	-1.730652
C	-0.702528	-0.144039	-3.096624
H	-0.296112	-1.170884	-3.118402
H	-1.800546	-0.248846	-3.155814
C	-0.195777	0.624287	-4.320266
H	-0.608016	1.648972	-4.305667
H	0.900706	0.737783	-4.245914
C	-0.541242	-0.042577	-5.654084
H	-0.149124	-1.075468	-5.656525
H	-1.638370	-0.133894	-5.746328
C	0.011282	0.708239	-6.868588
H	-0.385007	1.739451	-6.872395
H	1.107114	0.805648	-6.765187
C	-0.308995	0.037897	-8.206983
H	0.071819	-0.999169	-8.194705
H	-1.404716	-0.042696	-8.323865
C	0.277431	0.775512	-9.413756
H	-0.105131	1.811867	-9.429520
H	1.372342	0.859062	-9.290178
C	-0.027892	0.103501	-10.754852
H	0.345156	-0.936297	-10.734130
H	-1.122579	0.030228	-10.886234
C	0.578451	0.832929	-11.956639
H	0.206017	1.873062	-11.978763
H	1.673075	0.906716	-11.823293
C	0.279490	0.162240	-13.300368
H	0.648620	-0.877795	-13.275136
H	-0.814074	0.092840	-13.434995
C	0.897804	0.897628	-14.491110
H	0.521525	1.930417	-14.558512
H	1.993764	0.951476	-14.398316
C	-1.425652	3.030960	3.520824
F	-0.276092	3.726611	3.700074
F	-1.721995	3.080170	2.187867
F	-2.421500	3.689237	4.176453
H	-1.801898	-0.300593	2.306470
H	0.667781	0.395842	-15.442607

(11) **Pdt (ketone)**

49

C	-1.542649	-1.034985	1.848982
O	-0.830694	-2.027478	1.843685
C	-2.302741	-0.595072	3.096504
C	-1.914394	-1.357829	4.358087
H	-3.378675	-0.722321	2.873896
H	-2.167867	0.494125	3.219422
H	-2.520673	-1.032966	5.215335
H	-2.053902	-2.438094	4.219290
H	-0.855381	-1.197933	4.603627
C	-1.724087	-0.162841	0.611977
H	-2.794724	0.091699	0.512177
H	-1.223860	0.801975	0.824917
C	-1.177395	-0.773886	-0.675524
H	-0.119784	-1.041776	-0.524210
H	-1.697677	-1.726283	-0.872318
C	-1.316982	0.153145	-1.885664
H	-2.379827	0.421606	-2.027227

H	-0.788894	1.103059	-1.683741
C	-0.776227	-0.459522	-3.180698
H	0.284371	-0.732690	-3.037435
H	-1.307322	-1.407270	-3.383011
C	-0.902174	0.462132	-4.397064
H	-1.961915	0.743540	-4.534100
H	-0.361213	1.405266	-4.198517
C	-0.373979	-0.160305	-5.692649
H	0.681795	-0.453482	-5.551391
H	-0.923159	-1.097460	-5.895998
C	-0.481507	0.762622	-6.909953
H	-1.534358	1.070245	-7.043566
H	0.083286	1.692162	-6.713553
C	0.027435	0.123837	-8.205349
H	1.072537	-0.205268	-8.061792
H	-0.553235	-0.793837	-8.410595
C	-0.044304	1.049532	-9.422872
H	-1.086852	1.386757	-9.565968
H	0.544695	1.962673	-9.221654
C	0.458271	0.398348	-10.714666
H	1.494775	0.045909	-10.564469
H	-0.141240	-0.506363	-10.923422
C	0.413560	1.326248	-11.931443
H	-0.621589	1.683262	-12.081249
H	1.017878	2.228399	-11.724698
C	0.912675	0.670796	-13.222751
H	1.944551	0.309612	-13.069238
H	0.304739	-0.227379	-13.430383
C	0.872277	1.608300	-14.431130
H	-0.152749	1.960226	-14.626770
H	1.500235	2.497733	-14.265157
H	1.233512	1.110967	-15.343280

(12) **$AlEt_2OCH_2CF_3$**

23

O	0.075608	0.297577	1.281124
C	-0.331304	0.199716	-0.049348
Al	1.688470	0.261488	1.967827
C	3.212169	0.428178	0.712286
C	4.603349	0.629012	1.340236
C	1.719375	0.100363	3.935333
C	2.698529	1.032388	4.676338
H	-1.328958	0.652227	-0.184549
H	0.361149	0.680945	-0.767162
H	2.989776	1.249818	0.007565
H	3.205405	-0.482801	0.086447
H	4.861294	-0.185989	2.033931
H	5.398496	0.666003	0.578073
H	4.662604	1.566406	1.913713
H	1.956196	-0.951777	4.177786
H	0.688444	0.254197	4.295288
H	3.738805	0.880562	4.351063
H	2.673933	0.868170	5.765625
H	2.461273	2.094432	4.508430
C	-0.450864	-1.258109	-0.495228
F	0.734658	-1.925446	-0.331438
F	-1.390136	-1.943740	0.200146
F	-0.778217	-1.328644	-1.815115

(13) **$AlEt_3$**

22

Al	0.150145	-0.150198	-0.222434
C	1.980011	-0.930537	-0.142452
C	-0.131040	1.775986	0.199799

C	-1.418302	-1.315957	-0.614020
H	0.124000	1.913471	1.268225
H	0.636307	2.366672	-0.333408
C	-1.533538	2.341558	-0.082419
C	-2.203569	-1.686911	0.664664
H	-2.094780	-0.797620	-1.316211
H	-1.092580	-2.235569	-1.128805
H	1.939281	-1.786333	0.557933
H	2.187439	-1.400566	-1.122379
C	3.127904	0.018052	0.244989
H	-3.085310	-2.311702	0.446022
H	-1.584452	-2.253827	1.378684
H	-2.571621	-0.794379	1.196412
H	4.104310	-0.493221	0.278540
H	3.225532	0.851342	-0.468070
H	2.966721	0.470174	1.236129
H	-1.627629	3.401762	0.205836
H	-1.791570	2.276157	-1.150990
H	-2.314711	1.789230	0.463152

(14) **Int$_{3APM}$**

88

C	-0.169499	-0.684810	1.789680
O	-0.028664	1.141152	3.550550
C	-1.277729	1.636196	3.932258
O	0.506361	-1.580955	2.328101
Al	0.041024	-2.658210	3.937480
C	1.020110	-4.358289	3.578792
C	0.755140	-4.994247	2.200550
C	-1.962660	-2.570317	3.979050
C	-2.710250	-3.237421	2.809660
C	0.938246	-1.376196	5.248654
Al	1.423709	1.085282	4.617366
C	1.222252	2.025592	6.356239
C	2.522712	2.160649	7.171476
C	1.477996	-1.897154	6.585818
C	3.093335	0.948114	3.553646
C	4.294518	0.278568	4.246147
H	-2.082705	0.896176	3.758125
H	-1.330254	1.934256	4.996602
H	0.782773	-5.087803	4.374332
H	2.102159	-4.158896	3.689295
H	1.345582	-5.911260	2.033669
H	1.002715	-4.300541	1.380677
H	-0.304070	-5.269000	2.074156
H	-2.277502	-1.512031	4.067871
H	-2.296512	-3.026207	4.929673
H	-2.417815	-2.815427	1.832868
H	-2.490882	-4.314810	2.755847
H	-3.806426	-3.135185	2.883818
H	0.448173	1.528370	6.966899
H	0.817892	3.032343	6.141032
H	3.306641	2.685361	6.603372
H	2.372453	2.723406	8.107326
H	2.935869	1.178581	7.449531
H	3.363425	1.976796	3.251566
H	2.862164	0.421625	2.611065
H	4.580154	0.803391	5.170681
H	5.186923	0.252629	3.600136
H	4.076813	-0.764642	4.527594
H	0.167724	-0.598059	5.413345
H	2.223737	-2.689449	6.424354
H	1.953861	-1.118200	7.204503
H	0.668586	-2.336126	7.188416
H	1.776706	-0.998721	4.617764

C	0.325140	0.083601	0.622145
H	0.016605	1.132966	0.736540
H	1.422106	0.026668	0.583413
C	-0.294636	-0.502692	-0.671323
H	-0.000145	-1.561016	-0.765250
H	-1.395444	-0.485487	-0.596756
C	0.146971	0.268567	-1.918571
H	-0.167771	1.322491	-1.826608
H	1.249848	0.278664	-1.967151
C	-0.412169	-0.327551	-3.213427
H	-0.108041	-1.386941	-3.286486
H	-1.515859	-0.329477	-3.169957
C	0.045229	0.414493	-4.472494
H	-0.275258	1.469865	-4.413243
H	1.149420	0.433018	-4.502619
C	-0.483287	-0.206561	-5.768571
H	-0.168637	-1.264495	-5.818244
H	-1.587716	-0.219834	-5.743662
C	-0.014012	0.517440	-7.033262
H	-0.340574	1.572092	-6.994013
H	1.090479	0.542392	-7.049578
C	-0.522357	-0.123591	-8.327573
H	-0.198943	-1.179564	-8.361120
H	-1.626933	-0.145772	-8.314487
C	-0.046036	0.589347	-9.595885
H	-0.377211	1.643012	-9.569152
H	1.058447	0.619147	-9.603740
C	-0.541730	-0.064725	-10.888537
H	-0.211687	-1.118934	-10.912325
H	-1.646264	-0.093618	-10.882133
C	-0.062382	0.642453	-12.158745
H	-0.396454	1.695578	-12.139162
H	1.042197	0.675849	-12.163129
C	-0.550693	-0.017392	-13.451698
H	-0.215751	-1.069119	-13.469420
H	-1.654085	-0.050908	-13.446205
C	-0.065125	0.697359	-14.714246
H	-0.414906	1.741217	-14.738860
H	1.034960	0.717015	-14.760850
C	-1.646261	2.875944	3.121704
F	-0.741640	3.876812	3.280367
F	-1.714779	2.606897	1.782815
F	-2.863815	3.351723	3.501587
H	-1.226397	-0.549774	2.086805
H	-0.428744	0.202177	-15.626753

(15) **Pdt (Aldehyde)**

43

C	-0.183598	-0.662837	1.873468
O	-0.913049	-1.634742	1.909493
C	0.237805	0.059319	0.617958
H	-0.045114	1.122222	0.748562
H	1.345405	0.073007	0.612593
C	-0.320810	-0.517564	-0.679093
H	-0.028601	-1.577548	-0.755460
H	-1.421812	-0.518954	-0.629087
C	0.143675	0.243118	-1.923415
H	-0.158877	1.302774	-1.842984
H	1.248077	0.244568	-1.964218
C	-0.406373	-0.341861	-3.227062
H	-0.104976	-1.401851	-3.303911
H	-1.510396	-0.342937	-3.187327
C	0.055215	0.405557	-4.481026
H	-0.260296	1.462411	-4.415427
H	1.159779	0.420052	-4.510983

C -0.475815 -0.204546 -5.781272
H -0.165198 -1.263376 -5.837234
H -1.580432 -0.214518 -5.754627
C -0.006808 0.522872 -7.044137
H -0.331914 1.577950 -7.001380
H 1.097771 0.546374 -7.062655
C -0.518973 -0.115485 -8.338255
H -0.199233 -1.172662 -8.372200
H -1.623440 -0.134322 -8.322739
C -0.044109 0.593754 -9.608645
H -0.372844 1.648310 -9.584497
H 1.060374 0.621110 -9.619942
C -0.544380 -0.061893 -10.898588
H -0.217208 -1.117077 -10.921032
H -1.648946 -0.087861 -10.890780
C -0.063669 0.643239 -12.168934
H -0.394420 1.697450 -12.148453
H 1.040950 0.673436 -12.172720
C -0.552937 -0.013263 -13.462906
H -0.221009 -1.065966 -13.482201
H -1.656413 -0.043391 -13.458630
C -0.063078 0.703324 -14.722860
H -0.409652 1.748429 -14.744481
H 1.037251 0.719850 -14.766861
H 0.234720 -0.233963 2.823712
H -0.426488 0.211965 -15.637547

(C) Decomposition reaction of D_2 with Al_2Et_6

(1) **RC**

100

C 0.201248 1.721255 2.357844
O -0.413080 2.286778 3.405981
C -0.004470 1.816285 4.709378
O 1.102190 0.895822 2.515305
Al 2.494667 -0.539926 2.570918
C 3.453219 0.005118 4.238865
C 4.089227 1.407097 4.191097
C 3.464470 -0.447913 0.824577
C 2.907909 -1.321331 -0.314550
C 1.178135 -2.068623 2.778930
Al -1.335225 -2.613540 2.866143
C -1.429915 -3.978574 1.406605
C -1.083210 -3.457670 0.000453
C 1.840318 -3.432861 3.022957
C -1.473516 -3.143432 4.792929
C -1.212321 -2.017113 5.808475
C -2.056484 -0.797608 2.393687
C -3.585915 -0.817185 2.202251
H -0.020908 0.718816 4.750291
H 1.002230 2.180259 4.955878
H 4.239503 -0.743300 4.446155
H 2.765753 -0.068055 5.102726
H 4.609991 1.678461 5.125011
H 3.338478 2.194939 4.005550
H 4.827109 1.488596 3.377073
H 4.517466 -0.724597 1.016952
H 3.515484 0.607837 0.498917
H 2.921020 -2.390446 -0.048710
H 1.861669 -1.073888 -0.553781
H 3.480267 -1.219510 -1.252267
H -2.466513 -4.366284 1.409338
H -0.802961 -4.853426 1.650779
H -0.033271 -3.125598 -0.066102
H -1.220257 -4.220130 -0.784971

H	-1.707403	-2.593152	-0.279910
H	-0.810023	-4.001004	5.000823
H	-2.497064	-3.536822	4.941205
H	-0.176445	-1.638289	5.742031
H	-1.353027	-2.337760	6.854385
H	-1.882772	-1.157139	5.645869
H	0.596849	-2.047650	1.835071
H	-1.804085	-0.061374	3.176102
H	-1.577780	-0.441348	1.464100
H	-4.104425	-1.137498	3.120482
H	-4.000637	0.169910	1.933548
H	-3.885654	-1.517519	1.405832
H	2.496042	-3.704932	2.181779
H	2.466510	-3.408580	3.927571
H	1.123518	-4.260814	3.149877
H	0.557134	-1.750120	3.640778
C	-0.312228	2.203159	1.034582
H	-1.412832	2.195953	1.088868
H	-0.025441	3.265845	0.939314
C	0.202460	1.380389	-0.145149
H	1.301067	1.441324	-0.185875
H	-0.037291	0.319060	0.028377
C	-0.393762	1.820136	-1.482835
H	-1.495518	1.758561	-1.433729
H	-0.152539	2.882216	-1.667987
C	0.109603	0.972676	-2.654808
H	1.212059	1.026732	-2.696821
H	-0.133831	-0.088446	-2.467468
C	-0.472439	1.397154	-4.005318
H	-1.574042	1.322122	-3.968129
H	-0.245896	2.464319	-4.180455
C	0.053433	0.570929	-5.181922
H	1.155114	0.648387	-5.215412
H	-0.170073	-0.496731	-5.007461
C	-0.523267	0.995400	-6.535689
H	-1.623596	0.896780	-6.511284
H	-0.317722	2.068977	-6.698268
C	0.033316	0.191368	-7.713988
H	1.133771	0.290813	-7.732389
H	-0.170912	-0.882349	-7.552029
C	-0.531541	0.613043	-9.073601
H	-1.630337	0.496606	-9.066056
H	-0.341426	1.690380	-9.229576
C	0.054552	-0.177868	-10.246503
H	1.153507	-0.061567	-10.248402
H	-0.135313	-1.255155	-10.090404
C	-0.497986	0.239572	-11.612297
H	-1.595765	0.113816	-11.616781
H	-0.316032	1.318713	-11.765102
C	0.106869	-0.545053	-12.779862
H	1.204839	-0.419855	-12.771225
H	-0.076000	-1.624055	-12.626837
C	-0.436339	-0.130822	-14.150232
H	-1.533998	-0.258672	-14.162790
H	-0.255492	0.948579	-14.303991
C	-1.006410	2.360806	5.716931
F	-1.055420	3.714945	5.708160
F	-2.257332	1.896963	5.485062
F	-0.629702	1.960133	6.958623
C	0.175886	-0.915478	-15.314588
H	1.272417	-0.787695	-15.299014
H	-0.005705	-1.993291	-15.158905
C	-0.369999	-0.495505	-16.681095
H	-0.170818	0.569506	-16.877789
H	-1.460114	-0.642428	-16.735845
H	0.086897	-1.076769	-17.495783

(2) **TS_{1APP}**

100

C	3.618425	-0.122910	-2.494862
O	4.542775	-0.624998	-3.436610
C	5.903802	-0.552705	-3.034715
O	3.972836	-0.287195	-1.220023
Al	4.062461	0.827595	0.200105
C	2.421625	0.997633	1.311049
C	2.004704	-0.315758	2.000808
C	4.281891	2.691814	-0.999697
C	3.896436	2.555272	-2.338844
C	5.817302	0.604986	1.147927
C	6.051447	1.686636	2.214721
Al	8.227954	-0.583923	1.150265
C	8.355142	-0.937758	3.115909
C	7.197597	-1.687125	3.797194
C	9.248858	0.978517	0.415328
C	8.866518	1.473280	-0.989751
C	7.843748	-2.112356	-0.086183
C	6.500122	-2.854160	0.038637
H	9.284717	-1.529667	3.230441
H	6.564226	0.657304	0.328666
H	5.807790	-0.411851	1.583564
H	5.346160	2.848623	-0.794468
H	3.591090	3.221461	-0.332647
H	1.586320	1.386410	0.702970
H	9.201525	1.814340	1.135662
H	10.312689	0.672608	0.412109
H	8.667315	-2.831613	0.089864
H	7.999433	-1.776677	-1.127559
H	1.115852	-0.192203	2.641434
H	1.766855	-1.103063	1.267717
H	2.808029	-0.713469	2.641851
H	5.252992	1.669179	2.972360
H	7.005878	1.575006	2.752712
H	6.052988	2.694981	1.771346
H	9.507446	2.298081	-1.344391
H	8.932759	0.670086	-1.740449
H	7.829445	1.853977	-1.020338
H	6.425991	-3.716097	-0.646505
H	6.343939	-3.243397	1.056616
H	5.642435	-2.198381	-0.181204
H	6.176513	0.439689	-2.639028
H	6.146487	-1.308099	-2.273504
H	2.610678	1.773042	2.075845
H	8.560950	0.005093	3.652670
H	7.396726	-1.898943	4.861275
H	6.259991	-1.108517	3.761292
H	6.993606	-2.653951	3.310742
H	3.614121	1.091559	-2.657695
H	4.646239	2.573299	-3.135728
H	2.892589	2.854651	-2.652549
C	2.228510	-0.602058	-2.909209
H	2.086222	-0.356132	-3.972855
H	2.239407	-1.702187	-2.831007
C	1.107736	-0.018853	-2.052598
H	1.293203	-0.271304	-0.996964
H	1.125258	1.084521	-2.111563
C	-0.283263	-0.518530	-2.450568
H	-0.484809	-0.259649	-3.505219
H	-0.301229	-1.621570	-2.398063
C	-1.393433	0.049368	-1.561870
H	-1.175093	-0.198074	-0.507443
H	-1.380529	1.152792	-1.622699
C	-2.791472	-0.460572	-1.921338

H	-3.011235	-0.213744	-2.975579
H	-2.803549	-1.563554	-1.858835
C	-3.896082	0.107989	-1.026248
H	-3.668133	-0.130063	0.028320
H	-3.890496	1.210789	-1.095941
C	-5.294362	-0.413474	-1.368739
H	-5.525035	-0.174985	-2.422607
H	-5.298548	-1.516229	-1.299458
C	-6.395818	0.152679	-0.468228
H	-6.158689	-0.078492	0.585889
H	-6.397684	1.255105	-0.543509
C	-7.793262	-0.379225	-0.797582
H	-8.033212	-0.146861	-1.850758
H	-7.789848	-1.481719	-0.723647
C	-8.892056	0.183555	0.108286
H	-8.646923	-0.042895	1.161609
H	-8.900545	1.285703	0.029553
C	-10.288506	-0.357039	-0.210623
H	-10.535978	-0.129332	-1.263075
H	-10.278695	-1.459264	-0.133339
C	-11.385222	0.202649	0.699730
H	-11.133980	-0.020927	1.752258
H	-11.398535	1.304633	0.619057
C	-12.780816	-0.343916	0.388320
H	-13.034238	-0.119837	-0.663668
H	-12.767426	-1.446101	0.468038
C	6.763939	-0.805949	-4.261788
F	6.581928	0.144176	-5.217319
F	8.078648	-0.777499	-3.900992
F	6.518783	-2.010507	-4.829306
C	-13.877583	0.213139	1.300894
H	-13.621279	-0.009311	2.351443
H	-13.891622	1.313990	1.218814
C	-15.266767	-0.343502	0.983099
H	-15.289180	-1.439454	1.089509
H	-15.561581	-0.106308	-0.050905
H	-16.034147	0.072245	1.652752

(3) **TS_{1KPP}**

100

C	-0.035420	-0.091571	0.367845
O	-0.209356	0.428134	1.627986
C	0.475552	-0.243373	2.680127
O	1.057767	-0.738611	0.138562
Al	2.131306	-2.126115	-0.462717
C	3.355186	-2.551119	1.043195
C	4.383954	-1.435911	1.317797
C	2.784012	-1.843352	-2.321887
C	1.894327	-2.309528	-3.486900
C	0.489893	-3.741107	-0.519058
Al	-1.564649	-3.861073	-0.065346
C	-2.650854	-4.224559	-1.708891
C	-2.418790	-3.232644	-2.861956
C	1.225161	-5.002811	-0.972748
C	-1.840346	-4.857531	1.653724
C	-1.058421	-4.290914	2.851865
C	-1.594131	-1.734005	0.396816
C	-2.897897	-1.130018	0.852348
H	0.369017	-1.337587	2.605339
H	1.546538	0.008053	2.690036
H	3.881514	-3.499672	0.838448
H	2.760750	-2.742125	1.955678
H	5.045210	-1.669077	2.168491
H	3.894667	-0.474430	1.546226
H	5.033799	-1.258508	0.446090

H	3.771879	-2.332392	-2.393836
H	2.998396	-0.763075	-2.424757
H	1.721826	-3.396573	-3.456868
H	0.903928	-1.828572	-3.471254
H	2.337994	-2.083741	-4.470479
H	-3.722065	-4.240150	-1.440786
H	-2.429493	-5.251514	-2.054054
H	-1.359766	-3.195847	-3.168601
H	-2.999003	-3.478296	-3.768059
H	-2.704218	-2.205183	-2.578374
H	-1.555248	-5.913439	1.491588
H	-2.917091	-4.888230	1.896510
H	0.026705	-4.235298	2.650582
H	-1.170010	-4.894833	3.768296
H	-1.392435	-3.271568	3.110288
H	0.352632	-2.964183	-1.294053
H	-0.858612	-1.992431	1.159183
H	-1.268252	-1.593645	-0.633720
H	-3.372669	-1.739133	1.637230
H	-2.773485	-0.117512	1.279525
H	-3.614864	-1.058496	0.021146
H	2.291705	-4.863517	-1.226177
H	1.182782	-5.769160	-0.185103
H	0.739238	-5.428048	-1.862656
H	0.747062	-3.385340	0.495799
C	-0.616177	0.858362	-0.653756
H	-1.674963	1.031353	-0.410354
H	-0.103348	1.824969	-0.492091
C	-0.436100	0.419323	-2.102543
H	0.637699	0.300086	-2.315795
H	-0.893627	-0.573688	-2.258181
C	-1.055335	1.402027	-3.098417
H	-2.129780	1.523990	-2.873705
H	-0.599556	2.399151	-2.961868
C	-0.889061	0.963479	-4.555421
H	0.184537	0.821125	-4.773549
H	-1.361580	-0.025648	-4.694839
C	-1.482799	1.960205	-5.553789
H	-2.556544	2.100030	-5.334448
H	-1.011565	2.948390	-5.402145
C	-1.316723	1.545358	-7.017685
H	-0.244445	1.389000	-7.233129
H	-1.805335	0.567650	-7.179672
C	-1.886241	2.569860	-8.002678
H	-2.958697	2.725477	-7.787332
H	-1.398499	3.546706	-7.830741
C	-1.718557	2.177802	-9.472736
H	-0.647636	2.007934	-9.685021
H	-2.221350	1.210571	-9.653841
C	-2.266221	3.225745	-10.445465
H	-3.337055	3.395971	-10.232957
H	-1.763381	4.191956	-10.257768
C	-2.097856	2.849964	-11.919747
H	-1.028337	2.668908	-12.129990
H	-2.611853	1.891134	-12.113928
C	-2.628814	3.914520	-12.883676
H	-3.698088	4.096336	-12.672867
H	-2.114287	4.872447	-12.685724
C	-2.460657	3.548644	-14.360568
H	-1.392186	3.360179	-14.569855
H	-2.981863	2.595167	-14.562090
C	-2.981271	4.622529	-15.319575
H	-4.049693	4.812107	-15.110306
H	-2.459804	5.575892	-15.116984
C	-0.157108	0.196342	3.991597
F	-0.069521	1.534754	4.183482
F	-1.467638	-0.146960	4.059150

F	0.488602	-0.417555	5.020307
C	-2.814127	4.262278	-16.798485
H	-1.746843	4.070831	-17.005497
H	-3.337601	3.311470	-17.000688
C	-3.334254	5.346211	-17.744805
H	-2.804740	6.298864	-17.586367
H	-4.407134	5.533872	-17.581763
H	-3.201735	5.062846	-18.799333

(4) **Int$_{1APP}$**

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C	1.611586	-0.583494	-1.802577
O	2.511693	-1.317060	-2.708315
C	3.829625	-1.459305	-2.257070
O	1.885832	-0.894775	-0.486151
Al	1.999066	0.133735	0.956542
C	1.470407	-0.858863	2.589704
C	-0.029835	-1.221803	2.575211
C	1.776370	2.094509	0.701723
C	0.392637	2.614480	1.143375
Al	6.401875	-0.571614	0.426095
C	6.685869	-2.536966	0.325895
C	7.736020	-3.053083	-0.674186
C	4.620497	0.037204	1.180614
C	4.784824	0.774158	2.523923
C	7.805266	0.831143	0.358397
C	9.044368	0.546553	-0.508734
H	6.946394	-2.877023	1.346436
H	1.956468	2.351716	-0.356629
H	2.562863	2.623570	1.267706
H	1.704026	-0.265475	3.490013
H	4.191185	0.699041	0.403147
H	4.021983	-0.889889	1.283645
H	8.118408	1.040269	1.398730
H	7.315548	1.764143	0.023727
H	-0.332779	-1.781874	3.475433
H	-0.669789	-0.325830	2.527101
H	-0.284153	-1.847199	1.704954
H	0.196115	2.395674	2.204965
H	0.297121	3.705669	1.017195
H	-0.424113	2.153210	0.566031
H	3.834836	1.137790	2.949798
H	5.238230	0.120848	3.284985
H	5.440600	1.650289	2.413358
H	9.753144	1.390821	-0.512121
H	9.596649	-0.336216	-0.152316
H	8.772562	0.349990	-1.557340
H	3.872975	-1.634066	-1.169495
H	4.277340	-2.320730	-2.773618
H	2.071441	-1.780467	2.672955
H	5.707109	-3.009568	0.123042
H	7.815426	-4.152436	-0.666629
H	7.497419	-2.753457	-1.706473
H	8.738236	-2.655626	-0.454312
H	1.760685	0.498219	-2.003022
C	0.205521	-1.004955	-2.213772
H	0.098969	-0.856005	-3.300309
H	0.115285	-2.085180	-2.015409
C	-0.874639	-0.230762	-1.456581
H	-0.705672	-0.347027	-0.372094
H	-0.780135	0.848942	-1.671748
C	-2.297901	-0.694427	-1.775835
H	-2.500092	-0.560261	-2.853322
H	-2.373825	-1.779704	-1.583990
C	-3.369895	0.033307	-0.959624

H	-3.141988	-0.076655	0.116338
H	-3.322396	1.116925	-1.170511
C	-4.787944	-0.478205	-1.226921
H	-5.024204	-0.358139	-2.299494
H	-4.822739	-1.564780	-1.028966
C	-5.861880	0.219426	-0.387971
H	-5.608621	0.115631	0.682652
H	-5.844305	1.303712	-0.599305
C	-7.274660	-0.321960	-0.623998
H	-7.536973	-0.206855	-1.691236
H	-7.284511	-1.408861	-0.424580
C	-8.340974	0.358848	0.239113
H	-8.065464	0.253264	1.304199
H	-8.338933	1.444324	0.032276
C	-9.754004	-0.192473	0.030734
H	-10.039639	-0.077776	-1.030472
H	-9.754864	-1.279475	0.229094
C	-10.805742	0.482710	0.915697
H	-10.511561	0.372974	1.975278
H	-10.807312	1.569068	0.714002
C	-12.221382	-0.068198	0.727228
H	-12.521152	0.047522	-0.329985
H	-12.219416	-1.155431	0.924194
C	-13.262142	0.606532	1.625469
H	-12.960266	0.489731	2.682125
H	-13.261099	1.694001	1.429448
C	-14.681493	0.063111	1.444601
H	-14.987281	0.183034	0.389363
H	-14.684717	-1.024774	1.638768
C	4.715022	-0.252686	-2.569479
F	4.213529	0.922154	-2.126520
F	5.957761	-0.412181	-1.903590
F	5.015156	-0.112320	-3.869766
C	-15.716138	0.738940	2.349768
H	-15.408163	0.617747	3.403049
H	-15.710271	1.825766	2.156195
C	-17.132803	0.192846	2.163507
H	-17.175383	-0.885992	2.381050
H	-17.479046	0.333732	1.127613
H	-17.851683	0.696271	2.826954

(5) **Int$_{1KPP}$**

100

C	-0.196451	1.116271	3.209353
O	-0.205734	2.248128	4.145235
C	0.253498	1.992707	5.453912
O	0.934138	0.360708	3.412765
Al	2.122909	-0.888741	3.115314
C	3.321911	-1.091863	4.684097
C	4.343688	0.058537	4.798315
C	2.708341	-1.311363	1.255687
C	1.944797	-2.363312	0.431335
C	0.358859	-2.785813	3.633589
Al	-1.606847	-2.601925	4.039235
C	-2.896128	-3.007932	2.579749
C	-2.329911	-2.943355	1.150211
C	0.940145	-4.208810	3.644203
C	-2.123539	-2.391957	5.947397
C	-0.953511	-2.111601	6.907481
C	-1.451383	0.240803	3.455755
C	-2.798660	0.942390	3.311025
H	0.664281	0.977155	5.565131
H	1.051636	2.709689	5.707236
H	3.851330	-2.059026	4.627419
H	2.715173	-1.138095	5.606251

H	5.002296	-0.051474	5.675503
H	3.844025	1.036047	4.890736
H	4.998247	0.115881	3.913613
H	3.767913	-1.614157	1.337025
H	2.725687	-0.352804	0.705445
H	1.970076	-3.354797	0.909678
H	0.882155	-2.100316	0.299509
H	2.366582	-2.483712	-0.579975
H	-3.771622	-2.341762	2.676515
H	-3.297297	-4.020160	2.776842
H	-1.474648	-3.624549	1.016260
H	-3.078429	-3.212782	0.387435
H	-1.969061	-1.933599	0.895467
H	-2.658025	-3.308079	6.259251
H	-2.879189	-1.589804	6.026760
H	-0.214881	-2.928894	6.903919
H	-1.287783	-1.980565	7.948690
H	-0.410669	-1.192279	6.635591
H	0.473398	-2.331186	2.627680
H	-1.344407	-0.159167	4.481195
H	-1.385864	-0.595458	2.731350
H	-3.619090	0.283648	3.630129
H	-2.827971	1.847463	3.930422
H	-2.990335	1.231554	2.267740
H	2.021883	-4.232576	3.433094
H	0.796473	-4.689712	4.623993
H	0.450131	-4.845997	2.892689
H	0.840427	-2.167370	4.415981
C	-0.205372	1.813497	1.841921
H	-1.005961	2.569323	1.838709
H	0.747597	2.361426	1.776797
C	-0.352940	0.868202	0.651926
H	0.372464	0.044599	0.748658
H	-1.353736	0.401885	0.655907
C	-0.139251	1.560860	-0.695808
H	-0.893882	2.357848	-0.822453
H	0.841602	2.069142	-0.691579
C	-0.204697	0.599874	-1.885485
H	0.590581	-0.160047	-1.780969
H	-1.160317	0.044961	-1.857694
C	-0.067319	1.300489	-3.239293
H	-0.888221	2.031356	-3.353446
H	0.866783	1.890493	-3.251715
C	-0.074359	0.344195	-4.434000
H	0.775939	-0.355735	-4.345376
H	-0.986021	-0.279234	-4.398155
C	-0.006438	1.060740	-5.785395
H	-0.873729	1.739292	-5.878420
H	0.888750	1.708528	-5.810628
C	0.022704	0.113909	-6.987471
H	0.910686	-0.539900	-6.915851
H	-0.853792	-0.558098	-6.944474
C	0.034483	0.841273	-8.334635
H	-0.865068	1.479148	-8.409800
H	0.897945	1.530240	-8.370121
C	0.088871	-0.097234	-9.542750
H	1.003349	-0.714774	-9.484138
H	-0.758704	-0.804774	-9.493389
C	0.056968	0.635154	-10.886802
H	-0.865395	1.240228	-10.948261
H	0.894541	1.354650	-10.930425
C	0.129667	-0.297276	-12.098769
H	1.061378	-0.888951	-12.047964
H	-0.697628	-1.028496	-12.045955
C	0.069062	0.437114	-13.440564
H	-0.867007	1.021600	-13.493200
H	0.889990	1.175538	-13.490663

C	-0.843958	2.186908	6.494675
F	-1.419812	3.412548	6.417332
F	-1.849090	1.267506	6.384878
F	-0.317345	2.054144	7.746659
C	0.151741	-0.490702	-14.655833
H	1.091277	-1.067753	-14.606536
H	-0.663629	-1.233163	-14.600210
C	0.076463	0.255333	-15.989509
H	0.897089	0.983407	-16.084163
H	-0.869707	0.811239	-16.079830
H	0.142019	-0.432984	-16.844870

(6) **TS_{2APP}**

94

C	-0.072887	1.008930	2.444075
O	0.127769	1.950488	3.560853
C	-0.700740	1.708340	4.678642
O	0.915015	0.056718	2.425570
Al	2.159524	-0.636100	3.454496
C	3.438075	-1.653890	2.335427
C	2.721753	-2.706623	1.463012
C	1.683356	-1.023400	5.348683
C	0.577939	-2.092307	5.467808
C	3.555651	1.634145	3.850154
Al	2.994642	3.460765	4.485588
C	1.914466	3.687864	6.141063
C	2.491724	4.642275	7.206028
C	5.044595	1.461248	3.508162
C	3.808567	4.976425	3.487779
C	3.707702	6.385576	4.097660
H	-0.997500	0.649625	4.766191
H	-0.160890	1.992185	5.592665
H	4.212354	-2.135718	2.956021
H	3.975644	-0.946137	1.680537
H	3.418161	-3.233907	0.790036
H	1.945974	-2.243753	0.833685
H	2.222748	-3.476690	2.072767
H	1.362519	-0.098924	5.860451
H	2.585450	-1.359937	5.889304
H	-0.345129	-1.788866	4.946990
H	0.888404	-3.051637	5.023666
H	0.303065	-2.299816	6.514977
H	1.739251	2.692938	6.587984
H	0.919186	4.055771	5.830645
H	2.620818	5.660459	6.811222
H	1.834261	4.718941	8.087219
H	3.476339	4.310470	7.571087
H	3.380955	4.973799	2.467529
H	4.871303	4.709652	3.333037
H	2.661918	6.692744	4.251180
H	4.179052	7.150355	3.458845
H	4.203305	6.439602	5.078977
H	3.239866	0.945028	4.660707
H	5.286921	0.448462	3.150226
H	5.350266	2.165465	2.720510
H	5.684945	1.656972	4.381691
H	2.923735	1.481159	2.951132
C	-0.090673	1.809555	1.146262
H	-0.899511	2.555655	1.204011
H	0.863704	2.358004	1.067848
C	-0.275680	0.887573	-0.062383
H	0.516099	0.121039	-0.034737
H	-1.231287	0.342306	0.041802
C	-0.246601	1.595295	-1.418856
H	-1.076844	2.321088	-1.486316

H	0.683870	2.184862	-1.504338
C	-0.326886	0.607469	-2.587331
H	0.494789	-0.125278	-2.489351
H	-1.261484	0.023559	-2.507347
C	-0.253279	1.256393	-3.971720
H	-1.097873	1.957352	-4.097174
H	0.663712	1.869386	-4.038211
C	-0.261031	0.238826	-5.116695
H	0.582350	-0.462200	-4.981435
H	-1.177625	-0.375119	-5.054240
C	-0.170081	0.873466	-6.507009
H	-1.026263	1.555984	-6.653873
H	0.734403	1.506374	-6.558681
C	-0.134937	-0.145345	-7.649900
H	0.724939	-0.824010	-7.506128
H	-1.036296	-0.782738	-7.600306
C	-0.045527	0.499559	-9.035852
H	-0.910321	1.171883	-9.179785
H	0.850122	1.145729	-9.078043
C	0.006441	-0.505704	-10.189554
H	0.876184	-1.173325	-10.053960
H	-0.885678	-1.156678	-10.148481
C	0.085941	0.158757	-11.567053
H	-0.784772	0.826141	-11.698232
H	0.976207	0.812706	-11.603677
C	0.140605	-0.830212	-12.734293
H	1.015769	-1.493237	-12.611088
H	-0.746602	-1.488248	-12.697671
C	0.209075	-0.149199	-14.104183
H	-0.666598	0.514007	-14.224942
H	1.095029	0.510978	-14.138996
C	-1.978892	2.546271	4.642291
F	-1.713857	3.878263	4.624845
F	-2.745010	2.273255	3.549574
F	-2.733275	2.287826	5.747915
H	-1.062393	0.532085	2.600967
C	0.264477	-1.126441	-15.281621
H	1.142284	-1.785352	-15.164108
H	-0.618825	-1.787914	-15.245251
C	0.325680	-0.426090	-16.640870
H	1.215658	0.218285	-16.715604
H	-0.557725	0.212300	-16.798229
H	0.367099	-1.148488	-17.469444

(7) **TS_{2KPP}**

100

C	-0.236420	1.103544	2.364263
O	-0.185128	2.263388	3.353104
C	-1.256305	3.177223	3.238370
O	0.904626	0.409402	2.558645
Al	2.127752	-0.457142	3.473714
C	3.595455	-1.001973	2.254400
C	3.117162	-2.038195	1.215010
C	1.622468	-1.532572	5.073946
C	1.502290	-3.045640	4.800937
C	3.003455	1.669242	4.514159
Al	2.213685	3.409474	5.158995
C	1.575932	3.383671	7.041993
C	2.540750	2.699604	8.030596
C	4.475681	1.440547	4.896418
C	2.587031	5.019127	4.058809
C	2.287081	6.382992	4.703115
C	-1.514800	0.277451	2.691210
C	-1.412187	-1.219148	2.389346
H	-1.044207	3.996481	2.527174

H	-2.201143	2.694943	2.940249
H	4.451105	-1.410637	2.818617
H	3.977192	-0.106123	1.734478
H	3.908251	-2.309460	0.496279
H	2.265190	-1.659725	0.627399
H	2.784199	-2.973754	1.692404
H	0.682736	-1.146217	5.505864
H	2.391200	-1.369998	5.852324
H	0.713886	-3.272421	4.065217
H	2.440097	-3.460355	4.398722
H	1.261523	-3.619039	5.711577
H	0.603578	2.860254	7.057141
H	1.353959	4.412326	7.372155
H	3.514018	3.213857	8.084454
H	2.137646	2.675935	9.056687
H	2.745400	1.654250	7.747518
H	2.028775	4.910124	3.110868
H	3.650966	4.964068	3.760386
H	1.220550	6.487151	4.951901
H	2.550400	7.225975	4.043093
H	2.846397	6.522987	5.641611
H	2.327549	0.951216	5.027496
H	-2.371615	0.698966	2.140863
H	-1.724493	0.409456	3.764811
H	-2.368626	-1.714085	2.613062
H	-1.164513	-1.420845	1.339435
H	-0.640669	-1.692159	3.010671
H	4.871387	0.473052	4.546874
H	5.117287	2.220897	4.460049
H	4.617657	1.474420	5.986684
H	2.845180	1.689307	3.421470
C	-0.219509	1.725986	0.953094
H	-1.100947	2.372631	0.810535
H	0.672332	2.374125	0.919996
C	-0.156757	0.716830	-0.195018
H	0.661874	0.005671	-0.001726
H	-1.088798	0.127355	-0.231059
C	0.051867	1.391982	-1.553318
H	-0.753221	2.129995	-1.722411
H	0.993704	1.969340	-1.531918
C	0.084378	0.411032	-2.727965
H	0.921369	-0.296737	-2.591688
H	-0.836343	-0.200281	-2.717068
C	0.211221	1.103005	-4.087810
H	-0.625103	1.815640	-4.207337
H	1.132692	1.712667	-4.103897
C	0.220338	0.140809	-5.278159
H	1.080979	-0.546219	-5.189102
H	-0.682337	-0.495617	-5.238638
C	0.273702	0.854884	-6.631587
H	-0.588354	1.542141	-6.710722
H	1.174430	1.493846	-6.672301
C	0.271281	-0.091425	-7.834569
H	1.146392	-0.763435	-7.774165
H	-0.618185	-0.745252	-7.782046
C	0.282088	0.638446	-9.180544
H	-0.594054	1.310081	-9.235102
H	1.169878	1.294566	-9.232428
C	0.274336	-0.296238	-10.392579
H	1.156939	-0.959823	-10.348316
H	-0.607608	-0.959805	-10.335539
C	0.263367	0.444248	-11.732740
H	-0.619362	1.108140	-11.773419
H	1.144683	1.108702	-11.789109
C	0.252229	-0.482868	-12.950639
H	1.137730	-1.143221	-12.914692
H	-0.626666	-1.150405	-12.892331

C	0.231829	0.263499	-14.287259
H	-0.653587	0.924366	-14.322279
H	1.110409	0.931674	-14.345742
C	-1.529013	3.823773	4.585582
F	-1.845911	2.924401	5.547251
F	-0.444669	4.529795	5.034857
F	-2.559446	4.704889	4.479314
C	0.219277	-0.658828	-15.509377
H	1.104482	-1.317808	-15.474449
H	-0.658377	-1.326077	-15.449772
C	0.197103	0.101213	-16.837131
H	1.080292	0.751449	-16.937176
H	-0.695084	0.742463	-16.912538
H	0.188543	-0.583872	-17.697712

(8) **Int_{2KPP}**

94

C	-1.234150	-0.033184	3.019305
O	-0.583325	0.670071	4.253747
C	-1.535482	1.185376	5.182541
O	-1.426811	-1.334360	3.282807
Al	-0.681345	-2.680904	4.194886
C	-0.229020	-4.261433	3.094048
C	0.346977	-3.967658	1.698315
C	-1.326164	-2.707224	6.074749
C	-2.857659	-2.851359	6.181344
C	1.592096	-1.506822	4.420466
Al	1.396097	0.489734	4.772776
C	1.352420	0.906935	6.734479
C	2.692102	0.568499	7.423528
C	3.011137	-2.096519	4.361500
C	2.393254	1.705476	3.538794
C	3.736534	2.211741	4.100248
H	-2.470170	0.606871	5.142727
H	-1.118869	1.121709	6.195606
H	-1.140851	-4.879248	3.000077
H	0.475515	-4.885529	3.672784
H	0.577420	-4.887985	1.137150
H	1.282446	-3.387149	1.753956
H	-0.355577	-3.381470	1.086691
H	-1.007258	-1.775598	6.576931
H	-0.831308	-3.521636	6.631569
H	-3.380939	-2.048290	5.637641
H	-3.210131	-3.803554	5.754004
H	-3.210293	-2.820505	7.225357
H	0.551996	0.331242	7.237600
H	1.113006	1.971266	6.909065
H	3.531869	1.130530	6.985937
H	2.682381	0.795344	8.502688
H	2.940171	-0.501151	7.326952
H	1.743633	2.569457	3.308381
H	2.565656	1.206644	2.568194
H	3.598306	2.771113	5.039048
H	4.261798	2.884485	3.401341
H	4.427974	1.382627	4.323542
H	1.042930	-1.997705	5.258369
H	3.023410	-3.179907	4.158763
H	3.598721	-1.606916	3.570376
H	3.547249	-1.933404	5.308057
H	1.106342	-1.719916	3.443700
C	-0.339799	0.285194	1.832003
H	-0.159318	1.370957	1.810032
H	0.637717	-0.205830	1.960645
C	-0.979574	-0.169994	0.516819
H	-1.175495	-1.253165	0.562711

H	-1.963542	0.318755	0.401572
C	-0.107549	0.153142	-0.698836
H	0.104262	1.237046	-0.717023
H	0.871723	-0.345945	-0.588082
C	-0.741715	-0.258851	-2.029432
H	-0.917478	-1.349379	-2.030461
H	-1.738289	0.210083	-2.117205
C	0.101829	0.125008	-3.248104
H	0.283045	1.214868	-3.232366
H	1.096728	-0.348606	-3.169343
C	-0.538383	-0.257424	-4.585020
H	-0.691354	-1.350995	-4.619347
H	-1.545918	0.191912	-4.646629
C	0.281344	0.180697	-5.801568
H	0.437024	1.273791	-5.757766
H	1.288092	-0.270858	-5.746659
C	-0.363996	-0.181199	-7.141755
H	-0.498132	-1.276305	-7.199846
H	-1.379891	0.251137	-7.184343
C	0.436997	0.297503	-8.355483
H	0.569319	1.392754	-8.293147
H	1.453725	-0.132841	-8.315331
C	-0.209133	-0.055927	-9.697575
H	-0.322387	-1.152533	-9.770979
H	-1.233472	0.357066	-9.728358
C	0.575924	0.454575	-10.908779
H	0.682842	1.551893	-10.835730
H	1.602631	0.047779	-10.876383
C	-0.066308	0.098711	-12.252164
H	-0.159718	-0.999367	-12.332134
H	-1.098172	0.493012	-12.278400
C	0.707046	0.629873	-13.461861
H	0.793734	1.728888	-13.384940
H	1.741617	0.242538	-13.433278
C	-1.844916	2.654732	4.898634
F	-0.730464	3.422298	4.949426
F	-2.403563	2.835253	3.668820
F	-2.724253	3.122286	5.823515
H	-2.198012	0.499180	2.922560
C	0.070772	0.268181	-14.807024
H	-0.009482	-0.830076	-14.885261
H	-0.964683	0.650236	-14.831582
C	0.847485	0.813071	-16.007269
H	1.877187	0.423082	-16.023824
H	0.911616	1.911847	-15.972453
H	0.370739	0.536712	-16.959369

(9) **Int$_{2KPP}$**

100

C	-1.495009	-0.364514	2.750040
O	0.305185	1.492324	4.251317
C	0.714600	2.645088	3.588984
O	-0.941547	-1.420773	3.118155
Al	0.741263	-2.448746	2.952247
C	1.598499	-2.193581	1.155848
C	1.183224	-3.163337	0.035055
C	0.078779	-4.257124	3.473958
C	-1.186705	-4.715628	2.723248
C	1.671517	-1.403103	4.444477
Al	1.149820	0.741447	5.649445
C	-0.106918	0.159348	7.072509
C	0.410465	-0.940982	8.015229
C	2.858356	-2.106381	5.115038
C	2.947106	1.501157	6.034516
C	2.880731	2.781408	6.893671

C	-2.708743	0.123156	3.474898
C	-3.321537	-0.862077	4.461572
H	1.713589	3.012152	3.895384
H	0.741455	2.503484	2.491270
H	2.685223	-2.304483	1.338064
H	1.491971	-1.149758	0.808826
H	1.738588	-2.998260	-0.904302
H	0.111787	-3.080683	-0.210507
H	1.351472	-4.211274	0.328652
H	-0.116682	-4.263917	4.562097
H	0.885608	-4.996998	3.321583
H	-2.025313	-4.019551	2.886832
H	-1.020768	-4.765074	1.635026
H	-1.533098	-5.714294	3.039277
H	-1.061164	-0.150916	6.611695
H	-0.355916	1.064490	7.656832
H	1.348498	-0.644808	8.511262
H	-0.310494	-1.188141	8.811493
H	0.620993	-1.878844	7.475446
H	3.488850	1.703198	5.092750
H	3.555976	0.742405	6.555303
H	2.307923	3.583848	6.401584
H	3.880233	3.190052	7.116589
H	2.388284	2.594384	7.861430
H	0.808784	-1.285404	5.135745
H	-3.436064	0.472311	2.721049
H	-2.365610	1.048127	3.978369
H	-4.170010	-0.401026	4.984053
H	-3.680237	-1.766886	3.950876
H	-2.586000	-1.177672	5.212885
H	3.665265	-2.281436	4.387633
H	3.300252	-1.545468	5.954480
H	2.557582	-3.090450	5.504378
H	1.955950	-0.452944	3.952270
C	-1.005705	0.400772	1.559967
H	-1.381794	1.432844	1.598824
H	0.093086	0.423498	1.595120
C	-1.451752	-0.284674	0.248789
H	-1.155615	-1.344353	0.281749
H	-2.551994	-0.261929	0.170317
C	-0.826599	0.380265	-0.979608
H	-1.127485	1.441976	-1.019786
H	0.272031	0.373767	-0.866604
C	-1.199359	-0.310890	-2.293370
H	-0.893444	-1.370751	-2.244015
H	-2.297705	-0.312286	-2.411884
C	-0.556504	0.346134	-3.518323
H	-0.866789	1.405227	-3.569167
H	0.540649	0.356737	-3.389033
C	-0.900986	-0.345308	-4.839901
H	-0.584429	-1.402499	-4.791497
H	-1.998129	-0.361821	-4.969752
C	-0.257119	0.321409	-6.058969
H	-0.577894	1.377567	-6.107778
H	0.839325	0.344017	-5.923827
C	-0.587239	-0.367649	-7.385525
H	-0.262457	-1.422590	-7.339431
H	-1.683553	-0.393337	-7.521260
C	0.056662	0.307493	-8.599892
H	-0.270457	1.361831	-8.645956
H	1.152553	0.336484	-8.461211
C	-0.265410	-0.378988	-9.929759
H	0.064692	-1.432426	-9.885799
H	-1.361215	-0.410209	-10.068599
C	0.377869	0.302356	-11.140959
H	0.046693	1.355530	-11.184538
H	1.473441	0.335200	-11.000634

C	0.059976	-0.381906	-12.473023
H	0.393115	-1.434507	-12.430773
H	-1.035608	-0.416225	-12.613122
C	0.702207	0.303273	-13.682395
H	0.368787	1.355967	-13.724940
H	1.797893	0.338725	-13.542371
C	-0.257993	3.795269	3.842997
F	-1.533953	3.476268	3.465955
F	-0.308971	4.143375	5.156185
F	0.104755	4.902016	3.135973
C	0.386999	-0.378709	-15.016738
H	0.721969	-1.429634	-14.973707
H	-0.707748	-0.414666	-15.154930
C	1.032911	0.317495	-16.216474
H	2.129668	0.338820	-16.119766
H	0.689219	1.360245	-16.302360
H	0.791018	-0.192415	-17.160663

(10) **TS_{3APP}**

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C	-0.767943	-0.474077	1.949839
O	-0.256517	0.863287	3.462082
C	-1.345380	1.552267	4.012689
O	-0.134909	-1.546424	2.200373
Al	-0.216095	-2.759666	3.677014
C	0.695621	-4.414524	3.074036
C	0.102586	-4.999293	1.775759
C	-2.070328	-2.685478	4.408819
C	-3.137453	-3.356473	3.522004
C	1.115803	-1.405896	4.793688
Al	1.390093	0.695167	4.412321
C	1.284502	1.744376	6.110954
C	2.626845	1.796064	6.868483
C	1.847280	-2.045661	5.968680
C	2.892200	0.933843	3.123126
C	4.206451	0.240852	3.530969
H	-2.301878	1.037106	3.799826
H	-1.261532	1.652486	5.109115
H	0.660873	-5.173702	3.874854
H	1.768224	-4.196390	2.927077
H	0.640833	-5.899618	1.436118
H	0.140908	-4.271359	0.949403
H	-0.953418	-5.286409	1.900675
H	-2.351132	-1.629989	4.591439
H	-2.076736	-3.151394	5.410599
H	-3.176188	-2.910287	2.514524
H	-2.929231	-4.428529	3.381507
H	-4.152465	-3.279758	3.946270
H	0.505394	1.328543	6.777387
H	0.956567	2.774349	5.883594
H	3.419305	2.250968	6.253182
H	2.567508	2.384833	7.799375
H	2.980705	0.790765	7.148216
H	3.069512	2.014497	2.978825
H	2.575579	0.560200	2.132249
H	4.580794	0.610784	4.498606
H	5.015470	0.391894	2.796426
H	4.078387	-0.849405	3.637854
H	0.076986	-1.073287	4.931022
H	1.677738	-3.129610	6.081312
H	2.933545	-1.901961	5.873915
H	1.548122	-1.569848	6.913627
H	1.539213	-1.503778	3.784134
C	-0.362247	0.331232	0.760540
H	-0.812718	1.329087	0.814848

H	0.732059	0.442444	0.775997
C	-0.792883	-0.383635	-0.538857
H	-0.354720	-1.394581	-0.555896
H	-1.889278	-0.512643	-0.551236
C	-0.351830	0.395225	-1.780745
H	-0.788382	1.408785	-1.753088
H	0.743242	0.533516	-1.745782
C	-0.731967	-0.289361	-3.095824
H	-0.321245	-1.314634	-3.105351
H	-1.829644	-0.399317	-3.151167
C	-0.230765	0.465854	-4.329857
H	-0.644920	1.489878	-4.325352
H	0.865718	0.582375	-4.260073
C	-0.578737	-0.215800	-5.655451
H	-0.186352	-1.248539	-5.647535
H	-1.676018	-0.308246	-5.744711
C	-0.028253	0.522414	-6.878592
H	-0.423403	1.553980	-6.891609
H	1.067871	0.619701	-6.778340
C	-0.351646	-0.160228	-8.209930
H	0.026216	-1.198206	-8.187759
H	-1.447653	-0.238723	-8.325373
C	0.236583	0.563917	-9.423939
H	-0.142605	1.601301	-9.449594
H	1.331766	0.645153	-9.301189
C	-0.070570	-0.119705	-10.758613
H	0.296373	-1.161359	-10.726905
H	-1.165345	-0.187870	-10.891554
C	0.543029	0.594376	-11.966092
H	0.176560	1.636143	-11.998934
H	1.637446	0.662809	-11.829492
C	0.243725	-0.088795	-13.302912
H	0.603170	-1.132977	-13.266687
H	-0.850446	-0.149726	-13.444942
C	0.871208	0.619357	-14.506633
H	0.513427	1.664253	-14.543015
H	1.965552	0.679451	-14.364232
C	-1.490370	2.972283	3.459287
F	-0.351915	3.695484	3.592512
F	-1.817556	2.978636	2.132549
F	-2.484917	3.628428	4.118997
H	-1.807088	-0.379208	2.316138
C	0.574541	-0.061357	-15.845854
H	0.930119	-1.105701	-15.807079
H	-0.518753	-0.118252	-15.988516
C	1.211408	0.653850	-17.039155
H	2.307228	0.694843	-16.938340
H	0.848796	1.690576	-17.120039
H	0.982336	0.145186	-17.987221

(11) **Int$_{3APP}$**

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C	-0.507803	-0.581979	2.728887
O	-0.129529	1.123831	4.507385
C	-1.312575	1.693159	4.984539
O	0.135941	-1.546968	3.183065
Al	-0.296330	-2.664129	4.769502
C	0.511123	-4.414652	4.257235
C	0.090866	-4.947871	2.873701
C	-2.277279	-2.427823	4.980872
C	-3.169835	-2.986434	3.857174
C	0.793617	-1.514994	6.057813
Al	1.381325	0.938254	5.479668
C	1.340018	1.831936	7.253180
C	2.684341	1.837615	8.006325

C	1.395056	-2.134158	7.325116
C	2.973026	0.737146	4.311528
C	4.173839	-0.015752	4.913653
H	-2.187112	1.045783	4.781897
H	-1.299558	1.894507	6.072231
H	0.272848	-5.166600	5.031196
H	1.611073	-4.308879	4.292066
H	0.584650	-5.900188	2.615050
H	0.337215	-4.232006	2.072814
H	-0.994671	-5.125418	2.817368
H	-2.499107	-1.353401	5.133995
H	-2.567129	-2.896530	5.939722
H	-2.925019	-2.549802	2.873630
H	-3.044049	-4.074560	3.748821
H	-4.244293	-2.801499	4.027542
H	0.558541	1.378200	7.887972
H	1.007350	2.872934	7.084618
H	3.479736	2.317658	7.415059
H	2.624434	2.379639	8.964196
H	3.030139	0.817443	8.234750
H	3.282456	1.756155	4.014241
H	2.655351	0.246613	3.374900
H	4.543681	0.468219	5.830364
H	5.022906	-0.074536	4.213500
H	3.914202	-1.052221	5.184169
H	0.095963	-0.694069	6.318078
H	2.067712	-2.966730	7.071421
H	1.971203	-1.420262	7.936639
H	0.604463	-2.545862	7.970583
H	1.606748	-1.165836	5.379912
C	-0.021549	0.204139	1.568526
H	-0.363632	1.243539	1.668543
H	1.077363	0.182293	1.549391
C	-0.585584	-0.418338	0.266024
H	-0.256805	-1.468486	0.199593
H	-1.688268	-0.433356	0.305067
C	-0.124212	0.347080	-0.977303
H	-0.474455	1.392001	-0.916341
H	0.978896	0.391662	-0.984495
C	-0.613139	-0.288106	-2.281568
H	-0.282971	-1.341559	-2.317682
H	-1.717291	-0.314313	-2.287495
C	-0.113658	0.437056	-3.534351
H	-0.462256	1.484963	-3.516535
H	0.989870	0.483241	-3.510193
C	-0.559948	-0.227327	-4.839380
H	-0.227244	-1.280887	-4.841171
H	-1.663623	-0.258097	-4.876574
C	-0.028661	0.468458	-6.095359
H	-0.374605	1.517526	-6.108210
H	1.074221	0.513455	-6.045775
C	-0.445665	-0.220475	-7.397284
H	-0.111981	-1.273508	-7.372962
H	-1.548402	-0.253794	-7.456839
C	0.109443	0.453459	-8.654946
H	-0.232644	1.503389	-8.689317
H	1.211522	0.495949	-8.587600
C	-0.288908	-0.252435	-9.953610
H	0.045196	-1.304794	-9.912043
H	-1.390795	-0.287495	-10.027300
C	0.281304	0.407500	-11.212031
H	-0.056890	1.458236	-11.258971
H	1.382809	0.447107	-11.134343
C	-0.107462	-0.307539	-12.508656
H	0.226850	-1.359454	-12.458122
H	-1.208893	-0.343546	-12.589289
C	0.469960	0.345350	-13.767370

H	0.134959	1.397048	-13.820228
H	1.571452	0.382725	-13.686149
C	-1.598442	3.030257	4.303650
F	-0.607114	3.935384	4.515727
F	-1.733860	2.894829	2.950958
F	-2.757761	3.565913	4.775195
H	-1.540324	-0.404932	3.084152
C	0.084921	-0.371807	-15.064447
H	0.419373	-1.422371	-15.009396
H	-1.015531	-0.407781	-15.144941
C	0.669714	0.288333	-16.314807
H	1.770060	0.306988	-16.275613
H	0.325611	1.329989	-16.411566
H	0.377436	-0.246174	-17.230711

(12) **Pdt (Ketone)**

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C	-1.544405	-1.035008	1.848633
O	-0.832565	-2.028147	1.835832
C	-2.293611	-0.599033	3.103185
C	-1.908298	-1.378343	4.355733
H	-3.371995	-0.710491	2.885175
H	-2.144556	0.486988	3.236335
H	-2.501584	-1.049053	5.220237
H	-2.068770	-2.454988	4.210858
H	-0.844290	-1.239731	4.592886
C	-1.735276	-0.161745	0.614377
H	-2.810184	0.072837	0.511532
H	-1.255163	0.811793	0.831774
C	-1.173127	-0.759159	-0.673033
H	-0.110664	-1.006010	-0.519408
H	-1.673218	-1.721928	-0.872021
C	-1.327719	0.165428	-1.883594
H	-2.395140	0.413420	-2.027194
H	-0.817897	1.125452	-1.681814
C	-0.773397	-0.438844	-3.177217
H	0.291669	-0.693337	-3.031626
H	-1.287571	-1.395824	-3.379754
C	-0.911286	0.477255	-4.396700
H	-1.973528	0.750205	-4.531514
H	-0.376646	1.425235	-4.203982
C	-0.382580	-0.149230	-5.690313
H	0.672248	-0.445013	-5.546269
H	-0.934086	-1.085593	-5.891764
C	-0.484277	0.769691	-6.911099
H	-1.535457	1.081173	-7.048727
H	0.084106	1.697520	-6.717518
C	0.025181	0.124172	-8.202990
H	1.067883	-0.210426	-8.055506
H	-0.559679	-0.791046	-8.407298
C	-0.038328	1.046809	-9.423314
H	-1.078620	1.389524	-9.569211
H	0.555508	1.957199	-9.223224
C	0.463003	0.388389	-10.711847
H	1.498489	0.033851	-10.559848
H	-0.139157	-0.515554	-10.916371
C	0.420894	1.309720	-11.933896
H	-0.612355	1.672036	-12.082626
H	1.031553	2.208920	-11.733829
C	0.911805	0.641338	-13.221245
H	1.942345	0.272178	-13.070054
H	0.296503	-0.254155	-13.423963
C	0.880681	1.561783	-14.444042
H	-0.148232	1.936594	-14.593127
H	1.501872	2.454209	-14.245448

C	1.363122	0.888169	-15.732185
H	2.389572	0.511239	-15.580298
H	0.739629	-0.001469	-15.929707
C	1.332320	1.816323	-16.948001
H	1.974701	2.697097	-16.791933
H	0.311987	2.182493	-17.142142
H	1.681837	1.305616	-17.857460

(13) **Pdt (Aldehyde)**

49

C	-0.184735	-0.664313	1.878013
O	-0.915387	-1.635398	1.913925
C	0.238080	0.056781	0.622875
H	-0.043712	1.120061	0.752646
H	1.345568	0.069162	0.620037
C	-0.319831	-0.519148	-0.674886
H	-0.027381	-1.579007	-0.752738
H	-1.420726	-0.520623	-0.624081
C	0.144176	0.243798	-1.918100
H	-0.158433	1.303204	-1.835236
H	1.248456	0.246216	-1.958424
C	-0.405351	-0.339257	-3.223030
H	-0.103142	-1.398895	-3.300997
H	-1.509231	-0.341446	-3.183629
C	0.055592	0.409624	-4.476425
H	-0.261440	1.466000	-4.410293
H	1.159906	0.425660	-4.505684
C	-0.473142	-0.199715	-5.778045
H	-0.161922	-1.258315	-5.834930
H	-1.577697	-0.210786	-5.753029
C	-0.002950	0.529084	-7.040026
H	-0.329740	1.583595	-6.997399
H	1.101735	0.553781	-7.056833
C	-0.513127	-0.110337	-8.334678
H	-0.192745	-1.167333	-8.366748
H	-1.617717	-0.129888	-8.320257
C	-0.038265	0.596907	-9.606706
H	-0.367913	1.651166	-9.585215
H	1.066158	0.625185	-9.617688
C	-0.538739	-0.063937	-10.894206
H	-0.209498	-1.118478	-10.912476
H	-1.643262	-0.092670	-10.882846
C	-0.064941	0.635674	-12.171043
H	-0.399310	1.688603	-12.154881
H	1.039443	0.668765	-12.180055
C	-0.560872	-0.032831	-13.456291
H	-0.215111	-1.082014	-13.477683
H	-1.664743	-0.078685	-13.439411
C	-0.106415	0.674981	-14.735412
H	-0.457522	1.722615	-14.716797
H	0.997351	0.726394	-14.752979
H	0.233588	-0.235409	2.828233
C	-0.600511	-0.000017	-16.018408
H	-0.237620	-1.042304	-16.041216
H	-1.702246	-0.063462	-15.991617
C	-0.160733	0.724130	-17.292055
H	0.936992	0.777690	-17.360520
H	-0.543441	1.756399	-17.314017
H	-0.526857	0.213355	-18.194955

(D) Rate-determining transition states for D_3, D_4, and D_5 and corresponding reactants.

(1) **TS_{AP} (for D_3)**

97

C	3.594268	-0.197291	-2.542512
O	4.469062	-0.752886	-3.492373
C	5.880438	-0.828925	-3.162899
O	3.984462	-0.316637	-1.259367
Al	4.101946	0.828653	0.110249
C	2.524347	0.979592	1.314164
C	2.195822	-0.331866	2.053596
C	4.159594	2.730867	-1.100000
C	3.699240	2.558752	-2.401223
C	5.894580	0.700074	1.012010
C	6.098854	1.784912	2.081320
Al	8.139353	-0.652792	1.347220
C	7.899247	-1.127136	3.280168
C	6.543000	-1.686146	3.744251
C	9.423800	0.823838	0.914496
C	9.367717	1.404856	-0.507632
C	7.868470	-2.039567	-0.070955
C	6.609600	-2.922139	-0.012342
H	8.687876	-1.877241	3.486326
H	6.649134	0.745512	0.203477
H	5.868933	-0.317865	1.452854
H	5.222110	2.946644	-0.949494
H	3.473759	3.177225	-0.370398
H	1.641480	1.323798	0.747815
H	9.324939	1.634992	1.657028
H	10.432346	0.403537	1.095486
H	8.768081	-2.684590	-0.031560
H	7.935134	-1.542330	-1.055951
H	1.342821	-0.224835	2.744239
H	1.942817	-1.141290	1.350407
H	3.048848	-0.689166	2.653091
H	5.290370	1.759298	2.827860
H	7.047475	1.691083	2.633283
H	6.092423	2.790798	1.633093
H	10.145694	2.164745	-0.693396
H	9.495044	0.621987	-1.272609
H	8.398874	1.891837	-0.711878
H	6.569573	-3.662818	-0.830071
H	6.554150	-3.485248	0.932000
H	5.684268	-2.327363	-0.083101
H	5.967155	-1.168747	-2.120759
H	2.729374	1.778421	2.050074
H	8.175138	-0.256019	3.900752
H	6.549405	-1.989945	4.804628
H	5.737538	-0.940809	3.636887
H	6.238753	-2.568351	3.159217
H	3.551062	0.987083	-2.743333
H	4.388018	2.602649	-3.248455
H	2.648264	2.736231	-2.641700
C	2.190540	-0.722020	-2.865637
H	2.003668	-0.545005	-3.936328
H	2.225824	-1.814780	-2.721386
C	1.086661	-0.109392	-2.008547
H	1.309487	-0.293626	-0.945875
H	1.077369	0.988568	-2.134249
C	-0.305143	-0.657389	-2.332284
H	-0.531954	-0.485532	-3.399720
H	-0.305138	-1.753162	-2.193520
C	-1.408654	-0.036558	-1.471122
H	-1.171874	-0.198437	-0.404081
H	-1.411238	1.058907	-1.617913
C	-2.804226	-0.589335	-1.770230
H	-3.031841	-0.443636	-2.841677
H	-2.806368	-1.681831	-1.605692
C	-3.910868	0.051247	-0.927767
H	-3.680310	-0.087156	0.143913

H	-3.912698	1.142953	-1.098897
C	-5.305305	-0.508575	-1.220428
H	-5.531287	-0.379714	-2.294384
H	-5.305682	-1.598564	-1.039510
C	-6.415156	0.141635	-0.389603
H	-6.186379	0.018853	0.684427
H	-6.419080	1.230785	-0.575956
C	-7.807858	-0.425528	-0.676454
H	-8.034905	-0.307277	-1.751406
H	-7.804391	-1.513858	-0.485658
C	-8.919507	0.228073	0.149405
H	-8.689657	0.114531	1.224303
H	-8.926634	1.315714	-0.045587
C	-10.310676	-0.345190	-0.131808
H	-10.540980	-0.233534	-1.206948
H	-10.304021	-1.432705	0.064584
C	-11.424320	0.308100	0.692381
H	-11.191344	0.198257	1.766012
H	-11.431822	1.393968	0.493352
C	-12.808545	-0.276556	0.405417
H	-13.080461	-0.149907	-0.654101
H	-12.837751	-1.354944	0.626818
H	-13.588334	0.209281	1.010404
C	6.567243	0.526352	-3.309791
H	7.648276	0.421145	-3.140537
H	6.410662	0.934740	-4.320017
H	6.192613	1.247418	-2.570323
C	6.462980	-1.883672	-4.090899
H	5.936926	-2.839084	-3.962277
H	6.372479	-1.573905	-5.142643
H	7.526834	-2.039804	-3.861446

(2) **TS_{KP} (for D_3)**

97

C	-0.049935	-0.095414	0.430832
O	-0.227987	0.399344	1.684959
C	0.412583	-0.298334	2.800773
O	1.055005	-0.735276	0.171035
Al	2.129457	-2.054327	-0.506860
C	3.392050	-2.621322	0.919925
C	4.645472	-1.732641	1.039244
C	2.761565	-1.722817	-2.367709
C	1.878772	-2.179162	-3.541600
C	0.487751	-3.732443	-0.621672
Al	-1.551292	-3.840591	-0.160819
C	-2.674593	-4.114448	-1.798717
C	-2.442166	-3.087062	-2.919983
C	1.218429	-4.975173	-1.132728
C	-1.858658	-4.904613	1.512947
C	-1.001362	-4.473507	2.715036
C	-1.557682	-1.718851	0.388121
C	-2.875881	-1.148430	0.843980
H	0.600489	-1.338988	2.489319
H	3.698716	-3.665552	0.730099
H	2.857361	-2.646413	1.886637
H	5.332947	-2.073973	1.831213
H	4.387211	-0.686852	1.271824
H	5.221033	-1.715542	0.100251
H	3.756357	-2.196498	-2.450716
H	2.961206	-0.637965	-2.450630
H	1.723953	-3.269183	-3.533450
H	0.881061	-1.714570	-3.515518
H	2.317783	-1.925995	-4.520732
H	-3.741215	-4.117949	-1.512126
H	-2.481399	-5.132523	-2.185201

H	-1.387225	-3.057979	-3.241128
H	-3.040167	-3.289821	-3.825360
H	-2.704386	-2.065407	-2.596274
H	-1.665948	-5.969245	1.284449
H	-2.928268	-4.863062	1.785358
H	0.078457	-4.514838	2.489145
H	-1.156722	-5.103243	3.607937
H	-1.222402	-3.437158	3.022386
H	0.389626	-2.921188	-1.369871
H	-0.838042	-2.033786	1.143436
H	-1.242087	-1.590983	-0.646243
H	-3.365491	-1.794569	1.590361
H	-2.763565	-0.152562	1.313171
H	-3.577869	-1.044087	0.003501
H	2.283245	-4.822674	-1.383857
H	1.179485	-5.775060	-0.378673
H	0.727848	-5.361852	-2.037775
H	0.796201	-3.409882	0.392213
C	-0.614577	0.877466	-0.586033
H	-1.676572	1.048308	-0.355505
H	-0.101817	1.839180	-0.398755
C	-0.416353	0.467172	-2.040773
H	0.660497	0.362547	-2.245037
H	-0.859679	-0.528773	-2.217688
C	-1.035846	1.452658	-3.034093
H	-2.113640	1.562801	-2.819088
H	-0.590840	2.453293	-2.887525
C	-0.851290	1.020929	-4.491404
H	0.226050	0.893922	-4.700110
H	-1.307229	0.024381	-4.634733
C	-1.451174	2.004688	-5.499100
H	-2.528175	2.131847	-5.288065
H	-0.993635	3.000021	-5.352435
C	-1.269766	1.577170	-6.957909
H	-0.193457	1.439949	-7.166172
H	-1.736676	0.587088	-7.108807
C	-1.856023	2.573410	-7.962175
H	-2.932119	2.711294	-7.752959
H	-1.388287	3.562836	-7.807756
C	-1.675886	2.154230	-9.423571
H	-0.600388	2.009638	-9.631329
H	-2.150528	1.168882	-9.581891
C	-2.252576	3.160768	-10.423228
H	-3.327853	3.306113	-10.214795
H	-1.777275	4.145610	-10.262877
C	-2.073602	2.747344	-11.886439
H	-0.998642	2.598093	-12.093916
H	-2.552978	1.764934	-12.049038
C	-2.644497	3.759750	-12.883250
H	-3.719618	3.909581	-12.676246
H	-2.165332	4.742413	-12.720046
C	-2.466214	3.350416	-14.348159
H	-1.392021	3.200185	-14.553276
H	-2.946085	2.369432	-14.510583
C	-3.039016	4.371496	-15.333309
H	-4.118952	4.515443	-15.172577
H	-2.553860	5.353104	-15.214605
H	-2.896621	4.053515	-16.376619
C	-0.577720	-0.271298	3.953339
H	-1.513983	-0.775357	3.678225
H	-0.151152	-0.784539	4.826865
H	-0.809626	0.765210	4.237754
C	1.737790	0.380249	3.118973
H	2.237873	-0.140003	3.948724
H	2.403616	0.358111	2.247337
H	1.571435	1.426884	3.413040

(3) **RC (for D_3)**

97

C	0.128941	1.775774	2.405826
O	-0.507688	2.366014	3.406765
C	-0.125171	2.049812	4.809539
O	1.058061	0.974209	2.579780
Al	2.419740	-0.460793	2.594940
C	3.408820	0.016769	4.266479
C	4.193080	1.339091	4.182309
C	3.413050	-0.368205	0.857973
C	2.893937	-1.262688	-0.282365
C	1.132805	-2.024395	2.771527
Al	-1.318521	-2.704869	2.760433
C	-1.321472	-4.038443	1.266410
C	-0.962758	-3.483720	-0.123454
C	1.845584	-3.362086	3.023402
C	-1.498683	-3.334792	4.654905
C	-1.375007	-2.243677	5.731798
C	-2.111903	-0.903082	2.350640
C	-3.652439	-0.920059	2.320062
H	0.450036	1.114428	4.786975
H	4.105482	-0.804678	4.514515
H	2.703278	0.052467	5.118472
H	4.715146	1.596774	5.120001
H	3.533787	2.190647	3.941311
H	4.956931	1.304808	3.388167
H	4.467017	-0.626076	1.071577
H	3.453722	0.684438	0.520977
H	2.911151	-2.327970	-0.001917
H	1.851553	-1.029627	-0.550387
H	3.487375	-1.168175	-1.208151
H	-2.342287	-4.466434	1.239492
H	-0.667123	-4.893104	1.511764
H	0.075547	-3.113871	-0.160800
H	-1.055049	-4.238979	-0.922977
H	-1.611573	-2.638286	-0.404585
H	-0.771688	-4.142386	4.851961
H	-2.488757	-3.821687	4.738945
H	-0.384289	-1.756380	5.710989
H	-1.509544	-2.630674	6.756620
H	-2.123777	-1.446916	5.589360
H	0.580679	-2.011059	1.810248
H	-1.770696	-0.167126	3.099650
H	-1.731516	-0.543562	1.377716
H	-4.074300	-1.243386	3.286481
H	-4.092408	0.067652	2.095271
H	-4.034648	-1.618965	1.558327
H	2.543260	-3.593756	2.204173
H	2.438022	-3.319245	3.950108
H	1.165451	-4.224892	3.116169
H	0.484674	-1.723643	3.618918
C	-0.389262	2.190956	1.056157
H	-1.488946	2.146289	1.102117
H	-0.140972	3.260862	0.932441
C	0.159424	1.361327	-0.100604
H	1.257625	1.440708	-0.123117
H	-0.065592	0.298454	0.080587
C	-0.419943	1.782101	-1.451989
H	-1.521601	1.705002	-1.420725
H	-0.192372	2.847713	-1.635443
C	0.114006	0.941617	-2.615356
H	1.216527	1.009386	-2.637933
H	-0.119587	-0.122278	-2.433392
C	-0.452138	1.363452	-3.973814
H	-1.553746	1.281811	-3.949561

H	-0.230520	2.432618	-4.144184
C	0.089425	0.544118	-5.148362
H	1.190713	0.630605	-5.175692
H	-0.126853	-0.525763	-4.978759
C	-0.483620	0.967870	-6.503571
H	-1.584078	0.869105	-6.482071
H	-0.279318	2.041938	-6.666047
C	0.072657	0.166784	-7.683553
H	1.172843	0.266919	-7.705308
H	-0.130766	-0.907824	-7.524612
C	-0.500457	0.595712	-9.036684
H	-1.599487	0.483641	-9.019257
H	-0.308421	1.673885	-9.187456
C	0.067715	-0.185840	-10.223752
H	1.166496	-0.072074	-10.243572
H	-0.122607	-1.264561	-10.076510
C	-0.509320	0.249128	-11.573340
H	-1.607444	0.128692	-11.557063
H	-0.325570	1.329516	-11.717424
C	0.065042	-0.521962	-12.765266
H	1.161722	-0.398085	-12.781012
H	-0.116704	-1.601100	-12.618802
C	-0.522933	-0.078506	-14.106524
H	-1.614292	-0.223163	-14.127759
H	-0.327523	0.989627	-14.290551
H	-0.093929	-0.646228	-14.945797
C	0.738059	3.190801	5.320823
H	0.182253	4.140143	5.297577
H	1.037616	2.988084	6.358891
H	1.652775	3.295476	4.722060
C	-1.427674	1.863631	5.564850
H	-2.024214	2.786951	5.553239
H	-2.021948	1.048560	5.129339
H	-1.207839	1.603193	6.610100

(4) **TS_{AP} (for D_4)**

94

C	3.596252	-0.075573	-2.474280
O	4.526495	-0.558497	-3.406151
C	5.909505	-0.296654	-3.094720
O	3.941851	-0.233137	-1.186433
Al	4.091740	0.865821	0.219384
C	2.509040	1.003964	1.416060
C	2.158700	-0.324489	2.114287
C	4.211658	2.773584	-0.954484
C	3.778328	2.647565	-2.273755
C	5.898420	0.660969	1.073125
C	6.225432	1.756795	2.099371
Al	8.165398	-0.751191	1.079652
C	8.290593	-1.037223	3.057513
C	7.105011	-1.709809	3.770210
C	9.336859	0.670356	0.285382
C	9.056811	1.070284	-1.172348
C	7.628241	-2.285597	-0.091558
C	6.218717	-2.885236	0.065414
H	9.196091	-1.660244	3.196108
H	6.601843	0.664952	0.215566
H	5.872445	-0.345003	1.537453
H	5.277370	2.953638	-0.780440
H	3.525142	3.241974	-0.239317
H	1.636665	1.370962	0.846997
H	9.312905	1.564257	0.933284
H	10.375120	0.294885	0.366456
H	8.380368	-3.071251	0.120419
H	7.802921	-2.017266	-1.149042

H	1.296731	-0.229386	2.795531
H	1.909434	-1.112137	1.385535
H	3.000410	-0.705077	2.715390
H	5.483230	1.766747	2.912186
H	7.214514	1.640077	2.569844
H	6.210102	2.756252	1.636582
H	9.769566	1.818517	-1.559164
H	9.102493	0.201628	-1.848524
H	8.049756	1.507459	-1.291208
H	6.074347	-3.789333	-0.550284
H	6.009333	-3.172755	1.107903
H	5.435371	-2.172197	-0.234411
H	6.079193	0.796388	-3.059861
H	6.149622	-0.704007	-2.101637
H	2.711440	1.780803	2.175855
H	8.535212	-0.081753	3.554331
H	7.292570	-1.875251	4.844716
H	6.187964	-1.101581	3.701217
H	6.868215	-2.691716	3.331130
H	3.550176	1.125153	-2.630972
H	4.489622	2.702780	-3.101508
H	2.744410	2.882845	-2.538612
C	2.215785	-0.605036	-2.864757
H	2.051785	-0.378752	-3.929744
H	2.260305	-1.702879	-2.769683
C	1.087994	-0.041827	-2.003332
H	1.295025	-0.268797	-0.945543
H	1.072508	1.060692	-2.082405
C	-0.293436	-0.585645	-2.374374
H	-0.506739	-0.365804	-3.435728
H	-0.286380	-1.686600	-2.286326
C	-1.412295	-0.012944	-1.499855
H	-1.187545	-0.224037	-0.438875
H	-1.419485	1.088271	-1.594212
C	-2.801798	-0.557162	-1.840591
H	-3.021927	-0.356105	-2.904550
H	-2.799060	-1.656794	-1.733660
C	-3.916933	0.032999	-0.972942
H	-3.692015	-0.161370	0.091206
H	-3.922165	1.132316	-1.085506
C	-5.308079	-0.514876	-1.302080
H	-5.531544	-0.326281	-2.367646
H	-5.304886	-1.613342	-1.182731
C	-6.421464	0.084004	-0.438103
H	-6.193696	-0.098565	0.627589
H	-6.428158	1.181986	-0.562570
C	-7.812720	-0.469301	-0.757581
H	-8.040598	-0.289294	-1.823693
H	-7.806444	-1.566876	-0.630153
C	-8.924781	0.132800	0.105967
H	-8.693086	-0.042277	1.172125
H	-8.934430	1.229927	-0.025683
C	-10.315496	-0.425924	-0.205499
H	-10.548528	-0.251852	-1.271650
H	-10.306275	-1.523072	-0.073101
C	-11.428024	0.175797	0.658437
H	-11.191793	0.003918	1.723141
H	-11.438133	1.271450	0.523175
C	-12.812135	-0.393848	0.341778
H	-13.087308	-0.206083	-0.707728
H	-12.838712	-1.483404	0.500085
H	-13.590943	0.054381	0.976350
C	6.760838	-0.941330	-4.168504
H	7.824632	-0.755259	-3.961078
H	6.597844	-2.027748	-4.186757
H	6.523117	-0.536029	-5.161978

(5) **TS_{KP} (for D_4)**

94

C	-0.038500	-0.092244	0.407878
O	-0.199436	0.408142	1.664787
C	0.485471	-0.278802	2.738333
O	1.062696	-0.730151	0.143717
Al	2.140378	-2.080528	-0.467289
C	3.358427	-2.587389	1.018306
C	4.442066	-1.527008	1.297990
C	2.813053	-1.781716	-2.318433
C	1.933573	-2.219977	-3.501760
C	0.489143	-3.738838	-0.590268
Al	-1.557462	-3.835774	-0.151537
C	-2.659469	-4.109405	-1.804010
C	-2.417591	-3.083242	-2.924192
C	1.218853	-4.988412	-1.086154
C	-1.892127	-4.905996	1.512776
C	-1.082721	-4.455584	2.740841
C	-1.554776	-1.716865	0.400332
C	-2.856630	-1.141680	0.896109
H	0.197449	-1.345360	2.722890
H	1.571283	-0.224118	2.566535
H	3.836586	-3.556372	0.790972
H	2.763037	-2.762701	1.932725
H	5.107878	-1.809369	2.130548
H	4.000196	-0.551031	1.557924
H	5.083975	-1.359111	0.418304
H	3.796697	-2.279987	-2.386122
H	3.039005	-0.702061	-2.402409
H	1.749322	-3.305441	-3.491171
H	0.948399	-1.728603	-3.490226
H	2.391872	-1.983467	-4.476288
H	-3.729525	-4.116635	-1.530553
H	-2.458027	-5.127442	-2.186590
H	-1.358333	-3.047908	-3.230514
H	-3.001195	-3.291895	-3.837599
H	-2.691258	-2.062711	-2.606588
H	-1.668024	-5.965829	1.290541
H	-2.970251	-4.888838	1.751908
H	0.004015	-4.462319	2.545723
H	-1.243581	-5.094601	3.626143
H	-1.345762	-3.428354	3.045337
H	0.397870	-2.931137	-1.342963
H	-0.815795	-2.030887	1.137612
H	-1.262147	-1.577116	-0.639635
H	-3.325431	-1.788275	1.655031
H	-2.725832	-0.148123	1.365481
H	-3.582848	-1.031717	0.077290
H	2.287735	-4.843953	-1.325010
H	1.165408	-5.784236	-0.328775
H	0.737494	-5.376626	-1.995421
H	0.784198	-3.413284	0.426265
C	-0.615474	0.874008	-0.607817
H	-1.678134	1.036294	-0.373726
H	-0.110585	1.841059	-0.427016
C	-0.418606	0.458696	-2.061720
H	0.658761	0.365579	-2.269293
H	-0.850439	-0.543264	-2.232347
C	-1.053750	1.433916	-3.055244
H	-2.131865	1.531817	-2.835951
H	-0.620214	2.440117	-2.912276
C	-0.870699	1.003204	-4.513074
H	0.206844	0.883337	-4.725088
H	-1.320978	0.004100	-4.655910
C	-1.479311	1.985603	-5.517001

H	-2.556565	2.105439	-5.303053
H	-1.027768	2.983318	-5.367754
C	-1.298671	1.565855	-6.978167
H	-0.222390	1.430935	-7.188054
H	-1.764954	0.576390	-7.134770
C	-1.886093	2.568726	-7.975201
H	-2.962342	2.704006	-7.765122
H	-1.419408	3.557373	-7.812618
C	-1.705150	2.162585	-9.440170
H	-0.629791	2.016620	-9.647692
H	-2.182792	1.180457	-9.609025
C	-2.276663	3.181515	-10.430217
H	-3.351943	3.328013	-10.222630
H	-1.798665	4.163015	-10.257711
C	-2.095537	2.784521	-11.897699
H	-1.020786	2.631673	-12.103680
H	-2.580019	1.806945	-12.073826
C	-2.657313	3.812619	-12.883571
H	-3.732201	3.966276	-12.678140
H	-2.172886	4.790294	-12.706324
C	-2.476627	3.421044	-14.353023
H	-1.402777	3.265862	-14.556265
H	-2.962836	2.445726	-14.530012
C	-3.038549	4.459036	-15.326683
H	-4.117954	4.608860	-15.167735
H	-2.546625	5.435424	-15.193519
H	-2.894849	4.153712	-16.373585
C	0.077484	0.379713	4.038683
H	-1.007621	0.303664	4.193085
H	0.583054	-0.116121	4.879581
H	0.357584	1.442038	4.044923

(6) **RC (for D_4)**

94

C	-0.939379	1.985878	2.934436
O	-1.794239	2.317526	3.893804
C	-1.324421	2.193563	5.283303
O	0.221264	1.638551	3.186586
Al	2.037689	0.871345	3.335344
C	2.633134	1.701193	5.053531
C	2.746563	3.236434	5.015815
C	3.005619	1.361438	1.651746
C	2.992983	0.319628	0.518688
C	1.447869	-1.067935	3.476123
Al	-0.562447	-2.621223	3.451066
C	-0.139894	-3.709767	1.823752
C	-0.149240	-2.936817	0.493402
C	2.606566	-2.045343	3.719396
C	-0.402449	-3.414487	5.283643
C	-0.525157	-2.410136	6.442593
C	-2.022076	-1.254871	3.234274
C	-3.422604	-1.897720	3.224465
H	-0.919417	1.179872	5.415187
H	-0.506416	2.913071	5.432252
H	3.609751	1.270536	5.340632
H	1.941543	1.395169	5.860477
H	3.065196	3.672416	5.978088
H	1.785297	3.712001	4.753982
H	3.472331	3.569520	4.257033
H	4.052284	1.589750	1.925966
H	2.605523	2.323621	1.281000
H	3.469731	-0.623197	0.830780
H	1.969980	0.059201	0.204388
H	3.524300	0.661164	-0.386026
H	-0.891804	-4.520600	1.782207

H	0.826246	-4.228344	1.950994
H	0.635476	-2.161041	0.464843
H	0.023806	-3.584606	-0.383087
H	-1.110534	-2.422709	0.327683
H	0.535092	-3.987769	5.380469
H	-1.205655	-4.171279	5.367940
H	0.309952	-1.687997	6.446313
H	-0.522348	-2.893728	7.434380
H	-1.455582	-1.821639	6.375690
H	0.932719	-1.247649	2.510596
H	-1.970819	-0.510073	4.048739
H	-1.872909	-0.691799	2.296151
H	-3.624579	-2.441467	4.161893
H	-4.237384	-1.163052	3.099522
H	-3.527261	-2.629579	2.406871
H	3.343997	-1.988598	2.903910
H	3.136020	-1.797710	4.652221
H	2.296531	-3.099983	3.796601
H	0.731347	-1.041113	4.322338
C	-1.515630	2.089941	1.550305
H	-2.535408	1.675767	1.586321
H	-1.637604	3.165710	1.330268
C	-0.665381	1.407828	0.480668
H	0.331155	1.874489	0.451797
H	-0.502920	0.355163	0.764800
C	-1.306293	1.465452	-0.906711
H	-2.297599	0.979460	-0.875762
H	-1.489704	2.519231	-1.185604
C	-0.446724	0.801017	-1.985483
H	0.553021	1.270063	-1.990961
H	-0.283338	-0.259056	-1.721729
C	-1.057531	0.895367	-3.386083
H	-2.040758	0.392823	-3.392656
H	-1.257851	1.956932	-3.621651
C	-0.174854	0.300040	-4.486766
H	0.817488	0.784535	-4.455891
H	0.002821	-0.770101	-4.279124
C	-0.768858	0.459404	-5.888951
H	-1.750949	-0.044641	-5.930272
H	-0.970425	1.530446	-6.074545
C	0.125850	-0.080340	-7.008355
H	1.115022	0.408214	-6.949161
H	0.309100	-1.157799	-6.846394
C	-0.457728	0.133688	-8.407675
H	-1.440458	-0.366550	-8.474179
H	-0.655485	1.210950	-8.555258
C	0.443802	-0.368830	-9.538428
H	1.431593	0.121216	-9.460091
H	0.629565	-1.449758	-9.406036
C	-0.131572	-0.119553	-10.934705
H	-1.116369	-0.613923	-11.018119
H	-0.324198	0.961775	-11.061436
C	0.773497	-0.603719	-12.071247
H	1.758641	-0.113770	-11.981241
H	0.959880	-1.685012	-11.950386
C	0.192469	-0.334213	-13.460823
H	-0.778653	-0.837388	-13.589973
H	0.029080	0.743490	-13.620242
H	0.861302	-0.691144	-14.257601
C	-2.509632	2.458025	6.180943
H	-3.306897	1.723497	6.002959
H	-2.193286	2.376119	7.230778
H	-2.915100	3.466265	6.021573

(7) **TS_{AP} (for D_5)**

58

C	3.677823	-0.085918	-2.459283
O	4.515470	-0.634062	-3.452235
C	5.899479	-0.612829	-3.125193
O	4.111656	-0.261328	-1.210685
Al	4.089651	0.830610	0.228751
C	2.358902	0.914966	1.200816
C	2.059400	-0.366889	2.003020
C	4.315557	2.718031	-0.938612
C	3.953217	2.589491	-2.285210
C	5.802996	0.619142	1.244679
C	5.995603	1.660696	2.357131
Al	8.253949	-0.548852	1.126782
C	8.460447	-0.890110	3.086477
C	7.350515	-1.678301	3.802606
C	9.206567	1.030747	0.337905
C	8.794779	1.459454	-1.080790
C	7.839418	-2.084111	-0.090212
C	6.497242	-2.823285	0.060853
H	9.412811	-1.450053	3.171185
H	6.572672	0.719990	0.450106
H	5.808319	-0.413263	1.641167
H	5.372421	2.893132	-0.713248
H	3.602725	3.223325	-0.275850
H	1.541489	1.111323	0.484187
H	9.123687	1.886820	1.031062
H	10.283270	0.774279	0.339167
H	8.665547	-2.803176	0.075131
H	7.975778	-1.752931	-1.135772
H	1.105989	-0.307553	2.553744
H	1.999408	-1.251057	1.348884
H	2.845525	-0.574591	2.746663
H	5.180830	1.601713	3.095025
H	6.940028	1.539335	2.910437
H	5.991407	2.685742	1.953947
H	9.391265	2.303795	-1.465619
H	8.899512	0.635819	-1.804934
H	7.738806	1.783786	-1.119001
H	6.418774	-3.698712	-0.606452
H	6.348713	-3.192638	1.087445
H	5.640345	-2.170379	-0.167706
H	6.226261	0.367221	-2.741148
H	6.152881	-1.377995	-2.377061
H	2.367074	1.786642	1.880009
H	8.651471	0.059742	3.616073
H	7.590046	-1.883874	4.859504
H	6.393283	-1.131913	3.796331
H	7.164597	-2.651285	3.321125
H	3.718227	1.129868	-2.627890
H	4.714604	2.641155	-3.069646
H	2.945913	2.867966	-2.609232
C	2.245310	-0.490390	-2.761587
H	1.991953	-0.268188	-3.805622
H	2.135929	-1.569938	-2.586491
C	6.687073	-0.893824	-4.393463
F	6.490558	0.060886	-5.341112
F	8.017823	-0.907324	-4.094915
F	6.375210	-2.090294	-4.946312
H	1.561651	0.048282	-2.092650

(8) **TS_{KP} (for D_5)**

58

C	-0.023235	-0.112364	0.370083
O	-0.223733	0.451051	1.603650
C	0.445230	-0.188503	2.687768

O	1.071926	-0.771168	0.194266
Al	2.131001	-2.138540	-0.480946
C	3.408254	-2.586589	0.971264
C	4.431661	-1.467219	1.248313
C	2.668597	-1.782264	-2.358779
C	1.546190	-1.752263	-3.409101
C	0.494874	-3.757821	-0.516749
Al	-1.546926	-3.899159	-0.002488
C	-2.678322	-4.306091	-1.603352
C	-2.409353	-3.401323	-2.817788
C	1.212313	-4.996937	-1.054665
C	-1.762535	-4.858851	1.745940
C	-0.976748	-4.241943	2.916346
C	-1.596400	-1.761951	0.409982
C	-2.892546	-1.166460	0.899219
H	0.323114	-1.283046	2.650755
H	1.519202	0.048860	2.694732
H	3.937920	-3.524715	0.730877
H	2.837775	-2.804993	1.893037
H	5.114384	-1.714198	2.077821
H	3.937625	-0.517331	1.511755
H	5.059314	-1.262429	0.366601
H	3.431488	-2.525645	-2.649538
H	3.203550	-0.814582	-2.355054
H	1.043042	-2.728607	-3.497808
H	0.766487	-1.013992	-3.160361
H	1.914433	-1.494597	-4.415564
H	-3.742533	-4.238401	-1.314969
H	-2.527767	-5.363773	-1.887442
H	-1.365456	-3.478303	-3.164821
H	-3.047978	-3.639892	-3.685328
H	-2.586486	-2.337302	-2.583517
H	-1.451022	-5.910249	1.604661
H	-2.833623	-4.912819	2.008786
H	0.102678	-4.158507	2.694209
H	-1.053493	-4.827385	3.848193
H	-1.337236	-3.227298	3.157935
H	0.317884	-2.953024	-1.252977
H	-0.833752	-2.002335	1.151394
H	-1.299808	-1.616185	-0.628406
H	-3.320971	-1.757182	1.723689
H	-2.773120	-0.137357	1.285783
H	-3.644836	-1.138525	0.097245
H	2.271070	-4.847545	-1.333126
H	1.190212	-5.803103	-0.307095
H	0.698222	-5.375126	-1.950311
H	0.785843	-3.440779	0.501678
C	-0.583100	0.775943	-0.704625
H	-1.616405	1.062657	-0.478184
H	0.031459	1.689647	-0.756705
C	-0.189232	0.306972	3.978199
F	-0.082298	1.649638	4.123746
F	-1.504672	-0.014514	4.050359
F	0.442830	-0.280781	5.030509
H	-0.538128	0.267863	-1.674317

(9) **RC (for D_5)**

58

C	0.431047	1.736752	2.717883
O	-0.355702	2.383243	3.581817
C	-0.359155	1.875412	4.935331
O	1.133704	0.793050	3.100319
Al	2.489536	-0.589917	2.569653
C	3.806933	-0.250244	4.030024
C	4.385432	1.176357	4.060049

C	2.992724	-0.202241	0.670197
C	1.994698	-0.673423	-0.403112
C	1.257793	-2.181831	2.817210
Al	-1.270360	-2.677881	2.887398
C	-1.368921	-4.213111	1.611134
C	-0.810856	-3.957626	0.201002
C	1.959244	-3.534815	3.004946
C	-1.509417	-3.032097	4.845890
C	-1.352911	-1.823940	5.783990
C	-1.886913	-0.891742	2.192455
C	-3.387865	-0.891174	1.841791
H	-0.623362	0.809497	4.950674
H	0.623552	2.020215	5.404143
H	4.632550	-0.978904	3.937884
H	3.329630	-0.482190	4.999989
H	5.108171	1.330254	4.878996
H	3.595349	1.935572	4.190545
H	4.908096	1.423148	3.121738
H	3.968443	-0.693182	0.495635
H	3.216060	0.874142	0.543087
H	1.842645	-1.763159	-0.359566
H	0.996044	-0.222804	-0.275695
H	2.320911	-0.436986	-1.429856
H	-2.441844	-4.476939	1.539465
H	-0.891847	-5.105673	2.051399
H	0.277172	-3.781127	0.221577
H	-0.979604	-4.803724	-0.486368
H	-1.266597	-3.068956	-0.265683
H	-0.822759	-3.840248	5.155036
H	-2.521310	-3.462455	4.968393
H	-0.334823	-1.397580	5.731059
H	-1.528152	-2.070510	6.844891
H	-2.060465	-1.018142	5.525343
H	0.642057	-2.161888	1.894534
H	-1.688641	-0.099937	2.937014
H	-1.298826	-0.623282	1.295348
H	-4.009817	-1.131348	2.719545
H	-3.743849	0.080724	1.459253
H	-3.621867	-1.643554	1.071811
H	2.582158	-3.779074	2.130540
H	2.626060	-3.511847	3.879710
H	1.264115	-4.378432	3.147251
H	0.657619	-1.904816	3.707960
C	0.331029	2.251825	1.323447
H	-0.443956	1.662256	0.807618
H	0.030702	3.305171	1.312479
C	-1.411122	2.665243	5.699527
F	-1.137739	3.992241	5.717870
F	-2.645910	2.501134	5.170526
F	-1.436514	2.221989	6.982780
H	1.280680	2.098815	0.799528

(E) Two different possible orientations of alkyl chain concerning the $MgCl_2$ surface.

(1) **A (alkyl chain interacts with $MgCl_2$)**

105

C	6.835129	-0.628454	0.384862
O	6.036905	-0.162826	-0.447598
Ti	4.559967	1.010401	-1.165382
Cl	4.249792	2.199330	1.010929
Mg	2.415401	1.045667	2.079288
Cl	2.443750	2.129656	4.229611
Mg	0.556715	0.990033	5.277630
Cl	0.514589	2.107826	7.393797
Mg	-1.402647	0.939802	8.331498

Cl	-1.481847	0.326210	10.484297
O	7.579958	-1.709421	0.106360
C	7.466192	-2.290208	-1.212356
C	5.744465	2.629885	-1.627129
C	7.061670	2.927111	-0.931412
Cl	2.703288	-0.617699	0.116093
Cl	2.455270	1.936833	-2.324842
Cl	4.629620	-0.453806	-3.169284
Mg	2.593097	0.244239	-4.307091
Cl	2.933630	-0.702113	-6.482746
Mg	0.796203	-0.118996	-7.512904
Cl	1.035130	-1.070615	-9.683605
Mg	-1.059682	-0.250828	-10.632980
Cl	-2.842775	-1.605219	-9.659367
Mg	-2.906216	-0.516921	-7.539734
Cl	-4.949495	-1.441242	-6.573385
Mg	-4.796397	-0.489325	-4.386900
Cl	-1.252684	0.725417	-12.630854
Cl	-3.459290	1.698964	7.277153
Mg	-3.171457	0.583904	5.191682
Cl	-5.340738	1.015948	4.152414
Mg	-4.941559	0.058263	2.004001
Cl	-7.126242	0.446164	0.869162
Mg	-6.413764	-0.418002	-1.208498
Cl	-4.578031	-1.580435	-0.044478
Cl	-6.815837	-1.440936	-3.297897
Cl	-4.883134	1.169319	-2.321595
Cl	0.434759	1.982585	0.870581
Cl	0.860106	-1.113288	-3.128438
Cl	-3.231661	1.506353	0.859278
Cl	-2.829152	-1.503911	-3.194451
Mg	-2.901088	0.017092	-1.164230
Cl	-0.976365	-1.072214	0.011672
Cl	-1.226545	1.513705	-2.289553
Mg	-1.097721	0.050616	-4.346150
Cl	0.651052	1.501678	-5.441060
Cl	-0.932449	-1.544155	-6.298784
Mg	-1.214505	0.402168	2.065332
Cl	0.781915	-0.618518	3.211556
Cl	-1.440135	1.995381	4.003098
Cl	-2.945841	-1.093804	3.151147
Cl	-3.102177	1.115161	-5.447982
Mg	0.783344	0.430135	-1.104835
Cl	-1.179872	-0.659530	6.258443
Cl	-1.231407	1.193238	-8.454800
H	7.546381	-3.374966	-1.082480
H	6.517747	-2.019951	-1.693612
H	5.900193	2.229706	-2.658961
H	5.097995	3.520797	-1.706934
H	7.724225	2.048906	-0.921101
H	7.614500	3.743405	-1.425701
H	6.888058	3.240179	0.109715
C	8.621898	-1.808691	-2.088601
F	9.822644	-2.190099	-1.593010
F	8.484693	-2.335694	-3.326860
F	8.632258	-0.454365	-2.195825
C	6.945202	-0.145615	1.789290
H	7.925934	-0.402139	2.211043
H	6.813537	0.945958	1.789016
C	5.802330	-0.805114	2.599128
H	5.959139	-1.895451	2.626854
H	4.859690	-0.647133	2.048406
C	5.652239	-0.264169	4.020362
H	6.566218	-0.471778	4.601732
H	5.535664	0.832555	3.994436
C	4.440436	-0.895181	4.708885
H	4.521429	-1.995342	4.665469

H	3.530815	-0.647921	4.130315
C	4.228546	-0.462289	6.159143
H	5.103547	-0.765996	6.759365
H	4.174786	0.637281	6.220092
C	2.973151	-1.086399	6.771308
H	2.944130	-2.164154	6.532443
H	2.068857	-0.678511	6.262467
C	2.830072	-0.899181	8.280847
H	3.778931	-1.201853	8.758287
H	2.692681	0.169707	8.516689
C	1.688186	-1.720856	8.883070
H	1.810822	-2.778531	8.586011
H	0.725752	-1.400195	8.443338
C	1.595115	-1.627856	10.406669
H	2.580623	-1.861986	10.848991
H	1.358472	-0.589106	10.692344
C	0.532048	-2.557408	10.996417
H	0.804777	-3.608708	10.790068
H	-0.425444	-2.371783	10.480975
C	0.322279	-2.361517	12.498734
H	1.269169	-2.554097	13.036109
H	0.068377	-1.303253	12.682321
C	-0.782732	-3.247911	13.079152
H	-0.539932	-4.308518	12.889116
H	-1.721152	-3.045332	12.534997
C	-1.002689	-3.030367	14.577497
H	-0.087240	-3.248732	15.149864
H	-1.281695	-1.985969	14.786213
H	-1.803645	-3.674975	14.969541

(2) **B (alkyl chain away from $MgCl_2$)**

105

C	-4.169105	-4.583529	-2.008548
O	-3.250267	-3.740412	-2.048799
Ti	-2.618806	-1.857866	-2.172948
Cl	-0.600429	-2.649719	-3.349415
Mg	1.217123	-2.499582	-1.691097
Cl	2.887937	-3.915035	-2.667537
Mg	4.830196	-3.269987	-1.306286
Cl	6.577467	-4.436944	-2.431190
Mg	8.363079	-3.986796	-0.825840
Cl	9.742480	-5.548135	-0.019747
O	-5.406630	-4.095515	-1.812670
C	-6.544614	-4.967893	-1.772460
C	-4.152928	-1.341873	-3.496520
C	-3.559398	-1.681932	-4.866453
Cl	-1.879279	0.597753	-2.277581
Cl	-0.567662	-1.844960	-0.066580
Cl	-4.025661	-1.156157	-0.297091
Mg	-3.660816	1.240112	-0.480152
Cl	-5.665466	2.187455	0.432895
Mg	-4.999326	4.541037	0.485502
Cl	-6.854591	5.544509	1.592284
Mg	-6.213936	7.870698	1.232014
Cl	-4.431470	8.358717	2.825631
Mg	-2.687692	7.207858	1.683950
Cl	-0.749197	7.834004	3.041431
Mg	0.939348	6.578166	1.914189
Cl	3.000967	7.143922	3.190937
Mg	4.415888	5.728268	1.928894
Cl	4.010386	3.392740	2.586370
Cl	-7.631922	9.391303	0.419286
Cl	2.708371	5.680512	0.151199
Cl	6.513942	5.074496	1.045750
Mg	5.944547	2.659913	0.909297

Cl	7.905978	1.703635	-0.066436
Mg	7.210719	-0.645769	-0.106120
Cl	9.066610	-1.677222	-1.181720
Cl	-1.801784	1.499627	1.163938
Cl	1.791897	-0.094946	-2.050628
Cl	4.092570	2.467092	-0.770932
Cl	0.489475	4.156319	2.365394
Mg	2.215015	3.230532	0.755605
Cl	1.738952	0.833640	1.306018
Cl	0.429735	3.060742	-0.987520
Mg	3.579370	-0.011939	-0.204584
Cl	2.994611	-2.393192	0.287035
Cl	5.341511	-0.823862	-1.817182
Cl	5.376576	0.247682	1.561340
Mg	-1.356739	3.961274	0.549541
Cl	-3.166135	3.697287	-1.174202
Cl	-3.110116	4.756288	2.184379
Cl	-0.812489	6.377472	0.033524
Mg	-0.088435	0.581811	-0.470568
Cl	-4.321666	6.917410	-0.290711
Cl	6.485312	-2.992401	0.680813
H	-5.051470	-1.932497	-3.260722
H	-4.421286	-0.276185	-3.428334
H	-4.294994	-1.495211	-5.668224
H	-2.673886	-1.072295	-5.102166
H	-3.264816	-2.740407	-4.952039
H	-6.847608	-5.260749	-2.788361
H	-6.363649	-5.857520	-1.153846
C	-7.685837	-4.176148	-1.134965
F	-7.974941	-3.059515	-1.836564
F	-8.790432	-4.967208	-1.115479
F	-7.394228	-3.820329	0.133926
C	-3.898628	-6.045040	-2.167617
H	-2.999429	-6.129466	-2.793092
H	-4.724299	-6.527435	-2.714376
C	-3.658431	-6.792175	-0.834298
H	-4.514114	-6.654319	-0.152363
H	-2.784770	-6.351349	-0.329050
C	-3.436014	-8.282550	-1.100183
H	-4.317965	-8.686687	-1.629953
H	-2.585786	-8.400446	-1.794593
C	-3.181434	-9.125098	0.150837
H	-4.016980	-8.999310	0.861731
H	-2.276493	-8.761833	0.668529
C	-3.021232	-10.607707	-0.197241
H	-3.931741	-10.951126	-0.721413
H	-2.195932	-10.720206	-0.923063
C	-2.761418	-11.527205	0.997147
H	-3.570943	-11.409193	1.739337
H	-1.830175	-11.221537	1.506307
C	-2.661684	-12.995906	0.577140
H	-3.600549	-13.288324	0.072555
H	-1.866769	-13.100568	-0.183408
C	-2.386950	-13.972251	1.722102
H	-3.167395	-13.862989	2.496467
H	-1.431958	-13.709145	2.210984
C	-2.337323	-15.427344	1.249029
H	-3.299514	-15.682412	0.768952
H	-1.571517	-15.524411	0.458099
C	-2.045005	-16.441921	2.356332
H	-2.799586	-16.339622	3.157072
H	-1.071868	-16.205513	2.822877
C	-2.031432	-17.887449	1.852071
H	-3.009679	-18.120252	1.393402
H	-1.288028	-17.981913	1.039579
C	-1.725165	-18.924890	2.935376
H	-2.460240	-18.824596	3.752921

H	-0.741085	-18.702265	3.382990
C	-1.737196	-20.360455	2.405915
H	-2.722039	-20.619802	1.986815
H	-0.993079	-20.493699	1.605074
H	-1.509040	-21.088827	3.197533

(F) Binding of D_6, D_7, and D_8 with titanium on the $MgCl_2$ surface.

(1) **D_6**

17

C	1.760152	1.584806	0.252226
O	0.791012	1.352993	1.198783
C	0.928610	0.110223	1.897465
O	2.661098	0.802569	0.031706
H	0.882416	-0.744335	1.206734
H	1.877136	0.065585	2.452131
C	-0.225294	0.014267	2.882183
F	-1.432161	0.055126	2.265525
F	-0.139400	-1.170507	3.549930
F	-0.198088	1.010279	3.802731
C	1.523897	2.911369	-0.432430
H	1.518050	3.690408	0.347917
H	0.498196	2.898143	-0.835690
C	2.554015	3.208469	-1.517012
H	3.569111	3.240340	-1.099374
H	2.543486	2.433426	-2.295262
H	2.342400	4.177141	-1.989978

(2) **D_7**

23

C	1.762670	1.583573	0.253492
O	0.795580	1.346453	1.201748
C	0.932584	0.102836	1.898268
O	2.665832	0.804909	0.029480
H	0.884328	-0.751522	1.207434
H	1.880193	0.056048	2.453950
C	-0.221298	0.007796	2.882929
F	-1.427988	0.051024	2.265807
F	-0.137936	-1.177508	3.549918
F	-0.191954	1.002736	3.804717
C	1.515402	2.910137	-0.424436
H	1.507154	3.687769	0.358636
H	0.487929	2.894225	-0.825335
C	2.531312	3.236352	-1.516453
H	3.544758	3.233779	-1.084410
H	2.525509	2.433469	-2.271712
C	2.253976	4.584722	-2.187840
H	1.236929	4.576839	-2.616437
H	2.254693	5.380881	-1.422839
C	3.267341	4.925583	-3.281690
H	3.264015	4.165889	-4.078434
H	4.289120	4.973351	-2.875741
H	3.046697	5.897210	-3.746949

(3) **D_8**

29

C	1.772658	1.571458	0.248436
O	0.806412	1.334792	1.197326
C	0.938913	0.092118	1.894767
O	2.672328	0.790504	0.018461
H	0.882973	-0.762856	1.205200

H 1.888172 0.041780 2.447981
C -0.214217 0.009580 2.881859
F -1.421401 0.048813 2.265354
F -0.133133 -1.168294 3.562264
F -0.182425 1.015586 3.791276
C 1.525347 2.903044 -0.417694
H 1.514417 3.673088 0.372718
H 0.497746 2.888597 -0.818478
C 2.536423 3.244314 -1.508733
H 3.551256 3.248062 -1.079929
H 2.533966 2.447596 -2.270317
C 2.237203 4.594967 -2.163942
H 1.205867 4.589236 -2.560276
H 2.261779 5.389428 -1.395930
C 3.204661 4.953136 -3.293627
H 3.170512 4.163696 -4.065958
H 4.238601 4.952585 -2.905530
C 2.907244 6.308074 -3.942528
H 1.863680 6.314463 -4.302020
H 2.967464 7.098090 -3.173699
C 3.850140 6.641835 -5.099474
H 3.775301 5.889783 -5.900685
H 4.898365 6.663873 -4.763305
H 3.619312 7.622777 -5.540317

(4) **$Ti(Et)Cl_2$ on $MgCl_2$**

55

Ti -2.362791 -1.951127 -2.029822
Cl -0.537428 -2.736085 -3.470614
Mg 1.330417 -2.559907 -1.926651
Cl 3.059984 -3.828708 -2.979437
Mg 4.922133 -3.292669 -1.489657
Cl 6.729837 -4.407392 -2.559075
Mg 8.423755 -4.016105 -0.843081
Cl 9.766369 -5.591407 -0.009827
C -3.670688 -3.361678 -2.786569
C -4.035441 -2.290990 -3.782878
Cl -1.930493 0.524188 -2.447327
Cl -0.600718 -1.915722 -0.224294
Cl -4.150096 -1.126704 -0.510741
Mg -3.750841 1.246797 -0.611544
Cl -5.737184 2.195657 0.324447
Mg -5.066388 4.538773 0.387962
Cl -6.927687 5.536984 1.481968
Mg -6.270805 7.861067 1.154144
Cl -4.495229 8.292071 2.769453
Mg -2.743900 7.154655 1.630808
Cl -0.817996 7.743250 3.014142
Mg 0.877973 6.497571 1.891811
Cl 2.909682 7.041000 3.217410
Mg 4.347476 5.642181 1.968949
Cl 3.917054 3.289568 2.575391
Cl -7.653659 9.405347 0.330939
Cl 2.674929 5.616856 0.150900
Cl 6.455679 4.996617 1.116749
Mg 5.883263 2.587222 0.941455
Cl 7.872244 1.657010 0.013670
Mg 7.197514 -0.694934 -0.085303
Cl 9.120361 -1.685907 -1.068479
Cl -1.849253 1.430706 0.995613
Cl 1.776065 -0.114787 -2.168371
Cl 4.067170 2.413939 -0.791513
Cl 0.411574 4.060956 2.289849
Mg 2.167314 3.164447 0.703815
Cl 1.668502 0.743723 1.185356

Cl 0.403104 3.040144 -1.089602
Mg 3.560104 -0.076716 -0.288063
Cl 2.954095 -2.492398 0.084500
Cl 5.377826 -0.817429 -1.869180
Cl 5.295249 0.151104 1.531801
Mg -1.409728 3.922260 0.449852
Cl -3.206938 3.664479 -1.292016
Cl -3.171147 4.688267 2.083525
Cl -0.847343 6.333074 -0.019433
Mg -0.109608 0.589132 -0.637328
Cl -4.353012 6.891822 -0.365139
Cl 6.433459 -3.070547 0.585833
H -3.161544 -4.237606 -3.204501
H -4.463216 -3.633430 -2.080332
H -3.812828 -2.559798 -4.823031
H -5.067510 -1.932190 -3.684415
H -3.423237 -1.331122 -3.654170

(5) **D_6 binds to $Ti(Et)Cl_2$ on $MgCl_2$**

72

C 6.805423 -0.381857 0.434358
O 6.019128 0.173820 -0.357020
Ti 4.597611 1.240079 -1.236385
Cl 4.164354 2.410377 0.924616
Mg 2.485066 1.019464 1.989953
Cl 2.678574 1.701419 4.285113
Mg 0.659153 0.632802 5.187856
Cl 0.656943 1.419719 7.439443
Mg -1.224751 0.071756 8.233987
Cl -1.180716 -1.147869 10.102226
O 6.961566 -1.714530 0.460240
C 6.283313 -2.511158 -0.535589
C 5.665392 2.909807 -1.794429
C 6.971594 3.284075 -1.111239
Cl 2.807266 -0.560160 0.012687
Cl 2.436429 2.031716 -2.375700
Cl 4.705792 -0.260015 -3.194320
Mg 2.649858 0.339063 -4.359232
Cl 3.017495 -0.614453 -6.526954
Mg 0.865871 -0.109281 -7.564709
Cl 1.124523 -1.121057 -9.707297
Mg -0.977905 -0.359458 -10.684057
Cl -2.750338 -1.699369 -9.676084
Mg -2.833511 -0.540102 -7.596074
Cl -4.893265 -1.426398 -6.637342
Mg -4.749974 -0.441280 -4.464233
Cl -1.182535 0.571833 -12.701331
Cl -3.266774 1.100298 7.359392
Mg -3.068068 0.295025 5.131423
Cl -5.201014 0.971875 4.123243
Mg -4.896803 0.061908 1.934944
Cl -7.069790 0.506292 0.808830
Mg -6.379471 -0.345000 -1.287503
Cl -4.560094 -1.549749 -0.150409
Cl -6.794359 -1.347540 -3.385650
Cl -4.822343 1.223156 -2.387593
Cl 0.462012 1.953087 0.860106
Cl 0.936820 -1.061537 -3.196717
Cl -3.154936 1.490353 0.821660
Cl -2.787403 -1.467285 -3.274388
Mg -2.860688 0.037260 -1.238819
Cl -0.925448 -1.086516 -0.111005
Cl -1.183920 1.544550 -2.346749
Mg -1.044220 0.087817 -4.409041
Cl 0.686827 1.547536 -5.512484

Cl	-0.853862	-1.531199	-6.333421
Mg	-1.162726	0.305241	1.989418
Cl	0.859993	-0.774665	3.007346
Cl	-1.316523	1.779803	4.037511
Cl	-2.929367	-1.211449	2.989290
Cl	-3.044273	1.140158	-5.531376
Mg	0.825542	0.459902	-1.167432
Cl	-1.069205	-1.137085	5.945945
Cl	-1.169833	1.153535	-8.545941
H	6.015759	-3.455502	-0.049157
H	5.389530	-2.007206	-0.922480
H	5.827735	2.556149	-2.838412
H	4.952428	3.751578	-1.832847
H	7.689555	2.450326	-1.129612
H	7.459915	4.141806	-1.602669
H	6.796448	3.566239	-0.062011
C	7.243521	-2.798612	-1.692031
F	8.302201	-3.541897	-1.288968
F	6.588437	-3.479748	-2.657912
F	7.730839	-1.649693	-2.225468
C	7.593399	0.342577	1.476267
H	8.579010	-0.135083	1.569870
H	7.726946	1.375418	1.129212
C	6.862546	0.328051	2.836560
H	6.707568	-0.698482	3.194306
H	5.892401	0.837109	2.763027
H	7.465778	0.863547	3.580768

(6) **D_7 binds to Ti(Et)Cl_2 on $MgCl_2$**

78

C	6.694229	-0.595379	0.440954
O	5.973529	-0.077474	-0.430886
Ti	4.565574	1.104826	-1.243905
Cl	4.243768	2.339646	0.905079
Mg	2.462503	1.139918	1.987947
Cl	2.576303	2.134410	4.181067
Mg	0.635915	1.059847	5.190885
Cl	0.596070	2.058429	7.353270
Mg	-1.170713	0.659159	8.296916
Cl	-0.943593	-0.338480	10.281110
O	7.326155	-1.758936	0.220251
C	7.192341	-2.366538	-1.084020
C	5.766061	2.706135	-1.721143
C	7.083379	2.989535	-1.019839
Cl	2.737925	-0.528651	0.041403
Cl	2.451712	2.010505	-2.410758
Cl	4.640901	-0.377966	-3.231136
Mg	2.592710	0.299586	-4.369370
Cl	2.925883	-0.648716	-6.542158
Mg	0.763732	-0.117628	-7.551494
Cl	0.995690	-1.100126	-9.708732
Mg	-1.119540	-0.324044	-10.648209
Cl	-2.875181	-1.690978	-9.642143
Mg	-2.937418	-0.570889	-7.539522
Cl	-4.967711	-1.497686	-6.546262
Mg	-4.806411	-0.516913	-4.373614
Cl	-1.339992	0.633697	-12.651537
Cl	-3.284470	1.452936	7.364650
Mg	-3.048709	0.505274	5.190624
Cl	-5.229172	0.995245	4.188561
Mg	-4.880850	0.066616	2.016790
Cl	-7.077128	0.454929	0.910999
Mg	-6.393673	-0.416890	-1.176528
Cl	-4.539595	-1.570393	-0.034861
Cl	-6.810402	-1.465390	-3.251478

Cl -4.883613 1.166312 -2.323262
Cl 0.447337 2.048674 0.816007
Cl 0.879172 -1.066937 -3.169659
Cl -3.198643 1.524400 0.845259
Cl -2.814186 -1.500542 -3.195068
Mg -2.883600 0.032875 -1.180348
Cl -0.929007 -1.032498 -0.031817
Cl -1.235236 1.543913 -2.331785
Mg -1.106956 0.062981 -4.377061
Cl 0.615405 1.522711 -5.497706
Cl -0.935044 -1.555090 -6.305390
Mg -1.158652 0.430980 2.018853
Cl 0.887903 -0.552507 3.121510
Cl -1.393404 2.009359 3.979458
Cl -2.857246 -1.098077 3.107145
Cl -3.135848 1.090058 -5.468384
Mg 0.798667 0.497269 -1.167368
Cl -0.973414 -0.740218 6.101899
Cl -1.293305 1.148544 -8.489547
H 7.199445 -3.449841 -0.922550
H 6.269774 -2.049931 -1.586483
H 5.921735 2.290980 -2.747098
H 5.132881 3.605327 -1.814745
H 7.725324 2.096671 -0.984608
H 7.658231 3.783225 -1.525841
H 6.907172 3.327544 0.012998
C 8.388164 -1.987720 -1.958495
F 9.554327 -2.436747 -1.438013
F 8.229150 -2.536544 -3.184297
F 8.493976 -0.640730 -2.100431
C 6.845945 -0.069748 1.826885
H 7.847688 -0.305088 2.212322
H 6.709928 1.020208 1.794283
C 5.764743 -0.705165 2.736705
H 5.927016 -1.793558 2.788712
H 4.777967 -0.569076 2.258365
C 5.745491 -0.106309 4.144306
H 6.749348 -0.194096 4.592408
H 5.524760 0.971762 4.079888
C 4.716402 -0.793659 5.043530
H 4.949752 -1.859907 5.180987
H 3.705832 -0.728874 4.609912
H 4.679861 -0.322094 6.035189

(7) **D_8 binds to Ti(Et)Cl_2 on $MgCl_2$**

84

C 6.775108 -0.632918 0.415577
O 6.016417 -0.129408 -0.431623
Ti 4.583486 1.059152 -1.203972
Cl 4.282492 2.287215 0.959479
Mg 2.451019 1.145765 2.024397
Cl 2.462707 2.221429 4.182772
Mg 0.633025 1.006086 5.234065
Cl 0.463525 2.018200 7.387152
Mg -1.143543 0.425731 8.291393
Cl -0.642154 -0.741124 10.130393
O 7.452603 -1.763094 0.159315
C 7.315333 -2.354022 -1.152769
C 5.793764 2.656929 -1.672820
C 7.119195 2.928915 -0.982370
Cl 2.738259 -0.541054 0.076250
Cl 2.474987 1.984246 -2.370280
Cl 4.646952 -0.415783 -3.198573
Mg 2.598724 0.272165 -4.329632
Cl 2.930601 -0.682360 -6.501484

Mg	0.773417	-0.139506	-7.513782
Cl	1.002089	-1.123233	-9.671866
Mg	-1.109444	-0.336919	-10.609725
Cl	-2.870400	-1.696918	-9.603193
Mg	-2.932846	-0.568275	-7.505064
Cl	-4.972499	-1.476212	-6.516171
Mg	-4.810726	-0.485361	-4.347091
Cl	-1.332611	0.627350	-12.609807
Cl	-3.312319	1.207793	7.479621
Mg	-3.061349	0.456840	5.224609
Cl	-5.222321	1.040383	4.219199
Mg	-4.890249	0.111020	2.042644
Cl	-7.082727	0.508957	0.932641
Mg	-6.402676	-0.366242	-1.156169
Cl	-4.561584	-1.535012	-0.016459
Cl	-6.832646	-1.406353	-3.233726
Cl	-4.875407	1.201308	-2.300953
Cl	0.445943	2.052449	0.835887
Cl	0.874743	-1.080755	-3.131692
Cl	-3.195164	1.550636	0.869446
Cl	-2.828334	-1.486301	-3.165686
Mg	-2.887449	0.051147	-1.152730
Cl	-0.942814	-1.025817	-0.000372
Cl	-1.225182	1.546189	-2.306082
Mg	-1.103235	0.059322	-4.343551
Cl	0.632859	1.505119	-5.464247
Cl	-0.937835	-1.562913	-6.268681
Mg	-1.171087	0.444296	2.051215
Cl	0.879248	-0.554704	3.125677
Cl	-1.415337	1.979232	4.037516
Cl	-2.893141	-1.096837	3.111111
Cl	-3.123228	1.101656	-5.443403
Mg	0.800323	0.486742	-1.130926
Cl	-0.975969	-0.841298	6.051590
Cl	-1.275060	1.138646	-8.455145
H	7.349384	-3.439501	-1.009217
H	6.379386	-2.050726	-1.638628
H	5.938257	2.249603	-2.703607
H	5.164890	3.560226	-1.753775
H	7.760621	2.035266	-0.966957
H	7.690082	3.728249	-1.483855
H	6.955600	3.253574	0.056831
C	8.491217	-1.934261	-2.034751
F	9.673811	-2.361935	-1.533526
F	8.331894	-2.470145	-3.266355
F	8.562092	-0.583246	-2.159088
C	6.912634	-0.135011	1.813652
H	7.899344	-0.397638	2.217996
H	6.795315	0.957932	1.799395
C	5.783651	-0.768820	2.664802
H	5.934538	-1.859001	2.713393
H	4.828084	-0.617781	2.133523
C	5.671857	-0.189928	4.076301
H	6.609083	-0.362018	4.631460
H	5.536986	0.903751	4.016862
C	4.491300	-0.809777	4.829848
H	4.633761	-1.900846	4.919041
H	3.577779	-0.683506	4.218377
C	4.224998	-0.205243	6.210388
H	5.090856	-0.379856	6.869877
H	4.125186	0.887307	6.111027
C	2.967955	-0.785067	6.859145
H	3.077570	-1.854367	7.091526
H	2.104390	-0.740002	6.164231
H	2.686259	-0.260355	7.781506

(G) rate-determining transition states for D_1 and D_2 for the decomposition reactions with titanium, and corresponding reactant and product structures.

(1) **RC (for D_1)**

105

C 6.835129 -0.628454 0.384862
O 6.036905 -0.162826 -0.447598
Ti 4.559967 1.010401 -1.165382
Cl 4.249792 2.199330 1.010929
Mg 2.415401 1.045667 2.079288
Cl 2.443750 2.129656 4.229611
Mg 0.556715 0.990033 5.277630
Cl 0.514589 2.107826 7.393797
Mg -1.402647 0.939802 8.331498
Cl -1.481847 0.326210 10.484297
O 7.579958 -1.709421 0.106360
C 7.466192 -2.290208 -1.212356
C 5.744465 2.629885 -1.627129
C 7.061670 2.927111 -0.931412
Cl 2.703288 -0.617699 0.116093
Cl 2.455270 1.936833 -2.324842
Cl 4.629620 -0.453806 -3.169284
Mg 2.593097 0.244239 -4.307091
Cl 2.933630 -0.702113 -6.482746
Mg 0.796203 -0.118996 -7.512904
Cl 1.035130 -1.070615 -9.683605
Mg -1.059682 -0.250828 -10.632980
Cl -2.842775 -1.605219 -9.659367
Mg -2.906216 -0.516921 -7.539734
Cl -4.949495 -1.441242 -6.573385
Mg -4.796397 -0.489325 -4.386900
Cl -1.252684 0.725417 -12.630854
Cl -3.459290 1.698964 7.277153
Mg -3.171457 0.583904 5.191682
Cl -5.340738 1.015948 4.152414
Mg -4.941559 0.058263 2.004001
Cl -7.126242 0.446164 0.869162
Mg -6.413764 -0.418002 -1.208498
Cl -4.578031 -1.580435 -0.044478
Cl -6.815837 -1.440936 -3.297897
Cl -4.883134 1.169319 -2.321595
Cl 0.434759 1.982585 0.870581
Cl 0.860106 -1.113288 -3.128438
Cl -3.231661 1.506353 0.859278
Cl -2.829152 -1.503911 -3.194451
Mg -2.901088 0.017092 -1.164230
Cl -0.976365 -1.072214 0.011672
Cl -1.226545 1.513705 -2.289553
Mg -1.097721 0.050616 -4.346150
Cl 0.651052 1.501678 -5.441060
Cl -0.932449 -1.544155 -6.298784
Mg -1.214505 0.402168 2.065332
Cl 0.781915 -0.618518 3.211556
Cl -1.440135 1.995381 4.003098
Cl -2.945841 -1.093804 3.151147
Cl -3.102177 1.115161 -5.447982
Mg 0.783344 0.430135 -1.104835
Cl -1.179872 -0.659530 6.258443
Cl -1.231407 1.193238 -8.454800
H 7.546381 -3.374966 -1.082480
H 6.517747 -2.019951 -1.693612
H 5.900193 2.229706 -2.658961
H 5.097995 3.520797 -1.706934
H 7.724225 2.048906 -0.921101
H 7.614500 3.743405 -1.425701

H	6.888058	3.240179	0.109715
C	8.621898	-1.808691	-2.088601
F	9.822644	-2.190099	-1.593010
F	8.484693	-2.335694	-3.326860
F	8.632258	-0.454365	-2.195825
C	6.945202	-0.145615	1.789290
H	7.925934	-0.402139	2.211043
H	6.813537	0.945958	1.789016
C	5.802330	-0.805114	2.599128
H	5.959139	-1.895451	2.626854
H	4.859690	-0.647133	2.048406
C	5.652239	-0.264169	4.020362
H	6.566218	-0.471778	4.601732
H	5.535664	0.832555	3.994436
C	4.440436	-0.895181	4.708885
H	4.521429	-1.995342	4.665469
H	3.530815	-0.647921	4.130315
C	4.228546	-0.462289	6.159143
H	5.103547	-0.765996	6.759365
H	4.174786	0.637281	6.220092
C	2.973151	-1.086399	6.771308
H	2.944130	-2.164154	6.532443
H	2.068857	-0.678511	6.262467
C	2.830072	-0.899181	8.280847
H	3.778931	-1.201853	8.758287
H	2.692681	0.169707	8.516689
C	1.688186	-1.720856	8.883070
H	1.810822	-2.778531	8.586011
H	0.725752	-1.400195	8.443338
C	1.595115	-1.627856	10.406669
H	2.580623	-1.861986	10.848991
H	1.358472	-0.589106	10.692344
C	0.532048	-2.557408	10.996417
H	0.804777	-3.608708	10.790068
H	-0.425444	-2.371783	10.480975
C	0.322279	-2.361517	12.498734
H	1.269169	-2.554097	13.036109
H	0.068377	-1.303253	12.682321
C	-0.782732	-3.247911	13.079152
H	-0.539932	-4.308518	12.889116
H	-1.721152	-3.045332	12.534997
C	-1.002689	-3.030367	14.577497
H	-0.087240	-3.248732	15.149864
H	-1.281695	-1.985969	14.786213
H	-1.803645	-3.674975	14.969541

(2) **TS_{1AP} (for D_1)**

105

C	6.898172	0.031559	0.939686
O	5.769576	-0.011339	0.239131
Ti	4.456208	0.977349	-0.621017
Cl	3.934334	2.426706	1.330259
Mg	2.226228	1.126391	2.453923
Cl	2.111025	2.152539	4.624100
Mg	0.238501	0.879649	5.565353
Cl	0.075361	1.843630	7.751121
Mg	-1.865192	0.585398	8.513161
Cl	-2.066141	-0.257369	10.578116
O	7.725475	-1.069040	0.823834
C	7.710770	-1.791945	-0.411695
C	6.211020	2.417290	-0.980580
C	7.530283	2.087106	-0.556523
Cl	2.638745	-0.548329	0.470207
Cl	2.489579	2.036246	-1.938959
Cl	4.742115	-0.270668	-2.758905

Mg	2.729442	0.332030	-3.963540
Cl	3.181265	-0.601172	-6.128229
Mg	1.082657	-0.080404	-7.248428
Cl	1.426138	-1.072562	-9.389675
Mg	-0.626028	-0.286659	-10.449987
Cl	-2.432449	-1.640643	-9.527825
Mg	-2.596067	-0.526123	-7.428641
Cl	-4.669078	-1.460241	-6.553989
Mg	-4.636693	-0.481498	-4.373369
Cl	-0.763298	0.671493	-12.461341
Cl	-3.849054	1.458203	7.404225
Mg	-3.481426	0.426534	5.290526
Cl	-5.614252	0.866280	4.178699
Mg	-5.097928	-0.002284	2.015156
Cl	-7.209566	0.432455	0.770850
Mg	-6.406841	-0.416802	-1.277486
Cl	-4.625844	-1.599996	-0.049285
Cl	-6.719299	-1.409898	-3.395387
Cl	-4.823726	1.173984	-2.301090
Cl	0.266296	1.998632	1.154473
Cl	0.971247	-1.036987	-2.843951
Cl	-3.351650	1.475686	0.976197
Cl	-2.715444	-1.483822	-3.093373
Mg	-2.906520	0.019752	-1.054154
Cl	-1.016622	-1.061510	0.183321
Cl	-1.203647	1.553474	-2.097279
Mg	-0.953878	0.092675	-4.153679
Cl	0.824105	1.563213	-5.166722
Cl	-0.669285	-1.512831	-6.084559
Mg	-1.380699	0.368928	2.258831
Cl	0.603055	-0.628516	3.453251
Cl	-1.718465	1.902241	4.232842
Cl	-3.140545	-1.173268	3.206273
Cl	-2.910978	1.131012	-5.361026
Mg	0.747426	0.499486	-0.826393
Cl	-1.527001	-0.856331	6.364338
Cl	-0.903230	1.193274	-8.290786
H	7.441982	-2.836284	-0.199765
H	6.994385	-1.376010	-1.133042
H	5.996391	2.221950	-2.045152
H	5.783584	3.342043	-0.582516
H	8.194907	1.575071	-1.260109
H	8.050894	2.782598	0.111907
H	7.474802	1.062073	0.315948
C	9.107139	-1.775128	-1.023222
F	10.038527	-2.275787	-0.180848
F	9.111573	-2.521793	-2.154673
F	9.494192	-0.509748	-1.355385
C	6.777432	0.463285	2.389655
H	7.767308	0.392315	2.862527
H	6.456331	1.515054	2.407928
C	5.738678	-0.409363	3.110171
H	6.064114	-1.461645	3.089551
H	4.805539	-0.375465	2.520433
C	5.433455	0.015350	4.546168
H	6.317663	-0.143209	5.186074
H	5.209916	1.095795	4.582528
C	4.241003	-0.768391	5.099019
H	4.422935	-1.851173	4.984142
H	3.355241	-0.556195	4.469711
C	3.886797	-0.468761	6.555010
H	4.730118	-0.767545	7.201349
H	3.756898	0.617033	6.696598
C	2.630762	-1.214321	7.009920
H	2.676988	-2.261328	6.661807
H	1.740306	-0.801842	6.478778
C	2.373000	-1.193684	8.515523

H	3.295588	-1.521081	9.027047
H	2.182973	-0.160358	8.852152
C	1.219548	-2.106043	8.938429
H	1.388185	-3.115269	8.519963
H	0.277495	-1.751797	8.482081
C	1.032091	-2.210979	10.452459
H	1.992037	-2.495834	10.920414
H	0.763762	-1.220053	10.856015
C	-0.051018	-3.216850	10.848095
H	0.233682	-4.223777	10.491402
H	-0.987935	-2.950123	10.329921
C	-0.318588	-3.260629	12.353407
H	0.611841	-3.527266	12.888286
H	-0.594335	-2.247325	12.693362
C	-1.428226	-4.239960	12.745084
H	-1.167606	-5.250514	12.383582
H	-2.355110	-3.955084	12.218116
C	-1.687618	-4.284607	14.252259
H	-0.785054	-4.596855	14.801405
H	-1.979309	-3.293043	14.631616
H	-2.493121	-4.989849	14.506020

(3) **TS_{1KP} (for D_1)**

105

C	6.898172	0.031559	0.939686
O	5.769576	-0.011339	0.239131
Ti	4.456208	0.977349	-0.621017
Cl	3.934334	2.426706	1.330259
Mg	2.226228	1.126391	2.453923
Cl	2.111025	2.152539	4.624100
Mg	0.238501	0.879649	5.565353
Cl	0.075361	1.843630	7.751121
Mg	-1.865192	0.585398	8.513161
Cl	-2.066141	-0.257369	10.578116
O	7.725475	-1.069040	0.823834
C	7.710770	-1.791945	-0.411695
C	6.211020	2.417290	-0.980580
C	7.530283	2.087106	-0.556523
Cl	2.638745	-0.548329	0.470207
Cl	2.489579	2.036246	-1.938959
Cl	4.742115	-0.270668	-2.758905
Mg	2.729442	0.332030	-3.963540
Cl	3.181265	-0.601172	-6.128229
Mg	1.082657	-0.080404	-7.248428
Cl	1.426138	-1.072562	-9.389675
Mg	-0.626028	-0.286659	-10.449987
Cl	-2.432449	-1.640643	-9.527825
Mg	-2.596067	-0.526123	-7.428641
Cl	-4.669078	-1.460241	-6.553989
Mg	-4.636693	-0.481498	-4.373369
Cl	-0.763298	0.671493	-12.461341
Cl	-3.849054	1.458203	7.404225
Mg	-3.481426	0.426534	5.290526
Cl	-5.614252	0.866280	4.178699
Mg	-5.097928	-0.002284	2.015156
Cl	-7.209566	0.432455	0.770850
Mg	-6.406841	-0.416802	-1.277486
Cl	-4.625844	-1.599996	-0.049285
Cl	-6.719299	-1.409898	-3.395387
Cl	-4.823726	1.173984	-2.301090
Cl	0.266296	1.998632	1.154473
Cl	0.971247	-1.036987	-2.843951
Cl	-3.351650	1.475686	0.976197
Cl	-2.715444	-1.483822	-3.093373
Mg	-2.906520	0.019752	-1.054154

Cl	-1.016622	-1.061510	0.183321
Cl	-1.203647	1.553474	-2.097279
Mg	-0.953878	0.092675	-4.153679
Cl	0.824105	1.563213	-5.166722
Cl	-0.669285	-1.512831	-6.084559
Mg	-1.380699	0.368928	2.258831
Cl	0.603055	-0.628516	3.453251
Cl	-1.718465	1.902241	4.232842
Cl	-3.140545	-1.173268	3.206273
Cl	-2.910978	1.131012	-5.361026
Mg	0.747426	0.499486	-0.826393
Cl	-1.527001	-0.856331	6.364338
Cl	-0.903230	1.193274	-8.290786
H	7.441982	-2.836284	-0.199765
H	6.994385	-1.376010	-1.133042
H	5.996391	2.221950	-2.045152
H	5.783584	3.342043	-0.582516
H	8.194907	1.575071	-1.260109
H	8.050894	2.782598	0.111907
H	7.474802	1.062073	0.315948
C	9.107139	-1.775128	-1.023222
F	10.038527	-2.275787	-0.180848
F	9.111573	-2.521793	-2.154673
F	9.494192	-0.509748	-1.355385
C	6.777432	0.463285	2.389655
H	7.767308	0.392315	2.862527
H	6.456331	1.515054	2.407928
C	5.738678	-0.409363	3.110171
H	6.064114	-1.461645	3.089551
H	4.805539	-0.375465	2.520433
C	5.433455	0.015350	4.546168
H	6.317663	-0.143209	5.186074
H	5.209916	1.095795	4.582528
C	4.241003	-0.768391	5.099019
H	4.422935	-1.851173	4.984142
H	3.355241	-0.556195	4.469711
C	3.886797	-0.468761	6.555010
H	4.730118	-0.767545	7.201349
H	3.756898	0.617033	6.696598
C	2.630762	-1.214321	7.009920
H	2.676988	-2.261328	6.661807
H	1.740306	-0.801842	6.478778
C	2.373000	-1.193684	8.515523
H	3.295588	-1.521081	9.027047
H	2.182973	-0.160358	8.852152
C	1.219548	-2.106043	8.938429
H	1.388185	-3.115269	8.519963
H	0.277495	-1.751797	8.482081
C	1.032091	-2.210979	10.452459
H	1.992037	-2.495834	10.920414
H	0.763762	-1.220053	10.856015
C	-0.051018	-3.216850	10.848095
H	0.233682	-4.223777	10.491402
H	-0.987935	-2.950123	10.329921
C	-0.318588	-3.260629	12.353407
H	0.611841	-3.527266	12.888286
H	-0.594335	-2.247325	12.693362
C	-1.428226	-4.239960	12.745084
H	-1.167606	-5.250514	12.383582
H	-2.355110	-3.955084	12.218116
C	-1.687618	-4.284607	14.252259
H	-0.785054	-4.596855	14.801405
H	-1.979309	-3.293043	14.631616
H	-2.493121	-4.989849	14.506020

(4) **Int_{1AP} (for D_1)**

99

C 6.774981 1.296395 0.584636
O 5.489520 0.780342 0.847358
Ti 4.032471 -0.182313 1.145663
Cl 3.357201 1.199612 3.114315
Mg 1.273326 0.141886 3.757281
Cl 0.769267 1.174001 5.871280
Mg -1.397561 0.116436 6.310571
Cl -2.016838 1.202274 8.352414
Mg -4.135459 0.034676 8.683903
Cl -4.841629 -0.793628 10.640264
O 7.003507 1.289305 -0.816521
C 6.166495 2.189666 -1.528220
Cl 1.912200 -1.547572 1.850222
Cl 2.546154 0.977921 -0.487569
Cl 4.347723 -1.905694 -0.572661
Mg 3.177242 -0.806373 -2.418694
Cl 3.747583 -2.018489 -4.419956
Mg 2.193922 -0.984974 -5.975562
Cl 2.910709 -1.842214 -8.077566
Mg 1.303673 -0.632573 -9.473246
Cl -0.868739 -1.726096 -9.185074
Mg -1.373905 -0.807884 -7.043578
Cl -3.672084 -1.574032 -6.676130
Mg -4.032226 -0.635170 -4.511836
Cl 1.876002 0.503618 -11.308650
Cl -5.790247 1.032090 7.194143
Mg -4.997718 0.087727 5.166039
Cl -6.733410 0.855356 3.612577
Mg -5.867508 -0.061203 1.594615
Cl -7.553866 0.674058 -0.086068
Mg -6.451201 -0.335694 -1.911572
Cl -5.162243 -1.726260 -0.329336
Cl -6.382132 -1.316219 -4.058816
Cl -4.499394 1.038347 -2.510986
Cl -0.232397 1.218817 2.046492
Cl 0.933038 -1.878055 -1.785492
Cl -3.758320 1.163763 1.024943
Cl -2.592916 -1.860791 -2.861113
Mg -3.063930 -0.344889 -0.890598
Cl -1.652147 -1.647829 0.732020
Cl -1.006499 0.968640 -1.483038
Mg -0.432426 -0.523057 -3.462384
Cl 1.740425 0.666700 -3.984996
Cl 0.009867 -2.127590 -5.371722
Mg -2.282945 -0.173909 2.701749
Cl -0.741584 -1.399045 4.286909
Cl -2.893828 1.362995 4.592098
Cl -4.392187 -1.498328 3.168864
Cl -1.951218 0.783463 -5.019506
Mg 0.453509 -0.335002 0.153616
Cl -3.452927 -1.413026 6.621845
Cl 0.708728 0.682304 -7.325927
H 5.220535 2.394333 -1.001724
H 6.684616 3.142280 -1.735489
C 5.800502 1.576727 -2.869387
F 5.027082 0.410344 -2.677355
F 5.038863 2.416446 -3.593133
F 6.853898 1.198362 -3.595423
C 7.847970 0.456705 1.269179
H 8.814993 0.853437 0.927626
H 7.784999 0.678219 2.346586
C 7.742240 -1.064050 1.018642
H 8.711149 -1.434920 0.655508
H 7.027581 -1.261105 0.204617
C 7.353826 -1.885464 2.258953

H 7.443724 -2.956826 2.016667
H 8.082769 -1.691528 3.065756
C 5.949497 -1.631044 2.820119
H 5.214403 -1.945769 2.034302
H 5.819175 -0.554484 3.036306
C 5.613096 -2.411040 4.098931
H 5.835129 -3.480784 3.950563
H 6.276767 -2.060342 4.907886
C 4.149952 -2.223896 4.501582
H 3.510961 -2.698856 3.738828
H 3.928081 -1.141541 4.463067
C 3.738873 -2.741245 5.879293
H 3.869835 -3.835736 5.931613
H 4.396984 -2.308771 6.652674
C 2.282373 -2.374166 6.186239
H 1.624227 -2.801977 5.408950
H 2.178567 -1.273386 6.121846
C 1.791769 -2.819874 7.563961
H 1.831666 -3.921513 7.623986
H 2.487422 -2.445736 8.334995
C 0.371392 -2.359517 7.918831
H -0.334247 -2.695653 7.135689
H 0.354403 -1.249146 7.938079
C -0.084375 -2.887069 9.283234
H -0.038599 -3.990662 9.265286
H 0.643332 -2.566220 10.049508
C -1.486775 -2.454208 9.715564
H -2.218283 -2.766961 8.950291
H -1.528777 -1.351423 9.759602
C -1.888927 -3.027752 11.074998
H -1.891770 -4.128857 11.053760
H -1.183141 -2.710288 11.858470
H -2.891643 -2.684044 11.361696
H 6.782201 2.336695 0.964610

(5) **Int$_{1KP}$ (for D$_1$)**

105

C 6.743976 1.368387 0.644949
O 5.476457 0.763716 0.839754
Ti 4.029815 -0.202744 1.145031
Cl 3.357959 1.199959 3.110133
Mg 1.272307 0.145217 3.754644
Cl 0.762426 1.180917 5.866743
Mg -1.403469 0.120767 6.306062
Cl -2.026283 1.199614 8.351130
Mg -4.144076 0.024291 8.675891
Cl -4.854404 -0.810904 10.627880
O 6.984999 1.417673 -0.768862
C 6.070169 2.207842 -1.509699
C 6.690190 2.764920 1.286585
C 7.976311 3.575583 1.120887
Cl 1.904850 -1.554177 1.860497
Cl 2.545457 0.957481 -0.495094
Cl 4.328251 -1.943689 -0.563401
Mg 3.185600 -0.835510 -2.416003
Cl 3.747986 -2.050701 -4.418174
Mg 2.203625 -1.001641 -5.973571
Cl 2.915273 -1.852954 -8.080022
Mg 1.316036 -0.626584 -9.469987
Cl -0.859022 -1.715214 -9.186851
Mg -1.363697 -0.796627 -7.045744
Cl -3.668432 -1.548314 -6.687156
Mg -4.024796 -0.615465 -4.519911
Cl 1.886542 0.519758 -11.299698
Cl -5.799622 1.022312 7.186283

Mg	-5.001377	0.080872	5.159010
Cl	-6.732741	0.853825	3.604343
Mg	-5.865361	-0.059651	1.586243
Cl	-7.547456	0.688330	-0.092333
Mg	-6.446797	-0.317127	-1.921629
Cl	-5.166123	-1.720264	-0.342153
Cl	-6.380363	-1.285482	-4.074437
Cl	-4.488696	1.050960	-2.514776
Cl	-0.234263	1.212039	2.041291
Cl	0.928107	-1.894736	-1.788113
Cl	-3.754233	1.160642	1.021283
Cl	-2.596170	-1.856525	-2.871311
Mg	-3.060686	-0.345233	-0.896170
Cl	-1.655867	-1.655812	0.727941
Cl	-0.998696	0.960924	-1.484687
Mg	-0.424300	-0.530807	-3.464281
Cl	1.758263	0.646761	-3.982513
Cl	0.009935	-2.131916	-5.377989
Mg	-2.282568	-0.181590	2.699107
Cl	-0.742695	-1.400025	4.289494
Cl	-2.899770	1.360108	4.586397
Cl	-4.394452	-1.503025	3.162040
Cl	-1.933289	0.791148	-5.019170
Mg	0.454490	-0.350965	0.151715
Cl	-3.454292	-1.416926	6.616482
Cl	0.727545	0.681512	-7.318882
H	5.096372	2.319774	-1.008412
H	6.480699	3.208256	-1.731676
H	5.831902	3.307226	0.860156
H	6.446993	2.621540	2.350135
H	8.818907	3.121269	1.660200
H	8.266053	3.660813	0.063423
H	7.838392	4.590634	1.517333
C	5.792696	1.536582	-2.843987
F	5.081986	0.329879	-2.647544
F	5.005866	2.311152	-3.613899
F	6.888146	1.202845	-3.527614
C	7.839554	0.469434	1.237202
H	8.791627	0.847392	0.840133
H	7.858254	0.657806	2.322720
C	7.694355	-1.041673	0.959613
H	8.649188	-1.425169	0.572084
H	6.961416	-1.208465	0.156151
C	7.319910	-1.879968	2.194241
H	7.394220	-2.948277	1.933272
H	8.067632	-1.705993	2.988228
C	5.930871	-1.622376	2.790906
H	5.177518	-1.947255	2.026500
H	5.804506	-0.544657	3.002270
C	5.619917	-2.390837	4.083822
H	5.868263	-3.456797	3.952113
H	6.276694	-2.009990	4.884649
C	4.152501	-2.233260	4.485931
H	3.524875	-2.752618	3.742763
H	3.899110	-1.159914	4.409239
C	3.759807	-2.709398	5.883585
H	3.923587	-3.796650	5.976979
H	4.406828	-2.228042	6.637090
C	2.293835	-2.374282	6.182625
H	1.645548	-2.848948	5.424343
H	2.157123	-1.279923	6.077791
C	1.820389	-2.781188	7.578448
H	1.895223	-3.877869	7.679333
H	2.504925	-2.356718	8.333309
C	0.386011	-2.353855	7.918109
H	-0.307749	-2.730415	7.143391
H	0.336673	-1.243937	7.906765

C -0.060260 -2.856252 9.294906
H 0.027283 -3.957163 9.310378
H 0.646998 -2.484964 10.057518
C -1.482941 -2.465557 9.700629
H -2.193714 -2.823516 8.935539
H -1.565035 -1.364377 9.714653
C -1.880141 -3.017267 11.070544
H -1.843849 -4.118094 11.078654
H -1.195498 -2.654276 11.853231
H -2.897216 -2.701153 11.338025

(6) **RC (for D_2)**

111

C 6.858751 -0.606237 0.377476
O 6.054185 -0.146647 -0.452362
Ti 4.565375 1.014976 -1.165074
Cl 4.262294 2.207321 1.009117
Mg 2.436887 1.048766 2.089029
Cl 2.479058 2.135852 4.236563
Mg 0.592571 1.003308 5.293774
Cl 0.570005 2.128141 7.405603
Mg -1.353127 0.982601 8.357448
Cl -1.427050 0.394462 10.517470
O 7.607795 -1.683916 0.098037
C 7.491509 -2.268399 -1.218835
C 5.736996 2.639066 -1.642683
C 7.056906 2.948047 -0.957200
Cl 2.719092 -0.618879 0.132476
Cl 2.449764 1.927834 -2.315036
Cl 4.628012 -0.458560 -3.162382
Mg 2.583055 0.230359 -4.291455
Cl 2.915600 -0.718287 -6.466926
Mg 0.770643 -0.142774 -7.486484
Cl 0.999767 -1.097409 -9.656716
Mg -1.102418 -0.283429 -10.594835
Cl -2.877866 -1.640724 -9.610862
Mg -2.932514 -0.549882 -7.492490
Cl -4.968989 -1.477486 -6.513413
Mg -4.808182 -0.517413 -4.331448
Cl -1.307135 0.690361 -12.592556
Cl -3.411060 1.744592 7.308522
Mg -3.138370 0.611784 5.229972
Cl -5.310991 1.036185 4.197558
Mg -4.921863 0.062209 2.054408
Cl -7.113259 0.440796 0.930580
Mg -6.410881 -0.433548 -1.146608
Cl -4.568363 -1.588638 0.013845
Cl -6.821312 -1.467985 -3.228866
Cl -4.887041 1.149828 -2.275035
Cl 0.449100 1.979797 0.887146
Cl 0.858734 -1.128920 -3.100986
Cl -3.217316 1.503682 0.893232
Cl -2.832569 -1.525000 -3.146172
Mg -2.897102 0.003556 -1.122576
Cl -0.965186 -1.079472 0.048688
Cl -1.229090 1.497299 -2.260835
Mg -1.108381 0.028514 -4.312009
Cl 0.632242 1.480975 -5.418426
Cl -0.948825 -1.570326 -6.260541
Mg -1.194994 0.404300 2.095823
Cl 0.806762 -0.612276 3.236348
Cl -1.407867 2.009425 4.024536
Cl -2.922874 -1.082697 3.198625
Cl -3.121099 1.086469 -5.406166
Mg 0.788735 0.419550 -1.082127

Cl	-1.148914	-0.632200	6.292594
Cl	-1.265430	1.162701	-8.418931
H	7.573210	-3.352770	-1.086541
H	6.541680	-2.000415	-1.698650
H	5.888504	2.234483	-2.673498
H	5.084638	3.525603	-1.723098
H	7.724585	2.073711	-0.945533
H	7.601855	3.764316	-1.460196
H	6.888035	3.266625	0.082999
C	8.644746	-1.787337	-2.098471
F	9.847103	-2.164436	-1.603539
F	8.506739	-2.318561	-3.334840
F	8.651725	-0.433323	-2.210025
C	6.972249	-0.120554	1.780745
H	7.956335	-0.370532	2.198508
H	6.833610	0.970166	1.779883
C	5.836757	-0.787049	2.595228
H	5.999518	-1.876597	2.620311
H	4.890972	-0.633226	2.048722
C	5.688975	-0.250138	4.018333
H	6.604912	-0.456726	4.596945
H	5.568706	0.846242	3.995913
C	4.480277	-0.887583	4.706486
H	4.563379	-1.987295	4.656003
H	3.569010	-0.638684	4.131109
C	4.268670	-0.464956	6.159946
H	5.142000	-0.775756	6.758932
H	4.217430	0.634209	6.229426
C	3.009974	-1.090800	6.763545
H	2.976743	-2.165638	6.512310
H	2.109010	-0.673319	6.256581
C	2.861323	-0.920992	8.274547
H	3.802025	-1.244832	8.754191
H	2.738427	0.146602	8.523791
C	1.701168	-1.732527	8.855726
H	1.808947	-2.787870	8.545006
H	0.749159	-1.390322	8.410013
C	1.590930	-1.659489	10.379255
H	2.561903	-1.932106	10.831306
H	1.383358	-0.618124	10.678137
C	0.488922	-2.562235	10.939399
H	0.727876	-3.619013	10.719576
H	-0.454434	-2.335230	10.414220
C	0.262535	-2.383761	12.441765
H	1.190040	-2.630215	12.990324
H	0.054766	-1.318417	12.639964
C	-0.893262	-3.228305	12.983593
H	-0.699065	-4.296673	12.776209
H	-1.812585	-2.970500	12.428432
C	-1.140831	-3.042235	14.482549
H	-0.219258	-3.292014	15.039690
H	-1.340846	-1.975103	14.687326
C	-2.299400	-3.885284	15.023781
H	-3.222410	-3.620898	14.478856
H	-2.108538	-4.949470	14.798669
C	-2.521357	-3.710908	16.527733
H	-2.746962	-2.661901	16.775872
H	-1.622752	-3.999417	17.095931
H	-3.357561	-4.326751	16.891565

(7) **TS_{1AP} (for D_2)**

111

C	6.865160	-0.027226	0.904638
O	5.738131	0.008374	0.199860
Ti	4.458240	1.103074	-0.579276

Cl	3.917044	2.405826	1.467720
Mg	2.166855	1.053760	2.458871
Cl	1.994911	1.951067	4.681685
Mg	0.112820	0.618355	5.510141
Cl	-0.107896	1.498933	7.724815
Mg	-2.050149	0.203320	8.401298
Cl	-2.308900	-0.690527	10.436857
O	7.658204	-1.144526	0.727650
C	7.629917	-1.795969	-0.546718
C	6.241151	2.530778	-0.793788
C	7.555185	2.112000	-0.439195
Cl	2.608507	-0.478739	0.360598
Cl	2.509433	2.299915	-1.808916
Cl	4.754502	0.056107	-2.817526
Mg	2.776354	0.846110	-3.980550
Cl	3.273116	0.263885	-6.250387
Mg	1.175082	0.943632	-7.303025
Cl	1.535508	0.335365	-9.576317
Mg	-0.516848	1.301931	-10.486814
Cl	-2.374304	-0.168899	-9.877505
Mg	-2.518798	0.454320	-7.587604
Cl	-4.513534	-0.778092	-6.867257
Mg	-4.581808	-0.090758	-4.583132
Cl	-0.533779	2.596817	-12.302574
Cl	-4.012605	1.090655	7.274107
Mg	-3.590663	0.114253	5.143752
Cl	-5.726229	0.525821	4.028138
Mg	-5.134597	-0.153829	1.818709
Cl	-7.227644	0.348166	0.568371
Mg	-6.389913	-0.364838	-1.517809
Cl	-4.596091	-1.587309	-0.345511
Cl	-6.626485	-1.214032	-3.709839
Cl	-4.845222	1.349103	-2.383341
Cl	0.219253	1.997654	1.193211
Cl	1.009814	-0.657434	-3.057943
Cl	-3.408904	1.427972	0.914566
Cl	-2.637830	-1.143692	-3.388069
Mg	-2.904643	0.143260	-1.210394
Cl	-1.013228	-0.994334	-0.022633
Cl	-1.218656	1.800216	-2.069898
Mg	-0.912745	0.590409	-4.265452
Cl	0.858971	2.219654	-5.022487
Cl	-0.568423	-0.694677	-6.410254
Mg	-1.429541	0.276235	2.146515
Cl	0.540032	-0.770708	3.326356
Cl	-1.838490	1.675686	4.201079
Cl	-3.167758	-1.353290	2.972906
Cl	-2.905979	1.726264	-5.335036
Mg	0.741450	0.659419	-0.889537
Cl	-1.639336	-1.175612	6.211577
Cl	-0.832294	2.342827	-8.117199
H	7.352545	-2.847617	-0.389822
H	6.913319	-1.333006	-1.238771
H	5.997464	2.451473	-1.867866
H	5.856605	3.426036	-0.296747
H	8.176325	1.632299	-1.202747
H	8.124075	2.724560	0.269869
H	7.476116	1.020643	0.349417
C	9.022631	-1.759965	-1.166822
F	9.958651	-2.292199	-0.349194
F	9.018064	-2.465212	-2.324640
F	9.410281	-0.483910	-1.455475
C	6.747503	0.323717	2.375745
H	7.732987	0.206781	2.848670
H	6.448138	1.379870	2.449874
C	5.686165	-0.563079	3.044114
H	6.000282	-1.617596	2.991241

H	4.763383	-0.495571	2.441275
C	5.364454	-0.183011	4.488457
H	6.241511	-0.361621	5.133089
H	5.143723	0.896873	4.553812
C	4.165412	-0.977964	5.010503
H	4.346136	-2.058135	4.871599
H	3.283308	-0.749257	4.381467
C	3.808946	-0.707073	6.471014
H	4.657118	-1.006940	7.110650
H	3.669346	0.375272	6.628771
C	2.562434	-1.468309	6.924467
H	2.632051	-2.520918	6.597994
H	1.669917	-1.081636	6.377564
C	2.298265	-1.417286	8.428286
H	3.230124	-1.697063	8.951241
H	2.072528	-0.381790	8.734681
C	1.177091	-2.353820	8.882132
H	1.396119	-3.377047	8.526477
H	0.228245	-2.066529	8.392928
C	0.973479	-2.373594	10.397952
H	1.942179	-2.567691	10.893653
H	0.644008	-1.375259	10.732302
C	-0.054063	-3.411125	10.854561
H	0.302534	-4.424460	10.594299
H	-0.991804	-3.251972	10.296417
C	-0.357869	-3.336184	12.351915
H	0.568654	-3.512526	12.928632
H	-0.684820	-2.309902	12.591677
C	-1.437688	-4.321507	12.804170
H	-1.124932	-5.352669	12.557604
H	-2.357988	-4.132644	12.223356
C	-1.757639	-4.231922	14.298390
H	-0.838192	-4.420712	14.882321
H	-2.064014	-3.198709	14.541223
C	-2.851884	-5.201331	14.753893
H	-3.768528	-5.010129	14.169310
H	-2.546188	-6.233841	14.509845
C	-3.165135	-5.097658	16.248057
H	-3.503936	-4.083620	16.511948
H	-2.273124	-5.315466	16.856423
H	-3.954612	-5.802487	16.548768

(8) **TS_{1KP} (for D_2)**

111

C	6.654457	0.137250	0.776155
O	5.600810	-0.252241	0.083494
Ti	4.877441	1.447462	-0.405950
Cl	3.637322	1.871199	1.668850
Mg	1.605692	0.574340	1.171043
Cl	0.703425	0.147081	3.344530
Mg	-1.495226	-0.738680	2.682570
Cl	-2.409709	-1.326200	4.801729
Mg	-4.565264	-2.146390	3.992209
Cl	-5.461986	-4.039064	4.783387
O	7.885625	-0.154758	0.295555
C	7.995625	-0.636179	-1.053875
C	6.717298	2.360943	0.396211
C	7.122167	3.002211	1.705298
Cl	2.681687	0.169250	-1.113710
Cl	3.583274	3.543641	-1.428212
Cl	5.829883	1.506009	-2.724409
Mg	4.547527	3.231557	-3.843672
Cl	5.835756	3.552708	-5.850657
Mg	4.409673	5.184217	-6.968865
Cl	5.504856	5.480423	-9.065720

Mg	4.159611	7.360129	-9.852549
Cl	2.046086	6.396848	-10.601879
Mg	1.102264	6.027364	-8.449215
Cl	-1.166825	5.315042	-9.029160
Mg	-2.025582	4.955300	-6.829331
Cl	4.996259	9.271986	-10.641657
Cl	-5.912197	-0.206417	3.351331
Mg	-4.842033	0.216371	1.262066
Cl	-6.261752	1.894482	0.184667
Mg	-5.028722	2.177786	-1.852978
Cl	-6.397254	3.795299	-3.146009
Mg	-4.907106	3.923170	-4.982343
Cl	-3.881737	1.811296	-4.245593
Cl	-4.392578	4.329201	-7.256961
Cl	-2.935168	5.256525	-4.353477
Cl	0.370819	2.542754	0.195075
Cl	2.425271	2.043261	-4.401064
Cl	-2.883651	3.356115	-1.284407
Cl	-0.859752	2.922162	-5.911188
Mg	-1.778377	3.103012	-3.554813
Cl	-0.643017	1.016412	-2.738673
Cl	0.299985	4.351495	-2.910206
Mg	1.275788	4.224335	-5.228871
Cl	3.387345	5.409485	-4.531508
Cl	2.256793	3.945634	-7.535418
Mg	-1.719950	1.202250	-0.442134
Cl	-0.459889	-0.817744	0.334613
Cl	-2.694776	1.407499	1.875319
Cl	-3.839069	0.022678	-1.182963
Cl	0.038845	6.278796	-6.060171
Mg	1.495613	2.231330	-2.044741
Cl	-3.546715	-1.962703	1.634011
Cl	3.101097	7.342905	-7.466217
H	7.406600	-1.553546	-1.191321
H	7.668367	0.120192	-1.780027
H	7.556000	2.285089	-0.309812
H	5.969897	3.067500	-0.084693
H	6.318813	2.966452	2.454007
H	8.021616	2.528165	2.119768
H	7.376176	4.063074	1.543705
C	9.468501	-0.937869	-1.291325
F	9.952729	-1.841539	-0.406053
F	9.612989	-1.449330	-2.539556
F	10.230422	0.179847	-1.202366
C	6.635761	0.050435	2.279228
H	7.520469	0.572912	2.657509
H	5.745895	0.569477	2.655010
C	6.657423	-1.428812	2.766409
H	7.434603	-1.507405	3.540691
H	6.984672	-2.094012	1.950808
C	5.332484	-1.935110	3.345824
H	5.531338	-2.900710	3.841868
H	4.993473	-1.250833	4.143050
C	4.206201	-2.142179	2.330792
H	4.581888	-2.747926	1.487323
H	3.921664	-1.169546	1.885278
C	2.971924	-2.815282	2.935831
H	3.284523	-3.721844	3.482343
H	2.513304	-2.147534	3.684992
C	1.929245	-3.207934	1.888228
H	2.371210	-3.936155	1.185803
H	1.672531	-2.331764	1.262286
C	0.644689	-3.791818	2.479739
H	0.902984	-4.589199	3.197594
H	0.143008	-3.017343	3.097282
C	-0.329434	-4.338680	1.434475
H	0.179627	-5.114778	0.836475

H -0.588814 -3.537408 0.722221
C -1.615076 -4.913379 2.034075
H -1.381004 -5.801730 2.645622
H -2.047441 -4.180258 2.740439
C -2.669928 -5.261251 0.979906
H -2.280489 -6.046940 0.308100
H -2.837546 -4.373745 0.345475
C -4.005599 -5.700650 1.583467
H -3.888664 -6.679445 2.081282
H -4.293520 -4.999736 2.385387
C -5.145222 -5.771673 0.565044
H -4.881320 -6.473344 -0.247336
H -5.253874 -4.780422 0.085742
C -6.484665 -6.181313 1.183847
H -6.388330 -7.188631 1.627600
H -6.716665 -5.505268 2.025831
C -7.647475 -6.177762 0.187729
H -7.746308 -5.167496 -0.248020
H -7.407363 -6.848979 -0.655825
C -8.978982 -6.596593 0.814967
H -9.254095 -5.925981 1.643797
H -8.920040 -7.617333 1.223874
H -9.798885 -6.577601 0.081418

(9) **Int_{1AP} (for D_2)**

105

C 6.781727 1.320189 0.525192
O 5.504903 0.783433 0.781546
Ti 4.062694 -0.183487 1.126553
Cl 3.409107 1.250480 3.058224
Mg 1.347370 0.169997 3.736771
Cl 0.945626 1.153121 5.880186
Mg -1.268773 0.189653 6.306436
Cl -1.662998 1.119996 8.467996
Mg -3.936260 0.296041 8.747845
Cl -4.645592 -0.529409 10.704649
O 7.026808 1.292981 -0.872931
C 6.175396 2.159059 -1.610100
Cl 1.950242 -1.541715 1.877300
Cl 2.566128 0.945334 -0.515697
Cl 4.357676 -1.949174 -0.553890
Mg 3.170371 -0.873859 -2.407521
Cl 3.710851 -2.119803 -4.397650
Mg 2.137001 -1.119735 -5.955345
Cl 2.789512 -2.052113 -8.050313
Mg 1.212595 -0.809918 -9.450761
Cl -0.984091 -1.838474 -9.116576
Mg -1.437821 -0.870641 -6.984507
Cl -3.754119 -1.562525 -6.586125
Mg -4.069552 -0.593099 -4.429618
Cl 1.797167 0.293231 -11.303326
Cl -5.431505 1.567606 7.293566
Mg -4.876142 0.445598 5.260333
Cl -6.604720 1.212870 3.712057
Mg -5.820135 0.172939 1.700850
Cl -7.522873 0.857571 0.017645
Mg -6.452509 -0.207783 -1.802546
Cl -5.171471 -1.575993 -0.205227
Cl -6.427959 -1.222967 -3.935676
Cl -4.484521 1.122764 -2.455073
Cl -0.153388 1.268766 2.042959
Cl 0.911149 -1.910711 -1.738961
Cl -3.679008 1.312757 1.064133
Cl -2.642439 -1.827412 -2.776469
Mg -3.057084 -0.262866 -0.829487

Cl	-1.659392	-1.582342	0.790591
Cl	-0.974258	0.985806	-1.464051
Mg	-0.453045	-0.551033	-3.420017
Cl	1.734512	0.583419	-3.991522
Cl	-0.068464	-2.197475	-5.302753
Mg	-2.231512	-0.055672	2.739804
Cl	-0.715750	-1.335187	4.296118
Cl	-2.695122	1.549756	4.626165
Cl	-4.388043	-1.258464	3.271105
Cl	-1.957578	0.767051	-4.980715
Mg	0.473370	-0.334033	0.175584
Cl	-3.466284	-1.175556	6.653013
Cl	0.678816	0.557014	-7.319128
H	5.233534	2.377656	-1.081943
H	6.685392	3.106018	-1.858360
C	5.798255	1.495343	-2.923939
F	5.035089	0.332028	-2.681649
F	5.023671	2.304577	-3.668165
F	6.846637	1.098471	-3.648036
C	7.859599	0.512642	1.240370
H	8.825187	0.901486	0.885684
H	7.793345	0.773455	2.308846
C	7.761892	-1.017407	1.049682
H	8.732973	-1.397294	0.702136
H	7.048543	-1.251616	0.243986
C	7.378345	-1.788903	2.323491
H	7.500026	-2.867982	2.135471
H	8.092075	-1.535829	3.127420
C	5.959850	-1.548825	2.857055
H	5.241786	-1.947183	2.094945
H	5.789774	-0.464740	2.997179
C	5.654040	-2.241427	4.193804
H	5.969177	-3.296698	4.142604
H	6.267559	-1.768166	4.979360
C	4.172109	-2.155694	4.562736
H	3.592435	-2.779716	3.861611
H	3.843753	-1.113541	4.392260
C	3.802582	-2.533961	5.997766
H	4.161177	-3.551685	6.228868
H	4.314013	-1.854481	6.701197
C	2.288245	-2.459972	6.213718
H	1.789089	-3.212807	5.578940
H	1.926677	-1.475766	5.857664
C	1.828365	-2.624281	7.662512
H	2.221789	-3.575361	8.062178
H	2.265112	-1.823769	8.283612
C	0.305676	-2.629853	7.818450
H	-0.128889	-3.390793	7.146927
H	-0.097774	-1.657833	7.456239
C	-0.185209	-2.861839	9.249611
H	0.394216	-3.694710	9.686694
H	0.037104	-1.975888	9.868595
C	-1.674532	-3.202673	9.334119
H	-1.871993	-4.089197	8.704841
H	-2.271015	-2.386941	8.889845
C	-2.177785	-3.464000	10.755534
H	-1.488445	-4.160330	11.267865
H	-2.156519	-2.521908	11.328905
C	-3.597197	-4.038800	10.790446
H	-4.263596	-3.375788	10.215251
H	-3.601961	-5.017416	10.278562
C	-4.146016	-4.187535	12.209857
H	-4.215755	-3.205161	12.700259
H	-3.497015	-4.830301	12.826266
H	-5.152534	-4.631357	12.208196
H	6.764275	2.367085	0.886202

(10) **Int_{1KP} (for D_2)**

111

C	6.755717	1.389908	0.592291
O	5.499537	0.760708	0.771541
Ti	4.064187	-0.204403	1.122419
Cl	3.418447	1.257831	3.045945
Mg	1.356487	0.184146	3.732573
Cl	0.956419	1.168170	5.876223
Mg	-1.257119	0.201647	6.304943
Cl	-1.650742	1.126552	8.468868
Mg	-3.922579	0.297048	8.748583
Cl	-4.630866	-0.533951	10.703492
O	7.030687	1.410096	-0.816579
C	6.114733	2.158551	-1.598868
C	6.655173	2.799809	1.198114
C	7.926997	3.634784	1.046378
Cl	1.943709	-1.539377	1.884143
Cl	2.577346	0.929019	-0.528413
Cl	4.344010	-1.990674	-0.543208
Mg	3.185517	-0.904782	-2.405475
Cl	3.713919	-2.148276	-4.400925
Mg	2.146123	-1.130944	-5.954843
Cl	2.788106	-2.062945	-8.053804
Mg	1.214805	-0.810581	-9.448630
Cl	-0.984386	-1.832089	-9.112236
Mg	-1.430476	-0.864431	-6.978913
Cl	-3.748914	-1.551297	-6.581768
Mg	-4.061393	-0.582944	-4.425295
Cl	1.796852	0.292989	-11.301828
Cl	-5.420336	1.569564	7.297545
Mg	-4.865718	0.451035	5.261858
Cl	-6.598026	1.216086	3.716330
Mg	-5.811240	0.180913	1.703353
Cl	-7.514091	0.869653	0.021502
Mg	-6.444567	-0.195516	-1.799173
Cl	-5.164647	-1.565691	-0.203161
Cl	-6.421389	-1.210452	-3.931926
Cl	-4.475263	1.133829	-2.453068
Cl	-0.144902	1.279005	2.037315
Cl	0.910360	-1.918572	-1.737331
Cl	-3.671361	1.322754	1.065085
Cl	-2.637727	-1.820476	-2.774019
Mg	-3.048500	-0.253856	-0.828906
Cl	-1.655149	-1.574494	0.792405
Cl	-0.962526	0.989748	-1.465455
Mg	-0.440205	-0.551756	-3.417916
Cl	1.757848	0.568033	-3.989047
Cl	-0.064514	-2.198521	-5.301311
Mg	-2.221770	-0.043832	2.739543
Cl	-0.706372	-1.321300	4.297191
Cl	-2.687281	1.560995	4.627190
Cl	-4.376792	-1.249625	3.272396
Cl	-1.943537	0.772189	-4.976285
Mg	0.480321	-0.333990	0.173212
Cl	-3.451896	-1.168913	6.652448
Cl	0.692072	0.555319	-7.313955
H	5.141782	2.299189	-1.103451
H	6.527569	3.144617	-1.873269
H	5.796992	3.313255	0.737476
H	6.387257	2.675757	2.258178
H	8.767582	3.205954	1.609378
H	8.236106	3.711276	-0.006062
H	7.759376	4.652090	1.425150
C	5.830150	1.422908	-2.897585
F	5.109111	0.234473	-2.641627

F	5.048243	2.166973	-3.702975
F	6.921821	1.047906	-3.566122
C	7.852791	0.529596	1.237671
H	8.808046	0.904365	0.845171
H	7.847052	0.759899	2.315332
C	7.730112	-0.993560	1.019423
H	8.694430	-1.380523	0.660535
H	7.009684	-1.204138	0.214306
C	7.350288	-1.782956	2.284600
H	7.454049	-2.860351	2.076724
H	8.078641	-1.554155	3.082782
C	5.944037	-1.532834	2.844997
H	5.211016	-1.931003	2.095653
H	5.782034	-0.448254	2.986717
C	5.651424	-2.223474	4.186125
H	5.968912	-3.277996	4.135424
H	6.269091	-1.746072	4.965905
C	4.171372	-2.140357	4.563988
H	3.589148	-2.760009	3.861143
H	3.842233	-1.097053	4.401208
C	3.805384	-2.528685	5.997297
H	4.161183	-3.549474	6.218888
H	4.320575	-1.856652	6.704961
C	2.291393	-2.451572	6.216504
H	1.789330	-3.196957	5.575233
H	1.932948	-1.462986	5.869893
C	1.831070	-2.628246	7.663890
H	2.220726	-3.584526	8.054697
H	2.270285	-1.835234	8.292874
C	0.308054	-2.630139	7.818634
H	-0.127405	-3.389273	7.145573
H	-0.092843	-1.657003	7.456706
C	-0.185853	-2.862208	9.249108
H	0.399385	-3.688024	9.691757
H	0.025836	-1.972019	9.865629
C	-1.672600	-3.216134	9.329689
H	-1.858958	-4.109354	8.706525
H	-2.274638	-2.409668	8.876231
C	-2.179749	-3.470999	10.750955
H	-1.490020	-4.162352	11.269454
H	-2.163312	-2.525540	11.318911
C	-3.597742	-4.049510	10.785006
H	-4.264843	-3.389679	10.206940
H	-3.599370	-5.029462	10.275731
C	-4.148752	-4.196036	12.203834
H	-4.221387	-3.212779	12.691953
H	-3.499596	-4.836099	12.822843
H	-5.154338	-4.642005	12.201459

(H) n-hexane displaces alkyl chain of donors from $MgCl_2$ surface

(1) **n-hexane**

20

C	-0.294055	0.799159	-1.408175
H	-1.246758	1.253440	-1.084213
H	0.503660	1.445256	-1.001858
C	-0.169588	-0.597861	-0.793733
H	-0.969613	-1.244889	-1.197341
H	0.782214	-1.054953	-1.120467
C	-0.235768	-0.606070	0.735544
H	-1.188792	-0.151479	1.062191
H	0.562465	0.043130	1.139196
C	-0.107432	-2.002657	1.350157
H	-0.902111	-2.651673	0.942617
H	0.847436	-2.453472	1.027668

C -0.221550 0.794250 -2.936471
H 0.735647 0.377943 -3.287383
H -1.026357 0.180069 -3.369929
H -0.315892 1.808776 -3.351165
C -0.182250 -1.998028 2.878345
H -1.141414 -1.584987 3.227781
H -0.085056 -3.012231 3.293188
H 0.619744 -1.381064 3.313025

(2) **n-hexane displaces alkyl chain of D_1**

125

C -6.664835 -2.028119 -2.086826
O -5.437879 -1.814824 -2.001524
Ti -3.755497 -0.780061 -2.138928
Cl -2.689528 -2.715477 -3.244818
Mg -1.247046 -3.736899 -1.528031
Cl -0.559420 -5.807096 -2.583817
Mg 0.938224 -6.654068 -0.838331
Cl 1.470450 -8.840955 -1.620165
Mg 2.884598 -9.492373 0.262628
Cl 2.590241 -11.500476 1.218804
O -7.452241 -0.939133 -2.061060
C -8.878895 -1.073800 -2.130503
C -4.574232 0.516879 -3.558813
C -4.360292 -0.190033 -4.900625
Cl -1.586279 0.606569 -2.279228
Cl -2.215722 -1.991572 0.020636
Cl -4.394193 0.785543 -0.369420
Mg -2.532733 2.343106 -0.601102
Cl -3.409220 4.422610 0.197385
Mg -1.367233 5.774139 0.164961
Cl -2.167943 7.852645 1.010071
Mg -0.095918 9.125836 0.743584
Cl 1.424783 8.389314 2.509801
Mg 2.086455 6.346917 1.468607
Cl 3.981803 5.661186 2.852856
Mg 4.398729 3.512436 1.888058
Cl 6.286251 2.682174 3.283483
Mg 6.429358 0.588684 2.190474
Cl 4.557865 -0.847437 2.894261
Cl 0.046923 11.158069 -0.173700
Cl 5.180170 1.546193 0.293719
Cl 7.598878 -1.350990 1.499758
Mg 5.571105 -2.790619 1.389985
Cl 6.428518 -4.888121 0.621923
Mg 4.353950 -6.196058 0.644239
Cl 5.048755 -8.381282 -0.035671
Cl -0.992489 1.426712 1.127767
Cl 0.786776 -2.280846 -1.830810
Cl 4.141630 -1.825846 -0.430597
Cl 2.444897 2.021341 2.403722
Mg 3.164055 0.078737 0.939759
Cl 1.213993 -1.387776 1.506790
Cl 1.773653 1.019278 -0.918144
Mg 2.098224 -3.316948 0.119572
Cl 0.043173 -4.694585 0.551621
Cl 3.014457 -5.222840 -1.271524
Cl 3.508941 -4.155217 2.069108
Mg 0.973270 2.960604 0.473117
Cl -0.518914 3.843956 -1.351524
Cl 0.131619 4.800515 1.986266
Cl 2.987197 4.382133 -0.071163
Mg -0.263450 -0.483294 -0.383838
Cl 0.757474 7.066513 -0.600025
Cl 2.150470 -7.313694 1.397579

H	-5.639895	0.666379	-3.323536
H	-4.082073	1.501454	-3.540723
H	-4.809014	0.392578	-5.724044
H	-3.294018	-0.314615	-5.141745
H	-4.824084	-1.188855	-4.932637
H	-9.202514	-1.331758	-3.149479
H	-9.256552	-1.810791	-1.407780
C	-9.467724	0.289616	-1.769966
F	-9.035270	1.257101	-2.607366
F	-10.820321	0.207172	-1.871488
F	-9.156794	0.648482	-0.506856
C	-7.194627	-3.422406	-2.208010
H	-6.467762	-3.960055	-2.835476
H	-8.159989	-3.443667	-2.733391
C	-7.296621	-4.157896	-0.849000
H	-8.124437	-3.748040	-0.247211
H	-6.372166	-3.968094	-0.282529
C	-7.457991	-5.667200	-1.059846
H	-8.448378	-5.889798	-1.492425
H	-6.721214	-5.979197	-1.821302
C	-7.219596	-6.504846	0.203146
H	-8.095586	-6.461952	0.871259
H	-6.382568	-6.060360	0.769416
C	-6.858165	-7.957874	-0.128823
H	-7.729008	-8.479895	-0.560817
H	-6.093534	-7.942888	-0.927986
C	-6.289591	-8.757076	1.049105
H	-7.082853	-8.987841	1.780248
H	-5.557822	-8.125045	1.584208
C	-5.581738	-10.040972	0.602416
H	-6.310737	-10.739686	0.155648
H	-4.878422	-9.782529	-0.210183
C	-4.794383	-10.743506	1.712162
H	-5.486314	-11.167513	2.460962
H	-4.189827	-9.990947	2.251559
C	-3.855139	-11.831334	1.183167
H	-4.438638	-12.618879	0.674596
H	-3.211606	-11.386358	0.401804
C	-2.963157	-12.458300	2.258589
H	-3.575938	-13.078037	2.936752
H	-2.536873	-11.655274	2.885882
C	-1.815086	-13.294090	1.685135
H	-2.223863	-14.096738	1.044549
H	-1.203398	-12.657112	1.020844
C	-0.906018	-13.909155	2.752414
H	-1.503633	-14.575765	3.398847
H	-0.527950	-13.104677	3.406905
C	0.277588	-14.676252	2.158870
H	-0.065738	-15.485917	1.495286
H	0.923088	-14.006080	1.571168
C	-3.184319	-6.009355	0.887714
H	-4.027495	-6.164709	1.581661
H	-2.512588	-5.293499	1.386589
C	-2.441992	-7.331505	0.680258
H	-3.124917	-8.087905	0.255842
H	-1.670674	-7.177485	-0.101188
C	-1.778028	-7.875361	1.945165
H	-2.550210	-8.060747	2.712489
H	-1.110368	-7.101584	2.364313
C	-0.977860	-9.158233	1.712418
H	-1.640151	-9.938157	1.302894
H	-0.224176	-8.977157	0.924353
C	-0.279011	-9.672622	2.969482
H	-1.009568	-9.903029	3.760156
H	0.301354	-10.581827	2.758797
H	0.417487	-8.917750	3.365561
C	-3.701731	-5.405818	-0.418086

H -2.911506 -5.407836 -1.193147
H -4.504382 -6.011922 -0.862233
H -4.077139 -4.380836 -0.287193
H 0.898494 -15.130154 2.945340

(3) **n-hexane displaces alkyl chain of D_2**

131

C -6.635271 -2.061397 -2.116065
O -5.406846 -1.858875 -2.025038
Ti -3.719980 -0.829243 -2.153611
Cl -2.647185 -2.776173 -3.234468
Mg -1.238423 -3.796154 -1.488921
Cl -0.551652 -5.892393 -2.496087
Mg 0.914180 -6.720189 -0.712380
Cl 1.435513 -8.930172 -1.435593
Mg 2.834730 -9.546399 0.469683
Cl 2.559030 -11.538146 1.467119
O -7.412924 -0.965398 -2.107109
C -8.839872 -1.089473 -2.187639
C -4.520983 0.460834 -3.589105
C -4.294266 -0.256377 -4.923143
Cl -1.547924 0.550784 -2.282134
Cl -2.209783 -2.025064 0.031600
Cl -4.376768 0.752575 -0.403433
Mg -2.504125 2.298252 -0.618157
Cl -3.376758 4.380710 0.176425
Mg -1.332697 5.728305 0.142992
Cl -2.132892 7.809493 0.981274
Mg -0.060259 9.081873 0.716645
Cl 1.461413 8.348123 2.482933
Mg 2.119907 6.301326 1.449003
Cl 4.011971 5.616472 2.837638
Mg 4.424043 3.463335 1.881290
Cl 6.313828 2.643420 3.278110
Mg 6.449560 0.539216 2.205317
Cl 4.571619 -0.880625 2.925365
Cl 0.079045 11.117578 -0.193664
Cl 5.200680 1.480404 0.300266
Cl 7.608701 -1.413283 1.533408
Mg 5.575104 -2.846512 1.447527
Cl 6.417845 -4.962836 0.716018
Mg 4.330824 -6.254027 0.772351
Cl 5.006700 -8.461386 0.154872
Cl -0.974418 1.388010 1.123500
Cl 0.806500 -2.355978 -1.790459
Cl 4.150167 -1.902798 -0.386771
Cl 2.466579 1.981708 2.406208
Mg 3.182100 0.025829 0.957725
Cl 1.221642 -1.421456 1.536601
Cl 1.798475 0.957664 -0.909940
Mg 2.096885 -3.375241 0.181490
Cl 0.024177 -4.726186 0.624301
Cl 3.002930 -5.315356 -1.168035
Cl 3.500562 -4.185816 2.149777
Mg 0.999582 2.910697 0.467876
Cl -0.484208 3.791406 -1.365589
Cl 0.161894 4.760888 1.970212
Cl 3.017300 4.324948 -0.082254
Mg -0.243752 -0.533881 -0.372286
Cl 0.794598 7.017996 -0.622902
Cl 2.108503 -7.336990 1.544799
H -5.588612 0.614438 -3.366079
H -4.025881 1.443914 -3.571954
H -4.728759 0.323635 -5.755880
H -3.225961 -0.389024 -5.150539

H	-4.764115	-1.252320	-4.954418
H	-9.156982	-1.359323	-3.205508
H	-9.229528	-1.813670	-1.458463
C	-9.420176	0.283267	-1.850517
F	-8.973295	1.235308	-2.698029
F	-10.772524	0.210373	-1.961401
F	-9.115748	0.657006	-0.590099
C	-7.177788	-3.451642	-2.223071
H	-6.446569	-4.007030	-2.829307
H	-8.134676	-3.471512	-2.763930
C	-7.309926	-4.163440	-0.854304
H	-8.140068	-3.732694	-0.270692
H	-6.391266	-3.976968	-0.277709
C	-7.488920	-5.673484	-1.044929
H	-8.481582	-5.890692	-1.474930
H	-6.755452	-6.004331	-1.801758
C	-7.259766	-6.497903	0.228259
H	-8.133445	-6.435366	0.897744
H	-6.415544	-6.057701	0.787023
C	-6.918661	-7.959147	-0.087743
H	-7.798655	-8.475171	-0.508099
H	-6.159155	-7.963453	-0.892048
C	-6.352046	-8.751804	1.095325
H	-7.141327	-8.959838	1.837386
H	-5.603802	-8.125652	1.614413
C	-5.670840	-10.052166	0.656138
H	-6.416013	-10.743695	0.225103
H	-4.972656	-9.813185	-0.166852
C	-4.880802	-10.756753	1.762582
H	-5.568843	-11.168117	2.521816
H	-4.260573	-10.008112	2.289575
C	-3.960743	-11.856961	1.225934
H	-4.560121	-12.646966	0.740162
H	-3.334118	-11.423344	0.424377
C	-3.040937	-12.473854	2.283225
H	-3.630674	-13.090138	2.984192
H	-2.600121	-11.663848	2.891239
C	-1.903747	-13.304595	1.681116
H	-2.322286	-14.149605	1.105706
H	-1.358868	-12.680447	0.949625
C	-0.902963	-13.827469	2.713494
H	-1.415098	-14.502309	3.423393
H	-0.532425	-12.976885	3.312793
C	0.294680	-14.543698	2.083440
H	-0.056153	-15.425345	1.516620
H	0.767558	-13.867740	1.350156
C	-3.239034	-5.994058	0.913852
H	-4.089149	-6.124650	1.604581
H	-2.562667	-5.275866	1.403072
C	-2.510606	-7.328488	0.738936
H	-3.197507	-8.084164	0.319705
H	-1.728363	-7.197003	-0.035721
C	-1.867657	-7.858341	2.020596
H	-2.651869	-8.036027	2.777561
H	-1.206640	-7.080265	2.442307
C	-1.063258	-9.142752	1.812759
H	-1.717825	-9.927698	1.399596
H	-0.298108	-8.967214	1.034235
C	-0.382407	-9.644368	3.084863
H	-1.124529	-9.873660	3.864969
H	0.205775	-10.552502	2.891446
H	0.303251	-8.882993	3.487306
C	-3.739687	-5.412343	-0.408286
H	-2.944625	-5.439143	-1.178117
H	-4.545966	-6.018989	-0.845166
H	-4.104878	-4.380957	-0.301781
C	1.353484	-14.978366	3.100218

H 1.674423 -14.093210 3.675439
H 0.902616 -15.675798 3.828888
C 2.576171 -15.624915 2.445760
H 3.065686 -14.918189 1.758428
H 2.292547 -16.517165 1.864850
H 3.320504 -15.935057 3.194254

(4) **n-hexane displaces alkyl chain of D_6**

92

C 6.299248 -1.046817 -0.403337
O 5.884311 0.106907 -0.649450
Ti 4.495808 1.351915 -1.396118
Cl 4.323144 2.558785 0.808066
Mg 2.397732 1.585839 1.886948
Cl 2.259113 2.903330 3.913655
Mg 0.517018 1.671252 5.079531
Cl 0.301863 2.846131 7.155235
Mg -1.333684 1.353905 8.188474
Cl -1.157750 0.524639 10.260902
O 7.489238 -1.218173 0.171221
C 8.223992 -0.027368 0.521275
C 5.582414 2.995595 -2.035805
C 7.001136 3.140722 -1.496562
Cl 2.657337 -0.227665 0.012137
Cl 2.328242 2.178790 -2.515597
Cl 4.600366 -0.086352 -3.404771
Mg 2.489444 0.467535 -4.476147
Cl 2.873260 -0.502939 -6.636365
Mg 0.682039 -0.160482 -7.629175
Cl 0.981417 -1.218820 -9.743889
Mg -1.180040 -0.612855 -10.696724
Cl -2.834274 -2.070209 -9.643845
Mg -2.948220 -0.932599 -7.552363
Cl -4.816806 -2.059814 -6.455942
Mg -4.811450 -0.886965 -4.371983
Cl -1.447095 0.292197 -12.717901
Cl -3.495679 1.907471 7.199486
Mg -3.134301 0.863856 5.091711
Cl -5.338247 1.157023 4.072280
Mg -4.921471 0.124774 1.965125
Cl -7.132990 0.334349 0.835988
Mg -6.416043 -0.652947 -1.188210
Cl -4.500815 -1.630445 0.019165
Cl -6.773250 -1.858071 -3.195855
Cl -5.001652 0.927980 -2.444510
Cl 0.332006 2.307222 0.625900
Cl 0.889975 -0.969609 -3.196000
Cl -3.327972 1.591988 0.692381
Cl -2.747065 -1.633859 -3.147569
Mg -2.937036 -0.002681 -1.220509
Cl -0.924458 -0.883895 -0.011250
Cl -1.382575 1.543106 -2.458844
Mg -1.177145 -0.009688 -4.431770
Cl 0.434994 1.533068 -5.605896
Cl -0.869832 -1.680551 -6.294758
Mg -1.212019 0.706407 1.943380
Cl 0.870373 -0.073974 3.125346
Cl -1.583022 2.376849 3.781625
Cl -2.836731 -0.857646 3.118650
Cl -3.291334 0.794284 -5.575926
Mg 0.705777 0.657632 -1.246057
Cl -0.992129 -0.167682 6.100765
Cl -1.455191 0.901948 -8.578068
H 8.551900 0.506221 -0.380984
H 7.611980 0.640532 1.142829

H 5.573363 2.809877 -3.128811
H 4.965511 3.888634 -1.839061
H 7.622860 2.272737 -1.764837
H 7.502557 4.033669 -1.905744
H 7.004176 3.241771 -0.400593
C 9.442910 -0.487227 1.310302
F 10.238867 -1.298488 0.576739
F 10.162802 0.604560 1.669269
F 9.088943 -1.152938 2.435172
C 5.555084 -2.302368 -0.724464
H 4.502131 -2.105327 -0.470506
H 5.565711 -2.384485 -1.826317
C 6.076273 -3.576267 -0.063819
H 6.040683 -3.500560 1.031006
H 7.111451 -3.792500 -0.356617
C 4.493530 -0.261393 4.045586
H 3.797968 0.535721 3.718766
H 5.289949 0.281880 4.580397
C 3.744978 -1.177514 5.013844
H 2.933207 -1.695328 4.475062
H 4.430622 -1.965226 5.372645
C 3.167732 -0.439333 6.221420
H 2.498975 0.374176 5.859515
H 3.972785 0.093704 6.756258
C 2.391064 -1.325370 7.195913
H 1.508131 -1.741214 6.682312
H 3.021233 -2.188181 7.472079
C 1.958740 -0.577659 8.455718
H 1.403960 0.339346 8.202530
H 1.305355 -1.181031 9.099045
H 2.825576 -0.259243 9.053807
C 5.076482 -0.983204 2.832402
H 5.859991 -1.695025 3.131477
H 4.297946 -1.543289 2.291582
H 5.520893 -0.262415 2.130190
H 5.450118 -4.425341 -0.366850

(5) **n-hexane displaces alkyl chain of D_7**

98

C 6.438295 -0.940593 -0.295648
O 5.995372 0.191790 -0.588533
Ti 4.573326 1.374525 -1.368891
Cl 4.368692 2.648232 0.798880
Mg 2.476916 1.653350 1.917912
Cl 2.310427 3.004965 3.921649
Mg 0.604607 1.745339 5.118089
Cl 0.381197 2.927499 7.188952
Mg -1.239148 1.424804 8.235891
Cl -1.065749 0.621400 10.319050
O 7.625918 -1.060179 0.300458
C 8.323468 0.159168 0.628994
C 5.635022 3.015599 -2.052238
C 7.040632 3.222518 -1.499804
Cl 2.767484 -0.194104 0.079060
Cl 2.387010 2.136649 -2.506944
Cl 4.692001 -0.125661 -3.330035
Mg 2.577135 0.379594 -4.417437
Cl 2.964431 -0.619275 -6.562834
Mg 0.766312 -0.309099 -7.555366
Cl 1.079437 -1.369218 -9.666046
Mg -1.096244 -0.808017 -10.615473
Cl -2.721999 -2.291169 -9.551487
Mg -2.849985 -1.146566 -7.463749
Cl -4.685791 -2.305949 -6.343393
Mg -4.695732 -1.109064 -4.273120

Cl	-1.373897	0.082116	-12.642039
Cl	-3.411203	1.941151	7.245692
Mg	-3.039992	0.883653	5.147888
Cl	-5.248494	1.137940	4.121201
Mg	-4.819611	0.057716	2.040198
Cl	-7.033123	0.189240	0.903484
Mg	-6.298037	-0.851593	-1.088783
Cl	-4.358899	-1.744192	0.144586
Cl	-6.622061	-2.114557	-3.068011
Cl	-4.926523	0.735034	-2.382184
Cl	0.393935	2.303146	0.647074
Cl	1.001730	-1.049798	-3.103118
Cl	-3.251349	1.517214	0.731942
Cl	-2.615530	-1.784601	-3.035189
Mg	-2.835416	-0.116134	-1.142313
Cl	-0.801651	-0.922679	0.084764
Cl	-1.317572	1.433745	-2.418844
Mg	-1.083534	-0.154881	-4.358275
Cl	0.498815	1.397743	-5.561349
Cl	-0.756128	-1.843168	-6.201265
Mg	-1.117230	0.703017	2.003249
Cl	0.985786	-0.016292	3.191608
Cl	-1.510171	2.398147	3.814150
Cl	-2.717071	-0.864746	3.213147
Cl	-3.219458	0.590056	-5.505881
Mg	0.794106	0.622526	-1.192000
Cl	-0.878543	-0.106309	6.164079
Cl	-1.396123	0.708470	-8.507684
H	8.797268	0.581310	-0.267374
H	7.640073	0.898305	1.068747
H	5.648248	2.772385	-3.134533
H	4.993716	3.901906	-1.912379
H	7.683156	2.351583	-1.699933
H	7.532451	4.097689	-1.956173
H	7.019900	3.392650	-0.412746
C	9.398523	-0.206842	1.645371
F	10.268907	-1.118401	1.154827
F	10.091411	0.914800	1.964121
F	8.860954	-0.710555	2.782059
C	5.729046	-2.223411	-0.578764
H	4.654643	-2.009784	-0.469146
H	5.870589	-2.425531	-1.656997
C	6.145189	-3.432163	0.263574
H	6.065890	-3.176041	1.331896
H	7.203537	-3.674077	0.079812
C	5.267736	-4.652146	-0.035021
H	4.209242	-4.385004	0.127868
H	5.355776	-4.913965	-1.103315
C	5.631013	-5.862030	0.826595
H	5.516146	-5.636171	1.897958
H	6.674313	-6.171185	0.661493
H	4.987025	-6.722593	0.597226
C	4.608516	-0.081957	4.138642
H	3.903866	0.711655	3.824071
H	5.400334	0.462281	4.679306
C	3.873039	-1.020797	5.094777
H	3.074680	-1.550095	4.547171
H	4.571805	-1.797796	5.451416
C	3.273797	-0.303340	6.303786
H	2.592618	0.501024	5.944072
H	4.064738	0.240391	6.848886
C	2.505990	-1.211226	7.264757
H	1.634565	-1.638135	6.740733
H	3.149464	-2.064916	7.538292
C	2.050978	-0.481816	8.527276
H	1.488455	0.431154	8.277037
H	1.398028	-1.099452	9.157269

H 2.907181 -0.159125 9.138162
C 5.197683 -0.782260 2.916439
H 5.991393 -1.485909 3.206657
H 4.425331 -1.347030 2.371370
H 5.632171 -0.049700 2.220346

(6) **n-hexane displaces alkyl chain of D_8**

104

C 6.552886 -0.840240 -0.328619
O 6.069132 0.269604 -0.643624
Ti 4.608479 1.406110 -1.415873
Cl 4.355810 2.709966 0.738386
Mg 2.519836 1.653573 1.881254
Cl 2.249943 2.980571 3.892156
Mg 0.706244 1.529314 5.101728
Cl 0.482422 2.575462 7.237533
Mg -1.061966 0.964092 8.232828
Cl -0.831852 0.090353 10.280598
O 7.779608 -0.909658 0.193230
C 8.472620 0.337454 0.405251
C 5.602022 3.079743 -2.128754
C 7.006016 3.337474 -1.592779
Cl 2.860339 -0.190145 0.026696
Cl 2.399271 2.121528 -2.544464
Cl 4.753308 -0.106556 -3.361860
Mg 2.634577 0.373589 -4.454773
Cl 3.027320 -0.596841 -6.610239
Mg 0.821418 -0.303079 -7.593273
Cl 1.145755 -1.327098 -9.718164
Mg -1.033809 -0.776274 -10.662643
Cl -2.639426 -2.293352 -9.624260
Mg -2.781910 -1.187142 -7.515614
Cl -4.604997 -2.386687 -6.422490
Mg -4.596428 -1.260507 -4.311479
Cl -1.316999 0.134155 -12.679069
Cl -3.262347 1.437477 7.288013
Mg -2.885391 0.460328 5.153955
Cl -5.119001 0.653098 4.165721
Mg -4.678564 -0.336890 2.043506
Cl -6.916654 -0.274679 0.940905
Mg -6.155297 -1.189471 -1.099071
Cl -4.166237 -2.047112 0.082374
Cl -6.466358 -2.374722 -3.123808
Cl -4.868565 0.505592 -2.344071
Cl 0.391971 2.196846 0.644243
Cl 1.089977 -1.095306 -3.155932
Cl -3.195448 1.239820 0.772559
Cl -2.493956 -1.924847 -3.103833
Mg -2.733169 -0.311363 -1.161813
Cl -0.656769 -1.073122 0.025937
Cl -1.286861 1.319518 -2.420525
Mg -1.015351 -0.228712 -4.392553
Cl 0.530113 1.369365 -5.578901
Cl -0.677267 -1.881523 -6.268188
Mg -1.004703 0.488863 1.989451
Cl 1.170243 -0.139845 3.133165
Cl -1.462771 2.103849 3.858246
Cl -2.510481 -1.198522 3.157307
Cl -3.172592 0.501313 -5.505721
Mg 0.856623 0.562586 -1.229994
Cl -0.656759 -0.455640 6.099130
Cl -1.357493 0.702892 -8.526782
H 8.890028 0.707073 -0.540948
H 7.801179 1.093477 0.833721
H 5.612381 2.835730 -3.210617

H	4.932618	3.943870	-1.983460
H	7.679795	2.494524	-1.808995
H	7.456443	4.234939	-2.048466
H	6.994753	3.499448	-0.504153
C	9.606425	0.058286	1.382960
F	10.484546	-0.848158	0.896937
F	10.273247	1.218200	1.610257
F	9.140924	-0.403317	2.567842
C	5.854349	-2.149459	-0.495978
H	4.777845	-1.928892	-0.465951
H	6.056974	-2.489947	-1.528301
C	6.223252	-3.238671	0.520713
H	6.193064	-2.810797	1.534160
H	7.258433	-3.575144	0.357059
C	5.257336	-4.425624	0.451086
H	4.221258	-4.054199	0.547709
H	5.319781	-4.903196	-0.542499
C	5.518477	-5.467651	1.542366
H	5.465748	-4.975849	2.530484
H	6.549819	-5.852121	1.448175
C	4.823587	0.174403	4.137903
H	4.044625	0.914629	3.878853
H	5.564866	0.753605	4.712511
C	4.192270	-0.894684	5.030358
H	3.447884	-1.466893	4.450067
H	4.967168	-1.618200	5.337768
C	3.531737	-0.316754	6.282031
H	2.762140	0.427567	5.976946
H	4.266375	0.277948	6.852066
C	2.880615	-1.354814	7.196472
H	2.040472	-1.831497	6.663998
H	3.611913	-2.155597	7.399170
C	2.392838	-0.756018	8.514591
H	1.718906	0.096305	8.340637
H	1.840521	-1.482169	9.125092
H	3.231105	-0.372883	9.115822
C	5.467932	-0.381987	2.870365
H	6.320841	-1.032602	3.113288
H	4.745232	-0.976490	2.288605
H	5.831939	0.431025	2.224370
C	4.534157	-6.641343	1.513444
H	3.504712	-6.250525	1.589640
H	4.597378	-7.144283	0.533181
C	4.780841	-7.657078	2.630844
H	4.682344	-7.188164	3.622176
H	5.793499	-8.084275	2.565469
H	4.064487	-8.490018	2.583848

(I) Solvent phase calculations

(1) RC

72

C	0.951679	1.223420	0.097365
O	1.328251	1.293233	1.384186
C	1.590388	0.034687	2.042551
O	0.800685	0.151593	-0.489751
Al	1.371693	-1.666904	-1.191183
C	3.352395	-1.514350	-0.841017
C	3.990139	-0.141576	-1.119227
C	0.792249	-1.489676	-3.097961
C	-0.722897	-1.301278	-3.294049
C	0.279595	-2.874513	-0.017222
C	0.217860	-4.332273	-0.515078
H	0.693587	-0.599135	2.046813
H	2.416134	-0.497571	1.551394

H	3.829179	-2.267777	-1.496202
H	3.602573	-1.845624	0.184425
H	5.089294	-0.144129	-1.021316
H	3.625463	0.635794	-0.424258
H	3.758468	0.214670	-2.136134
H	1.129105	-2.384927	-3.653426
H	1.338149	-0.646370	-3.560805
H	-1.291302	-2.154039	-2.887995
H	-1.088494	-0.402024	-2.771307
H	-1.014922	-1.195613	-4.353646
H	-0.746784	-2.467280	0.046964
H	-0.188398	-4.392741	-1.537971
H	1.217752	-4.795648	-0.544200
H	-0.413774	-4.978480	0.118784
H	0.668183	-2.860272	1.018107
C	1.985977	0.362618	3.472428
F	0.997736	1.007407	4.140084
F	2.251807	-0.795117	4.131449
F	3.095174	1.139832	3.526344
C	0.743507	2.569987	-0.528018
H	1.743905	3.032446	-0.610499
H	0.187601	3.199810	0.184819
C	0.059145	2.503344	-1.893063
H	0.640868	1.847744	-2.559897
H	-0.927361	2.024969	-1.781175
C	-0.108469	3.881552	-2.536110
H	0.882138	4.354633	-2.659139
H	-0.682828	4.539927	-1.860080
C	-0.813230	3.809344	-3.893992
H	-0.239177	3.146673	-4.565740
H	-1.799403	3.328768	-3.763730
C	-1.004108	5.171218	-4.566334
H	-0.019154	5.649248	-4.714969
H	-1.568827	5.837212	-3.889235
C	-1.734842	5.079318	-5.909318
H	-1.163064	4.423880	-6.590546
H	-2.709610	4.581513	-5.756349
C	-1.965961	6.432969	-6.585676
H	-0.993370	6.927955	-6.759548
H	-2.526020	7.092739	-5.898619
C	-2.725993	6.323252	-7.910804
H	-2.160282	5.673211	-8.602349
H	-3.689620	5.811685	-7.733299
C	-2.991801	7.670462	-8.587192
H	-2.030294	8.180269	-8.779704
H	-3.549257	8.323417	-7.891557
C	-3.773345	7.547346	-9.898465
H	-3.214468	6.897531	-10.595858
H	-4.730455	7.030240	-9.702340
C	-4.057677	8.889586	-10.576979
H	-3.101732	9.403255	-10.787503
H	-4.606567	9.544015	-9.875649
C	-4.858692	8.761089	-11.876341
H	-4.308839	8.108556	-12.576791
H	-5.811278	8.244681	-11.663393
C	-5.144088	10.107158	-12.545395
H	-4.208551	10.629883	-12.800008
H	-5.720738	10.766990	-11.878144
H	-5.721188	9.984693	-13.474051

(2) $AlEt_3$

22

Al	0.150786	-0.149735	-0.223612
C	1.980477	-0.931600	-0.142503
C	-0.130705	1.776693	0.200338

C	-1.418724	-1.316315	-0.613483
H	0.123517	1.912570	1.269184
H	0.636160	2.366317	-0.334986
C	-1.533728	2.341905	-0.082413
C	-2.204351	-1.687509	0.664820
H	-2.093989	-0.796965	-1.316452
H	-1.092019	-2.235735	-1.128682
H	1.938966	-1.786205	0.559301
H	2.187108	-1.399646	-1.123522
C	3.128113	0.017950	0.244989
H	-3.086422	-2.312176	0.445866
H	-1.584133	-2.253228	1.378834
H	-2.571180	-0.794152	1.196294
H	4.105121	-0.493037	0.278705
H	3.225114	0.851343	-0.468439
H	2.966332	0.469880	1.236402
H	-1.628024	3.402452	0.206065
H	-1.791334	2.275682	-1.151224
H	-2.314536	1.789095	0.463714

(3) TS_{1KPM}

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C	-0.042476	-0.100032	0.357630
O	-0.208337	0.425408	1.616679
C	0.486711	-0.238203	2.667241
O	1.051348	-0.743518	0.122242
Al	2.128213	-2.130223	-0.475350
C	3.371785	-2.529267	1.021556
C	4.390608	-1.400307	1.276179
C	2.757363	-1.862769	-2.344909
C	1.853676	-2.342343	-3.493660
C	0.497674	-3.755507	-0.496808
Al	-1.552331	-3.882979	-0.024244
C	-2.649775	-4.278493	-1.652602
C	-2.430702	-3.304637	-2.823538
C	1.236619	-5.017890	-0.942366
C	-1.806102	-4.855328	1.711999
C	-1.019376	-4.264391	2.895176
C	-1.593450	-1.749948	0.407212
C	-2.898072	-1.149544	0.865091
H	0.390841	-1.333421	2.594188
H	1.555192	0.023813	2.673191
H	3.906570	-3.473593	0.819394
H	2.788829	-2.719090	1.941726
H	5.062795	-1.618629	2.122200
H	3.892824	-0.442337	1.500964
H	5.029809	-1.223405	0.396508
H	3.745626	-2.349676	-2.425320
H	2.967188	-0.782887	-2.460659
H	1.686046	-3.429807	-3.451931
H	0.861572	-1.865221	-3.468560
H	2.282857	-2.123387	-4.485142
H	-3.718730	-4.293741	-1.375558
H	-2.427084	-5.310140	-1.982549
H	-1.374706	-3.270386	-3.140481
H	-3.018833	-3.566094	-3.720031
H	-2.715781	-2.273291	-2.553760
H	-1.513869	-5.911309	1.563664
H	-2.880559	-4.890876	1.964108
H	0.063619	-4.202647	2.684237
H	-1.118273	-4.855442	3.821402
H	-1.360182	-3.244200	3.141419
H	0.346953	-2.988989	-1.279418
H	-0.851171	-1.994884	1.167368
H	-1.274936	-1.617822	-0.626714

H	-3.364350	-1.753862	1.658709
H	-2.777415	-0.132225	1.281752
H	-3.620436	-1.090380	0.037571
H	2.299952	-4.875162	-1.207141
H	1.206230	-5.775233	-0.145505
H	0.745293	-5.456519	-1.822785
H	0.760268	-3.386595	0.511844
C	-0.635817	0.842813	-0.663109
H	-1.692453	1.014924	-0.409944
H	-0.123413	1.811215	-0.510895
C	-0.469119	0.398867	-2.111960
H	0.602202	0.268967	-2.331553
H	-0.937760	-0.589645	-2.263135
C	-1.083714	1.387950	-3.104503
H	-2.155995	1.519898	-2.875163
H	-0.617950	2.380501	-2.968181
C	-0.927288	0.951597	-4.563223
H	0.143779	0.795922	-4.784764
H	-1.413241	-0.030582	-4.705009
C	-1.510000	1.960618	-5.555804
H	-2.581264	2.113939	-5.333310
H	-1.025129	2.941578	-5.400209
C	-1.352675	1.551726	-7.022301
H	-0.283464	1.378254	-7.239971
H	-1.858320	0.583699	-7.189916
C	-1.905123	2.592501	-7.999989
H	-2.974287	2.766158	-7.782009
H	-1.399498	3.559185	-7.822392
C	-1.746508	2.207190	-9.472793
H	-0.679452	2.016599	-9.687043
H	-2.269339	1.251875	-9.660182
C	-2.272731	3.272890	-10.438112
H	-3.339348	3.464972	-10.222993
H	-1.748765	4.226736	-10.245201
C	-2.114431	2.902222	-11.914809
H	-1.049402	2.698366	-12.127217
H	-2.649917	1.956175	-12.113622
C	-2.622299	3.983075	-12.872865
H	-3.686963	4.189059	-12.659931
H	-2.085653	4.928458	-12.672538
C	-2.465777	3.620046	-14.352186
H	-1.402682	3.409488	-14.562237
H	-3.006914	2.678952	-14.553175
C	-2.968762	4.713707	-15.296593
H	-4.037415	4.921360	-15.130002
H	-2.421034	5.656247	-15.139659
C	-0.145802	0.196544	3.980510
F	-0.066850	1.535456	4.172930
F	-1.453839	-0.155627	4.050843
F	0.506337	-0.413515	5.007445
H	-2.845036	4.428238	-16.351608

(4) TS_{1APM}

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C	1.500375	0.120031	-1.556323
O	2.453192	-0.304308	-2.511215
C	3.805375	-0.230143	-2.081908
O	1.833830	-0.118352	-0.289587
Al	1.861434	0.917057	1.197812
C	0.198360	0.947486	2.287484
C	-0.176321	-0.425829	2.877936
C	2.052928	2.840655	0.126632
C	1.709684	2.777649	-1.232588
C	3.598966	0.661594	2.173573
C	3.787137	1.681609	3.307733

Al	5.987251	-0.518148	2.186748
C	6.067371	-0.971368	4.135250
C	4.896864	-1.759410	4.747252
C	7.039312	1.070571	1.558922
C	6.722929	1.609409	0.153475
C	5.643391	-1.986393	0.866304
C	4.295009	-2.729289	0.909345
H	6.997983	-1.563098	4.242067
H	4.363685	0.774204	1.377403
H	3.588072	-0.380209	2.546830
H	3.105153	3.025658	0.368761
H	1.327727	3.317733	0.797422
H	-0.640860	1.344103	1.690065
H	6.948911	1.882030	2.303113
H	8.103406	0.768165	1.599897
H	6.460594	-2.714209	1.037021
H	5.833512	-1.601167	-0.152279
H	-1.079474	-0.382406	3.509299
H	-0.371256	-1.169097	2.088166
H	0.632753	-0.835365	3.504520
H	2.975209	1.598168	4.046216
H	4.734188	1.561838	3.857206
H	3.770318	2.714233	2.924722
H	7.371941	2.451458	-0.141519
H	6.834760	0.832052	-0.618563
H	5.684651	1.981280	0.082634
H	4.244599	-3.561714	0.186112
H	4.100109	-3.159826	1.903954
H	3.448355	-2.061202	0.684873
H	4.058199	0.750208	-1.644708
H	4.046151	-1.011871	-1.346754
H	0.345028	1.675551	3.106371
H	6.251792	-0.054511	4.722759
H	5.066761	-2.021136	5.805645
H	3.956422	-1.185340	4.711262
H	4.714174	-2.702957	4.209125
H	1.479032	1.347573	-1.643077
H	2.482250	2.873592	-2.002039
H	0.708268	3.074437	-1.557052
C	0.128435	-0.348169	-2.034502
H	-0.002212	-0.013307	-3.075173
H	0.159254	-1.450585	-2.050762
C	-1.018518	0.138330	-1.152698
H	-0.859103	-0.220250	-0.123674
H	-1.009492	1.241622	-1.098665
C	-2.392575	-0.326635	-1.640768
H	-2.569154	0.048309	-2.664745
H	-2.399107	-1.428600	-1.712420
C	-3.532058	0.128798	-0.725150
H	-3.347904	-0.248411	0.297012
H	-3.519882	1.231072	-0.648639
C	-4.915951	-0.329584	-1.192694
H	-5.101880	0.052367	-2.212872
H	-4.926606	-1.431300	-1.273339
C	-6.051078	0.120411	-0.268866
H	-5.864200	-0.263431	0.750432
H	-6.038388	1.222129	-0.185905
C	-7.437501	-0.334763	-0.733150
H	-7.626361	0.051918	-1.751068
H	-7.449158	-1.436172	-0.819203
C	-8.570513	0.110980	0.195447
H	-8.380383	-0.275710	1.213123
H	-8.558966	1.212439	0.281781
C	-9.957692	-0.344807	-0.266220
H	-10.149764	0.044481	-1.282549
H	-9.967771	-1.445994	-0.355596
C	-11.089591	0.096056	0.666187

H	-10.895678	-0.291903	1.682711
H	-11.080885	1.197410	0.754435
C	-12.476550	-0.362843	0.207240
H	-12.672471	0.026725	-0.808432
H	-12.484689	-1.464127	0.116614
C	-13.609406	0.073497	1.141280
H	-13.411863	-0.315910	2.155450
H	-13.600626	1.173726	1.230808
C	-14.989831	-0.392508	0.672511
H	-15.226521	0.009960	-0.325067
H	-15.035025	-1.490884	0.604861
C	4.685044	-0.428157	-3.305001
F	4.502292	0.549584	-4.232450
F	5.995389	-0.396458	-2.930068
F	4.461436	-1.616871	-3.917062
H	-15.783590	-0.067135	1.361277

(5) Int_{1KPM}

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C	-0.182753	1.121862	2.385924
O	-0.208760	2.266633	3.312525
C	0.242812	2.027022	4.627506
O	0.951917	0.380301	2.608097
Al	2.142968	-0.880518	2.366958
C	3.311313	-1.045051	3.963732
C	4.353205	0.089326	4.057101
C	2.765159	-1.344122	0.529422
C	1.997792	-2.389724	-0.299538
C	0.378490	-2.768501	2.894733
Al	-1.598723	-2.602029	3.249823
C	-2.846110	-3.023353	1.759240
C	-2.230291	-3.001837	0.348835
C	0.971702	-4.185564	2.945148
C	-2.167416	-2.354287	5.138970
C	-1.022265	-2.069516	6.127491
C	-1.433777	0.242258	2.632307
C	-2.784255	0.931707	2.463623
H	0.657500	1.014592	4.751466
H	1.034904	2.750472	4.880667
H	3.823051	-2.023419	3.950555
H	2.686134	-1.047208	4.874768
H	4.994485	-0.002422	4.949546
H	3.870826	1.078581	4.106525
H	5.023207	0.103152	3.182148
H	3.815477	-1.668923	0.641487
H	2.816272	-0.392737	-0.031464
H	1.988369	-3.374617	0.192549
H	0.945412	-2.103799	-0.459731
H	2.440415	-2.533154	-1.299001
H	-3.713668	-2.341859	1.810132
H	-3.265839	-4.025114	1.969282
H	-1.384271	-3.701754	0.260101
H	-2.957911	-3.273905	-0.433219
H	-1.841285	-2.004779	0.084660
H	-2.715444	-3.263922	5.446382
H	-2.919328	-1.545884	5.186070
H	-0.286402	-2.889071	6.149204
H	-1.383018	-1.929558	7.159224
H	-0.469318	-1.154250	5.861522
H	0.508923	-2.332036	1.882605
H	-1.334517	-0.144857	3.663037
H	-1.355432	-0.603699	1.920824
H	-3.602740	0.272968	2.787977
H	-2.825201	1.847726	3.066435
H	-2.969041	1.200769	1.413752

H	2.057062	-4.203593	2.753448
H	0.813181	-4.646659	3.932150
H	0.499821	-4.842265	2.198855
H	0.837129	-2.129871	3.674808
C	-0.186099	1.806964	1.012703
H	-1.002946	2.545265	0.990580
H	0.756969	2.372654	0.954072
C	-0.298733	0.847878	-0.169833
H	0.462784	0.057925	-0.070143
H	-1.278425	0.339155	-0.157303
C	-0.124295	1.540882	-1.523077
H	-0.917533	2.299278	-1.650540
H	0.831522	2.094605	-1.528115
C	-0.151712	0.569972	-2.706144
H	0.683956	-0.146161	-2.606459
H	-1.076667	-0.033516	-2.663663
C	-0.067701	1.269252	-4.065126
H	-0.926615	1.956553	-4.170730
H	0.835726	1.905167	-4.093037
C	-0.043197	0.308024	-5.255916
H	0.842208	-0.348322	-5.176652
H	-0.923125	-0.358919	-5.205423
C	-0.028451	1.021651	-6.610484
H	-0.927246	1.659344	-6.692699
H	0.836419	1.708740	-6.651359
C	0.026025	0.072306	-7.809919
H	0.939289	-0.546257	-7.744385
H	-0.824029	-0.632276	-7.756674
C	-0.001386	0.794660	-9.159797
H	-0.922083	1.402024	-9.227168
H	0.839369	1.510751	-9.207208
C	0.070502	-0.146810	-10.364763
H	1.000211	-0.741287	-10.307497
H	-0.760104	-0.874135	-10.309136
C	0.016175	0.578860	-11.711979
H	-0.919305	1.164157	-11.772524
H	0.839093	1.315379	-11.763682
C	0.102930	-0.357517	-12.920655
H	1.042431	-0.934444	-12.863719
H	-0.713594	-1.098805	-12.863220
C	0.033254	0.379884	-14.259833
H	-0.912920	0.935056	-14.357268
H	0.854818	1.107335	-14.355411
C	-0.864537	2.225001	5.655570
F	-1.444056	3.450246	5.564095
F	-1.867802	1.304387	5.545283
F	-0.351255	2.105107	6.915493
H	0.102539	-0.314760	-15.110108

(6) Int_{1APM}

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C	1.609218	-0.584168	-1.796366
O	2.508513	-1.322081	-2.701923
C	3.830902	-1.459128	-2.255673
O	1.879639	-0.900594	-0.479806
Al	2.010991	0.134360	0.960387
C	1.470952	-0.855789	2.591943
C	-0.030250	-1.215535	2.571391
C	1.785800	2.094492	0.700200
C	0.401115	2.614261	1.140095
Al	6.402155	-0.574950	0.441637
C	6.683538	-2.539402	0.329054
C	7.733557	-3.051280	-0.673442
C	4.615455	0.034736	1.182560
C	4.777444	0.773214	2.525466

C	7.801881	0.830628	0.363089
C	9.038012	0.545245	-0.508227
H	6.945096	-2.879775	1.349332
H	1.966656	2.349419	-0.358630
H	2.571968	2.623521	1.266758
H	1.702555	-0.261564	3.492287
H	4.194128	0.695788	0.400033
H	4.020901	-0.895130	1.283872
H	8.117474	1.039160	1.402796
H	7.309020	1.762067	0.028990
H	-0.338654	-1.775087	3.470340
H	-0.667973	-0.318102	2.519945
H	-0.282691	-1.840094	1.699827
H	0.203720	2.395511	2.201662
H	0.304935	3.705528	1.012965
H	-0.414384	2.151911	0.561688
H	3.826833	1.137076	2.950007
H	5.231046	0.120149	3.286448
H	5.432067	1.649978	2.413309
H	9.749369	1.387677	-0.511512
H	9.588336	-0.340608	-0.156224
H	8.761852	0.352801	-1.556520
H	3.878621	-1.630737	-1.167980
H	4.278558	-2.320882	-2.770977
H	2.070821	-1.778140	2.677404
H	5.704258	-3.010131	0.125020
H	7.815854	-4.150690	-0.667774
H	7.491127	-2.750572	-1.704516
H	8.734906	-2.650845	-0.454147
H	1.764877	0.496404	-1.993667
C	0.203383	-0.999681	-2.213910
H	0.100421	-0.843340	-3.299828
H	0.109639	-2.080919	-2.021897
C	-0.878757	-0.228241	-1.456803
H	-0.709332	-0.343917	-0.372411
H	-0.787033	0.851322	-1.672919
C	-2.300932	-0.696493	-1.776147
H	-2.503012	-0.563163	-2.853770
H	-2.373657	-1.781776	-1.582837
C	-3.372419	0.031510	-0.958951
H	-3.141572	-0.078448	0.116383
H	-3.323600	1.114734	-1.171304
C	-4.792997	-0.476497	-1.220321
H	-5.033460	-0.356442	-2.292038
H	-4.831110	-1.562515	-1.019658
C	-5.861839	0.226287	-0.378203
H	-5.607288	0.120209	0.691956
H	-5.840541	1.310488	-0.589896
C	-7.276711	-0.309734	-0.612512
H	-7.539981	-0.192189	-1.679220
H	-7.289924	-1.396758	-0.414129
C	-8.342805	0.370852	0.250845
H	-8.069777	0.262772	1.316237
H	-8.341302	1.456478	0.045347
C	-9.753223	-0.183884	0.035451
H	-10.033736	-0.065989	-1.026830
H	-9.749201	-1.271667	0.229831
C	-10.815245	0.480449	0.916315
H	-10.528154	0.368634	1.977626
H	-10.826231	1.567309	0.717486
C	-12.223071	-0.084945	0.714059
H	-12.514812	0.030901	-0.345591
H	-12.210520	-1.172829	0.908157
C	-13.283676	0.571522	1.603125
H	-12.988734	0.457293	2.660959
H	-13.297719	1.657801	1.406995
C	-14.685172	-0.005946	1.396451

H	-15.017884	0.124667	0.354656
H	-14.705884	-1.084827	1.617137
C	4.709982	-0.250851	-2.574800
F	4.208138	0.923407	-2.126338
F	5.955942	-0.407173	-1.925336
F	4.991177	-0.106165	-3.880725
H	-15.425853	0.482262	2.047257

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C	-0.410509	0.000001	-1.662305
C	-0.410502	0.000000	-0.327584
H	-0.410504	0.929476	-2.236787
H	-0.410503	-0.929476	-2.236785
H	-0.410505	0.929467	0.246873
H	-0.410506	-0.929467	0.246873