Supporting Information

New insights into cyclopropanation: Application in the synthesis of novel high-heating-value hydrocarbon fuel derived from furfural

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1. Experimental section

Materials: Furfural, cyclopentanone, dicyclopentadiene, tetrahydropyrrole, chloroiodomethane, bromoiodomethane, ammonia, aniline, 1,3-propanediamine, and diethylamine are purchased from Adamas. Dichloromethane, *n*-hexane and sodium hydroxide are obtained from Chron Chemicals. Tetrahydrofuran, N,N-dimethylformamide are obtained from Greagent. 5wt% Pd/C, 5wt% Pt/C, palladium nitrate, triethylaluminum, diethylzinc, and diiodomethane are purchased from Aladdin. ZSM-5 (H type, Si/Al=25) is purchased from Nankai Catalysts Company. Cyclopentadiene is prepared by distillation of dicyclopentadiene at 438 K. HZSM-5 is calcined in air at the temperature of 823 K for 12 h before used.

Synthesis of ZIF-8: According to the literature[1], a mixture of 2-methylimidazole (1.32 g), zinc nitrate tetrahydrate ($Zn(NO_3)_2 \cdot 4H_2O$, 0.60 g) and methanol (44 mL) is vigorously stirred at room temperature for 24 h. The generated precipitate is collected by centrifugation, washed with methanol and dried at 333 K for 12 h.

Synthesis of Pd/HZSM-5: The Pd/HZSM-5 catalyst is prepared by incipient wetness impregnation method. An appropriate amount of HZSM-5 and water is added into a flask, then $Pd(NO_3)_2$ solution is added gradually and stirred at room temperature for 30 minutes. After drying at 343 K overnight, the calcination and reduction of the samples are performed in 100 $mL \cdot min^{-1}$ of air and 50 $mL \cdot min^{-1}$ of 5 vol% H_2/Ar at 623 K for 3 h with 2 $K \cdot min^{-1}$ heating rate, respectively.

Synthesis of CPO (Hydrogenation/rearrangement): The hydrogenation/rearrangement reaction of FFA is carried out in a high-pressure batch reactor (50 mL, AHZN-50KJ, Shanghai Huotong Laboratory Equipment Co., Ltd.). In a typical reaction, 5.2 mmol FFA, 25 mg catalyst, and 30 mL water as the solvent are added into the reactor. The air residual inside the reactor is discharged by filling and releasing hydrogen for several times. The reaction is conducted at 433 K under 5 MPa hydrogen. The stirring speed is 500 rpm for eliminating the mass transfer limitation issue.

Synthesis of K-CPO (Knoevenagel condensation): The Knoevenagel condensation reaction is carried out at 293 K in a three-neck flask with 4 mL of methanol and 10 mmol catalyst. Then, the mixed solution of 100 mmol cycloketone and 150 mmol freshly prepared cyclopentadiene is added into the flash. The mixture is stirred for 1 h. After the reaction is completed, the mixture is washed by deionized water until the pH = 7. Finally, the product is purified using a chromatography column and concentrated using a rotary evaporator.

Synthesis of TCPP (Cyclopropanation): The cyclopropanation is conducted in a jacketed three-neck reactor at 253 K under a nitrogen atmosphere. Then, 30 mL solvent, 8 mmol diethylzinc /triethylaluminum, and 8 mmol diiodomethane /chloroiodomethane /bromoiodomethane are added to the reactor. After stirring for 20 minutes, 2.7 mmol olefin is added. The reactant is stirred for 6 h. After the reaction is completed, deionized water is slowly added to quench the reaction. The mixture is washed with saturated sodium chloride and deionized water. The product is further purified via vacuum distillation.

Analysis method: The liquid products generated from the reaction are analyzed using a Hefei Yaoke GC-9860 gas chromatograph equipped with an HP-5 capillary column (30 meters, inner diameter 0.25 mm, film thickness 0.25 μm) and a flame ionization detector (FID). Additionally, the reaction products are qualitatively analyzed using a Shimadzu GCMS-QP2020 gas chromatograph-mass spectrometer (GC-MS) with an Rtx-5MS capillary column (50 meters, inner diameter 0.25 mm, film thickness 0.25 μm). The ^{13}C NMR and ^{1}H NMR spectra of the K-CPO and TCPP are obtained by a Bruker AVANCE II 400 MHz spectrometer, and the solvent is $CDCl_3$.

Fuel performance evaluation method: The density of the fuel is measured using a Mettler Toledo DE40 densitometer according to the American standard ASTM D4052. The freezing point is determined by the cooling observation method according to the American standard ASTM D2386. The heat of combustion is measured using an IKA-C6000 isoperibol Package 2/10 oxygen bomb calorimeter according to the American standard ASTM D240-02.

2. Theoretical calculation section

The density functional theory (DFT) calculation methods: The mechanism of the cyclopropanation reaction is analyzed using quantum chemistry methods and the Gaussian software package[2]. Complete calculations are performed using the hybrid generalized gradient approximation Becke, 3-parameter, Lee-Yang-Parr (B3LYP)[3-5] method. Among them, the def2-svp[6] basis set is used for geometric optimization and vibration frequency analysis, and the def2-tzvp[7] basis set is used for single point energy calculation. The thermodynamic parameters are processed by the SMD implicit solvent model, and the solvent is selected as dichloromethane. In addition, the free energy of the system is corrected using the shermo[8] program. The temperature is set to 253.15 K, and the resonant frequency correction factor is set to 0.985. Finally, intrinsic reaction coordinate (IRC) calculations are performed to confirm that the optimized transition state correctly connects the relevant reactants and products. Activation energies (the reaction energy barriers) are estimated as the relative energies, including zero-point energy correction (ZPE), between the transition state and the reactant.

Molecular dynamics simulation methods: This study uses the GROMACS 2022.6 software package[9] for molecular dynamics simulations. The model is built using PACKMOL software[10], placing 1 olefin, 100 carbene molecules, and 1000 solvent molecules in a cubic simulation box with dimensions of 5×5×10 nm, with periodic boundary conditions applied in all three dimensions. The solute and solvent molecules are modeled using the GAFF force field, with charges assigned using RESP2.5 charges. After constructing the system, energy minimization is performed using the GROMACS software to ensure reasonable geometric configurations, employing the STEEP algorithm. Subsequently, a 5 ns NPT pre-equilibration simulation and a 50 ns NVT production simulation are conducted, with a time step of 1 fs for the molecular dynamics simulation. During the simulation, temperature and pressure are controlled using the V-rescale thermostat and Berendsen barostat, respectively. The PME method[11] is used to calculate electrostatic interactions within the system, with a cutoff radius set to 1.2 nm, and the LINCS algorithm[12] is used to constrain bonds involving hydrogen atoms. Finally, the VMD software[13] is used to post-process the dynamics trajectories to obtain the radial distribution function and dynamic configurations of the system.

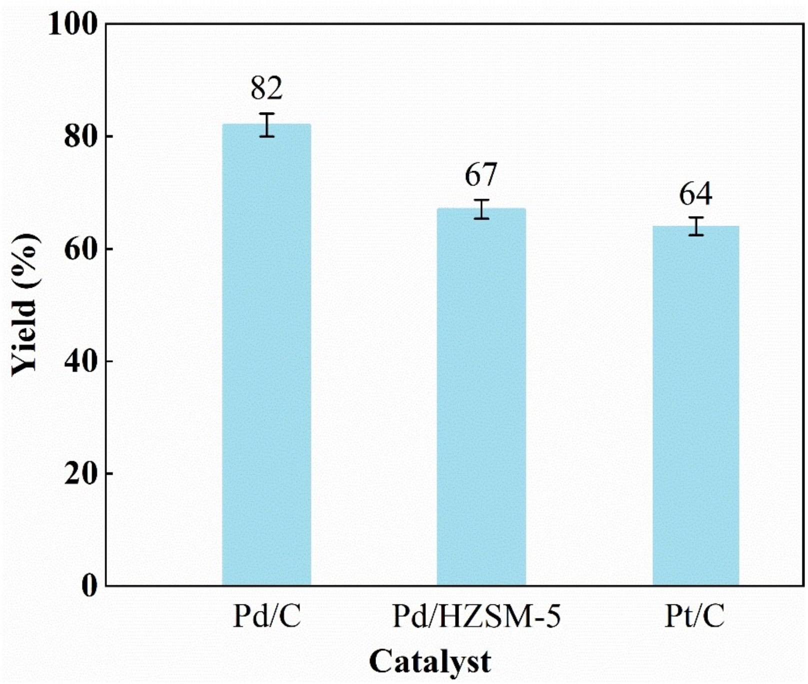

Figure S1. The effect of catalysts on the reaction of synthesizing cyclopentanone from furfural.

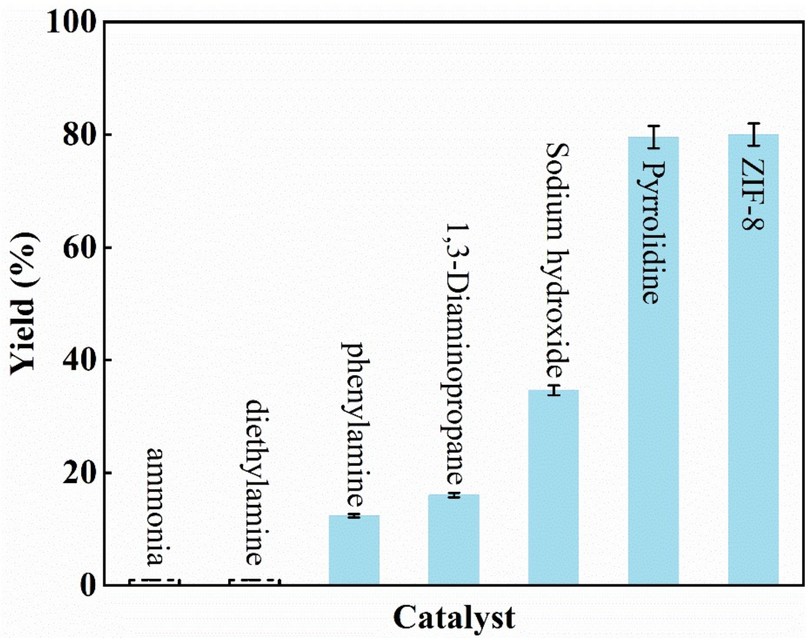

Figure S2. The effect of catalysts on Knoevenagel condensation.

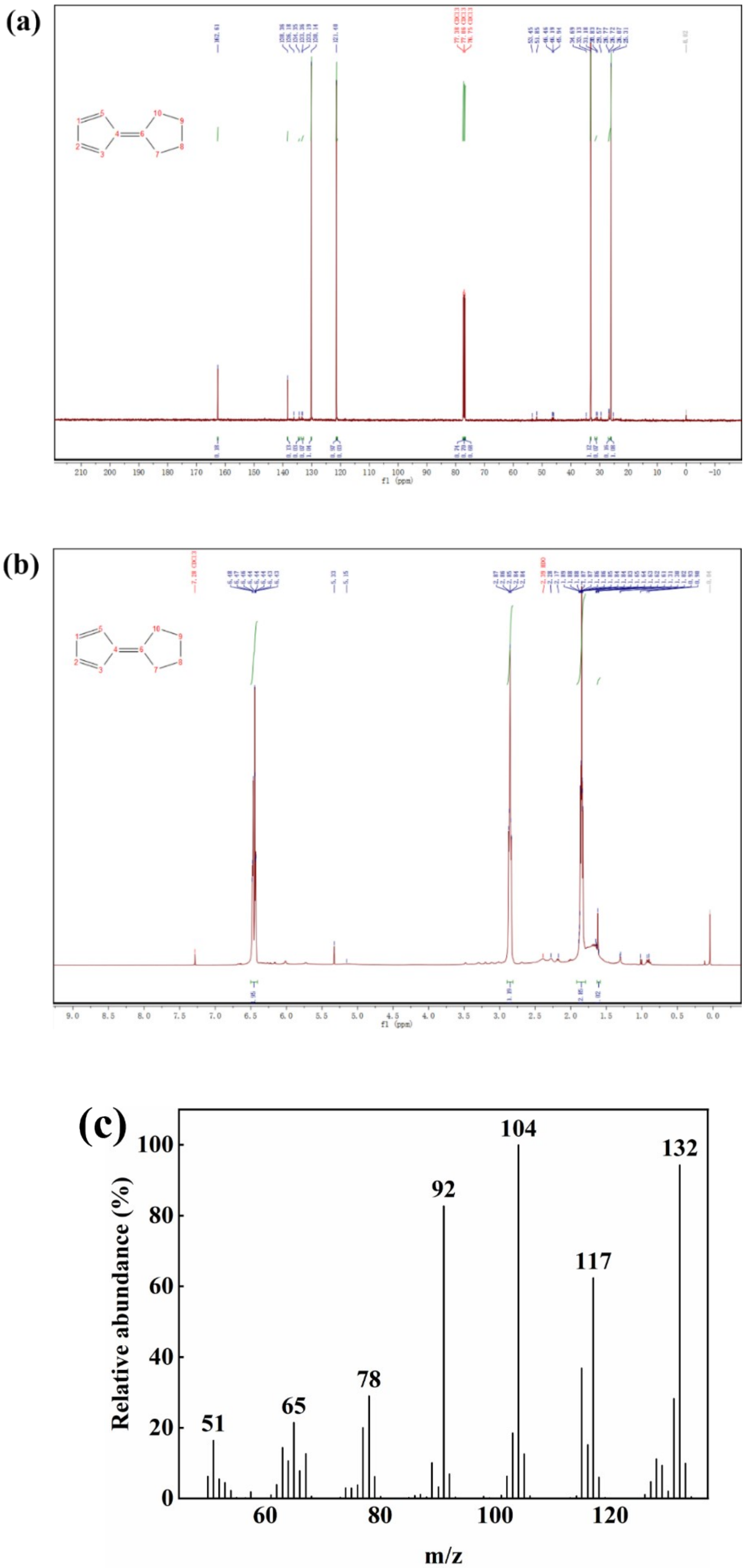

Figure S3. (a) ^{13}C-NMR and (b)^{1}H-NMR spectrum of K-CPO. (c) Mass spectrometry of K-CPO.

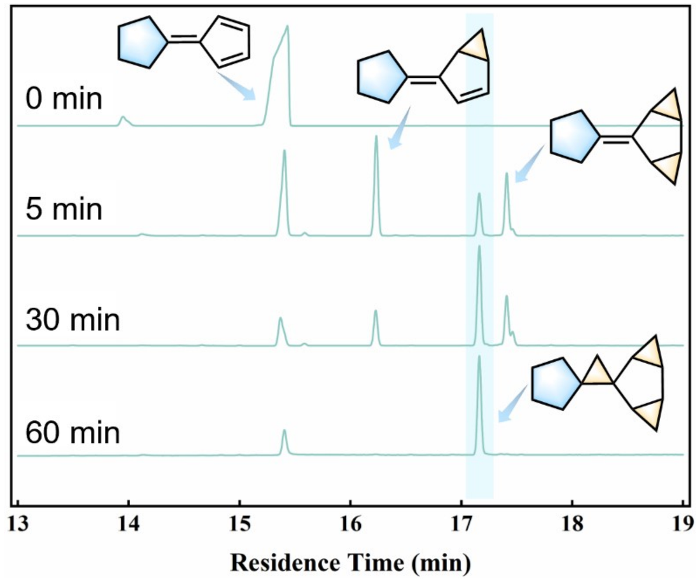

Figure S4. The change of product distribution of cyclopropanation reaction with time.

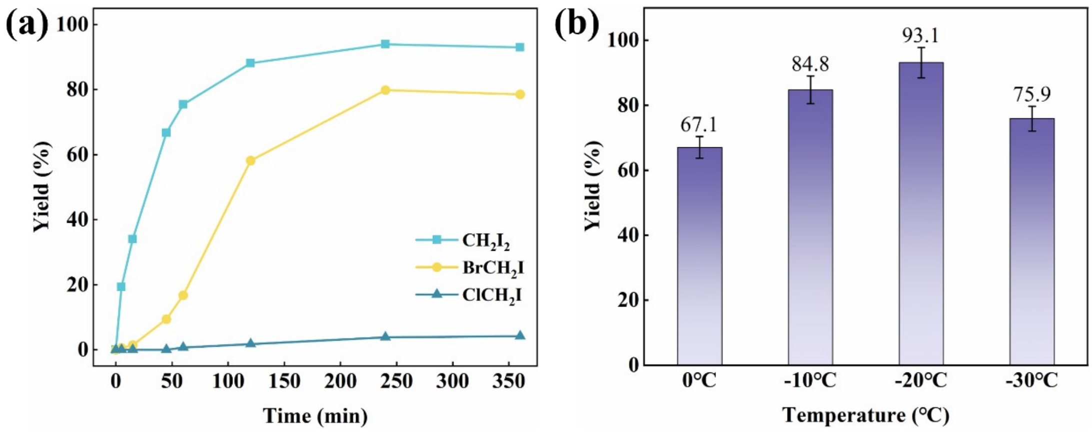

Figure S5. (a) The effect of halogenated iodomethanes on the cyclopropanation reaction. (b) The effect of temperature on the cyclopropanation reaction.

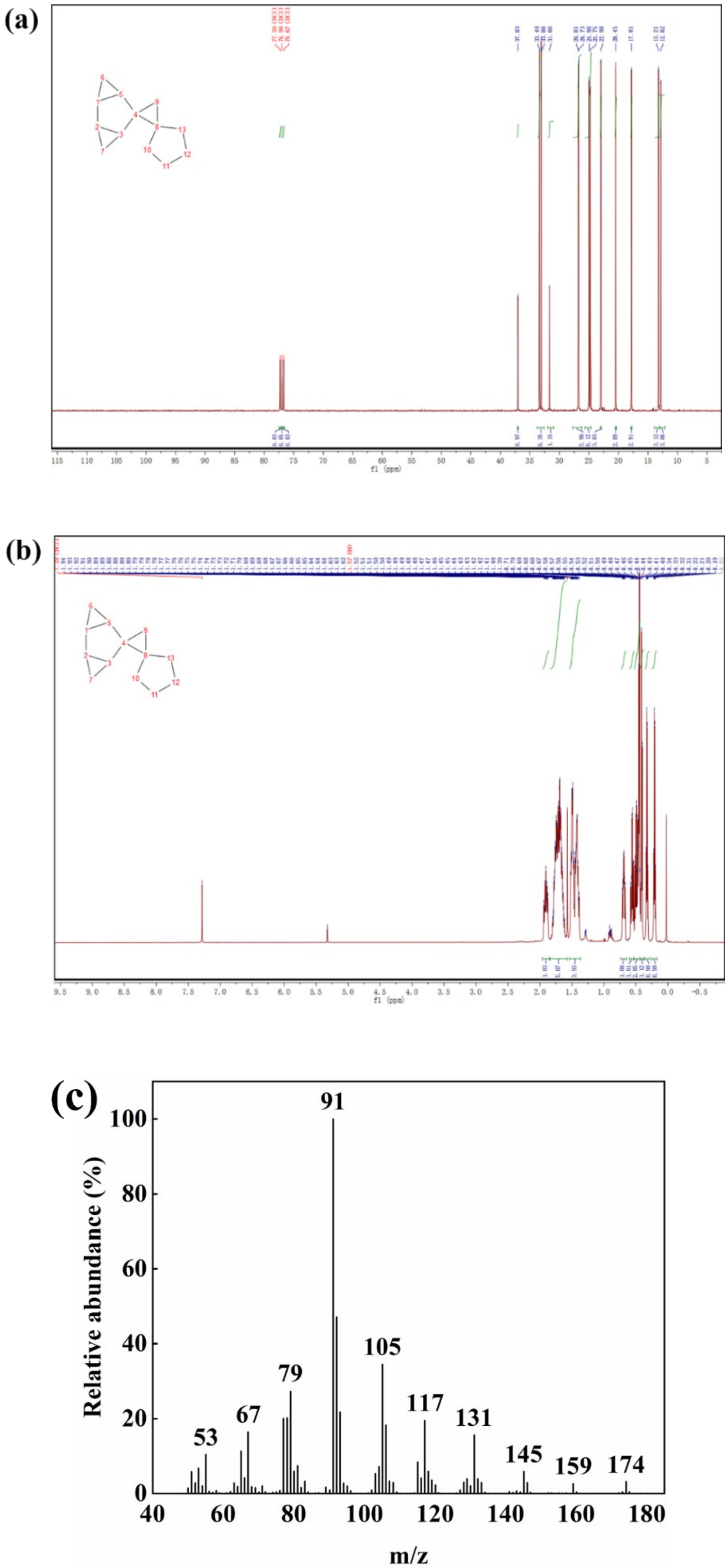

Figure S6. (a) ^{13}C-NMR and (b)^{1}H-NMR spectrum of TCPP. (c) Mass spectrometry of TCPP.

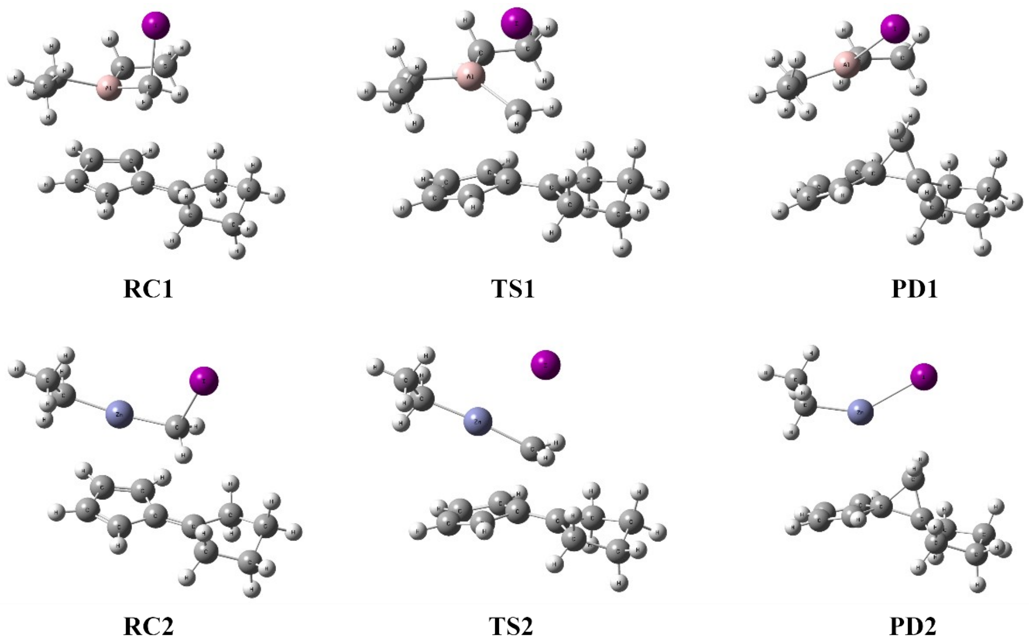

Figure S7. The geometric structures in the process of cyclopropanation using zinc carbenoid and aluminum carbenoid.

Table S1. The B3LYP/def2TZVP optimized cartesian coordinates (Å) of structures.

RC1			
Al	-1.002469	1.258272	0.565234
C	-1.432897	1.305849	2.509461
H	-1.036073	2.246623	2.939731
H	-2.533862	1.423316	2.56818
C	-1.968102	2.561649	-0.594849
H	-3.032084	2.443807	-0.302739
H	-1.712134	3.593344	-0.286802
I	-2.608157	-1.543023	-0.46233
C	3.843555	-2.496235	0.491329
C	3.227263	-1.209253	1.069132
C	3.160966	-0.252472	-0.098547
C	3.996168	-0.810103	-1.228414
C	4.786143	-1.97493	-0.603976
H	4.352012	-3.103967	1.254648
H	3.052426	-3.120412	0.041262
H	3.910399	-0.772811	1.8228
H	2.258099	-1.349985	1.570359
H	3.303347	-1.19434	-2.001177
H	4.61858	-0.046975	-1.719795
H	5.067004	-2.741683	-1.341355
H	5.716855	-1.594796	-0.148653
C	1.659802	1.496269	0.951621
C	1.189091	2.721242	0.524517
C	1.664543	2.959329	-0.83795
C	2.423715	1.892835	-1.228648
C	2.468579	0.925604	-0.131146
H	1.559253	1.07262	1.950599
H	0.646866	3.448924	1.131567
H	1.438501	3.848534	-1.427233
H	2.91353	1.763351	-2.193823
C	-0.635573	-0.529843	-0.255906
H	-0.245254	-0.538416	-1.283457
H	-0.057898	-1.24853	0.341477
C	-1.007214	0.116109	3.384044
H	-1.442951	-0.832103	3.024145
H	0.088515	-0.023582	3.391947
H	-1.316445	0.227071	4.440068
C	-1.848768	2.423425	-2.120282
H	-2.466921	3.161387	-2.665243
H	-0.810605	2.55911	-2.468435
H	-2.170388	1.425357	-2.464967

TS1			
Al	1.191809	-0.921007	0.531887
C	1.422642	-0.916307	2.504447
H	0.972147	-1.851297	2.892471
H	2.509185	-1.037572	2.686289
C	1.914474	-2.456134	-0.49921
H	2.939838	-2.61878	-0.110293
H	1.355733	-3.359741	-0.186269
I	2.423473	1.380652	-0.442392
C	-3.550171	2.506374	0.465932
C	-3.180227	1.127591	1.0373
C	-2.787055	0.304272	-0.162169
C	-3.262209	1.007027	-1.411456
C	-4.147768	2.163978	-0.907405
H	-4.240081	3.063652	1.116567
H	-2.640085	3.118107	0.342749
H	-4.079768	0.646802	1.469245
H	-2.421046	1.135513	1.833206
H	-2.37996	1.406196	-1.944423
H	-3.762532	0.320842	-2.111556
H	-4.162899	3.016015	-1.602753
H	-5.187101	1.814146	-0.78725
C	-1.912225	-1.721956	1.114212
C	-1.677192	-3.008212	0.738348
C	-1.754758	-3.105622	-0.725318
C	-2.033076	-1.879016	-1.240494
C	-2.161155	-0.929618	-0.113229
H	-1.947007	-1.325908	2.128017
H	-1.469071	-3.845684	1.406406
H	-1.608253	-4.025317	-1.293986
H	-2.15795	-1.616911	-2.290564
C	-0.220385	0.271961	-0.274423
H	-0.347968	0.411275	-1.353248
H	-0.538882	1.165302	0.276292
C	0.902158	0.283093	3.310154
H	1.359712	1.230092	2.97533
H	-0.190719	0.406436	3.208784
H	1.109212	0.193918	4.39272
C	1.955808	-2.378411	-2.032594
H	2.399714	-3.28096	-2.492526
H	0.947069	-2.265119	-2.465541
H	2.549971	-1.516627	-2.381989

PD1			
Al	-1.871607	0.260965	1.025558
C	-1.758143	-0.916917	2.614794
H	-1.337323	-0.308042	3.439855
H	-2.81762	-1.076305	2.900771
C	-3.230064	1.703849	1.088847
H	-4.165688	1.137775	1.278566
H	-3.058385	2.279634	2.019549
I	-1.944642	-1.00035	-1.255745
C	5.129683	-0.870731	0.592451
C	3.720215	-0.511713	1.083612
C	3.051213	-0.019245	-0.199241
C	4.13736	0.694934	-1.027396
C	5.479586	0.285044	-0.36309
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H	5.096308	-1.825612	0.040134
H	3.780886	0.307192	1.821183
H	3.186457	-1.351306	1.552969
H	4.084592	0.380023	-2.081052
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H	5.883344	1.131515	0.21622
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C	0.103485	1.788104	1.073109
C	0.316031	2.461515	-0.21126
C	1.174285	1.71411	-0.956197
C	1.57424	0.524631	-0.181414
H	0.971837	-0.05345	1.933407
H	-0.405979	2.230435	1.93357
H	-0.151926	3.401157	-0.505045
H	1.518029	1.930119	-1.968156
C	1.983934	-0.806593	-0.840819
H	1.917038	-0.816505	-1.932185
H	1.620856	-1.710712	-0.345297
C	-1.042687	-2.271881	2.543289
H	-1.471048	-2.918557	1.759055
H	0.030848	-2.16285	2.311197
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H	-2.567728	3.300688	-0.269414
H	-3.632784	2.108565	-1.030583

RC2			
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C	-4.415961	-2.506717	-0.584745
C	-4.448506	-1.011018	-0.950958
C	-3.600842	-0.332003	0.106617
C	-3.334222	-1.324593	1.220853
C	-4.297392	-2.4949	0.94742
H	-5.295646	-3.056299	-0.951656
H	-3.52266	-2.981664	-1.025792
H	-5.482375	-0.625912	-0.86937
H	-4.114411	-0.791017	-1.976187
H	-2.287132	-1.671753	1.135192
H	-3.435135	-0.882941	2.223733
H	-3.942499	-3.448192	1.366624
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C	-3.379368	1.930691	-1.011782
C	-2.767564	3.0978	-0.657616
C	-2.127744	2.920498	0.649847
C	-2.354709	1.645874	1.083741
C	-3.154468	0.953701	0.062962
H	-3.94122	1.738873	-1.925702
H	-2.749414	4.02079	-1.2398
H	-1.569562	3.694125	1.180153
H	-2.017634	1.204942	2.02167
C	1.003004	-0.597645	-0.277262
H	0.330749	-0.89122	0.541287
H	0.549804	-0.917813	-1.226116
I	2.72555	-1.9724	-0.044225
Zn	1.604255	1.3014	-0.235174
C	3.292012	3.551819	0.779875
H	2.988836	3.345972	1.82099
H	4.215004	2.973931	0.600537
H	3.574787	4.621177	0.738506

TS2			
C	-2.60623	-2.402948	-0.142624
H	-3.125203	-2.333718	-1.116675
H	-2.115341	-3.393023	-0.136048
C	3.921006	2.189468	-0.409377
C	3.455265	0.877999	-1.063469
C	2.865779	0.073297	0.067507
C	3.343488	0.657412	1.379428
C	4.373496	1.73758	0.988037
H	4.712745	2.692477	-0.983175
H	3.071736	2.888842	-0.328214
H	4.333069	0.312857	-1.433621
H	2.781829	0.997652	-1.924536
H	2.489429	1.112694	1.911585
H	3.741449	-0.118155	2.051557
H	4.420894	2.558133	1.718338
H	5.3795	1.289774	0.928803
C	1.902406	-1.812723	-1.342337
C	1.56032	-3.08921	-1.027361
C	1.485009	-3.223309	0.434195
C	1.784601	-2.028977	1.008956
C	2.091757	-1.065839	-0.075041
H	2.047387	-1.395371	-2.337834
H	1.366799	-3.896352	-1.735488
H	1.224751	-4.143052	0.960239
H	1.821419	-1.799543	2.073074
C	0.342437	0.296218	-0.078035
H	0.578701	0.82602	0.84963
H	0.632822	0.876695	-0.959347
I	-2.102084	1.908845	-0.07712
Zn	-1.187181	-1.005673	-0.127859
C	-3.625121	-2.312122	1.001042
H	-3.147043	-2.424818	1.989561
H	-4.145624	-1.339021	1.012861
H	-4.408724	-3.091779	0.93685

PD2			
C	2.230123	2.722245	-0.418822
H	2.485229	2.982861	-1.462148
H	1.160022	2.967389	-0.297724
C	-5.053534	-2.100658	-0.738786
C	-4.270586	-0.870289	-1.216672
C	-3.433718	-0.497898	0.012038
C	-4.233066	-0.942548	1.257292
C	-5.44899	-1.722889	0.698209
H	-5.91846	-2.338651	-1.378007
H	-4.39192	-2.984587	-0.731429
H	-4.974903	-0.054733	-1.456483
H	-3.657577	-1.055003	-2.111658
H	-3.607026	-1.581144	1.900937
H	-4.554911	-0.08629	1.86822
H	-5.711764	-2.595325	1.316385
H	-6.334395	-1.065476	0.671306
C	-2.539634	1.720544	-1.142768
C	-2.418072	2.993183	-0.676554
C	-2.366049	2.961789	0.787688
C	-2.461518	1.670682	1.206374
C	-2.584661	0.797914	0.01581
H	-2.60267	1.405442	-2.184898
H	-2.363355	3.899821	-1.282916
H	-2.263277	3.841432	1.426696
H	-2.448337	1.310199	2.235702
C	-1.955489	-0.610362	-0.026314
H	-1.429884	-0.9246	0.880696
H	-1.470903	-0.897298	-0.964396
I	2.913575	-1.783456	0.081053
Zn	2.414962	0.748552	-0.23669
C	3.081276	3.53834	0.558938
H	2.829228	3.319938	1.611199
H	4.159749	3.332904	0.442859
H	2.950291	4.629415	0.421932

K-CPO			
C	2.828058	-0.719682	-0.269463
C	1.415333	-1.228282	0.073601
C	0.530176	0.000105	0.000032
C	1.415499	1.228346	-0.07357
C	2.828168	0.719574	0.269435
H	3.624062	-1.347406	0.158138
H	2.967367	-0.709561	-1.364256
H	1.395205	-1.611134	1.111315
H	1.064329	-2.050332	-0.56834
H	1.395487	1.611002	-1.111353
H	1.064517	2.0504	0.568352
H	3.624224	1.347172	-0.158263
H	2.967613	0.709509	1.364206
C	-0.831686	0.000147	0.000045
C	-1.714747	-1.174072	0.047932
C	-3.006184	-0.732681	0.030536
C	-3.006321	0.732467	-0.030539
C	-1.714985	1.174159	-0.047927
H	-1.379183	2.210153	-0.091162
H	-3.90262	1.35489	-0.057382
H	-3.902381	-1.355249	0.057302
H	-1.378477	-2.209923	0.090947

MCPP			
C	-3.150679	0.534625	-0.412608
C	-1.808111	1.225081	-0.092684
C	-0.816454	0.078026	0.055286
C	-1.585715	-1.231788	0.128506
C	-3.055281	-0.809032	0.3327
H	-4.020287	1.132026	-0.118652
H	-3.227235	0.352861	-1.492845
H	-1.890004	1.781473	0.853599
H	-1.512877	1.952556	-0.857797
H	-1.481069	-1.786078	-0.816979
H	-1.217226	-1.899528	0.917525
H	-3.77081	-1.555388	-0.028358
H	-3.253576	-0.65416	1.401626
C	1.314269	1.431842	0.042966
C	2.629603	1.181271	0.204896
C	2.886171	-0.281737	0.354761
C	1.510609	-0.92809	0.267487
C	0.523615	0.195504	0.109971
H	0.881467	2.409607	-0.14299
H	3.419427	1.926087	0.19259
H	3.652554	-0.639619	1.03785
H	1.2507	-1.786967	0.880049
C	2.523204	-1.139285	-0.844146
H	2.97662	-2.125688	-0.90893
H	2.364929	-0.645692	-1.799505

DCPP			
C	1.002454	-0.025128	0.141417
C	1.887002	1.215018	0.063092
C	3.259146	0.6841	-0.407421
C	3.307468	-0.750737	0.15054
C	1.867422	-1.261935	-0.053715
H	1.98368	1.675859	1.057614
H	1.474762	1.987838	-0.596698
H	3.291226	0.652881	-1.504807
H	4.096921	1.306389	-0.074814
H	4.0615	-1.378425	-0.336638
H	3.544888	-0.722875	1.222512
H	1.756181	-1.648491	-1.07841
H	1.588575	-2.079345	0.620743
C	-2.659611	0.785664	0.191563
C	-1.223909	1.197953	0.600985
C	-0.315199	-0.024714	0.360467
C	-1.317851	-1.150489	0.454898
C	-2.401374	-0.571813	-0.477632
H	-3.526078	0.998657	0.811803
H	-1.039544	1.806435	1.485891
H	-1.73101	-1.102103	1.468835
H	-1.957476	-0.37316	-1.455182
C	-1.94763	1.893045	-0.544361
H	-2.267713	2.915946	-0.355422
H	-1.625689	1.718844	-1.568681
C	-2.252172	-2.075084	-0.289682
H	-1.993071	-2.597378	-1.209462
H	-2.891613	-2.656355	0.37182

TCPP			
C	0.333665	-0.000044	-0.401028
C	1.030946	1.231282	0.169112
C	2.202946	0.760167	1.007344
C	2.202977	-0.760052	1.007412
C	1.030981	-1.231293	0.169239
H	0.422053	2.069671	0.496304
H	2.444118	1.246245	1.94893
H	2.444206	-1.246037	1.949032
H	0.42213	-2.069691	0.496488
C	2.448327	-1.531618	-0.267661
H	2.793422	-2.558	-0.16483
H	2.852529	-1.023478	-1.138377
C	2.448281	1.531639	-0.267791
H	2.852505	1.023428	-1.138456
H	2.793331	2.558045	-0.165059
C	-2.794771	-0.78012	0.92366
C	-2.794519	0.78034	0.923651
C	-2.057879	1.196661	-0.372102
C	-1.168539	-0.000073	-0.698421
C	-2.057903	-1.196738	-0.371888
H	-2.260461	-1.158652	1.802264
H	-3.806978	-1.196012	0.966159
H	-2.259755	1.158683	1.802059
H	-3.806567	1.196577	0.966473
H	-2.778794	1.328438	-1.191389
H	-1.517824	2.142977	-0.274609
H	-2.778692	-1.328766	-1.191243
H	-1.517831	-2.143009	-0.274068
C	-0.185354	-0.000155	-1.832325
H	-0.066154	-0.913741	-2.41238
H	-0.066185	0.913352	-2.412512

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