Electronic Supplementary Information

Large Language Model Guided Automated Reaction Pathway Exploration

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Content

Original chemical logic from a Large Language Model

The original chemical logic could be classified into general chemical logic and specified chemical logic. The original chemical logic used in this program is constituted by general organic chemical (**Figure S1**) logic and general transition metal chemical logic (**Figure S2**). Both organic and transition metal chemical logic could be generated in detail by interacting with ChatGPT further, where Electrophilic active sites (**Figure S3**) and Bond strain active sites (**Figure S4**) are shown as examples. Then for each specified system performed with ARplorer, specified chemical logic associated with the system would be generated using ChatGPT (The specified chemical logic of three examples shown in this paper are shown in **Figure S5**, **Figure S6**, **Figure S7**). Both the general chemical logic and specified chemical logic constitute the system-specified chemical logic. All the chemical logic would be coded with SMARTS rules and used to guide the direction of automatic reaction search in ARplorer.

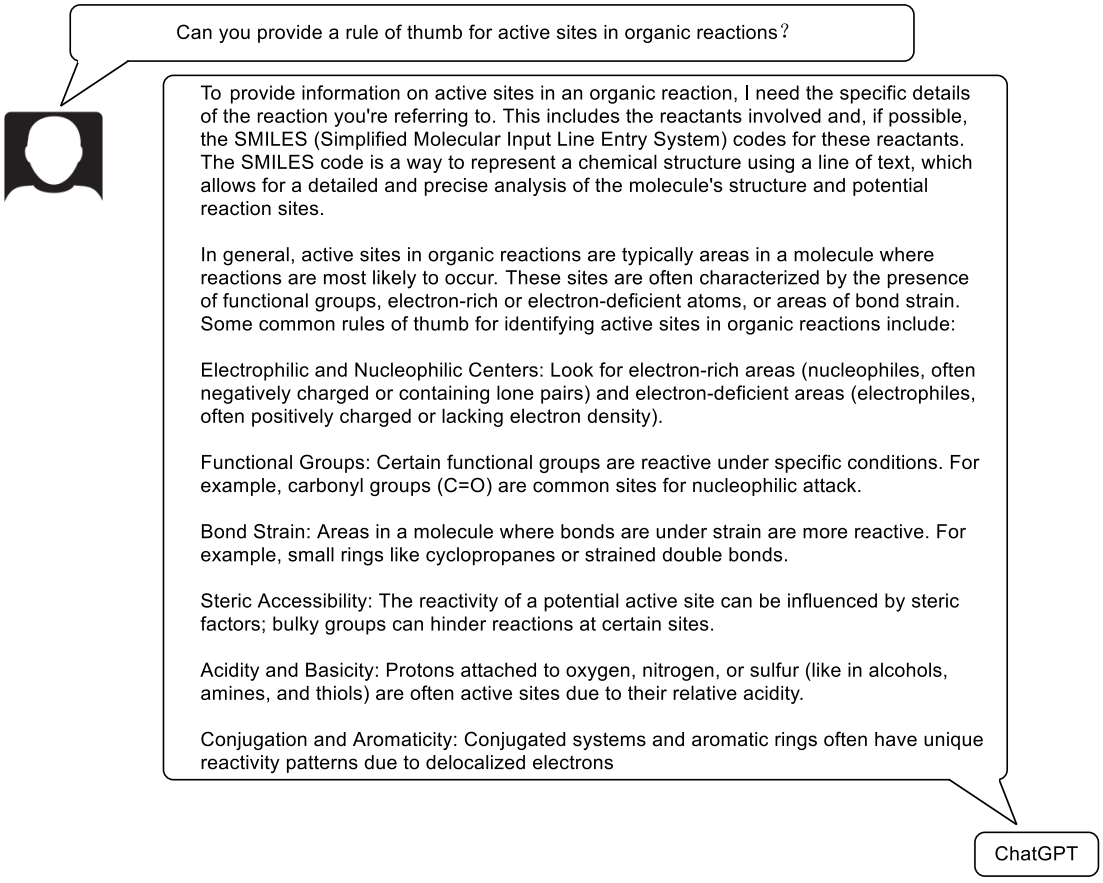

Figure S1. Create generalized organic chemical logic from ChatGPT

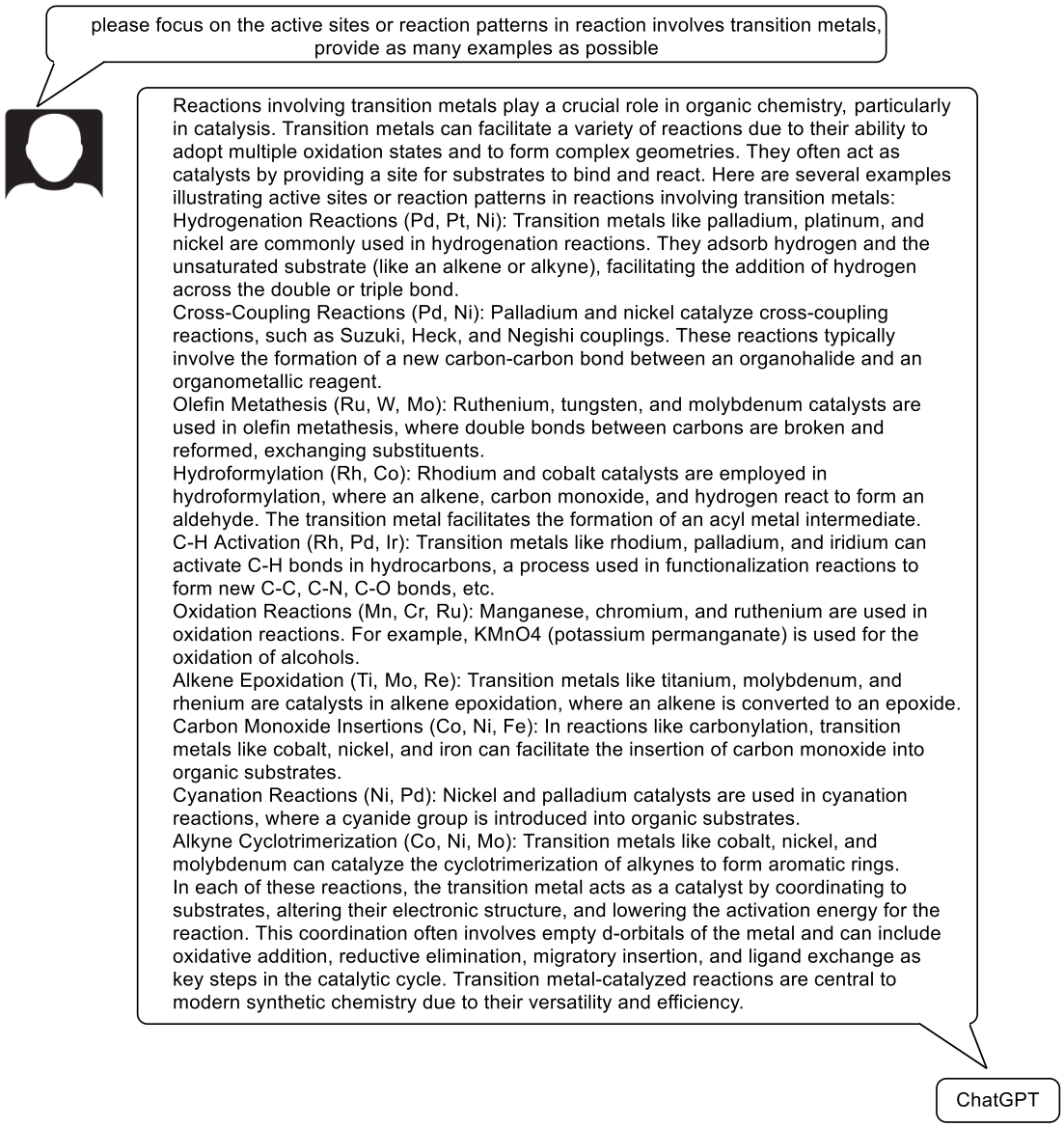

Figure S2. Create generalized chemical logic with transition metals from ChatGPT

Figure S3. Electrophilic active site in organic chemical logic from ChatGPT

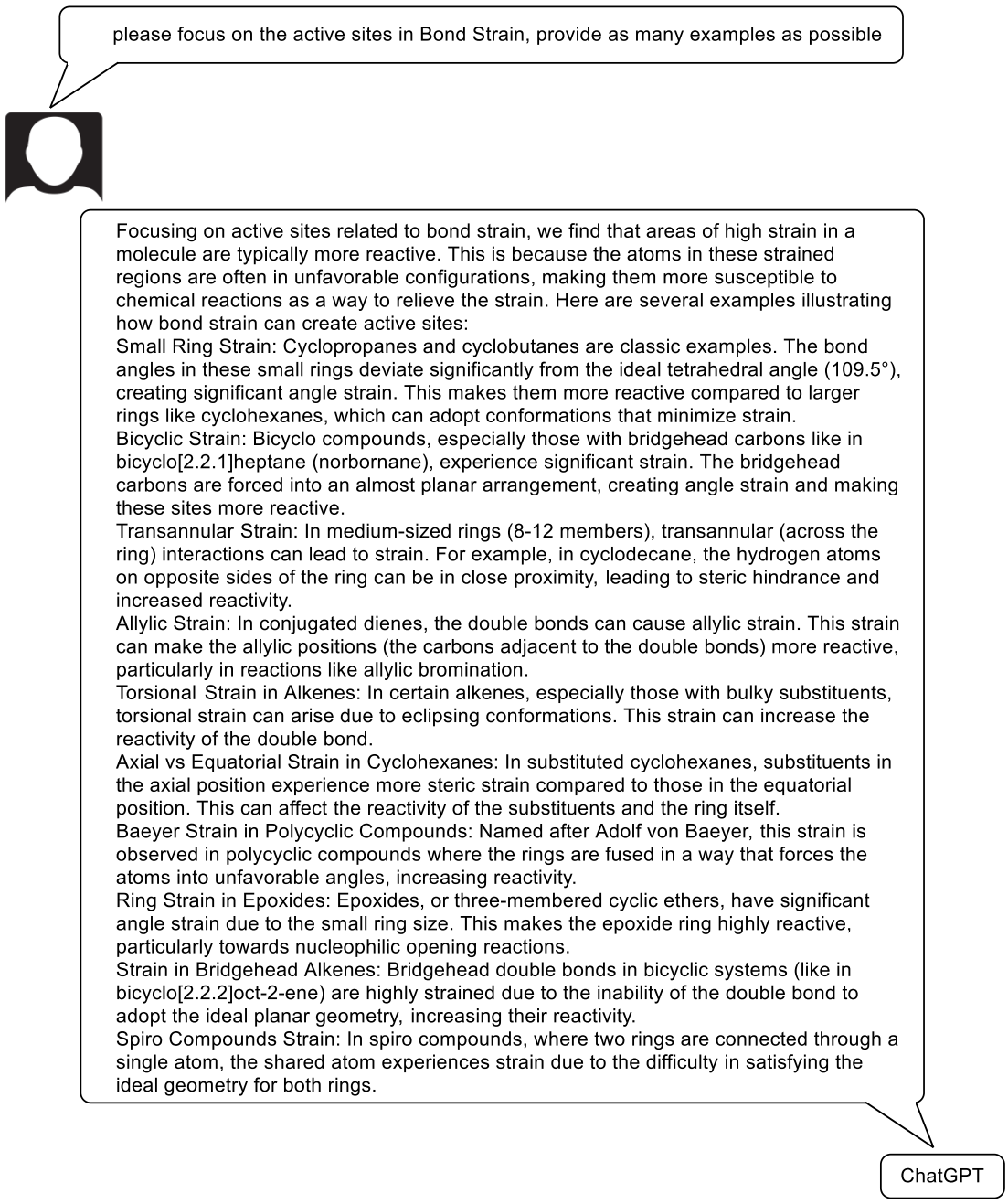

Figure S4. Bond strain active site in organic chemical logic from ChatGPT

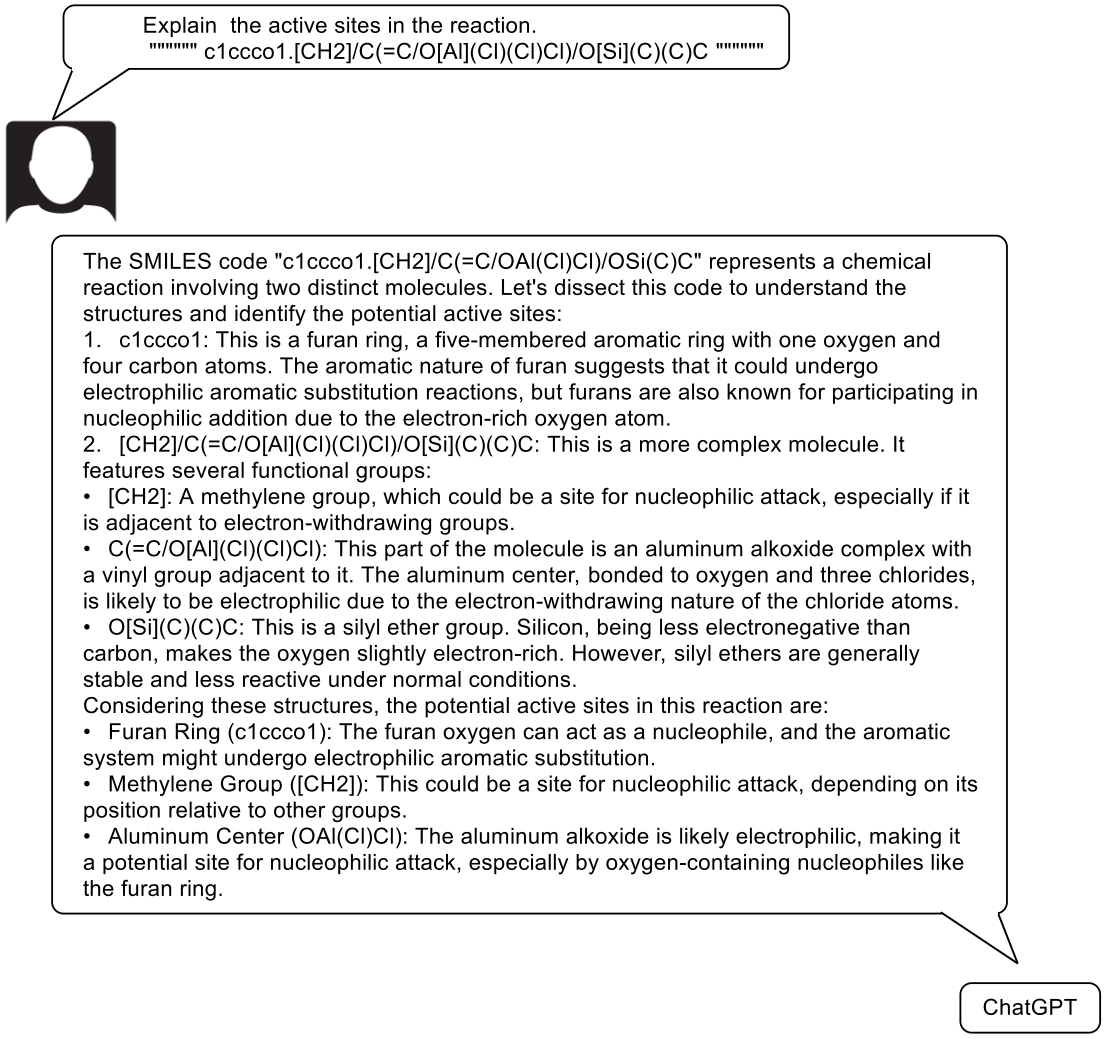

Figure S5. Specified chemical logic about example of cycloaddition reaction from ChatGPT

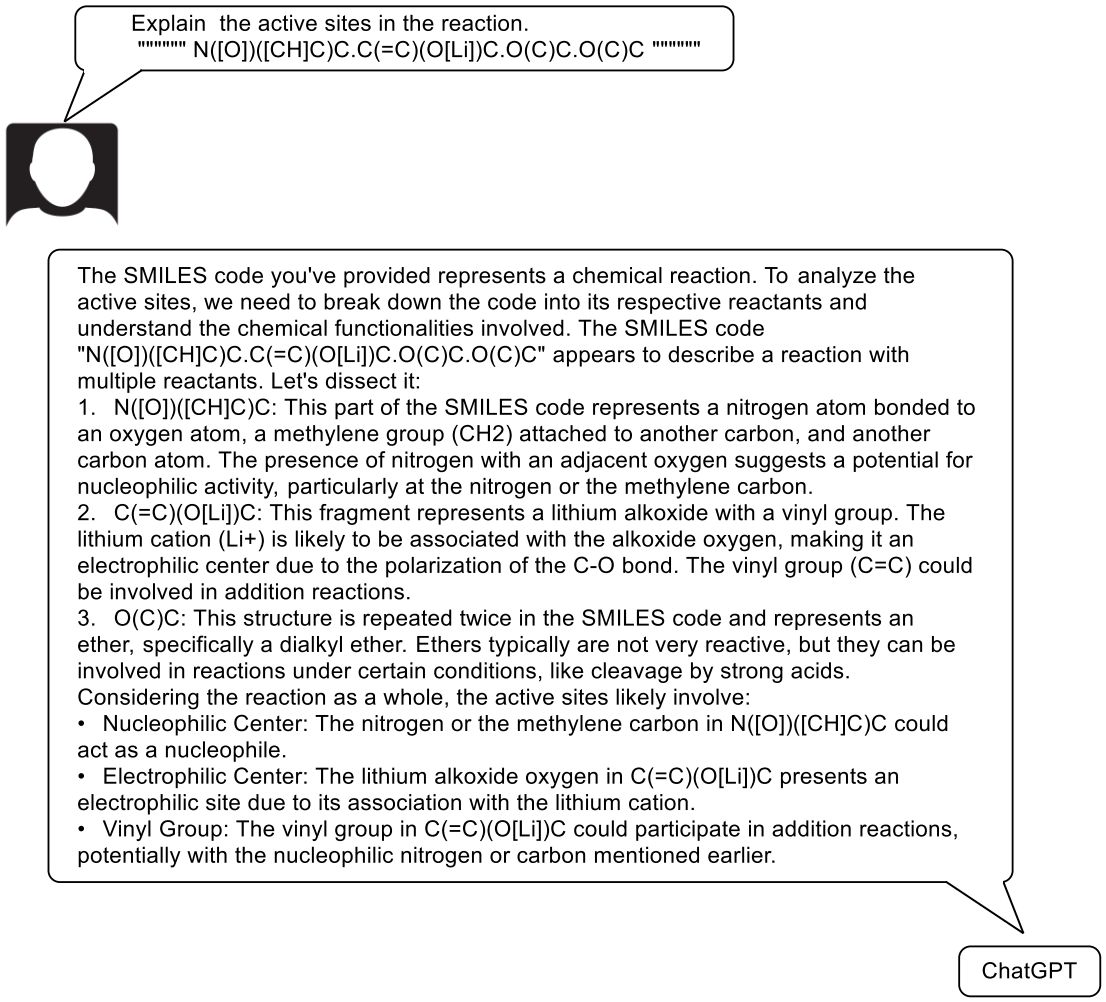

Figure S6. Specified chemical logic about example of asymmetric Mannich-type reaction from ChatGPT

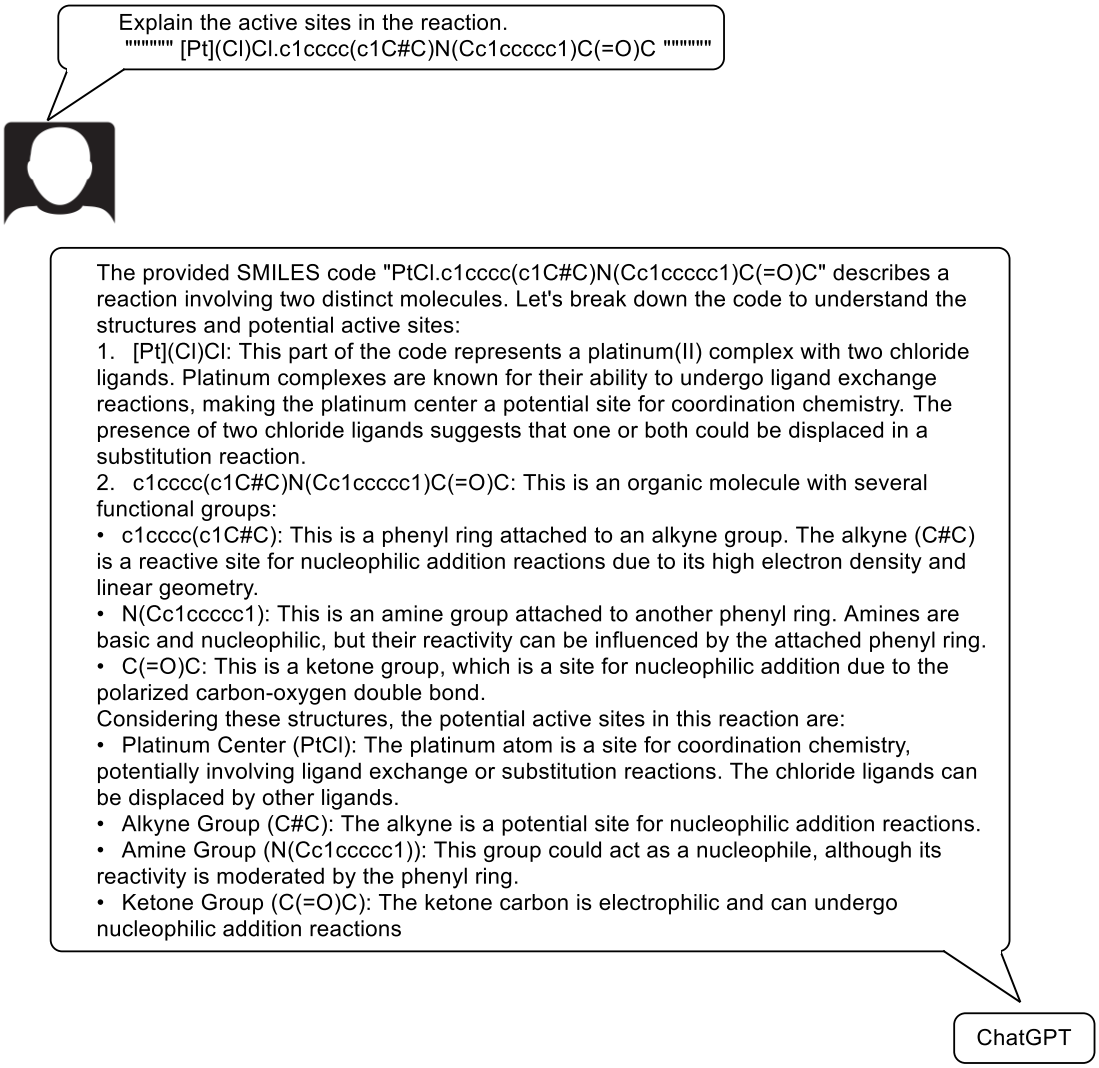

Figure S7. Specified chemical logic about example of asymmetric Mannich-type reaction from ChatGPT

Functions of customized potential U

Figure S8 shows the preparation and the mechanism to use U in optimizing structure and the main applications of U in this program.

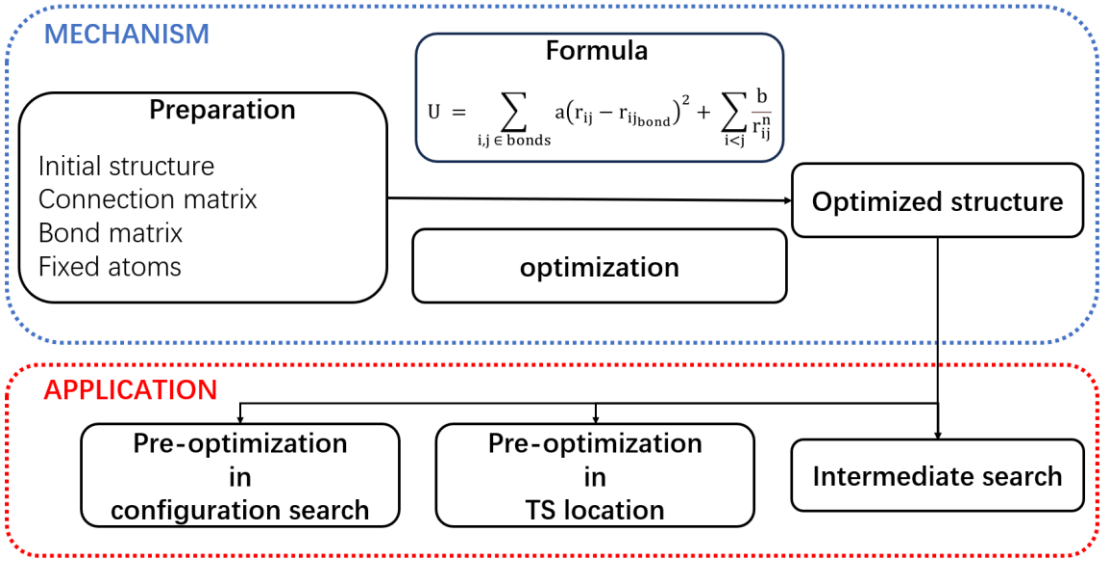

Figure S8. Functions of customized potential U.

Postprocessing

The postprocessing of the program is following. As shown in **Figure S9**, when the set of total reaction paths was got, it would be filtered by certain energy barrier which is set manually and a new set of filtered reaction paths forms. Then this set would be sorted by energy barrier and classified by the structure of final intermediate. Finally, a diagram of each filtered reaction path would be produced automatically.

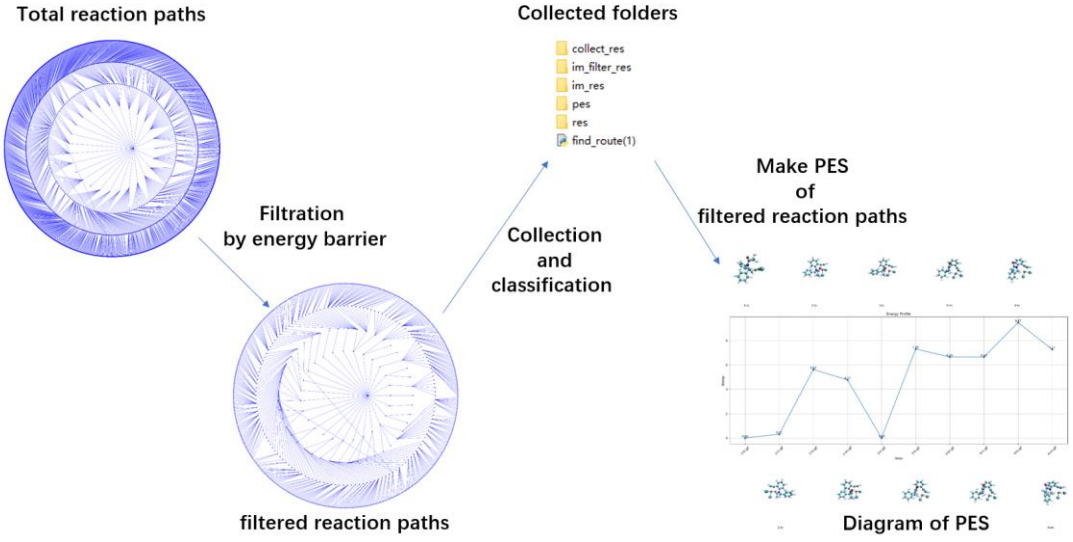

Figure S9. Workflow of postprocessing in the program.

Detail process of active-Learning Approach for Sampling Transition State Locations.

This method is a single-end method, as shown in **Figure S10-1**.

1. For a given IN (beginning from IM is similar), two probe structures were constructed in the first golden ratio point (the one is close to IN) of the range default reasonable distance (as described in **Response 2-11**). Then, both probe structures were optimised with the active site constrained.
2. Three consecutive probe points including the one with highest energy would be fitted into a quadratic function curve. The extreme point, which was close to one of the previous probes in terms of conformation space (0.1Å), would be guessed as the potential saddle point.
3. If a qualified TS was not obtained, this failed TS would be served as new probe point and the program return to step 2 until a qualified TS was found or reached the maximum step.

If a qualified TS could not be located when IN was a beginning point, similar process beginning from IM would be conducted.

Take a simple elementary reaction for an example. Active learning sampling took 7 probe points to locate the qualified TS. As for the normal scan method, the traditional scan should involve a twenty-step search to find the qualified TS (curve d) (**Figure S10-1**). Active learning sampling is more efficient.

It is worth noting that the quadratic function curve used here does not mean the shape around the TS is always quadratic-like. The quadratic curve is a way to explore the potential energy surface widely rather than search the potential energy surface step by step (we do not mean the normal scan method is not a good approach to locate TS). This method is different from other existing methods, and according to the result above, the active learning sample is a practical approach to efficiently locate TS.

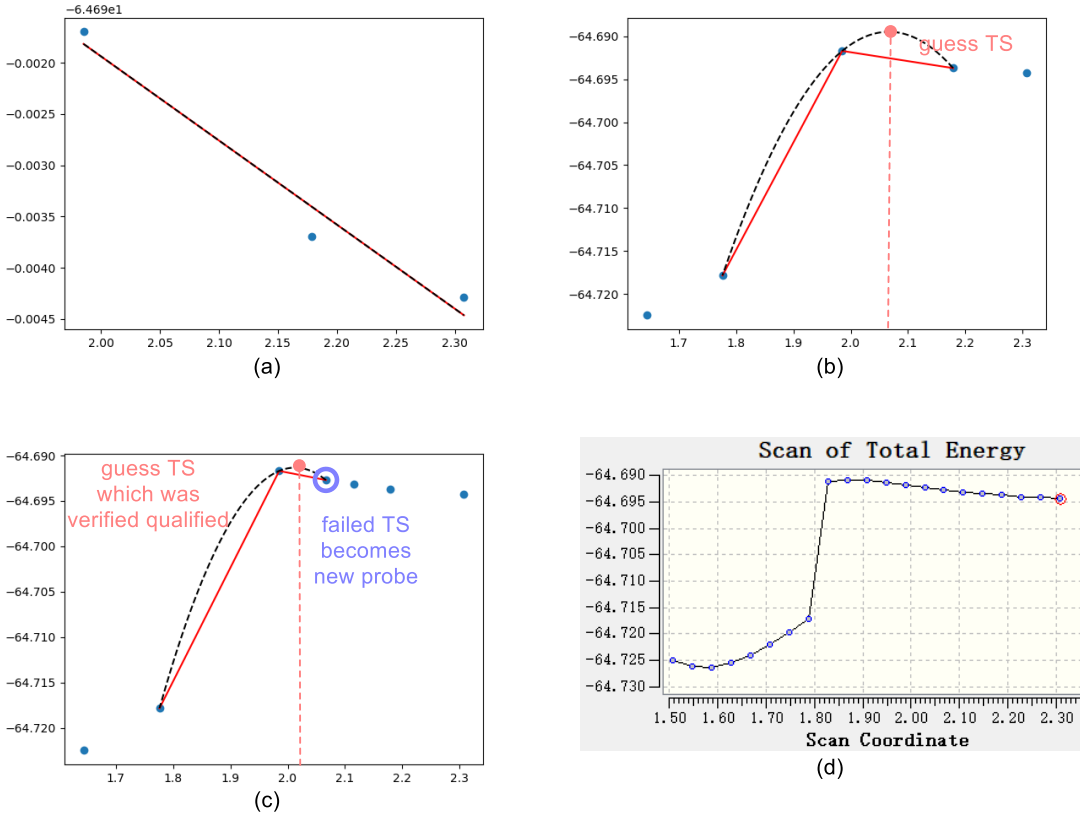

Figure 10-1. presentation of comparison between active learning sampling and normal scan approach for a simple elementary reaction. From (a) to (c) is a presentation of step 2 to step 4. (d) is the normal scan for TS location.

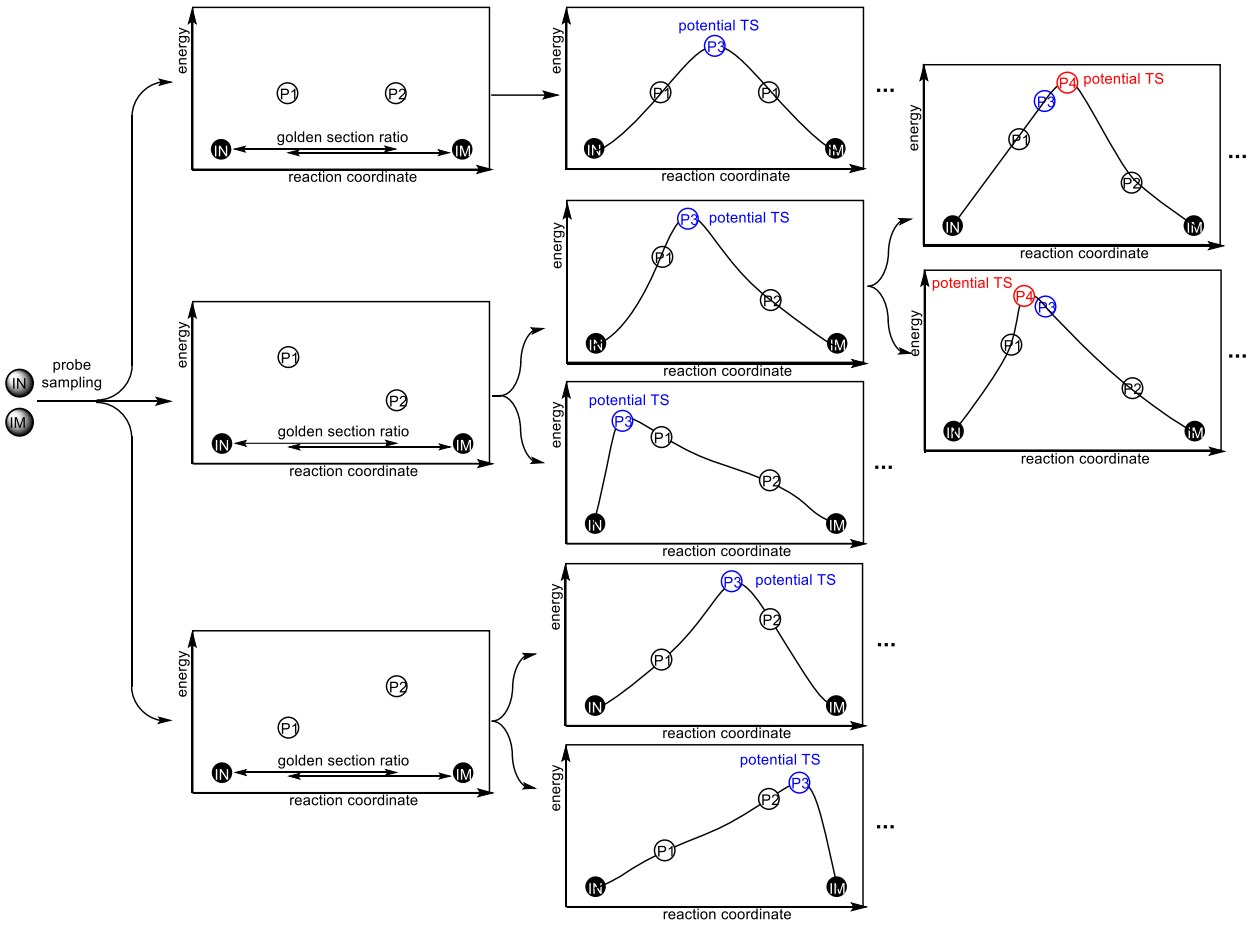

Figure S10-2. Detailed explanation of active-Learning Approach for Sampling Transition State Locations

Curation of Chemical Logic library

Table S1. Curated Chemical Logic Library(partial) from different reaction type

Reaction Type	Description	Extract SMARTS	Library
Michaelis–Arbuzov Reaction	A reaction where a trivalent phosphorus ester reacts with an alkyl halide to form a pentavalent phosphorus compound and another alkyl halide.	[P;H2,H1]~[C;H0][X;H0]	[$([P;H2,H1]~[C;H0][I,Cl,Br,F])]
Appel Reaction	Converts alcohols into alkyl halides using triphenylphosphine and a tetrahalomethane.	[O;H1]~[C;H0,H1]	[$(O[$([H])])]-[H] [$(O[$([H])]),$(O=*)]
Alder–Ene Reaction	A pericyclic reaction between an alkene with an allylic hydrogen and a compound containing a multiple bond, resulting in a new σ-bond and a shifted double bond.	[C;R]=[C;R],[C;R]=[C;R]	[$([CX3]~[$([CX3])])]-[!$([CX3])] [$([CX3]~[$([CX3])])]
Acyloin Condensation	A reductive coupling of two esters using metallic sodium to yield an α-hydroxyketone (acyloin).	[C;H1,H2]([O;H0])=[O;H0]	[$(C=[OX1])] [$(O[$([H])]),$(O=*)]

Acetoacetic Ester Synthesis	A method to synthesize methyl ketones by alkylating ethyl acetoacetate followed by hydrolysis and decarboxylation.	[C;H1,H2]([C;H0]=[O;H0])[C;H0]=[O;H0]	[$(O[$([H])]),$(O=*)]
Wittig Reaction	Transforms aldehydes or ketones into alkenes using a phosphonium ylide.	[P]=[C;H0],[#6][OX2]=O	[$(C=[OX1])] [$(O[$([H])]),$(O=*)]
Ullmann Reaction	A copper-catalyzed coupling of aryl halides to form biaryl compounds.	[C;R]([c;H0])[X;H0]	[$(C;R(-[c;H0])-[I,Br,Cl,F;H0))]
Ugi Reaction	A four-component condensation reaction involving an aldehyde, amine, carboxylic acid, and isocyanide to form α-aminoacyl amide derivatives.	[N;H2],[C;H0]=[O;H0]	[$(N[$([H])]),$(O[$([H])]),$(S[$([H])]),$(N=*),$(O=*),$(S=*),$([OX1]!#*)]
Swern Oxidation	Oxidizes primary and secondary alcohols to aldehydes and ketones using DMSO and oxalyl chloride under mild conditions.	[C;H0](=O)[O;H0],[C;H0]([O;H0])(=O)	[$(C=[OX1])] [$(O[$([H])]),$(O=*)]
Shi Epoxidation	An asymmetric epoxidation of alkenes using a fructose-derived organocatalyst and oxone as the oxidant.	[C;R]=[C;R],[O;H0]-[O;H0]	[$([CX3]~[$([CX3])])]-[!$([CX3])] [$([CX3]~[$([CX3])])]
Fischer Indole Synthesis	Produces indoles from phenylhydrazines and aldehydes	[C;H0]=[O;H0],[N;H2]~[c;H0]	[$(C=[OX1])] [$(N[$([H])]),$(O[$([H])]),$(S[$([H])]),$(N=*),$(O=*),$(S=*),$([OX1]!#*)]

	or ketones under acidic conditions.		
Fleming–Tamao Oxidation	Converts carbon–silicon bonds to carbon–oxygen bonds using peroxy acids or hydrogen peroxide.	[Si;H0]~[c;H0],[Si;H0]~[X;H0]	[$(Si;H0-[$([c;H0]),$(I,Cl,Br,F;H0)])]
Fischer Esterification	Forms esters by reacting carboxylic acids with alcohols in the presence of an acid catalyst.	[C;H0](=O)[O;H1],[C;H0][O;H1]	[$(C=[OX1])] [$(O[$([H])]),$(O=*)]
Friedländer Synthesis	Synthesizes quinoline derivatives from 2-aminobenzaldehydes and ketones.	[N;H2]~[C;H0]=[O;H0],[C;H0]=[C;H1]	[$(C=[OX1])] [$(N[$([H])]),$(O[$([H])]),$(S[$([H])]),$(N=*),$(O=*),$(S=*),$([OX1]!#*)]
Fukuyama Coupling Reaction	A palladium-catalyzed coupling of thioesters with organozinc reagents to form ketones.	[S;H0]~[C;H0]=[O;H0],[Zn;H0]~[C;H0]	[$(C=[OX1])] [$(N[$([H])]),$(O[$([H])]),$(S[$([H])]),$(N=*),$(O=*),$(S=*),$([OX1]!#*)]
Grignard Reaction	Forms carbon–carbon bonds by reacting organomagnesium halides with electrophilic carbon atoms.	[C;Mg],[#6][OX2]=O	[$(C=[OX1])] [$(O[$([H])]),$(O=*)]
Hofmann Rule	Predicts that in elimination reactions, the less substituted alkene will be the major product.	[N;H0]([C;H0])([C;H0])([C;H0])	[$(N;H0([C;H0])([C;H0])([C;H0]))]
Negishi Coupling Reaction	A palladium- or nickel-catalyzed cross-coupling of organozinc	[Zn;H0]-[C;H0],[*][X;H0]	[$(Zn;H0-[C;H0]),$(*-[X;H0])]

	compounds with organic halides to form carbon–carbon bonds.		
Sakurai Allylation Reaction	Adds allyl groups to aldehydes or ketones using allylsilanes in the presence of a Lewis acid.	[C;H0]=[C;H0],[Si;H0]~[C;H0]=[C;H0]	[$([CX3]~[$([CX3])])]-[!$([CX3])] [$([CX3]~[$([CX3])])]
Reformatsky Reaction	Forms β-hydroxy esters by reacting α-halo esters with aldehydes or ketones in the presence of zinc.	[C;H0][Br;H0],[C;H0][O;H0]	[$(C;H0-[Br;H0]),$(C;H0-[O;H0])]

TS benchmark

The ARplorer could discover reactions in different manual-unexplored systems rather than DFT-unexplored ones. It is easy to understand that a manual search of reaction pathways is generally incomplete and negligent. Besides, to verify the effectiveness of active learning sampling on TS location, our method was applied to the reaction database of RMG. From this database, some reactions involving the change of multiplicity were excluded, and 59 reactions were chosen. The result of active learning sampling on TS location on these 59 reactions is shown in **Table S2**. Active learning sampling on TS location used in ARplorer presented well in general situations of TS location. This test on the RMG database has been supplied with supporting information.

Table S2. Benchmark of active learning sampling on TS location

Entry	Reaction	Success (√) or failure (×)
1	[1+2] Cycloaddition	√
2	1,2-Insertion (CO)	√
3	1,2-Insertion (Carbene)	×
4	1,2-Elimination (NH_3)	√
5	1,2-Shift (C)	√
6	1,2-Shift (S)	√
7	1,2-Interchange	√
8	1,3-Insertion (ROR)	√
9	1,3-Insertion (RSR)	√
10	1,3-Insertion (CO_2)	×
11	1,3-Elimination (NH_3)	√
12	1,3-Sigmatropic Rearrangement	√
13	[2+2] Cycloaddition	√
14	6-Membered Central C-C Shift	√
15	Baeyer-Villiger Reaction Step1 (**Cat**)	√
16	Baeyer-Villiger Reaction Step2	√
17	Baeyer-Villiger Reaction Step2 (**Cat**)	√
18	Br atom Abstraction	√
19	Cl atom Abstraction	√
20	Cyclic-Formation (Ether)	√
21	Cyclic-Formation (Thioether)	√
22	Scission (Cyclopentadiene)	√
23	Diels-Alder Addition	√
24	Diels-Alder Addition (Aromatic)	√
25	F Atom Abstraction	√
26	Elimination (Peroxy Radical)	√
27	H Atom Abstraction	√
28	Intra-[2+2] Cycloaddition	√

29	Intra-5-Membered Conjugated Addition (C=C-C=C)	√
30	Intra-Diels-Alder (Monocyclic)	√
31	Concerted Intra-Diels-Alder (Monocyclic 1,2-Shift)	×
32	Intra-Ene Reaction	√
33	Intra-Halogen Migration	√
34	Intra-H Migration	√
35	Intra-OH Migration	√
36	Intra-Retro-Diels-Alder Reaction (Bicyclic)	√
37	Intra-RH-Addition (Endocyclic)	√
38	Intra-RH-Addition (Exocyclic)	√
39	Intra-R-Addition (Endocyclic)	√
40	Intra-R-Addition (Exocyclic)	√
41	Intra-R-Addition (ExoTetCyclic)	√
42	Intra-R-Addition (Exo Scission)	×
43	Intra-Substitution Cyclization (CS)	√
44	Intra-Substitution Isomerization (CS)	√
45	Intra-Substitution Cyclization (S)	√
46	Intra-Substitution Isomerization (S)	√
47	Ketoenol	√
48	Korcek Reaction Step1	√
49	Korcek Reaction Step2	×
50	Korcek Reaction Step1 (Cat)	√
51	Retroene	√
52	R-Addition (CO)	√
53	R-Addition (CS)	√
54	R-Addition (MultipleBond)	√
55	Singlet-Carbene Intra-Disproportionation	√
56	Substitution (S)	√
57	Substitution (O)	√
58	XY-Addition (MultipleBond)	√
59	XY-Elimination (Hydroxyl)	×
	Total number: 59; Succeed cases: 53; **Successful Rate: 90%**	

Comparsion between ARplorer and other existing programs of automated reaction pathways search

To show the distinct features of ARplorer, a comparison of ARplorer with other existing automated reaction pathways search programs (Kinbot, ADCR, GRRM and LASP) was performed through the pathways search of a representative organic reaction, the Claisen rearrangement of CH_2=CH-O-CH_2-CH=CH_2, and a transition metal-catalyzed reaction,

platinum-catalyzed annulation of alkynes to indoles. The results are shown in **Table S3-1** and **Table S3-2**.

ADCR is a MD-QM combined reaction pathways search program, GRRM is QM-based global reaction route mapping program, and LASP is based on large-scale atomistic simulation with neural network potential. ARplorer and Kinbot are rule-based automated reaction pathways search programs. As for the organic reaction (**Table S3-1**), It could be seen that the outcome yield (it means the obtained complete elementary reactions, including IN, TS, IM and PC, among the total searches) of the rule-based search is generally more efficient than the global search because the chemical logic or the rules could exclude many unimportant processes. LASP, based on machine learning potential, is also efficient in reaction pathways search; however, only limited elements were supported by LASP. The outcome yield of ARplorer is the highest among the tested programs, and it shows the efficiency of ARplorer in reaction pathway search.

As for the system with transition metal atoms, as shown in **Table S3-2**, the QM-based programs that use global search approaches, such as ADCR and GRRM, became heavily cost and made it difficult to obtain complete results of accessible reaction pathways for relatively larger systems. The Kinbot and LASP are limited, and the catalytic system with transition metal is unsupported in these two programs. According to the above comparison, ARplorer can be used as an automatic reaction pathway search program with broad applicability, high generality and high efficiency.

Table S3-1. Comparison between ARplorer and other programs
(Claisen rearrangement of CH_2=CH−O−CH_2−CH=CH_2)

Program	Total reactions	Outcome reaction	Outcome yield	Total number of TSs	Total number IMs	Costed Time (h)	Calculation level
ARplorer	427	156	36.5%	156	178	5	xTB (GFN-2)
ADCR	24949	221	0.8%	221	282	18.9	xTB (GFN-2)
GRRM	-	200	-	200	197	168	B3LYP /6-31G
Kinbot	220	64	29.1%	34	-	72	B3LYP /6-31G
LASP	1575	303	19.2%	303	2182	8	MLP

In ARplorer and ADCR, the reaction is specified to proceed in two reaction steps. In other programs, reaction steps could not be specified, and these programs were terminated at a given time. In ADCR, four of the twelve atoms were frozen. The site with "-" means this data could not be found.

Table S3-2. Comparison between ARplorer and existing programs
(platinum-catalyzed annulation of alkynes to indoles)

Program	result	Calculation level
ARplorer	As shown in Case 3 of the paper	xTB (GFN-2)
ADCR	Too costly and no output in 5 days	xTB

Kinbot	Transition metal elements are not supported	(GFN-2) B3LYP /6-31G
LASP	ML potential for transition metal was not found	MLP

Variance test of ChatGPT.

Three repeat consecutive rounds of production of chemical logic of case 2 were used to test the variance of the specific ChatGPT, as shown below in **Figure S11**, **S12**, **S13**. It could be seen that the variance introduced by this specific ChatGPT is minimal and does not significantly affect the extracted chemical logic

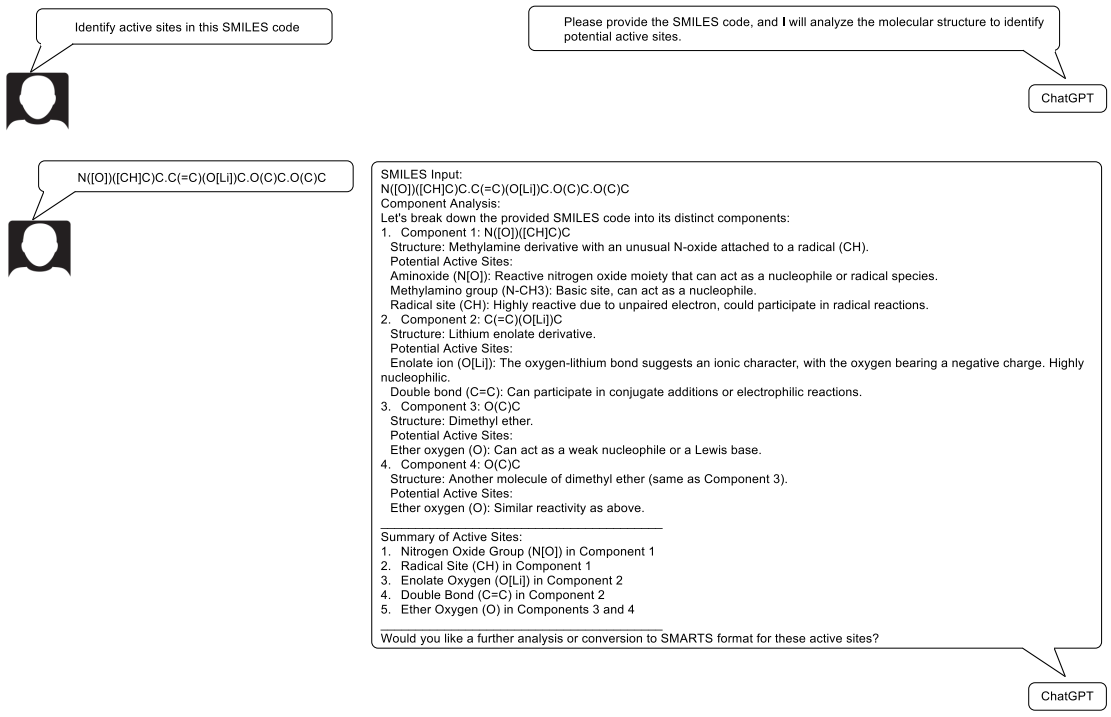

Figure S11. The first round of the variance test of the chemical logic of case 2.

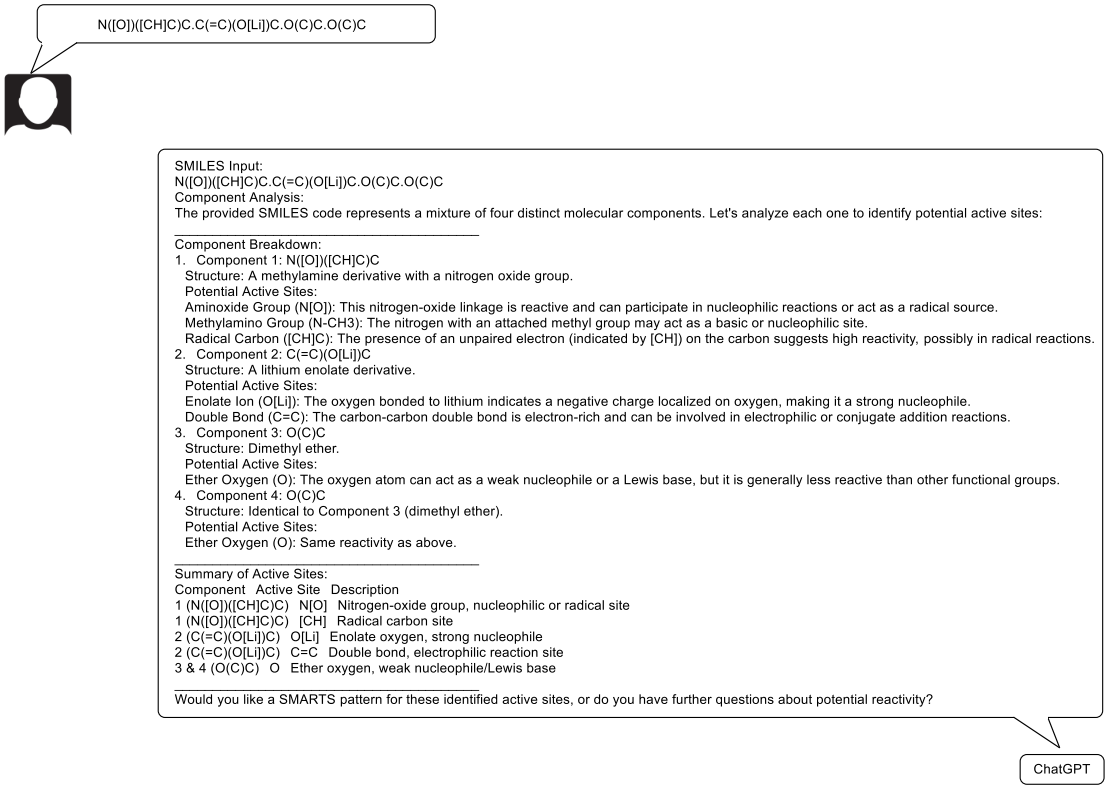

Figure S12. The second round of the variance test of the chemical logic of case 2.

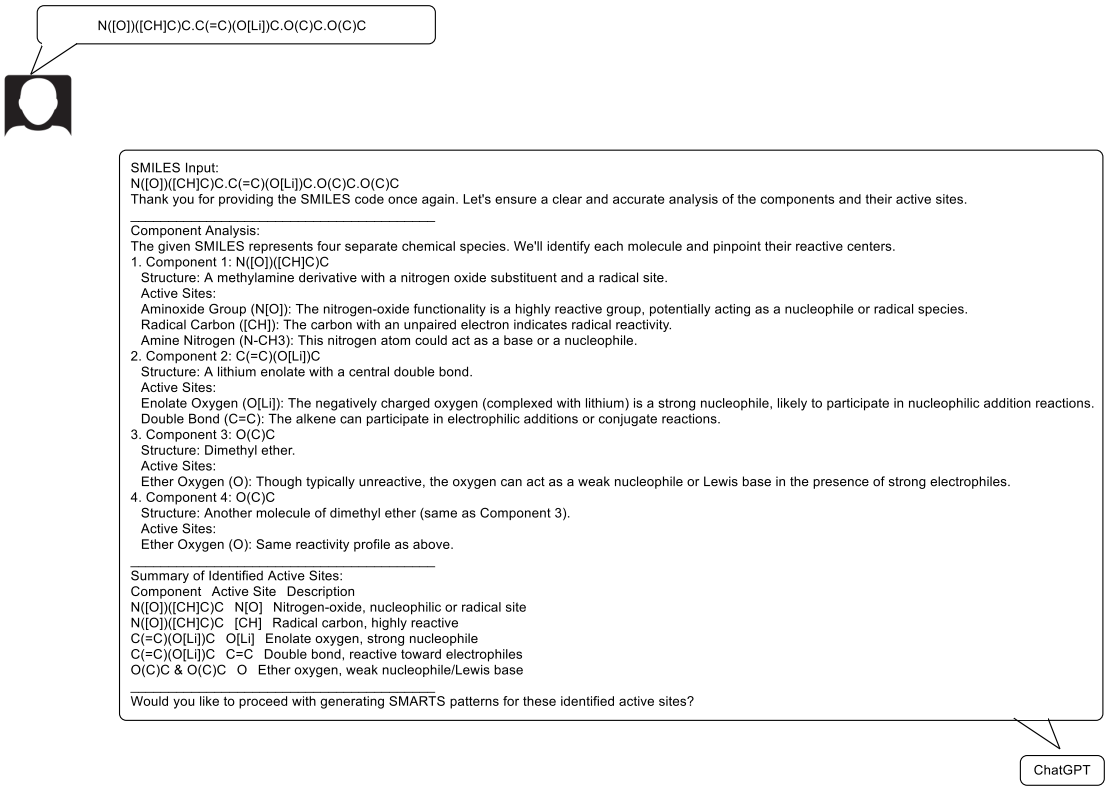

Figure S13. The third round of the variance test of the chemical logic of case 2.

To test if there is obvious stochasticity in ARplorer, a replicate run of case 2 and tests of change of energy threshold have been performed. The results are in Table 2, and the

corresponding PES are in Figure R1. No obvious stochasticity exists in the reaction pathways search with ARplorer. The parameters of the energy threshold mainly affect the total number of reactions found and barely affect the reaction with a low energy barrier.

Stochasticity test of ARplorer

To test if there is obvious stochasticity in ARplorer, a replicate run of case 2 and tests of change of energy threshold have been performed. The results are in **Table S4,** and the corresponding PES are in **Figure S14**. No obvious stochasticity exists in the reaction pathways search with ARplorer. The parameters of the energy threshold mainly affect the total number of reactions found and barely affect the reaction with a low energy barrier.

Table S4. Test of stochasticity (Case 2)

	IM_energy threshold (a.u.)	IRC_energy threshold (a.u.)	Number of reactions
original	0.08	0.2	156
Replication	0.08	0.2	156
Test1	0.04	0.1	29
Test2	0.08	0.1	55

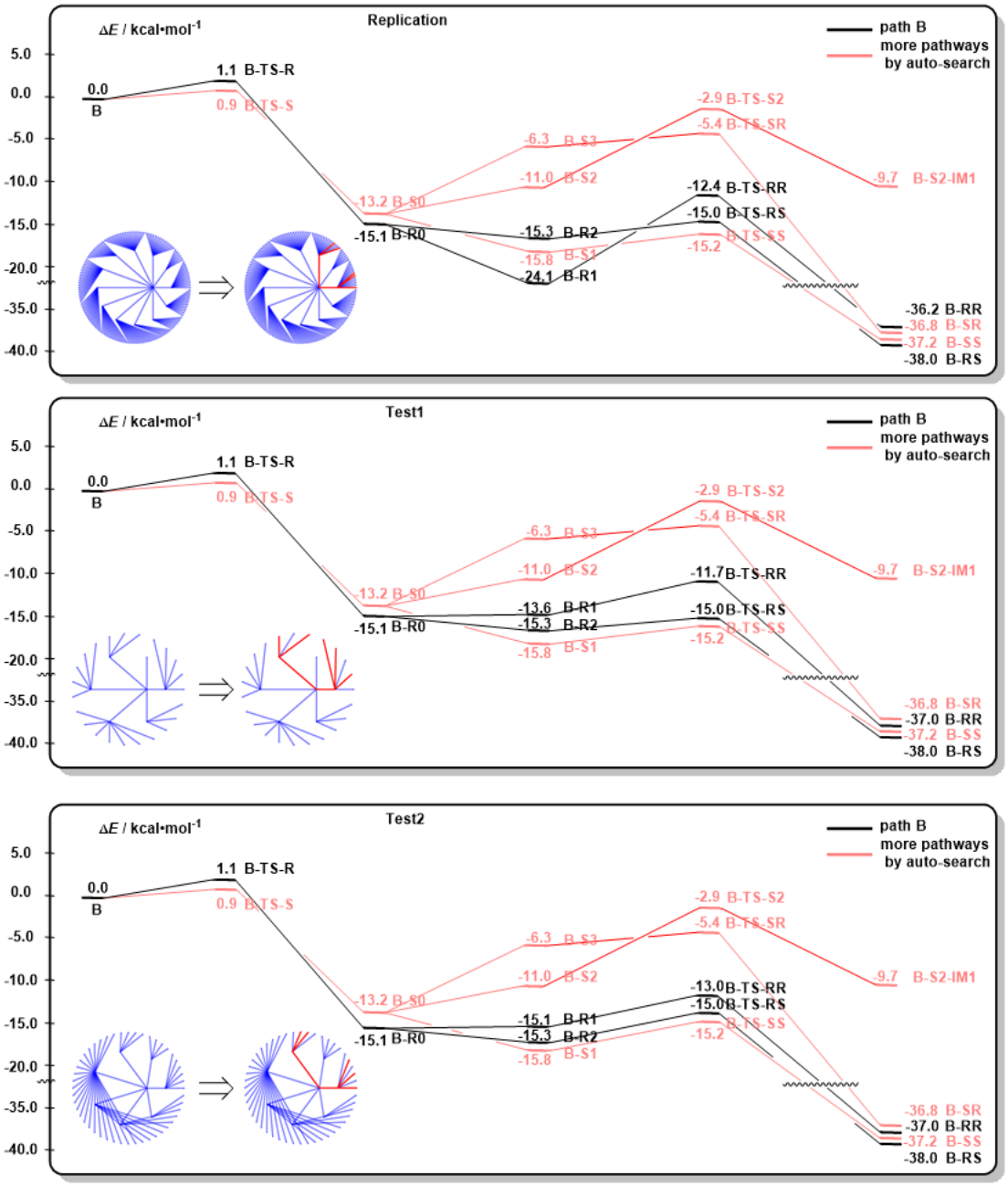

Figure S14 Reaction pathways with low energy barriers in replication test1 and test2.

Overview of the ARplorer workflow

To clarify the mechanism by which the chemical logic base and active-site library are integrated within ARplorer, an overview of the ARplorer workflow is presented in Figure S15. As depicted, the workflow begins with the systematic collection and curation of relevant documents, such as books, patents, and scientific literature (step 1). In step 2, text-mining and data-processing techniques are employed to extract key chemical logic terms, reaction types, and mechanistic details from these sources. The extracted information is then processed in to an active-site library (in SMARTS format). In Step 3, during the execution of ARplorer for comprehensive reaction pathway exploration, the system interacts with the active-site library at each iteration to identify the next possible reaction, which is subsequently filtered if it is not feasible.

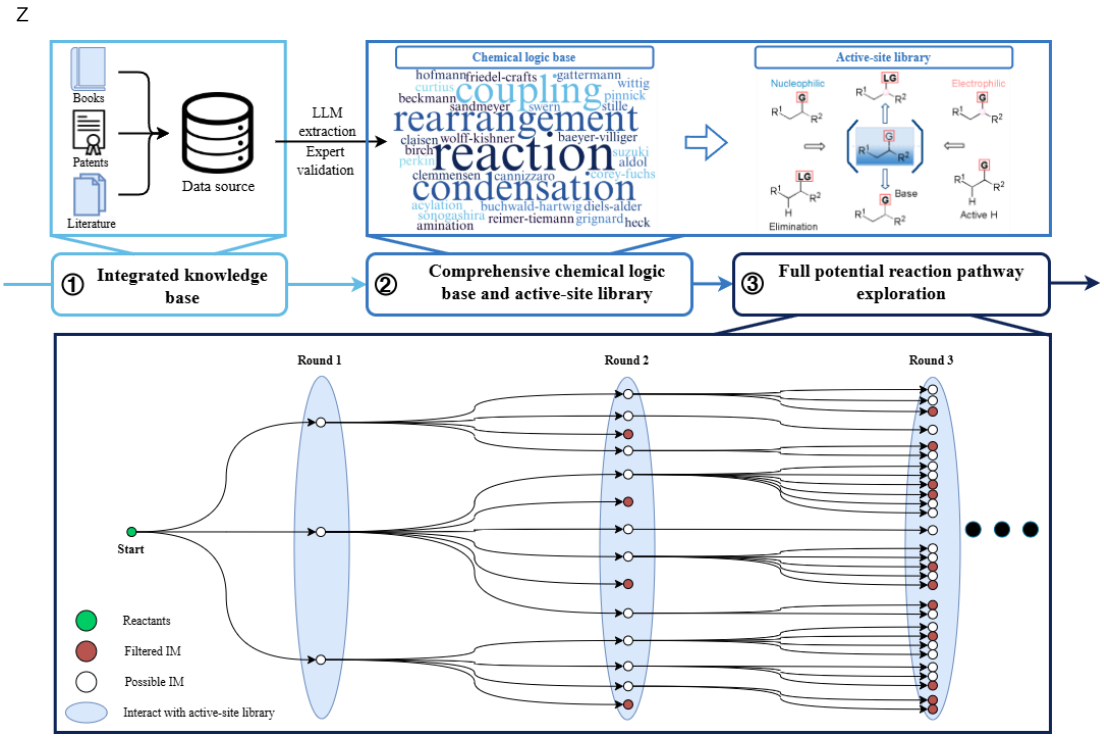

Figure S15 Overview of the ARplorer workflow

Design of Chain-of-through (COT) prompt

An effective strategy for designing Chain-of-Thought (COT) prompts to curate chemical knowledge bases involves structuring the prompts to mirror expert reasoning and reinforce scientific rigour. For instance, a well-designed COT prompt can sequentially guide the model through stages such as clarifying inputs[1], conducting structural analysis, decomposing functional groups, identifying reactive sites, and formulating reaction logic

based on explicit chemical principles. This approach not only improves the interpretability and transparency of the model's outputs but also reduces the risk of errors and unsupported inferences during knowledge extraction. By embedding domain-specific reasoning steps directly into the prompt design, this method provides a robust framework for the reliable curation and expansion of chemical knowledge bases. An example of CoT prompt design is shown below.

“””

1. Input Clarification
    - Prompt Example: “Verify the input reaction: Are all reactants specified? If not, list ambiguities.”
    - Purpose: Eliminates errors from misinterpreted or incomplete inputs.
2. Structural Analysis
    - Prompt Example: “Analyze the molecular structures: Identify bonds broken/formed and stereochemical constraints.”
    - Purpose: Grounds the model in explicit structural features.
3. Functional Group Decomposition
    - Prompt Example: “List all functional groups in reactants/products and their known reactivity patterns.”
    - *Anti-Hallucination Measure*: Limits proposals to documented group behaviors (e.g., “Carboxylates may undergo nucleophilic attack; avoid suggesting radical steps unless evidence exists”).
4. Reactive Site Identification
    - Prompt Example: “Rank potential reactive sites by electrophilicity/nucleophilicity, citing textbook rules (e.g., Markovnikov’s rule).”
    - Purpose: Prioritizes chemically logical sites over speculative ones.
5. Reaction Logic Formulation
    - Prompt Example: “Propose a mechanism only if all steps satisfy three criteria: (a) Orbital symmetry conservation, (b) Thermodynamic feasibility ($\Delta G < 0$), (c) No hypothetical intermediates.”
    - Validation: Requires self-checking before final output.

“”””

1. Liu, H., Yin, H., Luo, Z. & Wang, X. Integrating chemistry knowledge in large language models via prompt engineering. *Synth. Syst. Biotechnol.* **10**, 23–38 (2025).

DFT-optimized cartesian coordinates of all species involved in the cycloaddition reaction

A-IM1-TS1

C	0.4764	2.7820	-0.1171
C	1.8551	3.0314	-0.3492
C	2.5391	2.2875	0.5916
C	1.5621	1.7270	1.4094
O	0.3618	2.1272	1.0692
H	-0.3465	3.4262	-0.3831
H	2.2590	3.5842	-1.1736
H	3.5959	2.1428	0.6806
H	1.6605	1.0852	2.2668
C	-2.0061	1.5012	-2.2535
H	-1.5706	1.9435	-3.1291
H	-3.0638	1.3198	-2.2583
C	-1.2548	1.1438	-1.2123
C	0.2356	1.2946	-1.2788
H	0.5879	1.7262	-2.2245
O	0.9486	0.3586	-0.7806
O	-1.6736	0.6175	-0.0723
Si	-2.9303	-0.3698	0.4005
C	-2.7042	-0.3319	2.2809
H	-2.8089	0.6719	2.6826
H	-3.4395	-0.9620	2.7699
H	-1.7200	-0.6970	2.5553
C	-4.6164	0.3840	-0.0959
H	-4.8743	0.1793	-1.1316
H	-5.4117	-0.0306	0.5149
H	-4.6306	1.4617	0.0435
C	-2.6966	-2.0736	-0.4041
H	-1.6980	-2.4511	-0.1991
H	-3.4079	-2.8015	-0.0277
H	-2.8078	-2.0311	-1.4851

Al	1.5661	-1.1842	-0.1198
Cl	3.6189	-0.8319	-0.0180
Cl	0.7620	-1.5174	1.7727
Cl	0.9665	-2.5506	-1.5611

A-IM1

C	0.4203	2.7163	-0.2119
C	1.8215	2.9860	-0.3733
C	2.4609	2.2955	0.6282
C	1.4443	1.7597	1.4250
O	0.2633	2.1308	1.0181
H	-0.3686	3.4011	-0.4915
H	2.2592	3.5033	-1.2037
H	3.5130	2.1663	0.7792
H	1.5119	1.1546	2.3128
C	-2.0274	1.3458	-2.3430
H	-1.5815	1.7208	-3.2443
H	-3.0785	1.1285	-2.3580
C	-1.2999	1.1104	-1.2546
C	0.1965	1.3103	-1.2819
H	0.5454	1.6900	-2.2526
O	0.8997	0.3409	-0.7882
O	-1.7401	0.6734	-0.0841
Si	-2.9257	-0.3889	0.4098
C	-2.6862	-0.3075	2.2873
H	-2.8047	0.7028	2.6681
H	-3.4070	-0.9393	2.7950
H	-1.6939	-0.6508	2.5613
C	-4.6522	0.2624	-0.0923
H	-4.8970	0.0352	-1.1264
H	-5.4236	-0.1901	0.5220
H	-4.7257	1.3390	0.0365
C	-2.5986	-2.0887	-0.3691
H	-1.5779	-2.4040	-0.1666
H	-3.2628	-2.8515	0.0239
H	-2.7197	-2.0697	-1.4497
Al	1.5943	-1.1405	-0.1180
Cl	3.6372	-0.7057	-0.0281
Cl	0.8230	-1.4516	1.7989
Cl	1.0743	-2.6055	-1.4919

B

C	0.8826	2.8540	0.2282
C	2.1218	3.0796	-0.3328

C	2.9935	2.1710	0.2863
C	2.2313	1.4837	1.1958
O	0.9739	1.9285	1.1924
H	-0.0461	3.3814	0.1290
H	2.3556	3.7843	-1.1048
H	4.0342	2.0250	0.0866
H	2.4889	0.7157	1.8991
C	-1.7386	2.0854	-1.8957
H	-1.2717	2.8171	-2.5280
H	-2.8076	2.1020	-1.8166
C	-0.9940	1.1777	-1.2446
C	0.4588	1.1549	-1.4500
H	0.8598	1.8011	-2.2375
O	1.1746	0.2667	-0.9700
O	-1.4189	0.2072	-0.4518
Si	-2.8308	-0.1159	0.3932
C	-2.6468	0.7999	2.0524
H	-2.6472	1.8804	1.9271
H	-3.4531	0.5495	2.7338
H	-1.7116	0.5249	2.5313
C	-4.4004	0.4859	-0.5171
H	-4.3869	0.2216	-1.5711
H	-5.2764	0.0153	-0.0822
H	-4.5499	1.5594	-0.4375
C	-2.8564	-2.0043	0.4992
H	-1.9927	-2.3767	1.0391
H	-3.7453	-2.3524	1.0153
H	-2.8410	-2.4598	-0.4868
Al	1.2036	-1.3905	-0.1050
Cl	3.2699	-1.6311	-0.1016
Cl	0.4564	-1.3283	1.8271
Cl	0.2046	-2.5368	-1.5097

A-IM4

C	-0.4562	2.7952	0.1441
C	-1.8753	3.1470	0.2854
C	-2.5324	2.3335	-0.5736
C	-1.5007	1.6117	-1.2618
O	-0.3410	2.1981	-1.1055
H	0.3405	3.4901	0.3786
H	-2.2693	3.8007	1.0370
H	-3.5836	2.1680	-0.6926
H	-1.6154	0.8944	-2.0589
C	1.7256	1.1476	2.3596

H	1.2208	1.4949	3.2405
H	2.7535	0.8554	2.4556
C	1.0950	1.0465	1.1969
C	-0.3734	1.4038	1.0748
H	-0.8053	1.6474	2.0522
O	-1.0957	0.5126	0.3870
O	1.6069	0.6404	0.0406
Si	2.9147	-0.2912	-0.3930
C	2.7339	-0.2671	-2.2795
H	2.7497	0.7448	-2.6736
H	3.5396	-0.8194	-2.7510
H	1.7976	-0.7246	-2.5818
C	4.5402	0.5572	0.1496
H	4.7945	0.3466	1.1847
H	5.3718	0.2142	-0.4572
H	4.4807	1.6367	0.0390
C	2.7633	-2.0164	0.3881
H	1.8295	-2.4839	0.0867
H	3.5733	-2.6729	0.0872
H	2.7606	-1.9689	1.4743
Al	-1.5230	-1.2464	0.1003
Cl	-3.5895	-1.0566	-0.0844
Cl	-0.6578	-1.7834	-1.7107
Cl	-0.8132	-2.2015	1.7892

A-TS3

C	-0.8475	-2.8004	0.2287
C	-1.2500	-2.0061	1.2936
C	-2.5975	-1.7436	1.0861
C	-2.9255	-2.3503	-0.1283
O	-1.8994	-3.1227	-0.5379
H	0.0671	-3.3434	0.0844
H	-0.6189	-1.6432	2.0789
H	-3.2449	-1.1424	1.6896
H	-3.8929	-2.5673	-0.5426
C	-2.4147	-0.7581	-1.5269
H	-2.5013	-1.4185	-2.3719
H	-3.2443	-0.1020	-1.3326
C	-1.1642	-0.4073	-1.0730
C	-0.0246	-1.2117	-1.3923
H	-0.1492	-1.9900	-2.1529
O	1.1356	-0.9398	-1.0038
O	-0.9521	0.5366	-0.1671
Si	-1.5920	2.0459	0.1536

C	-0.6898	2.4993	1.7502
H	0.3821	2.5276	1.5818
H	-0.9966	3.4750	2.1120
H	-0.8722	1.7755	2.5388
C	-1.2235	3.1611	-1.3434
H	-1.7039	2.7999	-2.2503
H	-1.5604	4.1791	-1.1774
H	-0.1539	3.1944	-1.5296
C	-3.4858	1.9710	0.4268
H	-3.7825	1.1259	1.0410
H	-3.8185	2.8688	0.9375
H	-4.0422	1.9182	-0.5055
Al	2.3187	-0.0067	0.0269
Cl	4.0763	-1.0213	-0.3861
Cl	2.2583	1.9332	-0.6995
Cl	1.6504	-0.3313	1.9703

A-IM3

C	-0.4896	-2.6011	-0.0031
C	-0.9263	-1.9393	1.2700
C	-2.2460	-1.8067	1.1989
C	-2.6623	-2.3473	-0.1447
O	-1.6342	-3.2318	-0.4844
H	0.3539	-3.2845	0.0639
H	-0.2406	-1.6126	2.0274
H	-2.9250	-1.3704	1.9032
H	-3.6276	-2.8472	-0.2065
C	-2.5885	-1.1706	-1.2111
H	-2.6930	-1.6413	-2.1875
H	-3.3808	-0.4458	-1.0457
C	-1.2516	-0.5674	-1.0325
C	-0.0735	-1.4744	-1.1121
H	-0.0613	-2.0360	-2.0603
O	1.0975	-0.9120	-0.8366
O	-1.0765	0.5683	-0.5355
Si	-1.8158	1.9787	0.1244
C	-1.2707	1.8840	1.9320
H	-0.2395	1.5404	2.0004
H	-1.3245	2.8613	2.4010
H	-1.8808	1.2027	2.5204
C	-1.0696	3.3131	-0.9875
H	-1.4480	3.2670	-2.0066
H	-1.2814	4.3059	-0.6031
H	0.0123	3.1946	-1.0303

C	-3.7207	1.9035	-0.0455
H	-4.1685	1.0932	0.5252
H	-4.1478	2.8255	0.3369
H	-4.0486	1.8146	-1.0787
Al	2.2959	0.0598	-0.0528
Cl	4.1130	-0.8806	-0.3907
Cl	2.1850	1.9939	-0.8409
Cl	1.7827	0.0687	1.9993

A-IM3-TS1

C	-1.3232	-1.6629	0.5236
C	-2.0356	-0.8064	1.5359
C	-3.3000	-0.7166	1.1493
C	-3.4288	-1.5129	-0.1292
O	-2.3503	-2.4090	-0.0715
H	-0.5322	-2.3092	0.9007
H	-1.5424	-0.3637	2.3773
H	-4.1106	-0.1729	1.5920
H	-4.3603	-2.0623	-0.2624
C	-3.1680	-0.5652	-1.3567
H	-3.0925	-1.1995	-2.2393
H	-3.9624	0.1698	-1.4841
C	-1.8785	0.1037	-1.0554
C	-0.7320	-0.7230	-0.6146
H	-0.4021	-1.4122	-1.4052
O	0.2871	0.1008	-0.2172
O	-1.7847	1.3263	-0.9430
Si	-0.3351	2.1116	0.0600
C	0.5449	1.9702	1.7519
H	1.3910	1.2901	1.7270
H	0.9176	2.9496	2.0329
H	-0.1197	1.6431	2.5470
C	0.6531	2.7960	-1.4074
H	0.0103	3.0318	-2.2510
H	1.1596	3.7084	-1.1148
H	1.4119	2.0959	-1.7423
C	-1.6921	3.3938	0.5453
H	-2.4329	2.9821	1.2243
H	-1.2340	4.2397	1.0433
H	-2.2209	3.7675	-0.3237
Al	2.0294	-0.6208	-0.0148
Cl	2.0592	-1.9768	-1.6064
Cl	3.4415	0.8692	-0.1754
Cl	1.9331	-1.5780	1.8364

A-IM5

C	-1.5026	-1.3435	0.5799
C	-2.2339	-0.4913	1.5867
C	-3.4872	-0.3902	1.1722
C	-3.6009	-1.1848	-0.1112
O	-2.5278	-2.0993	-0.0220
H	-0.7311	-2.0032	0.9792
H	-1.7579	-0.0683	2.4490
H	-4.3037	0.1566	1.6014
H	-4.5328	-1.7370	-0.2366
C	-3.3298	-0.2545	-1.3193
H	-3.2899	-0.8704	-2.2200
H	-4.1056	0.5024	-1.4408
C	-1.9966	0.4220	-1.1301
C	-0.9070	-0.4372	-0.5434
H	-0.5961	-1.1338	-1.3366
O	0.2188	0.2988	-0.1391
O	-1.7935	1.5798	-1.4025
Si	0.2202	2.0201	0.1715
C	1.5046	2.0883	1.5773
H	2.4429	1.6204	1.2973
H	1.7214	3.1208	1.8317
H	1.1541	1.5962	2.4806
C	0.8791	2.8933	-1.3832
H	0.1250	2.9998	-2.1557
H	1.2305	3.8862	-1.1234
H	1.7201	2.3484	-1.8027
C	-1.3394	2.7878	0.9648
H	-2.0015	2.0578	1.4170
H	-1.0395	3.4879	1.7371
H	-1.9154	3.3362	0.2290
Al	1.9481	-0.8524	-0.0182
Cl	1.4897	-2.4529	-1.2578
Cl	3.4526	0.2867	-0.8316
Cl	1.9032	-1.3205	1.9880

A-TS2

C	-0.1915	2.0018	1.0985
C	-1.3877	2.4700	0.5611
C	-1.2393	2.3907	-0.8219
C	0.0488	1.9390	-1.0396
O	0.6973	1.8098	0.1159
H	0.1939	2.0516	2.0996

H	-2.2567	2.7666	1.1105
H	-1.9694	2.6176	-1.5707
H	0.6192	1.8322	-1.9424
C	-0.7963	-0.1437	1.2296
H	-1.6149	-0.0337	1.9183
H	0.1793	-0.3577	1.6359
C	-1.0459	-0.4332	-0.0861
C	0.0144	-0.6470	-1.0131
H	-0.2932	-0.8011	-2.0541
O	1.2256	-0.7644	-0.7211
O	-2.2705	-0.3928	-0.6404
Si	-3.7909	-0.7423	-0.0710
C	-4.4891	0.6714	1.0028
H	-4.4468	1.6212	0.4773
H	-5.5302	0.4857	1.2467
H	-3.9571	0.7888	1.9431
C	-4.7468	-0.8855	-1.7023
H	-4.6649	0.0224	-2.2915
H	-4.3778	-1.7046	-2.3112
H	-5.8003	-1.0628	-1.5162
C	-3.7518	-2.3684	0.9186
H	-3.1543	-2.2797	1.8221
H	-4.7474	-2.6793	1.2173
H	-3.3229	-3.1724	0.3268
Al	2.8795	-0.4491	-0.0243
Cl	3.5347	1.0894	-1.2510
Cl	2.6577	0.0961	1.9810
Cl	3.7531	-2.3064	-0.2431

A-IM2

C	0.2892	-1.6755	1.1209
C	1.4418	-2.3876	0.5331
C	1.2625	-2.3291	-0.8083
C	-0.0195	-1.7404	-1.0101
O	-0.6870	-1.6834	0.1257
H	-0.1184	-1.9719	2.0825
H	2.2853	-2.7438	1.0876
H	1.9278	-2.6399	-1.5882
H	-0.5933	-1.6940	-1.9201
C	0.7435	-0.1166	1.1889
H	1.6132	-0.0414	1.8335
H	-0.1235	0.3942	1.6100
C	1.0199	0.3209	-0.1816
C	-0.0061	0.6500	-1.0627

H	0.2860	0.9061	-2.0851
O	-1.2287	0.7949	-0.7349
O	2.2668	0.3051	-0.6620
Si	3.7602	0.7406	-0.0684
C	4.4920	-0.6264	1.0437
H	4.5037	-1.5860	0.5342
H	5.5188	-0.3906	1.3042
H	3.9492	-0.7517	1.9772
C	4.7444	0.8965	-1.6808
H	4.7175	-0.0248	-2.2544
H	4.3511	1.6863	-2.3131
H	5.7845	1.1262	-1.4769
C	3.6053	2.3753	0.8932
H	3.0270	2.2597	1.8063
H	4.5773	2.7677	1.1731
H	3.1087	3.1319	0.2916
Al	-2.8321	0.4196	-0.0383
Cl	-3.4899	-1.2001	-1.1725
Cl	-2.5600	-0.0289	2.0006
Cl	-3.8845	2.1828	-0.2784

A-IM2-TS1

C	0.3611	-1.6355	1.1540
C	1.4783	-2.3392	0.4681
C	1.1973	-2.2783	-0.8451
C	-0.1100	-1.6537	-0.9550
O	-0.6919	-1.6912	0.2494
H	0.0481	-1.9516	2.1449
H	2.3516	-2.7174	0.9582
H	1.7909	-2.5998	-1.6772
H	-0.7850	-1.7854	-1.7889
C	0.7641	-0.0614	1.2101
H	1.6313	0.0585	1.8521
H	-0.1286	0.4195	1.6188
C	1.0261	0.3236	-0.1699
C	-0.0321	0.3389	-1.1192
H	0.2827	0.4974	-2.1573
O	-1.2406	0.6756	-0.8226
O	2.2477	0.3171	-0.6528
Si	3.7755	0.7226	-0.0826
C	4.5076	-0.6478	1.0215
H	4.5450	-1.6000	0.4997
H	5.5262	-0.3974	1.3005
H	3.9522	-0.7943	1.9443

C	4.7116	0.8564	-1.7250
H	4.6714	-0.0736	-2.2845
H	4.2969	1.6355	-2.3574
H	5.7567	1.0923	-1.5564
C	3.6286	2.3667	0.8619
H	3.0977	2.2557	1.8041
H	4.6054	2.7812	1.0886
H	3.0894	3.1043	0.2733
Al	-2.8217	0.4238	-0.0534
Cl	-3.5858	-1.3110	-0.9257
Cl	-2.4846	0.2263	2.0224
Cl	-3.8487	2.1682	-0.4739

A-TS1

C	0.4764	2.7820	-0.1171
C	1.8551	3.0314	-0.3492
C	2.5391	2.2875	0.5916
C	1.5621	1.7270	1.4094
O	0.3618	2.1272	1.0692
H	-0.3465	3.4262	-0.3831
H	2.2590	3.5842	-1.1736
H	3.5959	2.1428	0.6806
H	1.6605	1.0852	2.2668
C	-2.0061	1.5012	-2.2535
H	-1.5706	1.9435	-3.1291
H	-3.0638	1.3198	-2.2583
C	-1.2548	1.1438	-1.2123
C	0.2356	1.2946	-1.2788
H	0.5879	1.7262	-2.2245
O	0.9486	0.3586	-0.7806
O	-1.6736	0.6175	-0.0723
Si	-2.9303	-0.3698	0.4005
C	-2.7042	-0.3319	2.2809
H	-2.8089	0.6719	2.6826
H	-3.4395	-0.9620	2.7699
H	-1.7200	-0.6970	2.5553
C	-4.6164	0.3840	-0.0959
H	-4.8743	0.1793	-1.1316
H	-5.4117	-0.0306	0.5149
H	-4.6306	1.4617	0.0435
C	-2.6966	-2.0736	-0.4041
H	-1.6980	-2.4511	-0.1991
H	-3.4079	-2.8015	-0.0277
H	-2.8078	-2.0311	-1.4851

Al	1.5661	-1.1842	-0.1198
Cl	3.6189	-0.8319	-0.0180
Cl	0.7620	-1.5174	1.7727
Cl	0.9665	-2.5506	-1.5611

A-IM1

C	0.4203	2.7163	-0.2119
C	1.8215	2.9860	-0.3733
C	2.4609	2.2955	0.6282
C	1.4443	1.7597	1.4250
O	0.2633	2.1308	1.0181
H	-0.3686	3.4011	-0.4915
H	2.2592	3.5033	-1.2037
H	3.5130	2.1663	0.7792
H	1.5119	1.1546	2.3128
C	-2.0274	1.3458	-2.3430
H	-1.5815	1.7208	-3.2443
H	-3.0785	1.1285	-2.3580
C	-1.2999	1.1104	-1.2546
C	0.1965	1.3103	-1.2819
H	0.5454	1.6900	-2.2526
O	0.8997	0.3409	-0.7882
O	-1.7401	0.6734	-0.0841
Si	-2.9257	-0.3889	0.4098
C	-2.6862	-0.3075	2.2873
H	-2.8047	0.7028	2.6681
H	-3.4070	-0.9393	2.7950
H	-1.6939	-0.6508	2.5613
C	-4.6522	0.2624	-0.0923
H	-4.8970	0.0352	-1.1264
H	-5.4236	-0.1901	0.5220
H	-4.7257	1.3390	0.0365
C	-2.5986	-2.0887	-0.3691
H	-1.5779	-2.4040	-0.1666
H	-3.2628	-2.8515	0.0239
H	-2.7197	-2.0697	-1.4497
Al	1.5943	-1.1405	-0.1180
Cl	3.6372	-0.7057	-0.0281
Cl	0.8230	-1.4516	1.7989
Cl	1.0743	-2.6055	-1.4919

A-IM1-TS2

C	-0.0394	2.5545	-0.5783
C	0.3899	2.2494	0.8147

C	-0.7039	1.9062	1.5081
C	-1.8156	2.0178	0.5757
O	-1.4638	2.7330	-0.4643
H	0.4113	3.4291	-1.0414
H	1.4193	2.2291	1.1203
H	-0.7728	1.5489	2.5140
H	-2.8627	2.0264	0.8405
C	-1.8150	0.1124	-2.5834
H	-1.3464	0.2566	-3.5383
H	-2.7542	-0.4096	-2.5626
C	-1.2317	0.5399	-1.4763
C	0.1217	1.2546	-1.4827
H	0.3230	1.5905	-2.5120
O	1.0901	0.4192	-1.0546
O	-1.7744	0.3398	-0.2318
Si	-2.4016	-1.1706	0.3594
C	-2.2925	-0.9795	2.2393
H	-2.8268	-0.1110	2.6151
H	-2.7215	-1.8538	2.7181
H	-1.2535	-0.9151	2.5525
C	-4.2287	-1.2246	-0.2067
H	-4.3442	-1.6373	-1.2052
H	-4.8086	-1.8537	0.4607
H	-4.6899	-0.2399	-0.2056
C	-1.3184	-2.5175	-0.4054
H	-0.2661	-2.2453	-0.3343
H	-1.4446	-3.4589	0.1195
H	-1.5408	-2.6908	-1.4552
Al	2.1866	-0.4417	-0.0443
Cl	3.7701	0.8711	0.3570
Cl	1.1927	-0.8373	1.7910
Cl	2.6527	-2.2074	-1.0283

A-IM9

C	0.1807	2.7057	0.6315
C	-0.2456	2.5022	-0.7994
C	0.7488	1.8885	-1.4216
C	1.8420	1.7102	-0.3970
O	1.6154	2.6707	0.5483
H	-0.1275	3.6405	1.0937
H	-1.2197	2.7558	-1.1654
H	0.8043	1.5248	-2.4254
H	2.8757	1.7286	-0.7420
C	1.2835	-0.2158	2.5409

H	0.7009	-0.1375	3.4391
H	2.0944	-0.9203	2.5399
C	0.9597	0.5043	1.4845
C	-0.2404	1.4431	1.4530
H	-0.4721	1.7338	2.4892
O	-1.2955	0.7805	0.9018
O	1.6652	0.3866	0.2806
Si	2.3742	-1.1705	-0.3771
C	2.3752	-0.9394	-2.2546
H	2.9081	-0.0521	-2.5868
H	2.8545	-1.7951	-2.7208
H	1.3529	-0.8970	-2.6256
C	4.1487	-1.0651	0.3268
H	4.1831	-1.1133	1.4121
H	4.7463	-1.8901	-0.0478
H	4.6522	-0.1471	0.0314
C	1.3004	-2.5612	0.3051
H	0.3025	-2.2171	0.5764
H	1.1645	-3.3210	-0.4587
H	1.7352	-3.0483	1.1739
Al	-2.1773	-0.3726	-0.0082
Cl	-3.9623	0.5200	-0.5677
Cl	-0.9977	-0.8188	-1.7281
Cl	-2.3041	-2.1217	1.1395

A-IM1-TS3

C	0.1633	2.0627	0.1195
C	0.9981	1.3577	-0.8890
C	2.0833	2.2424	-1.1549
C	1.9612	3.2872	-0.2953
O	0.8720	3.2435	0.4561
H	-0.8439	2.3147	-0.2355
H	0.5562	0.6647	-1.5875
H	2.8729	2.0802	-1.8586
H	2.5952	4.1474	-0.1672
C	1.8821	0.0722	2.5879
H	1.4572	0.3736	3.5261
H	2.7857	-0.5079	2.6116
C	1.2756	0.3798	1.4549
C	-0.0431	1.1197	1.3520
H	-0.2429	1.7295	2.2449
O	-1.0436	0.2421	1.1127
O	1.7182	0.0436	0.2144
Si	2.1537	-1.5710	-0.2793

C	2.1132	-1.4810	-2.1698
H	2.6709	-0.6359	-2.5636
H	2.5526	-2.3818	-2.5861
H	1.0921	-1.4203	-2.5366
C	3.9527	-1.7654	0.3390
H	4.0043	-2.1240	1.3631
H	4.4779	-2.4903	-0.2742
H	4.5065	-0.8317	0.2862
C	0.9327	-2.7601	0.5411
H	-0.0915	-2.4407	0.3532
H	1.0378	-3.7683	0.1538
H	1.0644	-2.8038	1.6198
Al	-2.2891	-0.2799	0.0257
Cl	-3.3528	1.4712	-0.4593
Cl	-1.3380	-0.8854	-1.7826
Cl	-3.2609	-1.8561	0.9271

A-IM10

C	0.6096	2.2289	-0.0228
C	1.4128	1.1224	-0.7198
C	2.7749	1.7304	-0.7926
C	2.7495	2.8793	-0.1185
O	1.5461	3.2257	0.3734
H	-0.1507	2.6863	-0.6600
H	0.9721	0.7618	-1.6478
H	3.6152	1.2755	-1.2727
H	3.5412	3.5811	0.0732
C	1.0158	-0.2966	2.5547
H	0.5059	0.0414	3.4369
H	1.6198	-1.1799	2.6423
C	0.8361	0.3470	1.4201
C	-0.0727	1.5277	1.1700
H	-0.1342	2.2004	2.0365
O	-1.3057	1.0683	0.8138
O	1.4067	-0.0188	0.2068
Si	1.9676	-1.6853	-0.2751
C	2.0024	-1.6334	-2.1649
H	2.6746	-0.8809	-2.5686
H	2.3306	-2.5951	-2.5474
H	1.0033	-1.4495	-2.5564
C	3.7234	-1.6848	0.4773
H	3.7265	-1.4915	1.5467
H	4.1943	-2.6506	0.3241
H	4.3659	-0.9387	0.0155

C	0.7387	-2.8939	0.4877
H	-0.2395	-2.4360	0.6456
H	0.5838	-3.7342	-0.1828
H	1.0713	-3.3004	1.4390
Al	-2.3504	0.0156	-0.0512
Cl	-4.0942	1.0183	-0.5162
Cl	-1.2510	-0.5012	-1.8140
Cl	-2.5721	-1.7326	1.0887

A-IM2-TS3

C	-0.0089	2.1631	0.9471
C	-1.1451	2.9400	0.3866
C	-1.2383	2.5623	-0.9027
C	-0.1167	1.6854	-1.1351
O	0.7781	1.8365	-0.1688
H	0.5915	2.5660	1.7559
H	-1.8032	3.5586	0.9620
H	-1.9872	2.8051	-1.6287
H	0.2530	1.3661	-2.0959
C	-0.6509	0.7467	1.3276
H	-1.4878	0.8926	2.0046
H	0.1497	0.1754	1.7973
C	-1.0869	0.1206	0.0558
C	-0.2316	-0.6833	-0.7026
H	-0.6660	-1.1556	-1.5901
O	0.9878	-0.8840	-0.4509
O	-2.3920	0.1871	-0.2637
Si	-3.6292	-0.9030	-0.0239
C	-3.8749	-1.1685	1.8467
H	-4.0889	-0.2341	2.3591
H	-4.7021	-1.8415	2.0471
H	-2.9886	-1.5999	2.3055
C	-5.0615	0.0379	-0.8351
H	-5.2138	1.0082	-0.3733
H	-4.8830	0.2025	-1.8930
H	-5.9864	-0.5200	-0.7414
C	-3.2423	-2.5608	-0.8735
H	-2.3413	-3.0139	-0.4676
H	-4.0499	-3.2729	-0.7393
H	-3.0958	-2.4384	-1.9433
Al	2.7078	-0.5302	-0.0231
Cl	3.3195	0.6532	-1.6187
Cl	2.7423	0.4158	1.8459
Cl	3.5180	-2.4303	0.0818

A-IM8

C	-0.0711	2.1481	0.9203
C	-1.1992	3.0401	0.4595
C	-1.4474	2.6718	-0.7914
C	-0.4396	1.5914	-1.0816
O	0.6457	1.9063	-0.2817
H	0.5869	2.4967	1.7084
H	-1.6998	3.7574	1.0778
H	-2.2058	2.9861	-1.4781
H	-0.1689	1.3910	-2.1128
C	-0.7380	0.7626	1.1685
H	-1.6455	0.8377	1.7597
H	-0.0258	0.0916	1.6466
C	-1.0539	0.3076	-0.2654
C	-0.1947	-0.7742	-0.7723
H	-0.6558	-1.4099	-1.5420
O	0.9906	-0.9088	-0.4986
O	-2.3777	0.1299	-0.5824
Si	-3.4652	-0.9642	0.0285
C	-4.1650	-0.3637	1.6990
H	-4.3616	0.7053	1.6835
H	-5.1035	-0.8598	1.9247
H	-3.4917	-0.5666	2.5282
C	-4.7893	-0.9445	-1.3285
H	-5.1852	0.0550	-1.4760
H	-4.3970	-1.2847	-2.2816
H	-5.6183	-1.5910	-1.0632
C	-2.6455	-2.6690	0.2609
H	-1.6903	-2.5802	0.7743
H	-3.2674	-3.3342	0.8508
H	-2.4609	-3.1633	-0.6887
Al	2.7461	-0.4569	0.0068
Cl	3.2453	0.5025	-1.7492
Cl	2.7692	0.6077	1.7811
Cl	3.4325	-2.3887	0.2910

A-IM3-TS2

C	-1.63851400	-3.00754600	-0.01910800
C	-0.93747200	-2.57533000	-1.13441600
C	-0.07951900	-1.58624600	-0.69616800
C	-0.28793200	-1.43903800	0.76033300
O	-1.31287100	-2.37612600	1.07460900
H	-2.36749000	-3.79701900	0.06276800

H	-1.04667000	-2.95009900	-2.13207800
H	0.74624600	-1.15626500	-1.22876000
H	0.66051600	-1.69723400	1.30720000
C	-0.68325700	-0.00820800	1.11422300
H	-1.59220800	-0.00666400	1.71159100
H	0.11584000	0.48578800	1.66854300
C	-0.90639100	0.73128100	-0.19974900
C	0.14233300	1.24003400	-0.88602900
H	-0.03657300	1.75980100	-1.82373900
O	1.39235200	1.07595000	-0.52621500
O	-2.15517000	0.94188700	-0.65166700
Si	-3.69344100	0.91408300	-0.06430800
C	-3.86209200	1.99115200	1.50025400
H	-4.90155100	2.22506000	1.70613100
H	-3.46031400	1.50764200	2.38696000
H	-3.33406900	2.93261500	1.37683000
C	-4.65597100	1.61806700	-1.53751000
H	-4.49326500	1.03207100	-2.43651800
H	-5.72163600	1.62434100	-1.33578500
H	-4.35562200	2.63797100	-1.75454600
C	-4.25681200	-0.87259000	0.31979800
H	-3.80831200	-1.26990800	1.22634700
H	-5.33295900	-0.91451100	0.45253700
H	-4.00420400	-1.54447600	-0.49725700
Al	2.95267500	0.46774700	-0.09378300
Cl	2.61547600	-0.88041900	1.56770900
Cl	3.55191200	-0.73090400	-1.69523300
Cl	4.17702100	1.99778600	0.53491900

A-IM6-TS

C	2.42469700	-2.77459400	-0.02281500
C	2.02529700	-1.71154400	1.03764400
C	0.62908000	-1.90626200	1.27509600
C	0.19780800	-2.48107600	0.03787500
O	1.18541900	-3.33336700	-0.43710600
H	3.11575100	-3.57773300	0.22659500
H	2.71988900	-1.39994000	1.80139600
H	-0.01208700	-1.35106900	1.94280400
H	-0.80576500	-2.84979100	-0.13577100
C	2.87318100	-1.68321700	-0.99506900
H	2.66547000	-1.85424700	-2.05006400
H	3.91098400	-1.39206000	-0.85370700
C	1.91517200	-0.71715500	-0.28041600
C	0.43286000	-1.01654300	-0.77273400

H	0.43287000	-1.33177700	-1.83161300
O	-0.45707300	-0.08879300	-0.53167400
O	2.29400800	0.54011700	-0.17715900
Si	1.65156500	2.08315300	0.00969300
C	0.56168000	2.24506800	1.55472500
H	0.97456400	1.70517800	2.40346400
H	0.46365900	3.28631800	1.84519800
H	-0.44000600	1.86362300	1.37309000
C	3.30035300	3.00006800	0.27424300
H	3.98415100	2.84478600	-0.55415600
H	3.13158800	4.06740400	0.36252200
H	3.80476900	2.67488200	1.17871700
C	0.84896100	2.63718500	-1.62136200
H	-0.11732400	2.16638800	-1.77019400
H	0.68977500	3.71056700	-1.61930800
H	1.47790800	2.39506800	-2.47433300
Al	-2.16484800	0.15306700	-0.06728000
Cl	-3.19702300	-1.38005900	-1.03948400
Cl	-2.13620200	-0.26794200	2.00458600
Cl	-2.69080200	2.08289300	-0.54518000

A-IM6

C	-2.93075400	-3.08098800	0.24952700
C	-1.78188900	-2.57854400	0.69160900
C	-1.82816300	-1.09222400	0.55353200
C	-3.19493800	-0.89514600	-0.13260200
O	-3.82452000	-2.16337700	-0.20999700
H	-3.27085000	-4.09962200	0.21787300
H	-0.96124200	-3.11533900	1.12113700
H	-1.57586000	-0.55166400	1.46184500
H	-3.89953400	-0.18046500	0.29227900
C	-2.48809800	-0.44509600	-1.42173500
H	-2.55093100	-1.19256700	-2.20976000
H	-2.78036000	0.52415600	-1.80857400
C	-1.11561800	-0.42490600	-0.70268400
C	-0.08079000	-1.35124600	-1.21378400
H	-0.43314900	-2.24161400	-1.75645100
O	1.10986900	-1.21121200	-1.00134400
O	-0.55289100	0.79736600	-0.45719700
Si	-1.10067300	2.22493700	0.18983400
C	-1.68626000	2.05019600	1.99815800
H	-0.94531200	1.52960500	2.59856400
H	-1.82513100	3.03041900	2.44367300
H	-2.63209500	1.52202900	2.09391600

C	0.44239400	3.30872900	0.04837000
H	0.80516800	3.36153000	-0.97284400
H	0.23515700	4.31977700	0.38253500
H	1.24965500	2.91524500	0.65774100
C	-2.54193500	2.95692700	-0.83288700
H	-3.48696100	2.44667500	-0.66487600
H	-2.69395500	3.99627000	-0.56033700
H	-2.33237900	2.93668000	-1.89901200
Al	2.44051500	-0.31795900	0.04254500
Cl	3.73628300	-1.92872600	0.17532200
Cl	2.97537000	1.17446200	-1.26122600
Cl	1.53288600	0.03160600	1.86912800

A-IM7

C	2.95030200	-1.54467100	-0.75885200
C	1.49153700	-1.71736500	-0.25196000
C	1.70140400	-1.75604700	1.23704500
C	3.00090000	-1.74272700	1.48609700
O	3.79699900	-1.68474500	0.37304600
H	3.26005400	-2.28246100	-1.50179700
H	0.98990300	-2.62128500	-0.60107700
H	0.89181200	-1.82133200	1.93324700
H	3.53494300	-1.78797600	2.41632100
C	3.05994100	-0.09837700	-1.30316200
H	3.13016200	-0.07777800	-2.39214600
H	3.93833000	0.40679400	-0.89909300
C	1.79658000	0.54720700	-0.86450500
C	0.72213400	-0.46095900	-0.73273800
H	0.38253500	-0.67624300	-1.77245800
O	-0.32043100	-0.00603100	0.00730800
O	1.66788200	1.73081000	-0.55095700
Si	0.20758100	2.50402400	0.24665400
C	0.04745100	1.90222400	2.03974900
H	-0.85065500	1.30398800	2.16028300
H	0.89146700	1.28329000	2.33510600
H	-0.01056900	2.74540900	2.72181400
C	1.09031400	4.19910900	0.31144300
H	1.37347300	4.55377100	-0.67505700
H	0.43958200	4.94833200	0.74851000
H	1.99321000	4.16601100	0.91405200
C	-1.15525000	2.66060500	-1.06200400
H	-1.75824900	1.76097200	-1.14382600
H	-1.82088900	3.47658900	-0.79837500
H	-0.73867300	2.87950200	-2.04351300

Al	-1.94707400	-0.80496900	-0.00724100
Cl	-2.19196200	-1.05204800	-2.09243100
Cl	-1.75754900	-2.66400500	0.91628500
Cl	-3.26390600	0.47466500	0.94068300

A-IM7-TS

C	-2.99654000	-1.50111300	0.64151400
C	-1.55707200	-1.62547300	0.06007000
C	-1.80118000	-1.33375300	-1.39452000
C	-3.10002600	-1.16718200	-1.58728000
O	-3.86728700	-1.29230300	-0.46278600
H	-3.34146300	-2.39064000	1.17370600
H	-1.10292200	-2.60804000	0.19441100
H	-1.01494400	-1.31336300	-2.11939900
H	-3.65266800	-0.96718200	-2.48593900
C	-3.01161000	-0.24871300	1.55188900
H	-2.98626500	-0.52149900	2.60752000
H	-3.89618400	0.36186000	1.37114500
C	-1.75720200	0.45140800	1.17263700
C	-0.72148800	-0.53872700	0.78070200
H	-0.31908500	-0.98399500	1.71085100
O	0.28714300	0.09976200	0.10453500
O	-1.57001700	1.64639500	1.02954100
Si	-0.11303400	2.18822800	-0.22363200
C	-1.20914100	3.75943300	-0.41444000
H	-1.48054000	4.18758600	0.54381400
H	-0.66694300	4.51443300	-0.97194000
H	-2.12994200	3.56111400	-0.95376700
C	1.27307400	2.67948200	0.97573800
H	0.87422200	3.14316500	1.87448800
H	1.88428000	1.83186000	1.27190700
H	1.92644900	3.40109300	0.49825100
C	0.10786200	1.71398300	-2.06103000
H	-0.79310100	1.26575000	-2.47393900
H	0.32856900	2.60134100	-2.64485800
H	0.92107300	1.00863300	-2.19950100
Al	1.95401900	-0.76778700	0.00931600
Cl	2.24245100	-1.18022200	2.04665800
Cl	1.55542900	-2.49957800	-1.07345500
Cl	3.34746800	0.47315300	-0.86196800

A-IM11

C	-3.07883100	-1.41580700	0.19638000
C	-1.70505500	-1.28099100	-0.51492100

C	-2.05864300	-0.41455200	-1.68992900
C	-3.35927700	-0.15859600	-1.65601600
O	-4.02505400	-0.70647700	-0.60448900
H	-3.42936800	-2.44900900	0.26945700
H	-1.29839800	-2.23669400	-0.85142600
H	-1.34943900	-0.10917400	-2.42962200
H	-3.97365500	0.40616600	-2.33306100
C	-2.94767300	-0.76450800	1.58083600
H	-2.92434900	-1.50986200	2.37702700
H	-3.78092900	-0.09004100	1.77834500
C	-1.63996400	-0.01737200	1.57470700
C	-0.75339100	-0.64673900	0.51891400
H	-0.23260100	-1.46854300	1.03945500
O	0.24623800	0.20650500	0.02229100
O	-1.32279200	0.90633200	2.26973300
Si	0.07057500	1.91227800	-0.19762100
C	-1.70571900	2.58039400	-0.05099400
H	-1.93850000	2.85683600	0.97101100
H	-1.78889300	3.47502100	-0.65928400
H	-2.46373600	1.88331000	-0.39080600
C	1.21624200	2.67240100	1.11074300
H	0.82927100	2.50637200	2.11304700
H	2.20700900	2.22693400	1.06075900
H	1.32422800	3.74253500	0.96711500
C	0.63642300	2.12295700	-2.00650400
H	-0.20034800	2.23387300	-2.69104500
H	1.25029500	3.01152400	-2.10630600
H	1.23490800	1.27840000	-2.33767300
Al	2.03782000	-0.76414000	-0.03188600
Cl	2.22487900	-1.16830300	1.98723600
Cl	1.47418400	-2.33559400	-1.25296000
Cl	3.49170200	0.45038400	-0.82106200

DFT-optimized cartesian coordinates of all species involved in the asymmetric Mannich-type reaction

B-TS-SR

N	-1.0929	-1.3631	0.9490
O	0.2833	-1.1968	0.7591
C	-1.7362	-1.3750	-0.3699
C	-1.5659	-0.3510	1.8591

C	-2.0104	-2.8355	-0.7319
H	-1.0052	-0.9638	-1.0883
H	-1.5191	0.6692	1.4331
H	-2.5862	-0.5745	2.1729
H	-0.9172	-0.3830	2.7323
H	-1.0948	-3.4025	-0.5964
H	-2.7701	-3.2463	-0.0712
H	-2.3419	-2.9310	-1.7638
C	-2.8105	0.9370	-0.5499
C	-3.0307	-0.5528	-0.5065
O	-1.8980	1.4563	-1.1589
H	-3.7559	-0.8223	0.2601
H	-3.4559	-0.8161	-1.4800
Li	1.3324	-0.0509	0.2125
O	1.7411	1.8193	0.1433
O	3.0289	-0.8987	-0.2457
C	2.9083	2.3359	0.7213
H	3.5368	2.8309	-0.0295
H	2.6724	3.0603	1.5098
H	3.4526	1.5026	1.1539
C	0.9447	2.8195	-0.4444
H	1.4780	3.3104	-1.2667
H	0.0488	2.3392	-0.8277
H	0.6624	3.5777	0.2953
C	4.2054	-0.5830	-0.9374
H	4.3221	-1.2121	-1.8281
H	4.1379	0.4569	-1.2452
H	5.0894	-0.7146	-0.2995
C	2.9867	-2.2455	0.1659
H	3.7804	-2.4579	0.8911
H	2.0080	-2.3781	0.6206
H	3.0933	-2.9182	-0.6916
C	-3.8843	1.7605	0.1261
H	-4.8398	1.5585	-0.3556
H	-3.9707	1.4855	1.1740
H	-3.6574	2.8206	0.0431

B-SR

N	-1.7770	-0.4984	0.8457
O	-0.6755	0.3745	0.6753
C	-2.3337	-0.6155	-0.5057
C	-2.6917	0.0479	1.8376
C	-3.7217	-1.2299	-0.5583
H	-1.6285	-1.2616	-1.0464

H	-3.2411	0.9358	1.5060
H	-3.4007	-0.7294	2.1176
H	-2.1003	0.3112	2.7137
H	-3.7342	-2.1828	-0.0334
H	-4.4643	-0.5716	-0.1137
H	-3.9975	-1.4010	-1.5961
C	-0.9000	1.3293	-0.4972
C	-2.2282	0.7906	-1.0965
O	0.1413	1.2233	-1.2848
H	-3.0814	1.4069	-0.8104
H	-2.1434	0.7728	-2.1793
Li	1.0206	0.0651	-0.3685
O	2.7426	0.7518	0.2139
O	1.3722	-1.8287	-0.2883
C	3.7298	0.3354	1.1158
H	4.7104	0.2664	0.6268
H	3.8089	1.0254	1.9643
H	3.4400	-0.6449	1.4823
C	2.9874	2.0344	-0.3099
H	3.9124	2.0478	-0.8982
H	2.1333	2.2562	-0.9434
H	3.0611	2.7772	0.4921
C	2.4070	-2.4500	-1.0004
H	2.0196	-3.2489	-1.6441
H	2.8742	-1.6872	-1.6157
H	3.1537	-2.8789	-0.3204
C	0.6794	-2.7188	0.5513
H	1.3455	-3.1315	1.3182
H	-0.1197	-2.1534	1.0221
H	0.2500	-3.5466	-0.0253
C	-1.0628	2.7346	0.1126
H	-1.2237	3.4422	-0.6960
H	-1.8934	2.7811	0.8117
H	-0.1418	2.9928	0.6286

B-S3

N	-0.8827	-1.3385	0.8781
O	0.5134	-1.2575	0.7560
C	-1.4323	-1.1784	-0.4656
C	-1.3073	-0.3018	1.7935
C	-1.0999	-2.4440	-1.2534
H	-0.9277	-0.3163	-0.9574
H	-1.1101	0.7128	1.4020
H	-2.3656	-0.4067	2.0302

H	-0.7321	-0.4331	2.7077
H	-0.0397	-2.6464	-1.1330
H	-1.6611	-3.2841	-0.8523
H	-1.3311	-2.3203	-2.3089
C	-3.3287	0.5226	-0.3421
C	-2.9467	-0.9308	-0.4773
O	-2.6455	1.4299	-0.7543
H	-3.4389	-1.5394	0.2805
H	-3.3298	-1.2425	-1.4546
Li	1.4860	-0.0091	0.2571
O	1.4820	1.9123	-0.0021
O	3.2857	-0.6677	-0.0898
C	2.6167	2.6304	0.3990
H	3.0889	3.1338	-0.4536
H	2.3607	3.3856	1.1511
H	3.3149	1.9214	0.8312
C	0.4858	2.7493	-0.5416
H	0.8364	3.2303	-1.4619
H	-0.3833	2.1341	-0.7615
H	0.1991	3.5258	0.1765
C	4.4550	-0.2865	-0.7617
H	4.6695	-0.9641	-1.5967
H	4.3022	0.7165	-1.1514
H	5.3194	-0.2835	-0.0846
C	3.3565	-1.9844	0.4089
H	4.1274	-2.0678	1.1830
H	2.3748	-2.1965	0.8236
H	3.5778	-2.6927	-0.3962
C	-4.6705	0.7644	0.3072
H	-5.4245	0.1212	-0.1402
H	-4.6026	0.5193	1.3654
H	-4.9606	1.8068	0.2027

B-TS-SS

N	1.6292	-1.2874	0.8186
O	0.2806	-0.9683	0.7966
C	2.4229	-0.1631	0.4262
C	1.8558	-2.5249	0.1037
C	3.9145	-0.4203	0.6331
H	2.1090	0.6424	1.0993
H	2.8942	-2.8339	0.2111
H	1.2135	-3.2758	0.5599
H	1.5961	-2.4671	-0.9662
H	4.0727	-0.8686	1.6105

H	4.3094	-1.0892	-0.1276
H	4.4657	0.5164	0.5881
C	1.2262	1.4756	-1.0905
C	2.1668	0.3387	-1.0634
O	0.0174	1.3581	-1.2617
H	1.7378	-0.4968	-1.6176
H	3.1293	0.6232	-1.4842
Li	-0.7549	0.0150	-0.1726
O	-2.1669	-1.0495	-0.9689
O	-1.8410	1.0526	1.0690
C	-2.2927	-2.2523	-0.2562
H	-3.2051	-2.2604	0.3508
H	-2.3067	-3.1134	-0.9352
H	-1.4200	-2.2956	0.3887
C	-3.2310	-0.8110	-1.8446
H	-4.1840	-0.7403	-1.3046
H	-3.0284	0.1335	-2.3413
H	-3.3128	-1.6071	-2.5964
C	-2.7726	2.0848	0.9260
H	-2.5059	2.9506	1.5461
H	-2.7640	2.3771	-0.1199
H	-3.7821	1.7540	1.2049
C	-1.7153	0.5927	2.3891
H	-2.6574	0.1641	2.7511
H	-0.9443	-0.1721	2.3503
H	-1.4088	1.4024	3.0617
C	1.8452	2.8400	-0.8879
H	2.5182	2.8244	-0.0342
H	2.4244	3.1110	-1.7696
H	1.0692	3.5845	-0.7318

B-SS

N	1.8351	0.0345	1.2291
O	0.9529	0.8749	0.5103
C	3.0589	0.0636	0.4171
C	1.2488	-1.2857	1.3893
C	4.0779	-1.0060	0.7710
H	3.4977	1.0517	0.6140
H	1.8975	-1.8744	2.0347
H	0.2868	-1.1519	1.8837
H	1.0872	-1.8050	0.4386
H	4.2931	-0.9849	1.8369
H	3.7239	-1.9967	0.4971
H	4.9996	-0.8118	0.2270

C	1.1792	0.7127	-0.9845
C	2.5724	0.0239	-1.0334
O	0.2025	0.0083	-1.5142
H	2.4361	-1.0017	-1.3784
H	3.2490	0.5372	-1.7115
Li	-1.0923	0.0717	-0.4346
O	-2.0838	-1.5957	-0.3018
O	-2.3170	1.2977	0.3837
C	-3.0269	-2.1470	0.5765
H	-3.9409	-2.4402	0.0442
H	-2.6228	-3.0281	1.0895
H	-3.2690	-1.3860	1.3127
C	-1.6732	-2.5033	-1.2961
H	-2.5136	-2.7849	-1.9408
H	-0.9155	-1.9842	-1.8740
H	-1.2477	-3.4080	-0.8469
C	-3.6847	1.4272	0.1047
H	-3.9038	2.3932	-0.3647
H	-3.9524	0.6288	-0.5806
H	-4.2843	1.3389	1.0196
C	-1.8494	2.2945	1.2599
H	-2.3499	2.2240	2.2328
H	-0.7837	2.1279	1.3796
H	-2.0198	3.2934	0.8437
C	1.2551	2.1598	-1.5031
H	2.0560	2.7054	-1.0122
H	1.4197	2.1346	-2.5758
H	0.3040	2.6459	-1.3014

B-S1

N	1.5271	-1.5997	0.3709
O	0.1761	-1.4559	0.1014
C	2.1466	-0.3085	0.4521
C	2.1222	-2.5233	-0.5747
C	3.6090	-0.3785	0.8755
H	1.5725	0.2155	1.2252
H	3.1228	-2.7966	-0.2428
H	1.4960	-3.4131	-0.5867
H	2.1715	-2.1264	-1.6009
H	3.7039	-1.0077	1.7568
H	4.2307	-0.7900	0.0839
H	3.9742	0.6167	1.1193
C	1.2731	1.7785	-0.6202
C	1.9877	0.5228	-0.8906

O	0.0666	1.7972	-0.3807
H	1.3408	-0.0980	-1.5208
H	2.9599	0.6776	-1.3538
Li	-0.7275	0.0383	-0.0737
O	-2.1470	-0.2661	-1.3471
O	-1.7636	0.2836	1.5530
C	-2.3679	-1.6382	-1.5447
H	-3.3101	-1.9578	-1.0852
H	-2.3894	-1.8836	-2.6133
H	-1.5342	-2.1374	-1.0616
C	-3.1465	0.5416	-1.8995
H	-4.1242	0.3320	-1.4470
H	-2.8687	1.5716	-1.6963
H	-3.2229	0.3923	-2.9846
C	-2.5456	1.3355	2.0396
H	-2.2132	1.6497	3.0373
H	-2.4273	2.1623	1.3457
H	-3.6052	1.0526	2.0963
C	-1.7786	-0.8530	2.3764
H	-2.7873	-1.2770	2.4488
H	-1.1073	-1.5602	1.8967
H	-1.4161	-0.6160	3.3835
C	2.0935	3.0465	-0.5871
H	2.9184	2.9348	0.1136
H	2.5148	3.2397	-1.5724
H	1.4752	3.8895	-0.2900

B-TS-RS

N	1.5015	-1.6262	0.7748
O	0.2272	-1.0911	0.7701
C	2.5126	-0.6913	0.3938
C	1.5237	-2.8746	0.0465
C	2.5638	0.4392	1.4151
H	3.4625	-1.2420	0.4235
H	1.1999	-2.7643	-1.0024
H	2.5268	-3.3017	0.0760
H	0.8285	-3.5524	0.5386
H	1.6342	1.0001	1.3790
H	2.6674	0.0103	2.4084
H	3.4072	1.0987	1.2261
C	1.5191	1.0658	-1.2596
C	2.3997	-0.1109	-1.0886
O	0.3112	0.9949	-1.4662
H	2.0107	-0.9298	-1.6971

H	3.4140	0.1379	-1.3983
Li	-0.6636	-0.0389	-0.2594
O	-2.3276	-0.8638	-0.8197
O	-1.4186	1.3344	0.9200
C	-2.5885	-1.9683	0.0070
H	-3.4403	-1.7754	0.6691
H	-2.7938	-2.8662	-0.5878
H	-1.6859	-2.1058	0.5952
C	-3.4018	-0.5300	-1.6509
H	-4.2909	-0.2615	-1.0653
H	-3.0915	0.3244	-2.2457
H	-3.6614	-1.3620	-2.3184
C	-2.1670	2.4953	0.7064
H	-1.7647	3.3398	1.2817
H	-2.1061	2.7212	-0.3544
H	-3.2185	2.3517	0.9878
C	-1.3891	0.9276	2.2631
H	-2.3958	0.6972	2.6303
H	-0.7734	0.0322	2.2748
H	-0.9451	1.7016	2.9008
C	2.2019	2.4157	-1.2805
H	1.4698	3.2047	-1.1292
H	2.9798	2.4803	-0.5270
H	2.6636	2.5556	-2.2582

B-RS

N	1.8108	-0.3171	1.2505
O	1.1374	0.6179	0.4310
C	2.9940	-0.7030	0.4751
C	0.9485	-1.4465	1.5537
C	4.1070	0.3030	0.7550
H	3.3196	-1.6984	0.7916
H	0.6406	-1.9974	0.6582
H	1.4858	-2.1085	2.2318
H	0.0617	-1.0625	2.0575
H	3.7706	1.3029	0.4961
H	4.3603	0.2883	1.8122
H	4.9926	0.0605	0.1726
C	1.2798	0.2220	-1.0137
C	2.5447	-0.6865	-0.9908
O	0.1887	-0.3926	-1.4317
H	2.2476	-1.6785	-1.3306
H	3.3201	-0.3048	-1.6499
Li	-1.0873	0.0615	-0.4346

O	-2.3984	-1.3458	-0.1484
O	-2.0324	1.5926	0.2237
C	-3.4329	-1.6026	0.7622
H	-4.3853	-1.7710	0.2434
H	-3.2094	-2.4823	1.3776
H	-3.5238	-0.7319	1.4053
C	-2.1700	-2.4229	-1.0257
H	-3.0460	-2.6045	-1.6589
H	-1.3205	-2.1325	-1.6350
H	-1.9351	-3.3367	-0.4684
C	-3.3554	1.9499	-0.0715
H	-3.3955	2.8854	-0.6412
H	-3.7818	1.1499	-0.6690
H	-3.9451	2.0738	0.8457
C	-1.3696	2.5688	0.9906
H	-1.8565	2.6957	1.9646
H	-0.3519	2.2176	1.1287
H	-1.3572	3.5332	0.4709
C	1.5462	1.5491	-1.7470
H	0.6785	2.1910	-1.6151
H	2.4302	2.0449	-1.3573
H	1.6717	1.3366	-2.8041

B-R2

N	-1.5196	1.6540	0.7114
O	-0.1961	1.3264	0.4825
C	-2.4086	0.5604	0.4501
C	-1.8574	2.8721	0.0052
C	-2.2258	-0.4970	1.5337
H	-3.4293	0.9582	0.5183
H	-1.7914	2.7704	-1.0907
H	-2.8665	3.1834	0.2770
H	-1.1479	3.6368	0.3152
H	-1.2086	-0.8758	1.5022
H	-2.3908	-0.0360	2.5045
H	-2.9280	-1.3166	1.4052
C	-1.5625	-1.3592	-1.0537
C	-2.2355	-0.0466	-1.0123
O	-0.3452	-1.4909	-0.9537
H	-1.5911	0.6681	-1.5342
H	-3.2150	-0.0962	-1.4850
Li	0.6264	-0.0484	-0.1747
O	2.1244	0.5630	-1.2454
O	1.6326	-0.8681	1.2926

C	2.4139	1.9016	-0.9364
H	3.3454	1.9838	-0.3650
H	2.4979	2.5069	-1.8469
H	1.5793	2.2442	-0.3327
C	3.1169	-0.0540	-2.0139
H	4.0784	-0.0709	-1.4846
H	2.7892	-1.0732	-2.1971
H	3.2545	0.4620	-2.9733
C	2.3968	-2.0313	1.4236
H	2.0621	-2.6330	2.2786
H	2.2633	-2.6021	0.5093
H	3.4615	-1.7976	1.5565
C	1.6789	-0.0380	2.4239
H	2.6984	0.3181	2.6130
H	1.0270	0.7992	2.1882
H	1.3118	-0.5622	3.3141
C	-2.4459	-2.5674	-1.2718
H	-1.9072	-3.4777	-1.0217
H	-3.3553	-2.4986	-0.6815
H	-2.7303	-2.6103	-2.3232

B-TS-RR

N	-1.7588	0.0226	-1.3117
O	-0.4247	0.1357	-0.9505
C	-2.6289	0.5056	-0.2510
C	-2.0192	-1.3456	-1.7149
C	-3.0323	1.9452	-0.5773
H	-3.5355	-0.1142	-0.2346
H	-1.7071	-2.0736	-0.9517
H	-3.0778	-1.4725	-1.9444
H	-1.4373	-1.5339	-2.6165
H	-2.1373	2.5524	-0.6798
H	-3.5712	1.9678	-1.5206
H	-3.6642	2.3610	0.2045
C	-1.1973	-0.7075	1.5325
C	-1.9814	0.5052	1.1697
O	-0.0108	-0.6704	1.8409
H	-2.8044	0.6181	1.8791
H	-1.3081	1.3598	1.2326
Li	0.7822	-0.0607	0.2426
O	2.1572	-1.2620	-0.3696
O	1.7982	1.5887	0.3698
C	2.0947	-1.3866	-1.7668
H	2.9627	-0.9188	-2.2457

H	2.0441	-2.4398	-2.0668
H	1.1846	-0.8711	-2.0595
C	3.2713	-1.8947	0.1924
H	4.2072	-1.4557	-0.1775
H	3.2075	-1.7560	1.2677
H	3.2745	-2.9686	-0.0351
C	2.8481	2.0729	1.1572
H	2.6121	3.0629	1.5687
H	2.9872	1.3696	1.9733
H	3.7782	2.1480	0.5788
C	1.4943	2.4205	-0.7210
H	2.3532	2.5202	-1.3942
H	0.6736	1.9264	-1.2352
H	1.1873	3.4174	-0.3830
C	-1.9942	-1.9752	1.7545
H	-2.2793	-1.9984	2.8083
H	-2.8958	-2.0035	1.1527
H	-1.3792	-2.8488	1.5570

B-RR

N	-1.8270	0.2914	-0.9298
O	-0.6447	-0.4138	-0.5356
C	-2.8266	0.1188	0.1336
C	-2.2752	-0.2006	-2.2165
C	-3.4914	1.4594	0.4273
H	-3.6012	-0.5987	-0.1839
H	-2.5678	-1.2593	-2.2031
H	-3.1272	0.3999	-2.5331
H	-1.4650	-0.0687	-2.9324
H	-2.7423	2.1855	0.7318
H	-3.9998	1.8355	-0.4578
H	-4.2193	1.3446	1.2267
C	-0.8793	-1.2320	0.7008
C	-2.0630	-0.4478	1.3234
O	0.2381	-1.2198	1.3810
H	-2.6788	-1.0828	1.9547
H	-1.6310	0.3520	1.9262
Li	1.0798	-0.0754	0.4023
O	2.7702	-0.7464	-0.2615
O	1.3459	1.8356	0.3096
C	3.7268	-0.3236	-1.1931
H	4.7313	-0.3062	-0.7502
H	3.7426	-0.9796	-2.0715
H	3.4532	0.6803	-1.5045

C	3.0003	-2.0554	0.2011
H	3.9522	-2.1182	0.7412
H	2.1724	-2.2771	0.8685
H	3.0111	-2.7680	-0.6310
C	2.4316	2.5030	0.8920
H	2.0997	3.1823	1.6860
H	3.0828	1.7459	1.3180
H	2.9861	3.0836	0.1434
C	0.4178	2.7177	-0.2727
H	0.8818	3.2907	-1.0846
H	-0.3929	2.1119	-0.6678
H	0.0243	3.4188	0.4729
C	-1.3134	-2.6488	0.2674
H	-1.3633	-3.2722	1.1554
H	-2.2808	-2.6481	-0.2286
H	-0.5593	-3.0543	-0.4025

B-R1

N	-1.5761	-0.0195	-1.4938
O	-0.2803	0.4163	-1.2586
C	-2.5029	0.5436	-0.5525
C	-1.6363	-1.4586	-1.5311
C	-2.7764	1.9961	-0.9348
H	-3.4350	-0.0332	-0.6152
H	-1.4477	-1.9064	-0.5395
H	-2.6189	-1.7745	-1.8874
H	-0.8715	-1.8109	-2.2186
H	-1.8285	2.5240	-0.9908
H	-3.2464	2.0315	-1.9138
H	-3.4241	2.4818	-0.2089
C	-1.4607	-0.7416	1.4630
C	-2.0049	0.5350	0.9454
O	-0.2551	-0.9462	1.5915
H	-2.8639	0.8422	1.5421
H	-1.2069	1.2772	0.9938
Li	0.6788	-0.0716	0.1195
O	2.1175	-1.2139	-0.4714
O	1.7012	1.4822	0.6914
C	2.3202	-1.1119	-1.8568
H	3.2851	-0.6425	-2.0829
H	2.2821	-2.0981	-2.3345
H	1.5074	-0.4894	-2.2206
C	3.0590	-2.0261	0.1700
H	4.0739	-1.6209	0.0625

H	2.7890	-2.0528	1.2214
H	3.0442	-3.0463	-0.2343
C	2.6264	1.7429	1.7082
H	2.4212	2.7059	2.1939
H	2.5313	0.9442	2.4381
H	3.6524	1.7592	1.3192
C	1.7088	2.4504	-0.3270
H	2.6925	2.5139	-0.8047
H	0.9701	2.1168	-1.0493
H	1.4386	3.4375	0.0671
C	-2.4740	-1.7322	1.9982
H	-2.7913	-1.4012	2.9877
H	-3.3508	-1.7800	1.3587
H	-2.0280	-2.7188	2.0950

B-TS-S2

N	1.8739	-0.9739	1.3122
O	0.6454	-0.2757	1.5156
C	2.5859	-0.3241	0.1768
C	1.6060	-2.3789	1.1647
C	2.4466	-1.0083	-1.1863
H	3.6477	-0.3605	0.4596
H	2.5503	-2.9014	1.0202
H	1.1527	-2.7263	2.0928
H	0.9197	-2.6097	0.3344
H	2.8939	-1.9997	-1.1725
H	1.4037	-1.0864	-1.4787
H	2.9643	-0.4085	-1.9312
C	1.1580	1.6335	-0.7205
C	2.1293	1.1319	0.1609
O	0.2399	0.9536	-1.2442
H	1.2007	0.7748	1.0895
H	2.8627	1.8426	0.5216
Li	-0.5052	-0.1287	0.0455
O	-1.5258	-1.5314	-0.7754
O	-1.8934	0.9862	0.7809
C	-2.2374	-2.5873	-0.1873
H	-3.3184	-2.4082	-0.2319
H	-2.0157	-3.5385	-0.6878
H	-1.9232	-2.6420	0.8509
C	-1.8398	-1.3489	-2.1324
H	-2.9036	-1.1213	-2.2629
H	-1.2435	-0.5108	-2.4742
H	-1.5919	-2.2434	-2.7162
C	-2.5985	1.9244	0.0147

H	-2.3811	2.9463	0.3451
H	-2.2633	1.8020	-1.0098
H	-3.6811	1.7545	0.0765
C	-2.1406	1.0992	2.1576
H	-3.1843	0.8556	2.3923
H	-1.4744	0.3971	2.6471
H	-1.9224	2.1117	2.5144
C	1.1457	3.1400	-0.9366
H	1.2566	3.6658	0.0084
H	1.9750	3.4217	-1.5830
H	0.2145	3.4367	-1.4127

B-S2-IM1

N	1.9531	-0.9745	1.3507
O	0.6745	-0.3101	1.5015
C	2.5724	-0.6376	0.0544
C	1.7226	-2.3781	1.5744
C	2.0102	-1.4061	-1.1492
H	3.6182	-0.9439	0.1916
H	2.6608	-2.9089	1.4318
H	1.3976	-2.5047	2.6074
H	0.9551	-2.8000	0.9098
H	2.2406	-2.4682	-1.0867
H	0.9348	-1.2674	-1.2171
H	2.4597	-1.0065	-2.0536
C	1.5109	1.5833	-0.6197
C	2.5556	0.8547	-0.1622
O	0.3207	1.1394	-0.8852
H	0.9406	0.6171	1.3883
H	3.4841	1.3634	0.0456
Li	-0.6338	0.0032	-0.0138
O	-1.6844	-1.2338	-1.0454
O	-2.0306	0.9201	0.9569
C	-2.5277	-2.3240	-0.7911
H	-3.5801	-2.0546	-0.9413
H	-2.2845	-3.1713	-1.4444
H	-2.3768	-2.6143	0.2450
C	-1.7821	-0.7654	-2.3686
H	-2.7998	-0.4265	-2.5904
H	-1.0928	0.0684	-2.4463
H	-1.5008	-1.5483	-3.0823
C	-2.2123	2.2387	0.5052
H	-2.0746	2.9562	1.3217
H	-1.4551	2.3979	-0.2562

H	-3.2107	2.3747	0.0744
C	-2.9121	0.5685	1.9874
H	-3.9549	0.6121	1.6494
H	-2.6698	-0.4477	2.2836
H	-2.7943	1.2324	2.8517
C	1.7076	3.0791	-0.8360
H	2.7315	3.3815	-0.6389
H	1.4516	3.3282	-1.8645
H	1.0370	3.6382	-0.1828

B-S2

N	1.5535	-1.4892	0.9301
O	0.2239	-1.1408	0.6799
C	2.4741	-0.5799	0.2676
C	1.7646	-2.8811	0.5845
C	2.3850	-0.5673	-1.2625
H	3.4799	-0.9121	0.5604
H	2.8023	-3.1502	0.7859
H	1.1104	-3.4758	1.2210
H	1.5234	-3.1144	-0.4639
H	2.7479	-1.5107	-1.6649
H	1.3443	-0.4368	-1.5549
H	2.9812	0.2389	-1.6819
C	1.5695	1.8080	-0.0367
C	2.2509	0.8431	0.8771
O	0.3939	1.7273	-0.3459
H	1.5912	0.6824	1.7307
H	3.2051	1.2489	1.2101
Li	-0.6550	0.1704	0.0260
O	-1.6806	-0.3954	-1.5371
O	-2.1456	0.5805	1.2163
C	-1.7998	-1.7939	-1.5002
H	-2.8176	-2.0992	-1.2329
H	-1.5342	-2.2385	-2.4670
H	-1.1034	-2.1181	-0.7307
C	-2.5335	0.2084	-2.4663
H	-3.5866	0.0077	-2.2311
H	-2.3520	1.2783	-2.4176
H	-2.3283	-0.1486	-3.4843
C	-3.1933	1.5041	1.2786
H	-3.1965	2.0385	2.2375
H	-3.0418	2.2170	0.4728
H	-4.1671	1.0126	1.1506
C	-2.2081	-0.3970	2.2241

H	-3.1258	-0.9907	2.1422
H	-1.3370	-1.0271	2.0611
H	-2.1639	0.0597	3.2194
C	2.4254	2.9401	-0.5574
H	2.6478	3.6186	0.2653
H	3.3699	2.5643	-0.9417
H	1.8992	3.4884	-1.3346

B-S0

N	-1.4709	-0.6871	-1.3714
O	-0.1405	-0.2998	-1.3785
C	-2.3099	0.4280	-1.0605
C	-1.6831	-1.8350	-0.5280
C	-3.7891	0.0560	-1.0234
H	-2.1557	1.1485	-1.8716
H	-2.6127	-2.3338	-0.8038
H	-0.8511	-2.5181	-0.6785
H	-1.7202	-1.5595	0.5411
H	-4.0435	-0.5044	-1.9195
H	-4.0329	-0.5510	-0.1559
H	-4.3978	0.9574	-0.9980
C	-1.4760	0.4571	1.4502
C	-1.8783	1.2276	0.2516
O	-0.2960	0.2129	1.7123
H	-2.7153	1.8846	0.4844
H	-1.0026	1.8021	-0.0533
Li	0.7569	0.0096	0.1004
O	2.1061	-1.3576	0.3179
O	1.9160	1.5421	-0.2284
C	2.3496	-2.0308	-0.8898
H	3.3486	-1.7998	-1.2782
H	2.2589	-3.1161	-0.7617
H	1.5897	-1.6710	-1.5780
C	2.9795	-1.7275	1.3460
H	4.0202	-1.4875	1.0908
H	2.6847	-1.1671	2.2282
H	2.9099	-2.8021	1.5587
C	2.8601	2.2495	0.5238
H	2.7484	3.3327	0.3835
H	2.6867	2.0020	1.5671
H	3.8838	1.9654	0.2484
C	2.0187	1.7775	-1.6098
H	3.0040	1.4845	-1.9883
H	1.2506	1.1617	-2.0673

H	1.8468	2.8353	-1.8421
C	-2.5560	0.1645	2.4729
H	-2.7344	1.0726	3.0503
H	-3.4907	-0.1229	2.0010
H	-2.2277	-0.6141	3.1574

B-R0

N	-1.5761	-0.0189	-1.4938
O	-0.2804	0.4169	-1.2584
C	-2.5031	0.5440	-0.5526
C	-1.6364	-1.4580	-1.5313
C	-2.7765	1.9967	-0.9346
H	-3.4352	-0.0327	-0.6156
H	-1.4485	-1.9058	-0.5396
H	-2.6187	-1.7738	-1.8883
H	-0.8710	-1.8103	-2.2183
H	-1.8287	2.5247	-0.9899
H	-3.2459	2.0323	-1.9138
H	-3.4247	2.4820	-0.2089
C	-1.4613	-0.7418	1.4629
C	-2.0053	0.5350	0.9454
O	-0.2558	-0.9466	1.5913
H	-2.8644	0.8422	1.5420
H	-1.2072	1.2770	0.9940
Li	0.6786	-0.0717	0.1200
O	2.1170	-1.2141	-0.4719
O	1.7010	1.4818	0.6928
C	2.3195	-1.1108	-1.8573
H	3.2841	-0.6407	-2.0831
H	2.2817	-2.0966	-2.3359
H	1.5063	-0.4883	-2.2204
C	3.0596	-2.0254	0.1687
H	4.0739	-1.6187	0.0616
H	2.7897	-2.0536	1.2201
H	3.0464	-3.0453	-0.2366
C	2.6279	1.7404	1.7086
H	2.4261	2.7044	2.1938
H	2.5311	0.9424	2.4392
H	3.6536	1.7533	1.3187
C	1.7103	2.4495	-0.3260
H	2.6939	2.5109	-0.8041
H	0.9706	2.1172	-1.0479
H	1.4422	3.4374	0.0678
C	-2.4748	-1.7322	1.9980

H	-2.7922	-1.4011	2.9875
H	-3.3516	-1.7800	1.3585
H	-2.0289	-2.7189	2.0949

B-TS-R

N	-1.2511	-0.1106	-1.5182
O	-0.0599	0.3425	-1.7520
C	-2.2399	0.6435	-1.1545
C	-1.4312	-1.5306	-1.7273
C	-2.1008	2.1246	-1.1946
H	-3.2168	0.1978	-1.0802
H	-2.3741	-1.8644	-1.3049
H	-1.4054	-1.7335	-2.8009
H	-0.6059	-2.0498	-1.2482
H	-1.0962	2.3977	-0.8813
H	-2.2367	2.4780	-2.2198
H	-2.8396	2.6029	-0.5603
C	-1.6861	-0.6481	1.3698
C	-2.2796	0.5706	1.3873
O	-0.4624	-0.8399	1.0409
H	-3.3115	0.6876	1.6706
H	-1.6801	1.4603	1.3261
Li	0.6365	-0.0540	-0.0781
O	2.1439	-1.2199	-0.3122
O	1.4397	1.5306	0.6560
C	3.1253	-1.1750	-1.3090
H	4.0850	-0.8246	-0.9087
H	3.2730	-2.1626	-1.7641
H	2.7668	-0.4794	-2.0610
C	2.4336	-2.1204	0.7219
H	3.3472	-1.8333	1.2563
H	1.5849	-2.0806	1.3958
H	2.5536	-3.1403	0.3360
C	1.4229	1.7141	2.0450
H	0.9295	2.6554	2.3151
H	0.8578	0.8817	2.4509
H	2.4389	1.7139	2.4594
C	2.0689	2.5687	-0.0405
H	3.1329	2.6369	0.2208
H	1.9644	2.3370	-1.0958
H	1.5930	3.5347	0.1708
C	-2.5205	-1.8834	1.6947
H	-2.5144	-2.0478	2.7718
H	-3.5528	-1.7580	1.3769

H	-2.0918	-2.7623	1.2173

B-TS-S

N	1.1840	-1.3575	1.0166
O	-0.0133	-1.2911	1.4478
C	2.1502	-0.6808	1.5204
C	1.4145	-2.2629	-0.0909
C	3.5463	-0.7418	1.0187
H	1.8913	-0.0069	2.3206
H	2.3010	-2.8727	0.0741
H	0.5300	-2.8869	-0.1893
H	1.5250	-1.6658	-0.9941
H	3.9893	-1.7272	1.1775
H	3.5750	-0.5220	-0.0473
H	4.1521	-0.0047	1.5353
C	1.5379	1.3020	-0.9875
C	1.9190	2.1212	0.0045
O	0.5252	0.4905	-0.9309
H	2.7706	2.7714	-0.0887
H	1.3586	2.1678	0.9244
Li	-0.6975	-0.1006	0.1382
O	-1.9687	-1.1074	-0.9163
O	-1.8252	1.2308	0.9318
C	-3.0620	-1.8994	-0.5518
H	-4.0073	-1.3545	-0.6665
H	-3.1093	-2.8137	-1.1581
H	-2.9228	-2.1644	0.4920
C	-1.9961	-0.7018	-2.2587
H	-2.8854	-0.0993	-2.4749
H	-1.1032	-0.1023	-2.4000
H	-1.9785	-1.5668	-2.9331
C	-1.7644	2.5270	0.4004
H	-1.4564	3.2529	1.1616
H	-1.0181	2.4977	-0.3861
H	-2.7344	2.8330	-0.0120
C	-2.6794	1.1208	2.0345
H	-3.7200	1.3330	1.7550
H	-2.5960	0.0991	2.3911
H	-2.3834	1.8087	2.8357
C	2.3261	1.2851	-2.2942
H	1.7088	1.6888	-3.0965
H	3.2328	1.8784	-2.2161
H	2.5884	0.2619	-2.5668

DFT-optimized cartesian coordinates of all species involved in the platinum-catalyzed reaction

c

Pt	-1.7202	0.0144	0.2318
Cl	-2.1176	-2.0866	-0.3777
Cl	-3.9385	0.1430	0.5935
C	1.1476	3.3043	-0.3213
C	2.3577	3.3600	-0.9865
C	2.9469	2.2008	-1.4680
C	2.3377	0.9716	-1.2768
C	1.1254	0.9021	-0.6069
C	0.5255	2.0722	-0.1320
H	0.6729	4.1998	0.0488
H	2.8424	4.3124	-1.1352
H	3.8889	2.2507	-1.9914
H	2.8013	0.0685	-1.6451
C	-0.7278	1.9457	0.5323
C	-1.7440	1.9841	1.2282
H	-2.5433	2.2909	1.8535
N	0.4883	-0.3607	-0.3400
C	1.0339	-1.0254	0.8755
C	2.5378	-1.0186	0.9377
H	0.6546	-2.0505	0.8589
H	0.6280	-0.5008	1.7495
C	3.2026	0.0443	1.5393
C	4.5850	0.0798	1.5707
C	5.3170	-0.9481	1.0010
C	4.6616	-2.0135	0.4070
C	3.2785	-2.0507	0.3750
H	2.6349	0.8474	1.9897
H	5.0902	0.9102	2.0413
H	6.3962	-0.9206	1.0245
H	5.2290	-2.8201	-0.0327
H	2.7664	-2.8758	-0.0956
C	0.4258	-1.2054	-1.4977
C	-0.1999	-0.5286	-2.6902
H	-0.9167	0.2392	-2.3902
H	-0.7092	-1.2859	-3.2809
H	0.5763	-0.0767	-3.3067
O	0.8538	-2.3238	-1.4976

C-TS1

Pt	2.6613	-0.1394	-0.1531
Cl	4.8278	0.1081	-0.0946
Cl	1.9997	1.5761	-1.3871
C	0.2089	1.3113	1.8555
C	-0.7557	1.9709	2.5993
C	-2.0865	1.5949	2.5151
C	-2.4836	0.5625	1.6761
C	-1.5304	-0.0920	0.9188
C	-0.1781	0.2786	1.0188
H	1.2523	1.5916	1.9082
H	-0.4685	2.7818	3.2506
H	-2.8306	2.1109	3.1020
H	-3.5236	0.2805	1.6111
C	0.6669	-0.5436	0.1720
C	0.1560	-1.4697	-0.5215
H	0.1961	-2.2776	-1.2075
N	-1.8265	-1.1214	-0.0188
C	-2.3338	-0.6381	-1.3152
C	-3.6306	0.1057	-1.1459
H	-2.4765	-1.5191	-1.9453
H	-1.5729	0.0139	-1.7498
C	-3.6407	1.4941	-1.0989
C	-4.8286	2.1758	-0.9004
C	-6.0126	1.4755	-0.7408
C	-6.0079	0.0911	-0.7855
C	-4.8219	-0.5924	-0.9873
H	-2.7160	2.0395	-1.2206
H	-4.8290	3.2549	-0.8689
H	-6.9389	2.0078	-0.5845
H	-6.9301	-0.4576	-0.6651
H	-4.8153	-1.6721	-1.0226
C	-2.2062	-2.3960	0.4018
C	-1.8728	-2.7053	1.8354
H	-0.8560	-2.4005	2.0701
H	-1.9883	-3.7730	2.0013
H	-2.5529	-2.1698	2.4953
O	-2.7085	-3.1821	-0.3625

C-IM3

Pt	-2.7093	-0.0054	-0.2167
Cl	-2.4632	1.8347	1.1292
Cl	-3.3941	-1.7190	-1.4346

C	-0.2662	-1.9050	1.4718
C	0.7364	-2.4430	2.2617
C	2.0242	-1.9248	2.2358
C	2.3609	-0.8639	1.4031
C	1.3685	-0.3665	0.5859
C	0.0568	-0.8498	0.6327
H	-1.2797	-2.2763	1.4959
H	0.5135	-3.2675	2.9211
H	2.7830	-2.3443	2.8778
H	3.3577	-0.4531	1.4145
C	-0.7664	-0.0399	-0.2646
C	0.0605	0.8406	-0.8609
H	-0.1412	1.6125	-1.5779
N	1.4459	0.7301	-0.3606
C	2.3811	0.5015	-1.5024
C	3.7575	0.0644	-1.0899
H	2.4316	1.4420	-2.0575
H	1.9140	-0.2635	-2.1263
C	4.0926	-1.2851	-1.1189
C	5.3571	-1.6991	-0.7400
C	6.2965	-0.7690	-0.3268
C	5.9712	0.5770	-0.3024
C	4.7085	0.9947	-0.6854
H	3.3601	-2.0118	-1.4386
H	5.6087	-2.7482	-0.7681
H	7.2828	-1.0920	-0.0301
H	6.7036	1.3055	0.0107
H	4.4599	2.0452	-0.6735
C	1.6094	2.1041	0.2928
C	0.9015	2.2513	1.5731
H	-0.1902	2.1835	1.4169
H	1.1293	3.2301	1.9871
H	1.1652	1.4725	2.2831
O	2.2222	2.9231	-0.3137

C-IM3-TS1

Pt	-2.4032	-0.4580	-0.3375
Cl	-2.7833	1.8040	-0.8186
Cl	-2.4558	-2.6142	0.0297
C	-0.1206	-0.6343	2.4992
C	0.8154	-0.5551	3.5065
C	2.0654	0.0321	3.2922
C	2.4124	0.5598	2.0659
C	1.4745	0.4838	1.0443

C	0.2046	-0.1098	1.2483
H	-1.0829	-1.0998	2.6482
H	0.5902	-0.9615	4.4807
H	2.7778	0.0643	4.1027
H	3.3862	0.9951	1.9018
C	-0.4917	-0.0503	-0.0154
C	0.3626	0.5471	-0.8905
H	0.2299	0.7737	-1.9326
N	1.5293	0.9528	-0.2498
C	2.7623	1.2405	-0.9390
C	3.6966	0.0510	-0.9539
H	3.2606	2.0910	-0.4599
H	2.5151	1.5303	-1.9657
C	3.1984	-1.2333	-1.1290
C	4.0575	-2.3174	-1.1378
C	5.4197	-2.1287	-0.9783
C	5.9214	-0.8500	-0.8075
C	5.0625	0.2348	-0.7911
H	2.1366	-1.3899	-1.2512
H	3.6593	-3.3119	-1.2693
H	6.0890	-2.9758	-0.9853
H	6.9828	-0.6958	-0.6810
H	5.4570	1.2320	-0.6533
C	0.5830	3.2270	-0.0064
C	-0.5113	2.9294	0.7210
H	-1.4450	2.5594	-0.0127
H	-0.9027	3.7843	1.2651
H	-0.4221	2.0442	1.3571
O	1.3878	3.7037	-0.6791

C-IM5

Pt	-2.3211	-0.8325	0.0494
Cl	-3.3477	1.2835	-0.0248
Cl	-1.7839	-2.9430	0.1292
C	-0.2478	1.6087	1.8427
C	0.6256	2.5260	2.3831
C	1.9046	2.7144	1.8464
C	2.3401	1.9850	0.7627
C	1.4631	1.0602	0.2042
C	0.1561	0.8689	0.7277
H	-1.2257	1.4472	2.2735
H	0.3310	3.1047	3.2465
H	2.5645	3.4369	2.3027
H	3.3364	2.1149	0.3685

C	-0.4640	-0.1258	-0.0916
C	0.4683	-0.4995	-1.0196
H	0.3953	-1.2343	-1.7994
N	1.6204	0.2259	-0.8617
C	2.8332	0.0608	-1.6156
C	3.9470	-0.5196	-0.7743
H	3.1435	1.0286	-2.0267
H	2.6179	-0.6093	-2.4541
C	3.6714	-1.5060	0.1639
C	4.6890	-2.0383	0.9347
C	5.9907	-1.5948	0.7727
C	6.2715	-0.6145	-0.1633
C	5.2530	-0.0772	-0.9309
H	2.6570	-1.8533	0.2948
H	4.4640	-2.8024	1.6635
H	6.7845	-2.0110	1.3750
H	7.2846	-0.2634	-0.2936
H	5.4750	0.6909	-1.6588
C	-0.4689	2.8332	-1.5559
C	-1.2665	3.3652	-0.6633
H	-2.3622	2.2432	-0.3580
H	-1.9233	4.1613	-0.9724
H	-0.9069	3.4123	0.3560
O	0.1638	2.3025	-2.3575

C-IM5-TS

Pt	2.1022	-0.5514	-0.3085
Cl	3.6574	0.9820	-0.9117
Cl	1.1420	-2.5927	-0.4345
C	-0.7253	3.4431	-1.1689
C	-2.0294	3.4322	-0.6676
C	0.1502	2.4117	-0.9115
C	-2.4926	2.3900	0.1069
C	-1.6162	1.3462	0.3767
C	-0.2921	1.3447	-0.1269
H	1.1531	2.4116	-1.3133
H	-0.4047	4.2767	-1.7749
H	-2.6883	4.2556	-0.8973
H	-3.5043	2.3798	0.4811
C	0.3064	0.1270	0.3421
C	-0.6637	-0.5341	1.0672
H	-0.5880	-1.4728	1.5827
N	-1.7990	0.2019	1.1129
C	-3.0421	-0.2033	1.7157

C	-4.0763	-0.5474	0.6674
H	-3.4132	0.6023	2.3579
H	-2.8429	-1.0783	2.3419
C	-5.3848	-0.1033	0.7915
C	-6.3268	-0.4256	-0.1702
C	-5.9647	-1.1882	-1.2669
C	-4.6591	-1.6314	-1.3968
C	-3.7184	-1.3151	-0.4335
H	-5.6706	0.4939	1.6462
H	-7.3432	-0.0768	-0.0638
H	-6.6983	-1.4361	-2.0192
H	-4.3717	-2.2269	-2.2500
H	-2.7008	-1.6624	-0.5386
C	2.0247	0.1748	1.6213
C	2.2787	1.6277	1.8479
H	1.8121	2.2674	1.1062
H	3.3576	1.7807	1.7946
H	1.9352	1.8852	2.8493
O	2.0483	-0.6895	2.4364

C-IM10

Pt	1.70068400	-0.78432200	-0.41949500
Cl	3.40890100	0.18622600	-1.45721100
Cl	0.04867800	-2.20669600	0.25570800
C	-0.32655400	3.36423500	-1.31350100
C	-1.68703200	3.20243700	-1.07785600
C	0.61241500	2.54958500	-0.70484500
C	-2.15585200	2.21527700	-0.22762400
C	-1.21922900	1.39767200	0.38041600
C	0.16402100	1.55725600	0.15998800
H	1.66291600	2.66770700	-0.91425100
H	0.00401800	4.13866400	-1.98811500
H	-2.39309000	3.85347800	-1.56978000
H	-3.21223700	2.08617600	-0.05740200
C	0.84950600	0.52369300	0.95980800
C	-0.24794200	-0.18444100	1.61236900
H	-0.13079800	-0.82973300	2.46551900
N	-1.41113200	0.36868100	1.30035600
C	-2.70008700	-0.03683900	1.80973200
C	-3.69087700	-0.35201400	0.71354200
H	-3.09683100	0.76569700	2.44274800
H	-2.54486300	-0.92382500	2.43077500
C	-5.00614200	0.08134100	0.81756200
C	-5.92021000	-0.21459600	-0.17858400

C	-5.52393100	-0.93884800	-1.28977800
C	-4.21354700	-1.37344300	-1.39647900
C	-3.29953300	-1.08630600	-0.39836800
H	-5.31822500	0.65089600	1.68200500
H	-6.94123800	0.12478500	-0.08754500
H	-6.23585700	-1.16522200	-2.06914700
H	-3.90068900	-1.94199400	-2.25892500
H	-2.28171900	-1.43518100	-0.47828100
C	2.12098600	0.66822600	1.77602400
C	2.97129500	1.87698300	1.50876700
H	3.44721500	1.78032900	0.53473000
H	3.73942700	1.94219200	2.27472900
H	2.35893800	2.77514200	1.51034900
O	2.36562800	-0.13076400	2.65240300

C-IM3-TS2

Pt	-2.6800	-0.1084	0.2014
Cl	-3.0361	-0.3633	-1.9929
Cl	-3.0565	0.1430	2.3797
C	-0.3713	2.3573	-0.6426
C	0.6055	3.2551	-1.0305
C	1.9461	2.8881	-1.0474
C	2.3565	1.6166	-0.6679
C	1.3845	0.7344	-0.2416
C	0.0228	1.0828	-0.2497
H	-1.4213	2.6115	-0.6449
H	0.3274	4.2516	-1.3365
H	2.6898	3.6012	-1.3676
H	3.3986	1.3456	-0.7037
C	-0.7589	-0.0633	0.1733
C	0.1410	-1.0901	0.4046
H	-0.0123	-1.9722	0.9999
N	1.5222	-0.6272	0.1673
C	2.5026	-0.9773	1.2083
C	3.9068	-0.5652	0.8643
H	2.4562	-2.0664	1.3135
H	2.1737	-0.5061	2.1379
C	4.5306	0.4623	1.5614
C	5.8255	0.8348	1.2444
C	6.5038	0.1875	0.2253
C	5.8886	-0.8410	-0.4696
C	4.5973	-1.2210	-0.1495
H	4.0009	0.9718	2.3532
H	6.3039	1.6316	1.7932

H	7.5127	0.4801	-0.0231
H	6.4179	-1.3536	-1.2584
H	4.1226	-2.0328	-0.6798
C	1.2869	-1.6910	-0.9473
C	0.9090	-1.1345	-2.2819
H	0.0041	-0.5355	-2.2623
H	0.7495	-1.9824	-2.9442
H	1.7295	-0.5338	-2.6741
O	1.7307	-2.7919	-0.7351

C-IM6

Pt	-2.54864600	-0.09455500	0.04586700
Cl	-2.82681600	-1.04348400	-1.95675900
Cl	-3.16802600	0.74618100	2.00058400
C	-0.32343100	2.41552900	-1.01622900
C	0.60968500	3.38282000	-1.28522900
C	1.93530200	3.24288000	-0.84421200
C	2.35985200	2.14308100	-0.13335900
C	1.42667200	1.14334100	0.14782100
C	0.07453800	1.27894900	-0.29195400
H	-1.35045500	2.49387100	-1.34264700
H	0.33394900	4.26586600	-1.83998000
H	2.64390200	4.02570600	-1.07014400
H	3.38280100	2.05421000	0.19418900
C	-0.65674100	0.16646200	0.15513000
C	0.31506100	-0.73563400	0.84629900
H	0.01116000	-0.96352900	1.87575700
N	1.57380600	-0.01184000	0.82517600
C	2.72797900	-0.44034600	1.57871800
C	3.99602800	-0.43713400	0.76017300
H	2.52734000	-1.45718400	1.92971000
H	2.85415700	0.20651100	2.45645700
C	5.12300100	0.24073100	1.20567400
C	6.28545900	0.23949700	0.45420200
C	6.32981600	-0.43499700	-0.75362700
C	5.21094700	-1.11684900	-1.20171000
C	4.05179500	-1.12126400	-0.44725800
H	5.09214200	0.77077800	2.14731600
H	7.15608100	0.76842900	0.81209100
H	7.23486900	-0.43290600	-1.34192100
H	5.24240700	-1.65117800	-2.13925000
H	3.18663500	-1.66652400	-0.79144100
C	0.57814300	-2.10570100	0.13610300
C	0.44005000	-2.07843000	-1.34155300

H	-0.62689200	-2.04969700	-1.58469600
H	0.87943400	-2.97045800	-1.78148200
H	0.87851500	-1.17605100	-1.76137900
O	0.91739000	-3.05039700	0.79057300

C-IM6-TS1

Pt	2.2173	-0.2714	-0.2032
Cl	2.8051	1.5324	-1.3413
Cl	4.3690	-0.8626	-0.1850
C	-1.1632	3.4773	0.6333
C	-2.4147	3.0329	1.0756
C	-0.2012	2.5912	0.2053
C	-2.7425	1.6944	1.1067
C	-1.7804	0.7885	0.6695
C	-0.5079	1.2287	0.2226
H	0.7651	2.9123	-0.1508
H	-0.9560	4.5358	0.6293
H	-3.1444	3.7597	1.3994
H	-3.7145	1.3624	1.4355
C	0.2477	0.0807	-0.1866
C	-0.6208	-1.0450	0.1170
H	-0.6128	-2.0141	-0.3613
N	-1.8287	-0.5749	0.6062
C	-2.9832	-1.3827	0.9066
C	-4.1636	-1.0398	0.0255
H	-3.2584	-1.2482	1.9598
H	-2.7047	-2.4316	0.7626
C	-5.4488	-1.0360	0.5496
C	-6.5317	-0.7312	-0.2562
C	-6.3372	-0.4199	-1.5909
C	-5.0571	-0.4200	-2.1182
C	-3.9745	-0.7317	-1.3153
H	-5.6036	-1.2753	1.5923
H	-7.5274	-0.7326	0.1611
H	-7.1812	-0.1772	-2.2184
H	-4.8988	-0.1784	-3.1582
H	-2.9785	-0.7291	-1.7339
C	0.7630	-1.0237	1.1078
C	0.5687	-0.5332	2.5155
H	0.2143	-1.3668	3.1231
H	-0.1343	0.2931	2.5751
H	1.5327	-0.2137	2.9146
O	1.5224	-1.9845	0.8276

C-TS2

Pt	-2.0947	-0.1228	-0.2121
Cl	-3.1427	-1.7542	-1.2305
Cl	-3.7511	0.7826	0.9170
C	1.0784	-2.0820	2.3794
C	1.9835	-1.1023	2.7550
C	0.3220	-1.9480	1.2256
C	2.1603	0.0402	1.9844
C	1.4350	0.1575	0.8211
C	0.5004	-0.8186	0.4412
H	-0.3925	-2.7014	0.9286
H	0.9552	-2.9570	2.9988
H	2.5551	-1.2169	3.6629
H	2.8508	0.8087	2.2971
C	-0.1567	-0.4459	-0.8144
C	0.4095	0.5487	-1.4103
H	0.3912	1.1641	-2.2785
N	1.4650	1.2820	-0.0768
C	2.7855	1.7552	-0.4876
C	3.7484	0.6015	-0.6279
H	3.1772	2.4678	0.2478
H	2.6869	2.2736	-1.4470
C	4.9295	0.5840	0.1007
C	5.8088	-0.4782	-0.0156
C	5.5104	-1.5361	-0.8561
C	4.3349	-1.5232	-1.5878
C	3.4607	-0.4573	-1.4803
H	5.1685	1.4061	0.7608
H	6.7251	-0.4798	0.5551
H	6.1927	-2.3679	-0.9419
H	4.0968	-2.3439	-2.2468
H	2.5436	-0.4552	-2.0509
C	0.4119	2.2205	0.2351
C	0.6200	3.6247	-0.2409
H	-0.2866	4.1887	-0.0367
H	0.8256	3.6545	-1.3089
H	1.4528	4.0906	0.2837
O	-0.5842	1.8433	0.8071

C-IM1-TS2

Pt	0.3650	-0.8553	-0.1456
Cl	1.4782	-2.8337	-0.4338
Cl	-1.2255	-2.1909	0.8739
C	-4.0416	0.3097	0.1444

C	-4.5089	0.4953	-1.1457
C	-3.6556	0.9240	-2.1491
C	-2.3178	1.1886	-1.8889
C	-1.8461	1.0118	-0.6010
C	-2.7097	0.5715	0.4125
H	-4.6935	-0.0315	0.9330
H	-5.5460	0.3007	-1.3727
H	-4.0314	1.0619	-3.1515
H	-1.6840	1.5217	-2.6972
C	-2.0160	0.4257	1.6622
C	-1.4727	-0.5917	2.1833
H	-0.9722	-0.8827	3.0764
N	-0.5218	1.1781	-0.0979
C	0.3511	2.0665	-0.8851
C	1.7848	1.7061	-0.6314
H	0.1371	3.1091	-0.6247
H	0.1379	1.9300	-1.9500
C	2.1246	0.3531	-0.7558
C	3.4266	-0.0714	-0.5105
C	4.3836	0.8544	-0.1271
C	4.0499	2.1936	-0.0054
C	2.7539	2.6204	-0.2537
H	1.4149	-0.3260	-1.3540
H	3.6838	-1.1135	-0.6274
H	5.3937	0.5300	0.0685
H	4.8003	2.9111	0.2892
H	2.4945	3.6637	-0.1516
C	-0.6613	1.8117	1.3205
C	0.5048	1.4399	2.2160
H	1.2862	2.1859	2.0727
H	0.9041	0.4458	1.9916
H	0.1831	1.4831	3.2521
O	-1.1896	2.9046	1.3619

C-IM4

Pt	0.7002	-0.2929	0.0586
Cl	2.1051	-2.0289	-0.2882
Cl	-0.8695	-0.1086	-2.4333
C	-3.9414	0.4023	0.4498
C	-4.5179	1.6370	0.4984
C	-3.7488	2.7951	0.2643
C	-2.4051	2.7101	0.0640
C	-1.7477	1.4478	0.0997
C	-2.5692	0.2498	0.1389

H	-4.5372	-0.4877	0.5699
H	-5.5763	1.7343	0.6826
H	-4.2332	3.7605	0.2633
H	-1.8167	3.6031	-0.0801
C	-1.9847	-1.0037	-0.1213
C	-0.8315	-1.1423	-0.9858
H	-0.6238	-2.1587	-1.3248
N	-0.4497	1.3180	0.2851
C	0.4796	2.4243	0.3414
C	1.8307	1.7310	0.3602
H	0.3229	3.0205	1.2502
H	0.3916	3.0857	-0.5304
C	2.7079	1.7917	-0.7277
C	3.9315	1.1463	-0.6704
C	4.3046	0.4415	0.4660
C	3.4542	0.3776	1.5557
C	2.2075	0.9979	1.5089
H	2.4318	2.3600	-1.6051
H	4.5973	1.1905	-1.5187
H	5.2590	-0.0601	0.4984
H	3.7490	-0.1622	2.4431
H	1.5854	1.0368	2.3999
C	-2.5189	-2.2467	0.5042
C	-1.4574	-3.2298	0.9352
H	-1.8234	-3.7908	1.7916
H	-0.5157	-2.7355	1.1755
H	-1.2795	-3.9385	0.1275
O	-3.6954	-2.4596	0.6835

C-IM1

Pt	0.8266	-0.8448	-0.0113
Cl	2.5974	-2.2112	-0.1650
Cl	-0.1350	-2.4508	1.2135
C	-4.5387	0.3256	-0.6841
C	-4.5782	-0.8729	-1.3706
C	-3.4080	-1.5724	-1.6187
C	-2.1969	-1.0744	-1.1695
C	-2.1475	0.1130	-0.4584
C	-3.3255	0.8368	-0.2249
H	-5.4440	0.8824	-0.4940
H	-5.5241	-1.2604	-1.7166
H	-3.4348	-2.5050	-2.1593
H	-1.2744	-1.6202	-1.3535
C	-3.2999	2.0740	0.4647

C	-3.2888	3.1285	1.0393
H	-3.2759	4.0454	1.5491
N	-0.8777	0.6272	-0.0240
C	-0.4333	1.7536	-0.8787
C	1.0422	2.0093	-0.7422
H	-0.9990	2.6523	-0.6074
H	-0.6732	1.4869	-1.9154
C	1.9220	0.9373	-0.9105
C	3.2912	1.1153	-0.7557
C	3.7846	2.3687	-0.4364
C	2.9165	3.4381	-0.2861
C	1.5512	3.2611	-0.4345
H	1.5436	-0.0154	-1.3912
H	3.9580	0.2764	-0.8881
H	4.8463	2.5109	-0.3070
H	3.3031	4.4150	-0.0387
H	0.8773	4.0924	-0.2930
C	-0.6752	0.8453	1.3678
C	-1.5818	0.0994	2.3065
H	-1.0264	-0.1253	3.2140
H	-1.9713	-0.8204	1.8822
H	-2.4057	0.7631	2.5687
O	0.1387	1.6579	1.7410

C-IM1-TS1

Pt	0.5888	-0.9493	-0.1043
Cl	2.1251	-2.5826	0.1511
Cl	-0.9071	-2.2801	0.9002
C	-4.4000	1.1742	-0.2783
C	-4.8355	0.0368	-0.9179
C	-3.9052	-0.8798	-1.3979
C	-2.5541	-0.6656	-1.2236
C	-2.0582	0.4745	-0.5938
C	-3.0356	1.4183	-0.1038
H	-5.1035	1.9050	0.0905
H	-5.8911	-0.1393	-1.0535
H	-4.2379	-1.7633	-1.9202
H	-1.8313	-1.3761	-1.6071
C	-2.4862	2.4637	0.6247
C	-1.3778	2.6541	1.2270
H	-0.9069	3.5539	1.5689
N	-0.7126	0.6308	-0.3681
C	-0.0827	1.6561	-1.2108
C	1.3857	1.7529	-0.9131

H	-0.5709	2.6294	-1.0909
H	-0.2185	1.3542	-2.2634
C	2.1178	0.5651	-0.8606
C	3.4628	0.5767	-0.5200
C	4.0853	1.7830	-0.2463
C	3.3711	2.9670	-0.3275
C	2.0249	2.9543	-0.6528
H	1.6748	-0.3732	-1.3144
H	4.0122	-0.3517	-0.4740
H	5.1293	1.7991	0.0265
H	3.8609	3.9067	-0.1204
H	1.4670	3.8787	-0.6914
C	-0.4903	1.3624	1.6088
C	-1.2700	0.4309	2.4827
H	-1.4567	0.9484	3.4243
H	-0.6736	-0.4577	2.6853
H	-2.2198	0.1404	2.0464
O	0.7018	1.5369	1.6695

C-IM2

Pt	0.5281	-0.9705	-0.3318
Cl	1.9976	-2.3775	0.6542
Cl	-1.1284	-2.0783	0.7090
C	-4.0101	1.5798	0.0499
C	-4.7725	0.5487	-0.3887
C	-4.1641	-0.5625	-1.0196
C	-2.8244	-0.5941	-1.2491
C	-1.9715	0.4955	-0.9169
C	-2.5909	1.5544	-0.1077
H	-4.4449	2.4320	0.5497
H	-5.8434	0.5631	-0.2574
H	-4.7840	-1.3808	-1.3516
H	-2.3708	-1.4147	-1.7846
C	-1.7624	2.2840	0.6572
C	-0.7905	2.4225	1.4931
H	-0.1901	3.2979	1.6673
N	-0.7000	0.4320	-1.2560
C	0.0260	1.6313	-1.6413
C	1.4059	1.6889	-1.0426
H	-0.5354	2.5430	-1.4128
H	0.1332	1.5784	-2.7388
C	2.1435	0.5072	-0.9297
C	3.4104	0.5197	-0.3619
C	3.9489	1.7139	0.0866

C	3.2265	2.8891	-0.0331
C	1.9590	2.8771	-0.5924
H	1.7901	-0.4326	-1.4563
H	3.9647	-0.4017	-0.2679
H	4.9311	1.7259	0.5332
H	3.6456	3.8195	0.3205
H	1.3941	3.7948	-0.6766
C	-0.3235	1.1041	2.1087
C	-1.2494	0.4273	3.0552
H	-2.0461	1.0782	3.3992
H	-0.6816	0.0303	3.8942
H	-1.6679	-0.4368	2.5263
O	0.7091	0.6382	1.6932

C-IM2-TS

Pt	0.3046	-0.5308	-0.6085
Cl	1.3036	-2.3208	-1.6475
Cl	-1.3045	-1.8953	0.2666
C	-4.1391	0.2493	0.0180
C	-4.5987	1.1899	-0.8985
C	-3.7218	2.1120	-1.4348
C	-2.3839	2.1286	-1.0670
C	-1.9062	1.2214	-0.1315
C	-2.8226	0.2719	0.4066
H	-4.8083	-0.4869	0.4355
H	-5.6364	1.1921	-1.1944
H	-4.0739	2.8341	-2.1566
H	-1.7172	2.8421	-1.5319
C	-2.1021	-0.6667	1.3028
C	-1.1527	0.0524	2.0199
H	-1.5354	0.8826	2.6041
N	-0.6026	1.1093	0.3407
C	0.2571	2.2703	0.4065
C	1.6903	1.8710	0.1713
H	0.1577	2.7465	1.3919
H	-0.0266	3.0254	-0.3433
C	1.9697	0.8592	-0.7613
C	3.2801	0.4448	-0.9811
C	4.3143	1.0357	-0.2769
C	4.0442	2.0363	0.6427
C	2.7410	2.4456	0.8701
H	1.1721	0.5597	-1.5594
H	3.4794	-0.3377	-1.6985
H	5.3303	0.7130	-0.4432

H	4.8513	2.4932	1.1954
H	2.5364	3.2148	1.6008
C	0.0602	-0.5992	2.5932
C	-0.1045	-1.0530	4.0189
H	-0.2585	-0.1891	4.6623
H	0.7792	-1.5966	4.3416
H	-0.9842	-1.6883	4.0964
O	1.0822	-0.7639	1.9699

C-IM8

Pt	-0.2175	0.7912	0.1210
Cl	-0.9224	2.8825	0.6856
Cl	1.3447	0.6639	1.7991
C	3.9929	-0.0814	-0.3359
C	4.3200	0.1485	-1.6660
C	3.3933	-0.0679	-2.6712
C	2.1108	-0.5193	-2.3833
C	1.7923	-0.7573	-1.0608
C	2.7310	-0.5474	-0.0359
H	4.7053	0.0969	0.4538
H	5.3059	0.5069	-1.9196
H	3.6626	0.1201	-3.6995
H	1.3998	-0.6616	-3.1853
C	2.1026	-0.8517	1.2867
C	0.9364	-1.7643	0.8108
H	1.3382	-2.7745	0.6465
N	0.5512	-1.1635	-0.4890
C	-0.4181	-1.8906	-1.3078
C	-1.7794	-1.2403	-1.2273
H	-0.4834	-2.9316	-0.9707
H	-0.0777	-1.9012	-2.3492
C	-1.8854	0.1615	-1.2146
C	-3.1345	0.7670	-1.0967
C	-4.2738	-0.0110	-0.9951
C	-4.1725	-1.3923	-1.0144
C	-2.9330	-2.0009	-1.1224
H	-1.0048	0.8208	-1.5055
H	-3.2022	1.8450	-1.0832
H	-5.2396	0.4600	-0.8975
H	-5.0600	-2.0010	-0.9311
H	-2.8612	-3.0791	-1.1169
C	-0.1765	-1.7931	1.8182
C	0.1235	-2.6117	3.0373
H	0.1328	-3.6691	2.7802

H	-0.6261	-2.4322	3.8022
H	1.1140	-2.3460	3.4019
O	-1.1947	-1.1501	1.6739

C-TS3

Pt	2.6099	-0.4642	-0.2910
Cl	0.8306	-1.5863	-1.1586
Cl	4.5466	0.5751	0.0167
C	0.7923	2.5999	0.4317
C	0.1227	3.5907	-0.2552
C	-1.1547	3.3500	-0.7423
C	-1.7721	2.1278	-0.5379
C	-1.1152	1.1146	0.1497
C	0.1878	1.3514	0.6298
H	1.7911	2.7570	0.8112
H	0.5927	4.5480	-0.4168
H	-1.6792	4.1223	-1.2842
H	-2.7723	1.9672	-0.9097
C	0.9090	0.3176	1.2665
C	1.8353	-0.4714	1.5938
H	2.1164	-1.1308	2.3928
N	-1.7278	-0.1276	0.3717
C	-2.5698	-0.6663	-0.6773
C	-4.0514	-0.4332	-0.4892
H	-2.3683	-1.7368	-0.7700
H	-2.2457	-0.2135	-1.6191
C	-4.5543	0.3607	0.5326
C	-5.9196	0.5579	0.6587
C	-6.7949	-0.0337	-0.2343
C	-6.2998	-0.8271	-1.2567
C	-4.9375	-1.0257	-1.3822
H	-3.8828	0.8274	1.2393
H	-6.2970	1.1768	1.4589
H	-7.8584	0.1212	-0.1347
H	-6.9769	-1.2927	-1.9568
H	-4.5508	-1.6445	-2.1787
C	-1.5413	-0.7707	1.5544
C	-2.3192	-2.0370	1.7727
H	-2.2081	-2.3303	2.8130
H	-1.8930	-2.8183	1.1447
H	-3.3720	-1.9199	1.5318
O	-0.7736	-0.3472	2.4123

C-IM11

Pt	3.0831	-0.1388	-0.0559
Cl	2.4767	0.3012	-2.1879
Cl	4.1187	-0.1620	1.9312
C	0.5084	1.6574	0.4938
C	-0.0143	2.9313	0.3388
C	-1.3104	3.0998	-0.1086
C	-2.0971	1.9949	-0.4114
C	-1.5617	0.7251	-0.2967
C	-0.2490	0.5432	0.1580
H	1.5129	1.5088	0.8790
H	0.5917	3.7905	0.5784
H	-1.7277	4.0882	-0.2202
H	-3.1184	2.1498	-0.7194
C	0.2575	-0.8195	0.2944
C	1.5303	-1.2484	0.3124
H	1.6910	-2.3245	0.4253
N	-2.3313	-0.4443	-0.5860
C	-3.5900	-0.3294	-1.2910
C	-4.7955	-0.1370	-0.3948
H	-3.7320	-1.2245	-1.9025
H	-3.5038	0.5153	-1.9808
C	-4.6747	0.1898	0.9484
C	-5.8067	0.3682	1.7267
C	-7.0653	0.2237	1.1714
C	-7.1915	-0.1011	-0.1695
C	-6.0630	-0.2823	-0.9473
H	-3.7005	0.3123	1.3984
H	-5.6995	0.6228	2.7700
H	-7.9454	0.3644	1.7796
H	-8.1700	-0.2149	-0.6102
H	-6.1618	-0.5352	-1.9929
C	-1.9269	-1.6169	-0.1040
C	-2.8187	-2.8104	-0.1038
H	-2.3723	-3.5734	0.5283
H	-2.9119	-3.2179	-1.1109
H	-3.8122	-2.5600	0.2628
O	-0.7517	-1.8080	0.3796

C-IM1-TS3

Pt	1.0191	-0.9215	-0.1680
Cl	1.2111	-2.3691	1.5326
Cl	3.0271	-1.6950	-0.8516
C	-4.4267	-0.5494	-0.7035
C	-4.3177	-1.8850	-1.0378

C	-3.0965	-2.5328	-0.9356
C	-1.9830	-1.8375	-0.4975
C	-2.0827	-0.4964	-0.1674
C	-3.3117	0.1653	-0.2642
H	-5.3756	-0.0392	-0.7720
H	-5.1894	-2.4255	-1.3735
H	-3.0095	-3.5778	-1.1875
H	-1.0248	-2.3445	-0.3899
C	-3.4466	1.5303	0.0814
C	-3.5787	2.6886	0.3690
H	-3.7044	3.6948	0.6388
N	-0.8981	0.1995	0.2661
C	-0.1000	0.7464	-0.8184
C	0.5472	2.0875	-0.6120
H	-0.7526	0.7868	-1.7013
H	0.9382	-0.1002	-1.4733
C	1.9291	2.2267	-0.5350
C	2.4929	3.4808	-0.3758
C	1.6861	4.6027	-0.2940
C	0.3099	4.4697	-0.3806
C	-0.2598	3.2203	-0.5458
H	2.5693	1.3536	-0.6027
H	3.5657	3.5780	-0.3167
H	2.1272	5.5795	-0.1677
H	-0.3233	5.3421	-0.3257
H	-1.3330	3.1142	-0.6134
C	-0.8881	0.5662	1.6301
C	0.3759	1.1695	2.1770
H	0.3513	1.0424	3.2571
H	0.4199	2.2336	1.9541
H	1.2710	0.6780	1.7827
O	-1.8604	0.3417	2.3024

C-IM12

Pt	0.8355	-1.0899	-0.2762
Cl	0.4128	-2.1207	1.7537
Cl	2.5495	-2.5406	-0.4262
C	-4.4089	0.2912	-0.6751
C	-4.5564	-1.0210	-1.0805
C	-3.4738	-1.8858	-1.0520
C	-2.2415	-1.4354	-0.6098
C	-2.0868	-0.1224	-0.1999
C	-3.1726	0.7607	-0.2314
H	-5.2465	0.9719	-0.6922

H	-5.5195	-1.3721	-1.4176
H	-3.5864	-2.9115	-1.3658
H	-1.3925	-2.1169	-0.5644
C	-3.0375	2.1092	0.1751
C	-2.9330	3.2570	0.5115
H	-2.8554	4.2564	0.8219
N	-0.7954	0.3361	0.2437
C	0.0810	0.7461	-0.7799
C	0.9790	1.9306	-0.6087
H	-0.4626	0.8097	-1.7316
H	1.2340	-0.9005	-1.7300
C	2.3628	1.7999	-0.5458
C	3.1633	2.9234	-0.4342
C	2.5927	4.1842	-0.3854
C	1.2164	4.3204	-0.4593
C	0.4108	3.2021	-0.5789
H	2.8109	0.8126	-0.5919
H	4.2352	2.8115	-0.3863
H	3.2179	5.0593	-0.2957
H	0.7667	5.3013	-0.4309
H	-0.6632	3.3073	-0.6390
C	-0.7299	0.6845	1.6287
C	0.5929	1.1487	2.1600
H	0.5831	0.9835	3.2357
H	0.7128	2.2151	1.9739
H	1.4329	0.6062	1.7247
O	-1.7228	0.5887	2.2946

C-IM13

Pt	1.0692	-0.8459	0.5069
Cl	2.0810	0.9721	1.6169
Cl	2.8895	-1.0580	-0.7970
C	-3.0282	0.4058	2.1000
C	-4.2413	0.8957	1.6574
C	-4.5293	0.9199	0.3015
C	-3.6008	0.4592	-0.6156
C	-2.3759	-0.0305	-0.1846
C	-2.0856	-0.0729	1.1865
H	-2.7927	0.3797	3.1526
H	-4.9646	1.2564	2.3721
H	-5.4781	1.2991	-0.0443
H	-3.8194	0.4777	-1.6713
C	-0.8551	-0.5765	1.6913
C	0.0261	-1.0168	2.4330

H	0.5873	-1.3704	3.2638
N	-1.4454	-0.5344	-1.1400
C	-0.1348	-0.0746	-1.1868
C	0.1964	1.3629	-1.0830
H	0.3970	-0.5159	-2.0307
H	0.6394	-2.2180	0.0063
C	-0.5549	2.3402	-0.4189
C	-0.1313	3.6555	-0.3924
C	1.0408	4.0356	-1.0231
C	1.7820	3.0880	-1.7119
C	1.3659	1.7745	-1.7466
H	-1.4701	2.0907	0.0896
H	-0.7206	4.3870	0.1401
H	1.3759	5.0606	-0.9756
H	2.6945	3.3719	-2.2134
H	1.9615	1.0432	-2.2729
C	-1.9024	-1.6426	-1.8775
C	-0.9425	-2.2622	-2.8499
H	-1.4509	-3.0975	-3.3249
H	-0.0579	-2.6330	-2.3339
H	-0.6395	-1.5521	-3.6158
O	-3.0264	-2.0458	-1.7145

C-IM13-TS1

Pt	-1.4400	-0.3261	-0.5071
Cl	-3.5429	0.3565	-1.2884
Cl	-2.3759	-1.8217	1.1291
C	2.8693	0.8297	-2.3544
C	4.2444	0.7285	-2.3024
C	4.8625	0.1224	-1.2166
C	4.1178	-0.4107	-0.1792
C	2.7342	-0.3279	-0.2293
C	2.1065	0.3227	-1.3020
H	2.3736	1.3090	-3.1834
H	4.8404	1.1307	-3.1069
H	5.9390	0.0603	-1.1788
H	4.6057	-0.8907	0.6521
C	0.6944	0.4380	-1.2835
C	-0.3891	0.8851	-1.7852
H	-0.7584	1.5785	-2.5111
N	1.8500	-0.8786	0.7109
C	0.5728	-0.3020	0.7441
C	0.4094	1.0808	1.2357
H	-0.1148	-0.9749	1.2640

H	-1.5448	-1.5034	-1.4247
C	1.4613	1.9118	1.6103
C	1.2027	3.2060	2.0254
C	-0.0944	3.6911	2.0557
C	-1.1501	2.8728	1.6810
C	-0.9004	1.5761	1.2773
H	2.4760	1.5435	1.5872
H	2.0226	3.8419	2.3232
H	-0.2861	4.7038	2.3746
H	-2.1633	3.2439	1.7099
H	-1.7526	0.9084	1.0396
C	2.1519	-2.1037	1.3204
C	1.1248	-2.6535	2.2697
H	1.5563	-3.5276	2.7512
H	0.2250	-2.9663	1.7401
H	0.8526	-1.9244	3.0299
O	3.2016	-2.6550	1.1026

C-IM14

Pt	-1.8208	-0.6552	0.1941
Cl	-2.3365	-0.4253	-2.0204
Cl	-1.5227	-0.8345	2.4907
C	2.9172	-2.5517	-0.6623
C	4.2722	-2.5976	-0.9430
C	5.0661	-1.4717	-0.7731
C	4.5388	-0.2729	-0.3184
C	3.1853	-0.2245	-0.0297
C	2.3799	-1.3611	-0.2032
H	2.2919	-3.4204	-0.7917
H	4.7136	-3.5157	-1.2989
H	6.1202	-1.5259	-0.9994
H	5.1588	0.5974	-0.1876
C	1.0076	-1.0107	0.1249
C	-0.1037	-1.6995	-0.0601
H	-0.1739	-2.7216	-0.4137
N	2.4288	0.8467	0.4512
C	1.0462	0.4251	0.6470
C	0.0264	1.2494	-0.1091
H	0.8015	0.4166	1.7189
H	-2.6598	-1.8877	0.2384
C	0.2519	1.5668	-1.4481
C	-0.6702	2.3177	-2.1529
C	-1.8311	2.7643	-1.5371
C	-2.0657	2.4709	-0.2059

C	-1.1473	1.7064	0.5212
H	1.1567	1.2239	-1.9285
H	-0.4851	2.5554	-3.1888
H	-2.5479	3.3467	-2.0952
H	-2.9470	2.8549	0.2885
H	-1.2446	1.6467	1.6011
C	2.9339	2.0693	0.8151
C	1.9557	3.0029	1.4878
H	2.5038	3.8802	1.8211
H	1.4881	2.5249	2.3457
H	1.1811	3.3147	0.7911
O	4.0867	2.3760	0.6107

C-IM13-TS2

Pt	1.9071	-0.5073	-0.2285
Cl	1.8803	-2.5918	-1.1857
Cl	2.3139	1.5517	0.6437
C	-0.5268	-1.8248	1.6313
C	-1.3626	-2.1794	2.6738
C	-2.6848	-1.7636	2.6744
C	-3.1793	-0.9824	1.6415
C	-2.3487	-0.6114	0.5974
C	-1.0127	-1.0463	0.5849
H	0.5082	-2.1530	1.5968
H	-0.9848	-2.7840	3.4833
H	-3.3408	-2.0469	3.4829
H	-4.2084	-0.6586	1.6465
C	-0.1797	-0.6566	-0.5024
C	0.0003	0.0230	-1.5220
H	0.2129	0.3577	-2.5035
N	-2.8359	0.1533	-0.5042
C	-2.1107	1.2099	-0.9775
C	-1.3340	2.0981	-0.2190
H	-2.2632	1.4520	-2.0193
H	3.2374	-0.9199	0.3395
C	-1.1957	2.0395	1.1901
C	-0.2107	2.7503	1.8185
C	0.6897	3.5193	1.0736
C	0.4308	3.7563	-0.2820
C	-0.5557	3.0588	-0.9183
H	-1.8711	1.4294	1.7681
H	-0.0894	2.6751	2.8880
H	1.4879	4.0469	1.5697
H	1.0523	4.4466	-0.8308

H	-0.7244	3.1929	-1.9772
C	-3.9381	-0.3827	-1.1879
C	-4.4723	0.4363	-2.3320
H	-5.4354	0.0204	-2.6170
H	-3.8069	0.3669	-3.1911
H	-4.5943	1.4800	-2.0527
O	-4.4293	-1.4245	-0.8354

C-IM15

Pt	1.9480	-0.1621	-0.1299
Cl	1.6253	-2.1126	-1.4682
Cl	1.9747	1.7726	0.9385
C	-0.0127	-2.6750	1.1147
C	-0.7881	-3.1557	2.1512
C	-2.1001	-2.7286	2.2763
C	-2.6415	-1.8260	1.3788
C	-1.8794	-1.3343	0.3239
C	-0.5487	-1.7726	0.1982
H	1.0163	-2.9935	1.0139
H	-0.3696	-3.8535	2.8592
H	-2.7105	-3.0914	3.0888
H	-3.6604	-1.4995	1.5002
C	0.2424	-1.2059	-0.8825
C	-0.1489	-0.0821	-1.5326
H	0.3383	0.2591	-2.4383
N	-2.3886	-0.3944	-0.5921
C	-1.4650	0.5747	-1.1743
C	-1.2332	1.7871	-0.2848
H	-1.8953	0.9250	-2.1176
H	3.3550	-0.3063	0.3722
C	-1.3501	1.7199	1.0961
C	-1.1028	2.8416	1.8684
C	-0.7293	4.0321	1.2725
C	-0.6077	4.1031	-0.1045
C	-0.8631	2.9878	-0.8793
H	-1.6314	0.7963	1.5787
H	-1.1919	2.7765	2.9420
H	-0.5264	4.9012	1.8791
H	-0.3107	5.0271	-0.5770
H	-0.7667	3.0462	-1.9548
C	-3.7305	-0.3855	-0.9101
C	-4.2379	0.8216	-1.6657
H	-5.3240	0.7969	-1.6249
H	-3.9415	0.7792	-2.7127

H	-3.8777	1.7473	-1.2232
O	-4.4680	-1.2929	-0.5982

C-IM1-TS4

Pt	-1.8367	-0.1975	-0.1143
Cl	-2.5035	-2.2664	-0.7880
Cl	-3.6294	-0.3493	1.3199
C	0.3922	3.6768	-0.4227
C	1.6700	4.1612	-0.6044
C	2.7524	3.3173	-0.4064
C	2.5598	2.0023	-0.0276
C	1.2759	1.4914	0.1626
C	0.1846	2.3503	-0.0348
H	-0.4679	4.3114	-0.5693
H	1.8234	5.1873	-0.8987
H	3.7573	3.6820	-0.5524
H	3.4165	1.3617	0.0999
C	-1.1555	1.9192	0.1499
C	-2.3862	1.9499	0.2324
H	-3.3955	2.2053	0.4314
N	1.1055	0.1624	0.5746
C	2.1536	-0.3917	1.4426
C	3.3724	-0.9038	0.7153
H	1.6988	-1.2224	1.9919
H	2.4380	0.3846	2.1580
C	4.6305	-0.7195	1.2785
C	5.7619	-1.2006	0.6444
C	5.6492	-1.8661	-0.5644
C	4.3996	-2.0555	-1.1291
C	3.2661	-1.5813	-0.4925
H	4.7227	-0.1979	2.2211
H	6.7323	-1.0530	1.0945
H	6.5318	-2.2389	-1.0617
H	4.3041	-2.5805	-2.0676
H	2.2965	-1.7515	-0.9321
C	0.1303	-0.7227	0.2124
C	-0.4361	-0.3121	-1.7586
H	-1.2327	0.0289	-2.4409
H	-0.1749	-1.3236	-2.0600
H	0.4124	0.3539	-1.8936
O	0.1997	-1.8877	0.4928

C-IM16

Pt	-1.6882	-0.2356	-0.2593

Cl	-1.8961	-2.3701	-0.9032
Cl	-3.3353	-0.6387	1.4442
C	0.1928	3.7249	-0.3853
C	1.4505	4.2423	-0.6200
C	2.5619	3.4393	-0.4228
C	2.4225	2.1447	0.0452
C	1.1647	1.6151	0.3243
C	0.0374	2.4168	0.0769
H	-0.6913	4.3179	-0.5603
H	1.5620	5.2559	-0.9709
H	3.5492	3.8195	-0.6343
H	3.3040	1.5381	0.1661
C	-1.2864	1.9111	0.2059
C	-2.5153	1.8088	0.1885
H	-3.5563	1.9434	0.3373
N	1.0487	0.3399	0.8994
C	2.2139	-0.1593	1.6476
C	3.2271	-0.8369	0.7594
H	1.8337	-0.8821	2.3767
H	2.6631	0.6760	2.1901
C	4.5856	-0.6440	0.9800
C	5.5217	-1.2796	0.1834
C	5.1082	-2.1079	-0.8458
C	3.7559	-2.3053	-1.0690
C	2.8184	-1.6767	-0.2690
H	4.9120	0.0012	1.7840
H	6.5746	-1.1253	0.3665
H	5.8382	-2.6010	-1.4696
H	3.4273	-2.9557	-1.8651
H	1.7659	-1.8482	-0.4413
C	-0.0086	-0.4993	0.8941
C	-0.5732	0.0077	-2.0104
H	-1.3185	-0.0050	-2.8098
H	0.1158	-0.8150	-2.1852
H	-0.0218	0.9442	-2.0673
O	-0.0934	-1.4907	1.5524

C-IM16-TS

Pt	-1.7570	-0.2458	0.0403
Cl	-0.6805	-2.2086	-0.6463
Cl	-3.9358	-1.1137	-0.1787
C	0.3052	3.6000	-0.5385
C	1.5313	4.0555	-0.9808
C	2.6747	3.2897	-0.7926

C	2.6159	2.0589	-0.1614
C	1.3914	1.5937	0.2924
C	0.2315	2.3723	0.1185
H	-0.5923	4.1810	-0.6796
H	1.6002	5.0120	-1.4747
H	3.6265	3.6545	-1.1462
H	3.5075	1.4674	-0.0358
C	-0.9938	1.8033	0.5639
C	-2.2435	1.7000	0.7519
H	-3.1470	2.1516	1.0912
N	1.1915	0.4022	0.9809
C	2.2860	-0.2949	1.6524
C	3.2688	-0.9065	0.6867
H	1.8256	-1.0789	2.2622
H	2.7940	0.4115	2.3184
C	4.6338	-0.7719	0.9111
C	5.5441	-1.3453	0.0409
C	5.0969	-2.0496	-1.0642
C	3.7377	-2.1858	-1.2903
C	2.8236	-1.6211	-0.4181
H	4.9857	-0.2213	1.7730
H	6.6027	-1.2393	0.2263
H	5.8078	-2.4941	-1.7445
H	3.3817	-2.7394	-2.1454
H	1.7652	-1.7462	-0.5945
C	-0.0749	0.0221	1.1952
C	-1.9569	0.2348	-1.9582
H	-2.2583	-0.6484	-2.5181
H	-0.9792	0.5834	-2.2997
H	-2.7131	1.0131	-2.0606
O	-0.5322	-0.6007	2.1241

C-IM17

Pt	-2.3608	-0.3906	0.0048
Cl	-1.6229	-1.7300	-1.7030
Cl	-3.0819	0.6478	1.9102
C	1.1952	3.2819	-1.1750
C	2.4488	3.8785	-1.1807
C	3.5083	3.3198	-0.4830
C	3.3561	2.1490	0.2503
C	2.1092	1.5606	0.2615
C	1.0297	2.1178	-0.4499
H	0.3719	3.7135	-1.7213
H	2.6013	4.7890	-1.7393

H	4.4741	3.8009	-0.5082
H	4.1886	1.7168	0.7817
C	-0.1095	1.2381	-0.2411
C	-1.3688	1.2004	-0.6686
H	-1.8464	1.9266	-1.3210
N	1.6928	0.4021	0.9177
C	2.5474	-0.4740	1.6844
C	3.5811	-1.1345	0.8060
H	1.8925	-1.2290	2.1325
H	3.0277	0.0970	2.4853
C	4.9202	-1.1478	1.1689
C	5.8596	-1.7545	0.3530
C	5.4677	-2.3452	-0.8357
C	4.1325	-2.3342	-1.2034
C	3.1926	-1.7338	-0.3859
H	5.2297	-0.6878	2.0972
H	6.8991	-1.7625	0.6456
H	6.2010	-2.8152	-1.4736
H	3.8206	-2.7969	-2.1275
H	2.1507	-1.7339	-0.6726
C	0.3935	0.1535	0.6500
C	-4.1378	-0.0600	-0.9239
H	-4.7674	-0.9029	-0.6217
H	-4.0207	-0.0610	-2.0060
H	-4.5891	0.8712	-0.5874
O	-0.2637	-0.7962	1.0695

C-IM17-TS

Pt	-2.2693	-0.3177	-0.0901
Cl	-3.1540	-1.4849	1.5853
Cl	-4.3050	0.5166	-0.5293
C	1.3467	3.4857	-0.2366
C	2.5937	4.0346	0.0250
C	3.6193	3.2633	0.5506
C	3.4373	1.9160	0.8379
C	2.1967	1.3720	0.5832
C	1.1486	2.1461	0.0433
H	0.5497	4.0861	-0.6457
H	2.7691	5.0786	-0.1844
H	4.5804	3.7155	0.7420
H	4.2428	1.3214	1.2381
C	0.0155	1.2543	-0.1083
C	-1.2450	1.3246	-0.5888
H	-1.6718	2.2439	-0.9714

N	1.7550	0.0606	0.7855
C	2.5517	-1.0194	1.3184
C	3.6966	-1.3667	0.3999
H	1.8774	-1.8759	1.4268
H	2.9263	-0.7386	2.3081
C	4.9843	-1.5186	0.8942
C	6.0280	-1.8351	0.0418
C	5.7937	-1.9945	-1.3129
C	4.5108	-1.8440	-1.8124
C	3.4671	-1.5341	-0.9599
H	5.1712	-1.3945	1.9516
H	7.0259	-1.9539	0.4368
H	6.6083	-2.2374	-1.9782
H	4.3225	-1.9714	-2.8679
H	2.4648	-1.4247	-1.3491
C	0.4759	-0.0488	0.3819
C	-1.7054	-0.1091	-2.1214
H	-2.1578	-1.0792	-2.3862
H	-0.6528	-0.1444	-2.3866
H	-2.2125	0.6588	-2.6964
O	-0.2260	-1.0777	0.4157

C-IM18

Pt	2.1094	-0.4763	0.1287
Cl	1.4239	-1.8046	-1.4915
Cl	4.0562	-0.1773	-0.8669
C	-1.1297	3.6166	-0.2554
C	-2.1911	3.9164	-1.0974
C	-2.9678	2.9104	-1.6516
C	-2.7146	1.5706	-1.3861
C	-1.6606	1.2764	-0.5466
C	-0.8673	2.2882	0.0224
H	-0.5270	4.4026	0.1722
H	-2.4144	4.9474	-1.3248
H	-3.7870	3.1707	-2.3044
H	-3.3247	0.7940	-1.8176
C	0.1561	1.6344	0.8240
C	1.1923	2.1779	1.4867
H	1.2950	3.2544	1.4912
N	-1.2049	0.0346	-0.1145
C	-1.7998	-1.2326	-0.4686
C	-3.2271	-1.3295	0.0040
H	-1.1861	-2.0059	0.0069
H	-1.7394	-1.3665	-1.5530

C	-4.2113	-1.8514	-0.8242
C	-5.5208	-1.9411	-0.3855
C	-5.8598	-1.5022	0.8828
C	-4.8828	-0.9812	1.7143
C	-3.5729	-0.8983	1.2785
H	-3.9493	-2.1934	-1.8154
H	-6.2782	-2.3510	-1.0370
H	-6.8822	-1.5678	1.2235
H	-5.1412	-0.6416	2.7064
H	-2.8103	-0.4994	1.9323
C	-0.1374	0.1725	0.7101
C	2.2298	1.3925	2.2154
H	1.7900	0.8636	3.0637
H	3.0356	2.0317	2.5668
H	2.6926	0.6090	1.5557
O	0.3694	-0.7709	1.3565

C-IM3-TS3

Pt	-2.6912	-0.1002	-0.2486
Cl	-2.3778	-1.5074	-1.9449
Cl	-3.6486	1.1356	1.3213
C	-0.1787	-1.6366	1.6799
C	0.8758	-2.1829	2.3908
C	2.1352	-1.5998	2.3550
C	2.3860	-0.4551	1.6094
C	1.3295	0.1022	0.9122
C	0.0542	-0.4908	0.9347
H	-1.1648	-2.0778	1.6873
H	0.7224	-3.0745	2.9790
H	2.9449	-2.0443	2.9130
H	3.3779	-0.0352	1.5969
C	-0.8180	0.3092	0.0906
C	-0.0534	1.3188	-0.4023
H	-0.3131	2.1320	-1.0539
N	1.2902	1.1973	0.0129
C	2.2180	0.4120	-1.6380
C	3.4501	-0.1427	-1.2228
H	2.2209	1.3459	-2.1783
H	1.4037	-0.2600	-1.8644
C	3.5333	-1.4961	-0.8364
C	4.7293	-2.0288	-0.4065
C	5.8624	-1.2304	-0.3254
C	5.7974	0.1102	-0.6902

C	4.6114	0.6520	-1.1313
H	2.6506	-2.1135	-0.9046
H	4.7844	-3.0699	-0.1268
H	6.7962	-1.6498	0.0168
H	6.6826	0.7260	-0.6295
H	4.5578	1.6911	-1.4227
C	1.9995	2.4369	0.1589
C	2.7866	2.6082	1.4181
H	2.9383	3.6723	1.5847
H	3.7640	2.1420	1.2987
H	2.2817	2.1615	2.2698
O	1.9217	3.2614	-0.7060

C-IM19

Pt	-2.1892	-0.0791	-0.1239
Cl	-2.2433	-2.2807	-0.3629
Cl	-3.1932	1.8842	0.0566
C	0.0897	0.1521	2.5010
C	1.0398	0.3072	3.4828
C	2.2969	0.8191	3.1632
C	2.6331	1.2068	1.8767
C	1.6839	1.0751	0.8720
C	0.4114	0.5230	1.1910
H	-0.8883	-0.2625	2.7021
H	0.8253	0.0233	4.5011
H	3.0384	0.9150	3.9421
H	3.6244	1.5784	1.6904
C	-0.3599	0.4218	0.0110
C	0.5326	0.8077	-1.1187
H	0.0924	1.5500	-1.7926
N	1.7235	1.3681	-0.4745
C	0.9316	-0.4421	-1.9637
C	1.9075	-1.2809	-1.1907
H	1.3838	-0.0889	-2.8900
H	0.0187	-0.9974	-2.1861
C	1.4683	-2.1350	-0.1866
C	2.3777	-2.8386	0.5820
C	3.7368	-2.6952	0.3584
C	4.1823	-1.8553	-0.6477
C	3.2726	-1.1509	-1.4167
H	0.4084	-2.2490	-0.0128
H	2.0239	-3.4995	1.3589
H	4.4467	-3.2406	0.9623
H	5.2411	-1.7483	-0.8345

H	3.6233	-0.4963	-2.2020
C	2.6136	2.0650	-1.2648
C	3.8107	2.6815	-0.5981
H	4.3148	3.3097	-1.3285
H	4.4976	1.9024	-0.2746
H	3.5118	3.2858	0.2542
O	2.3975	2.1733	-2.4503

C-TS4

Pt	-2.2338	0.3233	-0.2314
Cl	-3.4115	-1.5599	-0.6184
Cl	-1.6728	2.4135	0.4890
C	2.5481	-1.7330	-2.0663
C	3.7655	-2.2607	-1.6590
C	4.1256	-2.3335	-0.3203
C	3.2858	-1.8691	0.6899
C	2.0963	-1.3282	0.2759
C	1.7192	-1.2652	-1.0603
H	2.2651	-1.6933	-3.1052
H	4.4492	-2.6368	-2.4051
H	5.0759	-2.7694	-0.0532
H	3.5609	-1.9491	1.7292
C	0.4251	-0.6763	-1.0115
C	-0.6847	-0.1622	-1.3660
H	-0.9869	0.0560	-2.3930
N	0.9636	-0.7645	0.9822
C	1.1294	0.5886	1.5213
C	2.2152	1.3267	0.7841
H	1.3830	0.5244	2.5856
H	0.1826	1.1295	1.4023
C	1.9091	2.0671	-0.3504
C	2.9122	2.7086	-1.0548
C	4.2277	2.6201	-0.6320
C	4.5362	1.9012	0.5099
C	3.5342	1.2592	1.2150
H	0.8809	2.1512	-0.6664
H	2.6648	3.2845	-1.9336
H	5.0097	3.1200	-1.1834
H	5.5579	1.8428	0.8545
H	3.7803	0.7088	2.1119
C	0.1364	-1.7109	1.6251
C	-1.0220	-1.1428	2.3757
H	-1.5888	-1.9589	2.8154
H	-1.6757	-0.5971	1.6591

H	-0.7136	-0.4421	3.1465
O	0.3652	-2.8858	1.4937

C-IM20

Pt	-2.3049	0.3239	-0.2326
Cl	-3.5714	-1.4579	-0.7382
Cl	-1.6070	2.3202	0.6231
C	2.5380	-1.6442	-2.1256
C	3.7847	-2.1656	-1.7830
C	4.2124	-2.2907	-0.4687
C	3.4232	-1.8897	0.6158
C	2.2203	-1.3633	0.2530
C	1.7612	-1.2461	-1.0602
H	2.2177	-1.5682	-3.1510
H	4.4439	-2.4953	-2.5719
H	5.1842	-2.7154	-0.2717
H	3.7564	-2.0060	1.6338
C	0.4945	-0.6904	-0.6069
C	-0.6537	-0.2512	-1.1067
H	-0.7121	-0.2672	-2.1997
N	0.9962	-0.7854	0.8409
C	1.1962	0.5335	1.5005
C	2.2482	1.3220	0.7684
H	1.5093	0.3474	2.5309
H	0.2461	1.0782	1.4677
C	1.8967	2.0821	-0.3404
C	2.8683	2.7680	-1.0470
C	4.1939	2.7046	-0.6515
C	4.5460	1.9649	0.4644
C	3.5770	1.2758	1.1710
H	0.8601	2.1458	-0.6328
H	2.5880	3.3581	-1.9059
H	4.9509	3.2400	-1.2046
H	5.5757	1.9253	0.7863
H	3.8562	0.7065	2.0462
C	0.2236	-1.7853	1.6500
C	-1.0050	-1.2627	2.2632
H	-1.5180	-2.0690	2.7805
H	-1.6682	-0.8566	1.4570
H	-0.8129	-0.4401	2.9467
O	0.6517	-2.8976	1.6902

C-IM6-TS2

Pt	-1.9264	-0.4757	0.0412

Cl	-3.2106	1.0509	1.0027
Cl	-3.5877	-1.9578	0.1314
C	0.1824	4.3799	0.2184
C	1.4970	4.4216	-0.2515
C	-0.5065	3.1900	0.2870
C	2.1580	3.2840	-0.6693
C	1.4739	2.0747	-0.6098
C	0.1451	2.0247	-0.1187
H	-1.5226	3.1226	0.6423
H	-0.2935	5.2963	0.5299
H	2.0113	5.3700	-0.2947
H	3.1710	3.3487	-1.0368
C	-0.3231	0.6712	-0.1689
C	0.8620	-0.0756	-0.6961
H	0.5650	-0.0905	0.5198
N	1.8873	0.8180	-0.9927
C	3.2645	0.4374	-1.2105
C	3.7947	-0.4154	-0.0811
H	3.8545	1.3546	-1.2831
H	3.3606	-0.0931	-2.1621
C	3.4774	-0.1066	1.2362
C	3.9455	-0.8948	2.2723
C	4.7414	-1.9953	2.0026
C	5.0742	-2.2997	0.6938
C	4.6003	-1.5153	-0.3436
H	2.8716	0.7622	1.4570
H	3.6896	-0.6466	3.2910
H	5.1047	-2.6110	2.8107
H	5.7007	-3.1517	0.4778
H	4.8682	-1.7530	-1.3638
C	0.5544	-1.3968	-1.2208
C	1.4914	-2.1551	-2.1078
H	2.4169	-2.3746	-1.5777
H	1.7228	-1.5726	-2.9979
H	1.0154	-3.0857	-2.4057
O	-0.5645	-1.8570	-0.9434

C-IM9

Pt	-2.1857	-0.4603	0.1863
Cl	-3.5838	1.2618	0.3516
Cl	-3.8215	-1.6824	-0.6299
C	0.4891	4.2990	0.0639
C	1.7198	4.1401	-0.5875
C	-0.2641	3.2128	0.4356
C	2.2270	2.8968	-0.8908

C	1.4720	1.7833	-0.5273
C	0.2289	1.9386	0.1398
H	-1.2207	3.3175	0.9226
H	0.1345	5.2964	0.2725
H	2.2852	5.0191	-0.8580
H	3.1817	2.7982	-1.3846
C	-0.2729	0.6312	0.3637
C	0.6875	-0.2658	-0.1438
H	-0.9826	0.3851	1.2051
N	1.7315	0.4487	-0.6884
C	2.8734	-0.0799	-1.3869
C	4.0014	-0.4917	-0.4657
H	3.2358	0.6981	-2.0676
H	2.5629	-0.9290	-2.0010
C	4.1830	0.1240	0.7653
C	5.2302	-0.2554	1.5875
C	6.1079	-1.2469	1.1852
C	5.9361	-1.8596	-0.0449
C	4.8870	-1.4855	-0.8649
H	3.5061	0.9025	1.0861
H	5.3600	0.2283	2.5438
H	6.9240	-1.5412	1.8273
H	6.6178	-2.6326	-0.3656
H	4.7536	-1.9665	-1.8233
C	0.4281	-1.6783	-0.1022
C	1.5005	-2.7181	-0.2323
H	2.4342	-2.3894	0.2162
H	1.6724	-2.9414	-1.2849
H	1.1553	-3.6331	0.2439
O	-0.7471	-2.0457	0.0901