Supporting Information

Pd-catalyzed acylation and allylation of 2-alkynyl aniline with 1,2-diphenylcyclyrenone, gem-difluorinated cyclopropanes, respectively: a DFT study.

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1. Free energy profile of the entire acylation reaction

Because the free energy barrier of migratory insertion process is too high and the two-coordinated Pd center is not stable, path B and path C can be excluded. The correct route for this reaction is N-H deprotonation, C-N cyclization, oxidation addition of Pd(II) intermediate insert into cyclopropenone , cleavage of the four-membered palladacycle intermediate, protonation of ketene palladium intermediate and catalyst regeneration.

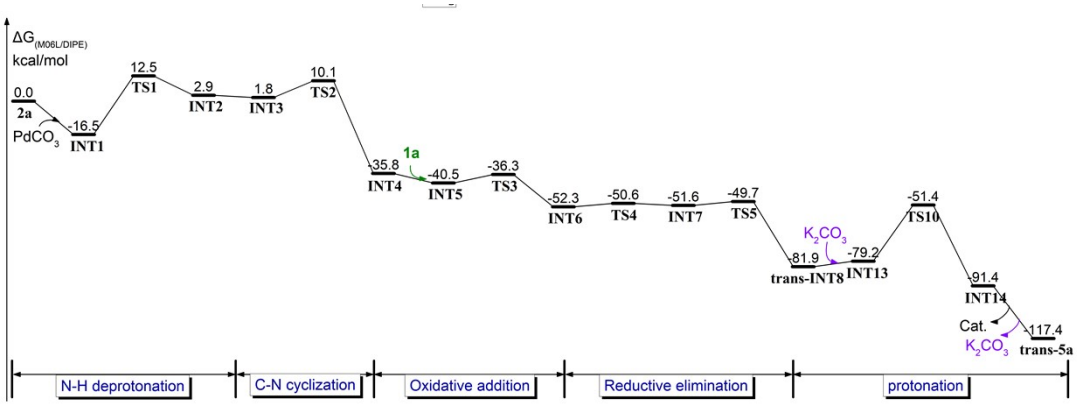


Figure S1. Calculated free energy profile for the entire acylation reaction. The energy values (kcal/mol) are calculated using M06-L method in diisopropyl ether.

Distortion-interaction analysis can be used to quantitatively study the reactivity and selectivity. This model has been applied to reactions of all types in both organic and inorganic chemistry, including substitutions and eliminations, cycloadditions, and several types of organometallic reactions.

The color coding scheme used for NCI gradient isosurfaces and RDG plots is as follows: red for steric repulsion ($\text{sign}(\lambda 2)\rho \gg 0$), dark blue for attractive interaction such as hydrogen-bonding ($\text{sign}(\lambda 2)\rho \ll 0$), and green for weak interaction such as van der Waals interaction ($\text{sign}(\lambda 2)\rho \approx 0$)

The ETS-NOCV method can be used to analyze the orbital interactions between fragments in depth. The NOCV theory can decompose the density change caused by orbital interaction into the contribution of each NOCV orbit, and the weight of the contribution is the eigenvalue of the NOCV orbit.

The Mayer bond orders reflects the number of electrons shared between two atoms in physical terms. There exists a positive correlation between the Mayer bond order and bond strength for analogous chemical bonds.

2. Free energy profile of other path in acylation reaction

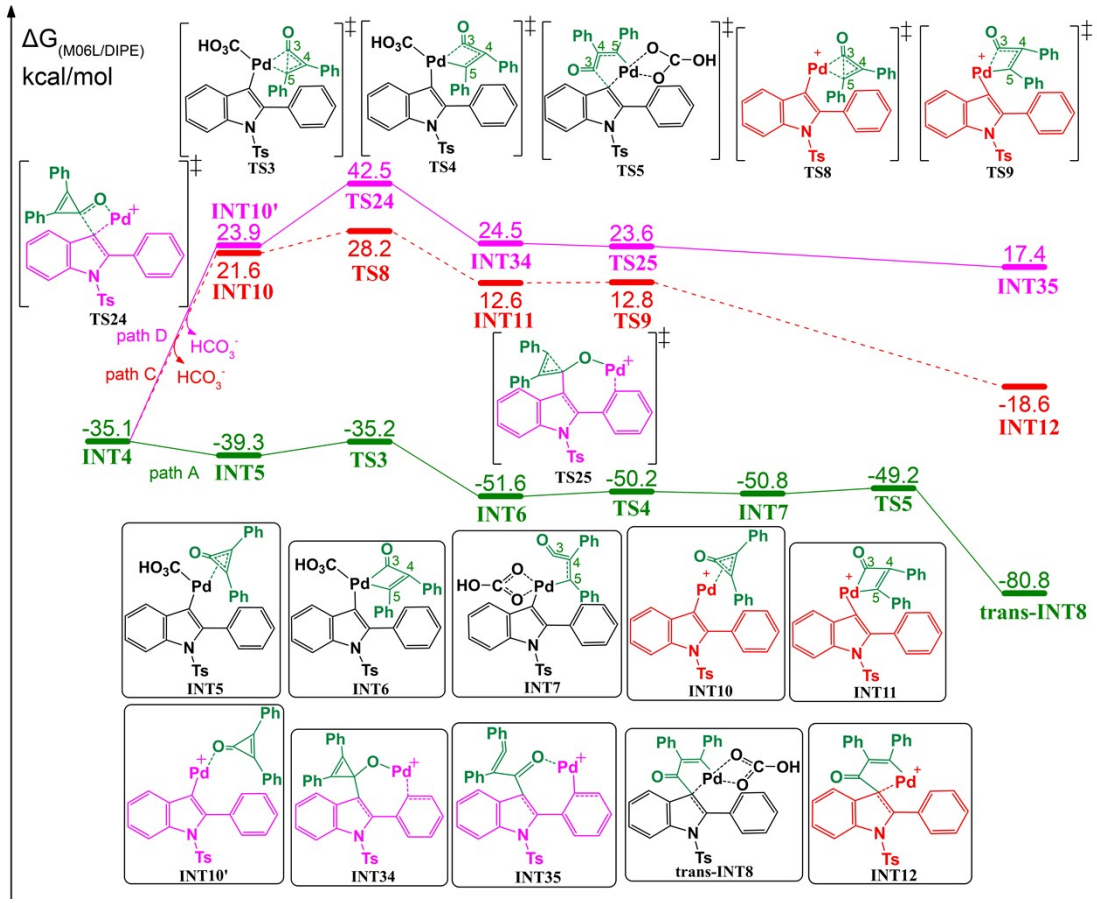


Figure S2. Calculated free energy profile for neutral Pd(II)-catalyzed (path A in green), cationic Pd(II)-catalyzed (path C in red) oxidative addition and cationic Pd(II)-catalyzed (path D in pink) migratory insertion to form vinylpalladium. The energy values (kcal/mol) are calculated using M06-L method in diisopropyl ether.

Another insertion type (path D in pink) cyclopropenone activation is considered and the calculated results are illustrated in Figure S2. As with path A and path C, it starts with the intermediate **INT4**. Ligand exchange undergoes between **2a** with HCO3-, and lone-pair-containing oxygen atom in **2a** coordinated with the Pd center to form the intermediate **INT10'** with absorbing free-energies by 59.6 kcal/mol. The Pd center attracted by C1(carbonyl) atom through the four-center transition state **TS24** to give the intermediate **INT34** with an energy barrier of 21.8 kcal/mol.The cleavage of C3-C5 bond in **INT34** leads to a free energy release of 6.7 kcal/mol in the formation of intermediate **INT35** through the transition state **TS25**.

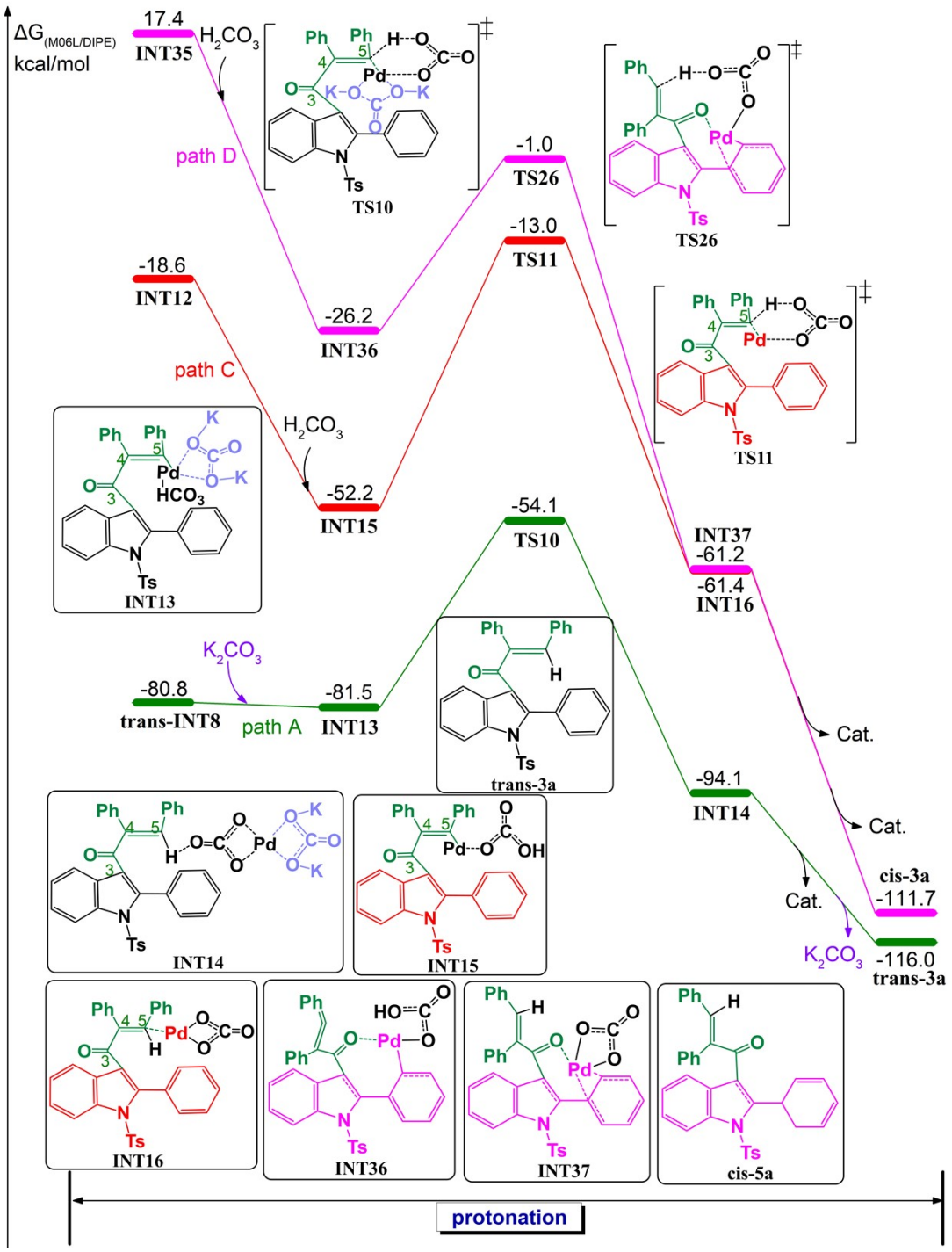


Figure S3. Calculated free energy profile for four-coordinated Pd(II)-catalyzed (path A in green) and two-coordinated Pd(II)-catalyzed (path C in red) (path D in pink) protonation to form final acylation product **trans-3a**. The energy values (kcal/mol) are calculated using M06-L method in diisopropyl ether.

The coordination of Pd center in **INT35** to HCO_3^- causes a free energy release of 12.4 kcal/mol in the generation of intermediate **INT36**. Subsequently, the vinyl-C5

atom abstracts the proton from HCO_3^- via **TS26** to generate the intermediate **INT37**, which has to overcome an energy barrier of 26.9 kcal/mol and is exothermal by 33.2 kcal/mol. With the removal of the Pd catalyst, the product **cis-INT3a** is formed.

According computational study can found the rate-determining step is **TS24** in path D. The computational results showed that the relative free energy of cationic Pd(II)-catalyzed migratory insertion transition state **TS24** is 15.2 kcal/mol and 78.7 kcal/mol higher than that of cationic Pd(II)-catalyzed oxidative addition transition state **TS8** and neutral Pd(II)-catalyzed oxidative addition transition state **TS3**, respectively. Therefore, path D can be excluded.

3. Pair and NOCV orbital information in TS3(Pd), TS8(Pd) and TS3(HCO_3^-)

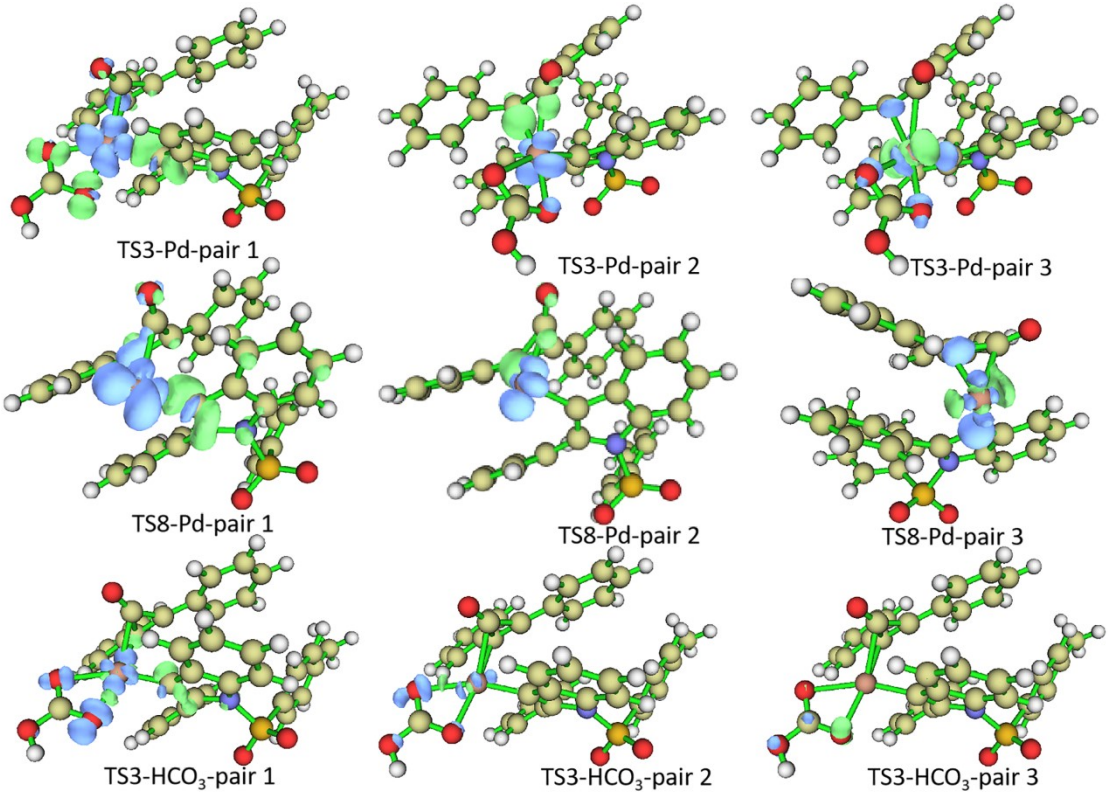


Figure S4. Isosurfaces of NOCV pair 1 and 2 density of **TS3(Pd)**, **TS8(Pd)**, **TS3(HCO_3^-)**.

Table S1. Pair and NOCV orbital information in TS3(Pd)

Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
1	-103.18	1	1.30670	-153.65	1016	-1.30670	-74.69
2	-23.53	2	0.54018	-106.43	1015	-0.54018	-62.87
3	-38.52	3	0.44046	-17.89	1014	-0.44046	69.57
4	-10.11	4	0.26084	-33.42	1013	-0.26084	5.36
5	-8.11	5	0.19300	1.61	1012	-0.19300	43.62
6	-11.03	6	0.17207	148.30	1011	-0.17207	212.39
7	-6.98	7	0.16326	73.24	1010	-0.16326	116.02
8	-5.10	8	0.13393	48.11	1009	-0.13393	86.19
9	-2.39	9	0.11262	-48.53	1008	-0.11262	-27.35
10	-1.16	10	0.07773	-17.48	1007	-0.07773	-2.60
11	-1.43	11	0.06613	92.68	1006	-0.06613	114.24
12	-1.03	12	0.05911	29.67	1005	-0.05911	47.16
13	-0.68	13	0.05289	2.17	1004	-0.05289	14.96
14	-0.61	14	0.04942	-5.19	1003	-0.04942	7.11
15	-0.40	15	0.04332	-17.62	1002	-0.04332	-8.31
16	-0.42	16	0.04128	11.10	1001	-0.04128	21.24
17	-0.36	17	0.03766	5.25	1000	-0.03766	14.74
18	-0.34	18	0.03391	2.47	999	-0.03391	12.43
19	-0.29	19	0.03262	28.49	998	-0.03262	37.47
20	-0.30	20	0.03039	-8.33	997	-0.03039	1.53
21	-0.23	21	0.02821	0.07	996	-0.02821	8.37
22	-0.26	22	0.02774	37.81	995	-0.02774	47.13
23	-0.15	23	0.02558	-36.93	994	-0.02558	-31.25
24	-0.17	24	0.02397	26.66	993	-0.02397	33.74
25	-0.14	25	0.02191	6.83	992	-0.02191	13.11
26	-0.12	26	0.02113	19.10	991	-0.02113	24.97
27	-0.11	27	0.02033	2.88	990	-0.02033	8.06
28	-0.14	28	0.01934	56.78	989	-0.01934	63.86
29	-0.10	29	0.01927	3.45	988	-0.01927	8.59
30	-0.09	30	0.01891	-41.81	987	-0.01891	-36.92
31	-0.10	31	0.01756	-7.67	986	-0.01756	-2.08
32	-0.09	32	0.01642	-19.08	985	-0.01642	-13.71
33	-0.09	33	0.01509	-63.92	984	-0.01509	-58.17
34	-0.10	34	0.01452	-35.65	983	-0.01452	-28.57
35	-0.08	35	0.01350	-15.36	982	-0.01350	-9.69
36	-0.08	36	0.01282	-89.68	981	-0.01282	-83.68
37	-0.09	37	0.01239	-6.30	980	-0.01239	0.62
38	-0.05	38	0.01229	8.13	979	-0.01229	12.19
39	-0.09	39	0.01184	-56.81	978	-0.01184	-48.93
40	-0.10	40	0.01141	38.78	977	-0.01141	47.27
41	-0.05	41	0.01110	45.33	976	-0.01110	50.22

42	**-0.05**	**42**	**0.01073**	**-25.92**	**975**	**-0.01073**	**-21.00**
43	**-0.04**	**43**	**0.01015**	**-46.61**	**974**	**-0.01015**	**-43.05**
44	**-0.03**	**44**	**0.00997**	**-14.97**	**973**	**-0.00997**	**-11.93**
45	**-0.03**	**45**	**0.00976**	**-47.74**	**972**	**-0.00976**	**-44.41**
46	**-0.04**	**46**	**0.00959**	**-25.22**	**971**	**-0.00959**	**-21.29**
47	**-0.05**	**47**	**0.00927**	**-34.83**	**970**	**-0.00927**	**-29.97**
48	**-0.05**	**48**	**0.00873**	**4.04**	**969**	**-0.00873**	**9.26**
49	**-0.02**	**49**	**0.00866**	**-35.66**	**968**	**-0.00866**	**-32.93**
50	**-0.03**	**50**	**0.00824**	**-85.76**	**967**	**-0.00824**	**-82.58**
51	**-0.02**	**51**	**0.00760**	**43.62**	**966**	**-0.00760**	**46.62**
52	**-0.02**	**52**	**0.00752**	**-16.89**	**965**	**-0.00752**	**-13.91**
53	**-0.03**	**53**	**0.00720**	**-64.62**	**964**	**-0.00720**	**-59.86**
54	**-0.03**	**54**	**0.00705**	**-16.36**	**963**	**-0.00705**	**-12.55**
55	**-0.02**	**55**	**0.00640**	**51.93**	**962**	**-0.00640**	**54.40**
56	**-0.02**	**56**	**0.00609**	**3.72**	**961**	**-0.00609**	**6.96**
57	**-0.01**	**57**	**0.00582**	**-18.23**	**960**	**-0.00582**	**-16.16**
58	**-0.01**	**58**	**0.00574**	**-34.37**	**959**	**-0.00574**	**-32.74**
59	**-0.02**	**59**	**0.00558**	**20.00**	**958**	**-0.00558**	**22.75**
60	**-0.02**	**60**	**0.00530**	**-7.99**	**957**	**-0.00530**	**-5.13**
61	**-0.01**	**61**	**0.00527**	**-38.00**	**956**	**-0.00527**	**-36.43**
62	**-0.01**	**62**	**0.00474**	**-28.46**	**955**	**-0.00474**	**-26.98**
63	**-0.01**	**63**	**0.00463**	**-27.25**	**954**	**-0.00463**	**-25.47**
64	**-0.01**	**64**	**0.00449**	**-23.81**	**953**	**-0.00449**	**-22.32**
65	**-0.01**	**65**	**0.00422**	**23.52**	**952**	**-0.00422**	**25.24**
66	**-0.01**	**66**	**0.00405**	**89.94**	**951**	**-0.00405**	**91.59**
67	**-0.00**	**67**	**0.00380**	**-6.87**	**950**	**-0.00380**	**-5.71**
68	**-0.00**	**68**	**0.00370**	**-7.56**	**949**	**-0.00370**	**-6.38**
69	**-0.01**	**69**	**0.00355**	**32.16**	**948**	**-0.00355**	**33.68**
70	**-0.00**	**70**	**0.00337**	**21.94**	**947**	**-0.00337**	**23.14**
71	**-0.00**	**71**	**0.00322**	**-41.29**	**946**	**-0.00322**	**-40.41**
72	**-0.00**	**72**	**0.00319**	**-8.06**	**945**	**-0.00319**	**-6.99**
73	**-0.00**	**73**	**0.00305**	**-40.66**	**944**	**-0.00305**	**-39.78**
74	**-0.00**	**74**	**0.00290**	**-28.91**	**943**	**-0.00290**	**-28.16**
75	**-0.00**	**75**	**0.00284**	**-34.18**	**942**	**-0.00284**	**-33.14**
76	**-0.00**	**76**	**0.00278**	**-7.80**	**941**	**-0.00278**	**-6.77**
77	**-0.00**	**77**	**0.00261**	**-28.88**	**940**	**-0.00261**	**-28.11**
78	**-0.00**	**78**	**0.00257**	**21.29**	**939**	**-0.00257**	**22.31**
79	**-0.00**	**79**	**0.00246**	**10.81**	**938**	**-0.00246**	**11.76**
80	**-0.00**	**80**	**0.00244**	**3.24**	**937**	**-0.00244**	**4.03**
81	**-0.00**	**81**	**0.00233**	**-17.57**	**936**	**-0.00233**	**-16.59**
82	**-0.00**	**82**	**0.00225**	**-14.28**	**935**	**-0.00225**	**-13.54**
83	**-0.00**	**83**	**0.00211**	**9.71**	**934**	**-0.00211**	**10.49**
84	**-0.00**	**84**	**0.00211**	**2.41**	**933**	**-0.00211**	**3.26**
85	**-0.00**	**85**	**0.00207**	**-73.09**	**932**	**-0.00207**	**-72.49**

86	-0.00	86	0.00199	-7.75	931	-0.00199	-6.86
87	-0.00	87	0.00193	-42.97	930	-0.00193	-42.14
88	-0.00	88	0.00190	-37.00	929	-0.00190	-36.25
89	-0.00	89	0.00188	-75.57	928	-0.00188	-75.02
90	-0.00	90	0.00179	-42.26	927	-0.00179	-41.61
91	-0.00	91	0.00168	-127.74	926	-0.00168	-126.84
92	-0.00	92	0.00165	-40.56	925	-0.00165	-39.96
93	-0.00	93	0.00164	-38.35	924	-0.00164	-37.89
94	-0.00	94	0.00155	-50.21	923	-0.00155	-49.56
95	-0.00	95	0.00147	-50.89	922	-0.00147	-50.38
96	-0.00	96	0.00133	-62.92	921	-0.00133	-62.47
97	-0.00	97	0.00133	-188.20	920	-0.00133	-187.52
98	-0.00	98	0.00127	-82.77	919	-0.00127	-82.25
99	-0.00	99	0.00124	-70.77	918	-0.00124	-70.14
100	-0.00	100	0.00117	-880.66	917	-0.00117	-878.93
101	-0.00	101	0.00111	-831.12	916	-0.00111	-829.37
102	-0.00	102	0.00108	-105.74	915	-0.00108	-105.24
103	-0.00	103	0.00106	-520.44	914	-0.00106	-519.31
104	-0.00	104	0.00103	-714.83	913	-0.00103	-713.48
105	-0.00	105	0.00100	-345.44	912	-0.00100	-344.74

Sum of NOCV eigenvalues: 0.00000

Sum of pair energies: -219.02 kcal/mol

NOCV orbitals with absolute eigenvalues smaller than 1.0E-03 are not shown

Note: All energies are given in kcal/mol

Table S2. Contribution of each basis function shell to NOCV pair 1/orbital 1 and 1016 in TS3(Pd)

Shell	Type	Atom	Orb. 1	Orb. 1016	Pair 1
3	P	1(C)	0.52 %	0.63 %	-0.14 %
4	S	1(C)	0.34 %	1.73 %	-1.82 %
5	P	1(C)	1.50 %	1.66 %	-0.21 %
6	S	1(C)	0.01 %	2.53 %	-3.29 %
7	P	1(C)	1.18 %	0.97 %	0.26 %
13	P	2(C)	0.58 %	0.19 %	0.51 %
14	S	2(C)	0.01 %	3.74 %	-4.88 %
15	P	2(C)	1.05 %	0.41 %	0.85 %
23	P	3(C)	0.42 %	0.58 %	-0.22 %
91	P	14(C)	0.50 %	0.21 %	0.39 %
139	P	21(C)	0.44 %	0.04 %	0.51 %
157	P	25(C)	0.34 %	0.76 %	-0.55 %
158	S	25(C)	0.00 %	0.42 %	-0.55 %

165	**P**	**26(O)**	**0.73 %**	**0.44 %**	**0.38 %**
167	**P**	**26(O)**	**0.86 %**	**0.52 %**	**0.44 %**
171	**P**	**27(C)**	**3.21 %**	**0.99 %**	**2.90 %**
172	**S**	**27(C)**	**3.34 %**	**3.22 %**	**0.16 %**
173	**P**	**27(C)**	**9.10 %**	**2.66 %**	**8.42 %**
174	**S**	**27(C)**	**15.18 %**	**6.26 %**	**11.66 %**
175	**P**	**27(C)**	**2.13 %**	**0.72 %**	**1.84 %**
181	**P**	**28(C)**	**0.57 %**	**0.05 %**	**0.69 %**
182	**S**	**28(C)**	**1.70 %**	**0.26 %**	**1.89 %**
183	**P**	**28(C)**	**1.96 %**	**0.47 %**	**1.95 %**
189	**P**	**29(C)**	**0.63 %**	**0.03 %**	**0.79 %**
190	**S**	**29(C)**	**0.74 %**	**0.24 %**	**0.65 %**
191	**P**	**29(C)**	**0.78 %**	**0.11 %**	**0.88 %**
197	**P**	**30(C)**	**0.53 %**	**0.04 %**	**0.64 %**
198	**S**	**30(C)**	**1.13 %**	**0.67 %**	**0.60 %**
199	**P**	**30(C)**	**0.57 %**	**0.21 %**	**0.46 %**
225	**P**	**34(C)**	**0.50 %**	**0.02 %**	**0.62 %**
227	**P**	**34(C)**	**0.68 %**	**0.02 %**	**0.86 %**
243	**P**	**38(C)**	**0.44 %**	**0.03 %**	**0.54 %**
245	**P**	**38(C)**	**1.06 %**	**0.06 %**	**1.30 %**
246	**S**	**38(C)**	**2.54 %**	**0.46 %**	**2.72 %**
247	**P**	**38(C)**	**2.07 %**	**0.23 %**	**2.39 %**
321	**P**	**50(N)**	**0.89 %**	**0.04 %**	**1.11 %**
323	**P**	**50(N)**	**1.60 %**	**0.14 %**	**1.91 %**
447	**P**	**69(O)**	**1.17 %**	**0.17 %**	**1.31 %**
448	**S**	**69(O)**	**0.00 %**	**0.56 %**	**-0.72 %**
449	**P**	**69(O)**	**2.82 %**	**0.40 %**	**3.17 %**
450	**S**	**69(O)**	**0.00 %**	**0.43 %**	**-0.56 %**
451	**P**	**69(O)**	**2.16 %**	**0.31 %**	**2.41 %**
455	**P**	**70(O)**	**1.86 %**	**0.36 %**	**1.96 %**
456	**S**	**70(O)**	**0.08 %**	**1.03 %**	**-1.24 %**
457	**P**	**70(O)**	**4.50 %**	**0.84 %**	**4.79 %**
458	**S**	**70(O)**	**0.08 %**	**0.85 %**	**-1.01 %**
459	**P**	**70(O)**	**3.82 %**	**0.70 %**	**4.08 %**
474	**S**	**73(Pd)**	**1.13 %**	**0.11 %**	**1.33 %**
476	**S**	**73(Pd)**	**1.70 %**	**0.22 %**	**1.94 %**
484	**D**	**73(Pd)**	**4.16 %**	**50.44 %**	**-60.48 %**
485	**D**	**73(Pd)**	**0.04 %**	**5.72 %**	**-7.43 %**
486	**D**	**73(Pd)**	**0.50 %**	**0.54 %**	**-0.06 %**

Table S3. Contribution of each atom to NOCV pair 1/orbitals 1 and 1016 in TS3(Pd)

Atom	Orb. 1	Orb. 1016	Pair 1
1(C):	3.59 %	7.68 %	-5.34 %
2(C):	2.10 %	4.47 %	-3.10 %
3(C):	0.67 %	0.88 %	-0.28 %
4(C):	0.39 %	0.13 %	0.35 %
5(C):	0.34 %	0.16 %	0.24 %
6(C):	0.05 %	0.05 %	0.01 %
7(H):	0.00 %	0.03 %	-0.04 %
8(C):	0.11 %	0.05 %	0.08 %
9(H):	0.00 %	0.00 %	0.00 %
10(C):	0.54 %	0.05 %	0.63 %
11(H):	0.00 %	0.01 %	-0.01 %
12(H):	0.00 %	0.01 %	-0.01 %
13(H):	0.00 %	0.00 %	0.00 %
14(C):	0.86 %	0.38 %	0.62 %
15(C):	0.74 %	0.41 %	0.44 %
16(C):	0.81 %	0.37 %	0.58 %
17(C):	0.09 %	0.08 %	0.01 %
18(H):	0.00 %	0.00 %	-0.00 %
19(C):	0.15 %	0.02 %	0.17 %
20(H):	0.04 %	0.03 %	0.01 %
21(C):	0.97 %	0.11 %	1.13 %
22(H):	0.00 %	0.01 %	-0.00 %
23(H):	0.00 %	0.00 %	0.00 %
24(H):	0.00 %	0.00 %	0.00 %
25(C):	0.67 %	2.04 %	-1.79 %
26(O):	1.97 %	1.20 %	1.01 %
27(C):	33.43 %	14.13 %	25.22 %
28(C):	4.77 %	0.83 %	5.15 %
29(C):	2.42 %	0.40 %	2.64 %
30(C):	2.69 %	1.00 %	2.20 %
31(C):	0.16 %	0.01 %	0.20 %
32(H):	0.07 %	0.01 %	0.08 %
33(C):	0.88 %	0.06 %	1.07 %
34(C):	1.48 %	0.08 %	1.83 %
35(H):	0.00 %	0.00 %	0.00 %
36(H):	0.12 %	0.02 %	0.14 %
37(H):	0.01 %	0.00 %	0.01 %
38(C):	6.53 %	0.86 %	7.40 %
39(C):	0.84 %	0.10 %	0.97 %
40(C):	0.39 %	0.03 %	0.46 %
41(C):	0.73 %	0.01 %	0.94 %

42(C):	0.16 %	0.01 %	0.20 %
43(H):	0.00 %	0.00 %	-0.00 %
44(C):	0.10 %	0.01 %	0.12 %
45(H):	0.05 %	0.01 %	0.04 %
46(C):	0.61 %	0.02 %	0.78 %
47(H):	0.01 %	0.00 %	0.01 %
48(H):	0.01 %	0.00 %	0.01 %
49(H):	0.00 %	0.00 %	0.00 %
50(N):	3.15 %	0.48 %	3.49 %
51(S):	0.14 %	0.20 %	-0.08 %
52(O):	0.10 %	0.01 %	0.12 %
53(O):	0.23 %	0.05 %	0.24 %
54(C):	0.25 %	0.05 %	0.26 %
55(C):	0.09 %	0.03 %	0.08 %
56(C):	0.10 %	0.00 %	0.13 %
57(C):	0.06 %	0.01 %	0.06 %
58(H):	0.00 %	0.00 %	0.00 %
59(C):	0.04 %	0.00 %	0.06 %
60(H):	0.00 %	0.00 %	0.00 %
61(C):	0.03 %	0.00 %	0.04 %
62(H):	0.00 %	0.00 %	0.01 %
63(H):	0.00 %	0.00 %	0.00 %
64(C):	0.00 %	0.00 %	0.00 %
65(H):	0.00 %	0.00 %	0.00 %
66(H):	0.00 %	0.00 %	0.00 %
67(H):	0.00 %	0.00 %	0.00 %
68(C):	0.14 %	0.14 %	0.00 %
69(O):	6.16 %	1.92 %	5.54 %
70(O):	10.35 %	3.87 %	8.47 %
71(O):	0.76 %	0.07 %	0.90 %
72(H):	0.07 %	0.02 %	0.06 %
73(Pd):	8.76 %	57.40 %	-63.56 %

Table S4. Contribution of each basis function shell to NOCV pair 2/orbitals 1 and 1015 in TS3(Pd)

Shell	Type	Atom	Orb. 2	Orb. 1015	Pair 2
3	P	1(C)	1.75 %	0.77 %	0.53 %
4	S	1(C)	2.01 %	1.40 %	0.33 %
5	P	1(C)	5.73 %	2.56 %	1.71 %
6	S	1(C)	22.23 %	12.29 %	5.37 %
7	P	1(C)	3.88 %	1.64 %	1.21 %
13	P	2(C)	0.51 %	0.38 %	0.07 %
14	S	2(C)	1.91 %	3.07 %	-0.63 %

15	P	2(C)	2.64 %	1.85 %	0.42 %
23	P	3(C)	0.68 %	0.90 %	-0.12 %
90	S	14(C)	0.95 %	0.45 %	0.27 %
91	P	14(C)	1.93 %	0.93 %	0.54 %
155	P	25(C)	1.27 %	1.14 %	0.07 %
156	S	25(C)	1.18 %	1.44 %	-0.14 %
157	P	25(C)	4.06 %	3.56 %	0.27 %
158	S	25(C)	15.78 %	12.30 %	1.88 %
159	P	25(C)	3.35 %	2.66 %	0.37 %
163	P	26(O)	0.59 %	0.34 %	0.13 %
165	P	26(O)	1.22 %	0.69 %	0.28 %
167	P	26(O)	2.50 %	1.59 %	0.49 %
182	S	28(C)	0.49 %	0.55 %	-0.03 %
455	P	70(O)	0.02 %	0.50 %	-0.26 %
457	P	70(O)	0.03 %	1.17 %	-0.61 %
459	P	70(O)	0.17 %	0.77 %	-0.33 %
480	P	73(Pd)	0.64 %	0.23 %	0.22 %
484	D	73(Pd)	15.17 %	30.23 %	-8.14 %
485	D	73(Pd)	0.17 %	7.98 %	-4.22 %
486	D	73(Pd)	1.16 %	1.81 %	-0.35 %

Table S5. Contribution of each atom to NOCV pair 2/orbitals 2 and 1015 in TS3(Pd)

Atom	Orb. 2	Orb. 1015	Pair 2
1(C):	36.05 %	18.89 %	9.27 %
2(C):	5.29 %	5.51 %	-0.12 %
3(C):	0.72 %	1.07 %	-0.19 %
4(C):	0.30 %	0.24 %	0.03 %
5(C):	0.49 %	0.50 %	-0.00 %
6(C):	0.03 %	0.02 %	0.00 %
7(H):	0.02 %	0.03 %	-0.01 %
8(C):	0.05 %	0.06 %	-0.01 %
9(H):	0.00 %	0.00 %	0.00 %
10(C):	0.14 %	0.17 %	-0.02 %
11(H):	0.00 %	0.00 %	-0.00 %
12(H):	0.01 %	0.01 %	-0.00 %
13(H):	0.00 %	0.00 %	-0.00 %
14(C):	3.39 %	1.45 %	1.05 %
15(C):	0.63 %	0.27 %	0.19 %
16(C):	0.45 %	0.24 %	0.11 %
17(C):	0.11 %	0.05 %	0.03 %
18(H):	0.01 %	0.00 %	0.00 %
19(C):	0.21 %	0.08 %	0.07 %

20(H):	**0.01 %**	**0.01 %**	**0.00 %**
21(C):	**0.10 %**	**0.12 %**	**-0.01 %**
22(H):	**0.04 %**	**0.01 %**	**0.02 %**
23(H):	**0.00 %**	**0.00 %**	**0.00 %**
24(H):	**0.00 %**	**0.00 %**	**0.00 %**
25(C):	**25.91 %**	**21.31 %**	**2.48 %**
26(O):	**4.37 %**	**2.64 %**	**0.94 %**
27(C):	**0.28 %**	**0.42 %**	**-0.08 %**
28(C):	**0.60 %**	**0.70 %**	**-0.05 %**
29(C):	**0.36 %**	**0.40 %**	**-0.02 %**
30(C):	**0.06 %**	**0.05 %**	**0.00 %**
31(C):	**0.05 %**	**0.06 %**	**-0.00 %**
32(H):	**0.39 %**	**0.36 %**	**0.02 %**
33(C):	**0.00 %**	**0.01 %**	**-0.00 %**
34(C):	**0.04 %**	**0.04 %**	**-0.00 %**
35(H):	**0.00 %**	**0.01 %**	**-0.00 %**
36(H):	**0.00 %**	**0.00 %**	**0.00 %**
37(H):	**0.00 %**	**0.00 %**	**-0.00 %**
38(C):	**0.03 %**	**0.16 %**	**-0.07 %**
39(C):	**0.16 %**	**0.15 %**	**0.01 %**
40(C):	**0.07 %**	**0.01 %**	**0.03 %**
41(C):	**0.22 %**	**0.21 %**	**0.00 %**
42(C):	**0.04 %**	**0.01 %**	**0.01 %**
43(H):	**0.00 %**	**0.00 %**	**0.00 %**
44(C):	**0.18 %**	**0.03 %**	**0.08 %**
45(H):	**0.13 %**	**0.28 %**	**-0.08 %**
46(C):	**0.03 %**	**0.01 %**	**0.01 %**
47(H):	**0.00 %**	**0.00 %**	**-0.00 %**
48(H):	**0.00 %**	**0.00 %**	**0.00 %**
49(H):	**0.00 %**	**0.00 %**	**-0.00 %**
50(N):	**0.04 %**	**0.05 %**	**-0.00 %**
51(S):	**0.01 %**	**0.02 %**	**-0.00 %**
52(O):	**0.00 %**	**0.00 %**	**0.00 %**
53(O):	**0.00 %**	**0.00 %**	**-0.00 %**
54(C):	**0.00 %**	**0.01 %**	**-0.00 %**
55(C):	**0.00 %**	**0.00 %**	**-0.00 %**
56(C):	**0.00 %**	**0.01 %**	**-0.00 %**
57(C):	**0.00 %**	**0.00 %**	**0.00 %**
58(H):	**0.00 %**	**0.00 %**	**0.00 %**
59(C):	**0.00 %**	**0.00 %**	**0.00 %**
60(H):	**0.00 %**	**0.00 %**	**0.00 %**
61(C):	**0.00 %**	**0.00 %**	**0.00 %**
62(H):	**0.00 %**	**0.00 %**	**-0.00 %**
63(H):	**0.00 %**	**0.00 %**	**0.00 %**

64(C):	0.00 %	0.00 %	0.00 %
65(H):	0.00 %	0.00 %	0.00 %
66(H):	0.00 %	0.00 %	-0.00 %
67(H):	0.00 %	0.00 %	-0.00 %
68(C):	0.16 %	0.24 %	-0.04 %
69(O):	0.09 %	0.08 %	0.01 %
70(O):	0.30 %	2.87 %	-1.39 %
71(O):	0.15 %	0.16 %	-0.00 %
72(H):	0.00 %	0.01 %	-0.00 %
73(Pd):	18.25 %	40.95 %	-12.26 %

Table S6. Contribution of each basis function shell to NOCV pair 3/orbitals 3 and 1014 in TS3(Pd):

Shell	Type	Atom	Orb. 3	Orb. 1014	Pair 3
3	P	1(C)	0.04 %	0.52 %	-0.21 %
4	S	1(C)	0.06 %	0.95 %	-0.39 %
5	P	1(C)	0.19 %	1.02 %	-0.37 %
6	S	1(C)	1.51 %	0.01 %	0.66 %
7	P	1(C)	0.12 %	2.20 %	-0.92 %
13	P	2(C)	0.04 %	0.53 %	-0.22 %
14	S	2(C)	0.04 %	0.71 %	-0.29 %
15	P	2(C)	2.98 %	2.13 %	0.37 %
22	S	3(C)	0.94 %	1.29 %	-0.15 %
23	P	3(C)	0.71 %	1.99 %	-0.56 %
91	P	14(C)	0.69 %	0.70 %	-0.01 %
158	S	25(C)	0.52 %	0.01 %	0.22 %
171	P	27(C)	0.09 %	0.78 %	-0.30 %
172	S	27(C)	0.71 %	2.80 %	-0.92 %
173	P	27(C)	0.09 %	1.44 %	-0.59 %
174	S	27(C)	1.62 %	0.02 %	0.70 %
175	P	27(C)	3.58 %	7.41 %	-1.68 %
182	S	28(C)	0.68 %	0.29 %	0.17 %
183	P	28(C)	2.37 %	1.95 %	0.19 %
190	S	29(C)	1.87 %	1.26 %	0.26 %
191	P	29(C)	0.47 %	0.52 %	-0.02 %
206	S	31(C)	0.64 %	0.65 %	-0.00 %
246	S	38(C)	0.94 %	0.43 %	0.22 %
247	P	38(C)	1.31 %	1.28 %	0.01 %
254	S	39(C)	0.75 %	0.55 %	0.09 %
443	P	68(C)	0.35 %	0.94 %	-0.26 %
448	S	69(O)	0.26 %	0.62 %	-0.16 %
449	P	69(O)	0.02 %	1.03 %	-0.45 %
451	P	69(O)	0.02 %	0.88 %	-0.38 %

455	P	70(O)	0.02 %	0.67 %	-0.29 %
456	S	70(O)	0.34 %	0.67 %	-0.14 %
457	P	70(O)	0.06 %	1.44 %	-0.61 %
459	P	70(O)	0.03 %	1.53 %	-0.66 %
466	S	71(O)	0.21 %	0.93 %	-0.32 %
473	S	73(Pd)	1.40 %	0.05 %	0.60 %
474	S	73(Pd)	9.80 %	2.09 %	3.39 %
475	S	73(Pd)	3.07 %	0.69 %	1.05 %
476	S	73(Pd)	51.54 %	36.06 %	6.82 %
477	S	73(Pd)	0.78 %	0.52 %	0.11 %
484	D	73(Pd)	2.79 %	7.77 %	-2.19 %
485	D	73(Pd)	0.17 %	2.42 %	-0.99 %

Table S7. Contribution of each atom to NOCV pair 3/orbitals 3 and 1014

Atom	Orb. 3	Orb. 1014	Pair 3
1(C):	1.96 %	4.85 %	-1.27 %
2(C):	3.12 %	3.65 %	-0.24 %
3(C):	1.67 %	3.49 %	-0.80 %
4(C):	0.03 %	0.22 %	-0.08 %
5(C):	0.09 %	0.29 %	-0.09 %
6(C):	0.03 %	0.04 %	-0.00 %
7(H):	0.05 %	0.10 %	-0.02 %
8(C):	0.01 %	0.03 %	-0.01 %
9(H):	0.01 %	0.01 %	0.00 %
10(C):	0.00 %	0.16 %	-0.07 %
11(H):	0.00 %	0.00 %	-0.00 %
12(H):	0.00 %	0.00 %	-0.00 %
13(H):	0.00 %	0.00 %	-0.00 %
14(C):	1.15 %	0.89 %	0.11 %
15(C):	0.14 %	0.18 %	-0.02 %
16(C):	0.39 %	0.25 %	0.06 %
17(C):	0.02 %	0.06 %	-0.02 %
18(H):	0.04 %	0.05 %	-0.01 %
19(C):	0.23 %	0.07 %	0.07 %
20(H):	0.11 %	0.19 %	-0.03 %
21(C):	0.10 %	0.06 %	0.02 %
22(H):	0.00 %	0.00 %	0.00 %
23(H):	0.00 %	0.01 %	-0.00 %
24(H):	0.00 %	0.00 %	-0.00 %
25(C):	0.74 %	0.88 %	-0.07 %
26(O):	0.35 %	0.33 %	0.01 %
27(C):	6.13 %	12.71 %	-2.89 %

28(C):	**3.06 %**	**2.31 %**	**0.33 %**
29(C):	**2.36 %**	**1.81 %**	**0.24 %**
30(C):	**0.32 %**	**0.56 %**	**-0.10 %**
31(C):	**0.80 %**	**0.78 %**	**0.01 %**
32(H):	**0.36 %**	**0.37 %**	**-0.01 %**
33(C):	**0.28 %**	**0.43 %**	**-0.07 %**
34(C):	**0.17 %**	**0.16 %**	**0.01 %**
35(H):	**0.00 %**	**0.00 %**	**-0.00 %**
36(H):	**0.00 %**	**0.01 %**	**-0.00 %**
37(H):	**0.00 %**	**0.00 %**	**-0.00 %**
38(C):	**2.26 %**	**1.90 %**	**0.16 %**
39(C):	**0.80 %**	**0.68 %**	**0.05 %**
40(C):	**0.05 %**	**0.15 %**	**-0.05 %**
41(C):	**0.15 %**	**0.12 %**	**0.01 %**
42(C):	**0.05 %**	**0.09 %**	**-0.02 %**
43(H):	**0.01 %**	**0.01 %**	**-0.00 %**
44(C):	**0.14 %**	**0.18 %**	**-0.02 %**
45(H):	**0.01 %**	**0.03 %**	**-0.01 %**
46(C):	**0.01 %**	**0.07 %**	**-0.03 %**
47(H):	**0.00 %**	**0.00 %**	**-0.00 %**
48(H):	**0.00 %**	**0.00 %**	**0.00 %**
49(H):	**0.00 %**	**0.00 %**	**-0.00 %**
50(N):	**0.11 %**	**0.22 %**	**-0.05 %**
51(S):	**0.03 %**	**0.23 %**	**-0.09 %**
52(O):	**0.00 %**	**0.01 %**	**-0.00 %**
53(O):	**0.00 %**	**0.05 %**	**-0.02 %**
54(C):	**0.02 %**	**0.03 %**	**-0.01 %**
55(C):	**0.00 %**	**0.00 %**	**-0.00 %**
56(C):	**0.02 %**	**0.01 %**	**0.00 %**
57(C):	**0.00 %**	**0.00 %**	**0.00 %**
58(H):	**0.00 %**	**0.00 %**	**0.00 %**
59(C):	**0.01 %**	**0.00 %**	**0.00 %**
60(H):	**0.01 %**	**0.01 %**	**0.00 %**
61(C):	**0.00 %**	**0.00 %**	**0.00 %**
62(H):	**0.00 %**	**0.00 %**	**0.00 %**
63(H):	**0.00 %**	**0.00 %**	**0.00 %**
64(C):	**0.00 %**	**0.00 %**	**0.00 %**
65(H):	**0.00 %**	**0.00 %**	**0.00 %**
66(H):	**0.00 %**	**0.00 %**	**-0.00 %**
67(H):	**0.00 %**	**0.00 %**	**0.00 %**
68(C):	**0.46 %**	**1.13 %**	**-0.30 %**
69(O):	**0.47 %**	**3.34 %**	**-1.26 %**
70(O):	**0.58 %**	**4.53 %**	**-1.74 %**
71(O):	**0.23 %**	**1.54 %**	**-0.58 %**

72(H):	0.03 %	0.11 %	-0.03 %
73(Pd):	70.83 %	50.60 %	8.91 %

Table S8. Pair and NOCV orbital information in TS8(Pd)

Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
1	-70.11	1	1.29731	-165.33	938	-1.29731	-111.29
2	-24.46	2	0.54395	-143.82	937	-0.54395	-98.86
3	-37.29	3	0.45497	-46.93	936	-0.45497	35.04
4	-10.19	4	0.24344	-61.25	935	-0.24344	-19.41
5	-7.65	5	0.18695	-32.23	934	-0.18695	8.69
6	-7.22	6	0.17176	13.35	933	-0.17176	55.42
7	-6.41	7	0.15728	37.81	932	-0.15728	78.55
8	-3.00	8	0.10625	20.49	931	-0.10625	48.74
9	-1.82	9	0.08533	-14.47	930	-0.08533	6.80
10	-1.09	10	0.06942	-51.15	929	-0.06942	-35.38
11	-0.43	11	0.04569	-55.20	928	-0.04569	-45.88
12	-0.34	12	0.03958	-51.67	927	-0.03958	-43.19
13	-0.34	13	0.03868	-69.93	926	-0.03868	-61.12
14	-0.52	14	0.03512	5.39	925	-0.03512	20.13
15	-0.23	15	0.03325	-64.58	924	-0.03325	-57.76
16	-0.20	16	0.02878	-46.33	923	-0.02878	-39.52
17	-0.20	17	0.02793	-28.07	922	-0.02793	-20.74
18	-0.17	18	0.02576	-47.56	921	-0.02576	-41.00
19	-0.18	19	0.02463	-33.51	920	-0.02463	-26.09
20	-0.16	20	0.02438	-46.58	919	-0.02438	-40.02
21	-0.11	21	0.02278	-46.63	918	-0.02278	-41.74
22	-0.13	22	0.02215	-30.09	917	-0.02215	-24.43
23	-0.10	23	0.02105	-59.36	916	-0.02105	-54.42
24	-0.11	24	0.01896	-54.69	915	-0.01896	-49.03
25	-0.06	25	0.01761	-66.07	914	-0.01761	-62.71
26	-0.09	26	0.01734	-29.12	913	-0.01734	-24.08
27	-0.06	27	0.01560	-26.66	912	-0.01560	-22.91
28	-0.05	28	0.01504	-93.69	911	-0.01504	-90.66
29	-0.07	29	0.01498	-79.19	910	-0.01498	-74.34
30	-0.05	30	0.01363	-72.21	909	-0.01363	-68.67
31	-0.05	31	0.01310	-38.18	908	-0.01310	-34.12
32	-0.06	32	0.01251	-66.95	907	-0.01251	-62.52
33	-0.05	33	0.01221	-50.42	906	-0.01221	-46.68
34	-0.07	34	0.01148	-56.17	905	-0.01148	-50.18
35	-0.04	35	0.01104	-48.96	904	-0.01104	-45.35
36	-0.06	36	0.01092	-74.23	903	-0.01092	-68.91

37	**-0.06**	**37**	**0.01066**	**-101.05**	**902**	**-0.01066**	**-95.50**
38	**-0.05**	**38**	**0.01045**	**-99.18**	**901**	**-0.01045**	**-94.59**
39	**-0.04**	**39**	**0.01009**	**-25.02**	**900**	**-0.01009**	**-20.99**
40	**-0.05**	**40**	**0.00994**	**-78.43**	**899**	**-0.00994**	**-73.73**
41	**-0.03**	**41**	**0.00936**	**-12.87**	**898**	**-0.00936**	**-9.61**
42	**-0.06**	**42**	**0.00911**	**-148.39**	**897**	**-0.00911**	**-142.06**
43	**-0.02**	**43**	**0.00816**	**-75.55**	**896**	**-0.00816**	**-72.89**
44	**-0.03**	**44**	**0.00788**	**-32.42**	**895**	**-0.00788**	**-28.12**
45	**-0.02**	**45**	**0.00757**	**-69.86**	**894**	**-0.00757**	**-67.72**
46	**-0.02**	**46**	**0.00729**	**-81.44**	**893**	**-0.00729**	**-79.27**
47	**-0.03**	**47**	**0.00719**	**16.74**	**892**	**-0.00719**	**20.99**
48	**-0.01**	**48**	**0.00690**	**-40.30**	**891**	**-0.00690**	**-38.13**
49	**-0.03**	**49**	**0.00681**	**-141.94**	**890**	**-0.00681**	**-137.37**
50	**-0.01**	**50**	**0.00648**	**-50.85**	**889**	**-0.00648**	**-49.10**
51	**-0.02**	**51**	**0.00620**	**-4.72**	**888**	**-0.00620**	**-1.91**
52	**-0.01**	**52**	**0.00602**	**-83.93**	**887**	**-0.00602**	**-81.44**
53	**-0.02**	**53**	**0.00562**	**104.02**	**886**	**-0.00562**	**106.70**
54	**-0.01**	**54**	**0.00537**	**-66.89**	**885**	**-0.00537**	**-65.28**
55	**-0.01**	**55**	**0.00519**	**-65.06**	**884**	**-0.00519**	**-63.40**
56	**-0.01**	**56**	**0.00504**	**-98.18**	**883**	**-0.00504**	**-96.01**
57	**-0.01**	**57**	**0.00498**	**-28.67**	**882**	**-0.00498**	**-27.02**
58	**-0.01**	**58**	**0.00477**	**9.87**	**881**	**-0.00477**	**11.60**
59	**-0.01**	**59**	**0.00453**	**-46.06**	**880**	**-0.00453**	**-44.95**
60	**-0.01**	**60**	**0.00425**	**-41.65**	**879**	**-0.00425**	**-40.28**
61	**-0.01**	**61**	**0.00409**	**-37.86**	**878**	**-0.00409**	**-36.48**
62	**-0.00**	**62**	**0.00390**	**-54.97**	**877**	**-0.00390**	**-53.82**
63	**-0.00**	**63**	**0.00366**	**-22.88**	**876**	**-0.00366**	**-21.86**
64	**-0.00**	**64**	**0.00358**	**-51.57**	**875**	**-0.00358**	**-50.72**
65	**-0.00**	**65**	**0.00348**	**-43.12**	**874**	**-0.00348**	**-42.08**
66	**-0.00**	**66**	**0.00341**	**-36.49**	**873**	**-0.00341**	**-35.29**
67	**-0.00**	**67**	**0.00336**	**-75.65**	**872**	**-0.00336**	**-74.88**
68	**-0.00**	**68**	**0.00333**	**-38.89**	**871**	**-0.00333**	**-37.81**
69	**-0.00**	**69**	**0.00328**	**-69.63**	**870**	**-0.00328**	**-68.77**
70	**-0.00**	**70**	**0.00316**	**-56.52**	**869**	**-0.00316**	**-55.67**
71	**-0.00**	**71**	**0.00312**	**-71.54**	**868**	**-0.00312**	**-70.72**
72	**-0.00**	**72**	**0.00306**	**-35.49**	**867**	**-0.00306**	**-34.42**
73	**-0.00**	**73**	**0.00298**	**-34.43**	**866**	**-0.00298**	**-33.39**
74	**-0.00**	**74**	**0.00292**	**-54.90**	**865**	**-0.00292**	**-53.85**
75	**-0.00**	**75**	**0.00282**	**-48.51**	**864**	**-0.00282**	**-47.47**
76	**-0.00**	**76**	**0.00269**	**-15.96**	**863**	**-0.00269**	**-14.91**
77	**-0.00**	**77**	**0.00256**	**-40.56**	**862**	**-0.00256**	**-39.62**
78	**-0.00**	**78**	**0.00254**	**-68.03**	**861**	**-0.00254**	**-67.24**
79	**-0.00**	**79**	**0.00245**	**-61.18**	**860**	**-0.00245**	**-60.27**
80	**-0.00**	**80**	**0.00243**	**-55.42**	**859**	**-0.00243**	**-54.68**

81	-0.00	81	0.00235	-63.63	858	-0.00235	-62.98
82	-0.00	82	0.00228	-59.15	857	-0.00228	-58.50
83	-0.00	83	0.00220	-92.21	856	-0.00220	-91.45
84	-0.00	84	0.00214	-69.33	855	-0.00214	-68.55
85	-0.00	85	0.00210	-67.32	854	-0.00210	-66.62
86	-0.00	86	0.00204	-52.21	853	-0.00204	-51.58
87	-0.00	87	0.00196	-55.02	852	-0.00196	-54.30
88	-0.00	88	0.00192	-31.48	851	-0.00192	-30.84
89	-0.00	89	0.00185	-61.14	850	-0.00185	-60.43
90	-0.00	90	0.00172	-58.97	849	-0.00172	-58.31
91	-0.00	91	0.00163	-78.03	848	-0.00163	-77.47
92	-0.00	92	0.00152	-61.26	847	-0.00152	-60.71
93	-0.00	93	0.00147	-52.43	846	-0.00147	-51.93
94	-0.00	94	0.00145	-139.66	845	-0.00145	-139.00
95	-0.00	95	0.00136	-66.25	844	-0.00136	-65.93
96	-0.00	96	0.00121	-185.82	843	-0.00121	-185.03
97	-0.00	97	0.00113	-1684.26	842	-0.00113	-1681.36
98	-0.00	98	0.00110	-672.18	841	-0.00110	-670.87
99	-0.00	99	0.00107	-202.47	840	-0.00107	-201.81
100	-0.00	100	0.00103	-771.11	839	-0.00103	-769.67

Sum of NOCV eigenvalues: 0.00000
Sum of pair energies: -173.79 kcal/mol
NOCV orbitals with absolute eigenvalues smaller than 1.0E-03 are not shown
Note: All energies are given in kcal/mol

Table S9. Contribution of each basis function shell to NOCV pair 1/orbitals 1 and 938 in TS8(Pd)

Shell	Type	Atom	Orb. 1	Orb. 938	Pair 1
3	P	1(C)	0.74 %	0.83 %	-0.12 %
4	S	1(C)	0.40 %	2.04 %	-2.12 %
5	P	1(C)	2.20 %	2.24 %	-0.06 %
6	S	1(C)	0.16 %	2.59 %	-3.15 %
7	P	1(C)	1.98 %	1.23 %	0.97 %
13	P	2(C)	0.62 %	0.21 %	0.53 %
14	S	2(C)	0.01 %	4.01 %	-5.19 %
15	P	2(C)	1.77 %	0.24 %	1.99 %
23	P	3(C)	0.92 %	0.83 %	0.12 %
91	P	14(C)	1.30 %	0.25 %	1.37 %
99	P	15(C)	0.59 %	0.11 %	0.63 %
105	P	16(C)	0.50 %	0.04 %	0.60 %
107	P	16(C)	0.85 %	0.14 %	0.93 %

137	**P**	**21(C)**	**0.74 %**	**0.03 %**	**0.92 %**
139	**P**	**21(C)**	**0.77 %**	**0.03 %**	**0.96 %**
157	**P**	**25(C)**	**0.47 %**	**0.74 %**	**-0.35 %**
165	**P**	**26(O)**	**0.96 %**	**0.52 %**	**0.57 %**
167	**P**	**26(O)**	**1.16 %**	**0.62 %**	**0.69 %**
171	**P**	**27(C)**	**3.47 %**	**1.55 %**	**2.49 %**
172	**S**	**27(C)**	**2.83 %**	**3.86 %**	**-1.34 %**
173	**P**	**27(C)**	**9.93 %**	**4.03 %**	**7.66 %**
174	**S**	**27(C)**	**13.06 %**	**9.17 %**	**5.05 %**
175	**P**	**27(C)**	**4.31 %**	**1.56 %**	**3.58 %**
181	**P**	**28(C)**	**0.51 %**	**0.13 %**	**0.50 %**
182	**S**	**28(C)**	**2.50 %**	**0.59 %**	**2.48 %**
183	**P**	**28(C)**	**2.06 %**	**0.63 %**	**1.86 %**
187	**P**	**29(C)**	**0.49 %**	**0.01 %**	**0.63 %**
189	**P**	**29(C)**	**1.24 %**	**0.01 %**	**1.60 %**
190	**S**	**29(C)**	**0.50 %**	**0.32 %**	**0.24 %**
191	**P**	**29(C)**	**1.24 %**	**0.06 %**	**1.54 %**
197	**P**	**30(C)**	**0.65 %**	**0.09 %**	**0.73 %**
198	**S**	**30(C)**	**0.87 %**	**0.99 %**	**-0.15 %**
199	**P**	**30(C)**	**0.74 %**	**0.33 %**	**0.53 %**
217	**P**	**33(C)**	**0.59 %**	**0.01 %**	**0.74 %**
219	**P**	**33(C)**	**0.56 %**	**0.02 %**	**0.70 %**
223	**P**	**34(C)**	**0.42 %**	**0.00 %**	**0.54 %**
225	**P**	**34(C)**	**1.02 %**	**0.00 %**	**1.32 %**
227	**P**	**34(C)**	**1.24 %**	**0.00 %**	**1.61 %**
243	**P**	**38(C)**	**0.68 %**	**0.03 %**	**0.85 %**
245	**P**	**38(C)**	**1.77 %**	**0.07 %**	**2.21 %**
246	**S**	**38(C)**	**2.22 %**	**0.65 %**	**2.03 %**
247	**P**	**38(C)**	**2.58 %**	**0.20 %**	**3.10 %**
253	**P**	**39(C)**	**0.50 %**	**0.01 %**	**0.65 %**
255	**P**	**39(C)**	**0.41 %**	**0.01 %**	**0.52 %**
269	**P**	**41(C)**	**0.49 %**	**0.01 %**	**0.62 %**
271	**P**	**41(C)**	**0.56 %**	**0.05 %**	**0.67 %**
301	**P**	**46(C)**	**0.52 %**	**0.00 %**	**0.67 %**
303	**P**	**46(C)**	**0.53 %**	**0.00 %**	**0.68 %**
319	**P**	**50(N)**	**0.52 %**	**0.04 %**	**0.62 %**
321	**P**	**50(N)**	**1.30 %**	**0.10 %**	**1.55 %**
323	**P**	**50(N)**	**2.10 %**	**0.24 %**	**2.42 %**
438	**S**	**68(Pd)**	**0.60 %**	**0.14 %**	**0.59 %**
440	**S**	**68(Pd)**	**0.46 %**	**0.06 %**	**0.52 %**
444	**P**	**68(Pd)**	**0.29 %**	**0.58 %**	**-0.38 %**
448	**D**	**68(Pd)**	**6.28 %**	**46.20 %**	**-51.79 %**
449	**D**	**68(Pd)**	**0.02 %**	**5.43 %**	**-7.01 %**

Table S10. Contribution of each atom to NOCV pair 1/orbitals 1and 938 in TS3(Pd)

Atom	Orb. 1	Orb. 938	Pair 1
1(C):	5.55 %	9.12 %	-4.63 %
2(C):	2.85 %	4.61 %	-2.28 %
3(C):	1.70 %	1.34 %	0.46 %
4(C):	0.62 %	0.16 %	0.59 %
5(C):	0.48 %	0.21 %	0.35 %
6(C):	0.10 %	0.05 %	0.06 %
7(H):	0.00 %	0.03 %	-0.04 %
8(C):	0.25 %	0.07 %	0.24 %
9(H):	0.01 %	0.00 %	0.01 %
10(C):	0.81 %	0.07 %	0.96 %
11(H):	0.00 %	0.01 %	-0.01 %
12(H):	0.00 %	0.01 %	-0.01 %
13(H):	0.00 %	0.00 %	0.00 %
14(C):	1.95 %	0.43 %	1.98 %
15(C):	1.40 %	0.62 %	1.01 %
16(C):	1.59 %	0.44 %	1.50 %
17(C):	0.28 %	0.14 %	0.17 %
18(H):	0.01 %	0.01 %	0.01 %
19(C):	0.32 %	0.03 %	0.37 %
20(H):	0.03 %	0.02 %	0.02 %
21(C):	1.81 %	0.07 %	2.26 %
22(H):	0.00 %	0.01 %	-0.01 %
23(H):	0.00 %	0.00 %	0.00 %
24(H):	0.00 %	0.00 %	0.00 %
25(C):	1.05 %	1.65 %	-0.78 %
26(O):	2.58 %	1.42 %	1.51 %
27(C):	34.01 %	20.51 %	17.51 %
28(C):	5.49 %	1.47 %	5.22 %
29(C):	3.48 %	0.40 %	3.99 %
30(C):	2.70 %	1.55 %	1.49 %
31(C):	0.14 %	0.01 %	0.16 %
32(H):	0.12 %	0.01 %	0.14 %
33(C):	1.41 %	0.05 %	1.76 %
34(C):	2.71 %	0.04 %	3.47 %
35(H):	0.00 %	0.00 %	0.00 %
36(H):	0.07 %	0.03 %	0.04 %
37(H):	0.01 %	0.00 %	0.01 %
38(C):	7.49 %	1.08 %	8.31 %
39(C):	1.32 %	0.16 %	1.50 %
40(C):	0.77 %	0.00 %	1.00 %

41(C):	1.36 %	0.08 %	1.66 %
42(C):	0.22 %	0.01 %	0.28 %
43(H):	0.00 %	0.00 %	-0.00 %
44(C):	0.34 %	0.03 %	0.40 %
45(H):	0.00 %	0.01 %	-0.01 %
46(C):	1.30 %	0.01 %	1.68 %
47(H):	0.02 %	0.00 %	0.02 %
48(H):	0.01 %	0.00 %	0.01 %
49(H):	0.00 %	0.00 %	0.00 %
50(N):	4.13 %	0.68 %	4.47 %
51(S):	0.14 %	0.22 %	-0.10 %
52(O):	0.15 %	0.01 %	0.19 %
53(O):	0.18 %	0.06 %	0.15 %
54(C):	0.26 %	0.10 %	0.21 %
55(C):	0.06 %	0.04 %	0.03 %
56(C):	0.18 %	0.01 %	0.22 %
57(C):	0.11 %	0.01 %	0.12 %
58(H):	0.00 %	0.00 %	0.00 %
59(C):	0.06 %	0.00 %	0.08 %
60(H):	0.01 %	0.00 %	0.01 %
61(C):	0.09 %	0.00 %	0.11 %
62(H):	0.00 %	0.00 %	0.01 %
63(H):	0.00 %	0.00 %	0.00 %
64(C):	0.01 %	0.00 %	0.01 %
65(H):	0.01 %	0.00 %	0.01 %
66(H):	0.00 %	0.00 %	0.00 %
67(H):	0.01 %	0.00 %	0.01 %
68(Pd):	8.23 %	52.87 %	-57.91 %

Table S11. Contribution of each basis function shell to NOCV pair 2/orbitals 2 and 937 in TS8(Pd)

Shell	Type	Atom	Orb. 2	Orb. 937	Pair 2
3	P	1(C)	1.90 %	0.77 %	0.62 %
4	S	1(C)	2.44 %	1.62 %	0.44 %
5	P	1(C)	6.40 %	2.64 %	2.04 %
6	S	1(C)	19.92 %	10.60 %	5.07 %
7	P	1(C)	3.28 %	0.94 %	1.27 %
13	P	2(C)	0.69 %	0.49 %	0.11 %
14	S	2(C)	1.89 %	3.66 %	-0.97 %
15	P	2(C)	3.78 %	2.38 %	0.76 %
23	P	3(C)	1.18 %	1.56 %	-0.21 %
91	P	14(C)	1.53 %	0.92 %	0.33 %
155	P	25(C)	1.27 %	1.27 %	-0.00 %

156	S	25(C)	0.98 %	1.22 %	-0.13 %
157	P	25(C)	3.81 %	3.79 %	0.01 %
158	S	25(C)	15.42 %	12.51 %	1.58 %
159	P	25(C)	3.76 %	3.20 %	0.31 %
163	P	26(O)	0.61 %	0.42 %	0.10 %
165	P	26(O)	1.25 %	0.84 %	0.22 %
167	P	26(O)	2.56 %	1.90 %	0.36 %
174	S	27(C)	0.53 %	0.29 %	0.13 %
175	P	27(C)	0.52 %	0.57 %	-0.02 %
182	S	28(C)	0.56 %	0.37 %	0.10 %
448	D	68(Pd)	16.27 %	31.55 %	-8.31 %
449	D	68(Pd)	0.19 %	8.46 %	-4.50 %
450	D	68(Pd)	0.74 %	1.49 %	-0.41 %

Table S12. Contribution of each atom to NOCV pair 2/orbitals 2 and 937 in TS8(Pd)

Atom	Orb. 2	Orb. 937	Pair 2
1(C):	34.48 %	16.84 %	9.59 %
2(C):	6.67 %	6.84 %	-0.10 %
3(C):	1.37 %	2.03 %	-0.36 %
4(C):	0.41 %	0.34 %	0.04 %
5(C):	0.72 %	0.66 %	0.03 %
6(C):	0.06 %	0.06 %	0.00 %
7(H):	0.10 %	0.11 %	-0.01 %
8(C):	0.10 %	0.11 %	-0.00 %
9(H):	0.01 %	0.01 %	0.00 %
10(C):	0.19 %	0.21 %	-0.01 %
11(H):	0.00 %	0.00 %	-0.00 %
12(H):	0.01 %	0.02 %	-0.01 %
13(H):	0.00 %	0.00 %	-0.00 %
14(C):	2.43 %	1.11 %	0.72 %
15(C):	0.66 %	0.38 %	0.15 %
16(C):	0.24 %	0.26 %	-0.01 %
17(C):	0.09 %	0.08 %	0.00 %
18(H):	0.00 %	0.00 %	0.00 %
19(C):	0.02 %	0.01 %	0.00 %
20(H):	0.01 %	0.01 %	0.00 %
21(C):	0.09 %	0.22 %	-0.07 %
22(H):	0.03 %	0.00 %	0.01 %
23(H):	0.00 %	0.00 %	-0.00 %
24(H):	0.00 %	0.00 %	0.00 %
25(C):	25.48 %	22.20 %	1.79 %
26(O):	4.47 %	3.17 %	0.71 %

27(C):	**1.16 %**	**0.92 %**	**0.13 %**
28(C):	**0.92 %**	**0.66 %**	**0.14 %**
29(C):	**0.16 %**	**0.12 %**	**0.02 %**
30(C):	**0.11 %**	**0.10 %**	**0.00 %**
31(C):	**0.09 %**	**0.08 %**	**0.00 %**
32(H):	**0.06 %**	**0.02 %**	**0.02 %**
33(C):	**0.04 %**	**0.05 %**	**-0.01 %**
34(C):	**0.01 %**	**0.01 %**	**0.00 %**
35(H):	**0.00 %**	**0.00 %**	**-0.00 %**
36(H):	**0.00 %**	**0.00 %**	**-0.00 %**
37(H):	**0.00 %**	**0.00 %**	**0.00 %**
38(C):	**0.19 %**	**0.19 %**	**-0.00 %**
39(C):	**0.10 %**	**0.10 %**	**0.00 %**
40(C):	**0.12 %**	**0.06 %**	**0.03 %**
41(C):	**0.19 %**	**0.42 %**	**-0.13 %**
42(C):	**0.05 %**	**0.06 %**	**-0.00 %**
43(H):	**0.00 %**	**0.00 %**	**-0.00 %**
44(C):	**0.19 %**	**0.08 %**	**0.06 %**
45(H):	**0.04 %**	**0.14 %**	**-0.06 %**
46(C):	**0.07 %**	**0.03 %**	**0.02 %**
47(H):	**0.00 %**	**0.00 %**	**-0.00 %**
48(H):	**0.00 %**	**0.00 %**	**0.00 %**
49(H):	**0.00 %**	**0.00 %**	**-0.00 %**
50(N):	**0.06 %**	**0.04 %**	**0.01 %**
51(S):	**0.00 %**	**0.00 %**	**0.00 %**
52(O):	**0.00 %**	**0.00 %**	**0.00 %**
53(O):	**0.00 %**	**0.00 %**	**0.00 %**
54(C):	**0.01 %**	**0.00 %**	**0.00 %**
55(C):	**0.00 %**	**0.00 %**	**0.00 %**
56(C):	**0.01 %**	**0.00 %**	**0.00 %**
57(C):	**0.00 %**	**0.00 %**	**0.00 %**
58(H):	**0.00 %**	**0.00 %**	**0.00 %**
59(C):	**0.00 %**	**0.00 %**	**0.00 %**
60(H):	**0.00 %**	**0.00 %**	**0.00 %**
61(C):	**0.00 %**	**0.00 %**	**0.00 %**
62(H):	**0.00 %**	**0.00 %**	**0.00 %**
63(H):	**0.00 %**	**0.00 %**	**0.00 %**
64(C):	**0.00 %**	**0.00 %**	**0.00 %**
65(H):	**0.00 %**	**0.00 %**	**0.00 %**
66(H):	**0.00 %**	**0.00 %**	**0.00 %**
67(H):	**0.00 %**	**0.00 %**	**0.00 %**
68(Pd):	**18.78 %**	**42.21 %**	**-12.75 %**

Table S13. Contribution of each basis function shell to NOCV pair 3/orbitals 3 and 936 in TS8(Pd)

Atom	Orb. 3	Orb. 936	Pair 3
1(C):	4.34 %	10.35 %	-2.73 %
2(C):	9.90 %	4.85 %	2.30 %
3(C):	1.44 %	4.97 %	-1.61 %
4(C):	0.18 %	0.30 %	-0.05 %
5(C):	0.24 %	0.58 %	-0.16 %
6(C):	0.13 %	0.06 %	0.03 %
7(H):	0.00 %	0.08 %	-0.03 %
8(C):	0.02 %	0.04 %	-0.01 %
9(H):	0.01 %	0.01 %	0.00 %
10(C):	0.03 %	0.26 %	-0.11 %
11(H):	0.01 %	0.01 %	0.00 %
12(H):	0.00 %	0.01 %	-0.00 %
13(H):	0.00 %	0.00 %	-0.00 %
14(C):	1.61 %	1.15 %	0.21 %
15(C):	0.22 %	1.03 %	-0.37 %
16(C):	0.10 %	0.17 %	-0.03 %
17(C):	0.04 %	0.27 %	-0.11 %
18(H):	0.01 %	0.03 %	-0.01 %
19(C):	0.07 %	0.08 %	-0.01 %
20(H):	0.00 %	0.16 %	-0.07 %
21(C):	0.09 %	0.16 %	-0.03 %
22(H):	0.01 %	0.01 %	-0.00 %
23(H):	0.00 %	0.01 %	-0.01 %
24(H):	0.00 %	0.00 %	-0.00 %
25(C):	1.04 %	0.97 %	0.03 %
26(O):	0.96 %	0.67 %	0.13 %
27(C):	2.44 %	17.93 %	-7.05 %
28(C):	0.93 %	0.50 %	0.20 %
29(C):	0.59 %	0.45 %	0.06 %
30(C):	0.08 %	1.58 %	-0.68 %
31(C):	0.33 %	0.33 %	-0.00 %
32(H):	0.12 %	0.19 %	-0.03 %
33(C):	0.01 %	0.09 %	-0.04 %
34(C):	0.04 %	0.07 %	-0.01 %
35(H):	0.00 %	0.00 %	0.00 %
36(H):	0.00 %	0.03 %	-0.01 %
37(H):	0.00 %	0.00 %	-0.00 %
38(C):	1.36 %	1.60 %	-0.11 %
39(C):	0.72 %	0.76 %	-0.02 %
40(C):	0.09 %	0.13 %	-0.02 %

41(C):	0.27 %	0.13 %	0.06 %
42(C):	0.04 %	0.09 %	-0.02 %
43(H):	0.02 %	0.04 %	-0.01 %
44(C):	0.15 %	0.05 %	0.04 %
45(H):	0.01 %	0.08 %	-0.03 %
46(C):	0.09 %	0.09 %	-0.00 %
47(H):	0.00 %	0.00 %	0.00 %
48(H):	0.00 %	0.00 %	-0.00 %
49(H):	0.00 %	0.00 %	0.00 %
50(N):	0.31 %	0.57 %	-0.12 %
51(S):	0.03 %	0.48 %	-0.20 %
52(O):	0.01 %	0.04 %	-0.02 %
53(O):	0.01 %	0.12 %	-0.05 %
54(C):	0.03 %	0.08 %	-0.03 %
55(C):	0.01 %	0.01 %	-0.00 %
56(C):	0.04 %	0.01 %	0.01 %
57(C):	0.00 %	0.00 %	-0.00 %
58(H):	0.00 %	0.00 %	0.00 %
59(C):	0.02 %	0.00 %	0.01 %
60(H):	0.01 %	0.00 %	0.00 %
61(C):	0.01 %	0.00 %	0.00 %
62(H):	0.00 %	0.00 %	-0.00 %
63(H):	0.00 %	0.00 %	-0.00 %
64(C):	0.00 %	0.00 %	0.00 %
65(H):	0.00 %	0.00 %	0.00 %
66(H):	0.00 %	0.00 %	-0.00 %
67(H):	0.00 %	0.00 %	0.00 %
68(Pd):	71.77 %	48.27 %	10.69 %

Table S14. Contribution of each atom to NOCV pair 3/orbitals 3 and 936 in TS8(Pd)

Atom	Orb. 3	Orb. 936	Pair 3
1(C):	4.34 %	10.35 %	-2.73 %
2(C):	9.90 %	4.85 %	2.30 %
3(C):	1.44 %	4.97 %	-1.61 %
4(C):	0.18 %	0.30 %	-0.05 %
5(C):	0.24 %	0.58 %	-0.16 %
6(C):	0.13 %	0.06 %	0.03 %
7(H):	0.00 %	0.08 %	-0.03 %
8(C):	0.02 %	0.04 %	-0.01 %
9(H):	0.01 %	0.01 %	0.00 %
10(C):	0.03 %	0.26 %	-0.11 %
11(H):	0.01 %	0.01 %	0.00 %
12(H):	0.00 %	0.01 %	-0.00 %

13(H):	**0.00 %**	**0.00 %**	**-0.00 %**
14(C):	**1.61 %**	**1.15 %**	**0.21 %**
15(C):	**0.22 %**	**1.03 %**	**-0.37 %**
16(C):	**0.10 %**	**0.17 %**	**-0.03 %**
17(C):	**0.04 %**	**0.27 %**	**-0.11 %**
18(H):	**0.01 %**	**0.03 %**	**-0.01 %**
19(C):	**0.07 %**	**0.08 %**	**-0.01 %**
20(H):	**0.00 %**	**0.16 %**	**-0.07 %**
21(C):	**0.09 %**	**0.16 %**	**-0.03 %**
22(H):	**0.01 %**	**0.01 %**	**-0.00 %**
23(H):	**0.00 %**	**0.01 %**	**-0.01 %**
24(H):	**0.00 %**	**0.00 %**	**-0.00 %**
25(C):	**1.04 %**	**0.97 %**	**0.03 %**
26(O):	**0.96 %**	**0.67 %**	**0.13 %**
27(C):	**2.44 %**	**17.93 %**	**-7.05 %**
28(C):	**0.93 %**	**0.50 %**	**0.20 %**
29(C):	**0.59 %**	**0.45 %**	**0.06 %**
30(C):	**0.08 %**	**1.58 %**	**-0.68 %**
31(C):	**0.33 %**	**0.33 %**	**-0.00 %**
32(H):	**0.12 %**	**0.19 %**	**-0.03 %**
33(C):	**0.01 %**	**0.09 %**	**-0.04 %**
34(C):	**0.04 %**	**0.07 %**	**-0.01 %**
35(H):	**0.00 %**	**0.00 %**	**0.00 %**
36(H):	**0.00 %**	**0.03 %**	**-0.01 %**
37(H):	**0.00 %**	**0.00 %**	**-0.00 %**
38(C):	**1.36 %**	**1.60 %**	**-0.11 %**
39(C):	**0.72 %**	**0.76 %**	**-0.02 %**
40(C):	**0.09 %**	**0.13 %**	**-0.02 %**
41(C):	**0.27 %**	**0.13 %**	**0.06 %**
42(C):	**0.04 %**	**0.09 %**	**-0.02 %**
43(H):	**0.02 %**	**0.04 %**	**-0.01 %**
44(C):	**0.15 %**	**0.05 %**	**0.04 %**
45(H):	**0.01 %**	**0.08 %**	**-0.03 %**
46(C):	**0.09 %**	**0.09 %**	**-0.00 %**
47(H):	**0.00 %**	**0.00 %**	**0.00 %**
48(H):	**0.00 %**	**0.00 %**	**-0.00 %**
49(H):	**0.00 %**	**0.00 %**	**0.00 %**
50(N):	**0.31 %**	**0.57 %**	**-0.12 %**
51(S):	**0.03 %**	**0.48 %**	**-0.20 %**
52(O):	**0.01 %**	**0.04 %**	**-0.02 %**
53(O):	**0.01 %**	**0.12 %**	**-0.05 %**
54(C):	**0.03 %**	**0.08 %**	**-0.03 %**
55(C):	**0.01 %**	**0.01 %**	**-0.00 %**
56(C):	**0.04 %**	**0.01 %**	**0.01 %**

57(C):	0.00 %	0.00 %	-0.00 %
58(H):	0.00 %	0.00 %	0.00 %
59(C):	0.02 %	0.00 %	0.01 %
60(H):	0.01 %	0.00 %	0.00 %
61(C):	0.01 %	0.00 %	0.00 %
62(H):	0.00 %	0.00 %	-0.00 %
63(H):	0.00 %	0.00 %	-0.00 %
64(C):	0.00 %	0.00 %	0.00 %
65(H):	0.00 %	0.00 %	0.00 %
66(H):	0.00 %	0.00 %	-0.00 %
67(H):	0.00 %	0.00 %	0.00 %
68(Pd):	71.77 %	48.27 %	10.69 %

Table S15. Pair and NOCV orbital information in TS3(HCO_3^-)

Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
1	-24.60	1	0.75068	-121.86	1016	-0.75068	-89.08
2	-13.51	2	0.31099	-57.19	1015	-0.31099	-13.76
3	-3.48	3	0.16789	-85.08	1014	-0.16789	-64.35
4	-2.86	4	0.11815	3.67	1013	-0.11815	27.90
5	-1.63	5	0.09183	9.36	1012	-0.09183	27.13
6	-1.81	6	0.08408	27.51	1011	-0.08408	49.08
7	-1.78	7	0.07769	10.01	1010	-0.07769	32.96
8	-1.07	8	0.06968	25.12	1009	-0.06968	40.52
9	-0.74	9	0.05986	9.01	1008	-0.05986	21.32
10	-0.73	10	0.05500	-74.33	1007	-0.05500	-61.11
11	-0.44	11	0.05349	-36.67	1006	-0.05349	-28.52
12	-0.45	12	0.04414	2.71	1005	-0.04414	12.95
13	-0.22	13	0.04239	-40.28	1004	-0.04239	-35.14
14	-0.38	14	0.04065	3.30	1003	-0.04065	12.54
15	-0.37	15	0.03716	8.49	1002	-0.03716	18.52
16	-0.16	16	0.03338	-40.04	1001	-0.03338	-35.24
17	-0.23	17	0.03215	-31.57	1000	-0.03215	-24.47
18	-0.09	18	0.02983	-67.02	999	-0.02983	-63.92
19	-0.12	19	0.02899	-43.05	998	-0.02899	-39.04
20	-0.12	20	0.02724	-60.05	997	-0.02724	-55.70
21	-0.20	21	0.02706	-10.52	996	-0.02706	-3.27
22	-0.12	22	0.02410	-58.06	995	-0.02410	-53.14
23	-0.13	23	0.02228	41.54	994	-0.02228	47.27
24	-0.09	24	0.02128	-45.65	993	-0.02128	-41.33
25	-0.19	25	0.02050	-68.33	992	-0.02050	-59.06
26	-0.09	26	0.01870	16.48	991	-0.01870	21.14

27	-0.06	27	0.01819	-39.05	990	-0.01819	-35.69
28	-0.06	28	0.01739	-35.14	989	-0.01739	-31.68
29	-0.07	29	0.01686	-14.14	988	-0.01686	-10.29
30	-0.06	30	0.01628	-44.55	987	-0.01628	-41.04
31	-0.04	31	0.01597	-58.38	986	-0.01597	-55.95
32	-0.07	32	0.01517	34.66	985	-0.01517	39.32
33	-0.05	33	0.01501	-28.17	984	-0.01501	-25.11
34	-0.03	34	0.01433	-58.29	983	-0.01433	-55.85
35	-0.05	35	0.01413	-28.38	982	-0.01413	-24.65
36	-0.05	36	0.01342	17.14	981	-0.01342	21.16
37	-0.03	37	0.01291	-26.00	980	-0.01291	-23.61
38	-0.03	38	0.01269	-31.57	979	-0.01269	-29.16
39	-0.03	39	0.01247	-44.58	978	-0.01247	-42.08
40	-0.04	40	0.01223	-39.88	977	-0.01223	-36.68
41	-0.04	41	0.01182	-20.91	976	-0.01182	-17.69
42	-0.03	42	0.01159	-38.89	975	-0.01159	-36.32
43	-0.02	43	0.01110	-55.24	974	-0.01110	-53.17
44	-0.04	44	0.01087	47.09	973	-0.01087	50.44
45	-0.03	45	0.01058	-48.39	972	-0.01058	-45.27
46	-0.02	46	0.01006	-26.80	971	-0.01006	-24.43
47	-0.02	47	0.00976	-51.08	970	-0.00976	-48.84
48	-0.02	48	0.00944	-46.33	969	-0.00944	-44.19
49	-0.02	49	0.00909	-43.74	968	-0.00909	-41.65
50	-0.02	50	0.00894	0.59	967	-0.00894	3.16
51	-0.02	51	0.00860	-26.50	966	-0.00860	-24.25
52	-0.02	52	0.00826	-36.09	965	-0.00826	-34.07
53	-0.01	53	0.00815	-47.59	964	-0.00815	-45.84
54	-0.01	54	0.00805	-54.96	963	-0.00805	-53.12
55	-0.02	55	0.00794	-23.11	962	-0.00794	-21.12
56	-0.01	56	0.00762	-26.33	961	-0.00762	-24.46
57	-0.01	57	0.00745	-5.08	960	-0.00745	-3.41
58	-0.01	58	0.00710	-30.62	959	-0.00710	-28.91
59	-0.01	59	0.00708	-47.34	958	-0.00708	-45.95
60	-0.02	60	0.00677	-1.92	957	-0.00677	0.47
61	-0.01	61	0.00674	-10.57	956	-0.00674	-8.81
62	-0.01	62	0.00642	-36.14	955	-0.00642	-34.80
63	-0.01	63	0.00620	-25.36	954	-0.00620	-23.68
64	-0.01	64	0.00611	-40.32	953	-0.00611	-38.51
65	-0.01	65	0.00596	-30.79	952	-0.00596	-29.42
66	-0.01	66	0.00590	-52.29	951	-0.00590	-51.03
67	-0.01	67	0.00574	-50.80	950	-0.00574	-49.16
68	-0.01	68	0.00551	-40.07	949	-0.00551	-38.38
69	-0.01	69	0.00535	-12.31	948	-0.00535	-10.98
70	-0.01	70	0.00521	-44.72	947	-0.00521	-43.21

71	**-0.01**	**71**	**0.00516**	**-28.27**	**946**	**-0.00516**	**-26.84**
72	**-0.01**	**72**	**0.00504**	**-48.93**	**945**	**-0.00504**	**-47.69**
73	**-0.01**	**73**	**0.00487**	**-36.35**	**944**	**-0.00487**	**-34.86**
74	**-0.01**	**74**	**0.00480**	**-29.66**	**943**	**-0.00480**	**-28.50**
75	**-0.01**	**75**	**0.00464**	**-32.00**	**942**	**-0.00464**	**-30.75**
76	**-0.01**	**76**	**0.00459**	**-11.54**	**941**	**-0.00459**	**-10.32**
77	**-0.01**	**77**	**0.00445**	**-34.20**	**940**	**-0.00445**	**-33.00**
78	**-0.01**	**78**	**0.00430**	**-43.89**	**939**	**-0.00430**	**-42.55**
79	**-0.00**	**79**	**0.00419**	**-57.81**	**938**	**-0.00419**	**-56.67**
80	**-0.01**	**80**	**0.00412**	**-81.09**	**937**	**-0.00412**	**-79.41**
81	**-0.01**	**81**	**0.00393**	**-188.91**	**936**	**-0.00393**	**-185.79**
82	**-0.00**	**82**	**0.00387**	**-48.93**	**935**	**-0.00387**	**-47.81**
83	**-0.00**	**83**	**0.00369**	**-13.15**	**934**	**-0.00369**	**-12.09**
84	**-0.00**	**84**	**0.00362**	**-20.12**	**933**	**-0.00362**	**-19.02**
85	**-0.01**	**85**	**0.00354**	**-92.22**	**932**	**-0.00354**	**-90.58**
86	**-0.00**	**86**	**0.00337**	**-37.90**	**931**	**-0.00337**	**-36.62**
87	**-0.00**	**87**	**0.00334**	**-50.21**	**930**	**-0.00334**	**-49.00**
88	**-0.00**	**88**	**0.00310**	**-51.74**	**929**	**-0.00310**	**-50.44**
89	**-0.01**	**89**	**0.00305**	**-132.58**	**928**	**-0.00305**	**-130.51**
90	**-0.00**	**90**	**0.00297**	**-40.63**	**927**	**-0.00297**	**-39.51**
91	**-0.00**	**91**	**0.00289**	**-64.57**	**926**	**-0.00289**	**-63.28**
92	**-0.00**	**92**	**0.00278**	**-55.88**	**925**	**-0.00278**	**-54.66**
93	**-0.00**	**93**	**0.00276**	**-33.45**	**924**	**-0.00276**	**-32.44**
94	**-0.00**	**94**	**0.00272**	**-85.53**	**923**	**-0.00272**	**-84.53**
95	**-0.00**	**95**	**0.00262**	**-34.47**	**922**	**-0.00262**	**-33.21**
96	**-0.01**	**96**	**0.00255**	**-278.77**	**921**	**-0.00255**	**-276.73**
97	**-0.00**	**97**	**0.00236**	**-100.64**	**920**	**-0.00236**	**-99.47**
98	**-0.00**	**98**	**0.00233**	**-64.96**	**919**	**-0.00233**	**-64.24**
99	**-0.00**	**99**	**0.00228**	**-65.05**	**918**	**-0.00228**	**-64.06**
100	**-0.00**	**100**	**0.00215**	**-29.58**	**917**	**-0.00215**	**-28.57**
101	**-0.00**	**101**	**0.00209**	**-305.65**	**916**	**-0.00209**	**-303.92**
102	**-0.00**	**102**	**0.00202**	**-44.69**	**915**	**-0.00202**	**-43.72**
103	**-0.00**	**103**	**0.00202**	**-199.86**	**914**	**-0.00202**	**-198.42**
104	**-0.00**	**104**	**0.00186**	**-186.79**	**913**	**-0.00186**	**-185.54**
105	**-0.00**	**105**	**0.00184**	**-59.22**	**912**	**-0.00184**	**-58.38**
106	**-0.00**	**106**	**0.00176**	**-71.46**	**911**	**-0.00176**	**-70.35**
107	**-0.00**	**107**	**0.00170**	**-45.90**	**910**	**-0.00170**	**-45.17**
108	**-0.00**	**108**	**0.00169**	**-71.85**	**909**	**-0.00169**	**-71.04**
109	**-0.00**	**109**	**0.00155**	**-51.23**	**908**	**-0.00155**	**-50.54**
110	**-0.00**	**110**	**0.00152**	**-41.02**	**907**	**-0.00152**	**-40.35**
111	**-0.00**	**111**	**0.00137**	**-85.36**	**906**	**-0.00137**	**-84.77**
112	**-0.00**	**112**	**0.00133**	**-220.39**	**905**	**-0.00133**	**-219.55**
113	**-0.00**	**113**	**0.00131**	**-64.19**	**904**	**-0.00131**	**-63.60**
114	**-0.00**	**114**	**0.00123**	**-179.43**	**903**	**-0.00123**	**-178.71**

115	-0.00	115	0.00111	-73.82	902	-0.00111	-73.38
116	-0.00	116	0.00110	-101.35	901	-0.00110	-100.65

Sum of NOCV eigenvalues: 0.00000

Sum of pair energies: -56.95 kcal/mol

NOCV orbitals with absolute eigenvalues smaller than 1.0E-03 are not shown

Note: All energies are given in kcal/mol

Table S16. Contribution of each basis function shell to NOCV pair 1/orbitals 1 and 1016 in TS3(HCO_3^-):

Shell	Type	Atom	Orb. 1	Orb. 1016	Pair 1
3	P	1(C)	0.56 %	0.10 %	0.35 %
5	P	1(C)	1.47 %	0.24 %	0.93 %
6	S	1(C)	2.80 %	1.18 %	1.22 %
7	P	1(C)	5.05 %	1.38 %	2.76 %
13	P	2(C)	0.66 %	0.34 %	0.24 %
14	S	2(C)	0.52 %	0.01 %	0.38 %
23	P	3(C)	0.61 %	0.02 %	0.45 %
91	P	14(C)	0.82 %	0.50 %	0.24 %
167	P	26(O)	0.54 %	0.20 %	0.26 %
171	P	27(C)	1.29 %	0.49 %	0.60 %
173	P	27(C)	3.58 %	1.32 %	1.70 %
174	S	27(C)	8.83 %	3.35 %	4.11 %
175	P	27(C)	1.73 %	1.75 %	-0.01 %
182	S	28(C)	1.25 %	0.21 %	0.78 %
183	P	28(C)	1.22 %	0.43 %	0.59 %
190	S	29(C)	0.69 %	0.23 %	0.34 %
191	P	29(C)	0.68 %	0.07 %	0.46 %
227	P	34(C)	0.61 %	0.04 %	0.43 %
243	P	38(C)	0.55 %	0.04 %	0.38 %
245	P	38(C)	1.39 %	0.09 %	0.97 %
246	S	38(C)	1.29 %	0.24 %	0.79 %
247	P	38(C)	3.02 %	0.23 %	2.09 %
254	S	39(C)	0.66 %	0.30 %	0.27 %
255	P	39(C)	0.57 %	0.21 %	0.27 %
271	P	41(C)	0.52 %	0.16 %	0.27 %
321	P	50(N)	0.86 %	0.07 %	0.60 %
323	P	50(N)	1.69 %	0.12 %	1.18 %
438	S	68(Pd)	1.76 %	0.83 %	0.70 %
440	S	68(Pd)	3.94 %	2.77 %	0.88 %
441	S	68(Pd)	2.70 %	1.29 %	1.06 %
444	P	68(Pd)	2.36 %	0.53 %	1.37 %

445	P	68(Pd)	0.50 %	0.37 %	0.10 %
446	P	68(Pd)	0.85 %	0.47 %	0.28 %
448	D	68(Pd)	14.92 %	31.64 %	-12.55 %
449	D	68(Pd)	0.89 %	1.57 %	-0.51 %
450	D	68(Pd)	1.35 %	0.43 %	0.69 %
457	P	69(C)	0.62 %	2.70 %	-1.56 %
461	P	70(O)	0.45 %	1.30 %	-0.64 %
463	P	70(O)	1.24 %	2.67 %	-1.07 %
464	S	70(O)	0.01 %	1.35 %	-1.01 %
465	P	70(O)	0.82 %	4.05 %	-2.43 %
469	P	71(O)	0.85 %	3.77 %	-2.19 %
470	S	71(O)	0.26 %	1.90 %	-1.23 %
471	P	71(O)	2.48 %	7.54 %	-3.80 %
472	S	71(O)	0.05 %	1.45 %	-1.05 %
473	P	71(O)	1.91 %	10.06 %	-6.12 %
479	P	72(O)	0.12 %	0.70 %	-0.43 %
481	P	72(O)	0.03 %	1.10 %	-0.80 %
485	S	73(H)	0.23 %	0.66 %	-0.33 %

Table S17. Contribution of each atom to NOCV pair 1/orbitals 1 and 1016 in TS3(HCO_3^-)

Atom	Orb. 1	Orb. 1016	Pair 1
1(C):	10.32 %	3.08 %	5.44 %
2(C):	1.93 %	0.74 %	0.89 %
3(C):	1.04 %	0.07 %	0.73 %
4(C):	0.54 %	0.08 %	0.35 %
5(C):	0.34 %	0.07 %	0.20 %
6(C):	0.09 %	0.02 %	0.05 %
7(H):	0.03 %	0.01 %	0.02 %
8(C):	0.10 %	0.02 %	0.06 %
9(H):	0.00 %	0.00 %	0.00 %
10(C):	0.61 %	0.03 %	0.44 %
11(H):	0.01 %	0.00 %	0.01 %
12(H):	0.01 %	0.00 %	0.00 %
13(H):	0.00 %	0.00 %	0.00 %
14(C):	0.98 %	0.55 %	0.32 %
15(C):	0.27 %	0.15 %	0.09 %
16(C):	0.41 %	0.30 %	0.08 %
17(C):	0.08 %	0.04 %	0.03 %
18(H):	0.00 %	0.00 %	0.00 %
19(C):	0.33 %	0.26 %	0.06 %
20(H):	0.31 %	0.10 %	0.16 %
21(C):	0.15 %	0.06 %	0.06 %
22(H):	0.03 %	0.00 %	0.02 %

23(H):	**0.00 %**	**0.00 %**	**0.00 %**
24(H):	**0.00 %**	**0.00 %**	**0.00 %**
25(C):	**0.78 %**	**0.66 %**	**0.08 %**
26(O):	**1.17 %**	**0.41 %**	**0.57 %**
27(C):	**16.07 %**	**7.40 %**	**6.51 %**
28(C):	**3.10 %**	**0.82 %**	**1.71 %**
29(C):	**1.99 %**	**0.45 %**	**1.16 %**
30(C):	**1.22 %**	**0.31 %**	**0.69 %**
31(C):	**0.27 %**	**0.04 %**	**0.17 %**
32(H):	**0.01 %**	**0.00 %**	**0.01 %**
33(C):	**0.55 %**	**0.17 %**	**0.29 %**
34(C):	**1.26 %**	**0.17 %**	**0.82 %**
35(H):	**0.00 %**	**0.00 %**	**0.00 %**
36(H):	**0.09 %**	**0.02 %**	**0.05 %**
37(H):	**0.00 %**	**0.00 %**	**0.00 %**
38(C):	**6.47 %**	**0.74 %**	**4.30 %**
39(C):	**1.53 %**	**0.57 %**	**0.72 %**
40(C):	**0.69 %**	**0.05 %**	**0.48 %**
41(C):	**1.16 %**	**0.35 %**	**0.61 %**
42(C):	**0.19 %**	**0.02 %**	**0.13 %**
43(H):	**0.00 %**	**0.00 %**	**0.00 %**
44(C):	**0.08 %**	**0.21 %**	**-0.10 %**
45(H):	**0.20 %**	**0.14 %**	**0.04 %**
46(C):	**0.95 %**	**0.07 %**	**0.66 %**
47(H):	**0.01 %**	**0.00 %**	**0.01 %**
48(H):	**0.01 %**	**0.00 %**	**0.01 %**
49(H):	**0.00 %**	**0.00 %**	**0.00 %**
50(N):	**3.03 %**	**0.42 %**	**1.96 %**
51(S):	**0.22 %**	**0.14 %**	**0.06 %**
52(O):	**0.14 %**	**0.02 %**	**0.09 %**
53(O):	**0.16 %**	**0.05 %**	**0.08 %**
54(C):	**0.29 %**	**0.05 %**	**0.18 %**
55(C):	**0.09 %**	**0.01 %**	**0.06 %**
56(C):	**0.26 %**	**0.02 %**	**0.18 %**
57(C):	**0.06 %**	**0.00 %**	**0.04 %**
58(H):	**0.00 %**	**0.00 %**	**0.00 %**
59(C):	**0.15 %**	**0.01 %**	**0.11 %**
60(H):	**0.01 %**	**0.00 %**	**0.00 %**
61(C):	**0.05 %**	**0.00 %**	**0.04 %**
62(H):	**0.01 %**	**0.00 %**	**0.00 %**
63(H):	**0.01 %**	**0.00 %**	**0.00 %**
64(C):	**0.00 %**	**0.00 %**	**0.00 %**
65(H):	**0.00 %**	**0.00 %**	**0.00 %**
66(H):	**0.00 %**	**0.00 %**	**0.00 %**

67(H):	0.01 %	0.00 %	0.00 %
68(Pd):	30.22 %	40.29 %	-7.56 %
69(C):	1.01 %	3.04 %	-1.52 %
70(O):	2.54 %	9.63 %	-5.32 %
71(O):	5.58 %	24.93 %	-14.53 %
72(O):	0.51 %	2.22 %	-1.28 %
73(H):	0.24 %	0.98 %	-0.56 %

Table S18. Contribution of each basis function shell to NOCV pair 2/orbitals 2 and 1015 in TS3(HCO_3^-):

Shell	Type	Atom	Orb. 2	Orb. 1015	Pair 2
7	P	1(C)	2.69 %	0.97 %	0.53 %
14	S	2(C)	6.64 %	2.66 %	1.24 %
15	P	2(C)	0.40 %	0.59 %	-0.06 %
22	S	3(C)	1.23 %	0.82 %	0.13 %
23	P	3(C)	1.61 %	0.88 %	0.23 %
90	S	14(C)	1.50 %	0.77 %	0.23 %
91	P	14(C)	1.41 %	0.86 %	0.17 %
107	P	16(C)	0.55 %	0.43 %	0.04 %
126	S	19(C)	0.54 %	0.38 %	0.05 %
173	P	27(C)	0.54 %	0.10 %	0.14 %
175	P	27(C)	5.91 %	3.89 %	0.63 %
183	P	28(C)	1.26 %	0.87 %	0.12 %
247	P	38(C)	1.52 %	1.04 %	0.15 %
437	S	68(Pd)	0.51 %	0.27 %	0.08 %
438	S	68(Pd)	3.02 %	2.06 %	0.30 %
439	S	68(Pd)	1.57 %	1.05 %	0.16 %
440	S	68(Pd)	33.82 %	29.27 %	1.42 %
441	S	68(Pd)	0.95 %	0.78 %	0.05 %
444	P	68(Pd)	2.23 %	0.57 %	0.52 %
445	P	68(Pd)	1.01 %	0.88 %	0.04 %
446	P	68(Pd)	3.47 %	2.30 %	0.36 %
447	P	68(Pd)	0.86 %	0.60 %	0.08 %
448	D	68(Pd)	0.51 %	4.29 %	-1.17 %
449	D	68(Pd)	0.27 %	0.73 %	-0.14 %
456	S	69(C)	0.92 %	0.58 %	0.11 %
457	P	69(C)	7.49 %	11.66 %	-1.30 %
461	P	70(O)	0.43 %	1.32 %	-0.28 %
462	S	70(O)	0.27 %	1.02 %	-0.23 %
463	P	70(O)	1.51 %	2.19 %	-0.21 %
464	S	70(O)	0.61 %	0.05 %	0.17 %
465	P	70(O)	0.83 %	4.90 %	-1.27 %
472	S	71(O)	0.56 %	0.87 %	-0.10 %

473	P	71(O)	0.35 %	1.80 %	-0.45 %
480	S	72(O)	3.67 %	9.15 %	-1.70 %
481	P	72(O)	0.23 %	1.52 %	-0.40 %
485	S	73(H)	0.53 %	1.19 %	-0.21 %

Table S19. Contribution of each atom to NOCV pair 2/orbitals 2 and 1015 in TS3(HCO_3^-)

Atom	Orb. 2	Orb. 1015	Pair 2
1(C):	2.93 %	1.02 %	0.59 %
2(C):	7.20 %	3.33 %	1.20 %
3(C):	2.90 %	1.70 %	0.37 %
4(C):	0.28 %	0.15 %	0.04 %
5(C):	0.08 %	0.04 %	0.01 %
6(C):	0.04 %	0.02 %	0.01 %
7(H):	0.04 %	0.02 %	0.01 %
8(C):	0.02 %	0.01 %	0.00 %
9(H):	0.01 %	0.01 %	0.00 %
10(C):	0.02 %	0.01 %	0.00 %
11(H):	0.00 %	0.00 %	0.00 %
12(H):	0.00 %	0.00 %	0.00 %
13(H):	0.00 %	0.00 %	0.00 %
14(C):	2.92 %	1.64 %	0.40 %
15(C):	0.53 %	0.28 %	0.08 %
16(C):	1.07 %	0.63 %	0.14 %
17(C):	0.03 %	0.02 %	0.00 %
18(H):	0.01 %	0.01 %	0.00 %
19(C):	0.73 %	0.48 %	0.08 %
20(H):	0.01 %	0.07 %	-0.02 %
21(C):	0.13 %	0.05 %	0.02 %
22(H):	0.00 %	0.00 %	-0.00 %
23(H):	0.02 %	0.01 %	0.00 %
24(H):	0.00 %	0.00 %	0.00 %
25(C):	0.22 %	0.05 %	0.05 %
26(O):	0.11 %	0.02 %	0.03 %
27(C):	7.31 %	4.19 %	0.97 %
28(C):	1.37 %	0.93 %	0.14 %
29(C):	0.58 %	0.49 %	0.03 %
30(C):	0.12 %	0.08 %	0.01 %
31(C):	0.07 %	0.05 %	0.01 %
32(H):	0.27 %	0.16 %	0.03 %
33(C):	0.06 %	0.03 %	0.01 %
34(C):	0.03 %	0.01 %	0.00 %
35(H):	0.00 %	0.00 %	0.00 %

36(H):	0.03 %	0.01 %	0.01 %
37(H):	0.00 %	0.00 %	-0.00 %
38(C):	1.73 %	1.13 %	0.19 %
39(C):	0.46 %	0.39 %	0.02 %
40(C):	0.11 %	0.05 %	0.02 %
41(C):	0.40 %	0.29 %	0.03 %
42(C):	0.01 %	0.00 %	0.00 %
43(H):	0.03 %	0.02 %	0.00 %
44(C):	0.06 %	0.06 %	0.00 %
45(H):	0.01 %	0.00 %	0.00 %
46(C):	0.07 %	0.02 %	0.02 %
47(H):	0.00 %	0.00 %	0.00 %
48(H):	0.01 %	0.01 %	0.00 %
49(H):	0.00 %	0.00 %	-0.00 %
50(N):	0.24 %	0.08 %	0.05 %
51(S):	0.30 %	0.14 %	0.05 %
52(O):	0.02 %	0.00 %	0.01 %
53(O):	0.10 %	0.01 %	0.03 %
54(C):	0.04 %	0.02 %	0.00 %
55(C):	0.00 %	0.00 %	-0.00 %
56(C):	0.02 %	0.02 %	-0.00 %
57(C):	0.00 %	0.00 %	0.00 %
58(H):	0.00 %	0.00 %	0.00 %
59(C):	0.00 %	0.00 %	0.00 %
60(H):	0.01 %	0.01 %	0.00 %
61(C):	0.00 %	0.00 %	-0.00 %
62(H):	0.00 %	0.00 %	0.00 %
63(H):	0.00 %	0.00 %	0.00 %
64(C):	0.00 %	0.00 %	0.00 %
65(H):	0.00 %	0.00 %	0.00 %
66(H):	0.00 %	0.00 %	0.00 %
67(H):	0.00 %	0.00 %	0.00 %
68(Pd):	48.56 %	43.00 %	1.73 %
69(C):	8.94 %	12.69 %	-1.17 %
70(O):	3.67 %	9.58 %	-1.84 %
71(O):	1.51 %	3.98 %	-0.77 %
72(O):	4.01 %	11.48 %	-2.32 %
73(H):	0.53 %	1.47 %	-0.29 %

Table S20. Contribution of each basis function shell to NOCV pair/orbitals:

Shell	Type	Atom	Orb. 3	Orb. 1014	Pair 3
6	S	1(C)	15.08 %	13.61 %	0.25 %

7	P	1(C)	0.58 %	0.62 %	-0.01 %
14	S	2(C)	1.35 %	1.30 %	0.01 %
15	P	2(C)	3.01 %	3.07 %	-0.01 %
23	P	3(C)	1.68 %	1.52 %	0.03 %
30	S	4(C)	0.56 %	0.53 %	0.01 %
38	S	5(C)	1.34 %	1.21 %	0.02 %
91	P	14(C)	2.10 %	1.85 %	0.04 %
99	P	15(C)	0.59 %	0.52 %	0.01 %
107	P	16(C)	0.70 %	0.64 %	0.01 %
158	S	25(C)	11.94 %	11.35 %	0.10 %
159	P	25(C)	2.91 %	2.67 %	0.04 %
174	S	27(C)	0.52 %	0.42 %	0.02 %
175	P	27(C)	0.67 %	0.66 %	0.00 %
182	S	28(C)	0.66 %	0.67 %	-0.00 %
246	S	38(C)	3.42 %	3.30 %	0.02 %
247	P	38(C)	1.09 %	0.94 %	0.03 %
255	P	39(C)	4.92 %	4.37 %	0.09 %
262	S	40(C)	3.11 %	2.80 %	0.05 %
263	P	40(C)	0.97 %	0.89 %	0.01 %
271	P	41(C)	4.55 %	3.95 %	0.10 %
278	S	42(C)	0.86 %	0.78 %	0.01 %
290	S	44(C)	2.17 %	1.91 %	0.04 %
291	P	44(C)	0.60 %	0.52 %	0.01 %
295	S	45(H)	1.65 %	1.48 %	0.03 %
302	S	46(C)	0.84 %	0.75 %	0.02 %
440	S	68(Pd)	2.09 %	1.71 %	0.06 %
441	S	68(Pd)	1.68 %	1.64 %	0.01 %
444	P	68(Pd)	0.89 %	0.62 %	0.05 %
446	P	68(Pd)	4.38 %	4.02 %	0.06 %
449	D	68(Pd)	1.57 %	1.20 %	0.06 %
450	D	68(Pd)	0.89 %	0.80 %	0.01 %
453	P	69(C)	0.06 %	0.80 %	-0.12 %
455	P	69(C)	0.01 %	1.08 %	-0.18 %
457	P	69(C)	4.07 %	7.53 %	-0.58 %
463	P	70(O)	0.69 %	0.01 %	0.11 %
465	P	70(O)	0.67 %	0.08 %	0.10 %
469	P	71(O)	1.16 %	0.18 %	0.16 %
471	P	71(O)	3.86 %	0.09 %	0.63 %
473	P	71(O)	0.49 %	2.87 %	-0.40 %
477	P	72(O)	0.15 %	0.75 %	-0.10 %
479	P	72(O)	0.54 %	1.23 %	-0.12 %
481	P	72(O)	0.08 %	5.54 %	-0.92 %

Table S21. Contribution of each atom to NOCV pair 3/orbitals 3 and 1014 in TS3(HCO_3^-)

Atom	Orb. 3	Orb. 1014	Pair 3
1(C):	15.94 %	14.59 %	0.23 %
2(C):	4.44 %	4.50 %	-0.01 %
3(C):	1.69 %	1.53 %	0.03 %
4(C):	0.61 %	0.55 %	0.01 %
5(C):	1.69 %	1.51 %	0.03 %
6(C):	0.08 %	0.08 %	-0.00 %
7(H):	0.05 %	0.05 %	0.00 %
8(C):	0.28 %	0.26 %	0.00 %
9(H):	0.01 %	0.01 %	0.00 %
10(C):	0.09 %	0.03 %	0.01 %
11(H):	0.00 %	0.00 %	0.00 %
12(H):	0.01 %	0.01 %	0.00 %
13(H):	0.00 %	0.00 %	0.00 %
14(C):	2.18 %	1.90 %	0.05 %
15(C):	0.64 %	0.54 %	0.02 %
16(C):	1.04 %	0.98 %	0.01 %
17(C):	0.25 %	0.23 %	0.00 %
18(H):	0.02 %	0.02 %	0.00 %
19(C):	0.17 %	0.15 %	0.00 %
20(H):	0.15 %	0.15 %	0.00 %
21(C):	0.16 %	0.12 %	0.01 %
22(H):	0.01 %	0.01 %	0.00 %
23(H):	0.07 %	0.06 %	0.00 %
24(H):	0.00 %	0.00 %	0.00 %
25(C):	15.12 %	14.30 %	0.14 %
26(O):	0.67 %	0.67 %	-0.00 %
27(C):	1.22 %	1.10 %	0.02 %
28(C):	1.06 %	1.06 %	0.00 %
29(C):	0.15 %	0.11 %	0.01 %
30(C):	0.39 %	0.30 %	0.01 %
31(C):	0.11 %	0.10 %	0.00 %
32(H):	0.01 %	0.01 %	0.00 %
33(C):	0.10 %	0.08 %	0.00 %
34(C):	0.04 %	0.02 %	0.00 %
35(H):	0.00 %	0.00 %	-0.00 %
36(H):	0.00 %	0.00 %	0.00 %
37(H):	0.00 %	0.00 %	0.00 %
38(C):	4.52 %	4.26 %	0.04 %
39(C):	5.30 %	4.70 %	0.10 %
40(C):	4.10 %	3.70 %	0.07 %

41(C):	**4.71 %**	**4.07 %**	**0.11 %**
42(C):	**1.21 %**	**1.08 %**	**0.02 %**
43(H):	**0.10 %**	**0.09 %**	**0.00 %**
44(C):	**2.78 %**	**2.44 %**	**0.06 %**
45(H):	**1.75 %**	**1.59 %**	**0.03 %**
46(C):	**1.16 %**	**1.00 %**	**0.03 %**
47(H):	**0.02 %**	**0.01 %**	**0.00 %**
48(H):	**0.01 %**	**0.01 %**	**-0.00 %**
49(H):	**0.03 %**	**0.02 %**	**0.00 %**
50(N):	**0.02 %**	**0.02 %**	**0.00 %**
51(S):	**0.02 %**	**0.02 %**	**-0.00 %**
52(O):	**0.00 %**	**0.00 %**	**0.00 %**
53(O):	**0.00 %**	**0.00 %**	**0.00 %**
54(C):	**0.02 %**	**0.02 %**	**0.00 %**
55(C):	**0.02 %**	**0.01 %**	**0.00 %**
56(C):	**0.01 %**	**0.01 %**	**0.00 %**
57(C):	**0.01 %**	**0.01 %**	**0.00 %**
58(H):	**0.00 %**	**0.00 %**	**0.00 %**
59(C):	**0.00 %**	**0.00 %**	**0.00 %**
60(H):	**0.00 %**	**0.00 %**	**0.00 %**
61(C):	**0.01 %**	**0.00 %**	**0.00 %**
62(H):	**0.00 %**	**0.00 %**	**0.00 %**
63(H):	**0.00 %**	**0.00 %**	**0.00 %**
64(C):	**0.00 %**	**0.00 %**	**0.00 %**
65(H):	**0.00 %**	**0.00 %**	**0.00 %**
66(H):	**0.00 %**	**0.00 %**	**0.00 %**
67(H):	**0.00 %**	**0.00 %**	**0.00 %**
68(Pd):	**12.86 %**	**11.00 %**	**0.31 %**
69(C):	**4.44 %**	**9.48 %**	**-0.85 %**
70(O):	**1.70 %**	**0.21 %**	**0.25 %**
71(O):	**5.65 %**	**3.22 %**	**0.41 %**
72(O):	**1.01 %**	**7.87 %**	**-1.15 %**
73(H):	**0.08 %**	**0.11 %**	**-0.01 %**

4. Free energy profile of other path in allylation reaction

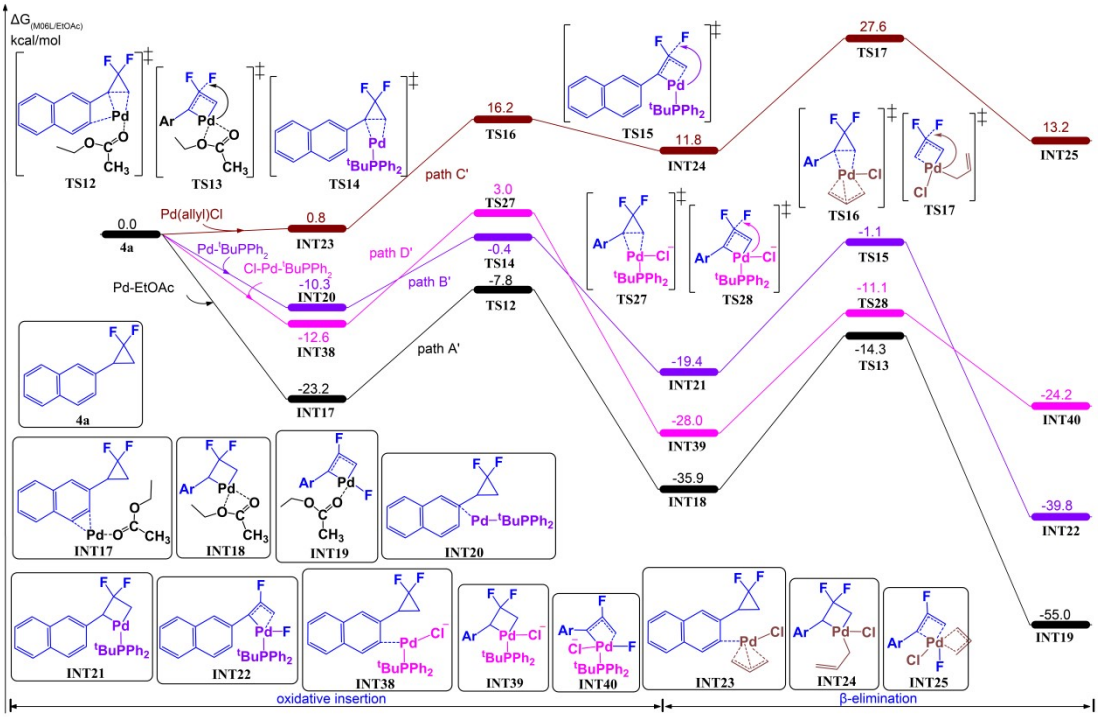


Figure S5. Calculated free energy profile for oxidative addition and β-elimination steps catalyzed by Pd(0)-EtOAc (path A' in black), Pd(0)-^{t}BuPPh$_2$ (path B' in purpul), [Pd(II)(allyl)Cl] (path C' in brown) and [Pd(0)(^{t}BuPPh$_2$)Cl]$^-$ (path D' in pink) in allylation reaction. The energy values (kcal/mol) are calculated using M06-L method in ethyl acetate.

We also considered the effect of forth ligand [Pd(0)(^{t}BuPPh$_2$)Cl]$^-$ on oxidative addition and β-elimination steps. The calculated free energy profiles are shown in Figure S4. Regant gem-difluorinated cyclopropane (**4a**) is acted as the relative zero. According to experimental conditions, [Pd(0)(^{t}BuPPh$_2$)Cl]$^-$ (path D' in pink) can be considered as potential active species, which coordinates **4a** to form the corresponding intermediate **INT38**. Palladium(0) catalyst inserts into the C3'-C5' bond of cyclopropane via the transition state **TS27** to yield four-membered cyclopallad(II)butane **INT39**, which requires a 15.6 kcal/mol activation energy barrier. Subsequent β-fluoride elimination via transition state **TS28** with an overall activation free energy barrier of 16.9 kcal/mol causes to form the intermediate **INT40**.

The rate-determining step is β-fluoride elimination in path D'. The computational results showed that the relative free energy of **TS24** is 10.0 kcal/mol and 38.7 kcal/mol lower than that of **TS15** and **TS17**, respectively, but the relative free energy of **TS24** is 3.2 kcal/mol higher than that of **TS13**. Therefore, path D' can be excluded.

5. NCI and RDG analysis for TS13,TS15,TS17 and TS28 allylation reaction

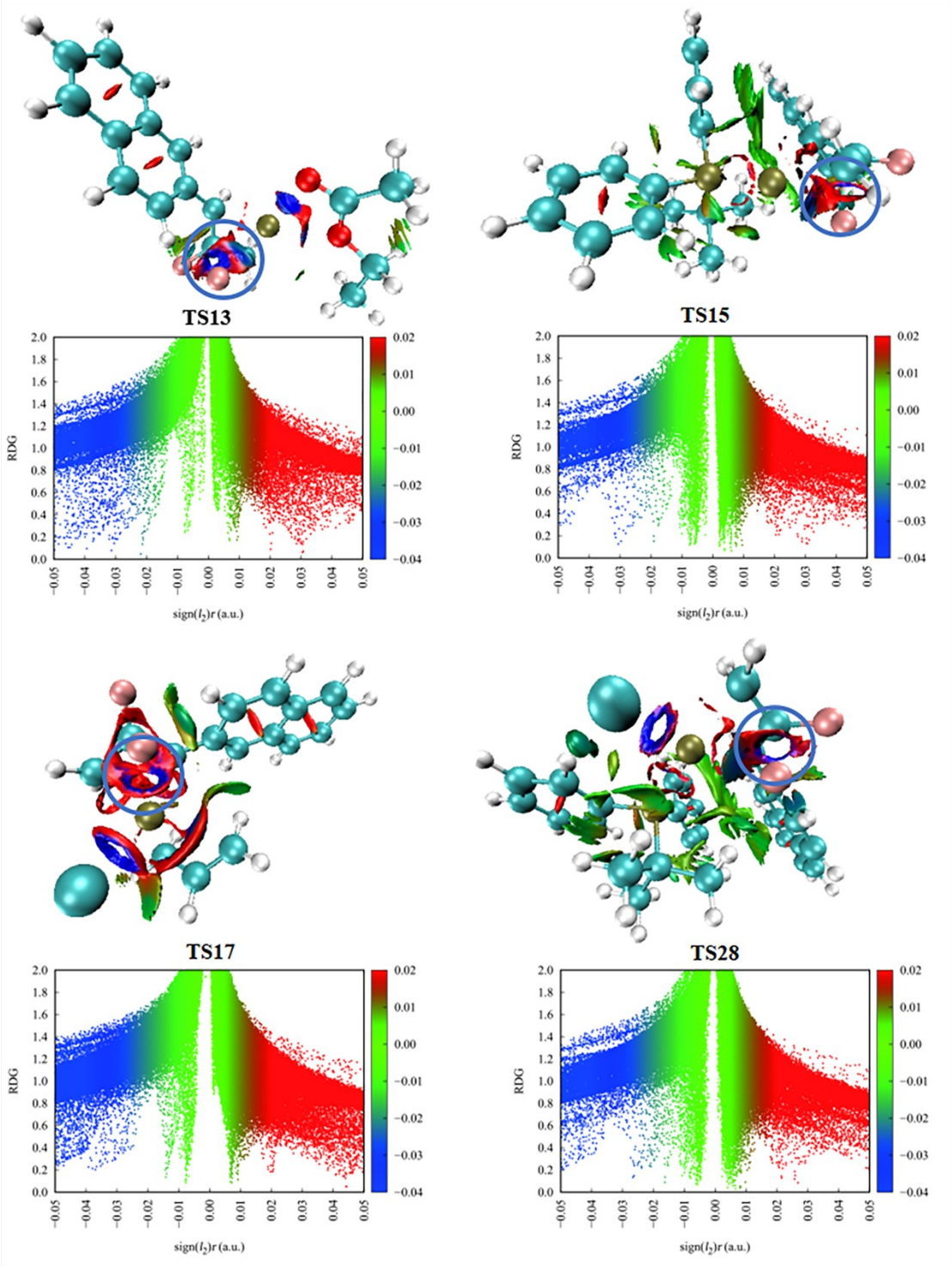


Figure S6. Noncovalent interaction (NCI) gradient isosurfaces (above) and reduced density gradient (RDG) (below) i**n TS13, TS15, TS17 and TS28** (blue, strong attraction; green, weak interaction; red, steric effect).

According to Fig. S6, it is evident that a repulsive interaction exists between the two benzene rings of naphthalenyl in these four transition states. In **TS13**, the red region is predominantly localized between the Pd atom and the C(carbonyl) atom of the ester group, whereas the blue region is observed between the Pd atom and these two oxygen atoms of the ester group. There is a repulsive force between the F2 and F1 atoms, as well as between the C3' and C5' atoms. Additionally, there is a strong attractive force between the F2 atoms and both the C4' and Pd atoms. These interactions also can be observed in **TS15**, **TS17**, and **TS28**. The green region primarily encompasses the benzene ring located between the F2 atom and the naphthalene group. In **TS15**, a repulsive force is observed between the Pd and P atoms, with negligible strong attraction between the Pd atom and the ligand, and only weak interactions between the **4a** and the ligand (covered in green). In **TS17**, there is significant attraction between the Pd and Cl atoms, accompanied by both strong attraction and repulsion between the Pd atom and the allyl group of the ligand. Additionally, within the ligand, there is a weak interaction between the Cl atom and the allyl group. In **TS28**, strong attraction persists between the Pd and Cl atoms, while there is almost nothing but repulsion between the Pd and P atoms. Furthermore, numerous weak interactions are present between the **4a** and the ligand. A detailed examination reveals that the strongest interaction occurs between F2 atoms and C3 in **TS13**, as indicated by the largest blue area (circled in blue in Figure S6)

6. Pair and NOCV orbital information in TS13, TS15, TS17 and TS28.

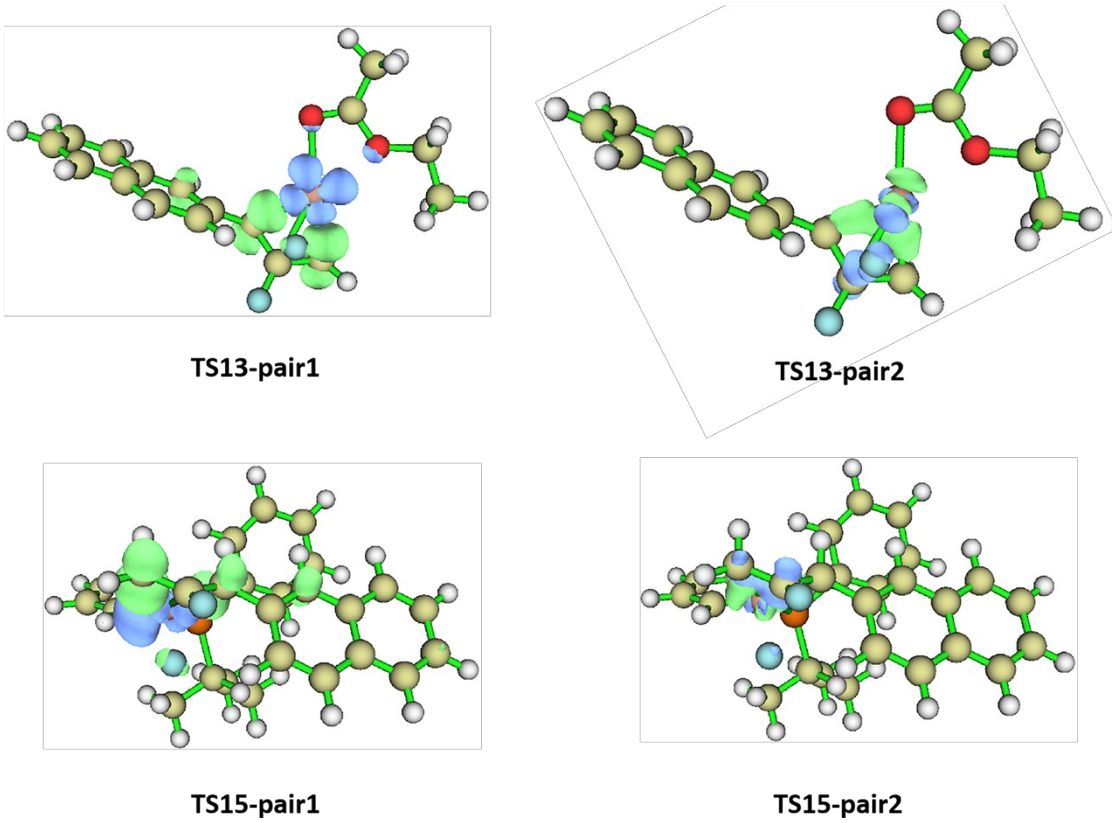


Figure S7. Isosurfaces of NOCV pair 1 and 2 density of **TS13** and **TS15.**

In **TS13**, **TS15**, **TS17** and **TS28**, **4a** is used as one fragment and the corresponding ligand is used as the other fragment. According to Figure S7 and Table S23, electrons in the NOCV pair 1 of **TS13** mainly transfer from Pd (-46.1%) atom to C3' (13.79 %) and C5' (16.89 %) atoms. However, some electrons are also lost from the two oxygen (-4.06 % and -2.40 %) atoms in the ligand. In the NOCV pair 2, and the electrons in the Pd atom get a little feedback (1.32 %). According to Table S26, electrons in pair1 of **TS15** mainly flow from P (-46.58 %) atom to a benzene ring carbon atom (12.45 %) connected to P atom, allyl C3' (5.61 %) and C5' (5.77 %) atoms.

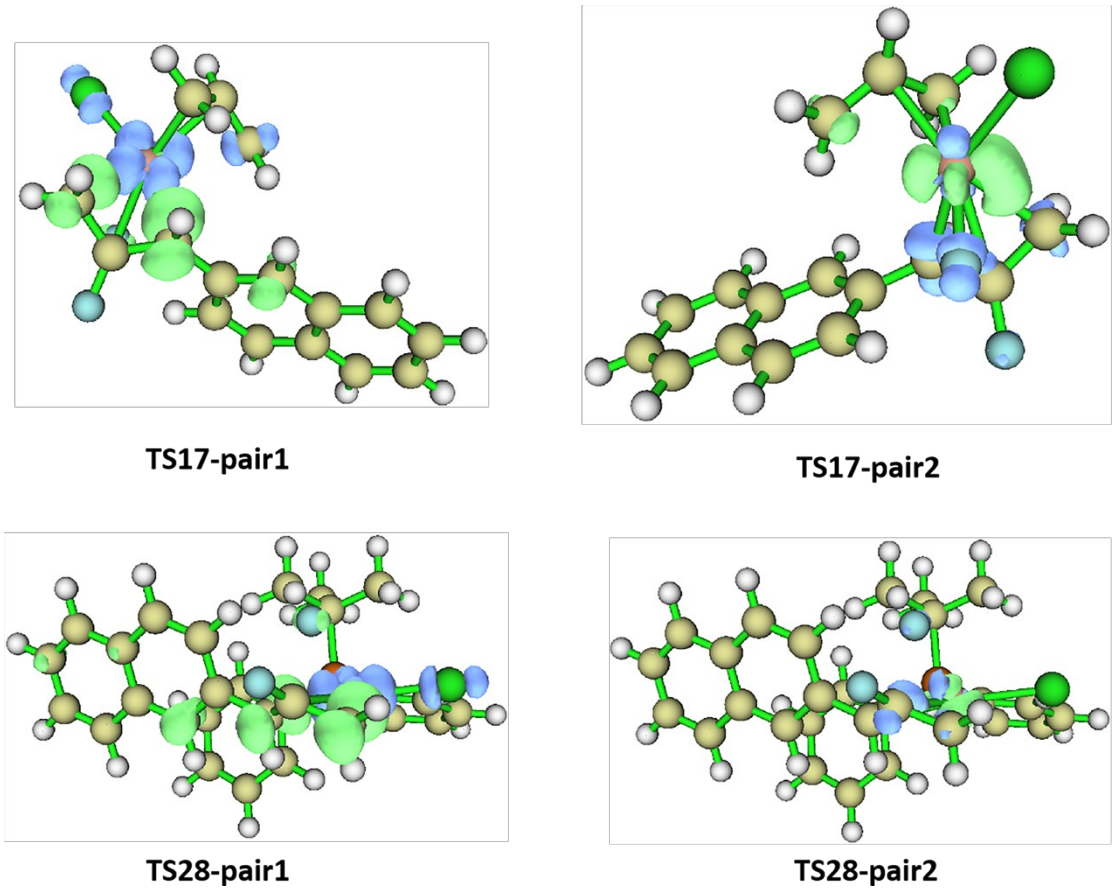


Figure S8. Isosurfaces of NOCV pair 1 and 2 density of **TS17** and **TS28.**

In combination with Figure S8 and Table S27, it can be found that electrons in the NOCV pair 1 of **TS17** mainly transfer from Pd(-27.07 %) and the two terminal carbon atoms of the allyl group in the ligand (-5.04 % and -5.04 %) to the central C atom (9.58 %) within the allyl group of the ligand, C4' (6.09 %), C5' (5.42 %) and the two carbon atoms (6.87 % and 4.09 %) in the naphthalene group. From Table S31, it can be found that the electrons in the NOCV pair 1 of **TS28** mainly provide from the P (-23.07 %) atom, the C27 (-7.42%) atom connected with P atom, Pd (-5.58%), C40 (-5.16 %) and C43 (-4.76 %) atoms to the C3 (11.66 %), C2 (7.24 %) and allyl C3' (9.55 %) and C5' (5.60 %) atoms.

Table S22. Pair and NOCV orbital information in TS13

Pair Energy |	Orbital	Eigenvalue	Energy |	Orbital	Eigenvalue	Energy
1********	1	1.11184	-15387.14	624	-1.11184	0.00
2-5837.79	2	0.38212	-15277.36	623	-0.38212	0.00
3-3681.62	3	0.30803	-11952.23	622	-0.30803	0.00
4-2495.59	4	0.20939	-11918.52	621	-0.20939	0.00
5-1125.87	5	0.17573	-6406.86	620	-0.17573	0.00
6-6774.31	6	0.13925	-6393.05	619	-0.13925	42254.52
7-4622.87	7	0.09529	-6355.79	618	-0.09529	42157.12
8-3274.33	8	0.08417	-6325.66	617	-0.08417	32575.87
9-1980.07	9	0.05230	-6321.99	616	-0.05230	31539.17
10-1766.97	10	0.04676	-6318.22	615	-0.04676	31470.35
11-1245.70	11	0.03899	-6315.94	614	-0.03899	25632.53
12-1045.65	12	0.03299	-6315.65	613	-0.03299	25379.04
13 -959.72	13	0.03036	-6315.15	612	-0.03036	25293.61
14 -605.80	14	0.02809	-6310.18	611	-0.02809	15259.65
15 -562.85	15	0.02610	-6309.53	610	-0.02610	15256.16
16 -517.55	16	0.02405	-6309.40	609	-0.02405	15213.54
17 -494.06	17	0.02296	-6309.18	608	-0.02296	15213.09
18 -480.18	18	0.02238	-6309.00	607	-0.02238	15144.79
19 -442.69	19	0.02064	-6308.72	606	-0.02064	15137.64
20 -416.30	20	0.01942	-6306.72	605	-0.01942	15134.98
21 -402.12	21	0.01877	-6302.35	604	-0.01877	15126.45
22 -315.68	22	0.01832	-2107.44	603	-0.01832	15120.67
23 -290.52	23	0.01771	-1296.87	602	-0.01771	15107.68
24 -280.94	24	0.01713	-1292.04	601	-0.01713	15106.07
25 -257.80	25	0.01577	-1271.47	600	-0.01577	15079.99
26 -246.18	26	0.01557	-762.21	599	-0.01557	15044.52
27 -233.08	27	0.01481	-694.95	598	-0.01481	15041.35
28 -225.62	28	0.01440	-640.12	597	-0.01440	15029.74
29 -214.46	29	0.01374	-618.45	596	-0.01374	14990.95
30 -208.69	30	0.01356	-527.34	595	-0.01356	14859.98
31 -64.33	31	0.01333	-504.61	594	-0.01333	4322.28
32 -61.25	32	0.01291	-486.98	593	-0.01291	4258.15
33 -57.26	33	0.01214	-474.59	592	-0.01214	4240.66
34 -55.28	34	0.01182	-464.21	591	-0.01182	4211.93
35 -52.87	35	0.01152	-458.94	590	-0.01152	4130.66
36 -51.76	36	0.01144	-449.94	589	-0.01144	4074.47

37	-46.61	37	0.01110	-432.05	588	-0.01110	3767.55
38	-42.29	38	0.01060	-408.47	587	-0.01060	3582.63
39	-38.10	39	0.00987	-392.68	586	-0.00987	3467.66
40	-36.37	40	0.00977	-368.00	585	-0.00977	3353.82
41	-33.16	41	0.00919	-364.23	584	-0.00919	3242.07
42	-30.76	42	0.00861	-350.74	583	-0.00861	3222.00
43	-29.20	43	0.00848	-348.65	582	-0.00848	3094.73
44	-28.43	44	0.00827	-347.58	581	-0.00827	3090.33
45	-26.91	45	0.00794	-311.86	580	-0.00794	3078.09
46	-24.69	46	0.00777	-309.86	579	-0.00777	2866.84
47	-22.84	47	0.00747	-300.80	578	-0.00747	2757.35
48	-21.74	48	0.00722	-296.79	577	-0.00722	2715.75
49	-21.26	49	0.00719	-291.98	576	-0.00719	2666.57
50	-19.51	50	0.00661	-290.13	575	-0.00661	2660.98
51	-17.48	51	0.00595	-285.38	574	-0.00595	2651.39
52	-15.77	52	0.00540	-276.69	573	-0.00540	2642.02
53	-15.28	53	0.00529	-268.38	572	-0.00529	2618.56
54	-14.72	54	0.00512	-266.56	571	-0.00512	2607.81
55	-13.27	55	0.00468	-257.31	570	-0.00468	2576.37
56	-13.02	56	0.00462	-248.31	569	-0.00462	2568.66
57	-12.55	57	0.00449	-247.71	568	-0.00449	2550.61
58	-11.83	58	0.00423	-245.38	567	-0.00423	2548.00
59	-11.01	59	0.00396	-240.76	566	-0.00396	2542.15
60	-9.78	60	0.00353	-238.62	565	-0.00353	2530.31
61	-9.38	61	0.00340	-236.97	564	-0.00340	2519.88
62	-8.40	62	0.00306	-235.17	563	-0.00306	2513.46
63	-8.22	63	0.00300	-229.68	562	-0.00300	2509.59
64	-7.93	64	0.00292	-228.89	561	-0.00292	2486.97
65	-7.39	65	0.00278	-226.76	560	-0.00278	2434.30
66	-3.58	66	0.00135	-217.73	559	-0.00135	2424.87
67	-3.16	67	0.00121	-216.11	558	-0.00121	2401.83
Sum of NOCV eigenvalues:			0.00000				

Table S23. Contribution of each basis function shell to NOCV pair1/orbitals 1 and 624 in TS13

Shell	Type	Atom	Orb. 1	Orb. 624	Pair 1
5	P	1(C)	0.48 %	0.00 %	0.53 %
7	P	1(C)	0.56 %	0.00 %	0.62 %
18	S	2(C)	1.85 %	0.01 %	2.05 %
27	P	3(C)	0.47 %	0.02 %	0.50 %
28	S	3(C)	1.87 %	0.06 %	2.01 %
29	P	3(C)	1.94 %	0.33 %	1.78 %

38	**S**	**4(C)**	**3.59 %**	**0.28 %**	**3.67 %**
39	**P**	**4(C)**	**0.78 %**	**0.20 %**	**0.65 %**
83	**S**	**10(C)**	**0.44 %**	**1.08 %**	**-0.71 %**
84	**P**	**10(C)**	**1.27 %**	**0.03 %**	**1.37 %**
90	**P**	**11(C)**	**1.14 %**	**0.03 %**	**1.22 %**
92	**P**	**11(C)**	**1.15 %**	**0.07 %**	**1.20 %**
93	**S**	**11(C)**	**0.89 %**	**0.03 %**	**0.95 %**
112	**P**	**14(C)**	**1.27 %**	**0.16 %**	**1.23 %**
113	**S**	**14(C)**	**0.05 %**	**0.96 %**	**-1.01 %**
114	**P**	**14(C)**	**1.94 %**	**1.34 %**	**0.67 %**
123	**S**	**15(C)**	**2.18 %**	**1.01 %**	**1.30 %**
124	**P**	**15(C)**	**0.68 %**	**0.15 %**	**0.59 %**
138	**P**	**18(C)**	**1.97 %**	**0.89 %**	**1.21 %**
139	**S**	**18(C)**	**0.78 %**	**1.98 %**	**-1.34 %**
140	**P**	**18(C)**	**5.75 %**	**2.52 %**	**3.59 %**
141	**S**	**18(C)**	**3.36 %**	**2.62 %**	**0.82 %**
142	**P**	**18(C)**	**5.51 %**	**2.25 %**	**3.63 %**
143	**S**	**18(C)**	**5.51 %**	**0.00 %**	**6.12 %**
144	**P**	**18(C)**	**0.32 %**	**0.51 %**	**-0.21 %**
152	**P**	**19(C)**	**0.67 %**	**0.08 %**	**0.65 %**
154	**P**	**19(C)**	**0.69 %**	**0.18 %**	**0.57 %**
158	**P**	**20(C)**	**1.86 %**	**0.71 %**	**1.28 %**
159	**S**	**20(C)**	**0.87 %**	**1.54 %**	**-0.75 %**
160	**P**	**20(C)**	**5.52 %**	**2.06 %**	**3.86 %**
161	**S**	**20(C)**	**3.31 %**	**2.42 %**	**0.98 %**
162	**P**	**20(C)**	**4.39 %**	**1.86 %**	**2.81 %**
163	**S**	**20(C)**	**11.25 %**	**3.67 %**	**8.42 %**
179	**S**	**23(H)**	**1.14 %**	**0.26 %**	**0.99 %**
205	**S**	**26(Pd)**	**4.54 %**	**0.50 %**	**4.49 %**
210	**P**	**26(Pd)**	**1.33 %**	**1.51 %**	**-0.20 %**
212	**D**	**26(Pd)**	**5.69 %**	**45.56 %**	**-44.33 %**
213	**D**	**26(Pd)**	**0.01 %**	**5.55 %**	**-6.16 %**
214	**D**	**26(Pd)**	**0.58 %**	**0.53 %**	**0.05 %**
263	**S**	**34(O)**	**0.00 %**	**0.51 %**	**-0.56 %**
265	**S**	**34(O)**	**0.00 %**	**1.64 %**	**-1.82 %**
267	**S**	**34(O)**	**0.13 %**	**1.30 %**	**-1.30 %**
268	**P**	**34(O)**	**0.55 %**	**0.38 %**	**0.19 %**
276	**P**	**35(C)**	**0.00 %**	**0.54 %**	**-0.60 %**
277	**S**	**35(C)**	**0.39 %**	**1.91 %**	**-1.69 %**
285	**S**	**36(O)**	**0.00 %**	**0.46 %**	**-0.51 %**
287	**S**	**36(O)**	**0.13 %**	**0.97 %**	**-0.94 %**
297	**S**	**37(C)**	**0.08 %**	**0.89 %**	**-0.90 %**

Table S24. Contribution of each atom to NOCV pair1/orbitals 1 and 624 in TS13

Atom	Orb. 1	Orb. 624	Pair 1
1(C):	1.28 %	0.20 %	1.21 %
2(C):	2.06 %	0.04 %	2.25 %
3(C):	4.91 %	0.42 %	4.99 %
4(C):	4.58 %	0.52 %	4.52 %
5(C):	1.10 %	0.48 %	0.69 %
6(C):	0.09 %	0.64 %	-0.61 %
7(H):	0.02 %	0.00 %	0.02 %
8(H):	0.00 %	0.00 %	0.00 %
9(H):	0.00 %	0.00 %	0.00 %
10(C):	2.01 %	1.13 %	0.97 %
11(C):	4.14 %	0.61 %	3.93 %
12(H):	0.01 %	0.01 %	0.01 %
13(H):	0.00 %	0.00 %	0.00 %
14(C):	3.99 %	2.63 %	1.52 %
15(C):	3.50 %	1.26 %	2.50 %
16(H):	0.20 %	0.07 %	0.15 %
17(H):	0.22 %	0.08 %	0.15 %
18(C):	23.35 %	10.95 %	13.79 %
19(C):	2.08 %	0.35 %	1.92 %
20(C):	27.73 %	12.54 %	16.89 %
21(H):	0.27 %	0.09 %	0.20 %
22(H):	0.08 %	0.03 %	0.05 %
23(H):	1.68 %	0.33 %	1.50 %
24(F):	0.51 %	0.03 %	0.54 %
25(F):	0.82 %	0.07 %	0.83 %
26(Pd):	12.88 %	54.34 %	-46.10 %
27(C):	0.11 %	0.57 %	-0.51 %
28(H):	0.03 %	0.02 %	0.01 %
29(H):	0.04 %	0.06 %	-0.03 %
30(H):	0.01 %	0.07 %	-0.06 %
31(C):	0.14 %	1.01 %	-0.97 %
32(H):	0.02 %	0.02 %	0.01 %
33(H):	0.02 %	0.08 %	-0.06 %
34(O):	0.78 %	4.43 %	-4.06 %
35(C):	0.81 %	3.08 %	-2.52 %
36(O):	0.40 %	2.56 %	-2.40 %
37(C):	0.10 %	1.14 %	-1.16 %
38(H):	0.00 %	0.04 %	-0.05 %
39(H):	0.01 %	0.02 %	-0.02 %
40(H):	0.01 %	0.08 %	-0.08 %

Table S25. Contribution of each basis function shell to NOCV pair 2/orbitals 2 and 623 in TS13

Shell	Type	Atom	Orb. 2	Orb. 623	Pair 2
18	S	2(C)	1.55 %	2.40 %	-0.33 %
19	P	2(C)	0.63 %	0.86 %	-0.09 %
29	P	3(C)	4.05 %	5.42 %	-0.52 %
38	S	4(C)	0.54 %	0.22 %	0.12 %
39	P	4(C)	1.27 %	2.11 %	-0.32 %
58	S	6(C)	0.77 %	0.74 %	0.01 %
83	S	10(C)	3.94 %	4.25 %	-0.12 %
84	P	10(C)	9.51 %	10.91 %	-0.53 %
93	S	11(C)	0.40 %	0.51 %	-0.04 %
94	P	11(C)	0.24 %	0.97 %	-0.28 %
113	S	14(C)	19.40 %	17.65 %	0.67 %
114	P	14(C)	7.06 %	9.41 %	-0.90 %
124	P	15(C)	16.49 %	18.49 %	-0.76 %
143	S	18(C)	6.72 %	6.05 %	0.26 %
153	S	19(C)	3.38 %	2.42 %	0.36 %
163	S	20(C)	5.51 %	3.42 %	0.80 %
169	S	21(H)	0.64 %	0.52 %	0.05 %
204	S	26(Pd)	2.13 %	1.74 %	0.15 %
205	S	26(Pd)	6.76 %	4.42 %	0.89 %
212	D	26(Pd)	0.71 %	0.31 %	0.15 %
214	D	26(Pd)	0.51 %	0.43 %	0.03 %
278	P	35(C)	1.07 %	0.83 %	0.09 %
297	S	37(C)	1.69 %	1.42 %	0.10 %

Table S26. Contribution of each atom to NOCV pair 2/orbitals 2 and 623 in TS13

Atom	Orb. 2	Orb. 623	Pair 2
1(C):	0.18 %	0.23 %	-0.02 %
2(C):	2.19 %	3.26 %	-0.41 %
3(C):	4.15 %	5.43 %	-0.49 %
4(C):	1.82 %	2.34 %	-0.20 %
5(C):	0.32 %	0.32 %	-0.00 %
6(C):	0.78 %	0.75 %	0.01 %
7(H):	0.07 %	0.06 %	0.00 %
8(H):	0.00 %	0.00 %	-0.00 %
9(H):	0.03 %	0.03 %	0.00 %
10(C):	13.46 %	15.17 %	-0.65 %

11(C):	0.66 %	1.50 %	-0.32 %
12(H):	0.01 %	0.01 %	0.00 %
13(H):	0.00 %	0.00 %	-0.00 %
14(C):	26.50 %	27.08 %	-0.22 %
15(C):	16.56 %	18.59 %	-0.78 %
16(H):	0.09 %	0.07 %	0.01 %
17(H):	0.40 %	0.28 %	0.05 %
18(C):	7.09 %	6.20 %	0.34 %
19(C):	3.92 %	3.12 %	0.30 %
20(C):	5.88 %	3.66 %	0.85 %
21(H):	0.69 %	0.56 %	0.05 %
22(H):	0.17 %	0.14 %	0.01 %
23(H):	0.10 %	0.06 %	0.02 %
24(F):	0.03 %	0.09 %	-0.02 %
25(F):	0.10 %	0.24 %	-0.05 %
26(Pd):	10.93 %	7.48 %	1.32 %
27(C):	0.33 %	0.31 %	0.01 %
28(H):	0.01 %	0.01 %	0.00 %
29(H):	0.00 %	0.00 %	-0.00 %
30(H):	0.01 %	0.00 %	0.00 %
31(C):	0.24 %	0.23 %	0.00 %
32(H):	0.00 %	0.00 %	-0.00 %
33(H):	0.00 %	0.00 %	-0.00 %
34(O):	0.12 %	0.12 %	-0.00 %
35(C):	1.14 %	0.97 %	0.07 %
36(O):	0.16 %	0.13 %	0.01 %
37(C):	1.83 %	1.54 %	0.11 %
38(H):	0.00 %	0.00 %	-0.00 %
39(H):	0.01 %	0.01 %	-0.00 %
40(H):	0.01 %	0.00 %	0.00 %

Table S27. Pair and NOCV orbital information in TS15

Pair Energy |	Orbital	Eigenvalue Energy	|	Orbital	Eigenvalue	Energy
1********	1	1.22630	-48178.99	951	-1.22630	0.00
2-4803.71	2	0.31229	-15382.36	950	-0.31229	0.00
3-3645.76	3	0.23848	-15287.19	949	-0.23848	0.00
4-1380.83	4	0.21602	-6392.04	948	-0.21602	0.00
5-1060.16	5	0.16754	-6327.97	947	-0.16754	0.00
6 -755.61	6	0.11944	-6326.33	946	-0.11944	0.00
7 -668.90	7	0.10580	-6322.38	945	-0.10580	0.00
8 -621.33	8	0.09830	-6321.09	944	-0.09830	0.00

9	-467.07	9	0.07392	-6318.56	943	-0.07392	0.00
10	-382.38	10	0.06053	-6317.12	942	-0.06053	0.00
11	-303.64	11	0.04807	-6316.30	941	-0.04807	0.00
12	-4948.63	12	0.04526	-6316.09	940	-0.04526	103032.01
13	-2021.51	13	0.04162	-6315.93	939	-0.04162	42256.68
14	-1936.68	14	0.03995	-6315.53	938	-0.03995	42167.88
15	-1494.00	15	0.03842	-6315.47	937	-0.03842	32567.02
16	-1072.69	16	0.03356	-6314.65	936	-0.03356	25644.72
17	-987.15	17	0.03106	-6314.14	935	-0.03106	25465.68
18	-953.03	18	0.03010	-6314.13	934	-0.03010	25347.98
19	-635.27	19	0.02944	-6314.06	933	-0.02944	15262.65
20	-605.24	20	0.02806	-6313.88	932	-0.02806	15256.43
21	-530.87	21	0.02462	-6313.50	931	-0.02462	15252.29
22	-511.13	22	0.02371	-6310.87	930	-0.02371	15249.92
23	-496.83	23	0.02307	-6310.42	929	-0.02307	15222.31
24	-480.38	24	0.02232	-6310.25	928	-0.02232	15214.95
25	-443.98	25	0.02064	-6309.93	927	-0.02064	15198.32
26	-436.07	26	0.02028	-6309.67	926	-0.02028	15192.05
27	-403.44	27	0.01878	-6307.49	925	-0.01878	15178.65
28	-372.76	28	0.01735	-6306.16	924	-0.01735	15175.27
29	-355.85	29	0.01657	-6303.92	923	-0.01657	15168.12
30	-338.88	30	0.01579	-6301.68	922	-0.01579	15161.96
31	-329.28	31	0.01535	-6300.98	921	-0.01535	15156.90
32	-310.02	32	0.01446	-6299.40	920	-0.01446	15147.28
33	-275.58	33	0.01432	-4098.57	919	-0.01432	15144.34
34	-246.70	34	0.01366	-2913.13	918	-0.01366	15142.15
35	-236.48	35	0.01310	-2912.52	917	-0.01310	15135.75
36	-230.78	36	0.01279	-2910.53	916	-0.01279	15129.63
37	-220.09	37	0.01277	-2110.88	915	-0.01277	15124.95
38	-202.66	38	0.01234	-1299.64	914	-0.01234	15124.13
39	-196.04	39	0.01195	-1294.72	913	-0.01195	15115.40
40	-194.51	40	0.01187	-1275.66	912	-0.01187	15113.23
41	-170.81	41	0.01077	-756.53	911	-0.01077	15100.21
42	-164.98	42	0.01051	-628.70	910	-0.01051	15065.44
43	-158.50	43	0.01021	-528.15	909	-0.01021	14996.37
44	-155.00	44	0.00999	-521.88	908	-0.00999	14991.42
45	-146.45	45	0.00947	-518.16	907	-0.00947	14938.40
46	-139.93	46	0.00908	-503.59	906	-0.00908	14913.08
47	-134.82	47	0.00876	-490.25	905	-0.00876	14896.40
48	-83.21	48	0.00871	-485.31	904	-0.00871	9067.69
49	-79.50	49	0.00836	-464.91	903	-0.00836	9043.73
50	-77.21	50	0.00813	-461.31	902	-0.00813	9040.90
51	-38.67	51	0.00758	-452.74	901	-0.00758	4647.80
52	-35.48	52	0.00742	-451.91	900	-0.00742	4327.85

53	**-34.31**	**53**	**0.00726**	**-450.50**	**899**	**-0.00726**	**4275.94**
54	**-33.08**	**54**	**0.00706**	**-450.00**	**898**	**-0.00706**	**4233.41**
55	**-32.44**	**55**	**0.00697**	**-433.03**	**897**	**-0.00697**	**4222.48**
56	**-30.68**	**56**	**0.00674**	**-409.65**	**896**	**-0.00674**	**4141.37**
57	**-29.48**	**57**	**0.00656**	**-407.46**	**895**	**-0.00656**	**4084.81**
58	**-22.12**	**58**	**0.00631**	**-407.16**	**894**	**-0.00631**	**3099.00**
59	**-21.55**	**59**	**0.00618**	**-391.59**	**893**	**-0.00618**	**3092.37**
60	**-20.99**	**60**	**0.00607**	**-368.78**	**892**	**-0.00607**	**3090.64**
61	**-19.87**	**61**	**0.00576**	**-363.48**	**891**	**-0.00576**	**3088.65**
62	**-19.65**	**62**	**0.00571**	**-363.08**	**890**	**-0.00571**	**3079.87**
63	**-17.56**	**63**	**0.00542**	**-361.96**	**889**	**-0.00542**	**2875.72**
64	**-16.36**	**64**	**0.00524**	**-358.26**	**888**	**-0.00524**	**2765.44**
65	**-15.92**	**65**	**0.00520**	**-351.61**	**887**	**-0.00520**	**2709.42**
66	**-15.18**	**66**	**0.00499**	**-345.88**	**886**	**-0.00499**	**2692.97**
67	**-14.78**	**67**	**0.00490**	**-344.34**	**885**	**-0.00490**	**2672.74**
68	**-14.00**	**68**	**0.00471**	**-318.11**	**884**	**-0.00471**	**2656.55**
69	**-13.50**	**69**	**0.00456**	**-309.26**	**883**	**-0.00456**	**2648.75**
70	**-13.05**	**70**	**0.00443**	**-304.78**	**882**	**-0.00443**	**2643.42**
71	**-12.85**	**71**	**0.00438**	**-297.85**	**881**	**-0.00438**	**2637.20**
72	**-12.47**	**72**	**0.00427**	**-291.80**	**880**	**-0.00427**	**2630.49**
73	**-12.03**	**73**	**0.00414**	**-291.32**	**879**	**-0.00414**	**2617.47**
74	**-11.60**	**74**	**0.00400**	**-283.11**	**878**	**-0.00400**	**2613.06**
75	**-11.01**	**75**	**0.00385**	**-275.10**	**877**	**-0.00385**	**2581.84**
76	**-10.79**	**76**	**0.00378**	**-272.95**	**876**	**-0.00378**	**2577.46**
77	**-10.42**	**77**	**0.00368**	**-269.53**	**875**	**-0.00368**	**2560.79**
78	**-10.17**	**78**	**0.00360**	**-266.97**	**874**	**-0.00360**	**2556.50**
79	**-9.99**	**79**	**0.00354**	**-266.09**	**873**	**-0.00354**	**2555.45**
80	**-9.56**	**80**	**0.00339**	**-264.35**	**872**	**-0.00339**	**2551.84**
81	**-8.86**	**81**	**0.00316**	**-258.67**	**871**	**-0.00316**	**2548.18**
82	**-8.22**	**82**	**0.00295**	**-256.80**	**870**	**-0.00295**	**2526.43**
83	**-7.82**	**83**	**0.00282**	**-254.55**	**869**	**-0.00282**	**2520.67**
84	**-7.56**	**84**	**0.00273**	**-252.08**	**868**	**-0.00273**	**2516.45**
85	**-7.29**	**85**	**0.00265**	**-247.81**	**867**	**-0.00265**	**2507.85**
86	**-6.72**	**86**	**0.00244**	**-246.25**	**866**	**-0.00244**	**2504.19**
87	**-6.40**	**87**	**0.00235**	**-245.25**	**865**	**-0.00235**	**2482.88**
88	**-5.75**	**88**	**0.00212**	**-242.69**	**864**	**-0.00212**	**2465.81**
89	**-4.71**	**89**	**0.00176**	**-239.04**	**863**	**-0.00176**	**2439.96**
90	**-4.23**	**90**	**0.00158**	**-238.40**	**862**	**-0.00158**	**2437.31**
91	**-3.99**	**91**	**0.00150**	**-236.31**	**861**	**-0.00150**	**2429.16**
92	**-3.47**	**92**	**0.00131**	**-230.76**	**860**	**-0.00131**	**2423.26**
93	**-3.21**	**93**	**0.00122**	**-227.06**	**859**	**-0.00122**	**2415.64**
94	**-2.90**	**94**	**0.00110**	**-225.56**	**858**	**-0.00110**	**2398.98**
95	**-2.75**	**95**	**0.00105**	**-221.35**	**857**	**-0.00105**	**2396.27**
Sum of NOCV eigenvalues:			**0.00000**				

Table S28. Contribution of each basis function shell to NOCV pair 1 orbitals 1 and 951 in TS15

Shell	Type	Atom	Orb. 1	Orb. 951	Pair 1
8	S	1(C)	1.67 %	0.66 %	1.25 %
18	S	2(C)	0.52 %	0.04 %	0.59 %
29	P	3(C)	1.68 %	0.58 %	1.35 %
48	S	5(C)	0.63 %	0.05 %	0.70 %
58	S	6(C)	1.26 %	0.07 %	1.46 %
83	S	10(C)	1.12 %	0.00 %	1.37 %
113	S	14(C)	1.70 %	0.00 %	2.08 %
123	S	15(C)	0.64 %	0.10 %	0.66 %
140	P	18(C)	0.75 %	0.35 %	0.49 %
141	S	18(C)	0.66 %	0.39 %	0.33 %
142	P	18(C)	0.84 %	0.34 %	0.60 %
143	S	18(C)	1.99 %	0.03 %	2.40 %
144	P	18(C)	2.17 %	0.69 %	1.82 %
153	S	19(C)	0.77 %	0.15 %	0.76 %
160	P	20(C)	0.59 %	0.04 %	0.68 %
162	P	20(C)	0.61 %	0.05 %	0.69 %
163	S	20(C)	3.55 %	0.57 %	3.65 %
205	S	26(Pd)	3.55 %	0.98 %	3.15 %
212	D	26(Pd)	0.87 %	3.33 %	-3.01 %
220	S	27(P)	0.48 %	0.02 %	0.56 %
221	S	27(P)	14.64 %	55.75 %	-50.42 %
222	P	27(P)	13.78 %	10.76 %	3.71 %
227	P	27(P)	0.21 %	0.61 %	-0.48 %
236	S	28(C)	8.95 %	0.13 %	10.82 %
237	P	28(C)	2.43 %	1.07 %	1.67 %
246	S	29(C)	0.17 %	2.45 %	-2.79 %
247	P	29(C)	3.44 %	1.31 %	2.61 %
256	S	30(C)	0.41 %	0.80 %	-0.48 %
257	P	30(C)	2.86 %	1.77 %	1.34 %
266	S	31(C)	4.58 %	0.16 %	5.42 %
281	S	33(C)	0.56 %	0.83 %	-0.34 %
282	P	33(C)	0.71 %	0.21 %	0.61 %
296	S	35(C)	1.34 %	1.14 %	0.25 %
321	S	39(C)	1.10 %	0.55 %	0.68 %
322	P	39(C)	1.06 %	0.53 %	0.65 %
331	S	40(C)	0.00 %	0.46 %	-0.56 %
332	P	40(C)	0.63 %	0.85 %	-0.27 %
381	S	46(C)	0.89 %	0.29 %	0.74 %

406	S	50(C)	1.60 %	2.48 %	-1.08 %
407	P	50(C)	2.94 %	1.18 %	2.16 %
416	S	51(C)	0.98 %	0.07 %	1.13 %
441	S	55(C)	2.74 %	2.04 %	0.86 %

Table S29. Contribution of each atom to NOCV pair 1/orbitals 1 and 951 in TS15

Atom	Orb. 1	Orb. 951	Pair 1
1(C):	1.90 %	0.68 %	1.50 %
2(C):	0.68 %	0.11 %	0.70 %
3(C):	1.84 %	0.72 %	1.38 %
4(C):	0.22 %	0.10 %	0.14 %
5(C):	0.81 %	0.09 %	0.88 %
6(C):	1.38 %	0.09 %	1.58 %
7(H):	0.00 %	0.00 %	0.00 %
8(H):	0.00 %	0.00 %	0.00 %
9(H):	0.00 %	0.00 %	0.00 %
10(C):	1.19 %	0.37 %	1.00 %
11(C):	0.68 %	0.17 %	0.63 %
12(H):	0.00 %	0.00 %	0.00 %
13(H):	0.00 %	0.00 %	0.01 %
14(C):	2.22 %	0.50 %	2.10 %
15(C):	0.88 %	0.42 %	0.57 %
16(H):	0.01 %	0.01 %	0.01 %
17(H):	0.01 %	0.00 %	0.01 %
18(C):	6.81 %	2.23 %	5.61 %
19(C):	1.11 %	0.22 %	1.09 %
20(C):	5.45 %	0.75 %	5.77 %
21(H):	0.07 %	0.02 %	0.06 %
22(H):	0.02 %	0.00 %	0.02 %
23(H):	0.21 %	0.02 %	0.23 %
24(F):	0.08 %	0.02 %	0.07 %
25(F):	0.14 %	0.03 %	0.13 %
26(Pd):	4.98 %	5.44 %	-0.56 %
27(P):	29.28 %	67.27 %	-46.58 %
28(C):	11.43 %	1.28 %	12.45 %
29(C):	3.63 %	3.90 %	-0.33 %
30(C):	3.29 %	2.63 %	0.81 %
31(C):	4.63 %	0.20 %	5.43 %
32(H):	0.18 %	0.21 %	-0.03 %
33(C):	1.27 %	1.06 %	0.26 %
34(H):	0.10 %	0.03 %	0.08 %
35(C):	1.53 %	1.30 %	0.29 %
36(H):	0.00 %	0.00 %	-0.00 %

37(H):	0.03 %	0.01 %	0.02 %
38(H):	0.01 %	0.02 %	-0.01 %
39(C):	2.19 %	1.10 %	1.33 %
40(C):	0.63 %	1.35 %	-0.88 %
41(C):	0.37 %	0.17 %	0.25 %
42(C):	0.29 %	0.45 %	-0.20 %
43(H):	0.02 %	0.05 %	-0.04 %
44(C):	0.17 %	0.43 %	-0.32 %
45(H):	0.01 %	0.02 %	-0.00 %
46(C):	0.94 %	0.33 %	0.75 %
47(H):	0.00 %	0.00 %	-0.00 %
48(H):	0.00 %	0.00 %	0.00 %
49(H):	0.00 %	0.00 %	0.00 %
50(C):	4.57 %	3.68 %	1.09 %
51(C):	1.06 %	0.09 %	1.19 %
52(H):	0.00 %	0.01 %	-0.00 %
53(H):	0.00 %	0.02 %	-0.02 %
54(H):	0.00 %	0.02 %	-0.02 %
55(C):	3.01 %	2.19 %	1.00 %
56(H):	0.00 %	0.01 %	-0.01 %
57(H):	0.01 %	0.02 %	-0.02 %
58(H):	0.07 %	0.00 %	0.09 %
59(C):	0.34 %	0.07 %	0.33 %
60(H):	0.04 %	0.02 %	0.03 %
61(H):	0.10 %	0.04 %	0.08 %
62(H):	0.09 %	0.03 %	0.07 %

Table S30. Contribution of each basis function shell to NOCV pair 2/orbitals 2 and 950 in TS15

Shell	Type	Atom	Orb. 2	Orb. 950	Pair 2
8	S	1(C)	0.87 %	0.96 %	-0.03 %
18	S	2(C)	0.67 %	0.38 %	0.09 %
28	S	3(C)	3.01 %	2.63 %	0.12 %
29	P	3(C)	3.93 %	4.22 %	-0.09 %
38	S	4(C)	2.95 %	2.71 %	0.08 %
39	P	4(C)	1.12 %	1.22 %	-0.03 %
83	S	10(C)	0.47 %	0.59 %	-0.04 %
84	P	10(C)	6.38 %	7.08 %	-0.22 %
93	S	11(C)	1.81 %	1.46 %	0.11 %
94	P	11(C)	0.71 %	0.45 %	0.08 %
113	S	14(C)	0.94 %	1.47 %	-0.17 %
114	P	14(C)	3.24 %	3.84 %	-0.19 %
123	S	15(C)	0.56 %	0.52 %	0.01 %

124	P	15(C)	7.38 %	8.25 %	-0.27 %
143	S	18(C)	2.16 %	2.67 %	-0.16 %
144	P	18(C)	8.56 %	7.21 %	0.42 %
153	S	19(C)	2.09 %	1.97 %	0.04 %
154	P	19(C)	1.01 %	0.76 %	0.08 %
163	S	20(C)	9.74 %	7.23 %	0.78 %
204	S	26(Pd)	1.30 %	1.09 %	0.07 %
205	S	26(Pd)	1.31 %	1.11 %	0.06 %
221	S	27(P)	8.06 %	12.21 %	-1.30 %
222	P	27(P)	6.75 %	6.05 %	0.22 %
237	P	28(C)	0.40 %	0.60 %	-0.06 %
246	S	29(C)	2.02 %	1.94 %	0.02 %
256	S	30(C)	2.12 %	1.62 %	0.16 %
257	P	30(C)	1.55 %	1.16 %	0.12 %
266	S	31(C)	1.26 %	0.95 %	0.10 %
281	S	33(C)	3.12 %	2.79 %	0.10 %
321	S	39(C)	0.61 %	0.15 %	0.15 %
332	P	40(C)	0.95 %	0.64 %	0.10 %
351	S	42(C)	1.28 %	0.89 %	0.12 %
406	S	50(C)	0.20 %	1.08 %	-0.27 %
407	P	50(C)	1.92 %	2.17 %	-0.08 %
441	S	55(C)	2.66 %	3.46 %	-0.25 %
466	S	59(C)	0.47 %	0.58 %	-0.03 %

Table S31. Contribution of each atom to NOCV pair 2/orbitals 2 and 950 in TS15

Atom	Orb. 2	Orb. 950	Pair 2
1(C):	0.90 %	1.00 %	-0.03 %
2(C):	0.71 %	0.45 %	0.08 %
3(C):	6.94 %	6.86 %	0.03 %
4(C):	4.07 %	3.93 %	0.04 %
5(C):	0.38 %	0.36 %	0.00 %
6(C):	0.30 %	0.32 %	-0.01 %
7(H):	0.01 %	0.01 %	-0.00 %
8(H):	0.00 %	0.00 %	-0.00 %
9(H):	0.00 %	0.00 %	-0.00 %
10(C):	6.85 %	7.67 %	-0.26 %
11(C):	2.52 %	1.93 %	0.19 %
12(H):	0.01 %	0.00 %	0.00 %
13(H):	0.00 %	0.00 %	-0.00 %
14(C):	4.22 %	5.33 %	-0.35 %
15(C):	7.94 %	8.78 %	-0.26 %
16(H):	0.01 %	0.00 %	0.00 %
17(H):	0.01 %	0.01 %	0.00 %

18(C):	**10.79 %**	**9.92 %**	**0.27 %**
19(C):	**3.15 %**	**2.98 %**	**0.05 %**
20(C):	**10.23 %**	**7.67 %**	**0.80 %**
21(H):	**0.35 %**	**0.27 %**	**0.03 %**
22(H):	**0.04 %**	**0.03 %**	**0.00 %**
23(H):	**0.17 %**	**0.14 %**	**0.01 %**
24(F):	**0.01 %**	**0.06 %**	**-0.02 %**
25(F):	**0.02 %**	**0.07 %**	**-0.02 %**
26(Pd):	**3.80 %**	**3.08 %**	**0.22 %**
27(P):	**15.09 %**	**18.64 %**	**-1.11 %**
28(C):	**0.41 %**	**0.66 %**	**-0.08 %**
29(C):	**2.25 %**	**2.14 %**	**0.03 %**
30(C):	**3.68 %**	**2.79 %**	**0.28 %**
31(C):	**1.31 %**	**1.00 %**	**0.10 %**
32(H):	**0.15 %**	**0.09 %**	**0.02 %**
33(C):	**3.43 %**	**3.00 %**	**0.13 %**
34(H):	**0.02 %**	**0.02 %**	**-0.00 %**
35(C):	**0.43 %**	**0.47 %**	**-0.01 %**
36(H):	**0.00 %**	**0.00 %**	**-0.00 %**
37(H):	**0.00 %**	**0.00 %**	**-0.00 %**
38(H):	**0.00 %**	**0.00 %**	**-0.00 %**
39(C):	**0.65 %**	**0.17 %**	**0.15 %**
40(C):	**1.06 %**	**0.65 %**	**0.13 %**
41(C):	**0.21 %**	**0.11 %**	**0.03 %**
42(C):	**1.49 %**	**1.01 %**	**0.15 %**
43(H):	**0.00 %**	**0.00 %**	**-0.00 %**
44(C):	**0.15 %**	**0.14 %**	**0.00 %**
45(H):	**0.01 %**	**0.01 %**	**-0.00 %**
46(C):	**0.06 %**	**0.03 %**	**0.01 %**
47(H):	**0.00 %**	**0.00 %**	**0.00 %**
48(H):	**0.00 %**	**0.00 %**	**-0.00 %**
49(H):	**0.00 %**	**0.00 %**	**0.00 %**
50(C):	**2.14 %**	**3.27 %**	**-0.35 %**
51(C):	**0.30 %**	**0.21 %**	**0.03 %**
52(H):	**0.00 %**	**0.00 %**	**-0.00 %**
53(H):	**0.01 %**	**0.01 %**	**0.00 %**
54(H):	**0.00 %**	**0.00 %**	**-0.00 %**
55(C):	**2.83 %**	**3.67 %**	**-0.26 %**
56(H):	**0.03 %**	**0.02 %**	**0.00 %**
57(H):	**0.01 %**	**0.00 %**	**0.00 %**
58(H):	**0.00 %**	**0.00 %**	**-0.00 %**
59(C):	**0.58 %**	**0.70 %**	**-0.04 %**
60(H):	**0.00 %**	**0.00 %**	**-0.00 %**
61(H):	**0.26 %**	**0.24 %**	**0.00 %**

62(H):	0.05 %	0.05 %	-0.00 %

Table S32. Pair and NOCV orbital information in TS17

Pair Energy |	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
1********	1	1.09057	-63448.31	567	-1.09057	0.00
2********	2	0.68776	-15402.23	566	-0.68776	0.00
3-3622.33	3	0.23624	-15332.92	565	-0.23624	0.00
4-1211.53	4	0.18880	-6417.04	564	-0.18880	0.00
5 -816.01	5	0.12875	-6338.07	563	-0.12875	0.00
6********	6	0.08505	-6335.15	562	-0.08505	135961.91
7-3737.21	7	0.07698	-6332.83	561	-0.07698	42217.66
8-3547.02	8	0.07317	-6330.02	560	-0.07317	42145.07
9-2752.11	9	0.07087	-6328.92	559	-0.07087	32506.75
10-2159.73	10	0.06769	-6327.71	558	-0.06769	25580.41
11-1689.13	11	0.05327	-6322.39	557	-0.05327	25386.81
12-1577.04	12	0.04986	-6321.86	556	-0.04986	25308.10
13-1059.45	13	0.04598	-6318.78	555	-0.04598	16723.00
14 -821.01	14	0.03588	-6314.96	554	-0.03588	16566.96
15 -800.09	15	0.03505	-6314.63	553	-0.03505	16510.18
16 -723.87	16	0.03356	-6314.53	552	-0.03356	15252.12
17 -677.38	17	0.03141	-6314.08	551	-0.03141	15250.22
18 -630.56	18	0.02929	-6313.84	550	-0.02929	15216.82
19 -595.12	19	0.02765	-6313.23	549	-0.02765	15208.98
20 -516.78	20	0.02455	-5855.03	548	-0.02455	15199.42
21 -431.59	21	0.02207	-4415.67	547	-0.02207	15137.03
22 -419.00	22	0.02144	-4412.76	546	-0.02144	15133.38
23 -413.33	23	0.02117	-4412.66	545	-0.02117	15112.95
24 -306.96	24	0.01778	-2160.58	544	-0.01778	15105.38
25 -283.30	25	0.01722	-1345.51	543	-0.01722	15101.93
26 -265.60	26	0.01617	-1336.03	542	-0.01617	15091.42
27 -252.00	27	0.01536	-1334.03	541	-0.01536	15074.72
28 -219.05	28	0.01385	-778.68	540	-0.01385	15037.05
29 -202.16	29	0.01287	-677.32	539	-0.01287	15024.92
30 -189.40	30	0.01221	-534.91	538	-0.01221	14978.35
31 -178.70	31	0.01162	-515.33	537	-0.01162	14860.13
32 -76.70	32	0.01135	-499.00	536	-0.01135	6256.09
33 -53.74	33	0.01117	-496.38	535	-0.01117	4316.00
34 -51.07	34	0.01086	-471.50	534	-0.01086	4232.39
35 -46.83	35	0.01004	-458.39	533	-0.01004	4205.77
36 -42.85	36	0.00926	-440.72	532	-0.00926	4183.94
37 -39.03	37	0.00857	-439.58	531	-0.00857	4113.17
38 -37.18	38	0.00829	-419.47	530	-0.00829	4067.20

39	-28.53	39	0.00815	-418.33	529	-0.00815	3083.82
40	-27.31	40	0.00790	-375.54	528	-0.00790	3081.52
41	-26.36	41	0.00765	-375.27	527	-0.00765	3071.96
42	-23.75	42	0.00738	-360.62	526	-0.00738	2858.02
43	-21.02	43	0.00676	-357.19	525	-0.00676	2753.09
44	-20.38	44	0.00671	-342.61	524	-0.00671	2696.85
45	-19.54	45	0.00656	-321.24	523	-0.00656	2658.79
46	-18.35	46	0.00622	-304.44	522	-0.00622	2646.68
47	-17.61	47	0.00605	-303.57	521	-0.00605	2606.75
48	-16.80	48	0.00579	-301.96	520	-0.00579	2599.24
49	-14.78	49	0.00515	-292.95	519	-0.00515	2574.90
50	-14.07	50	0.00493	-286.78	518	-0.00493	2565.90
51	-13.25	51	0.00467	-281.10	517	-0.00467	2558.90
52	-12.28	52	0.00436	-268.48	516	-0.00436	2546.23
53	-11.64	53	0.00415	-264.05	515	-0.00415	2542.55
54	-9.80	54	0.00353	-259.20	514	-0.00353	2521.59
55	-9.29	55	0.00336	-253.21	513	-0.00336	2515.69
56	-7.80	56	0.00285	-249.27	512	-0.00285	2485.47
57	-6.35	57	0.00234	-243.40	511	-0.00234	2475.84
58	-5.63	58	0.00209	-241.35	510	-0.00209	2447.06
59	-4.87	59	0.00183	-238.71	509	-0.00183	2418.16
60	-3.43	60	0.00131	-235.43	508	-0.00131	2377.85
61	-3.14	61	0.00121	-231.70	507	-0.00121	2368.56
62	-2.82	62	0.00109	-226.99	506	-0.00109	2359.86
Sum of NOCV eigenvalues:		-0.00000					

Table S33. Contribution of each basis function shell to NOCV pair 1/orbitals 1 and 567 in TS17

Shell	Type	Atom	Orb. 1	Orb. 567	Pair 1
18	S	2(C)	3.88 %	1.05 %	3.10 %
19	P	2(C)	1.22 %	0.36 %	0.94 %
28	S	3(C)	5.81 %	2.20 %	3.94 %
29	P	3(C)	3.90 %	1.60 %	2.51 %
38	S	4(C)	0.49 %	0.00 %	0.53 %
39	P	4(C)	1.10 %	0.76 %	0.37 %
48	S	5(C)	2.15 %	1.03 %	1.23 %
49	P	5(C)	0.72 %	0.10 %	0.68 %
58	S	6(C)	1.35 %	0.47 %	0.96 %
84	P	10(C)	1.08 %	0.69 %	0.43 %
92	P	11(C)	0.50 %	0.06 %	0.48 %
93	S	11(C)	0.53 %	0.04 %	0.53 %
94	P	11(C)	0.11 %	0.72 %	-0.67 %
112	P	14(C)	1.03 %	0.36 %	0.72 %

114	P	14(C)	1.28 %	1.00 %	0.30 %
123	S	15(C)	2.25 %	1.45 %	0.87 %
124	P	15(C)	0.94 %	0.40 %	0.59 %
138	P	18(C)	0.71 %	0.31 %	0.44 %
140	P	18(C)	2.08 %	0.92 %	1.27 %
141	S	18(C)	3.13 %	2.07 %	1.16 %
142	P	18(C)	2.54 %	1.07 %	1.59 %
143	S	18(C)	2.94 %	0.63 %	2.52 %
144	P	18(C)	0.51 %	1.08 %	-0.62 %
152	P	19(C)	0.53 %	0.25 %	0.31 %
153	S	19(C)	11.09 %	6.84 %	4.63 %
154	P	19(C)	0.53 %	0.29 %	0.26 %
158	P	20(C)	0.69 %	0.78 %	-0.10 %
159	S	20(C)	0.32 %	1.28 %	-1.04 %
160	P	20(C)	2.02 %	2.17 %	-0.16 %
161	S	20(C)	1.34 %	2.06 %	-0.78 %
162	P	20(C)	1.69 %	2.02 %	-0.36 %
204	S	26(Pd)	0.00 %	0.46 %	-0.50 %
205	S	26(Pd)	3.50 %	1.46 %	2.23 %
206	S	26(Pd)	0.13 %	0.54 %	-0.44 %
210	P	26(Pd)	0.23 %	0.74 %	-0.57 %
211	P	26(Pd)	1.23 %	0.63 %	0.66 %
212	D	26(Pd)	1.98 %	25.86 %	-26.04 %
213	D	26(Pd)	0.01 %	2.45 %	-2.66 %
221	S	27(Cl)	0.78 %	0.03 %	0.82 %
226	P	27(Cl)	0.40 %	2.04 %	-1.78 %
227	P	27(Cl)	0.30 %	1.77 %	-1.60 %
236	S	28(C)	12.69 %	2.81 %	10.77 %
237	P	28(C)	0.89 %	1.76 %	-0.95 %
248	P	30(C)	0.01 %	0.72 %	-0.78 %
250	P	30(C)	0.00 %	1.01 %	-1.10 %
251	S	30(C)	0.19 %	2.65 %	-2.68 %
266	S	32(C)	10.40 %	14.64 %	-4.62 %
267	P	32(C)	0.79 %	1.01 %	-0.24 %

Table S34. Contribution of each atom to NOCV pair 1/orbitals 1 and 567 in TS17

Atom	Orb. 1	Orb. 567	Pair 1
1(C):	1.04 %	0.39 %	0.71 %
2(C):	5.17 %	1.42 %	4.09 %
3(C):	10.12 %	3.82 %	6.87 %
4(C):	1.70 %	0.79 %	0.99 %
5(C):	3.20 %	1.14 %	2.25 %
6(C):	1.80 %	0.57 %	1.34 %

7(H):	0.00 %	0.00 %	-0.00 %
8(H):	0.00 %	0.00 %	0.00 %
9(H):	0.00 %	0.00 %	0.00 %
10(C):	1.20 %	0.81 %	0.43 %
11(C):	2.07 %	1.00 %	1.17 %
12(H):	0.00 %	0.00 %	0.00 %
13(H):	0.00 %	0.00 %	0.00 %
14(C):	2.61 %	1.64 %	1.05 %
15(C):	3.50 %	1.94 %	1.71 %
16(H):	0.04 %	0.02 %	0.02 %
17(H):	0.25 %	0.13 %	0.13 %
18(C):	12.08 %	6.50 %	6.09 %
19(C):	12.43 %	7.46 %	5.42 %
20(C):	6.72 %	8.57 %	-2.01 %
21(H):	0.11 %	0.02 %	0.10 %
22(H):	0.07 %	0.04 %	0.03 %
23(H):	0.28 %	0.12 %	0.18 %
24(F):	0.19 %	0.10 %	0.10 %
25(F):	0.48 %	0.11 %	0.41 %
26(Pd):	7.51 %	32.34 %	-27.07 %
27(Cl):	1.64 %	4.77 %	-3.42 %
28(C):	13.67 %	5.16 %	9.28 %
29(H):	0.01 %	0.02 %	-0.00 %
30(C):	0.35 %	4.97 %	-5.04 %
31(H):	0.06 %	0.01 %	0.05 %
32(C):	11.25 %	15.87 %	-5.04 %
33(H):	0.24 %	0.02 %	0.24 %
34(H):	0.01 %	0.22 %	-0.23 %
35(H):	0.16 %	0.04 %	0.13 %

Table S35. Contribution of each basis function shell to NOCV pair 2/orbitals 2 and 566 in TS17

Shell	Type	Atom	Orb. 2	Orb. 566	Pair 2
8	S	1(C)	1.41 %	1.04 %	0.25 %
9	P	1(C)	0.69 %	0.80 %	-0.07 %
18	S	2(C)	1.40 %	0.06 %	0.91 %
19	P	2(C)	0.88 %	1.30 %	-0.29 %
28	S	3(C)	23.18 %	15.21 %	5.48 %
29	P	3(C)	2.70 %	5.96 %	-2.24 %
38	S	4(C)	0.64 %	2.38 %	-1.20 %
39	P	4(C)	4.31 %	6.11 %	-1.24 %
48	S	5(C)	0.44 %	0.88 %	-0.31 %
49	P	5(C)	1.87 %	2.22 %	-0.24 %

58	S	6(C)	1.67 %	1.29 %	0.26 %
59	P	6(C)	0.81 %	0.92 %	-0.07 %
84	P	10(C)	5.61 %	10.06 %	-3.06 %
93	S	11(C)	2.19 %	0.54 %	1.13 %
94	P	11(C)	0.59 %	5.59 %	-3.44 %
113	S	14(C)	1.35 %	0.31 %	0.71 %
114	P	14(C)	2.09 %	6.22 %	-2.84 %
123	S	15(C)	0.74 %	0.47 %	0.18 %
124	P	15(C)	6.00 %	12.35 %	-4.37 %
142	P	18(C)	0.13 %	0.62 %	-0.34 %
143	S	18(C)	1.11 %	2.10 %	-0.68 %
144	P	18(C)	3.43 %	0.55 %	1.98 %
153	S	19(C)	0.90 %	0.01 %	0.61 %
154	P	19(C)	2.15 %	0.87 %	0.88 %
163	S	20(C)	11.97 %	5.11 %	4.72 %
164	P	20(C)	0.50 %	0.31 %	0.13 %
204	S	26(Pd)	0.73 %	0.54 %	0.13 %
205	S	26(Pd)	2.00 %	1.18 %	0.57 %
212	D	26(Pd)	1.78 %	1.33 %	0.31 %
236	S	28(C)	4.68 %	3.33 %	0.93 %
237	P	28(C)	0.97 %	0.54 %	0.29 %
257	S	31(H)	0.84 %	0.51 %	0.23 %
264	S	32(C)	0.57 %	0.34 %	0.15 %
266	S	32(C)	3.18 %	2.00 %	0.82 %
267	P	32(C)	0.55 %	0.31 %	0.16 %

Table S36. Contribution of each atom to NOCV pair 2/orbitals 2 and 566 in TS17

Atom	Orb. 2	Orb. 566	Pair 2
1(C):	2.10 %	1.87 %	0.16 %
2(C):	2.27 %	1.36 %	0.63 %
3(C):	25.89 %	21.23 %	3.21 %
4(C):	4.96 %	8.51 %	-2.44 %
5(C):	2.31 %	3.13 %	-0.56 %
6(C):	2.48 %	2.21 %	0.18 %
7(H):	0.01 %	0.03 %	-0.01 %
8(H):	0.00 %	0.00 %	-0.00 %
9(H):	0.00 %	0.01 %	-0.00 %
10(C):	5.64 %	10.28 %	-3.19 %
11(C):	2.92 %	6.35 %	-2.36 %
12(H):	0.00 %	0.00 %	0.00 %
13(H):	0.00 %	0.00 %	-0.00 %
14(C):	3.80 %	6.88 %	-2.12 %
15(C):	6.76 %	12.90 %	-4.22 %

16(H):	0.07 %	0.09 %	-0.01 %
17(H):	0.03 %	0.08 %	-0.03 %
18(C):	4.74 %	3.82 %	0.63 %
19(C):	3.17 %	1.32 %	1.28 %
20(C):	12.86 %	6.31 %	4.50 %
21(H):	0.02 %	0.02 %	-0.00 %
22(H):	0.15 %	0.17 %	-0.01 %
23(H):	0.11 %	0.01 %	0.07 %
24(F):	0.05 %	0.37 %	-0.22 %
25(F):	0.35 %	0.89 %	-0.37 %
26(Pd):	5.52 %	3.50 %	1.39 %
27(Cl):	0.40 %	0.21 %	0.13 %
28(C):	5.85 %	3.92 %	1.33 %
29(H):	0.06 %	0.01 %	0.03 %
30(C):	0.83 %	0.39 %	0.30 %
31(H):	0.85 %	0.52 %	0.23 %
32(C):	5.14 %	3.28 %	1.28 %
33(H):	0.11 %	0.05 %	0.04 %
34(H):	0.11 %	0.05 %	0.04 %
35(H):	0.41 %	0.23 %	0.12 %

Table S37. Pair and NOCV orbital information in TS28

Pair Energy |	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
1********	1	1.30058	-63425.97	981	-1.30058	0.00
2********	2	0.33144	-48165.31	980	-0.33144	0.00
3-3735.91	3	0.24313	-15365.78	979	-0.24313	0.00
4-3133.25	4	0.20520	-15269.04	978	-0.20520	0.00
5-1070.99	5	0.16803	-6373.74	977	-0.16803	0.00
6 -795.82	6	0.12606	-6313.00	976	-0.12606	0.00
7 -705.41	7	0.11179	-6309.85	975	-0.11179	0.00
8 -613.82	8	0.09732	-6307.37	974	-0.09732	0.00
9 -572.43	9	0.09079	-6305.29	973	-0.09079	0.00
10 -475.98	10	0.07549	-6304.99	972	-0.07549	0.00
11 -429.25	11	0.06808	-6304.70	971	-0.06808	0.00
12 -359.37	12	0.05700	-6304.42	970	-0.05700	0.00
13-7340.02	13	0.05157	-6304.17	969	-0.05157	136031.84
14-5295.28	14	0.04843	-6303.94	968	-0.04843	103034.10
15-2235.12	15	0.04600	-6303.78	967	-0.04600	42280.49
16-2184.60	16	0.04506	-6303.56	966	-0.04506	42181.93
17-1606.71	17	0.04132	-6303.48	965	-0.04132	32580.41
18-1179.96	18	0.03692	-6303.09	964	-0.03692	25656.60

19	-1131.12	19	0.03556	-6302.61	963	-0.03556	25507.29
20	-1089.56	20	0.03439	-6302.00	962	-0.03439	25376.78
21	-726.54	21	0.03148	-6301.28	961	-0.03148	16776.69
22	-706.71	22	0.03069	-6301.07	960	-0.03069	16722.80
23	-669.49	23	0.02925	-6301.06	959	-0.02925	16585.99
24	-601.70	24	0.02789	-6300.78	958	-0.02789	15273.50
25	-592.60	25	0.02748	-6300.65	957	-0.02748	15264.34
26	-577.55	26	0.02679	-6298.22	956	-0.02679	15264.17
27	-534.18	27	0.02478	-6296.48	955	-0.02478	15263.52
28	-524.05	28	0.02433	-6296.25	954	-0.02433	15244.41
29	-508.67	29	0.02364	-6291.13	953	-0.02364	15224.25
30	-484.00	30	0.02251	-6291.10	952	-0.02251	15209.27
31	-464.31	31	0.02160	-6290.03	951	-0.02160	15204.25
32	-455.63	32	0.02121	-6286.68	950	-0.02121	15191.19
33	-438.93	33	0.02044	-6285.38	949	-0.02044	15189.18
34	-410.76	34	0.01955	-5832.79	948	-0.01955	15181.35
35	-373.58	35	0.01909	-4393.00	947	-0.01909	15175.00
36	-354.85	36	0.01814	-4390.77	946	-0.01814	15170.48
37	-340.17	37	0.01740	-4390.55	945	-0.01740	15159.08
38	-313.33	38	0.01628	-4084.47	944	-0.01628	15156.72
39	-286.73	39	0.01588	-2899.11	943	-0.01588	15153.44
40	-279.53	40	0.01549	-2898.54	942	-0.01549	15149.98
41	-259.57	41	0.01439	-2896.30	941	-0.01439	15147.23
42	-237.05	42	0.01375	-2094.85	940	-0.01375	15141.74
43	-214.92	43	0.01309	-1283.53	939	-0.01309	15138.48
44	-211.88	44	0.01291	-1278.21	938	-0.01291	15133.70
45	-196.34	45	0.01199	-1258.96	937	-0.01199	15122.57
46	-186.47	46	0.01177	-738.75	936	-0.01177	15108.04
47	-181.70	47	0.01158	-610.08	935	-0.01158	15075.18
48	-175.39	48	0.01130	-516.81	934	-0.01130	15009.89
49	-167.94	49	0.01083	-510.17	933	-0.01083	15002.48
50	-164.89	50	0.01067	-505.85	932	-0.01067	14950.66
51	-159.21	51	0.01033	-489.50	931	-0.01033	14927.80
52	-153.27	52	0.00996	-477.13	930	-0.00996	14909.10
53	-88.34	53	0.00924	-470.28	929	-0.00924	9091.81
54	-87.68	54	0.00922	-453.74	928	-0.00922	9057.78
55	-84.95	55	0.00895	-449.54	927	-0.00895	9044.01
56	-58.20	56	0.00861	-441.29	926	-0.00861	6320.61
57	-42.32	57	0.00832	-439.41	925	-0.00832	4650.23
58	-38.67	58	0.00809	-438.07	924	-0.00809	4340.57
59	-37.33	59	0.00788	-437.27	923	-0.00788	4302.90
60	-35.88	60	0.00766	-421.62	922	-0.00766	4263.07
61	-33.69	61	0.00722	-418.61	921	-0.00722	4245.49
62	-32.57	62	0.00715	-397.94	920	-0.00715	4159.87

63	**-31.06**	**63**	**0.00690**	**-393.83**	**919**	**-0.00690**	**4107.30**
64	**-23.74**	**64**	**0.00678**	**-392.58**	**918**	**-0.00678**	**3108.91**
65	**-23.34**	**65**	**0.00670**	**-378.45**	**917**	**-0.00670**	**3105.73**
66	**-22.65**	**66**	**0.00655**	**-357.67**	**916**	**-0.00655**	**3101.32**
67	**-22.09**	**67**	**0.00640**	**-351.62**	**915**	**-0.00640**	**3100.54**
68	**-21.73**	**68**	**0.00632**	**-350.25**	**914**	**-0.00632**	**3088.87**
69	**-19.04**	**69**	**0.00589**	**-349.90**	**913**	**-0.00589**	**2881.50**
70	**-17.91**	**70**	**0.00574**	**-345.67**	**912**	**-0.00574**	**2773.37**
71	**-17.32**	**71**	**0.00565**	**-340.82**	**911**	**-0.00565**	**2722.90**
72	**-16.31**	**72**	**0.00537**	**-332.11**	**910**	**-0.00537**	**2707.28**
73	**-15.94**	**73**	**0.00529**	**-329.74**	**909**	**-0.00529**	**2682.83**
74	**-15.42**	**74**	**0.00519**	**-305.44**	**908**	**-0.00519**	**2665.25**
75	**-14.72**	**75**	**0.00498**	**-294.79**	**907**	**-0.00498**	**2661.53**
76	**-14.51**	**76**	**0.00491**	**-292.74**	**906**	**-0.00491**	**2661.05**
77	**-13.82**	**77**	**0.00470**	**-287.42**	**905**	**-0.00470**	**2651.03**
78	**-13.43**	**78**	**0.00459**	**-280.33**	**904**	**-0.00459**	**2647.17**
79	**-13.18**	**79**	**0.00451**	**-278.80**	**903**	**-0.00451**	**2643.35**
80	**-12.84**	**80**	**0.00444**	**-266.85**	**902**	**-0.00444**	**2627.89**
81	**-12.27**	**81**	**0.00429**	**-261.53**	**901**	**-0.00429**	**2595.86**
82	**-12.15**	**82**	**0.00427**	**-260.11**	**900**	**-0.00427**	**2587.56**
83	**-11.32**	**83**	**0.00400**	**-257.39**	**899**	**-0.00400**	**2571.80**
84	**-10.74**	**84**	**0.00380**	**-253.50**	**898**	**-0.00380**	**2569.92**
85	**-10.13**	**85**	**0.00359**	**-252.49**	**897**	**-0.00359**	**2568.08**
86	**-9.59**	**86**	**0.00341**	**-252.23**	**896**	**-0.00341**	**2562.33**
87	**-9.33**	**87**	**0.00333**	**-247.87**	**895**	**-0.00333**	**2557.71**
88	**-8.95**	**88**	**0.00322**	**-245.00**	**894**	**-0.00322**	**2539.35**
89	**-8.08**	**89**	**0.00291**	**-241.75**	**893**	**-0.00291**	**2537.22**
90	**-7.83**	**90**	**0.00282**	**-240.22**	**892**	**-0.00282**	**2534.46**
91	**-6.72**	**91**	**0.00244**	**-235.32**	**891**	**-0.00244**	**2521.61**
92	**-5.97**	**92**	**0.00217**	**-233.11**	**890**	**-0.00217**	**2518.28**
93	**-5.69**	**93**	**0.00208**	**-231.84**	**889**	**-0.00208**	**2507.96**
94	**-4.33**	**94**	**0.00160**	**-231.39**	**888**	**-0.00160**	**2480.51**
95	**-3.97**	**95**	**0.00148**	**-228.19**	**887**	**-0.00148**	**2458.48**
96	**-3.66**	**96**	**0.00137**	**-226.89**	**886**	**-0.00137**	**2451.55**
97	**-3.58**	**97**	**0.00134**	**-223.60**	**885**	**-0.00134**	**2443.56**
98	**-3.32**	**98**	**0.00125**	**-219.84**	**884**	**-0.00125**	**2440.87**
99	**-3.13**	**99**	**0.00118**	**-214.34**	**883**	**-0.00118**	**2429.56**
100	**-2.99**	**100**	**0.00113**	**-212.70**	**882**	**-0.00113**	**2418.39**
101	**-2.77**	**101**	**0.00106**	**-209.28**	**881**	**-0.00106**	**2413.40**
Sum of NOCV eigenvalues:			**0.00000**				

Table S38. Contribution of each basis function shell to NOCV pair 1/orbitals 1 and 981 in TS28

Shell	Type	Atom	Orb. 1	Orb. 981	Pair 1
18	S	2(C)	5.77 %	0.37 %	7.02 %
28	S	3(C)	6.71 %	0.56 %	8.00 %
29	P	3(C)	2.61 %	0.17 %	3.17 %
38	S	4(C)	7.39 %	0.68 %	8.72 %
39	P	4(C)	0.41 %	0.02 %	0.51 %
49	P	5(C)	0.68 %	0.23 %	0.58 %
84	P	10(C)	2.31 %	0.09 %	2.89 %
93	S	11(C)	2.52 %	0.22 %	2.99 %
123	S	15(C)	1.98 %	0.36 %	2.11 %
124	P	15(C)	1.59 %	0.01 %	2.05 %
138	P	18(C)	0.54 %	0.14 %	0.52 %
140	P	18(C)	1.51 %	0.39 %	1.46 %
141	S	18(C)	1.14 %	0.52 %	0.81 %
142	P	18(C)	1.86 %	0.41 %	1.88 %
143	S	18(C)	3.65 %	0.00 %	4.74 %
158	P	20(C)	0.50 %	0.10 %	0.51 %
160	P	20(C)	1.42 %	0.29 %	1.47 %
161	S	20(C)	0.75 %	0.33 %	0.55 %
162	P	20(C)	1.45 %	0.32 %	1.47 %
163	S	20(C)	1.47 %	0.22 %	1.63 %
179	S	23(H)	1.15 %	0.13 %	1.33 %
206	S	26(P)	0.38 %	0.59 %	-0.26 %
207	S	26(P)	4.48 %	13.82 %	-12.15 %
208	P	26(P)	2.79 %	8.00 %	-6.78 %
213	P	26(P)	0.16 %	2.87 %	-3.52 %
222	S	27(C)	0.39 %	0.62 %	-0.30 %
223	P	27(C)	3.33 %	8.80 %	-7.11 %
233	P	28(C)	0.26 %	1.66 %	-1.82 %
242	S	29(C)	0.65 %	0.64 %	0.01 %
243	P	29(C)	1.27 %	0.15 %	1.46 %
253	P	30(C)	0.35 %	1.56 %	-1.57 %
258	S	31(H)	0.20 %	0.68 %	-0.62 %
267	S	32(C)	0.03 %	0.85 %	-1.07 %
268	P	32(C)	0.76 %	0.51 %	0.33 %
282	S	34(C)	0.68 %	0.09 %	0.77 %
283	P	34(C)	0.37 %	1.00 %	-0.81 %
307	S	38(C)	0.19 %	2.48 %	-2.98 %
308	P	38(C)	1.52 %	0.96 %	0.73 %
318	P	39(C)	1.09 %	3.39 %	-2.99 %
327	S	40(C)	3.54 %	5.14 %	-2.07 %

328	P	40(C)	2.69 %	4.94 %	-2.92 %
337	S	41(C)	5.32 %	3.28 %	2.65 %
338	P	41(C)	0.44 %	1.12 %	-0.89 %
352	S	43(C)	3.69 %	5.74 %	-2.66 %
353	P	43(C)	1.02 %	2.60 %	-2.06 %
367	S	45(C)	2.55 %	0.63 %	2.50 %
368	P	45(C)	0.18 %	0.87 %	-0.91 %
393	P	49(C)	0.40 %	1.62 %	-1.58 %
402	S	50(C)	0.01 %	0.85 %	-1.08 %
427	S	54(C)	0.19 %	1.21 %	-1.33 %
452	S	58(C)	0.02 %	1.01 %	-1.29 %
463	S	60(H)	0.78 %	0.10 %	0.89 %
480	P	62(Pd)	2.65 %	0.27 %	3.09 %
481	D	62(Pd)	0.81 %	6.76 %	-7.73 %
482	D	62(Pd)	0.00 %	0.79 %	-1.03 %
490	S	63(Cl)	0.00 %	0.86 %	-1.12 %
496	P	63(Cl)	0.06 %	0.64 %	-0.75 %

Table S39. Contribution of each atom to NOCV pair 1/orbitals 1 and 981 in TS28

Atom	Orb. 1	Orb. 981	Pair 1
1(C):	0.52 %	0.04 %	0.61 %
2(C):	5.95 %	0.39 %	7.24 %
3(C):	9.69 %	0.73 %	11.66 %
4(C):	7.85 %	0.71 %	9.28 %
5(C):	1.31 %	0.23 %	1.40 %
6(C):	0.42 %	0.26 %	0.21 %
7(H):	0.00 %	0.00 %	0.00 %
8(H):	0.00 %	0.00 %	0.00 %
9(H):	0.00 %	0.00 %	0.00 %
10(C):	2.62 %	0.37 %	2.93 %
11(C):	3.71 %	0.30 %	4.44 %
12(H):	0.01 %	0.00 %	0.01 %
13(H):	0.00 %	0.00 %	0.00 %
14(C):	0.71 %	0.53 %	0.24 %
15(C):	3.81 %	0.39 %	4.44 %
16(H):	0.20 %	0.03 %	0.23 %
17(H):	0.09 %	0.02 %	0.10 %
18(C):	9.30 %	1.96 %	9.55 %
19(C):	0.47 %	0.14 %	0.43 %
20(C):	5.80 %	1.49 %	5.60 %
21(H):	0.21 %	0.04 %	0.22 %
22(H):	0.13 %	0.03 %	0.13 %
23(H):	1.30 %	0.14 %	1.51 %

24(F):	**0.15 %**	**0.01 %**	**0.19 %**
25(F):	**0.25 %**	**0.02 %**	**0.30 %**
26(P):	**8.00 %**	**25.74 %**	**-23.07 %**
27(C):	**3.79 %**	**9.50 %**	**-7.42 %**
28(C):	**0.30 %**	**1.83 %**	**-2.00 %**
29(C):	**1.93 %**	**0.89 %**	**1.35 %**
30(C):	**0.54 %**	**1.82 %**	**-1.67 %**
31(H):	**0.20 %**	**0.69 %**	**-0.63 %**
32(C):	**0.79 %**	**1.38 %**	**-0.76 %**
33(H):	**0.04 %**	**0.33 %**	**-0.38 %**
34(C):	**1.05 %**	**1.12 %**	**-0.08 %**
35(H):	**0.01 %**	**0.00 %**	**0.01 %**
36(H):	**0.01 %**	**0.00 %**	**0.01 %**
37(H):	**0.00 %**	**0.00 %**	**-0.00 %**
38(C):	**1.79 %**	**3.80 %**	**-2.62 %**
39(C):	**1.18 %**	**3.80 %**	**-3.40 %**
40(C):	**6.24 %**	**10.21 %**	**-5.16 %**
41(C):	**5.77 %**	**4.42 %**	**1.75 %**
42(H):	**0.08 %**	**0.01 %**	**0.09 %**
43(C):	**4.73 %**	**8.38 %**	**-4.76 %**
44(H):	**0.03 %**	**0.04 %**	**-0.02 %**
45(C):	**2.74 %**	**1.71 %**	**1.34 %**
46(H):	**0.05 %**	**0.02 %**	**0.05 %**
47(H):	**0.00 %**	**0.00 %**	**-0.00 %**
48(H):	**0.01 %**	**0.00 %**	**0.01 %**
49(C):	**0.55 %**	**1.71 %**	**-1.51 %**
50(C):	**0.02 %**	**0.90 %**	**-1.13 %**
51(H):	**0.00 %**	**0.03 %**	**-0.03 %**
52(H):	**0.00 %**	**0.01 %**	**-0.01 %**
53(H):	**0.01 %**	**0.01 %**	**-0.00 %**
54(C):	**0.39 %**	**1.41 %**	**-1.33 %**
55(H):	**0.04 %**	**0.30 %**	**-0.35 %**
56(H):	**0.07 %**	**0.03 %**	**0.04 %**
57(H):	**0.01 %**	**0.05 %**	**-0.05 %**
58(C):	**0.06 %**	**1.08 %**	**-1.33 %**
59(H):	**0.02 %**	**0.03 %**	**-0.02 %**
60(H):	**0.78 %**	**0.11 %**	**0.87 %**
61(H):	**0.00 %**	**0.00 %**	**0.00 %**
62(Pd):	**4.05 %**	**8.34 %**	**-5.58 %**
63(Cl):	**0.23 %**	**2.45 %**	**-2.89 %**

Table S40. Contribution of each basis function shell to NOCV pair 2/orbitals 2 and 980 in TS28

Shell	Type	Atom	Orb. 2	Orb. 980	Pair 2
8	S	1(C)	0.80 %	0.90 %	-0.03 %
29	P	3(C)	1.84 %	1.91 %	-0.02 %
38	S	4(C)	0.53 %	0.41 %	0.04 %
39	P	4(C)	0.61 %	0.68 %	-0.02 %
83	S	10(C)	0.79 %	0.88 %	-0.03 %
84	P	10(C)	3.20 %	3.41 %	-0.07 %
113	S	14(C)	1.51 %	1.58 %	-0.02 %
114	P	14(C)	2.87 %	3.04 %	-0.06 %
124	P	15(C)	4.45 %	4.73 %	-0.09 %
143	S	18(C)	1.57 %	2.13 %	-0.18 %
144	P	18(C)	3.02 %	2.44 %	0.19 %
163	S	20(C)	4.46 %	2.97 %	0.49 %
207	S	26(P)	19.94 %	26.26 %	-2.10 %
208	P	26(P)	6.80 %	6.93 %	-0.04 %
222	S	27(C)	0.03 %	0.65 %	-0.21 %
232	S	28(C)	6.98 %	6.04 %	0.31 %
233	P	28(C)	0.95 %	0.95 %	0.00 %
242	S	29(C)	3.50 %	2.39 %	0.37 %
243	P	29(C)	4.05 %	2.54 %	0.50 %
252	S	30(C)	2.36 %	2.34 %	0.01 %
253	P	30(C)	0.52 %	0.35 %	0.06 %
267	S	32(C)	8.09 %	6.43 %	0.55 %
268	P	32(C)	1.04 %	0.62 %	0.14 %
307	S	38(C)	1.07 %	0.85 %	0.07 %
317	S	39(C)	0.48 %	0.75 %	-0.09 %
328	P	40(C)	1.88 %	1.63 %	0.08 %
352	S	43(C)	4.44 %	4.35 %	0.03 %
393	P	49(C)	2.17 %	2.07 %	0.03 %
402	S	50(C)	0.54 %	0.29 %	0.08 %
427	S	54(C)	3.10 %	3.53 %	-0.14 %

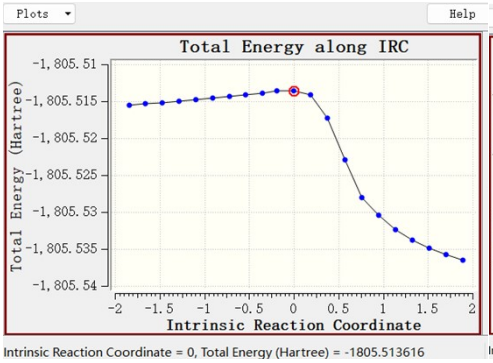
Table S41. Contribution of each atom to NOCV pair 2/orbitals 2 and 980 in TS28

Atom	Orb. 2	Orb. 980	Pair 2
1(C):	0.85 %	0.95 %	-0.03 %
2(C):	0.26 %	0.26 %	-0.00 %
3(C):	2.19 %	2.29 %	-0.03 %
4(C):	1.14 %	1.09 %	0.02 %
5(C):	0.12 %	0.13 %	-0.01 %

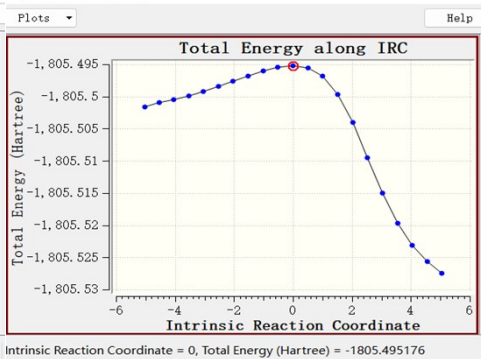
6(C):	0.03 %	0.05 %	-0.01 %
7(H):	0.01 %	0.01 %	0.00 %
8(H):	0.00 %	0.00 %	-0.00 %
9(H):	0.00 %	0.00 %	0.00 %
10(C):	3.99 %	4.30 %	-0.10 %
11(C):	0.46 %	0.38 %	0.03 %
12(H):	0.00 %	0.00 %	0.00 %
13(H):	0.00 %	0.00 %	0.00 %
14(C):	4.39 %	4.63 %	-0.08 %
15(C):	4.50 %	4.78 %	-0.09 %
16(H):	0.02 %	0.01 %	0.00 %
17(H):	0.04 %	0.03 %	0.00 %
18(C):	4.63 %	4.60 %	0.01 %
19(C):	0.38 %	0.31 %	0.02 %
20(C):	4.73 %	3.17 %	0.52 %
21(H):	0.38 %	0.26 %	0.04 %
22(H):	0.00 %	0.00 %	0.00 %
23(H):	0.11 %	0.07 %	0.01 %
24(F):	0.00 %	0.02 %	-0.01 %
25(F):	0.02 %	0.05 %	-0.01 %
26(P):	26.89 %	33.32 %	-2.13 %
27(C):	0.06 %	0.96 %	-0.30 %
28(C):	7.93 %	6.99 %	0.31 %
29(C):	7.56 %	4.94 %	0.87 %
30(C):	2.88 %	2.69 %	0.06 %
31(H):	0.01 %	0.00 %	0.00 %
32(C):	9.13 %	7.05 %	0.69 %
33(H):	0.00 %	0.00 %	0.00 %
34(C):	0.23 %	0.11 %	0.04 %
35(H):	0.00 %	0.00 %	-0.00 %
36(H):	0.00 %	0.00 %	-0.00 %
37(H):	0.00 %	0.00 %	0.00 %
38(C):	1.40 %	1.14 %	0.09 %
39(C):	0.66 %	1.06 %	-0.13 %
40(C):	1.94 %	1.79 %	0.05 %
41(C):	0.29 %	0.38 %	-0.03 %
42(H):	0.03 %	0.04 %	-0.00 %
43(C):	4.71 %	4.60 %	0.04 %
44(H):	0.11 %	0.08 %	0.01 %
45(C):	0.03 %	0.02 %	0.00 %
46(H):	0.00 %	0.00 %	-0.00 %
47(H):	0.00 %	0.00 %	-0.00 %
48(H):	0.00 %	0.00 %	-0.00 %
49(C):	2.26 %	2.09 %	0.06 %

50(C):	**0.57 %**	**0.32 %**	**0.08 %**
51(H):	**0.00 %**	**0.00 %**	**-0.00 %**
52(H):	**0.01 %**	**0.01 %**	**0.00 %**
53(H):	**0.00 %**	**0.01 %**	**-0.00 %**
54(C):	**3.27 %**	**3.72 %**	**-0.15 %**
55(H):	**0.02 %**	**0.02 %**	**0.00 %**
56(H):	**0.00 %**	**0.00 %**	**0.00 %**
57(H):	**0.00 %**	**0.00 %**	**0.00 %**
58(C):	**0.10 %**	**0.07 %**	**0.01 %**
59(H):	**0.00 %**	**0.00 %**	**-0.00 %**
60(H):	**0.35 %**	**0.29 %**	**0.02 %**
61(H):	**0.04 %**	**0.02 %**	**0.00 %**
62(Pd):	**1.12 %**	**0.82 %**	**0.10 %**
63(Cl):	**0.14 %**	**0.06 %**	**0.03 %**

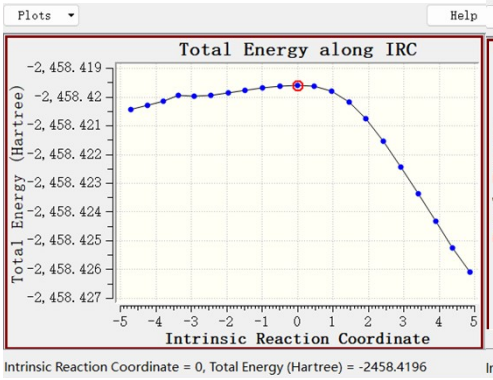
7. IRC diagrams for all transition states



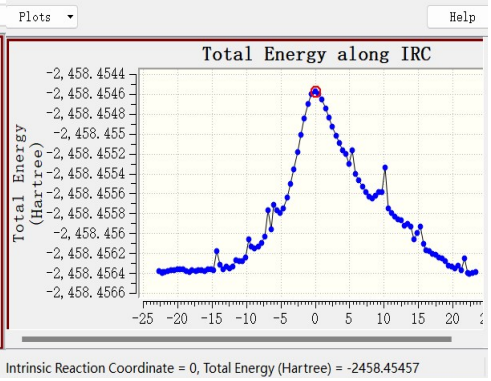
TS1



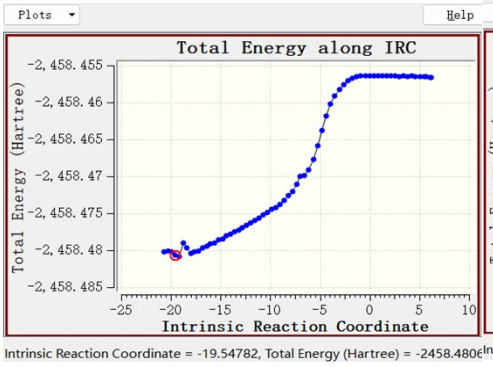
TS2



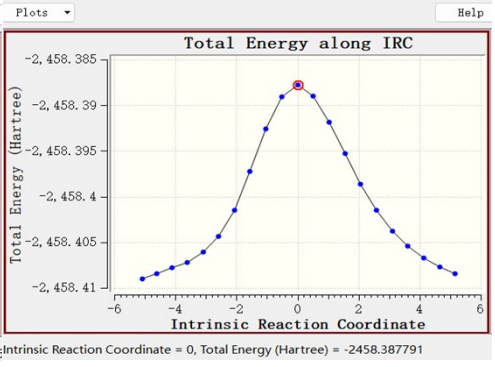
TS3



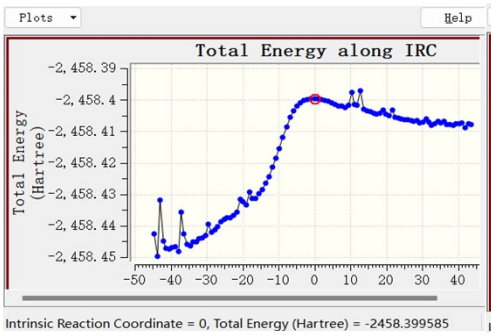
TS4



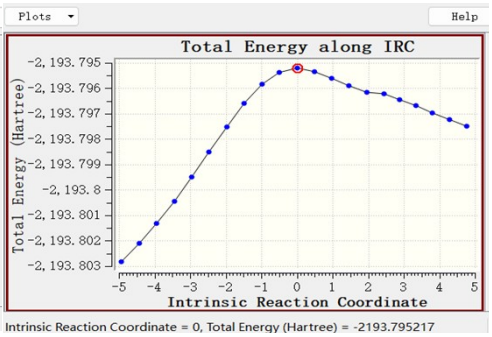
TS5



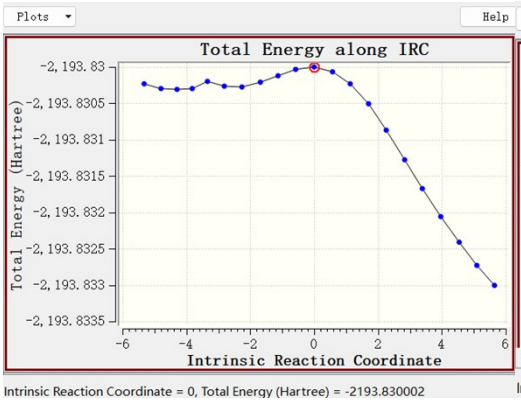
TS6



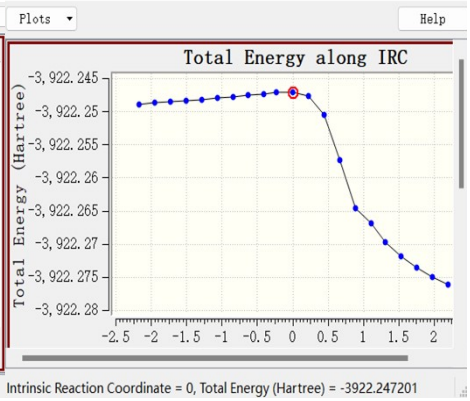
TS7



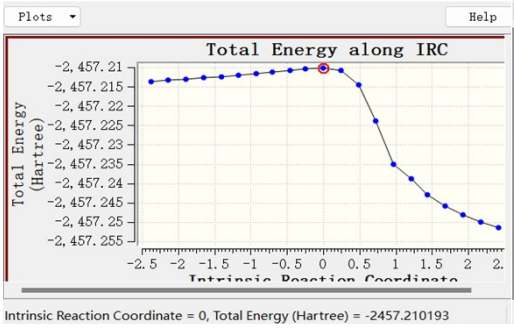
TS8



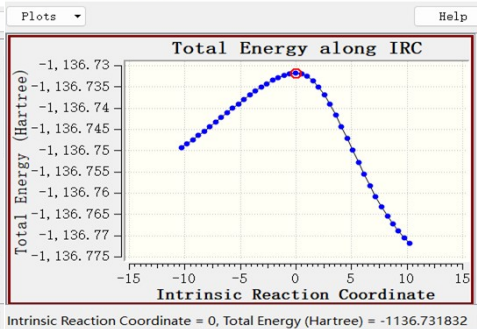
TS9



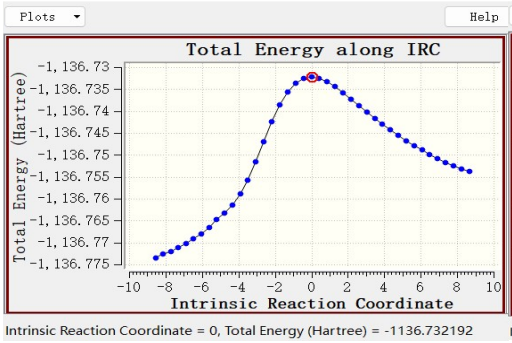
TS10



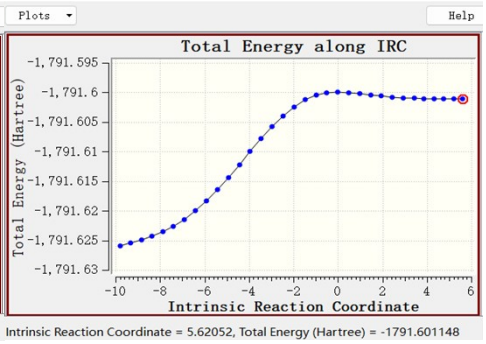
TS11



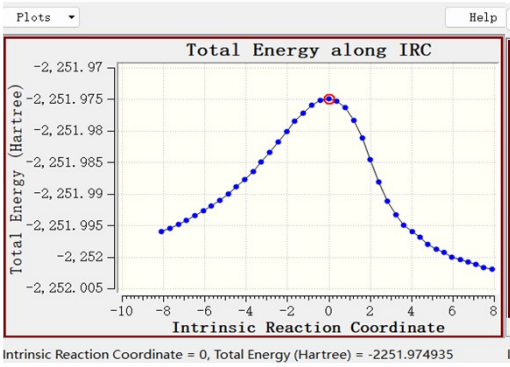
TS12



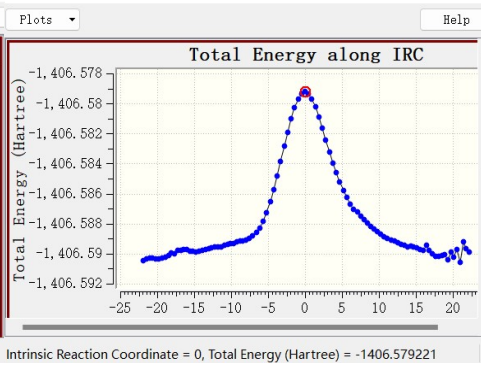
TS13



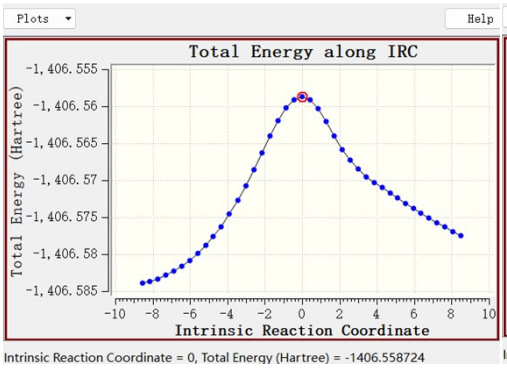
TS14



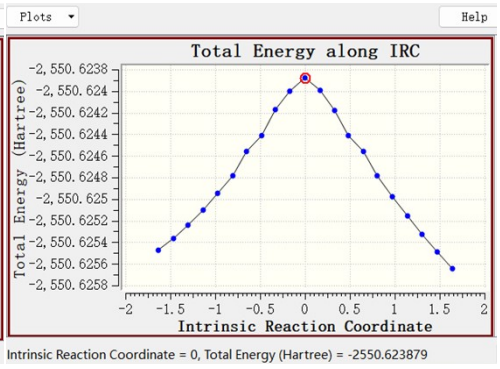
TS15



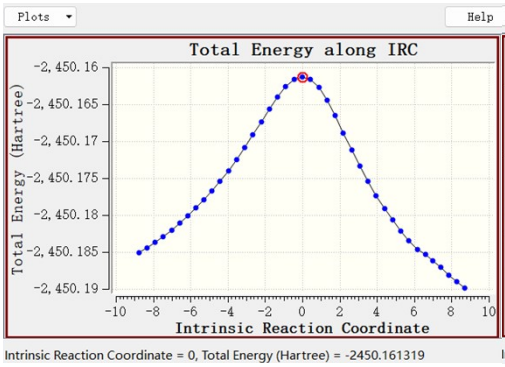
TS16



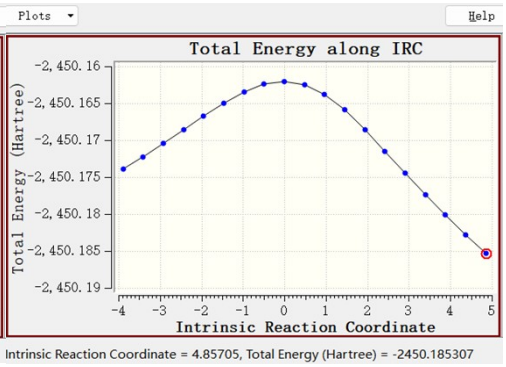
TS17



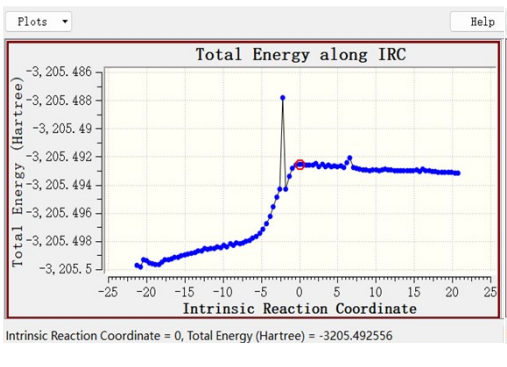
TS18



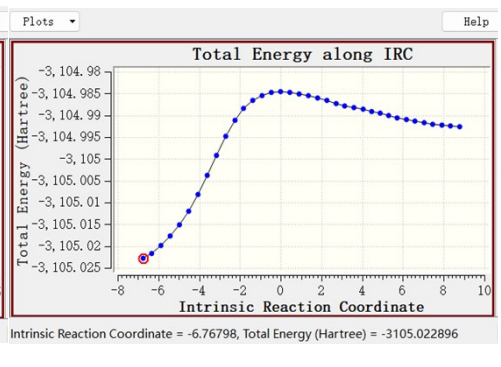
TS19



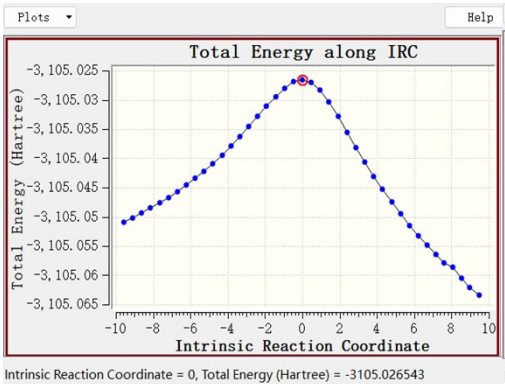
TS20



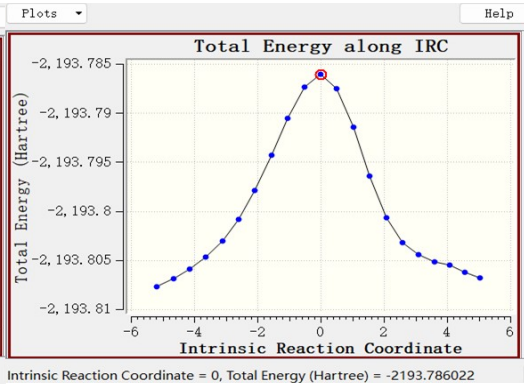
TS21



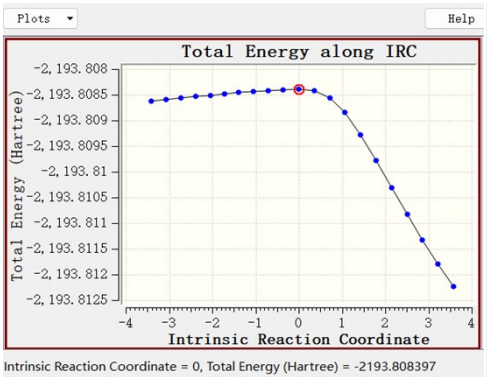
TS22



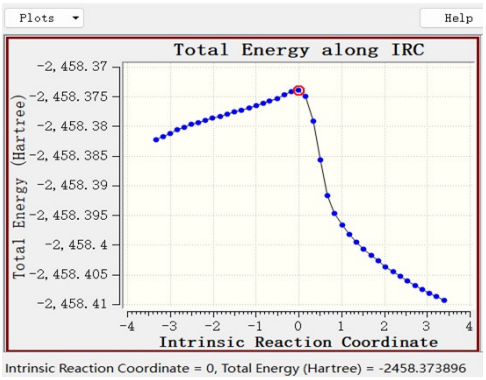
TS23



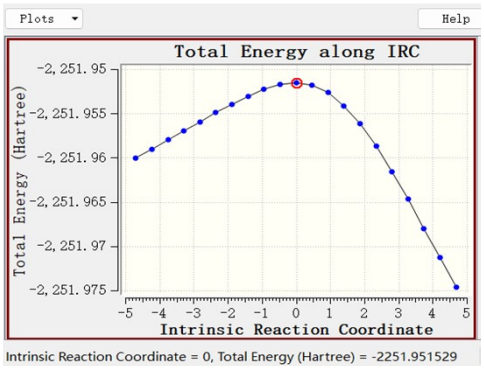
TS24



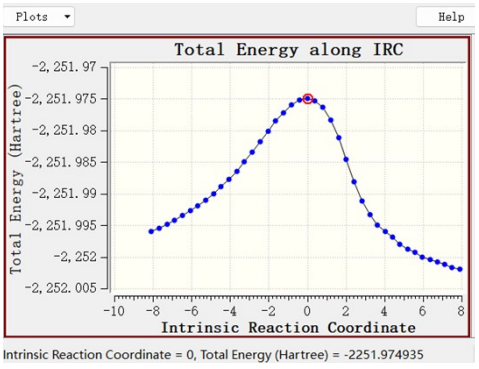
TS25



TS26



TS27



TS28

8. Calculated absolute energies and free energies of all involving acylation reaction structures at the M06L-D3/6-311++G(d,p)-SDD-SMD(diisopropyl ether) //B3LYP-D3/6-31G(d)-SDD-SMD(diisopropyl ether) level of theory

Geometry	$E_{(elec\text{-}B3LYP\text{-}D3)}$[1]	$G_{(corr\text{-}B3LYP\text{-}D3)}$[2]	$H_{(corr\text{-}B3LYP\text{-}D3)}$[3]	$E_{(solv\text{-}M06\text{-}L)}$[4]
2a-acylation	**-1413.803599**	**0.279715**	**0.350744**	**-759.905437**
INT1	**-1805.549476**	**0.291086**	**0.374247**	**-1805.770102**
TS1	**-1805.513616**	**0.285971**	**0.367891**	**-1805.733781**
INT2	**-1805.526577**	**0.289886**	**0.372639**	**-1805.751158**
INT3	**-1805.513551**	**0.289042**	**0.373579**	**-1805.738957**
TS2	**-1805.495176**	**0.287815**	**0.372036**	**-1805.723206**
INT4	**-1805.582310**	**0.291798**	**0.374090**	**-1805.801536**
INT5	**-2458.429132**	**0.484674**	**0.593566**	**-2458.72149**
TS3	**-2458.419600**	**0.484255**	**0.592025**	**-2458.714559**
INT6	**-2458.456631**	**0.486241**	**0.593738**	**-2458.74264**
TS4	**-2458.454830**	**0.486227**	**0.592613**	**-2458.740453**
INT7	**-2458.456741**	**0.486227**	**0.593937**	**-2458.741039**
TS5	**-2458.456382**	**0.485909**	**0.592791**	**-2458.739051**
trans-INT8	**-2458.507853**	**0.486543**	**0.594692**	**-2458.790509**
INT5'	**-2458.413350**	**0.485195**	**0.593323**	**-2458.700817**
TS6	**-2458.387791**	**0.486671**	**0.592074**	**-2458.67335**
INT9	**-2458.418567**	**0.486024**	**0.592704**	**-2458.705711**
TS7	**-2458.399584**	**0.484812**	**0.591794**	**-2458.684033**
cis-INT8	**-2458.487547**	**0.486277**	**0.594057**	**-2458.766541**
INT10	**-2193.811610**	**0.461353**	**0.559142**	**-2194.041409**
TS8	**-2193.795217**	**0.459666**	**0.558601**	**-2194.029193**
INT11	**-2193.830375**	**0.462401**	**0.560610**	**-2194.056725**

TS9	**-2193.830002**	**0.461702**	**0.559394**	**-2194.05573**
INT12	**-2193.889486**	**0.463224**	**0.561415**	**-2194.107314**
1a	**-652.806083**	**0.164683**	**0.216166**	**-652.885062**
$PdCO_3$	**-391.687699**	**-0.012577**	**0.021563**	**-391.78965**
HCO_3^-	**-264.488580**	**0.000503**	**0.030734**	**-264.560235**
INT13	**-3922.291786**	**0.497055**	**0.621114**	**-3922.659357**
TS10	**-3922.247227**	**0.493048**	**0.616043**	**-3922.611799**
INT14	**-3922.330116**	**0.498644**	**0.622231**	**-3922.681061**
trans-3a	**-2066.726535**	**0.475123**	**0.570814**	**-1314.531412**
INT15	**-2458.460029**	**0.486133**	**0.594708**	**-2458.743547**
TS11	**-2458.396307**	**0.483139**	**0.587832**	**-2458.677946**
INT16	**-2458.474687**	**0.486763**	**0.594348**	**-2458.758779**
K_2CO_3	**-1463.717966**	**-0.016409**	**0.024232**	**-1463.841903**
$PdCO_3$-K_2CO_3	**-1855.537773**	**-0.005353**	**0.047754**	**-1855.77662**
INT10'	**-2193.814682**	**0.463621**	**0.561124**	**-2194.039993**
TS24	**-2193.786022**	**0.462143**	**0.558432**	**-2194.008808**
INT34	**-2193.810128**	**0.461269**	**0.560013**	**-2194.036649**
TS25	**-2193.808397**	**0.459083**	**0.558579**	**-2194.035845**
INT35	**-2193.823072**	**0.461155**	**0.560051**	**-2194.047913**
INT36	**-2458.409600**	**0.483049**	**0.592688**	**-2458.699014**
TS26	**-2458.373896**	**0.481834**	**0.587528**	**-2458.657605**
INT37	**-2458.482727**	**0.489129**	**0.594960**	**-2458.76084**
cis-3a	**-2066.719853**	**0.475413**	**0.570733**	**-2066.903953**

1The electronic energy calculated by B3LYP-D3(BJ) in diIsopropyl ether solvent.
2The thermal correction to Gibbs free energy calculated by B3LYP-D3(BJ) in diIsopropyl ether solvent.
3The thermal correction to enthalpy calculated by B3LYP-D3(BJ) in diIsopropyl ether solvent.
4The electronic energy calculated by M06-L in diIsopropyl ether solvent.

9. Calculated absolute energies and free energies of all involving allylation reaction structures at the M06L-D3/6-311++G(d,p)-SDD-SMD(ethyl acetate) //B3LYP-D3/6-31G(d)-SDD-SMD(ethyl acetate) level of theory

Geometry	$E_{(elec\text{-}B3LYP\text{-}D3)}$[1]	$G_{(corr\text{-}B3LYP\text{-}D3)}$[2]	$H_{(corr\text{-}B3LYP\text{-}D3)}$[3]	$E_{(solv\text{-}M06\text{-}L)}$[4]
4a	**-701.081363**	**0.157302**	**0.206801**	**-701.173134**
INT17	**-1136.758452**	**0.265176**	**0.337914**	**-1136.925713**
TS12	**-1136.731832**	**0.26376**	**0.335729**	**-1136.899925**
INT18	**-1136.784128**	**0.265178**	**0.337024**	**-1136.946637**
TS13	**-1136.732192**	**0.26253**	**0.334942**	**-1136.909288**
INT19	**-1136.810201**	**0.265517**	**0.337450**	**-1136.977887**
INT20	**-1791.615608**	**0.444795**	**0.535526**	**-1791.789917**
TS14	**-1791.599985**	**0.443972**	**0.533592**	**-1791.77347**
INT21	**-1791.636871**	**0.44524**	**0.534322**	**-1791.805389**
TS15	**-1791.595598**	**0.443078**	**0.532488**	**-1791.774878**
INT22	**-1791.667715**	**0.444891**	**0.534834**	**-1791.838658**
INT23	**-1406.600466**	**0.221548**	**0.288420**	**-1406.751984**
TS16	**-1406.579221**	**0.220122**	**0.285934**	**-1406.726241**
INT24	**-1406.591149**	**0.221026**	**0.287276**	**-1406.734655**
TS17	**-1406.558724**	**0.220009**	**0.285592**	**-1406.708662**
INT25	**-1406.584967**	**0.219432**	**0.287345**	**-1406.730267**
INT26	**-2550.626537**	**0.571503**	**0.690237**	**-2550.907024**
TS18	**-2550.623879**	**0.568323**	**0.684343**	**-2550.903703**
INT27	**-2550.627854**	**0.561804**	**0.689093**	**-2550.909787**
TS19	**-2450.137541**	**0.559931**	**0.672815**	**-2450.399911**
INT28	**-2450.203278**	**0.560957**	**0.674541**	**-2450.460094**
TS20	**-2450.162028**	**0.561566**	**0.673699**	**-2450.418839**
INT29	**-2450.231099**	**0.564647**	**0.677037**	**-2450.481349**

2a-allylation	**-1413.805178**	**0.279623**	**0.350636**	**-1413.932578**
INT30	**-3205.514767**	**0.754165**	**0.888893**	**-3205.800858**
TS21	**-3205.492556**	**0.748534**	**0.883907**	**-3205.782337**
INT31	**-3205.498337**	**0.751208**	**0.886869**	**-3205.785938**
TS22	**-3104.984628**	**0.736737**	**0.869945**	**-3105.252770**
INT32	**-3105.062184**	**0.744237**	**0.871542**	**-3105.326083**
TS23	**-3105.026543**	**0.742734**	**0.871364**	**-3105.291679**
INT33	**-3105.087882**	**0.744788**	**0.874506**	**-3105.344910**
INT38	**-2251.984839**	**0.445291**	**0.538054**	**-2252.173610**
TS27	**-2251.951529**	**0.442158**	**0.535874**	**-2252.145098**
INT39	**-2252.013585**	**0.445432**	**0.536161**	**-2252.199744**
TS28	**-2251.974935**	**0.44291**	**0.535470**	**-2252.170133**
INT40	**-2251.999266**	**0.444611**	**0.537735**	**-2252.193296**
Pd(0)-^{t}BuPPh$_2$	**-1090.495911**	**0.263237**	**0.327477**	**-1090.578935**
[Pd(II)(allyl)Cl]	**-705.496587**	**0.040345**	**0.079287**	**-705.558087**
Pd(0)-EtOAc	**-435.626067**	**0.084781**	**0.130206**	**-435.695132**
HF	**-100.424814**	**-0.007573**	**0.012173**	**-100.470087**

[1]The electronic energy calculated by B3LYP-D3(BJ) in ethyl acetate solvent.
[2]The thermal correction to Gibbs free energy calculated by B3LYP-D3(BJ) in ethyl acetate solvent.
[3]The thermal correction to enthalpy calculated by B3LYP-D3(BJ) in ethyl acetate solvent.
[4]The electronic energy calculated by M06-L in ethyl acetate solvent.

10. Cartesian coordinates of the acylation structures (optimization in diIsopropyl ether)

2a			
C	-0.14253900	-0.80380200	2.56604800
C	-1.47036800	-1.10167000	2.23032700
C	-1.73125900	-1.71124600	0.99246300
C	-0.70353600	-1.98761100	0.09756000
C	0.60908100	-1.66046900	0.45131500
C	0.90371600	-1.07726800	1.68534200
H	0.07705300	-0.34186200	3.52501600
H	-2.75585100	-1.94899200	0.71879800
H	-0.91017800	-2.44356900	-0.86468000
H	1.92823300	-0.83786500	1.94884000
O	3.17654100	-2.06045100	-0.08781800
O	1.42643800	-2.69923600	-1.84381600
H	-3.19103600	-1.65577000	3.41616500
S	1.90152400	-1.82260700	-0.76893300
N	2.01476700	-0.27360500	-1.49324200
H	1.13106000	-0.08353300	-1.96798900
C	2.46954000	0.82107000	-0.70373100
C	3.82759400	0.91935700	-0.39075900
C	1.56126800	1.80843700	-0.24217500
C	4.29587300	1.98671400	0.37396800
H	4.50048900	0.15040100	-0.75204400
C	2.05961500	2.89520600	0.50292600
C	3.41343200	2.97971800	0.81283500
H	5.35332700	2.05104100	0.61381900
H	1.36534800	3.65606300	0.84602400
H	3.78138300	3.81886200	1.39624700
C	0.16841200	1.66842100	-0.49392700
C	-1.01642700	1.46478500	-0.68087500
C	-2.40266700	1.18173100	-0.83994400
C	-3.35222100	1.75331000	0.03175900
C	-2.83746700	0.28418500	-1.83619500
C	-4.70086800	1.42495100	-0.08943600
H	-3.01887700	2.44219300	0.80202900
C	-4.18820500	-0.03672700	-1.94943100
H	-2.10886000	-0.15842100	-2.50882700
C	-5.12300800	0.52860400	-1.07645400
H	-5.42445200	1.86846200	0.58922400
H	-4.51232900	-0.73110700	-2.71978300
H	-6.17542600	0.27391500	-1.16643100
C	-2.61157900	-0.76142900	3.15514800
H	-2.25948300	-0.30163900	4.08385500
H	-3.30229100	-0.06136600	2.66785100

INT1			
C	-1.28746200	-3.33712600	-0.01598900
C	-2.34193400	-2.76196200	-0.74106600
C	-2.03407100	-1.87515100	-1.78381900
C	-0.71405500	-1.55699500	-2.09408700
C	0.31423400	-2.14894900	-1.35697300
C	0.04089200	-3.04202300	-0.31734800
H	-1.50895700	-4.02874600	0.79305400
H	-2.83947700	-1.41811000	-2.35165800
H	-0.47998300	-0.86341900	-2.89487400
H	0.85189200	-3.50030600	0.23833000
O	2.87437900	-2.79586400	-1.31308500
O	2.07839000	-1.03499300	-2.99194200
H	-4.09231000	-3.99910900	-0.97711700
S	2.00656700	-1.67197300	-1.67607200
N	2.32868300	-0.42502800	-0.56264900
H	1.83798000	0.43023700	-0.83856500
C	2.40413300	-0.73369700	0.82039800
C	3.53403400	-1.40734800	1.29549100
C	1.36928400	-0.39903000	1.73187100
C	3.64902700	-1.74137900	2.64380800
H	4.31373600	-1.66255600	0.58799800
C	1.51665500	-0.70868200	3.09902700
C	2.64417600	-1.38597300	3.54943300
H	4.53469400	-2.26546400	2.99075900
H	0.72667900	-0.42804600	3.78894400
H	2.74147500	-1.63191100	4.60257700
C	0.15353500	0.22331300	1.29865500
C	-1.00857300	0.54627000	0.98560900
C	-2.43055200	0.54584800	0.76973100
C	-3.26757700	-0.06265900	1.72456000
C	-2.98950400	1.12712200	-0.38348500
C	-4.64531900	-0.08766900	1.52035500
H	-2.83130000	-0.51354800	2.61064100
C	-4.36830100	1.09295800	-0.57719600
H	-2.33914200	1.58789400	-1.12050800
C	-5.19839400	0.48886800	0.37260900

H	-5.28817500	-0.55975700	2.25773400	H	-1.43092100	-0.18367900	-2.61402500
H	-4.79512000	1.53972400	-1.47045300	C	-3.79727200	-2.40846900	-0.43983800
H	-6.27357600	0.46846900	0.21898500	H	-2.02870700	-3.57187200	0.03109800
C	-3.77544700	-3.10583800	-0.42174100	C	-4.31383900	-1.38620900	-1.21992100
H	-3.90819000	-3.31939600	0.64408100	H	-3.88214800	0.19522000	-2.63023200
H	-4.45157100	-2.28948400	-0.69286400	H	-4.45236300	-3.03648700	0.15584100
C	1.24602100	3.37105100	-1.42685500	H	-5.38213900	-1.19149700	-1.22245900
O	1.00944100	3.97732000	-0.27611900	C	-3.98936200	2.81817700	-1.06599100
O	0.82155900	2.08280400	-1.33510300	H	-4.21161900	2.87850600	-2.13644000
O	1.74518400	3.83573600	-2.42482300	H	-4.53179000	1.95987300	-0.65106300
Pd	0.22389300	2.29162100	0.54215800	C	-0.23953000	-0.01078800	2.94356600
TS1				O	-1.41546900	-0.48966200	2.68539600
C	-1.57935900	2.71788000	-1.85822300	O	0.69832300	-0.61756600	2.05220400
C	-2.50784300	2.69555500	-0.80779700	O	0.12135500	0.78550300	3.77529100
C	-2.03007200	2.56217700	0.50609200	Pd	-0.81621400	-1.43020000	0.91194900
C	-0.66737700	2.44820000	0.76843300	INT2			
C	0.23234700	2.44898600	-0.30134200	C	-2.05547400	2.76835700	-1.76713900
C	-0.21093700	2.58789100	-1.61619600	C	-3.01872000	2.55048900	-0.77013700
H	-1.93037600	2.83832700	-2.88037200	C	-2.58219000	2.28994900	0.53684600
H	-2.73295500	2.55021600	1.33533500	C	-1.22406600	2.22539900	0.84379700
H	-0.30559000	2.37129700	1.78849000	C	-0.29017600	2.41725500	-0.17485300
H	0.50483200	2.60072600	-2.43179700	C	-0.69284500	2.70353700	-1.48012400
O	2.74476800	2.61935600	-1.15449100	H	-2.37576100	2.98716400	-2.78275200
O	2.28353800	2.75771900	1.34193700	H	-3.31138100	2.12835600	1.32670100
H	-4.39824300	3.71733700	-0.58804000	H	-0.90003300	2.03581100	1.86069000
S	1.97361300	2.18214100	0.02383100	H	0.04333600	2.85923900	-2.26274500
N	1.94015300	0.51410100	0.12948700	O	2.19706300	3.39264500	-0.31765500
H	1.24185500	0.00446700	1.30242400	O	1.58484600	1.91406400	1.63520800
C	2.88013300	-0.28156600	-0.45811800	H	-4.98772800	3.41123100	-0.54393200
C	4.24307800	0.04099700	-0.67630400	S	1.45277500	2.21797100	0.17362500
C	2.45668400	-1.62161200	-0.81930700	N	1.70931000	0.83321600	-0.66528400
C	5.13309400	-0.93775500	-1.07958500	H	0.99855700	0.38750500	2.11605200
H	4.59250800	1.04467100	-0.46904400	C	2.90129500	0.25459000	-0.76280200
C	3.41114800	-2.62302200	-1.16255600	C	4.18518700	0.84903800	-0.51317200
C	4.73577600	-2.27969400	-1.29974400	C	2.89512700	-1.18595600	-1.10413400
H	6.18073100	-0.67285100	-1.19674600	C	5.32978200	0.10068500	-0.59723600
H	3.06317000	-3.63189700	-1.36266400	H	4.23213100	1.90742100	-0.28338800
H	5.47163500	-3.02335000	-1.58807600	C	4.12427200	-1.92111000	-1.15879700
C	1.09915700	-1.85603500	-0.94491800	C	5.31368500	-1.29339800	-0.91916500
C	-0.14418000	-1.96766800	-0.99259300	H	6.28704400	0.58294100	-0.41632800
C	-1.54882200	-1.86088300	-1.25069900	H	4.08138300	-2.97738400	-1.40547800
C	-2.09631800	-0.81693100	-2.03913200	H	6.24918700	-1.84093300	-0.97252600
C	-2.41086200	-2.66937000	-0.44078300	C	1.66487900	-1.75895500	-1.22260400
C	-3.46248200	-0.60246000	-2.02542900	C	0.42524900	-1.93224900	-1.07243300

C	-0.96551500	-1.99236600	-1.39324200	H	4.27665700	0.01067000	-2.15776000
C	-1.63267400	-0.94935500	-2.09989500	H	5.33192800	2.25864500	-2.13532000
C	-1.73375300	-2.97498500	-0.68084300	C	1.81890800	-0.54277900	-1.20656100
C	-3.01105100	-0.91724600	-2.11514100	C	0.87123300	-1.39730200	-0.98098000
H	-1.03975000	-0.18366100	-2.58659500	C	-0.47836600	-1.76660900	-1.30896900
C	-3.14773700	-2.89755300	-0.71324400	C	-1.29978300	-0.80731500	-1.94226300
H	-1.25086300	-3.87319400	-0.30295300	C	-1.00224100	-3.03339600	-0.98489700
C	-3.77159700	-1.88449300	-1.41639400	C	-2.61277300	-1.12774200	-2.26397200
H	-3.52075800	-0.12522900	-2.65559800	H	-0.90010400	0.17896400	-2.14883200
H	-3.72901000	-3.65758600	-0.20063600	C	-2.32444900	-3.33598200	-1.29429400
H	-4.85595600	-1.83095000	-1.44369200	H	-0.37021700	-3.75995400	-0.48364100
C	-4.49398500	2.59355500	-1.08414200	C	-3.12754300	-2.38774900	-1.93756800
H	-4.67664600	2.74076000	-2.15359400	H	-3.24418500	-0.38759800	-2.74484500
H	-4.98777400	1.66350000	-0.77656800	H	-2.73055900	-4.30925000	-1.03519400
C	-0.67852500	-0.31215400	3.01793600	H	-4.16036100	-2.62682300	-2.17577900
O	-1.56667900	-1.09135300	2.51339000	C	-5.78884400	-0.17254200	-0.10116300
O	0.55079300	-0.49586100	2.28648700	H	-6.59412500	0.33462900	0.44691500
O	-0.72582200	0.47929700	3.93103700	H	-6.06910800	-0.16895700	-1.16110700
Pd	-0.50074300	-1.59833900	0.75774200	C	0.75832200	-1.15170700	2.56476200
INT3				O	1.45486800	-0.04288300	2.20913200
C	-4.16458700	1.70821700	-0.56623400	O	1.25011800	-2.26059300	2.06237400
C	-4.46745700	0.52144100	0.11907200	O	-0.21782400	-1.11103800	3.30362300
C	-3.51961700	0.00095700	1.01200300	Pd	2.18920400	-2.15070500	0.26040200
C	-2.29482200	0.63238600	1.21502000	TS2			
C	-2.01924200	1.80528700	0.50899800	C	4.29763900	-1.52399000	-0.22887000
C	-2.94543700	2.35661600	-0.37801100	C	3.89944700	-2.15164600	-1.41545700
H	-4.89101500	2.12789400	-1.25815100	C	2.96513000	-1.50005500	-2.24061500
H	-3.73528900	-0.91843500	1.54959800	C	2.44760200	-0.25559700	-1.89755600
H	-1.57432600	0.21414600	1.91072500	C	2.85856800	0.33893900	-0.69946000
H	-2.71205500	3.27428500	-0.90782900	C	3.78170800	-0.28089200	0.13900100
O	-0.51084500	3.97099700	0.20260300	H	5.01160900	-2.01691100	0.42545800
O	0.01384000	2.39611600	2.11769600	H	2.64448000	-1.97535300	-3.16439200
H	-5.75894800	-1.21141800	0.24252400	H	1.72626100	0.23985700	-2.53944900
S	-0.42708900	2.58736800	0.71008400	H	4.07181300	0.19030700	1.07107600
N	0.48150200	1.55591800	-0.21382600	O	2.63591200	2.24804900	1.13267900
H	0.92719100	0.75803100	2.43057000	O	2.58376300	2.92066700	-1.30742500
C	1.67089100	1.84082100	-0.70490300	H	3.67346000	-4.16730400	-2.16627200
C	2.34084800	3.12036400	-0.72082800	S	2.23758500	1.94805200	-0.25399800
C	2.42032500	0.68980300	-1.27075700	N	0.57629600	1.64698300	-0.35871200
C	3.60775100	3.23465300	-1.21825500	H	-5.51264300	-2.01258400	1.43209600
H	1.81601600	3.98556900	-0.33505700	C	-0.31467200	2.64047500	-0.10706000
C	3.75099800	0.87537700	-1.76378600	C	-0.14686300	4.04691800	-0.21507200
C	4.32870100	2.11274100	-1.74755300	C	-1.63966700	2.12747800	0.18103000
H	4.08987400	4.20869400	-1.21645600	C	-1.26967200	4.84915100	-0.16467500

H	0.83325300	4.47151800	-0.39444000
C	-2.77209700	2.96938200	0.16097200
C	-2.58069900	4.32573700	0.00805900
H	-1.14804100	5.92264200	-0.28205400
H	-3.75648100	2.54207900	0.32483000
H	-3.42650600	5.00544300	0.03443100
C	-1.56816800	0.74994800	0.41155200
C	-0.46887100	-0.02918600	0.48362400
C	0.47579800	-0.69713700	1.34643200
C	0.97801700	-0.04115700	2.48946400
C	0.88061700	-2.01611500	1.06573700
C	1.84902800	-0.70872000	3.34355200
H	0.68782900	0.98411600	2.68863500
C	1.75779500	-2.67476200	1.92177100
H	0.50412700	-2.50865500	0.17461000
C	2.23822400	-2.02372500	3.06227500
H	2.23044900	-0.20356800	4.22602500
H	2.06874500	-3.69122900	1.70002900
H	2.92184200	-2.53883800	3.73164200
C	4.46290300	-3.49201800	-1.81605800
H	5.18062100	-3.38179300	-2.63974300
H	4.98406000	-3.97576400	-0.98380600
C	-4.76784800	-2.19938600	-0.28841400
O	-4.72168700	-1.67101000	0.97700100
O	-3.76773500	-1.82113100	-1.03045100
O	-5.67728600	-2.93488000	-0.63872500
Pd	-2.06820800	-0.87471900	-0.50803800
INT4			
C	2.79668700	0.40322600	2.92184200
C	3.60524000	-0.74403700	2.98822000
C	4.18551800	-1.22682200	1.80660900
C	3.96155200	-0.59819800	0.58267900
C	3.14864000	0.53637900	0.55040700
C	2.55938600	1.04775100	1.71179800
H	2.35161500	0.79806100	3.83162100
H	4.82206600	-2.10671200	1.84245400
H	4.41454700	-0.97517500	-0.32723400
H	1.94356500	1.93976800	1.66778800
O	2.36190800	2.67955600	-0.80102200
O	3.76777900	0.92874400	-2.00876200
H	4.64575400	-2.16443000	4.24946200
S	2.75495400	1.28697700	-1.01559400
N	1.29721700	0.46922200	-1.49260800
H	-3.42577400	-3.00196300	0.07628200
C	1.32910800	-0.93078100	-1.76392700
C	2.28866200	-1.68264900	-2.44032900
C	0.15497100	-1.52561700	-1.22605700
C	2.04326500	-3.04864300	-2.59402700
H	3.18123600	-1.22185200	-2.84418600
C	-0.07262500	-2.89707400	-1.40765800
C	0.87585400	-3.65060700	-2.09163100
H	2.76948700	-3.65540100	-3.12759600
H	-0.97742700	-3.35410200	-1.01799100
H	0.71470900	-4.71411000	-2.24363200
C	-0.57782500	-0.48625300	-0.54325500
C	0.11788400	0.68635700	-0.73142800
C	-0.58833400	1.90205000	-0.41410200
C	-0.59516400	3.07697500	-1.18173500
C	-1.54446400	1.75044600	0.65648000
C	-1.57076500	4.03844900	-0.94934700
H	0.12848300	3.19998600	-1.97829100
C	-2.53454100	2.75174200	0.85441300
H	-1.23684800	1.16800300	1.53553800
C	-2.55990900	3.87154700	0.04414000
H	-1.58561600	4.93371300	-1.56541200
H	-3.24507000	2.63598700	1.66732000
H	-3.31468300	4.63852500	0.18799500
C	3.82476000	-1.44300300	4.30611900
H	4.05125300	-0.72586300	5.10353900
H	2.92126100	-1.98835800	4.60947300
C	-4.63732200	-1.54480800	0.79762400
O	-3.58548900	-2.05754200	-0.10720000
O	-4.40205800	-0.31136200	0.99681500
O	-5.48566100	-2.31773600	1.17495400
Pd	-2.38768800	-0.26900300	0.21155100
INT5			
C	-2.67150100	0.27742700	1.58397700
C	-1.63360700	-0.61023700	1.94522300
C	-0.25810100	-0.72151400	2.38440400
C	0.17289500	-1.92654000	2.96728400
C	0.64683900	0.34334400	2.23284300
C	1.49291300	-2.06111700	3.39107000
H	-0.52733100	-2.74912500	3.07057400
C	1.96441800	0.20293700	2.65584300
H	0.31474200	1.26613200	1.77422400
C	2.38917000	-1.00013700	3.23122200
H	1.82507000	-2.99541500	3.83378500
H	2.66494200	1.02245300	2.52778800

H	3.42090900	-1.11021900	3.55416800	C	5.30405900	2.43740900	-0.16373000
C	-3.08793900	1.66024200	1.42862300	H	4.13986700	2.29771600	-1.98198800
C	-2.19432100	2.67782800	1.04811300	C	5.34894300	0.45513900	1.21071700
C	-4.44396200	1.96631900	1.65370700	H	4.22905200	-1.23453000	0.48706700
C	-2.65140600	3.98607800	0.91905300	C	5.74396500	1.78746600	0.99659700
H	-1.16126200	2.44013100	0.82278800	H	5.59908500	3.46708500	-0.34673400
C	-4.89030300	3.27917600	1.52882200	H	5.68174600	-0.06352000	2.10643200
H	-5.12932900	1.17010400	1.92762300	C	6.62249800	2.48819900	2.00239400
C	-3.99504300	4.28962700	1.16286300	H	7.58224900	1.96815100	2.11325800
H	-1.95974300	4.76639800	0.61707400	H	6.83025200	3.52136100	1.70755700
H	-5.93528900	3.51383600	1.70966000	H	6.15108800	2.50549600	2.99307800
H	-4.34618800	5.31285900	1.06011100	Pd	-2.39715000	-0.82055700	-0.34903100
C	-3.00035600	-1.00154900	2.19326600	C	-4.23092600	-1.07179200	-2.02247600
O	-3.80605900	-1.75786800	2.69566500	O	-4.58481100	-0.71072800	-0.87157700
C	-0.46854600	-1.13827200	-0.65470100	O	-2.99694300	-1.29653800	-2.31546700
C	0.17400200	-2.40440500	-0.41241200	O	-5.15749800	-1.22483900	-2.97214700
C	-0.30219000	-3.63191700	0.07384100	H	-4.70699800	-1.51433700	-3.78846000
C	1.55211800	-2.24613500	-0.70215400	TS3			
C	0.59640100	-4.67537000	0.26304000	C	-1.95377600	0.70323100	1.35442200
H	-1.35791300	-3.74989400	0.30359800	C	-0.96079100	-0.01035300	2.03250700
C	2.45922300	-3.29290000	-0.51105600	C	0.33329600	0.02322700	2.65831900
C	1.96217200	-4.50166900	-0.02513800	C	0.70259700	-1.06491500	3.47677900
H	0.24388200	-5.63192600	0.63903300	C	1.27545300	1.03211600	2.37165100
H	3.51004800	-3.18343200	-0.74466800	C	1.98336100	-1.12676800	4.01615400
H	2.65178300	-5.32702300	0.12952100	H	-0.01666300	-1.85532800	3.66779500
C	0.47256700	-0.23923400	-1.07599500	C	2.55516200	0.95824200	2.91081500
C	0.29736100	1.20104200	-1.31910500	H	1.00583200	1.84702300	1.71084200
C	1.12434800	2.15345200	-0.70057500	C	2.90874600	-0.11539500	3.73679500
C	-0.76077900	1.64884100	-2.12843900	H	2.26439200	-1.96517200	4.64650000
C	0.90705500	3.51711500	-0.89378100	H	3.28138100	1.73201200	2.68202400
H	1.93116700	1.82154800	-0.05788400	H	3.90934700	-0.16734800	4.15736600
C	-0.98351600	3.01395900	-2.31068200	C	-2.27930400	2.12212500	1.16523200
H	-1.39596600	0.92058200	-2.62352100	C	-1.54846200	3.11535600	1.84699100
C	-0.14826600	3.95316300	-1.70047300	C	-3.34702700	2.51460800	0.33575400
H	1.56097100	4.23826300	-0.41002500	C	-1.86456300	4.46109000	1.68465200
H	-1.80724000	3.34316900	-2.93820800	H	-0.74751500	2.83139900	2.51998400
H	-0.31786800	5.01568800	-1.85277100	C	-3.65351700	3.86388700	0.17173100
N	1.74497300	-0.90369800	-1.10478900	H	-3.93655900	1.76162100	-0.17640600
S	3.09640300	-0.38190900	-2.04676700	C	-2.91220400	4.84082900	0.83989900
O	2.61131900	0.58378400	-3.03060000	H	-1.29312400	5.21497400	2.21922800
O	3.79756600	-1.59330900	-2.47584000	H	-4.47676200	4.15019200	-0.47667700
C	4.11259100	0.46729300	-0.84748700	H	-3.15354000	5.89241800	0.71082100
C	4.49032700	1.78661300	-1.09220300	C	-2.20101200	-0.66766700	2.16323000
C	4.53878500	-0.21213000	0.29815000	O	-2.93424800	-1.38573800	2.80641800

C	-0.80222400	-1.26570100	-0.47553900	O	-3.63910500	-1.65937200	-1.72642500
C	-0.22601000	-2.50918600	-0.02185300	O	-5.86469300	-1.49781500	-2.07606900
C	-0.73674600	-3.56667200	0.74716800	H	-5.58284500	-2.08054300	-2.80648800
C	1.12974300	-2.53153100	-0.43558200	INT6			
C	0.10290900	-4.62498500	1.07796100	C	1.84305600	0.61543600	-0.06945400
H	-1.76905800	-3.54071600	1.08409200	C	1.25374100	0.99770400	-1.26206100
C	1.97508900	-3.59606800	-0.11123200	C	0.90809600	2.29012600	-1.88808500
C	1.44228000	-4.63683400	0.64898800	C	0.80255100	2.39923500	-3.28581300
H	-0.27775900	-5.45060200	1.67308500	C	0.62300800	3.41751100	-1.09619000
H	3.00459400	-3.62188100	-0.44296100	C	0.44382800	3.61164000	-3.87531400
H	2.08298900	-5.47326900	0.91473400	H	1.00771700	1.53716600	-3.91302200
C	0.17447700	-0.54236600	-1.10793800	C	0.26414900	4.62539900	-1.69057900
C	0.09833300	0.85990300	-1.54224600	H	0.68263400	3.34488900	-0.01638100
C	1.04001900	1.80575600	-1.10345500	C	0.17748600	4.73019900	-3.08187100
C	-0.98918000	1.29671600	-2.31682400	H	0.37629800	3.68097800	-4.95756900
C	0.88977500	3.15506400	-1.41869000	H	0.04714900	5.48611400	-1.06363600
H	1.87410500	1.48287900	-0.49210300	H	-0.10150600	5.67350800	-3.54302300
C	-1.14147200	2.64885300	-2.62386800	C	2.57604400	1.34005100	0.95009000
H	-1.70782400	0.56820500	-2.68013700	C	3.25347500	2.54117300	0.64284400
C	-0.20513400	3.58316400	-2.17510100	C	2.69481600	0.80552700	2.24946800
H	1.62430400	3.87383100	-1.06442200	C	3.99870800	3.19487200	1.61820900
H	-1.99237300	2.97148600	-3.21775600	H	3.20512800	2.94504300	-0.36217100
H	-0.32740200	4.63644000	-2.41245900	C	3.42547200	1.47536100	3.22551700
N	1.38292200	-1.31047300	-1.10496900	H	2.18175500	-0.11860100	2.49082600
S	2.66564200	-1.08918900	-2.24058100	C	4.07824100	2.67107600	2.91358100
O	2.13993500	-0.32305800	-3.36912700	H	4.52220800	4.11340200	1.36820400
O	3.26745300	-2.40699100	-2.45276800	H	3.48760800	1.06288200	4.22825700
C	3.81958900	-0.07205600	-1.33309800	H	4.65477900	3.19011900	3.67440700
C	4.29902700	1.09544100	-1.92508700	O	0.57716600	-0.80538900	-2.84158200
C	4.24434200	-0.47531700	-0.06411800	C	-0.01990000	-1.67021300	0.20321200
C	5.22080400	1.87454400	-1.22516300	C	-0.72028100	-2.78348400	-0.42206100
H	3.94298000	1.39558600	-2.90443600	C	-0.33958100	-3.72562000	-1.39158700
C	5.16291600	0.31700400	0.61663900	C	-2.02270300	-2.84318300	0.12936100
H	3.85286100	-1.37736500	0.39537400	C	-1.25653400	-4.69280900	-1.78894200
C	5.66428600	1.50187900	0.05070600	H	0.65958200	-3.70333900	-1.80999900
H	5.59680000	2.78754300	-1.67896100	C	-2.94037200	-3.82924800	-0.24761000
H	5.49534900	0.01338300	1.60583200	C	-2.54061400	-4.74402000	-1.21967200
C	6.63851600	2.35836500	0.82044200	H	-0.97287900	-5.42525900	-2.54001200
H	7.43397700	1.75079300	1.26735500	H	-3.92517000	-3.87747000	0.19517700
H	7.10395600	3.11490000	0.18113100	H	-3.23766700	-5.51657100	-1.53280100
H	6.13304600	2.88271100	1.64259300	C	-0.88504300	-1.08191900	1.08742200
Pd	-2.66370800	-0.69159800	-0.10283200	C	-0.68393900	0.05167500	2.01934000
C	-4.77768100	-1.19001000	-1.35890000	C	-0.72126600	1.37562000	1.56360600
O	-4.90613600	-0.44887300	-0.34958600	C	-0.46682100	-0.19642500	3.38308200

C	-0.52904200	2.43447800	2.45271000	H	0.05951200	4.17233500	-4.66684900
H	-0.91693500	1.57297000	0.51636100	H	-0.12411100	5.53950500	-0.58894200
C	-0.26579700	0.86124700	4.26873300	H	-0.36764100	5.99527000	-3.02500000
H	-0.46213500	-1.22157800	3.74211500	C	2.62352700	1.38695200	0.68461400
C	-0.29370800	2.18014000	3.80438200	C	3.30556900	2.54806600	0.25737000
H	-0.56841600	3.45729000	2.08716100	C	2.81028300	0.93675600	2.00805900
H	-0.09278600	0.65756000	5.32205400	C	4.13286900	3.23928600	1.13632300
H	-0.13838300	3.00393100	4.49591300	H	3.19976500	2.88970500	-0.76620400
N	-2.12570100	-1.80422800	1.08901500	C	3.61375500	1.65105200	2.89093000
S	-3.61757400	-0.96926500	1.38669700	H	2.29026200	0.04533900	2.34056100
O	-3.55373600	-0.41637900	2.73793200	C	4.27931100	2.80099600	2.45727100
O	-4.68818000	-1.90410300	1.03438300	H	4.66436100	4.12215100	0.79244500
C	-3.55219300	0.37336500	0.20707400	H	3.72518300	1.30599600	3.91468500
C	-3.85541400	1.66269800	0.64363500	H	4.91763400	3.35113600	3.14336700
C	-3.16447300	0.12286300	-1.11301400	O	0.10026600	-0.61762900	-2.88563100
C	-3.77487700	2.71669700	-0.26528600	C	0.03363600	-1.69123700	0.08248700
H	-4.11760700	1.83877400	1.68093100	C	-0.67020100	-2.76507100	-0.60255900
C	-3.07360800	1.19217200	-1.99933900	C	-0.29279400	-3.62862800	-1.64257800
H	-2.91625400	-0.88092700	-1.44248300	C	-1.96294100	-2.87890600	-0.03771300
C	-3.38249800	2.50147700	-1.59400800	C	-1.20589700	-4.57271200	-2.10060900
H	-4.00562800	3.72489400	0.06875700	H	0.70401600	-3.56270400	-2.06531600
H	-2.74945800	1.00953900	-3.02046400	C	-2.87894700	-3.83932600	-0.47889800
C	-3.31013200	3.64139100	-2.57761200	C	-2.48340300	-4.67454200	-1.52272600
H	-2.48725000	3.50416200	-3.28569200	H	-0.92622800	-5.24659000	-2.90612800
H	-4.24000300	3.70649500	-3.15892000	H	-3.85781200	-3.93046100	-0.02939700
H	-3.16901800	4.60190500	-2.07203600	H	-3.17894100	-5.42646800	-1.88570400
C	3.87760100	-2.82752700	-0.86386100	C	-0.82020700	-1.18411600	1.02663600
O	4.04322500	-1.57349800	-0.76664500	C	-0.58052500	-0.13549100	2.04551100
O	2.75368500	-3.38823700	-0.65004000	C	-0.68164600	1.22339400	1.72244800
O	4.93918200	-3.56918600	-1.20608800	C	-0.23621000	-0.50343200	3.35494000
H	4.64689300	-4.49962400	-1.23410400	C	-0.43261100	2.19996900	2.68839800
C	1.00135600	-0.26520200	-1.87916300	H	-0.96577300	1.51047700	0.71713600
Pd	1.91918900	-1.35854300	-0.23252700	C	0.01730200	0.47266100	4.31823500
TS4				H	-0.17303300	-1.55726500	3.61039100
C	1.79836600	0.61454300	-0.23317900	C	-0.07816900	1.82769300	3.98581900
C	1.05721700	1.09303600	-1.31245000	H	-0.51827500	3.25123200	2.42588400
C	0.68517500	2.45385600	-1.78810900	H	0.28603600	0.17660600	5.32875100
C	0.53910300	2.71537000	-3.15993000	H	0.11959600	2.58790900	4.73677200
C	0.43436600	3.48483600	-0.86667300	N	-2.05372700	-1.91739500	1.00139100
C	0.16139800	3.98411400	-3.60164100	S	-3.53964200	-1.15089600	1.44029700
H	0.73050100	1.93048500	-3.88688100	O	-3.41243800	-0.70227800	2.82536300
C	0.06276100	4.75147800	-1.31339400	O	-4.60914100	-2.08029000	1.07017100
H	0.54215900	3.29483000	0.19450100	C	-3.56661000	0.28139900	0.36891100
C	-0.07495300	5.00729300	-2.68076700	C	-3.86077600	1.52903700	0.91767700

C	-3.25456600	0.13660000	-0.98669100	O	-0.55444400	-0.40109700	-2.80380600
C	-3.84282500	2.64981200	0.08815500	C	0.18092800	-1.74165900	-0.06147500
H	-4.06849100	1.62314100	1.97775900	C	-0.47023200	-2.79266700	-0.82465300
C	-3.22554900	1.27055900	-1.79306600	C	-0.04593900	-3.55624000	-1.92218300
H	-3.01881200	-0.83764900	-1.40315300	C	-1.76454100	-2.99965400	-0.28857400
C	-3.52326300	2.54135600	-1.27240300	C	-0.91315200	-4.49845700	-2.46552700
H	-4.06602900	3.62626400	0.50999000	H	0.95126000	-3.40925300	-2.32697000
H	-2.96079500	1.17045700	-2.84245400	C	-2.63785000	-3.95326900	-0.82107300
C	-3.51363700	3.75383300	-2.16792300	C	-2.19405400	-4.69067800	-1.91851700
H	-2.71542400	3.69089700	-2.91387800	H	-0.59701600	-5.09770500	-3.31528800
H	-4.46590500	3.84037000	-2.70866500	H	-3.61987500	-4.11447900	-0.39905300
H	-3.37385600	4.67592500	-1.59512700	H	-2.85569300	-5.43675200	-2.35043100
C	3.93701500	-2.82239000	-0.80244700	C	-0.70106800	-1.34501500	0.91066900
O	4.11169600	-1.56817400	-0.77868200	C	-0.47808300	-0.37199100	2.00695400
O	2.80091500	-3.36145400	-0.59406200	C	-0.74295400	0.99215300	1.83338800
O	5.00214700	-3.59676700	-1.06025300	C	0.05107400	-0.81406700	3.22879500
H	4.69753300	-4.52309000	-1.03619100	C	-0.48969200	1.89958800	2.86353000
C	0.60877000	-0.02179800	-2.02544200	H	-1.15008900	1.33933500	0.89187000
Pd	1.96563500	-1.33662600	-0.30238300	C	0.30792200	0.09346900	4.25704200
INT7				H	0.25634600	-1.87182900	3.36534800
C	1.67051000	0.67195600	-0.43522900	C	0.03780600	1.45341700	4.07656600
C	0.72736300	1.19457800	-1.33727600	H	-0.70569300	2.95467800	2.71607300
C	0.31242700	2.61067600	-1.60847500	H	0.71742900	-0.26131000	5.19903500
C	0.10169900	3.05012600	-2.92424800	H	0.23731700	2.15989500	4.87787600
C	0.10813700	3.50372000	-0.54462500	N	-1.90079400	-2.12311100	0.81801000
C	-0.30589900	4.36235900	-3.17273700	S	-3.40985100	-1.52965000	1.39769500
H	0.26999000	2.37332700	-3.75851500	O	-3.24766100	-1.22534800	2.81796400
C	-0.28902500	4.81491500	-0.79892900	O	-4.42621100	-2.49164500	0.96666500
H	0.27670600	3.17466900	0.47344400	C	-3.59378500	0.00586600	0.49932200
C	-0.49968200	5.24862100	-2.11133700	C	-3.95261300	1.15775200	1.19838000
H	-0.46037500	4.69135500	-4.19654000	C	-3.33573400	0.03856700	-0.87458600
H	-0.43716900	5.49883200	0.03221700	C	-4.04784000	2.36406600	0.50516500
H	-0.81219800	6.27097400	-2.30452100	H	-4.11857500	1.11582500	2.26914200
C	2.56294000	1.55625100	0.32201400	C	-3.42334500	1.25548300	-1.54475100
C	3.22464200	2.63393600	-0.30409200	H	-3.05305400	-0.86262700	-1.40936000
C	2.80857600	1.30286800	1.68695600	C	-3.78092500	2.43492000	-0.86909900
C	4.10927900	3.42913500	0.41837100	H	-4.31815900	3.26726900	1.04592200
H	3.05956400	2.82789900	-1.35866300	H	-3.20905000	1.29433300	-2.60953400
C	3.66077700	2.13020700	2.41268900	C	-3.88594200	3.73967600	-1.61666300
H	2.30072600	0.47773900	2.17427000	H	-3.11357700	3.81906600	-2.38814900
C	4.31946700	3.18863000	1.78021600	H	-4.86109200	3.82073600	-2.11569400
H	4.63063300	4.24187300	-0.07950100	H	-3.78598200	4.59735800	-0.94419800
H	3.81920400	1.93951800	3.47032100	C	4.23906900	-2.56307000	-0.55357500
H	4.99983400	3.82090000	2.34428400	O	4.31219900	-1.30438800	-0.64884900

O	3.13910100	-3.18090700	-0.36701000
O	5.38027100	-3.26716500	-0.65752800
H	5.14499600	-4.20798100	-0.55550000
C	0.04381300	0.24602300	-2.06003300
Pd	2.08665800	-1.22687500	-0.32502100
TS5			
C	1.58480400	0.89771200	-0.50606000
C	0.47643700	1.18722500	-1.30695700
C	-0.19409900	2.49987500	-1.59205800
C	-0.63692200	2.80581400	-2.88791100
C	-0.41942800	3.42037100	-0.55535400
C	-1.29038300	4.01244800	-3.14458700
H	-0.46447600	2.10559200	-3.70144900
C	-1.06624200	4.62639500	-0.81794100
H	-0.07961200	3.19245400	0.44774400
C	-1.50615700	4.92641500	-2.11080400
H	-1.62265500	4.23855700	-4.15398400
H	-1.22987300	5.33205300	-0.00806100
H	-2.01330500	5.86625900	-2.31058500
C	2.37451800	1.98065700	0.09592200
C	2.83868800	3.06445600	-0.67595000
C	2.69094100	1.92839500	1.46715900
C	3.60501700	4.06650200	-0.08673200
H	2.60692800	3.10679000	-1.73552500
C	3.42332300	2.95590700	2.05716100
H	2.33348900	1.09540500	2.06334200
C	3.88939000	4.02157500	1.28207000
H	3.97455200	4.88808100	-0.69414400
H	3.64110400	2.91631300	3.12087500
H	4.47704000	4.81214500	1.74088400
C	-0.16718800	0.10517300	-1.88553600
O	-0.79303900	-0.52810500	-2.62529000
C	0.50726500	-1.67129000	-0.15674400
C	0.03999100	-2.82967100	-0.89582200
C	0.60632200	-3.54879500	-1.95727800
C	-1.23941200	-3.19069600	-0.40749900
C	-0.10320500	-4.61067800	-2.50773200
H	1.58871200	-3.27130600	-2.32880900
C	-1.95945400	-4.25831500	-0.95366700
C	-1.37127000	-4.95611400	-2.00808500
H	0.32490800	-5.18145900	-3.32730200
H	-2.93169200	-4.53767400	-0.57336200
H	-1.91049000	-5.79143000	-2.44668600
C	-0.46673400	-1.37414300	0.77755400
C	-0.37862300	-0.37668500	1.87171000
C	-0.95019400	0.89753300	1.76985100
C	0.36034700	-0.70369100	3.01996200
C	-0.79900900	1.82427000	2.80327100
H	-1.50468600	1.16939100	0.88032100
C	0.50790400	0.22176100	4.05322500
H	0.81220300	-1.68825200	3.09576700
C	-0.07221800	1.48927500	3.94704900
H	-1.24956200	2.80876700	2.70883500
H	1.07789000	-0.04627400	4.93868100
H	0.04508100	2.21183300	4.75024200
N	-1.53847300	-2.29762100	0.65278400
S	-3.08217900	-2.07176800	1.38510000
O	-2.86775200	-1.83290200	2.81044600
O	-3.91047700	-3.19490100	0.94430000
C	-3.63376200	-0.55429600	0.62199100
C	-4.17706800	0.44770000	1.42550100
C	-3.46149900	-0.37416100	-0.75297900
C	-4.53782900	1.65837700	0.83586300
H	-4.27608600	0.29708700	2.49479000
C	-3.81427400	0.84755700	-1.31918300
H	-3.03151000	-1.15943600	-1.36608800
C	-4.35327400	1.88246500	-0.53606900
H	-4.94948900	2.44934400	1.45711300
H	-3.65957300	1.00628900	-2.38293800
C	-4.73596300	3.19737800	-1.16614100
H	-4.70779400	4.01476500	-0.43820700
H	-4.06508000	3.45186200	-1.99244000
H	-5.75646300	3.14894000	-1.56959700
Pd	2.32949900	-0.89178700	-0.28764400
C	4.66341900	-1.90044500	-0.26270600
O	4.57329300	-0.64804700	-0.39723800
O	3.64388700	-2.66115400	-0.15640500
O	5.89350900	-2.44415300	-0.23277000
H	5.77731900	-3.40571300	-0.12019900
trans-INT8			
C	-2.25662400	-0.14391100	0.08295600
C	-2.12172400	0.69108100	1.15276600
C	-2.97597000	1.87421900	1.43103200
C	-3.53743800	2.08732500	2.70041800
C	-3.21722300	2.81606700	0.41627200
C	-4.33516700	3.20747400	2.94086500
H	-3.34593300	1.37469300	3.49468600
C	-4.01239300	3.93471400	0.65978400

H	-2.77415000	2.66542200	-0.56375400
C	-4.57734800	4.13307800	1.92299300
H	-4.76883200	3.35567700	3.92667500
H	-4.18861200	4.65339000	-0.13658100
H	-5.19874500	5.00445400	2.11316700
C	-3.37488300	-0.16088700	-0.86814700
C	-4.70432800	-0.15427100	-0.39995100
C	-3.14777500	-0.20895800	-2.25658300
C	-5.76986900	-0.18000500	-1.29619000
H	-4.88973400	-0.12274500	0.66900100
C	-4.21665900	-0.21725900	-3.15011100
H	-2.12913300	-0.23254800	-2.62898600
C	-5.53037100	-0.20524100	-2.67368000
H	-6.78921800	-0.17709400	-0.91954100
H	-4.02381900	-0.24422600	-4.21924700
H	-6.36343500	-0.22199300	-3.37139100
C	-1.00167100	0.37740400	2.05773500
O	-0.87939200	0.77137600	3.21277500
C	0.05784200	-0.51742800	1.46633600
C	0.87442700	-1.44197000	2.23445100
C	0.66240800	-2.04016600	3.48123300
C	2.02750400	-1.74205900	1.47648800
C	1.61134900	-2.93986200	3.95281500
H	-0.21913600	-1.78553200	4.05960200
C	2.97406700	-2.66319600	1.93489800
C	2.74707900	-3.24449000	3.18198600
H	1.47605200	-3.41221500	4.92131900
H	3.84712500	-2.91677500	1.35188000
H	3.47559300	-3.95402700	3.56444700
C	0.77474700	-0.20921300	0.26586300
C	0.70031200	1.08656800	-0.47758800
C	0.99268700	2.25455900	0.24153000
C	0.35037700	1.17668100	-1.82934400
C	0.93224600	3.49871700	-0.38612100
H	1.26853400	2.18681600	1.28970300
C	0.28614900	2.42245400	-2.45302900
H	0.13517300	0.27299900	-2.38582500
C	0.57668800	3.58517500	-1.73386100
H	1.15895200	4.39722100	0.18054000
H	0.00607100	2.48308800	-3.50104200
H	0.52321800	4.55457000	-2.22178200
N	1.97074200	-0.96482700	0.29355900
S	3.10849100	-0.97818200	-1.01685100
O	2.34241300	-1.01467000	-2.25971100
O	4.06505300	-2.03450800	-0.69226900
C	3.88562500	0.61302500	-0.83958100
C	3.77918600	1.54724300	-1.86772900
C	4.57800300	0.89394800	0.34293700
C	4.37230700	2.79735600	-1.69730400
H	3.22081700	1.31074100	-2.76550400
C	5.15806600	2.14820000	0.49211100
H	4.64998700	0.15414000	1.13459000
C	5.06431200	3.11793600	-0.52197800
H	4.28340100	3.53777000	-2.48740900
H	5.68993100	2.38361900	1.41030100
C	5.71295400	4.46739300	-0.34503200
H	5.31595800	5.20166200	-1.05305900
H	5.56279100	4.85108000	0.67042400
H	6.79683400	4.40010300	-0.50861300
Pd	-0.91961200	-1.59627200	-0.15845500
C	-0.92464500	-3.84817600	-1.27163300
O	-1.95951600	-3.10695700	-1.30933900
O	0.13733700	-3.49552200	-0.67480400
O	-0.99411700	-5.03229300	-1.89467700
H	-0.12829400	-5.46762700	-1.78141100
INT5’			
C	3.10590400	-1.50900000	-1.16001400
C	3.99892800	-0.68526700	-0.43592900
C	4.06519900	-0.83690000	0.95955600
C	3.24675700	-1.74144600	1.62798900
C	2.36101600	-2.54230700	0.89509500
C	2.30600500	-2.45615100	-0.49523000
H	3.11301700	-1.47998400	-2.24603000
H	4.75355500	-0.21970100	1.53045400
H	3.27039100	-1.81117400	2.70988000
H	1.61623700	-3.07628500	-1.05691900
O	0.46393400	-4.42455100	0.92427800
O	1.38614500	-3.60974600	3.15273400
H	5.94469300	0.10455600	-0.89660000
S	1.01161300	-3.35615500	1.75931700
N	-0.20780100	-2.03151100	1.79294700
C	0.34433100	-0.91498200	2.50144600
C	0.59294800	-0.79697400	3.86390900
C	0.65850900	0.11041700	1.58379800
C	1.15496900	0.40250200	4.31390000
H	0.36411400	-1.60958800	4.54348900
C	1.22298300	1.30375800	2.04955000
C	1.46232800	1.43941300	3.41735900

H	1.34687600	0.53485000	5.37500000	H	0.05524500	6.15539000	2.98959200
H	1.46060900	2.10733500	1.36129400	H	3.03676100	3.66725500	-1.88537900
H	1.88622800	2.36580100	3.79588700	C	2.84237900	2.11980200	-2.97838000
C	0.27402500	-0.36031100	0.25747300	O	2.54124400	2.83213400	-1.81014100
C	-0.37623500	-1.55736900	0.41787700	O	2.26865800	0.97189000	-3.02519000
C	-1.18060600	-2.34830600	-0.51517400	O	3.59574100	2.62376600	-3.80178300
C	-2.19299500	-3.19410500	-0.02199400	Pd	1.14999400	0.33763600	-1.36509900
C	-1.03200200	-2.23036700	-1.91050800	TS6			
C	-3.03273500	-3.88383400	-0.89363200	C	3.38851100	-1.16511100	-0.71190400
H	-2.31968000	-3.29560300	1.05022500	C	4.12421400	-0.16696400	-0.02690200
C	-1.87478000	-2.92025500	-2.78004500	C	4.03652600	-0.11202800	1.37280200
H	-0.25686500	-1.58776500	-2.31640100	C	3.22581100	-0.99454400	2.08137000
C	-2.88199500	-3.74983400	-2.27706100	C	2.50369900	-1.97143100	1.38712100
H	-3.80958800	-4.52783300	-0.48972800	C	2.58929400	-2.07917500	-0.00274300
H	-1.74056700	-2.81000500	-3.85298900	H	3.54637400	-1.30511100	-1.77688500
H	-3.53734300	-4.28920600	-2.95578600	H	4.60354700	0.64005200	1.91413700
C	4.89326400	0.30346500	-1.13755800	H	3.13862000	-0.91798300	3.15932400
H	4.76935900	0.26325300	-2.22142300	H	2.04791900	-2.85612300	-0.53055800
H	4.67080000	1.32603700	-0.81162600	O	0.84480700	-4.05929300	1.49861400
C	-2.75559600	1.53030600	-0.73166800	O	1.41275100	-2.85392800	3.66796900
C	-1.79681300	2.43828200	-0.32260800	H	5.97472800	0.90272100	-0.27650200
C	-1.49298100	1.52410900	-1.33195900	S	1.18410600	-2.83860000	2.22400600
O	-0.68621900	1.03090600	-2.16222300	N	-0.15147800	-1.65794600	1.94922500
C	-4.05039300	0.92544400	-0.56465400	C	0.17330900	-0.39194500	2.53963300
C	-4.30494600	-0.30901200	-1.19344900	C	0.34121500	-0.08298900	3.88648100
C	-5.03909700	1.52702600	0.23647300	C	0.34027600	0.56154300	1.51835100
C	-5.53500000	-0.93446900	-1.01184800	C	0.70029200	1.23081500	4.19991700
H	-3.53231100	-0.77523600	-1.79719800	H	0.21161500	-0.83632700	4.65391200
C	-6.27000600	0.89966300	0.40136400	C	0.70924800	1.86905200	1.84806300
H	-4.83832700	2.48246700	0.71233400	C	0.88838100	2.19211200	3.19306000
C	-6.51671500	-0.33083000	-0.21954900	H	0.83229800	1.51063500	5.24120900
H	-5.72392500	-1.89368900	-1.48411000	H	0.84855300	2.61233600	1.07131800
H	-7.03693700	1.36328100	1.01507000	H	1.16658800	3.20616000	3.46669200
H	-7.47684100	-0.82078200	-0.08208100	C	0.05098700	-0.09385200	0.24271600
C	-1.33678700	3.46807100	0.56906100	C	-0.31226200	-1.40527300	0.54203000
C	-0.08303500	4.05934700	0.31604900	C	-0.86906100	-2.45350100	-0.30882400
C	-2.08571400	3.85335300	1.69578500	C	-1.78364100	-3.37198300	0.24411000
C	0.40961800	5.02864100	1.18557000	C	-0.57208900	-2.53961300	-1.68302300
H	0.49450100	3.74224900	-0.54867300	C	-2.39320800	-4.33234300	-0.55745500
C	-1.57917500	4.81506900	2.56455700	H	-2.02404300	-3.30938900	1.29950700
H	-3.04369600	3.38101800	1.89114000	C	-1.17986800	-3.50593400	-2.47995600
C	-0.33476700	5.40328200	2.30922500	H	0.14264500	-1.84876100	-2.12082700
H	1.37561200	5.48715200	0.99404200	C	-2.09490500	-4.40458300	-1.92126600
H	-2.14962600	5.10743600	3.44133100	H	-3.10446300	-5.02519600	-0.11689400

H	-0.93576400	-3.55863900	-3.53726900	H	3.50224700	-0.81048400	-3.08950300
H	-2.56738800	-5.15905100	-2.54435500	H	6.17116100	-0.03095800	0.19146400
C	5.00461700	0.79759800	-0.77513100	H	4.81138900	-1.50283400	1.65413300
H	5.17080700	0.47822900	-1.80668600	H	2.14492800	-2.29377600	-1.63587800
H	4.53724500	1.78811200	-0.80819200	O	1.59386600	-3.89709100	0.38859000
C	-2.56423600	0.82413400	-0.66552600	O	3.02972000	-3.26669100	2.39271300
C	-1.92836500	1.94992800	-0.26194600	H	6.76927500	0.20070700	-2.55314200
C	-1.17103000	0.96770500	-0.98217100	S	2.31916300	-2.89414300	1.16873800
O	-0.40612000	0.95541100	-2.05891300	N	1.13714400	-1.67592800	1.64801600
C	-3.80391900	0.09689800	-0.78607900	C	1.70776200	-0.51963300	2.25069500
C	-3.85850600	-1.08102400	-1.55348300	C	2.58364100	-0.44421500	3.33271600
C	-4.96805200	0.55736400	-0.13975800	C	1.23711100	0.62420500	1.57248200
C	-5.05356500	-1.78654300	-1.66540100	C	2.99423000	0.82519300	3.73876100
H	-2.96261700	-1.43707200	-2.04888300	H	2.92516300	-1.33944600	3.83656600
C	-6.15899300	-0.15331100	-0.25558300	C	1.65299900	1.89255800	2.00788000
H	-4.92993500	1.47159200	0.44411700	C	2.53380800	1.97835800	3.08310300
C	-6.20368600	-1.32711400	-1.01648200	H	3.67031800	0.91923100	4.58391600
H	-5.08411400	-2.69889000	-2.25395600	H	1.29932800	2.79339200	1.52315500
H	-7.05334300	0.20479800	0.24676800	H	2.86199900	2.95589900	3.42545700
H	-7.13403200	-1.88220200	-1.10178000	C	0.33648900	0.16764000	0.51745800
C	-1.97235900	3.26715000	0.32499500	C	0.27786800	-1.20539000	0.59512100
C	-1.02272300	4.22755700	-0.07583100	C	-0.63831000	-2.18941100	-0.02015600
C	-2.92848100	3.60292000	1.30069100	C	-1.26865500	-3.13950200	0.83751100
C	-1.03826400	5.50107800	0.48664000	C	-0.76946100	-2.37019400	-1.43072400
H	-0.28674900	3.96461500	-0.83038900	C	-1.97803600	-4.20274400	0.31519300
C	-2.92919700	4.87500500	1.86827400	H	-1.15843500	-3.02312900	1.91007500
H	-3.64356300	2.85523800	1.62982100	C	-1.47757700	-3.49202100	-1.94288900
C	-1.98803400	5.82614800	1.46113900	H	-0.15203200	-1.77977900	-2.09748300
H	-0.30833200	6.24039100	0.16883000	C	-2.08288200	-4.38891100	-1.08173900
H	-3.66240300	5.12572500	2.62981500	H	-2.44815800	-4.91399900	0.98829500
H	-1.99420500	6.81884500	1.90300100	H	-1.52339400	-3.63308100	-3.01847600
H	3.07715600	3.54729400	-2.49036200	H	-2.62463300	-5.24469900	-1.47431700
C	3.00326800	1.79337000	-3.20049800	C	5.75654900	0.60216400	-2.41984400
O	2.65626200	2.71294400	-2.21629000	H	5.31245300	0.72880300	-3.41199800
O	2.51711100	0.61761100	-3.00024400	H	5.86158900	1.59247100	-1.96078000
O	3.72110900	2.14704800	-4.12867600	C	-1.13393100	2.27789100	0.16091500
Pd	1.32236800	0.21752600	-1.33647500	C	-0.09052700	2.47795000	-0.60409500
INT9				C	-0.46735300	1.02992800	-0.38992900
C	3.79069400	-0.95816800	-2.05219300	O	-1.00501900	0.40824200	-1.49661500
C	4.92723000	-0.30853300	-1.54959900	C	-2.18611100	2.69178800	1.05124100
C	5.28918500	-0.52363600	-0.20962300	C	-2.97438600	1.71945200	1.69408200
C	4.53372500	-1.34784300	0.61810700	C	-2.42776400	4.05552200	1.30657400
C	3.40060300	-1.97477700	0.09000400	C	-3.98522800	2.10351400	2.57160500
C	3.01987300	-1.79019400	-1.24085500	H	-2.78768900	0.66894700	1.49145300

C	-3.44072000	4.43288900	2.18397900	C	-0.92149200	3.32768500	-1.02837000
H	-1.81938900	4.80784100	0.81181900	C	-1.74553800	4.11891200	-1.82164600
C	-4.22176600	3.45947100	2.81743400	H	-3.34751200	4.17759200	-3.27058800
H	-4.59260700	1.34611100	3.05957700	H	-0.17312100	3.79197300	-0.40146200
H	-3.62479600	5.48681700	2.37475200	H	-1.62459400	5.19860200	-1.80432700
H	-5.01380800	3.75817900	3.49879400	C	-0.40656200	0.83451100	-0.37787600
C	0.91881500	3.27064700	-1.25838900	C	-0.98613800	-0.33556400	-0.81551700
C	2.03023300	2.63421800	-1.84222100	C	-0.57587600	-1.73603700	-0.58980000
C	0.83064500	4.67557900	-1.29187100	C	-0.14861600	-2.51713500	-1.68229700
C	3.03197400	3.39017000	-2.44614700	C	-0.63780800	-2.32936500	0.68699500
H	2.10165800	1.55085400	-1.80591000	C	0.21862700	-3.84766700	-1.50014800
C	1.83633600	5.42452800	-1.89814700	H	-0.12534100	-2.07273000	-2.67258300
H	-0.02996300	5.16673300	-0.84625600	C	-0.30631400	-3.68094600	0.85654000
C	2.93837600	4.78532400	-2.47652300	H	-0.99985900	-1.74591100	1.52580400
H	3.88627400	2.89128100	-2.89495000	C	0.13326200	-4.43605700	-0.23011300
H	1.76116400	6.50838800	-1.92209500	H	0.54638800	-4.43683200	-2.35235200
H	3.72025000	5.37305200	-2.94999800	H	-0.36797600	-4.12538200	1.84491400
H	-4.71465500	-2.61886600	-0.97255900	H	0.40389500	-5.47912400	-0.09213300
C	-5.03881000	-0.61340900	-1.05087700	C	-5.65751000	0.25793400	3.76600500
O	-4.30519000	-1.81150200	-0.60750800	H	-5.49166700	-0.56456600	4.46834900
O	-4.18254800	0.32233600	-1.18147600	H	-5.16278400	1.15137200	4.16737300
O	-6.23325500	-0.68747800	-1.20701500	C	2.22851100	1.17845700	-0.25227400
Pd	-2.41818700	-0.87749600	-1.05425600	C	1.72371400	2.13125800	0.47831800
TS7				C	0.81106900	0.92407400	0.49573700
C	-4.49557400	-1.28839600	2.12587000	O	0.83246000	0.19284700	1.64094200
C	-5.13710900	-0.07045300	2.38939600	C	3.22688100	0.68010900	-1.17344300
C	-5.29117700	0.85129300	1.33952400	C	2.95786900	-0.40956200	-2.02200500
C	-4.81562700	0.57560600	0.06219800	C	4.48988800	1.30297700	-1.22954500
C	-4.17231600	-0.64635200	-0.16431200	C	3.93467800	-0.87341200	-2.90098800
C	-4.00667200	-1.58590200	0.85403700	H	1.97853100	-0.87684200	-1.99420000
H	-4.37531300	-2.01560400	2.92425300	C	5.46232400	0.82837700	-2.10597100
H	-5.79386700	1.79658300	1.52774700	H	4.70412900	2.13888100	-0.57028900
H	-4.94197400	1.29073200	-0.74305900	C	5.18925600	-0.25954000	-2.94280800
H	-3.51014400	-2.52833800	0.65349700	H	3.71462600	-1.71315100	-3.55446000
O	-3.09379200	-2.38409100	-1.85148300	H	6.43810200	1.30531700	-2.13456900
O	-4.32598900	-0.38483300	-2.81086300	H	5.95160900	-0.62475800	-3.62520600
H	-6.73336700	0.47097900	3.73884500	C	1.79360700	3.44645000	1.07000700
S	-3.48414300	-0.97945000	-1.77297100	C	0.87966600	3.81265600	2.07492900
N	-2.00583200	-0.03790000	-1.76833300	C	2.76684000	4.37108900	0.64529100
C	-2.07566500	1.37270900	-1.89037300	C	0.94431600	5.08044100	2.64865700
C	-2.89741200	2.16110900	-2.70105300	H	0.12830000	3.09720300	2.39597700
C	-1.08455000	1.93243900	-1.04977300	C	2.82221900	5.63728800	1.22142900
C	-2.72264600	3.54209400	-2.64929100	H	3.46211800	4.09266200	-0.14115000
H	-3.63735600	1.71334300	-3.34971500	C	1.91338400	5.99451400	2.22369000

H	0.23863300	5.35626900	3.42714500	C	2.10403400	-2.87632400	2.65980400
H	3.57289000	6.34863400	0.88824300	H	2.29278200	-1.47952400	4.29600600
H	1.96076200	6.98346500	2.67123800	H	1.88785700	-4.01204700	0.83567100
H	2.81122400	-3.64470400	-0.13381300	H	2.18712100	-3.75516900	3.29362600
C	2.79610500	-3.60538700	1.88922900	C	5.78187700	-4.22706400	-1.31331600
O	3.09096800	-3.01059100	0.55579500	H	5.67897900	-4.96728100	-0.51360000
O	2.34057200	-2.67937800	2.62790300	H	5.14071200	-4.52947600	-2.14859200
O	3.01874600	-4.78173400	2.04585200	C	-2.94545000	-0.01219800	-0.19457100
Pd	1.91329100	-1.28713400	0.98882000	C	-1.91912800	0.91296500	-0.17930800
cis-INT8				C	-0.63873200	0.32586400	-0.51632700
C	5.47508400	-2.52196400	0.53243900	O	-0.60908100	-0.92235400	-0.79732500
C	5.43837000	-2.84053000	-0.83214100	C	-4.32882600	0.22761000	0.22622000
C	5.08871200	-1.83586600	-1.75148100	C	-4.61241400	0.82922000	1.46957600
C	4.78185200	-0.54817700	-1.32662200	C	-5.40149900	-0.18588400	-0.58967300
C	4.81442600	-0.27167400	0.04369300	C	-5.93106500	1.01155600	1.87901300
C	5.16360200	-1.24082300	0.98282600	H	-3.79397400	1.14944400	2.10607600
H	5.73388100	-3.28956800	1.25626200	C	-6.71881600	0.02137600	-0.18386100
H	5.05414500	-2.06928100	-2.81226400	H	-5.19254100	-0.65626400	-1.54587400
H	4.50834500	0.22045300	-2.04279500	C	-6.98765300	0.61474500	1.05291000
H	5.15862700	-1.00549900	2.04055100	H	-6.13509600	1.47071200	2.84249000
O	4.41319400	1.41959700	2.05667500	H	-7.53554700	-0.28748300	-0.83059900
O	5.18291100	2.34759500	-0.17310100	H	-8.01509400	0.76528000	1.37290500
H	6.81999100	-4.26598600	-1.66987300	C	-2.07982300	2.33770200	0.22264100
S	4.41483400	1.36892000	0.59575200	C	-3.01205500	3.16124600	-0.42749200
N	2.76100000	1.56008700	0.04600600	C	-1.30819000	2.87728800	1.26373700
C	2.28246600	2.63039000	-0.74537200	C	-3.16129300	4.49623900	-0.05314900
C	2.88756400	3.82495400	-1.15387900	H	-3.61641600	2.74851900	-1.23046200
C	0.94888600	2.31667400	-1.09930600	C	-1.45465800	4.21406900	1.63459800
C	2.13174800	4.68986400	-1.94049800	H	-0.58912400	2.24649200	1.77866200
H	3.90100500	4.07041800	-0.87179500	C	-2.37988300	5.02786300	0.97628400
C	0.21615900	3.19661900	-1.91022100	H	-3.88417700	5.12279600	-0.56894400
C	0.81313500	4.38063900	-2.32121200	H	-0.84609200	4.61901500	2.43875100
H	2.57792100	5.62520200	-2.26664000	H	-2.49206800	6.06972300	1.26426600
H	-0.80286300	2.95871800	-2.19355900	H	-4.81644100	-3.05564000	0.07401800
H	0.25443600	5.07803100	-2.93889100	C	-3.35408600	-4.33214500	-0.64603800
C	0.63786500	1.03232100	-0.51413900	O	-4.14284300	-3.04511000	-0.63251100
C	1.75787600	0.58726500	0.17099500	O	-2.17161500	-4.02467600	-0.96997000
C	1.89230200	-0.61091100	1.02482500	O	-3.94694200	-5.34523000	-0.36976700
C	2.06195000	-0.46940300	2.41205200	Pd	-2.41047600	-1.84572800	-0.65012700
C	1.82472200	-1.89668200	0.46508900	$PdCO_3$			
C	2.16589300	-1.59883800	3.22353000	C	-1.52189500	-0.00008600	0.00003600
H	2.11894000	0.52251300	2.84615700	O	-0.73612700	1.08029300	-0.00000100
C	1.93396900	-3.02215800	1.28057200	O	-0.73569800	-1.07983400	-0.00000100
H	1.70372200	-2.00747100	-0.60500500	O	-2.73073500	-0.00029200	-0.00001700

Pd	0.92938800	-0.00001800	-0.00000100
HCO_3^-			
C	-0.18187000	0.00004100	-0.01303900
O	-0.68496600	1.13577300	0.01122600
O	-0.68584800	-1.13529400	0.01127900
O	1.30647500	-0.00050600	-0.11381900
H	1.60593400	-0.00002900	0.80874500
CO_3^{2-}			
C	-1.35384200	-0.04737600	0.00000000
H	-1.73461100	-1.07324400	-0.00011400
H	-1.73960800	0.47908000	-0.88185500
H	-1.73959000	0.47887500	0.88198500
C	0.18724800	-0.00056100	-0.00000700
O	0.71419700	1.15332000	0.00000100
O	0.81247500	-1.10295600	0.00000200
INT10			
C	3.17998800	1.11484100	1.21147400
C	1.96348600	1.67383700	1.57993700
C	0.63791100	1.48676700	2.10212900
C	-0.18682000	2.61413800	2.27898600
C	0.12028900	0.19325600	2.32416500
C	-1.50942000	2.44844000	2.68177400
H	0.21416100	3.60332000	2.08421500
C	-1.20537000	0.03670100	2.70924200
H	0.75069800	-0.67517300	2.16051600
C	-2.01816700	1.16392300	2.89204000
H	-2.14609700	3.31732000	2.81728600
H	-1.61439700	-0.95787100	2.86065000
H	-3.05340900	1.03446500	3.19063100
C	3.94628800	-0.12071000	1.11512700
C	3.64952700	-1.23448700	1.93605400
C	4.96138600	-0.22508300	0.13123100
C	4.34645300	-2.42139600	1.76614500
H	2.88863900	-1.13942800	2.70383300
C	5.63752500	-1.43868100	-0.04108600
H	5.24396200	0.65026700	-0.44787000
C	5.33179900	-2.52922700	0.77088800
H	4.12692500	-3.27154600	2.40505400
H	6.41667300	-1.51518300	-0.79342700
H	5.86745600	-3.46535500	0.64335700
C	2.98045700	2.52910200	1.01846500
O	3.36467800	3.62008400	0.64808800
C	0.58645700	0.84185500	-1.41029600
C	-0.15446100	2.05806600	-1.24605400
C	0.22045100	3.39668000	-1.03646500
C	-1.53070200	1.72210700	-1.41866000
C	-0.76857900	4.37048500	-1.01779400
H	1.26270500	3.65549200	-0.87768200
C	-2.51664700	2.70924800	-1.45799600
C	-2.11576700	4.02717800	-1.23863600
H	-0.50123400	5.40907100	-0.84811600
H	-3.55127600	2.47569200	-1.67284300
H	-2.86935300	4.80933100	-1.25117100
C	-0.32480800	-0.19511300	-1.54494500
C	0.22190800	-1.50935400	-1.33010000
C	-0.32763500	-2.50932100	-0.50475100
C	1.57756500	-1.66195500	-1.81777400
C	0.45034600	-3.59284500	-0.13109000
H	-1.32767200	-2.39410000	-0.10791600
C	2.34106600	-2.79173200	-1.41172300
H	1.84042300	-1.17616400	-2.75823000
C	1.79015100	-3.73227600	-0.56533300
H	0.02754100	-4.34471500	0.52962600
H	3.34876500	-2.91124200	-1.79648800
H	2.36798800	-4.59666800	-0.25371200
N	-1.62501200	0.31562100	-1.56465400
S	-3.04076900	-0.57795200	-2.03154300
O	-2.52711700	-1.80707500	-2.63145700
O	-3.87863000	0.35699000	-2.77691400
C	-3.81714200	-0.96372900	-0.47305400
C	-3.91532600	-2.30047200	-0.08116100
C	-4.35352600	0.06542900	0.30824500
C	-4.54050000	-2.60290700	1.12884900
H	-3.52153700	-3.08840000	-0.71401300
C	-4.97684000	-0.26087800	1.50768500
H	-4.28634500	1.10093100	-0.00396300
C	-5.07824300	-1.59431600	1.94019900
H	-4.62156700	-3.64102200	1.43898100
H	-5.40009800	0.53243300	2.11798800
C	-5.77587500	-1.92062700	3.23561600
H	-6.86203300	-1.80365300	3.12765300
H	-5.58162600	-2.94983700	3.55225200
H	-5.45833200	-1.24594700	4.03910000
Pd	2.34416600	0.19965600	-0.78422100
TS8			
C	2.59978200	0.14968300	0.82747800
C	1.62537900	0.89145400	1.52104700
C	0.50428900	0.82915800	2.41892300

C	0.12967000	2.00583400	3.10455300
C	-0.31452800	-0.31717100	2.50134600
C	-1.02996800	2.02292000	3.87117500
H	0.74696100	2.89499400	3.02229100
C	-1.47791800	-0.28519400	3.26098500
H	-0.05260900	-1.20922100	1.94570300
C	-1.83470500	0.88058500	3.94958900
H	-1.31364800	2.92706600	4.40108300
H	-2.11325000	-1.16403800	3.30967800
H	-2.74416300	0.90003600	4.54343900
C	3.17824200	-1.18731200	0.90671100
C	2.66326000	-2.17587900	1.76897100
C	4.31686000	-1.48867800	0.13049600
C	3.25998800	-3.43155800	1.83052000
H	1.81413500	-1.95359600	2.40357000
C	4.90083900	-2.75010900	0.18478800
H	4.75018200	-0.72281000	-0.51038300
C	4.37055800	-3.72605600	1.03353500
H	2.85661000	-4.18354400	2.50235600
H	5.77439600	-2.96871800	-0.42203400
H	4.82801700	-4.70991300	1.08241900
C	2.66714000	1.79354200	1.24516700
O	3.31967100	2.76762200	1.50758800
C	0.83211600	1.35157600	-1.16406500
C	0.09191400	2.54365400	-0.82073800
C	0.46504300	3.82211200	-0.38124900
C	-1.27880000	2.22864700	-0.99459500
C	-0.53085900	4.76062100	-0.13246700
H	1.51131100	4.06336400	-0.22108900
C	-2.27880600	3.17807800	-0.77947000
C	-1.88355900	4.44141900	-0.33873100
H	-0.26029500	5.75223300	0.21787400
H	-3.32218500	2.95399300	-0.95567600
H	-2.64517900	5.19325000	-0.15466500
C	-0.06725500	0.32153400	-1.40308900
C	0.25577800	-1.10236700	-1.49141900
C	-0.39767600	-2.03735000	-0.66891500
C	1.31170700	-1.53436400	-2.31526400
C	0.01631400	-3.36585300	-0.65163400
H	-1.20231300	-1.70996300	-0.02175200
C	1.72674100	-2.86599200	-2.28851200
H	1.77270600	-0.83084000	-3.00329700
C	1.08495300	-3.78253900	-1.45385400
H	-0.48774400	-4.07682700	-0.00303900
H	2.54322000	-3.18836000	-2.92796100
H	1.40950600	-4.81865800	-1.43237500
N	-1.36073900	0.85762700	-1.35650200
S	-2.74971300	0.13419600	-2.16278200
O	-2.21500700	-0.81104600	-3.13731800
O	-3.58355600	1.25872800	-2.57885100
C	-3.53946400	-0.75485300	-0.83780900
C	-3.79986100	-2.11396100	-1.01555600
C	-3.90146300	-0.08447100	0.33590200
C	-4.43547300	-2.81349500	0.00978400
H	-3.49659300	-2.61556200	-1.92792500
C	-4.52838800	-0.80538400	1.34633800
H	-3.68801700	0.97043500	0.47455500
C	-4.80914300	-2.17563400	1.20039800
H	-4.64235600	-3.87210600	-0.12013900
H	-4.80989700	-0.29608700	2.26416000
C	-5.50994500	-2.92809500	2.30239600
H	-6.55661900	-2.60767700	2.38311700
H	-5.50339500	-4.00713800	2.12194800
H	-5.04025500	-2.73823100	3.27494100
Pd	2.75927400	1.11256400	-1.01205500
INT11			
C	1.84498700	-1.14044800	-0.61851500
C	1.66938400	-0.08667800	-1.49425400
C	2.35870200	1.20459700	-1.66983100
C	2.30184800	1.87929900	-2.90188000
C	3.03461600	1.79837400	-0.58774600
C	2.92579100	3.11733900	-3.05139200
H	1.77771500	1.43734900	-3.74384200
C	3.65195600	3.03642500	-0.74573100
H	3.06647400	1.29673700	0.37293200
C	3.60425500	3.69782500	-1.97696200
H	2.88204800	3.62673100	-4.00952800
H	4.16853200	3.48816000	0.09632400
H	4.08842700	4.66270900	-2.09583600
C	2.87355800	-1.54462300	0.30792400
C	4.22965600	-1.26205900	0.01360400
C	2.55435200	-2.27574000	1.47357000
C	5.22796800	-1.68788500	0.88093500
H	4.48549000	-0.71434400	-0.88712500
C	3.56232500	-2.68508700	2.33847700
H	1.51549400	-2.47583600	1.70874500
C	4.89825300	-2.39454900	2.04446600
H	6.26685500	-1.47071000	0.65143700

H	3.30568000	-3.22612200	3.24410800	C	0.55556800	-0.50410000	-2.28697400
H	5.68446200	-2.71970600	2.71957400	Pd	0.48735200	-2.44311100	-1.19062600
O	-0.17111400	-0.22843900	-3.17065200	TS9			
C	-1.11130900	-1.53504500	-0.44254800	C	1.79612700	-1.14451800	-0.65618300
C	-2.34832000	-1.65968200	-1.18211500	C	1.62613500	-0.04382200	-1.47903400
C	-2.68078000	-2.23263000	-2.41893400	C	2.35403100	1.23889400	-1.61791700
C	-3.35408400	-1.05544100	-0.38765400	C	2.36724600	1.91951400	-2.84691700
C	-4.00558000	-2.19821100	-2.83742200	C	3.00112600	1.80711800	-0.50658000
H	-1.91585900	-2.68592600	-3.04419900	C	3.02753800	3.14227500	-2.96407200
C	-4.69190100	-1.04131200	-0.79611300	H	1.87127100	1.49470600	-3.71518200
C	-4.99671200	-1.61296800	-2.02941600	C	3.65946000	3.02803800	-0.63290700
H	-4.28029300	-2.63244800	-3.79422400	H	2.98608500	1.29631500	0.44923700
H	-5.46176900	-0.59949800	-0.17944300	C	3.67740300	3.69850300	-1.85977600
H	-6.02831400	-1.60800600	-2.36860200	H	3.03630100	3.65671600	-3.92044900
C	-1.34832000	-0.86645500	0.73080400	H	4.15643100	3.45902600	0.23150800
C	-0.42937700	-0.51630100	1.83606700	H	4.19133600	4.65067400	-1.95294500
C	0.49613000	0.52694500	1.70013200	C	2.87051600	-1.53869300	0.22575400
C	-0.48166000	-1.24145700	3.03660700	C	4.21004600	-1.22308300	-0.10790800
C	1.37586200	0.82441400	2.74184200	C	2.60505100	-2.28701300	1.39442900
H	0.50691700	1.12067800	0.79363700	C	5.24545400	-1.63974500	0.71912700
C	0.40402700	-0.94658700	4.07204200	H	4.42438700	-0.66125000	-1.01066800
H	-1.22071000	-2.02854400	3.15332400	C	3.64905000	-2.68091900	2.22332900
C	1.33861200	0.08344500	3.92407700	H	1.57802500	-2.50787100	1.66147400
H	2.08239200	1.64206300	2.62967000	C	4.96839200	-2.36218400	1.88696500
H	0.35973500	-1.51426700	4.99714900	H	6.27179300	-1.40151400	0.45656800
H	2.02565000	0.31398400	4.73344700	H	3.43337500	-3.23238100	3.13336400
N	-2.73867400	-0.57995200	0.79648400	H	5.78318700	-2.67694600	2.53256600
S	-3.30338900	0.84629700	1.65139700	O	-0.27527200	-0.08979900	-3.11340800
O	-4.69256200	1.02589700	1.23366500	C	-1.12397200	-1.54125000	-0.46447700
O	-2.97140600	0.66398600	3.06056800	C	-2.36152300	-1.63362300	-1.21126400
C	-2.25862100	2.11634200	0.95550500	C	-2.69775300	-2.18412200	-2.45741100
C	-1.60695600	2.99461900	1.82128900	C	-3.36232700	-1.01985500	-0.41729600
C	-2.07166700	2.17867800	-0.42889600	C	-4.01848900	-2.11736200	-2.88566900
C	-0.75127200	3.95373200	1.28274200	H	-1.93847200	-2.65039500	-3.08071000
H	-1.74262200	2.90713700	2.89343600	C	-4.69594700	-0.97059100	-0.83621900
C	-1.19704900	3.13183700	-0.94288100	C	-5.00326800	-1.52026100	-2.07900600
H	-2.57829100	1.48797200	-1.09565600	H	-4.29496000	-2.53598100	-3.84893300
C	-0.52634800	4.03390400	-0.09942500	H	-5.46112800	-0.52040500	-0.21978600
H	-0.23704300	4.64008100	1.95015300	H	-6.03194700	-1.48923800	-2.42570500
H	-1.02873700	3.17417300	-2.01561800	C	-1.36341000	-0.88644200	0.71756500
C	0.39709000	5.07825100	-0.67192100	C	-0.44243300	-0.57414200	1.83323500
H	0.84197100	4.74660100	-1.61478700	C	0.47212600	0.48247900	1.73448500
H	-0.15371200	6.00703100	-0.87272600	C	-0.47874000	-1.34860500	3.00276000
H	1.20703400	5.32186000	0.02322200	C	1.35311000	0.74916700	2.78360200

H	0.47443400	1.10857300	0.84988100	C	-5.28249800	-1.26048300	-2.33286600
C	0.40822200	-1.08464200	4.04583300	H	-4.56190100	-1.88307300	-0.39433200
H	-1.20815900	-2.14840600	3.09136300	C	-3.98768900	0.47415200	-3.43980400
C	1.32912100	-0.03768000	3.93611100	H	-2.25911300	1.19230800	-2.36448000
H	2.04926600	1.57919900	2.70139400	C	-5.07517700	-0.40827600	-3.42357700
H	0.37497500	-1.68918600	4.94778700	H	-6.13142300	-1.93743500	-2.32432100
H	2.01645100	0.16948700	4.75156300	H	-3.83912300	1.13918100	-4.28521300
N	-2.74727500	-0.57373600	0.77865100	H	-5.76573200	-0.42776200	-4.26176900
S	-3.29626000	0.83822200	1.66200100	O	-1.03632100	-0.44297000	3.09449900
O	-2.94525400	0.63389300	3.06352600	C	-0.04746700	-1.16073300	1.07059500
O	-4.69038600	1.02909200	1.26640000	C	0.73280000	-2.28731900	1.54509500
C	-2.25557100	2.11509300	0.97158400	C	0.48481100	-3.22624700	2.55491700
C	-1.59144000	2.98132400	1.83976400	C	1.90075500	-2.37095600	0.75257600
C	-2.08149300	2.19132000	-0.41383900	C	1.41233900	-4.24166000	2.75163100
C	-0.73450900	3.94073300	1.30284700	H	-0.40284000	-3.13852300	3.17215200
H	-1.71760400	2.88407700	2.91224300	C	2.82455500	-3.40482500	0.92977400
C	-1.20531700	3.14361400	-0.92643900	C	2.56086700	-4.32563800	1.94375700
H	-2.60007800	1.51109100	-1.08209100	H	1.25315000	-4.97557500	3.53562000
C	-0.52065300	4.03280400	-0.08018600	H	3.71109500	-3.48757400	0.31836600
H	-0.21036900	4.61745100	1.97234700	H	3.27211900	-5.12887600	2.11242100
H	-1.04652900	3.19561900	-2.00034100	C	0.71874900	-0.51090500	0.03828500
C	0.40604300	5.07432500	-0.65266200	C	0.65502500	0.94759400	-0.28341100
H	0.87369100	4.72836900	-1.57950700	C	0.85246700	1.84291800	0.77841300
H	-0.14841500	5.99366400	-0.88452800	C	0.38011800	1.44204500	-1.56485500
H	1.19900300	5.33872000	0.05404400	C	0.77440400	3.21832600	0.55788000
C	0.49532800	-0.33254200	-2.27302800	H	1.06973800	1.46394900	1.77265800
Pd	0.47147700	-2.48686200	-1.15849600	C	0.29800100	2.81747900	-1.77913400
INT12				H	0.24173000	0.75210500	-2.38833100
C	-2.35314800	-0.37983900	-0.16410400	C	0.49423700	3.70762800	-0.71933500
C	-2.25622400	0.09105200	1.09276200	H	0.92902600	3.90335100	1.38611500
C	-3.20047500	1.07318300	1.67454200	H	0.08345200	3.19320000	-2.77565500
C	-3.73228900	0.89371700	2.96226200	H	0.42876700	4.77841900	-0.88966400
C	-3.57305000	2.20390200	0.92815500	N	1.88229900	-1.27581200	-0.14930100
C	-4.63138300	1.82499300	3.48224900	S	3.08078700	-0.90225600	-1.37524600
H	-3.44202600	0.03030200	3.54932500	O	2.32308600	-0.60494200	-2.58937900
C	-4.47027700	3.13172000	1.45406000	O	4.01993800	-2.01857300	-1.33263600
H	-3.14353400	2.36034900	-0.05708500	C	3.82292800	0.56944500	-0.72143900
C	-5.00437000	2.94292700	2.73158500	C	3.74323800	1.75867400	-1.44509200
H	-5.04222000	1.67532500	4.47692900	C	4.45271600	0.50110400	0.52667200
H	-4.74755700	4.00443100	0.86909000	C	4.29728800	2.91054800	-0.89080600
H	-5.70468000	3.66554600	3.14146800	H	3.24125000	1.78653600	-2.40464900
C	-3.30467800	-0.34494600	-1.25703900	C	4.99170900	1.66547700	1.06040900
C	-4.40507700	-1.23783200	-1.25351800	H	4.50747700	-0.43420800	1.07568700
C	-3.09944800	0.50595000	-2.37101800	C	4.91972200	2.88595400	0.36505100

H	4.23231700	3.84601800	-1.43913000	H	-0.19450000	0.86747800	3.28694400
H	5.47323400	1.63158400	2.03383900	H	-3.35295100	3.66885400	2.43698600
C	5.51698600	4.13637900	0.95661400	H	-1.55775000	2.84272700	3.95122000
H	5.35810800	4.17996100	2.03965300	C	-1.76964500	-2.49134100	5.07297400
H	6.60149600	4.16264000	0.78613800	H	-2.12355100	-3.47076200	5.42125400
H	5.08927500	5.03769900	0.50669000	H	-0.71642900	-2.61239800	4.79274700
C	-1.12482800	-0.47153500	1.87804300	C	1.48744300	1.04595000	-0.47243300
Pd	-1.02365700	-1.62989200	-0.86648500	C	0.37876400	1.44464000	-1.13423200
INT13				C	-0.33130300	0.45601600	-2.03072100
C	-2.42985900	-2.61856300	2.64238000	O	0.26596200	0.00386700	-3.00851800
C	-2.58509000	-2.01089200	3.89873900	C	2.37530100	1.95355000	0.29098100
C	-3.49276800	-0.95135600	4.02893600	C	3.06765300	2.99150700	-0.36389000
C	-4.22659600	-0.49458700	2.93553900	C	2.61207500	1.76294700	1.66671100
C	-4.04926500	-1.12286900	1.70335000	C	3.95322000	3.81764900	0.33378200
C	-3.16019200	-2.18893600	1.53965700	H	2.89818400	3.14534200	-1.42528000
H	-1.70217700	-3.40986100	2.49800700	C	3.49117900	2.59091800	2.36873000
H	-3.61322100	-0.45948400	4.99064400	H	2.09162700	0.96096400	2.18205400
H	-4.89895800	0.35034600	3.02706800	C	4.17014200	3.62416300	1.70591800
H	-2.98689100	-2.64806000	0.57213500	H	4.46549600	4.62155600	-0.19005500
O	-5.82200900	-1.65492000	-0.20030400	H	3.64179700	2.43710200	3.43484700
O	-5.65157500	0.71996800	0.65052000	H	4.84368900	4.27899200	2.25358400
H	-1.82516900	-1.79634300	5.91736600	C	-0.18398800	2.82383800	-1.14997200
S	-5.00865900	-0.55257200	0.31682300	C	-0.77477500	3.31665800	-2.32915100
N	-3.80631300	-0.24452000	-0.91597700	C	-0.17366300	3.65923700	-0.01895800
C	-3.82031700	-0.84527200	-2.19644000	C	-1.32118900	4.59930400	-2.37924400
C	-4.85215500	-1.46973400	-2.90569100	H	-0.80008100	2.69243700	-3.21823800
C	-2.53408200	-0.65875700	-2.75169800	C	-0.71675900	4.94118200	-0.06955300
C	-4.56070600	-1.93370000	-4.18575500	H	0.22808800	3.28474500	0.91438700
H	-5.83837700	-1.58953700	-2.48102600	C	-1.29227000	5.42047100	-1.24972700
C	-2.26796400	-1.13314300	-4.04701700	H	-1.76983800	4.95550000	-3.30325200
C	-3.28334500	-1.77134200	-4.75018900	H	-0.70818400	5.56012400	0.82435900
H	-5.34328200	-2.42649700	-4.75667100	H	-1.72099500	6.41877500	-1.28591900
H	-1.28257000	-0.99568900	-4.47198600	H	1.80448600	-1.98465900	1.42679700
H	-3.08851300	-2.14537600	-5.75206000	C	0.30876100	-2.71141600	0.47775100
C	-1.73664600	0.07818300	-1.78920800	O	1.15771500	-2.70430300	1.57003600
C	-2.53563900	0.32445500	-0.68468800	O	0.47699700	-1.76328200	-0.39357000
C	-2.24783400	1.03760600	0.57603300	O	-0.54157000	-3.59163500	0.42264400
C	-1.22181300	0.58789400	1.42139100	Pd	2.27657200	-0.78283100	-0.55565500
C	-3.00938400	2.15461100	0.94990900	C	4.74195200	-1.40724200	-0.55750100
C	-0.97770800	1.23597600	2.63004700	O	5.98268300	-1.59332800	-0.38534300
H	-0.63750800	-0.27212900	1.12167600	K	5.59302300	-4.24937200	-0.47211300
C	-2.75935600	2.80193700	2.16003100	O	3.85761700	-2.36426900	-0.55566800
H	-3.79335500	2.51199500	0.29267900	O	4.25198200	-0.19167100	-0.71614800
C	-1.74726900	2.34226600	3.00489200	K	6.14747800	1.07477400	0.43649300

TS10			
C	-3.10119000	-0.46440100	3.55231400
C	-3.83954300	0.62536700	4.03672500
C	-4.85361600	1.16455200	3.23001600
C	-5.12222500	0.63817100	1.96938900
C	-4.36526000	-0.44793700	1.52538200
C	-3.35382600	-1.01892900	2.30027200
H	-2.29399200	-0.87933200	4.14946500
H	-5.43001500	2.01444800	3.58645500
H	-5.88301300	1.07551100	1.33228900
H	-2.71295100	-1.82193000	1.93571400
O	-5.33603600	-2.47458000	0.10144600
O	-5.46872000	-0.14824500	-0.87427900
H	-4.37208500	1.76973400	5.79863400
S	-4.75828100	-1.13970400	-0.06429600
N	-3.18945600	-1.39504900	-0.77408000
C	-2.72228800	-2.61757200	-1.31848500
C	-3.27315500	-3.90372200	-1.32750000
C	-1.47181200	-2.34220100	-1.91185600
C	-2.53745800	-4.90993300	-1.94754300
H	-4.22693600	-4.11354900	-0.86756500
C	-0.74729200	-3.37271200	-2.52678500
C	-1.28909100	-4.65195600	-2.54091400
H	-2.94369200	-5.91786700	-1.96721900
H	0.21409600	-3.15577500	-2.97507100
H	-0.74170500	-5.46324100	-3.01395700
C	-1.18013900	-0.94062200	-1.69267200
C	-2.24746000	-0.38307300	-1.00858300
C	-2.51300600	1.03141100	-0.63500200
C	-2.09793600	1.54222900	0.60317300
C	-3.21759800	1.85513400	-1.52410900
C	-2.40701800	2.85711800	0.95185800
H	-1.55108500	0.89275000	1.27683500
C	-3.52053800	3.17029700	-1.17166900
H	-3.53727800	1.45864600	-2.48242400
C	-3.12309900	3.67142700	0.07018800
H	-2.09079400	3.24112600	1.91836700
H	-4.06710000	3.80091100	-1.86744400
H	-3.36597100	4.69465000	0.34634600
C	-3.51328800	1.23625300	5.37726900
H	-3.19375000	0.47472200	6.09712800
H	-2.69082700	1.95869200	5.28288200
C	1.14019800	0.88334800	-0.26357100
C	0.53247300	0.98906300	-1.48823000
C	0.05319300	-0.29837700	-2.13262300
O	0.76168300	-0.78572600	-3.01604400
C	1.86121300	1.98561600	0.42334800
C	2.72045100	2.87204700	-0.25742300
C	1.75030400	2.10860800	1.82255400
C	3.41283400	3.87011000	0.43173000
H	2.84497900	2.77234000	-1.33028600
C	2.45027900	3.10120500	2.51453700
H	1.11129300	1.41161300	2.35720200
C	3.28009300	3.99428100	1.82405500
H	4.05126300	4.55834000	-0.11840200
H	2.33835400	3.18479700	3.59290000
H	3.80651000	4.78214000	2.35762900
C	0.31804700	2.21825700	-2.28616400
C	0.41870500	2.20386100	-3.69084500
C	-0.05427800	3.41918500	-1.65271900
C	0.18076200	3.36219800	-4.43074200
H	0.69892600	1.28722500	-4.19679500
C	-0.30665100	4.56787000	-2.39633300
H	-0.18116300	3.43602700	-0.57785600
C	-0.18297100	4.54815800	-3.78896700
H	0.27502800	3.33361000	-5.51314900
H	-0.61282400	5.47761800	-1.88664000
H	-0.37833700	5.44662800	-4.36864000
H	0.59928400	0.11017900	0.52860100
C	-0.07232000	-1.86842300	1.22873200
O	-0.12985300	-0.61858800	1.59637800
O	0.91169100	-2.21946100	0.37632100
O	-0.85611500	-2.75905900	1.60665200
Pd	2.36905600	-0.93071800	-0.01825800
C	4.85767300	-1.12229900	0.12936100
O	6.07529100	-1.14819400	0.45337800
K	5.89395400	-3.80403400	1.00427700
O	4.07027200	-2.17067200	0.22473000
O	4.24778000	-0.02831100	-0.26564500
K	5.60230500	1.50743900	1.32623000
INT14			
C	-3.09485800	-0.12228800	2.74808200
C	-3.36848500	1.11186600	3.36276300
C	-4.07192400	2.08601500	2.64034300
C	-4.46135700	1.86146100	1.32048300
C	-4.14901400	0.63600400	0.73155700
C	-3.48505900	-0.37356100	1.43634600

H	-2.57150800	-0.90903000	3.28219900	C	1.57877500	1.56072400	3.79581500
H	-4.30070000	3.04137100	3.10542900	H	0.51806600	0.06168200	2.67181400
H	-4.96167000	2.63443800	0.74790000	C	2.33417900	2.73834700	3.74240400
H	-3.25380400	-1.33588200	0.98986300	H	3.14601800	4.27288800	2.45406200
O	-5.51584500	-0.70195200	-1.14707900	H	1.36255900	1.09125000	4.75168100
O	-4.79928400	1.67989400	-1.62163300	H	2.70451800	3.19411200	4.65695400
H	-3.35680300	2.26217400	5.20100300	C	2.32808500	1.80138200	-1.67305300
S	-4.55607600	0.38820900	-0.98325500	C	3.68029500	1.45279300	-1.53023100
N	-3.04459600	-0.22448300	-1.60703000	C	2.00091700	2.98360300	-2.35360800
C	-2.78010100	-1.55664600	-2.00941600	C	4.68669700	2.27365600	-2.04687800
C	-3.61986500	-2.66608200	-2.15911000	H	3.94215800	0.52946800	-1.01867000
C	-1.39367900	-1.63317900	-2.27500200	C	3.00765700	3.80812600	-2.86181000
C	-3.03692000	-3.85480300	-2.58901600	H	0.95710600	3.26179500	-2.46743300
H	-4.67727700	-2.60802300	-1.94723300	C	4.35260900	3.45814600	-2.70986900
C	-0.83286400	-2.84174600	-2.71110800	H	5.72938600	1.98467900	-1.93499700
C	-1.66072000	-3.94592600	-2.86505200	H	2.73957600	4.72558600	-3.37922000
H	-3.66642600	-4.73183300	-2.71021100	H	5.13273400	4.10008700	-3.11020300
H	0.22857200	-2.90072700	-2.91779300	H	0.11599300	0.11084500	0.41026500
H	-1.24163200	-4.89239300	-3.19539500	C	-1.05987500	-2.93557700	2.07922800
C	-0.81787400	-0.34171700	-1.96634800	O	-0.12550800	-2.22668200	2.72159800
C	-1.84645900	0.49997600	-1.57362100	O	-0.57399100	-3.39781600	0.93480300
C	-1.79748500	1.96708400	-1.33609600	O	-2.20066200	-3.12005200	2.49301000
C	-1.66681700	2.51098800	-0.05228700	Pd	1.22507800	-2.52927400	1.24675700
C	-1.83641100	2.82441500	-2.44503700	C	3.48784300	-1.92529400	0.35996700
C	-1.56467500	3.89127800	0.11919300	O	4.55461000	-1.46429300	-0.13735500
H	-1.63616600	1.85686600	0.81092700	K	3.53199600	-1.97965800	-2.67598900
C	-1.73972900	4.20614500	-2.27127500	O	2.66938400	-2.71275700	-0.29201900
H	-1.94578500	2.40406300	-3.44042400	O	3.07588600	-1.60580400	1.56616100
C	-1.59972300	4.74180800	-0.98821900	K	4.64747200	0.40977900	1.92770600
H	-1.45546300	4.29742300	1.12099800	trans-3a			
H	-1.77367800	4.86131500	-3.13754600	C	3.22552000	-3.53578400	0.08589400
H	-1.52036100	5.81717400	-0.85241700	C	3.49600600	-3.40698300	-1.28375300
C	-2.87881400	1.37964000	4.76355800	C	3.74966800	-2.12643100	-1.80445700
H	-3.06646800	0.52228500	5.41972000	C	3.72613400	-1.00080100	-0.98795100
H	-1.79390100	1.55142100	4.76203700	C	3.43509500	-1.16572900	0.36917400
C	0.88032400	0.84682700	0.17721100	C	3.18817200	-2.42160700	0.92144500
C	1.24345600	0.93522200	-1.12470500	H	3.02727900	-4.51883100	0.50412600
C	0.60531300	-0.01347400	-2.09048500	H	3.96677100	-2.01181300	-2.86311100
O	1.30651400	-0.56433700	-2.95696800	H	3.91867200	-0.01493900	-1.40022200
C	1.38195800	1.55382200	1.36138800	H	2.94705700	-2.51843600	1.97355400
C	2.11803400	2.75857800	1.32286100	O	2.91890000	-0.10158800	2.75001700
C	1.09650600	0.98085600	2.62105000	O	4.61264500	1.04504000	1.25469300
C	2.58896800	3.34063000	2.50248200	H	4.20271100	-4.51188100	-3.00528000
H	2.30858100	3.24709300	0.37535800	S	3.38056500	0.27313600	1.41437900

N	2.12691200	1.23814800	0.66910900
C	2.34530900	2.49443400	0.05212300
C	3.37524600	3.43061500	0.20063400
C	1.23481800	2.74027900	-0.78835300
C	3.28111900	4.60795500	-0.53762100
H	4.21128200	3.25264900	0.86144800
C	1.15920300	3.93734300	-1.51651500
C	2.18983000	4.86063600	-1.38929500
H	4.07070700	5.34861100	-0.44455800
H	0.31083500	4.11741500	-2.16690100
H	2.15183200	5.79101800	-1.94935800
C	0.32395200	1.62509200	-0.65030600
C	0.89148800	0.71973700	0.22503300
C	0.38993100	-0.61476700	0.60334700
C	0.15958800	-0.96248000	1.94309800
C	0.10089500	-1.54397400	-0.40858400
C	-0.34446900	-2.22300100	2.26181900
H	0.37696000	-0.24699800	2.72737100
C	-0.39371100	-2.80609100	-0.08510300
H	0.28126300	-1.27570600	-1.44469700
C	-0.61781700	-3.14893700	1.25098200
H	-0.52835700	-2.47960600	3.30141500
H	-0.60772200	-3.51776800	-0.87742400
H	-1.00642100	-4.13170100	1.50402900
C	3.47727800	-4.61121200	-2.19070200
H	3.69779000	-5.53231900	-1.64148000
H	2.48615400	-4.73044500	-2.64921900
C	-2.34644200	1.11750400	0.59516500
C	-2.16361600	0.90002300	-0.72953200
C	-0.96116100	1.52122600	-1.38298600
O	-1.04112600	1.98922800	-2.51908300
C	-3.48365700	0.77303200	1.45923200
C	-4.81181000	0.66100000	1.00352800
C	-3.23065000	0.58007000	2.83129000
C	-5.83965700	0.34131000	1.88754700
H	-5.03786100	0.83956900	-0.04133500
C	-4.25783000	0.24450100	3.71175200
H	-2.21337300	0.68143600	3.20104600
C	-5.56776900	0.12196500	3.24205000
H	-6.85910400	0.26633200	1.51820400
H	-4.03721800	0.08725900	4.76434000
H	-6.37296700	-0.13132700	3.92665000
C	-3.08095500	0.10812100	-1.59360900
C	-3.64473700	0.62731200	-2.77018700
C	-3.37667300	-1.21798900	-1.23017300
C	-4.49196100	-0.15962500	-3.55427700
H	-3.41564400	1.64376400	-3.06538400
C	-4.21931100	-2.00145300	-2.01658200
H	-2.93997200	-1.62649500	-0.32514000
C	-4.78225400	-1.47404400	-3.18266800
H	-4.92603000	0.25905400	-4.45880200
H	-4.43535500	-3.02462800	-1.71929900
H	-5.44055500	-2.08346200	-3.79663700
H	-1.53815100	1.62310800	1.11905900

INT15

C	-4.51876200	-2.46660400	-1.50442800
C	-4.95347900	-2.71599100	-0.19566600
C	-4.88364900	-1.67662700	0.74850200
C	-4.38562700	-0.42490700	0.40399900
C	-3.93944100	-0.21999200	-0.90498000
C	-4.00586500	-1.22324500	-1.86968800
H	-4.56835300	-3.25860400	-2.24663400
H	-5.22549200	-1.85225200	1.76508300
H	-4.33416800	0.37188700	1.13990200
H	-3.64221500	-1.04125500	-2.87432100
O	-2.75427800	1.32678400	-2.71149100
O	-4.28136500	2.40625100	-1.00024800
H	-6.28487000	-4.00781500	0.91801200
S	-3.30409500	1.37985400	-1.35896500
N	-1.97961100	1.59328300	-0.22820900
C	-1.87147500	2.67440500	0.67944900
C	-2.52223500	3.91208200	0.71697300
C	-0.86735800	2.32859500	1.61045500
C	-2.15843000	4.79252400	1.73134800
H	-3.26470000	4.18539600	-0.01809600
C	-0.51500800	3.23701200	2.62117900
C	-1.17071000	4.46058400	2.67539700
H	-2.64312100	5.76362900	1.78046700
H	0.26091400	2.97741600	3.32912200
H	-0.90554900	5.17740000	3.44760400
C	-0.34453100	1.02865000	1.23132800
C	-1.03749900	0.61084100	0.09964700
C	-0.89620700	-0.62202800	-0.70237500
C	-0.53737700	-0.55046400	-2.05912800
C	-1.13609400	-1.87532000	-0.12089600
C	-0.41104800	-1.71747300	-2.81261900
H	-0.39124700	0.41624200	-2.52599400
C	-1.00577300	-3.03959900	-0.87604500

H	-1.43777600	-1.93268300	0.91836500
C	-0.64092600	-2.96459600	-2.22262600
H	-0.13631300	-1.64998100	-3.86171400
H	-1.19283300	-4.00234200	-0.41005100
H	-0.54594600	-3.87222600	-2.81275600
C	-5.45432900	-4.07979400	0.20724300
H	-5.79068300	-4.65778700	-0.65935300
H	-4.65579700	-4.65301800	0.69769100
C	2.43547100	-0.55649200	0.45336900
C	1.49198500	-0.81804700	1.35197200
C	0.75641900	0.37966100	1.94453200
O	1.13416700	0.78044200	3.04266100
C	3.44687400	-1.12385300	-0.39875200
C	4.80086600	-0.76712200	-0.11385800
C	3.14042800	-1.75778500	-1.64310100
C	5.80783500	-1.02968300	-1.06604700
H	5.07122800	-0.42714900	0.88276800
C	4.15209000	-2.03263700	-2.53909900
H	2.10808500	-2.01238300	-1.85763300
C	5.48524500	-1.65452600	-2.26007200
H	6.83657300	-0.76580600	-0.84032100
H	3.92205600	-2.53230500	-3.47583500
H	6.26394300	-1.86965600	-2.98615900
C	1.21795600	-2.15861000	1.93459500
C	0.44097300	-2.27767700	3.10181000
C	1.68320100	-3.33785100	1.32404300
C	0.14030800	-3.53172800	3.63507000
H	0.07802800	-1.38988700	3.60655100
C	1.38601300	-4.58725600	1.86196200
H	2.26381400	-3.28519700	0.41063100
C	0.60917000	-4.69310700	3.01971600
H	-0.46084600	-3.59544300	4.53813400
H	1.75582700	-5.48242500	1.36881700
H	0.37426600	-5.66895600	3.43583400
H	1.11614800	1.64671900	-1.42955600
C	1.39180200	3.40072400	-0.71146300
O	0.78767200	2.54561800	-1.60685900
O	2.29058600	2.86043300	0.08147000
O	1.07835000	4.57418100	-0.71517400
Pd	3.24621500	1.10229900	-0.25506500

TS11

C	4.84176900	2.57697800	-1.06413100
C	5.40091100	2.57988300	0.22130400
C	5.33194800	1.40530800	0.99029200
C	4.71688200	0.25928500	0.49752700
C	4.15406300	0.29905000	-0.78126200
C	4.21231100	1.44327100	-1.57446300
H	4.88731900	3.47710400	-1.67116900
H	5.76822200	1.39007200	1.98562900
H	4.66798900	-0.64463800	1.09710000
H	3.75323800	1.45118700	-2.55623100
O	2.73215000	-0.85922300	-2.69778600
O	4.28635100	-2.29793900	-1.29844100
H	6.86577800	3.58862500	1.45505800
S	3.37136400	-1.16556200	-1.42294700
N	2.11864000	-1.45563400	-0.23739400
C	2.00444600	-2.60294300	0.59036300
C	2.73631200	-3.79353400	0.63186500
C	0.91637500	-2.36967700	1.46000500
C	2.35952500	-4.74148100	1.57974300
H	3.55198900	-3.98148900	-0.04999400
C	0.54852400	-3.34275800	2.39850700
C	1.28076000	-4.52278400	2.45430700
H	2.91198300	-5.67558400	1.63291200
H	-0.28996000	-3.16093200	3.05952700
H	1.01247500	-5.28871600	3.17695000
C	0.35798500	-1.07801100	1.11764000
C	1.11933400	-0.54161600	0.08706100
C	1.05058900	0.82475400	-0.47786600
C	0.63437800	1.06387200	-1.79591400
C	1.41627400	1.90213600	0.34564400
C	0.58536100	2.37315000	-2.27581000
H	0.33718400	0.22353400	-2.41032400
C	1.37910600	3.20542800	-0.14538400
H	1.74089100	1.70957000	1.36311200
C	0.96190000	3.44277500	-1.45736700
H	0.25504200	2.55653400	-3.29473700
H	1.66655100	4.03208700	0.49771000
H	0.92686400	4.45919100	-1.84099200
C	6.03254200	3.82760100	0.78547100
H	6.40464300	4.48430600	-0.00769100
H	5.29876600	4.40010000	1.36926400
C	-2.40482300	0.11409700	-0.14592400
C	-1.66405500	0.53328900	0.96384900
C	-0.86074200	-0.54204700	1.68728200
O	-1.35864100	-0.95762600	2.73670500
C	-3.57874200	0.81706800	-0.70422500
C	-4.62609900	1.26369200	0.13476600

C	-3.71489200	0.96228600	-2.10213300	C	0.92716000	2.42608300	-0.66063700
C	-5.76885800	1.84766300	-0.41299400	C	1.82393400	5.03738600	-0.38906900
H	-4.52214000	1.16602500	1.21223100	H	3.25474500	4.29341200	1.04890800
C	-4.85016100	1.56240200	-2.63738200	C	0.29402500	3.43755300	-1.39726600
H	-2.92066500	0.60035600	-2.74810800	C	0.75805500	4.74016600	-1.25922400
C	-5.88036000	2.00478300	-1.79652300	H	2.16128800	6.06540000	-0.28982300
H	-6.56695000	2.18673500	0.24174800	H	-0.54390000	3.19470400	-2.04172900
H	-4.93885700	1.68192700	-3.71370300	H	0.28519200	5.54115900	-1.82033600
H	-6.76669000	2.46751400	-2.22161500	C	0.65724300	1.01452300	-0.52461000
C	-1.61546300	1.88611000	1.50758600	C	1.54552700	0.48956400	0.38835400
C	-1.16718800	2.12172000	2.82934800	C	1.66467300	-0.92226100	0.79044300
C	-1.92254200	3.00236700	0.69378000	C	1.61262800	-1.31382200	2.13884800
C	-1.06694600	3.41810600	3.32178100	C	1.76077400	-1.90658300	-0.20776600
H	-0.92751700	1.28498000	3.47386800	C	1.66349900	-2.66549700	2.47646100
C	-1.80170200	4.29456700	1.18811800	H	1.53685200	-0.55941000	2.91316600
H	-2.20598400	2.85405100	-0.33997400	C	1.81577600	-3.25692100	0.13528500
C	-1.38280400	4.50882700	2.50534600	H	1.81867300	-1.60586300	-1.24930000
H	-0.73943600	3.57900200	4.34479500	C	1.76831300	-3.63953900	1.47770500
H	-2.02430000	5.13818300	0.54136800	H	1.62045100	-2.95903400	3.52164400
H	-1.29553500	5.52083100	2.89110100	H	1.89465000	-4.00630500	-0.64699600
H	-1.76416100	-0.51903300	-0.94798900	H	1.81244500	-4.69141400	1.74681100
C	-1.02109700	-2.59994900	-1.36651000	C	6.22886100	-2.63262400	-2.58261600
O	-1.13751600	-1.46352600	-1.95764600	H	6.45517700	-3.61111900	-2.14826800
O	-1.86830200	-2.88033300	-0.30999300	H	5.50707100	-2.77944000	-3.39590100
O	-0.23457900	-3.51721900	-1.61939500	C	-1.55198100	-0.43242300	0.80858700
Pd	-3.38051400	-1.71239500	0.07694200	C	-1.35838600	-0.63457000	-0.56211400
INT16				C	-0.38785900	0.29480900	-1.28636300
C	5.52088000	-2.06443200	-0.21540000	O	-0.51715500	0.48564700	-2.48711400
C	5.68816300	-1.67567000	-1.55070300	C	-2.65858400	-0.91677200	1.64154500
C	5.33542400	-0.36540400	-1.92251700	C	-3.82264000	-1.54407100	1.10355900
C	4.82862600	0.53398400	-0.99236400	C	-2.67208700	-0.52651600	3.00956100
C	4.66495200	0.10706600	0.33041300	C	-4.95156500	-1.73840500	1.91795200
C	5.00509700	-1.18250000	0.73381600	H	-3.82318000	-1.96749900	0.10721200
H	5.78445200	-3.07406400	0.08728900	C	-3.78259700	-0.75705200	3.79920700
H	5.46018400	-0.05009200	-2.95519300	H	-1.79436200	-0.03528800	3.42003900
H	4.55569700	1.54209100	-1.28931700	C	-4.93442500	-1.35317500	3.25080400
H	4.84962900	-1.49403200	1.76040700	H	-5.82934900	-2.21531000	1.49314000
O	3.80020000	0.56570100	2.79971300	H	-3.77198500	-0.46154400	4.84415000
O	4.66432300	2.52534900	1.44294600	H	-5.80686500	-1.51703900	3.87641600
H	7.14770000	-2.24115500	-3.03662300	C	-1.80731900	-1.83831800	-1.31112200
S	3.97182800	1.23992500	1.51441900	C	-2.42266300	-1.75126600	-2.57116800
N	2.37306200	1.53240000	0.86189000	C	-1.56872600	-3.10441800	-0.74805100
C	1.99568600	2.73658700	0.21223700	C	-2.80540400	-2.91235500	-3.24304400
C	2.45198100	4.05008900	0.36764900	H	-2.60800900	-0.77742200	-3.00730500

C	-1.94623900	-4.26113100	-1.42836800	H	-4.60493400	3.57099500	2.24410600
H	-1.07597000	-3.17521000	0.21619200	S	0.67292900	2.65614300	-1.58541300
C	-2.56911900	-4.16801500	-2.67618200	N	0.85895900	1.01867200	-1.38778000
H	-3.29104700	-2.83384000	-4.21176000	H	2.36752200	1.34616600	0.69284500
H	-1.75177200	-5.23372400	-0.98434600	C	1.29218700	0.17375600	-2.29901600
H	-2.86736400	-5.06923100	-3.20510900	C	1.87151900	0.46866200	-3.58838900
H	-0.87589800	0.24703200	1.31796800	C	1.17668100	-1.25908900	-1.93637000
C	-4.31476800	2.61812200	-1.09029100	C	2.34916600	-0.53767200	-4.37932700
O	-4.89520000	1.78079800	-0.23057800	H	1.94010000	1.50139900	-3.90498800
O	-3.05612200	2.22234800	-1.31740800	C	1.72436000	-2.26846700	-2.80125500
O	-4.83707100	3.58897100	-1.59972200	C	2.29006600	-1.91870300	-3.99150600
Pd	-3.22344500	0.65271700	-0.06476700	H	2.80006800	-0.28689600	-5.33603200
K_2CO_3				H	1.64966900	-3.30653600	-2.49153600
C	0.00011700	0.82461700	0.00157600	H	2.68953100	-2.67652200	-4.65808500
O	0.00068000	-0.51455300	0.00586200	C	0.48365800	-1.58953100	-0.81239400
K	-2.51022200	-0.63061400	0.00825000	C	-0.22144600	-1.78780700	0.23996100
O	-1.12655100	1.44507300	-0.05080100	C	-1.60104300	-1.72556000	0.69035500
O	1.12555800	1.44619700	0.04961900	C	-2.44414700	-0.72631200	0.16396700
K	2.51031700	-0.63051500	-0.01071800	C	-2.11135200	-2.64392900	1.62748600
$PdCO_3$-K_2CO_3				C	-3.78182500	-0.67530500	0.54942200
C	3.50017300	-0.00009000	0.00729300	H	-2.04098300	0.00266200	-0.53181000
O	2.72896000	1.09014400	-0.01760700	C	-3.44680500	-2.57665200	2.01545800
O	2.72882300	-1.09029500	0.02518600	H	-1.45520100	-3.40484000	2.04069100
O	4.72146400	0.00000300	0.01306000	C	-4.28587200	-1.59690700	1.47273900
Pd	1.03789400	-0.00000200	-0.00512400	H	-4.42714700	0.09277700	0.13519600
C	-1.48399500	0.00002300	-0.01109400	H	-3.83517100	-3.28884700	2.73787500
O	-2.75132500	-0.00008100	-0.00788000	H	-5.32875800	-1.54828300	1.77365800
K	-2.81225400	2.67397800	0.01628100	C	-4.53577700	2.72088600	1.55392500
O	-0.77465200	1.10168500	-0.03145900	H	-5.41598900	2.73883200	0.90328100
O	-0.77487200	-1.10153400	0.00695200	H	-4.57894500	1.80848800	2.16150400
K	-2.81234300	-2.67391900	0.00227200	C	1.61047500	0.45446200	2.19914700
INT10’				O	2.36712700	0.44280700	1.06539200
C	-3.26302100	2.81383700	-0.64006300	O	1.27887300	-0.73511000	2.62352200
C	-3.25448900	2.77003600	0.76085100	O	1.31084300	1.49642200	2.77000500
C	-2.01664500	2.74950900	1.42486000	Pd	1.35757200	-2.29853600	1.32745600
C	-0.81953300	2.76365600	0.71787500	TS24			
C	-0.86050700	2.80047800	-0.67894900	C	3.49745100	0.04359200	-1.69423800
C	-2.07173800	2.82483800	-1.36903100	C	3.83689900	1.40530100	-1.47056000
H	-4.21184000	2.83466500	-1.17012400	C	3.96881700	1.85345700	-0.14870000
H	-1.99156000	2.70749100	2.51087900	C	3.73850600	0.99981600	0.92811500
H	0.12591800	2.72415700	1.24709000	C	3.39136900	-0.33508100	0.69159900
H	-2.08260900	2.84970000	-2.45385800	C	3.29672500	-0.83566600	-0.60863500
O	0.43838700	3.08884000	-2.97923700	H	3.58238000	-0.36769400	-2.70059100
O	1.75087900	3.31569400	-0.81416600	H	4.23474800	2.88880700	0.04171700

H	3.80230400	1.37158700	1.94451700	C	-5.20458700	-3.37407100	0.37395700
H	3.07272600	-1.88206900	-0.78429900	H	-3.78954300	-4.60818700	-0.69371500
O	2.74236500	-2.71922000	1.70330100	H	-6.43582300	-1.90248200	1.36521000
O	3.11398000	-0.77810100	3.31858800	H	-5.86103600	-4.20337200	0.62242300
H	5.19296600	2.35665600	-2.82951700	C	-2.87793300	2.52660000	-0.25182400
S	2.68483700	-1.29882100	2.02537200	C	-2.45185200	3.61270000	-1.04116700
N	0.94617800	-0.76924700	1.84535000	C	-3.73165800	2.75556900	0.84309600
C	0.84456200	0.64877200	2.02817600	C	-2.87807000	4.90291100	-0.74012300
C	1.06124600	1.38321900	3.19054700	H	-1.79911200	3.43108500	-1.89059000
C	0.49216400	1.25607700	0.80824800	C	-4.14175600	4.05141800	1.14665400
C	0.93183300	2.77132300	3.10131300	H	-4.04202200	1.92228100	1.46597000
H	1.32752200	0.89406500	4.11959000	C	-3.71937000	5.12473400	0.35589000
C	0.36890200	2.64563700	0.73346100	H	-2.55483800	5.73729000	-1.35604500
C	0.59720300	3.39439700	1.88748700	H	-4.79088600	4.22620400	1.99977900
H	1.08671400	3.37597800	3.98979100	H	-4.04541000	6.13357700	0.59281200
H	0.09620200	3.12685400	-0.19856700	Pd	1.12334200	0.32633500	-1.95920500
H	0.49754600	4.47521800	1.85079300	INT34			
C	0.26822700	0.17750200	-0.15000100	C	4.14478500	0.68960300	-1.96271200
C	0.49505300	-1.03896700	0.51761500	C	4.94253800	1.68080100	-1.36937000
C	0.26690900	-2.41579100	0.11007200	C	5.20348700	1.60072300	0.00789100
C	-0.10191600	-3.35830100	1.09415800	C	4.68443300	0.56711200	0.78260800
C	0.33692000	-2.83353200	-1.23548200	C	3.89689500	-0.40449800	0.15914800
C	-0.40842600	-4.66720100	0.73679400	C	3.61745500	-0.35617900	-1.20991000
H	-0.17194600	-3.04492900	2.12939300	H	3.93936400	0.73383700	-3.02886100
C	0.04159600	-4.14599200	-1.58501000	H	5.82166800	2.35948000	0.48017000
H	0.63196100	-2.12488900	-2.00403800	H	4.88853600	0.51054900	1.84564300
C	-0.33598000	-5.06709900	-0.60009900	H	3.01326100	-1.12679400	-1.67718300
H	-0.70474900	-5.37649200	1.50348500	O	2.94252400	-2.87337000	0.31164200
H	0.10701000	-4.45409100	-2.62444000	O	3.76718500	-1.76378800	2.45150200
H	-0.56673600	-6.09221400	-0.87546900	H	5.51596700	3.74593900	-1.65111300
C	4.11356900	2.32391500	-2.62997500	S	3.13981600	-1.68273400	1.13510700
H	3.62026800	1.98397000	-3.54625400	N	1.51923300	-1.02110100	1.43345400
H	3.78939200	3.34690000	-2.41430700	C	1.45048000	0.22653800	2.10739300
C	-2.62929400	-0.14517500	-0.56798200	C	2.16004300	0.66312200	3.22616900
C	-2.41659800	1.19658200	-0.56395900	C	0.49366500	1.03499800	1.45668000
C	-1.44526300	0.35795300	-1.18594800	C	1.88915600	1.94818800	3.69334000
O	-0.82990700	0.28179900	-2.36821100	H	2.88226500	0.02455200	3.71740000
C	-3.50815100	-1.24133300	-0.25297100	C	0.23281200	2.32391700	1.95061100
C	-3.19502500	-2.54427900	-0.68251500	C	0.93896500	2.76916000	3.06259700
C	-4.68686900	-1.01527200	0.48540600	H	2.41848000	2.31442800	4.56807000
C	-4.04050100	-3.60343900	-0.36656800	H	-0.49522800	2.96995200	1.47725000
H	-2.28974600	-2.71460600	-1.25328500	H	0.74896800	3.76485400	3.45228600
C	-5.52801900	-2.07920900	0.79564800	C	-0.03474500	0.27181000	0.33815400
H	-4.93586500	-0.00722800	0.80135900	C	0.61318000	-0.96947200	0.34529700

C	0.28525800	-2.19553600	-0.36758500
C	0.10297700	-3.39456200	0.36546300
C	0.15702500	-2.23817100	-1.80025800
C	-0.25265200	-4.56709400	-0.27901600
H	0.22281400	-3.37443400	1.44277600
C	-0.14209900	-3.47577900	-2.44431300
H	0.57213700	-1.42034000	-2.38069200
C	-0.39319400	-4.61158200	-1.68403000
H	-0.41969900	-5.46828800	0.30322800
H	-0.14388300	-3.52052900	-3.52915200
H	-0.65358200	-5.54572500	-2.17232900
C	5.53558500	2.79446400	-2.19386400
H	6.58585500	2.57885800	-2.43118900
H	5.00304900	2.92452200	-3.14126200
C	-2.54538200	0.86087800	0.30708200
C	-2.03803200	1.89959000	-0.26760700
C	-1.20182500	0.61230500	-0.48699500
O	-1.27861200	0.15985600	-1.74642600
C	-3.43563300	0.07095300	1.10973600
C	-3.17228400	-1.29624400	1.32590600
C	-4.58351500	0.65912600	1.67795100
C	-4.05416500	-2.06562700	2.08147700
H	-2.26630700	-1.73634400	0.91696500
C	-5.45903300	-0.12004700	2.42842600
H	-4.78172400	1.71508900	1.51924100
C	-5.19913600	-1.48083100	2.63038500
H	-3.84410400	-3.11807000	2.24985900
H	-6.34666600	0.33378700	2.85948100
H	-5.88534300	-2.08116400	3.22063800
C	-1.97649600	3.25704000	-0.74233200
C	-0.84113600	3.71522100	-1.43422500
C	-3.04624300	4.13656800	-0.48617000
C	-0.77995300	5.03723500	-1.86613600
H	-0.01856200	3.03226700	-1.62529200
C	-2.97342500	5.45685300	-0.92107600
H	-3.92155600	3.77917200	0.04842800
C	-1.84346900	5.90893000	-1.61114400
H	0.09673800	5.38905800	-2.40208300
H	-3.79923800	6.13438200	-0.72407700
H	-1.79308900	6.93944200	-1.95084700
Pd	-1.95475000	-1.69621100	-1.85422700
TS25			
C	4.25033300	1.15776200	-1.96610500
C	4.89356800	2.24498400	-1.35356500
C	5.06725900	2.22743100	0.03945500
C	4.60001900	1.16764100	0.81176200
C	3.95715700	0.10551300	0.17040300
C	3.77643900	0.08481200	-1.21595000
H	4.12500800	1.14785000	-3.04538900
H	5.57711000	3.05456300	0.52597700
H	4.74132500	1.15643200	1.88625600
H	3.29649600	-0.76003000	-1.69871700
O	3.24865000	-2.44278200	0.33974300
O	3.82328400	-1.20547300	2.49034600
H	6.32974700	3.79934300	-1.79632800
S	3.27390500	-1.22007600	1.13730100
N	1.57838200	-0.71725500	1.33007800
C	1.34402100	0.53117800	1.96546100
C	1.96035500	1.07997300	3.09047900
C	0.32030200	1.20256600	1.26572200
C	1.52941500	2.33861800	3.50657900
H	2.73360200	0.54386800	3.62480000
C	-0.09817000	2.46911000	1.70361800
C	0.51575200	3.02752800	2.81965000
H	1.98488300	2.78897900	4.38359800
H	-0.87462300	3.01435700	1.18067300
H	0.20352000	4.00797000	3.16713600
C	-0.09103300	0.34648800	0.16351200
C	0.70446300	-0.81136100	0.22293200
C	0.54164700	-2.07982000	-0.46298500
C	0.51088400	-3.28357700	0.28491100
C	0.40846200	-2.15273600	-1.89244800
C	0.30411100	-4.49961400	-0.34364500
H	0.62411400	-3.23443200	1.36194100
C	0.26673400	-3.42525300	-2.52207800
H	0.70910500	-1.29328600	-2.48361200
C	0.16719600	-4.57676100	-1.74617600
H	0.25323500	-5.40735500	0.24992700
H	0.27737000	-3.48570500	-3.60617900
H	0.02601100	-5.54149300	-2.22415300
C	5.37175600	3.41963300	-2.16773200
H	5.49006400	3.15843500	-3.22385700
H	4.65084400	4.24626300	-2.10916900
C	-2.65676300	0.46372100	0.39419400
C	-2.39187900	1.52342200	-0.28209000
C	-1.29588200	0.50169200	-0.64362400
O	-1.40022900	0.03477500	-1.86479900
C	-3.09185900	-0.41923500	1.42545300

C	-2.94128500	-1.81660200	1.31715800
C	-3.66607100	0.13361200	2.59191700
C	-3.37785300	-2.64568900	2.34465100
H	-2.46775000	-2.23797200	0.43255700
C	-4.10545400	-0.70675800	3.60921200
H	-3.75900200	1.21122900	2.68440600
C	-3.96289200	-2.09381500	3.48934400
H	-3.25683200	-3.72150000	2.25792900
H	-4.55259300	-0.28025300	4.50217500
H	-4.30011100	-2.74349300	4.29173700
C	-2.74261900	2.82409200	-0.80324400
C	-1.88236900	3.48897800	-1.69274300
C	-3.94068300	3.43561500	-0.38850800
C	-2.21835400	4.75688900	-2.16073700
H	-0.96235200	3.00742400	-2.01088900
C	-4.26593900	4.70356800	-0.86137900
H	-4.60274400	2.91399400	0.29677900
C	-3.40742800	5.36514200	-1.74654900
H	-1.55408800	5.27062300	-2.84940500
H	-5.19011800	5.17668600	-0.54236200
H	-3.66706300	6.35355600	-2.11473500
Pd	-1.75565200	-1.93975500	-2.00373700
INT35			
C	4.39619100	0.68125100	-2.33566900
C	5.20754600	1.71901300	-1.84449700
C	5.42147100	1.80931600	-0.46175900
C	4.83599100	0.90302800	0.42083600
C	4.03157100	-0.11117900	-0.10121200
C	3.80323100	-0.23690700	-1.47641100
H	4.23545000	0.58900400	-3.40661900
H	6.05711600	2.59734700	-0.06784200
H	5.01012800	0.97386600	1.48832000
H	3.19426300	-1.04768300	-1.86245900
O	3.00897900	-2.51736200	0.32400500
O	3.79850100	-1.17201900	2.33584300
H	6.61134600	3.29947100	-2.31405300
S	3.21364500	-1.24034100	0.99880000
N	1.60964500	-0.49918300	1.17376100
C	1.53440400	0.80446300	1.72911300
C	2.26844600	1.37981100	2.76888300
C	0.51951600	1.50915900	1.05147900
C	1.95986200	2.69291000	3.11999100
H	3.03779000	0.82435300	3.28846900
C	0.22622700	2.83104100	1.41917200
C	0.95207800	3.41157500	2.45386100
H	2.50932400	3.16518200	3.92901200
H	-0.54276300	3.39430800	0.90229700
H	0.73762400	4.43423100	2.74997900
C	-0.02793200	0.62266700	0.03715400
C	0.66168600	-0.59959700	0.13207600
C	0.29714600	-1.90078500	-0.40011700
C	0.18116800	-3.00099700	0.47280700
C	-0.01705600	-2.07940700	-1.79036600
C	-0.29425100	-4.22490100	0.01632800
H	0.42834500	-2.86983600	1.51947600
C	-0.46088100	-3.35685000	-2.24857300
H	0.36068000	-1.35080500	-2.50313600
C	-0.63749000	-4.40197800	-1.33384200
H	-0.40075600	-5.05094200	0.71297800
H	-0.55951300	-3.53923400	-3.31495000
H	-0.99754200	-5.36556500	-1.68243900
C	5.81990800	2.71624100	-2.79434200
H	6.24414300	2.21744600	-3.67312100
H	5.05947100	3.41996800	-3.15806100
C	-2.71982400	0.60594000	0.90065100
C	-2.41882400	1.55647600	0.07864900
C	-1.25023200	0.86964200	-0.69612000
O	-1.53849100	0.43196600	-1.83542500
C	-2.76316300	-0.58872800	1.58834500
C	-3.50349300	-1.69048100	1.05574500
C	-1.95938200	-0.77180000	2.75289000
C	-3.41389800	-2.93277700	1.66290500
H	-4.14392500	-1.53081700	0.19320800
C	-1.87730700	-2.02453100	3.33492400
H	-1.39872800	0.07019900	3.14480400
C	-2.59541500	-3.10200000	2.78948300
H	-3.96981700	-3.77485100	1.26312400
H	-1.25369900	-2.17654200	4.21013800
H	-2.52072500	-4.08156400	3.25251400
C	-2.97370500	2.86998900	-0.25694700
C	-2.36953700	3.65733200	-1.24920800
C	-4.10258900	3.35389800	0.42787200
C	-2.89230900	4.91370000	-1.55442800
H	-1.49627300	3.28890900	-1.77922100
C	-4.61848200	4.60795400	0.11699900
H	-4.56620300	2.74326400	1.19832500
C	-4.01519200	5.39040200	-0.87448800
H	-2.42149300	5.51845900	-2.32387800

H	-5.49187200	4.97709900	0.64682900
H	-4.42112700	6.36884000	-1.11486900
Pd	-2.11678000	-1.63026900	-1.86009700
INT36			
C	3.74342200	-0.68929800	-2.40343500
C	4.68825800	0.23892300	-1.94219100
C	5.11514100	0.15878700	-0.60639800
C	4.59587400	-0.79749200	0.26081800
C	3.64045400	-1.69601300	-0.22472700
C	3.20903700	-1.65559700	-1.55260300
H	3.41435800	-0.65201800	-3.43842900
H	5.85556700	0.86393400	-0.23775800
H	4.91515100	-0.84221300	1.29559000
H	2.47124200	-2.36514400	-1.91020600
O	2.16317800	-3.86582500	0.18844300
O	3.60960100	-3.01484500	2.10007600
H	6.32224900	1.35512700	-2.81393100
S	2.78524300	-2.76337400	0.91781200
N	1.46308400	-1.69002600	1.46748000
C	1.93090800	-0.52383400	2.13850500
C	2.73932100	-0.45068200	3.27211900
C	1.43976600	0.61882500	1.47774600
C	3.08755800	0.81746400	3.73506400
H	3.08610300	-1.34960000	3.76486900
C	1.81283400	1.88576800	1.95406400
C	2.63764900	1.97109600	3.07428900
H	3.71310200	0.90935700	4.61827500
H	1.48002400	2.79114600	1.46400400
H	2.92915700	2.94998700	3.44476300
C	0.58979300	0.15437700	0.37502300
C	0.60755600	-1.24824500	0.41068600
C	-0.20321100	-2.23441800	-0.27431100
C	-0.72803500	-3.32840600	0.45710700
C	-0.48943300	-2.14369800	-1.67642800
C	-1.55636600	-4.25512500	-0.15478100
H	-0.49522100	-3.41236000	1.51266500
C	-1.30698100	-3.13385700	-2.28991000
H	0.13981000	-1.51452700	-2.29658700
C	-1.87133200	-4.15023900	-1.52388300
H	-1.97680400	-5.06666900	0.43219400
H	-1.45612700	-3.10586300	-3.36538200
H	-2.52961200	-4.87842700	-1.98847100
C	5.22693800	1.31873400	-2.84656900
H	4.91987000	1.16715800	-3.88593300
H	4.86292600	2.30455100	-2.52807100
C	-1.33160100	2.25710000	0.87281500
C	-0.47056600	2.44514600	-0.06854200
C	-0.19638100	0.99342100	-0.49309900
O	-0.76911100	0.63859800	-1.56730800
C	-2.21411600	1.78423400	1.82967000
C	-3.57359200	1.54894600	1.47862000
C	-1.76292900	1.48211900	3.14784600
C	-4.44017900	0.99823500	2.41173800
H	-3.91038000	1.77670900	0.47523600
C	-2.64905400	0.94100900	4.06503400
H	-0.72525400	1.66418800	3.40797600
C	-3.98289300	0.69305700	3.70008000
H	-5.46527000	0.79624000	2.11849800
H	-2.30806800	0.70143100	5.06810100
H	-4.66546700	0.26039000	4.42641800
C	0.13735100	3.61105500	-0.72237900
C	1.20262200	3.43221100	-1.61799800
C	-0.31035500	4.90978500	-0.42760400
C	1.80752600	4.53831600	-2.21439200
H	1.55790900	2.42974800	-1.84024800
C	0.29779600	6.01009300	-1.02573200
H	-1.13725300	5.04528300	0.26460100
C	1.35802400	5.82792600	-1.92067700
H	2.62930800	4.39231000	-2.91019400
H	-0.05694700	7.01141800	-0.79740800
H	1.82907000	6.68843800	-2.38787900
Pd	-2.24561300	-0.87087100	-1.51255200
C	-4.96835800	-0.12199800	-0.88947000
O	-3.94433400	0.41886900	-1.43744300
O	-5.99318900	0.42194700	-0.48156600
O	-4.83386800	-1.50396900	-0.76145200
H	-5.63958400	-1.82087900	-0.31522500
TS26			
C	-3.29968400	-2.15869200	-2.06691000
C	-3.48313900	-3.47277700	-1.61041100
C	-3.85866300	-3.67553900	-0.27239100
C	-4.03248100	-2.60514200	0.59880900
C	-3.83642700	-1.30871800	0.11356500
C	-3.47166900	-1.06963500	-1.21395400
H	-3.02300300	-1.98358500	-3.10289600
H	-4.01079100	-4.68776500	0.09272300
H	-4.31495300	-2.76779100	1.63234700
H	-3.33783600	-0.05641000	-1.57707700

O	-4.33460900	1.26930900	0.51875400	H	5.69162800	-3.51132200	2.09517000
O	-4.54243900	-0.32315100	2.49235100	H	7.65614700	-1.98743400	2.19284000
H	-4.18463000	-5.27687000	-2.56414000	C	1.87811200	-1.95675400	-1.40386200
S	-3.91128800	0.07055300	1.23595200	C	0.60224600	-2.38185600	-1.82259300
N	-2.17878900	0.28099400	1.62678200	C	2.99954300	-2.70192600	-1.81788700
C	-1.53908200	-0.87650000	2.15171500	C	0.45076600	-3.53033700	-2.59744200
C	-1.96017900	-1.71410400	3.18456300	H	-0.28286200	-1.82006900	-1.53771600
C	-0.33297400	-1.07621100	1.45243600	C	2.84438100	-3.84660900	-2.59564900
C	-1.13787000	-2.79174000	3.50691600	H	3.99295000	-2.37223700	-1.53485500
H	-2.88424800	-1.52737700	3.71592800	C	1.56983200	-4.27084500	-2.98555000
C	0.48384300	-2.15997800	1.80275600	H	-0.54396400	-3.84115900	-2.90420100
C	0.06817900	-3.01148200	2.82194900	H	3.72336100	-4.40532200	-2.90620300
H	-1.43082700	-3.46101600	4.31052600	H	1.45238900	-5.16287500	-3.59494400
H	1.42262300	-2.33103800	1.29628300	Pd	0.34350700	3.11362900	-0.70359000
H	0.69631500	-3.85310600	3.09952100	C	3.16928900	3.07676000	-0.18947700
C	-0.21513100	0.01068200	0.48320400	O	2.20808900	3.84354900	-0.70091800
C	-1.33914000	0.82459200	0.63312600	O	4.31735600	3.11319500	-0.62796800
C	-1.68804100	2.14731200	0.07411000	O	2.79085500	2.29837500	0.82993200
C	-2.19222100	3.14199600	0.96541300	H	2.94444400	1.21409100	0.53350600
C	-1.72617600	2.40206200	-1.32740500	INT37			
C	-2.67419900	4.34089700	0.47660600	C	0.40325200	3.77256500	-2.47747400
H	-2.18602800	2.93897500	2.03052900	C	-0.55128000	4.69915300	-2.03345800
C	-2.26541300	3.62282800	-1.80650300	C	-0.56519600	5.05769900	-0.67580200
H	-1.50866700	1.60093200	-2.02651200	C	0.35106700	4.51906900	0.22101900
C	-2.71058000	4.58749700	-0.91542600	C	1.29208000	3.60217500	-0.25724400
H	-3.03949000	5.09458800	1.16737700	C	1.32819900	3.21353900	-1.59853200
H	-2.31949800	3.78908500	-2.87770000	H	0.42805500	3.48881700	-3.52605700
H	-3.10508000	5.52878500	-1.28598300	H	-1.30152900	5.77263700	-0.31863000
C	-3.28261900	-4.65392300	-2.52546400	H	0.34480200	4.80834600	1.26562900
H	-3.04348000	-4.34095900	-3.54628400	H	2.07321800	2.50621500	-1.94755300
H	-2.46742900	-5.29246200	-2.16318400	O	3.62195100	2.41546100	0.10179900
C	3.05837100	-0.21621000	0.11236800	O	2.65699800	3.75758900	2.02720200
C	2.03677000	-0.75052000	-0.57050900	H	-1.44327400	6.39436700	-3.02516100
C	0.88181000	0.21958800	-0.43739000	S	2.47554300	2.89426900	0.86402400
O	0.99623900	1.22301000	-1.19964700	N	1.60592200	1.46858000	1.49549000
C	4.28969200	-0.73871900	0.66082100	C	0.45405500	1.73069400	2.28975700
C	5.40633300	0.12682300	0.75548800	C	0.26999200	2.65437600	3.32201200
C	4.41361400	-2.05730300	1.16306000	C	-0.54941200	0.81255600	1.92017800
C	6.61252300	-0.33275800	1.27820700	C	-0.95471100	2.63820600	3.98612000
H	5.30778900	1.15023100	0.40022700	H	1.05346700	3.34237900	3.60773800
C	5.61252400	-2.49673700	1.71277000	C	-1.75369900	0.77894300	2.63767200
H	3.56590500	-2.73247400	1.10320600	C	-1.95168300	1.70505500	3.65546500
C	6.71926700	-1.63917800	1.76585900	H	-1.12475100	3.34246300	4.79529800
H	7.46766000	0.33645200	1.32442100	H	-2.50418300	0.02969000	2.41924500

H	-2.88256000	1.69373400	4.21517300
C	0.00477200	-0.03057400	0.87462800
C	1.32359600	0.35957800	0.66865200
C	2.38627300	-0.23246500	-0.17374400
C	3.72407000	-0.26782000	0.31058800
C	2.15296300	-0.56005600	-1.54052500
C	4.77252800	-0.56916000	-0.54170400
H	3.90901800	-0.03312200	1.35222700
C	3.23666900	-0.83726100	-2.39527500
H	1.15722600	-0.44076800	-1.95736000
C	4.53496900	-0.83481200	-1.89948700
H	5.78589400	-0.59084300	-0.15396100
H	3.04261400	-1.05010000	-3.44188600
H	5.36784700	-1.05310500	-2.56091800
C	-1.55339000	5.30368100	-2.98283400
H	-1.43889100	4.91324800	-3.99858100
H	-2.57695500	5.09614200	-2.64866700
C	-2.84489300	-2.24322500	0.27223800
C	-2.16026200	-1.09313400	0.02744200
C	-0.68984600	-1.15014800	0.24719200
O	-0.10035300	-2.19232100	-0.13466400
C	-4.25765900	-2.56185700	0.05434600
C	-4.85738800	-3.52151300	0.89396600
C	-5.02724400	-2.00462900	-0.98738400
C	-6.19358100	-3.88073900	0.72935300
H	-4.26682700	-3.97912000	1.68384000
C	-6.35641500	-2.37966300	-1.16097800
H	-4.57491400	-1.29607300	-1.67141500
C	-6.94809700	-3.30873400	-0.29807200
H	-6.64179500	-4.61399100	1.39411200
H	-6.93284800	-1.94979000	-1.97562100
H	-7.98762300	-3.59416700	-0.43512700
C	-2.73504600	0.18379900	-0.47856000
C	-3.87110400	0.76886400	0.10596000
C	-2.14670100	0.81586500	-1.58554700
C	-4.40782000	1.94649500	-0.40911200
H	-4.33929500	0.28958200	0.95932400
C	-2.69288500	1.98805900	-2.11007300
H	-1.27222100	0.37302500	-2.05623000
C	-3.82363600	2.55764200	-1.52263000
H	-5.28521600	2.38606100	0.05747700
H	-2.23492100	2.45276100	-2.97713100
H	-4.25009100	3.47030400	-1.93020100
Pd	1.92701100	-2.61433500	-0.22801400
C	3.21875500	-4.69762100	0.00406300
O	1.90346400	-4.58960900	0.20473300
O	3.86881000	-5.72026500	0.11002900
O	3.71186300	-3.50099900	-0.33343000
H	-2.26653600	-3.05413500	0.71159200
cis-3a			
C	-2.67939000	3.87373200	0.55646100
C	-2.99640400	3.99201900	-0.80422300
C	-3.42074800	2.84756700	-1.50045300
C	-3.51652500	1.61391500	-0.86519800
C	-3.16998600	1.52973300	0.48612000
C	-2.75867600	2.64695100	1.21149700
H	-2.35094800	4.74963800	1.10924300
H	-3.67796000	2.92553500	-2.55343700
H	-3.84092000	0.73411300	-1.41248100
H	-2.48278600	2.55078000	2.25506000
O	-2.71813100	0.05133600	2.65011800
O	-4.61580600	-0.60801300	1.10528000
H	-3.55462800	5.40611900	-2.34597600
S	-3.28057000	-0.04541400	1.30425100
N	-2.21097900	-1.04707400	0.35119100
C	-2.59285200	-2.22599700	-0.33362100
C	-3.76032800	-2.99685300	-0.27333000
C	-1.50130900	-2.59238000	-1.15456700
C	-3.81717400	-4.13463400	-1.07378800
H	-4.58512200	-2.72568500	0.36904600
C	-1.58174000	-3.74780400	-1.94774400
C	-2.74386000	-4.50793800	-1.90314300
H	-4.71384400	-4.74784800	-1.04836200
H	-0.74662100	-4.02198500	-2.58077000
H	-2.82439800	-5.40357700	-2.51313300
C	-0.44021400	-1.63149900	-0.93289100
C	-0.89985700	-0.69622500	-0.01993500
C	-0.23417100	0.52887400	0.47224700
C	0.10026200	0.68857600	1.82469200
C	0.07847300	1.55010200	-0.43927000
C	0.72843600	1.85786600	2.25700900
H	-0.13623000	-0.09614200	2.53291000
C	0.70288900	2.71616500	-0.00403700
H	-0.18659200	1.42765600	-1.48432700
C	1.02648900	2.87375800	1.34657500
H	0.98678300	1.97042200	3.30628400
H	0.94012100	3.49937300	-0.71820400
H	1.51909200	3.78119100	1.68498800

C	-2.84523300	5.31183800	-1.51703800
H	-2.99447400	6.15611900	-0.83589700
H	-1.83488700	5.40544600	-1.93820400
C	2.65315200	-0.06031200	-1.54908300
C	2.10395400	-1.11238500	-0.90342100
C	0.88863400	-1.72638800	-1.56896100
O	1.01994700	-2.32056200	-2.63603900
C	3.73815000	0.83785200	-1.12168300
C	3.95183700	1.17349800	0.22875000
C	4.54649500	1.44802900	-2.09763500
C	4.95874500	2.06587800	0.58775600
H	3.30795000	0.74870000	0.99037700
C	5.56181000	2.33437800	-1.73637700
H	4.37901500	1.21551500	-3.14696100
C	5.77408300	2.64468300	-0.39106600
H	5.10277500	2.31775400	1.63540500
H	6.18255700	2.78618700	-2.50591200
H	6.56020600	3.33956500	-0.10740100
C	2.66529400	-1.80174600	0.28967900
C	1.86949200	-2.29010400	1.34115100
C	4.05202900	-2.04898300	0.34176700
C	2.44358200	-2.96231200	2.42194700
H	0.79706000	-2.14509900	1.32260100
C	4.62300500	-2.71965600	1.41988000
H	4.67950700	-1.71311200	-0.47712100
C	3.82153600	-3.17566300	2.47124900
H	1.80568000	-3.32127300	3.22557900
H	5.69555400	-2.89563400	1.43419300
H	4.26632800	-3.70113400	3.31218500
H	2.20539000	0.20424000	-2.50683500

11. Cartesian coordinates of the allylation structures (optimization in ethyl acetate)

4a			
C	4.35048700	0.31017100	0.19125700
C	3.31668300	1.21387800	0.07020500
C	1.97250500	0.76688100	-0.04280100
C	1.70256300	-0.64049700	-0.02950000
C	2.79134800	-1.54709200	0.09620000
C	4.08448100	-1.08284500	0.20433000
H	1.07323800	2.73297900	-0.17677700
H	5.37515200	0.66188700	0.27741200
H	3.51526100	2.28316400	0.05982500
C	0.87647500	1.66341000	-0.16927500
C	0.35870600	-1.08498500	-0.14439300
H	2.58523800	-2.61494000	0.10597000
H	4.90841600	-1.78506900	0.30062100
C	-0.69485400	-0.19712000	-0.26888100
C	-0.41431600	1.20144400	-0.27775400
H	0.16531100	-2.15553200	-0.13739900
H	-1.22845200	1.91304000	-0.36178400
C	-2.07965400	-0.73447300	-0.39637800
C	-3.28188300	-0.07403900	0.18795600
C	-3.16815200	-0.04623400	-1.27888600
H	-2.14308600	-1.81989700	-0.39316700
H	-3.81616200	-0.69745700	-1.85801300
H	-2.90248600	0.89975600	-1.74289500
F	-4.23195400	-0.84632300	0.77793600
F	-3.14790900	1.07866500	0.89692300
INT17			
C	1.58147600	3.96034900	-0.08800000
C	0.78188400	3.36130800	-1.04624700
C	-0.04896700	2.26366200	-0.71778800
C	-0.04320300	1.76729000	0.62308200
C	0.76953200	2.40802100	1.58729400
C	1.57035900	3.48277200	1.24059400
H	-0.88553100	1.99722100	-2.70650000
H	2.21383700	4.80312400	-0.35484700
H	0.77997800	3.73128600	-2.06939700
C	-0.89576600	1.62783700	-1.68358500
C	-0.88883900	0.64504100	0.96995700
H	0.76200800	2.03473400	2.60918200
H	2.19225800	3.96178500	1.99252400
C	-1.76412900	0.06063500	0.00815100
C	-1.70607100	0.57655100	-1.34662900
H	-1.07112300	0.47426800	2.03054300
H	-2.35131600	0.13984600	-2.10181300
C	-2.94190200	-0.73701500	0.48556900
C	-4.34066500	-0.45377700	0.05547000
C	-3.73669200	-1.71099000	-0.42656300
H	-2.86497400	-1.06929400	1.51753900
H	-4.06586500	-2.64402200	0.02155900
H	-3.45431400	-1.76475600	-1.47435500
F	-5.34167600	-0.49159800	0.97637300
F	-4.58870800	0.55274700	-0.82517100
C	4.31331400	1.13986700	-0.11108700
H	3.89165000	1.42630200	0.85709600
H	3.66230700	1.53247100	-0.89829000
H	5.30409400	1.59656900	-0.21290200
C	4.43965900	-0.36560100	-0.21794700
H	4.84475000	-0.66890400	-1.18884200
H	5.07118100	-0.77539600	0.57700100
O	3.09269200	-0.90501800	-0.08020300
C	2.84453800	-2.20917100	-0.11879100
O	1.67205700	-2.58147700	-0.00976100
C	3.97239000	-3.18642700	-0.28436700
H	4.51620400	-2.99193400	-1.21544300
H	4.68601900	-3.08994000	0.54199400
H	3.56999800	-4.19958100	-0.30130700
Pd	0.02201700	-1.15074500	0.17740200
TS12			
C	-3.32208900	-3.32129700	0.03763100
C	-2.35528000	-3.07532400	-0.91792000
C	-1.15450100	-2.40100900	-0.58293900
C	-0.94724100	-1.96911400	0.76832300
C	-1.96147100	-2.23472900	1.72931500
C	-3.12021000	-2.89526700	1.37321700
H	-0.28571300	-2.46144500	-2.56890100
H	-4.23815200	-3.84043600	-0.23132500
H	-2.50317200	-3.39798500	-1.94639900
C	-0.13198900	-2.13808600	-1.54160700

C	0.26277300	-1.30706200	1.11298200
H	-1.80674500	-1.90926300	2.75590700
H	-3.88366500	-3.09238900	2.12167600
C	1.26885900	-1.06402800	0.15582700
C	1.03467700	-1.50494000	-1.19715500
H	0.44415400	-1.06829800	2.15796700
H	1.79784600	-1.33356200	-1.94627800
C	2.54728600	-0.45572600	0.60074600
C	3.84230800	-0.46848400	-0.09756500
C	3.33781800	0.89971300	-0.24047900
H	2.67440500	-0.34691100	1.67469800
H	3.77561900	1.65931500	0.39802400
H	3.02613300	1.19551800	-1.23911700
F	4.94900200	-0.66313200	0.67958100
F	3.98308700	-1.21854200	-1.23035100
C	-3.84518400	0.23579800	-0.79975500
H	-3.57313800	-0.35792000	0.07730200
H	-3.28063600	-0.13724200	-1.65941700
H	-4.91444800	0.10026100	-0.99762600
C	-3.55858300	1.70362600	-0.56531600
H	-3.81057600	2.31031000	-1.44163400
H	-4.10686400	2.08449400	0.30240500
O	-2.12799000	1.81348200	-0.31111900
C	-1.55317400	2.97696900	-0.01654800
O	-0.33901700	2.99060000	0.19462100
C	-2.38262700	4.22823700	0.05966700
H	-2.91390900	4.40313900	-0.88224100
H	-3.13397100	4.13878600	0.85289100
H	-1.73064400	5.07547700	0.27405100
Pd	0.87048900	1.13532400	0.19383400

INT18

C	-5.54865300	0.86884800	-0.31051400
C	-4.60739200	0.47376000	-1.23810900
C	-3.36841300	-0.08180600	-0.82321700
C	-3.10555700	-0.23286500	0.57782500
C	-4.09727500	0.18351000	1.50915000
C	-5.28977600	0.72231900	1.07580500
H	-2.55103400	-0.37422200	-2.80846200
H	-6.49357600	1.29374000	-0.63886200
H	-4.80144800	0.58433000	-2.30278400
C	-2.36113500	-0.48709500	-1.74318000
C	-1.86174200	-0.77550600	0.99062400
H	-3.89677000	0.07007200	2.57227100
H	-6.03879700	1.03767500	1.79759000
C	-0.88448400	-1.16318100	0.08397200
C	-1.16290700	-1.00374700	-1.31136500
H	-1.67117900	-0.87357100	2.05772500
H	-0.40884300	-1.29015600	-2.03367300
C	0.42882000	-1.62698300	0.59967300
C	1.25112200	-2.74073700	0.00594400
C	2.62680100	-2.18519000	0.21043300
H	0.42185500	-1.75065600	1.68733900
H	3.03910000	-2.42020100	1.19548100
H	3.33300100	-2.37733300	-0.60214900
F	1.01683500	-3.99126900	0.58345000
F	0.99885500	-2.93751700	-1.34411400
C	-0.89317500	2.57125100	0.30297400
H	-0.90016500	2.05904600	1.26928800
H	-1.11200300	1.84047800	-0.48041300
H	-1.68377200	3.32949300	0.30465800
C	0.43938300	3.24220100	0.05802400
H	0.46912800	3.74846500	-0.91136800
H	0.69267900	3.95391800	0.84910000
O	1.45358800	2.18485200	0.05268400
C	2.75742500	2.42225600	-0.16914900
O	3.48183200	1.42967900	-0.17759100
C	3.23575900	3.82335300	-0.38081500
H	2.74153800	4.26551700	-1.25288300
H	2.99178700	4.44347000	0.48922300
H	4.31491400	3.81402900	-0.53599400
Pd	1.92557000	-0.26029500	0.22958000

TS13

C	-6.19941000	1.26118700	0.45993100
C	-5.29101400	0.63598900	1.28832400
C	-4.04625400	0.17476400	0.78467200
C	-3.74434900	0.36983300	-0.60432900
C	-4.70198700	1.01922000	-1.43227100
C	-5.90178200	1.45475400	-0.91276900
H	-3.30148700	-0.60271800	2.66482600
H	-7.14953600	1.60872900	0.85708500
H	-5.51607800	0.48695600	2.34192900
C	-3.07947200	-0.46945800	1.60827900
C	-2.50358700	-0.09568500	-1.10824900
H	-4.47033800	1.16499000	-2.48496600
H	-6.62639400	1.94878400	-1.55471900
C	-1.58422100	-0.73631100	-0.28968500
C	-1.88359400	-0.90901700	1.09745400
H	-2.28120500	0.04929700	-2.16388200

H	-1.11857100	-1.36326700	1.71908700
C	-0.31505200	-1.20981700	-0.86033000
C	0.44265100	-2.32042700	-0.36063800
C	1.78482800	-2.28180800	-0.83264400
H	-0.20700900	-1.06567800	-1.93902900
H	2.53229200	-2.88361400	-0.31946200
H	1.91943100	-2.18926000	-1.91310800
F	-0.12910200	-3.38027300	0.22837800
Pd	1.52653800	-0.23784000	-0.36504800
F	0.88903900	-1.70493900	1.57766300
C	5.25670800	-0.33295600	0.18634900
H	5.11588400	-0.65305100	-0.85138000
H	4.67551500	-0.99051400	0.84111200
H	6.31745100	-0.42988800	0.44194900
C	4.82913900	1.10694500	0.36446000
H	4.93723500	1.44124200	1.40000000
H	5.36975500	1.78565300	-0.30137600
O	3.40797700	1.16035400	0.01160800
C	2.63685700	2.25560700	0.14574400
O	1.44091300	2.07129200	-0.06844000
C	3.25374300	3.56059500	0.52738500
H	3.67432200	3.49193000	1.53744300
H	4.06865000	3.81611400	-0.15837500
H	2.48955900	4.33819100	0.50527500

INT19

C	-5.30700200	-0.75306700	0.47674700
C	-4.26395100	-1.47663200	1.01582000
C	-2.96037100	-1.39352900	0.45881700
C	-2.74316900	-0.54648800	-0.67733000
C	-3.84057500	0.18402300	-1.21313500
C	-5.09344300	0.08424800	-0.64748400
H	-2.00961500	-2.74423000	1.86121600
H	-6.30011900	-0.82267200	0.91219800
H	-4.42509000	-2.11922600	1.87811200
C	-1.85080400	-2.10423800	0.99666700
C	-1.43479000	-0.43904600	-1.21213800
H	-3.67237400	0.82241200	-2.07750100
H	-5.92511700	0.64685500	-1.06294800
C	-0.36299800	-1.13161600	-0.66940800
C	-0.59378700	-1.98024700	0.45734000
H	-1.27249100	0.22719800	-2.05601000
H	0.23916300	-2.51002700	0.90316000
C	0.98292600	-0.85214200	-1.19484700
C	2.13233300	-1.66799400	-1.07870400
C	3.41496500	-1.10600400	-1.30971700
H	1.02283100	-0.12200900	-2.00202800
H	4.28668300	-1.69244300	-1.02789900
H	3.54859200	-0.42872800	-2.15188500
F	2.05293400	-2.88319100	-0.48643300
Pd	2.43433500	0.03363700	0.16446900
F	3.92702500	0.92954200	1.16811200
C	-0.72197600	3.34976400	-1.88574600
H	-0.59170900	2.46717400	-2.52045600
H	0.20208900	3.93663100	-1.90785800
H	-1.53208600	3.95976900	-2.30009900
C	-1.07178600	2.94771500	-0.46899300
H	-1.19114100	3.82265400	0.17776000
H	-1.98522200	2.34744800	-0.43643300
O	0.03794000	2.14401700	0.02883600
C	-0.00789000	1.56867100	1.22536300
O	0.94461200	0.86576400	1.57278600
C	-1.20178800	1.76985800	2.11249700
H	-1.38502400	2.83477100	2.28945900
H	-2.09319700	1.35075800	1.63177800
H	-1.03098900	1.26130100	3.06128800

INT20

P	1.63983800	-0.53556300	-0.50175800
C	2.39952700	1.11593300	-0.14202200
C	1.60043400	2.26663300	-0.24014400
C	3.75559500	1.26170000	0.19695200
C	2.14595600	3.53337100	-0.01924300
H	0.54502500	2.17037700	-0.47967900
C	4.29863900	2.52768000	0.42388400
H	4.38875900	0.38450900	0.29210100
C	3.49577600	3.66696500	0.31336900
H	1.50822400	4.40968800	-0.09467100
H	5.34890000	2.62331100	0.68766300
H	3.91971800	4.65170900	0.49270800
C	2.58525500	-1.63315100	0.65375900
C	3.27005100	-2.80699000	0.30651700
C	2.51611500	-1.28260300	2.01718100
C	3.87773900	-3.59769400	1.28851900
H	3.34063300	-3.12611100	-0.72551700
C	3.12724800	-2.06629900	2.99343300
H	1.97852100	-0.38518000	2.31340900
C	3.81276800	-3.23134400	2.63224400
H	4.40486300	-4.50142800	0.99331600
H	3.06425100	-1.77010800	4.03742800

H	4.28671600	-3.84644700	3.39252600	C	2.22277300	2.34895700	-0.73280900
C	2.18094100	-0.86394700	-2.30293800	C	-0.10306800	2.79439600	-2.21057600
C	1.58181300	-2.20888500	-2.76064500	H	-0.48099400	0.68823100	-1.95683900
H	1.78860100	-2.35350200	-3.82945900	C	1.91397900	3.63445400	-1.17966100
H	1.99652500	-3.06852000	-2.22665000	H	3.11696600	2.19373300	-0.13722700
H	0.49391300	-2.22180400	-2.62164200	C	0.75057700	3.86023000	-1.92112300
C	1.53898000	0.25584200	-3.14996500	H	-1.02002500	2.96414900	-2.76758400
H	0.44919200	0.27936200	-3.02946500	H	2.57890500	4.46107100	-0.94235200
H	1.93277200	1.24431100	-2.89125100	H	0.50581600	4.86350300	-2.26002800
H	1.75980100	0.07388600	-4.21003200	C	2.40507500	-0.14493300	1.24593900
C	3.70373200	-0.83264800	-2.51476300	C	3.46967100	-0.86017100	1.81674700
H	3.92566400	-1.02215100	-3.57358700	C	1.71356800	0.77664300	2.05828200
H	4.12152600	0.14679700	-2.26023300	C	3.84298000	-0.64974300	3.14776900
H	4.23262200	-1.58804900	-1.92693800	H	4.01936700	-1.59057700	1.23569800
C	-1.52717200	4.61862800	0.57756000	C	2.08596300	0.98392600	3.38563000
C	-2.12927000	3.87324000	-0.41908300	H	0.88002900	1.33976800	1.64916000
C	-2.37653400	2.48928300	-0.24180000	C	3.15512700	0.27181800	3.93807200
C	-1.98166600	1.86674600	0.98540500	H	4.67597800	-1.21135500	3.56310700
C	-1.37711300	2.65638000	1.99427800	H	1.54015000	1.70503700	3.98923700
C	-1.15126800	4.00466900	1.79500000	H	3.44643500	0.43355700	4.97248500
H	-3.26892500	2.15226200	-2.19257400	C	3.13492300	-1.02652500	-1.60827300
H	-1.34241500	5.67919000	0.42857300	C	3.40134200	-2.52651800	-1.37167600
H	-2.42079300	4.34130200	-1.35667200	H	4.14622400	-2.88106700	-2.09674800
C	-2.98201400	1.68343300	-1.25438300	H	3.78895400	-2.74099300	-0.37160900
C	-2.20727200	0.45805400	1.16382400	H	2.48620900	-3.11473500	-1.50659300
H	-1.07900300	2.17821200	2.92449500	C	2.59292300	-0.86059900	-3.04371800
H	-0.67809400	4.59695100	2.57358500	H	1.64207100	-1.39113200	-3.17822200
C	-2.84984200	-0.31288700	0.17038500	H	2.43779900	0.19099300	-3.30535700
C	-3.20172000	0.34072900	-1.06596000	H	3.31745900	-1.28088800	-3.75347400
H	-2.06605000	0.04338100	2.15981000	C	4.43113200	-0.21349500	-1.46107700
H	-3.68425600	-0.23445800	-1.84858500	H	5.18364500	-0.60014900	-2.16163500
C	-3.35270600	-1.67922100	0.51839400	H	4.27231500	0.84258800	-1.70152400
C	-4.74475200	-2.11974400	0.21655200	H	4.85495400	-0.27391800	-0.45409600
C	-3.66386600	-2.76653300	-0.54960600	C	-2.61691800	4.53792400	0.40377400
H	-2.95919900	-2.07734500	1.45007900	C	-3.14948300	3.58555400	-0.43887400
H	-3.39504000	-3.78811500	-0.29780800	C	-2.98064100	2.20197600	-0.16858700
H	-3.55511100	-2.49211100	-1.59527000	C	-2.26019700	1.80444200	1.00527600
F	-5.43635000	-2.82718400	1.14860200	C	-1.72738900	2.81137700	1.85804000
F	-5.59421600	-1.26628600	-0.41499700	C	-1.89662300	4.14608600	1.56085000
Pd	-0.61808800	-0.54194100	-0.15613000	H	-4.02853400	1.48155200	-1.92212500
TS14				H	-2.74491100	5.59433200	0.18334800
P	1.72468600	-0.46027400	-0.45023400	H	-3.69928900	3.88136000	-1.32958300
C	1.37194100	1.26732800	-1.02021900	C	-3.47714200	1.18765300	-1.03194500
C	0.20337400	1.50876700	-1.75854400	C	-2.06885800	0.42513900	1.26328600

H	-1.17877900	2.50707300	2.74639700	C	2.39265700	2.22313500	-2.63045000
H	-1.47815400	4.90632900	2.21511800	H	2.59767700	1.18496700	-2.92333700
C	-2.53409900	-0.54878500	0.39080600	H	1.42374800	2.51087200	-3.05367800
C	-3.26393100	-0.14444100	-0.76723500	H	3.16233300	2.85693900	-3.08960500
H	-1.49288900	0.13224200	2.13741700	C	2.18424000	3.87289300	-0.73394300
H	-3.64256700	-0.89576200	-1.45067100	H	3.04736000	4.47142800	-1.05462900
C	-2.24281000	-1.97712700	0.70030000	H	1.30311400	4.28070400	-1.23667500
C	-3.10680500	-3.10509800	0.31243600	H	2.06657800	4.01050600	0.34708500
C	-1.91928600	-3.20658000	-0.54868200	C	-5.46141500	-0.08466900	0.44575600
H	-1.72666000	-2.16171300	1.64082700	C	-4.85640600	-1.10034400	-0.26556500
H	-1.23877700	-4.03103000	-0.33723700	C	-3.49879900	-1.43959800	-0.03127500
H	-2.07583800	-2.92484400	-1.58880400	C	-2.76359200	-0.72031900	0.96661700
F	-3.28601200	-4.08463100	1.24458900	C	-3.41648300	0.31711700	1.68769900
F	-4.30729900	-2.85039700	-0.27820600	C	-4.73330200	0.63134400	1.42912700
Pd	-0.12402000	-1.76225900	-0.34783200	H	-3.37995500	-3.02101100	-1.50889000
INT21				H	-6.49990300	0.17189500	0.25360100
P	1.12758500	1.19493500	-0.39969200	H	-5.41094000	-1.64968300	-1.02319400
C	-0.50140300	1.71863300	-1.08424800	C	-2.82342700	-2.45783800	-0.76286600
C	-1.21440600	0.75551800	-1.81896600	C	-1.39907500	-1.03636300	1.17757000
C	-1.07743200	2.99280700	-0.91983400	H	-2.85141600	0.86569400	2.43772400
C	-2.46721300	1.04670500	-2.36111400	H	-5.22030000	1.43200700	1.97979900
H	-0.79528800	-0.23831500	-1.94736600	C	-0.74078800	-1.99894400	0.42363500
C	-2.33137900	3.28227400	-1.46035900	C	-1.49428700	-2.72960400	-0.54841600
H	-0.56120800	3.76490900	-0.36170900	H	-0.84703200	-0.47287500	1.92422000
C	-3.03158300	2.30984000	-2.17888800	H	-1.00604500	-3.50871100	-1.12301600
H	-3.00567100	0.27916500	-2.90941600	C	0.71666300	-2.16611200	0.60761000
H	-2.76208800	4.26949300	-1.31506800	C	1.44240500	-3.43346000	0.22024900
H	-4.01173300	2.53557000	-2.59024600	C	1.94565100	-3.14795100	-1.15956600
C	1.07069400	1.50161300	1.41866600	H	1.08295100	-1.74575300	1.54578000
C	2.06926400	0.88275700	2.19500000	H	2.96841900	-3.49600200	-1.33616100
C	0.06455100	2.22451800	2.07885600	H	1.25360300	-3.49331600	-1.93447900
C	2.07818400	1.00962800	3.58455000	F	2.50908400	-3.61557200	1.09327900
H	2.83106000	0.27733500	1.71194000	F	0.66878700	-4.58971200	0.35451500
C	0.06823600	2.34103300	3.47159600	Pd	1.67447200	-1.09298300	-0.89971500
H	-0.74599500	2.67641900	1.52060600	TS15			
C	1.07602000	1.74020700	4.22841500	C	5.79917380	1.99144755	-0.98256086
H	2.85924900	0.52344800	4.16306100	C	5.31076280	0.80113655	-1.48020586
H	-0.72436100	2.89938200	3.96300700	C	4.21998680	0.14466655	-0.85194386
H	1.07439200	1.82953700	5.31138900	C	3.62856180	0.74007055	0.31118414
C	2.42430700	2.40048600	-1.10062500	C	4.15731080	1.96630355	0.80192214
C	3.80072000	1.96374900	-0.56234400	C	5.21769980	2.57863955	0.16959014
H	4.58317300	2.55784600	-1.05214100	H	4.12349080	-1.53057245	-2.22373386
H	3.88666800	2.12882000	0.51664600	H	6.63504880	2.48406055	-1.47233586
H	4.00567900	0.90515100	-0.76442400	H	5.75681580	0.34796155	-2.36255986

C	3.68268380	-1.08228145	-1.33617286
C	2.53304580	0.09105655	0.93378914
H	3.70525580	2.41284355	1.68324214
H	5.61382780	3.51536655	0.55289214
C	2.02904680	-1.10827645	0.44773914
C	2.62152380	-1.69152545	-0.71525186
H	2.08180280	0.55308155	1.80840114
H	2.17826080	-2.59973645	-1.10501186
C	0.89602180	-1.73761545	1.13605114
C	0.60300080	-3.16090445	1.08641914
C	-0.68282420	-3.46037045	1.57235314
H	0.64761580	-1.28589745	2.09873814
H	-1.10074420	-4.44829345	1.39322914
H	-1.00805120	-2.95024945	2.47975714
F	1.59632180	-4.07028945	0.97332714
F	0.25957880	-3.42539145	-0.84466386
Pd	-1.08411420	-1.65024445	0.32790414
P	-1.34708420	0.53428055	-0.44053286
C	-3.11774920	0.99586255	-0.22971886
C	-4.07924020	-0.02704145	-0.29827686
C	-3.54231220	2.31652455	-0.01488586
C	-5.43804820	0.26409955	-0.16366086
H	-3.76131020	-1.05634145	-0.45893986
C	-4.90129820	2.60589855	0.12266414
H	-2.81263620	3.11837555	0.04983214
C	-5.85049620	1.58235555	0.04714214
H	-6.17037720	-0.53693845	-0.21796186
H	-5.21853120	3.63205255	0.28867814
H	-6.90721220	1.81114755	0.15645314
C	-0.47685020	1.76507055	0.61886214
C	0.43848680	2.73497855	0.18874014
C	-0.73963120	1.65362955	1.99848514
C	1.06539180	3.57860255	1.11180514
H	0.68730580	2.84396255	-0.85847386
C	-0.11535420	2.49506655	2.91680714
H	-1.43511320	0.89565655	2.35188014
C	0.79280480	3.46361855	2.47451014
H	1.77611480	4.31925755	0.75629914
H	-0.33431220	2.39312655	3.97643214
H	1.28434880	4.11889655	3.18854214
C	-0.99764220	0.83044055	-2.27932586
C	-1.37347720	2.24359255	-2.75759486
H	-1.17314320	2.32117655	-3.83429086
H	-2.43813720	2.44820255	-2.60248986
H	-0.80271820	3.03180755	-2.25977886
C	0.48455680	0.50993455	-2.54986286
H	0.72511980	-0.51425845	-2.25190786
H	0.68172280	0.60520355	-3.62568686
H	1.17233380	1.17845755	-2.02592386
C	-1.86403320	-0.19617345	-3.04101686
H	-1.65633820	-0.10651445	-4.11498586
H	-1.63406820	-1.22545845	-2.74137286
H	-2.93516920	-0.02014845	-2.89386386

INT22

C	6.22690700	-1.19703800	0.57994600
C	5.37232500	-0.41054500	1.32372000
C	4.22962400	0.18438700	0.72592700
C	3.97361200	-0.04420600	-0.66495900
C	4.87584000	-0.85566300	-1.40545500
C	5.97680800	-1.41978700	-0.79781600
H	3.49572600	1.15571000	2.51926600
H	7.09760000	-1.64896400	1.04765600
H	5.56129900	-0.23628100	2.38058600
C	3.31129600	0.98430500	1.46117900
C	2.81432500	0.52208500	-1.25445900
H	4.67621000	-1.03093500	-2.45987100
H	6.65829200	-2.04075700	-1.37325700
C	1.93310500	1.30065000	-0.52456700
C	2.20063500	1.52469200	0.86029800
H	2.61840400	0.32606300	-2.30594100
H	1.50552200	2.11567400	1.44481300
C	0.73546100	1.85406200	-1.19151300
C	0.29088200	3.19964400	-0.98819700
C	-0.90426300	3.66862200	-1.51607400
H	0.56508200	1.47930300	-2.20098700
H	-1.30317400	4.61733600	-1.16875000
H	-1.25444500	3.29923000	-2.47657000
F	0.88758700	3.94091200	-0.02367100
F	-3.18692800	2.22814600	0.19983200
Pd	-1.27037100	1.77974300	-0.37368400
P	-1.38976600	-0.43261700	0.42213900
C	-2.84110000	-1.33847700	-0.26965700
C	-3.97356000	-0.60947400	-0.67090400
C	-2.85888200	-2.74109100	-0.36320800
C	-5.09745900	-1.27675400	-1.16444900
H	-3.97632300	0.47172000	-0.56452400
C	-3.98498800	-3.40060900	-0.85815000
H	-1.99246800	-3.32067000	-0.06080300

C	-5.10534600	-2.66984100	-1.26355600	H	0.10154400	0.28531800	-2.02722600
H	-5.96775500	-0.70283500	-1.47230400	H	1.24629500	2.06832600	1.73027300
H	-3.98497400	-4.48527400	-0.92791300	C	2.25270800	0.70076800	-0.46651300
H	-5.97977800	-3.18505400	-1.65261400	C	3.41556600	1.56490300	-0.10628800
C	0.02300000	-1.50083700	-0.08394700	C	3.27733100	0.30295200	0.63851200
C	1.07628200	-1.88292800	0.76025500	H	2.38648500	0.16894800	-1.40422800
C	0.07358700	-1.89248300	-1.43542900	H	3.95904700	-0.51047900	0.40850800
C	2.12304500	-2.67382800	0.27982200	H	2.93005800	0.36203800	1.66623400
H	1.10376700	-1.56565400	1.79422200	F	4.41669900	1.70216200	-1.01380200
C	1.12100000	-2.67931600	-1.91329100	F	3.22187400	2.75185000	0.52334200
H	-0.71915100	-1.59491600	-2.11648200	Pd	-0.12399700	-1.47487200	0.06709100
C	2.14544500	-3.08341100	-1.05276500	Cl	-1.32055700	-1.10184600	2.10477600
H	2.93069000	-2.95285900	0.95039600	C	1.01337200	-3.19743800	-0.57301900
H	1.13400000	-2.97738300	-2.95838700	H	2.01614200	-3.26123900	-0.15417500
H	2.96457100	-3.69332000	-1.42282800	C	0.76794400	-2.40137000	-1.70786700
C	-1.65212900	-0.51131900	2.30472300	H	-0.12677300	-2.55641600	-2.31020900
C	-1.59198800	-1.94347100	2.86118200	C	-0.10671400	-3.60898200	0.19517000
H	-1.83549800	-1.91502900	3.93143600	H	0.04539900	-4.04136600	1.18067800
H	-2.32704000	-2.59245500	2.37346400	H	1.59903500	-1.91235400	-2.21061600
H	-0.60771200	-2.40650400	2.75862600	H	-1.04428900	-3.87125100	-0.29484600
C	-0.61250500	0.40200300	2.98325300	TS16			
H	-0.73147500	1.43935000	2.65016900	C	-5.42481900	-0.60801800	0.04981700
H	-0.76649200	0.37538900	4.06980600	C	-4.63668300	0.22381100	0.81710300
H	0.42018400	0.10168400	2.78518300	C	-3.29318000	0.49288800	0.44622000
C	-3.05969800	0.06584800	2.57223200	C	-2.76657300	-0.11348900	-0.74134800
H	-3.17907200	0.20713600	3.65421700	C	-3.60474300	-0.96555300	-1.51258700
H	-3.21038400	1.02692400	2.07235200	C	-4.90443800	-1.20792500	-1.12485300
H	-3.84553600	-0.61840600	2.23610400	H	-2.83992400	1.79926400	2.11358100
INT23				H	-6.45168900	-0.80827300	0.34360200
C	-4.17177000	1.97706500	-0.42398800	H	-5.03318500	0.68379400	1.71901100
C	-3.19409200	2.30004300	0.49469800	C	-2.44451800	1.34200400	1.21005900
C	-1.85321600	1.88466900	0.29674400	C	-1.42351800	0.15011800	-1.10562800
C	-1.52651300	1.12305800	-0.86626100	H	-3.20171600	-1.42204700	-2.41377300
C	-2.54727400	0.81244100	-1.79965800	H	-5.53753800	-1.86092000	-1.71954600
C	-3.84471300	1.23001700	-1.58116700	C	-0.61372400	0.98550500	-0.34632700
H	-1.06292100	2.78123800	2.10118200	C	-1.14723200	1.58487300	0.83363700
H	-5.19760600	2.29717900	-0.26364300	H	-1.02578100	-0.31771100	-2.00332800
H	-3.43937500	2.87353600	1.38516700	H	-0.52010600	2.22369400	1.44157600
C	-0.81302800	2.20237000	1.21559500	C	0.76515200	1.21410300	-0.82106100
C	-0.17062900	0.69823400	-1.05917000	C	1.60523800	2.38380500	-0.49933900
H	-2.29189900	0.23760300	-2.68700700	C	2.34942600	1.39938300	0.29530800
H	-4.62184500	0.98724000	-2.30086100	H	0.99326200	0.83698200	-1.81336900
C	0.83667500	1.04193100	-0.14631300	H	3.33877100	1.13720600	-0.07207200
C	0.48216200	1.79951800	1.01078200	H	2.19507100	1.46200100	1.36816400

F	2.27261200	2.90606600	-1.57415500
F	1.03290200	3.41987800	0.17676800
Pd	1.63312300	-0.78978300	0.14930000
Cl	0.89881100	-0.73683100	2.46825100
C	2.70152600	-2.43184400	-0.81469400
H	3.74740900	-2.51570700	-0.52385400
C	2.31573000	-1.48744700	-1.79474400
H	1.36997300	-1.60841900	-2.32248300
C	1.69991500	-2.97641800	0.01188400
H	1.97261300	-3.53266100	0.90413300
H	3.07918900	-0.91874900	-2.32150200
H	0.69522000	-3.15053700	-0.37238000
INT24			
C	-5.58326200	-0.50409800	0.05433900
C	-4.75755900	0.34774700	0.75952200
C	-3.40658800	0.52988100	0.37042200
C	-2.91070900	-0.18446200	-0.77037000
C	-3.78692200	-1.05383400	-1.47777400
C	-5.09454100	-1.21066500	-1.07300600
H	-2.90037500	1.94754800	1.92925400
H	-6.61667600	-0.63727300	0.36271000
H	-5.13201500	0.88926900	1.62466400
C	-2.52176300	1.40167800	1.06883200
C	-1.56174800	-0.00312400	-1.15425800
H	-3.40604700	-1.59251300	-2.34218500
H	-5.75764500	-1.87771500	-1.61693800
C	-0.70827800	0.84645800	-0.45335400
C	-1.21786400	1.55854700	0.67827700
H	-1.18550200	-0.54702000	-2.01807300
H	-0.56770900	2.22749300	1.22828500
C	0.67922900	0.93788100	-0.90683700
C	1.63215300	2.01842400	-0.45601100
C	2.25437400	1.38823300	0.74654200
H	0.83494000	0.63556000	-1.93989300
H	3.34180000	1.45715300	0.79817700
H	1.74278800	1.61495900	1.68042200
F	2.57136300	2.22705100	-1.44621900
F	1.04107500	3.24571200	-0.23550300
Pd	1.70370800	-0.55858600	0.26734300
Cl	0.59663800	-1.02105900	2.40349900
C	3.00579100	-2.21818800	-0.74042600
H	3.83137900	-2.51995700	-0.09625600
C	3.03389700	-0.89618800	-1.33039600
H	2.49193600	-0.74871300	-2.26409600
C	1.86406900	-2.97473700	-0.74191900
H	1.78459800	-3.87283500	-0.13717600
H	3.96068900	-0.32931500	-1.26611000
H	1.03078600	-2.74984800	-1.40602000
TS17			
C	-5.95766400	-0.51883400	-0.56774200
C	-5.04354600	0.31994700	-1.17040300
C	-3.73366700	0.46071400	-0.64292100
C	-3.37314400	-0.28325300	0.52951100
C	-4.33931100	-1.13841000	1.12899500
C	-5.60261800	-1.25383300	0.59170200
H	-3.03116400	1.87699500	-2.12444600
H	-6.95771500	-0.61997700	-0.98057300
H	-5.31399600	0.88428100	-2.05957100
C	-2.75901400	1.31256300	-1.23588700
C	-2.06355700	-0.14569400	1.05056700
H	-4.06301700	-1.69971200	2.01842300
H	-6.33409600	-1.91004100	1.05537100
C	-1.12539400	0.69064600	0.45540400
C	-1.49515500	1.42754800	-0.71283600
H	-1.79369000	-0.71340700	1.93873400
H	-0.76062800	2.06506200	-1.18750400
C	0.21969300	0.74530700	1.02708200
C	1.17315300	1.81216900	0.83003500
C	2.49225100	1.39506500	1.22436100
H	0.33555700	0.26202700	1.99604600
H	3.34395000	1.97395300	0.87758600
H	2.58192700	0.95332800	2.21570500
F	0.80704400	3.08931400	0.68429600
F	1.46122500	1.62630700	-1.00446500
Pd	1.93467100	-0.25754900	-0.01796800
Cl	4.19619000	-0.63012000	-0.90873700
C	1.64419500	-2.52768300	-0.23036900
H	2.44640400	-2.96800300	-0.81636400
C	0.46472900	-2.20414800	-0.84900100
H	-0.39511800	-1.83056300	-0.30021900
C	1.96028800	-2.01850500	1.08910800
H	2.94164000	-2.24607300	1.49796900
H	0.32535100	-2.40376500	-1.90773200
H	1.16262600	-1.94699700	1.82753000
INT25			
C	-6.09631400	-0.30459600	-0.64349800
C	-5.10707400	0.51054300	-1.15415900
C	-3.80690600	0.50966600	-0.58772300

C	-3.53599200	-0.35544600	0.52462900	H	-5.89223200	-3.14256300	-1.36797300
C	-4.57685600	-1.18489000	1.02761800	H	-7.21530000	-4.81293500	-0.10777400
C	-5.82984400	-1.15907700	0.45588800	C	-1.81202800	-2.81406600	-1.18276100
H	-2.95415900	1.95696400	-1.95665500	C	-1.17388000	-3.77101700	-0.32791300
H	-7.08924300	-0.29459600	-1.08468600	H	-3.70630400	-2.14116300	-1.93297900
H	-5.31108300	1.16449800	-1.99828500	H	-0.09923800	-3.74224500	-0.20866200
C	-2.75439100	1.32623400	-1.09402900	C	-1.10293200	-1.74267100	-1.86948100
C	-2.23674800	-0.35941900	1.08528700	C	0.22369900	-1.51923300	-2.00097100
H	-4.36574700	-1.83695400	1.87174800	C	0.86929900	-0.33457100	-2.54403000
H	-6.62066300	-1.79383200	0.84577600	H	-1.72804300	-0.97770700	-2.32108200
C	-1.23455400	0.47553800	0.59785100	H	1.79405500	-0.55640200	-3.08377800
C	-1.50642100	1.31979400	-0.52617100	H	0.18558500	0.27646600	-3.13982800
H	-2.03118200	-1.02007400	1.92497900	F	1.11670800	-2.44610700	-1.52282000
H	-0.69704000	1.89635600	-0.95495100	Pd	1.42629100	0.78014100	-0.93138700
C	0.07426600	0.40852600	1.22769600	C	-3.71416000	5.37150500	0.31118000
C	1.04086300	1.44119800	1.29005400	C	-3.08280400	5.82802400	1.47564700
C	2.36873700	1.18187000	1.64069000	C	-1.77398500	5.39165000	1.75021700
H	0.20809300	-0.36931700	1.97426800	C	-1.10738800	4.52692000	0.89003400
H	3.11096400	1.95583100	1.47293000	C	-1.77260400	4.08490100	-0.26023100
H	2.59505400	0.41627800	2.37536000	C	-3.06870500	4.49675800	-0.56373300
F	0.75258500	2.63164500	0.76101100	H	-4.72485300	5.69957300	0.08446900
F	1.49459700	1.28913300	-1.45636400	H	-1.27285800	5.73685200	2.65074700
Pd	1.96810200	-0.17587700	-0.09998700	H	-0.09637500	4.19439400	1.10908000
Cl	4.35202100	-0.15917100	-0.67593300	H	-3.56153700	4.14326400	-1.46314700
C	1.96741200	-2.37212200	-0.49510300	O	-1.78609000	2.53882500	-2.44803000
H	2.81280400	-2.64603600	-1.12093200	O	0.40264200	3.55572700	-1.67261200
C	0.77861800	-1.98833300	-1.09794600	H	-3.69446400	6.43922100	3.45493400
H	-0.13859500	-1.85186500	-0.53138200	S	-0.90748700	2.98321600	-1.36121300
C	2.20090600	-2.06433700	0.88570300	N	-0.55618700	1.59537200	-0.33887500
H	3.19283600	-2.24054500	1.29243700	C	-1.64095300	0.79787700	0.19951500
H	0.68948800	-1.98582200	-2.18066500	C	-2.97708700	0.96575200	-0.18175600
H	1.38258600	-2.15252100	1.59777900	C	-1.32450100	-0.20644600	1.15359000
INT26				C	-3.99038800	0.20463100	0.40119800
C	-5.48347400	-5.72973500	0.82709200	H	-3.24700600	1.68254000	-0.94211100
C	-4.10995900	-5.71596100	0.95408700	C	-2.36723300	-0.95556000	1.73312500
C	-3.32538200	-4.76862200	0.24559400	C	-3.69280500	-0.75107300	1.37139900
C	-3.97911600	-3.82373400	-0.61187800	H	-5.01667700	0.36523200	0.08391300
C	-5.39756300	-3.86310700	-0.72050300	H	-2.10585900	-1.72457700	2.45249400
C	-6.13231200	-4.79325100	-0.01738100	H	-4.47848500	-1.35152400	1.81907100
H	-1.40523400	-5.41747100	1.01052200	C	0.01283200	-0.54966400	1.50438300
H	-6.07469500	-6.45863500	1.37514000	C	1.12273200	-0.94183200	1.81056300
H	-3.60858000	-6.43093200	1.60268100	C	2.45407800	-1.37307600	2.08865800
C	-1.90822100	-4.70720600	0.35796500	C	3.08414000	-1.04544200	3.30496700
C	-3.19689900	-2.86846800	-1.30500300	C	3.16033000	-2.12267900	1.12577700

C	4.39328500	-1.45850800	3.54856200	H	-0.25317700	-3.78208200	-0.26082300
H	2.54353300	-0.46297800	4.04489700	C	-1.20184100	-1.67543500	-1.81800600
C	4.46806900	-2.53250600	1.37999900	C	0.13071700	-1.50397800	-1.97073900
H	2.67694700	-2.36235800	0.18578700	C	0.79956700	-0.33235300	-2.50723600
C	5.08901300	-2.20283400	2.58942400	H	-1.80075300	-0.86787900	-2.22890500
H	4.87206300	-1.19838700	4.48869300	H	1.71331800	-0.56020200	-3.06155300
H	5.00372400	-3.10672000	0.62922200	H	0.12588000	0.32405000	-3.06243700
H	6.10830400	-2.52533000	2.78439100	F	0.99948400	-2.47198700	-1.53431200
C	-3.77604800	6.78063700	2.41632100	Pd	1.43087200	0.71579800	-0.88403500
H	-3.31572600	7.77615100	2.36755800	C	-3.56629500	5.49583100	0.16728900
H	-4.83717200	6.88917300	2.17155500	C	-2.96638200	5.94916500	1.34925700
F	1.66158900	2.10134600	0.77340100	C	-1.70157500	5.44400300	1.69920000
H	0.10777600	1.95378300	0.41149200	C	-1.04802600	4.51536900	0.89664800
C	7.68603900	-1.39351000	-1.12242200	C	-1.68017000	4.07606300	-0.27280000
H	7.81076800	-1.13611400	-2.17923300	C	-2.93155100	4.55913000	-0.65005800
H	7.27309200	-2.40550200	-1.05393400	H	-4.54372200	5.87548900	-0.11837700
H	8.67152000	-1.38681800	-0.64387500	H	-1.22435800	5.78475100	2.61452800
C	6.78443600	-0.39691000	-0.42506800	H	-0.07333300	4.12825900	1.17833600
H	6.63731100	-0.66041100	0.62566500	H	-3.40138100	4.20604800	-1.56202800
H	7.18361400	0.62066700	-0.48782200	O	-1.72026200	2.46479800	-2.40449700
O	5.50048400	-0.43830900	-1.11234200	O	0.48345500	3.46790500	-1.66511900
C	4.45556600	0.24482600	-0.66288100	H	-3.61607700	6.66478900	3.28193100
O	3.42598000	0.13953100	-1.34684100	S	-0.82802300	2.90360800	-1.31941500
C	4.57697700	1.07786900	0.57464400	N	-0.48246600	1.58856100	-0.26443200
H	4.82833800	0.43905700	1.42797600	C	-1.55920000	0.81835000	0.28987800
H	5.38514900	1.80859200	0.45386700	C	-2.91240700	1.03026000	-0.01894900
H	3.63336500	1.58887300	0.76916500	C	-1.24078900	-0.21540600	1.21614000
TS18				C	-3.92072900	0.29091800	0.59759100
C	-5.69761400	-5.60931100	0.75680900	H	-3.19803100	1.76825400	-0.75315000
C	-4.32317800	-5.65346400	0.86577500	C	-2.27772000	-0.94614300	1.82854200
C	-3.51180500	-4.70091400	0.19569300	C	-3.61161700	-0.69672700	1.53267800
C	-4.14015500	-3.68901500	-0.60237500	H	-4.95508800	0.49051800	0.33178900
C	-5.56009100	-3.66899900	-0.69285700	H	-2.00674600	-1.73550100	2.52222000
C	-6.32093000	-4.60677100	-0.02894700	H	-4.39491200	-1.28227400	2.00378200
H	-1.60896700	-5.46158200	0.89850300	C	0.09886400	-0.60114900	1.51105500
H	-6.30940100	-6.34338800	1.27450900	C	1.20560200	-1.02791700	1.78304600
H	-3.84158900	-6.41962100	1.46924000	C	2.53583500	-1.48364200	2.02518100
C	-2.09176800	-4.70071600	0.28933700	C	3.19902900	-1.17399500	3.22896500
C	-3.33037200	-2.73185100	-1.25992000	C	3.21086600	-2.23078800	1.03824200
H	-6.03480800	-2.89776400	-1.29511000	C	4.51092100	-1.59856500	3.43492300
H	-7.40484200	-4.58167800	-0.10509700	H	2.68142600	-0.59518800	3.98800600
C	-1.94262200	-2.74217700	-1.16066400	C	4.52265200	-2.64987700	1.25375700
C	-1.32996100	-3.76269900	-0.36284500	H	2.70039200	-2.46001600	0.10953900
H	-3.81829300	-1.95549200	-1.84448500	C	5.17719200	-2.33567500	2.44954300

H	5.01524400	-1.35237400	4.36542000	H	0.92502500	1.06073900	-3.21614300
H	5.03515600	-3.21975000	0.48380400	H	-0.60386200	0.12608000	-2.89717300
H	6.19939900	-2.66582100	2.61399000	F	2.49389400	-0.44154500	-1.88493300
C	-3.64527000	6.96871400	2.22897600	Pd	0.12636200	1.57228300	-0.88168500
H	-3.13790300	7.94001400	2.16004200	C	-6.70856800	0.48759800	-0.00423300
H	-4.69123500	7.11665000	1.94258400	C	-6.76176200	0.97867900	1.30656300
F	1.46751600	2.17882800	0.99311900	C	-5.61509500	1.59293200	1.83875600
H	0.38445900	1.98401800	0.54377900	C	-4.44865200	1.71912300	1.09127700
C	7.69490300	-1.41236600	-1.15563700	C	-4.42259200	1.20703800	-0.21111000
H	7.81050500	-1.17113200	-2.21724800	C	-5.54576700	0.59722700	-0.76836500
H	7.29200100	-2.42680500	-1.06742100	H	-7.58470600	0.00937500	-0.43444100
H	8.68320100	-1.38822700	-0.68358600	H	-5.63839700	1.97848200	2.85506600
C	6.78890300	-0.41293500	-0.46870700	H	-3.57292600	2.19463900	1.51915800
H	6.64832000	-0.66222100	0.58628100	H	-5.50760500	0.20985400	-1.78089000
H	7.17791200	0.60719300	-0.55007100	O	-3.13981200	0.67076300	-2.47803300
O	5.50072300	-0.47560100	-1.14927100	O	-2.62196800	2.83375800	-1.27299300
C	4.44789400	0.18817400	-0.69582300	H	-7.80398800	0.45101700	3.12474800
O	3.40984000	0.05748900	-1.36237800	S	-2.94177300	1.39661000	-1.20660000
C	4.56491200	1.03346100	0.53533900	N	-1.70217900	0.70786500	-0.27375900
H	4.79671400	0.39898900	1.39748700	C	-1.79013500	-0.66316200	0.09425600
H	5.37907500	1.75759400	0.42108700	C	-2.76077400	-1.55927100	-0.38906500
H	3.62935100	1.56031500	0.72177100	C	-0.83384500	-1.16504800	1.02750700
INT27				C	-2.84239400	-2.86711300	0.08783600
C	2.34868700	-7.69982100	0.81879000	H	-3.45652700	-1.24471200	-1.15338500
C	3.11259700	-6.56538000	0.63847500	C	-0.93488600	-2.48886500	1.49261000
C	2.56115000	-5.41076300	0.02439100	C	-1.94034300	-3.33753000	1.04326800
C	1.19552100	-5.43900000	-0.41114600	H	-3.61773000	-3.52072100	-0.30295100
C	0.43339700	-6.62395100	-0.20990900	H	-0.18896100	-2.84514400	2.19617300
C	0.99678500	-7.72842400	0.39126200	H	-1.99746700	-4.35785400	1.41000800
H	4.34525500	-4.18926000	0.15157100	C	0.28115300	-0.38467500	1.45124200
H	2.78055000	-8.57801500	1.29142400	C	1.29351200	0.19840500	1.79387500
H	4.14916500	-6.53990900	0.96674300	C	2.49085500	0.92317300	2.07238400
C	3.30851700	-4.21639400	-0.17603200	C	2.67094800	1.59872800	3.29474800
C	0.64430800	-4.28488200	-1.01670200	C	3.49928400	0.99439800	1.08852600
H	-0.60303100	-6.64091300	-0.53910300	C	3.83333300	2.33460600	3.52252300
H	0.40599000	-8.62829600	0.54098600	H	1.89364600	1.54775700	4.05129300
C	1.38279200	-3.11806400	-1.19892600	C	4.65702900	1.73322900	1.32592100
C	2.74859900	-3.10921900	-0.76450800	H	3.35071500	0.48303300	0.14359300
H	-0.39570000	-4.31160300	-1.33017000	C	4.82814500	2.40563800	2.54099000
H	3.34493000	-2.21713600	-0.89987900	H	3.96300100	2.85465000	4.46774100
C	0.70063000	-1.96998700	-1.77497400	H	5.42464400	1.78597900	0.55885600
C	1.16659400	-0.73364200	-2.07042500	H	5.73326200	2.97860200	2.72381000
C	0.38770700	0.39735300	-2.53389000	C	-8.01825600	0.86897100	2.13386800
H	-0.35803800	-2.10355700	-1.97532700	H	-8.46775800	1.85799900	2.29266700

H	-8.76696600	0.23456700	1.64898600	C	3.58929800	2.08590200	-1.41162200
F	-1.27785400	2.44133000	1.64157500	C	2.87181900	2.44980100	-0.27529300
H	-1.47775500	1.72525700	0.99091800	C	3.04407900	1.72405900	0.90753700
C	5.64409200	5.20079500	-1.00843600	C	3.92468900	0.64284100	0.95272200
H	5.48358000	5.53767000	-2.03767800	H	5.33059300	-0.54477100	-0.15495200
H	6.23268800	4.27763300	-1.02812800	H	3.45578100	2.65326500	-2.33009600
H	6.21749900	5.96790600	-0.47662000	H	2.19635400	3.29717300	-0.29411200
C	4.32521300	4.98269000	-0.29835900	H	4.05838700	0.09107500	1.87726900
H	4.47580700	4.62597000	0.72400800	O	2.86381300	1.69396100	3.53949900
H	3.72231100	5.89593500	-0.27724700	O	1.85971100	3.63412300	2.26735700
O	3.60409000	3.96297500	-1.05284100	H	6.09136500	-0.03410700	-2.40367600
C	2.43338300	3.50068000	-0.64430900	S	2.09071500	2.17713700	2.36537500
O	1.91067600	2.64234200	-1.37244500	N	0.65692000	1.46240500	2.15682000
C	1.81354200	4.03431100	0.61374300	C	-1.06111500	1.54794400	0.35349400
H	2.47571900	3.85752400	1.46674100	C	-0.63618700	2.59519400	-0.50555400
H	1.66019400	5.11567300	0.52195300	C	-0.54457900	3.91787800	-0.02227400
H	0.85189400	3.55585300	0.80827300	C	-0.24930300	2.30619200	-1.83385100
TS19				C	-0.07973900	4.92892600	-0.85875100
C	6.11215300	-3.26485000	-0.88357600	H	-0.79948800	4.12180800	1.01108600
C	5.26129400	-2.91381000	-1.91145400	C	0.19251400	3.33069000	-2.66479400
C	3.88021800	-2.69879400	-1.66667900	H	-0.30223500	1.28316800	-2.19025800
C	3.37492800	-2.87003600	-0.33638200	C	0.28183100	4.64094400	-2.17987700
C	4.27705100	-3.23195900	0.70260100	H	0.00477200	5.94332100	-0.47972100
C	5.61586600	-3.42053600	0.43611700	H	0.48395500	3.10614800	-3.68700100
H	3.35545800	-2.16443000	-3.69896200	C	0.28405700	0.22952600	2.60917300
H	7.16944100	-3.42055100	-1.08079800	C	0.92863600	-0.60230700	3.56408300
H	5.64036400	-2.78738600	-2.92258900	C	-0.94812500	-0.27036400	2.05243300
C	2.97516400	-2.29805400	-2.68899300	C	0.36860900	-1.81508400	3.95088200
C	1.99625900	-2.66586700	-0.09387000	H	1.85918900	-0.26531400	4.00263200
H	3.89102600	-3.34739500	1.71260400	C	-1.50978200	-1.47825800	2.48787200
H	6.29828500	-3.69009500	1.23766700	C	-0.85705700	-2.26431400	3.43206200
C	1.12253500	-2.27277800	-1.10391800	H	0.89288000	-2.42078300	4.68736500
C	1.64677700	-2.07685600	-2.42184400	H	-2.45171300	-1.80118100	2.05280600
H	1.61902100	-2.80609200	0.91653100	H	-1.28581000	-3.20723900	3.75925600
H	0.98054800	-1.77147000	-3.21868500	C	-1.48796500	0.52845900	0.98393700
C	-0.28290300	-2.11912900	-0.76132200	H	0.63938400	5.43582400	-2.82876700
C	-1.28375400	-1.51987000	-1.44010600	C	5.24095900	0.61428800	-2.63562900
C	-2.66441500	-1.39096100	-1.00986200	H	4.58815400	0.06667500	-3.32815100
H	-0.57656400	-2.51089500	0.20752200	H	5.61476800	1.49565900	-3.17033000
H	-3.36540200	-1.43846400	-1.84717500	Pd	-3.15684900	0.43305600	-0.18914600
H	-2.92449900	-2.08900600	-0.21260500	C	-6.26913400	-3.04732900	1.34007700
F	-1.03675100	-0.91425100	-2.64475700	H	-5.97422300	-2.46729600	2.22064800
C	4.64265200	0.29455900	-0.19238700	H	-5.39461100	-3.58630900	0.96092000
C	4.48593900	1.00612500	-1.38920600	H	-7.02406100	-3.78064500	1.64339200

C	-6.85111000	-2.14677000	0.27243000	H	-6.07904000	0.56127400	-1.16265200
H	-7.12825900	-2.70836300	-0.62484800	O	-4.92534200	2.50067100	0.35698600
H	-7.72217900	-1.59410800	0.63735300	O	-3.27438500	1.38675900	1.93142900
O	-5.80631900	-1.18413400	-0.07913200	H	-7.50463500	-4.14775100	1.22847900
C	-5.97410600	-0.28755400	-1.03776100	S	-4.01619600	1.38734800	0.65913400
O	-5.03408500	0.48326300	-1.27881800	N	-2.88150800	1.31829700	-0.67220900
C	-7.25946000	-0.22146900	-1.80427600	C	-2.20754800	2.56186200	-0.90085400
H	-7.42049600	-1.16108300	-2.34546000	C	-2.72651100	3.84867500	-1.05694400
H	-8.10580400	-0.08129500	-1.12330000	C	-0.82324800	2.29486800	-1.00806000
H	-7.21499600	0.60482600	-2.51383900	C	-1.82407000	4.88437800	-1.31242000
INT28				H	-3.78870900	4.03968500	-0.98303700
C	9.07256800	-0.56138600	1.37140900	C	0.06120200	3.34960800	-1.28137000
C	8.45055300	0.04067500	0.29789600	C	-0.44473900	4.64032600	-1.42295800
C	7.12557700	-0.31675200	-0.06590300	H	-2.20360600	5.89497000	-1.43811700
C	6.43708600	-1.31449000	0.69967100	H	1.12409100	3.14820700	-1.37742900
C	7.10624100	-1.91612800	1.80200800	H	0.23111900	5.46610700	-1.63073900
C	8.39338000	-1.54876300	2.12948200	C	-0.59969000	0.86599200	-0.83394500
H	6.95889100	1.04148700	-1.74539200	C	-1.83153600	0.30944300	-0.62582400
H	10.08751300	-0.28151700	1.64093100	C	-2.15807500	-1.12429900	-0.54322800
H	8.96754400	0.79861900	-0.28623300	C	-1.48127400	-1.95307100	0.36781300
C	6.44561100	0.27860200	-1.16444100	C	-3.08867900	-1.70591700	-1.42083600
C	5.11448100	-1.66946400	0.33492400	C	-1.73208000	-3.32605300	0.40361600
H	6.58386200	-2.67369100	2.38187600	H	-0.75959900	-1.50751000	1.04447100
H	8.89480700	-2.01626300	2.97285500	C	-3.34012700	-3.07647100	-1.38382400
C	4.46675100	-1.08657600	-0.74742500	H	-3.61272400	-1.07387100	-2.13081900
C	5.16481700	-0.08818000	-1.49884500	C	-2.66384500	-3.89280400	-0.47040400
H	4.59944600	-2.42380200	0.92652200	H	-1.20435600	-3.95149600	1.11955300
H	4.67480100	0.38642000	-2.33946600	H	-4.06412500	-3.50894600	-2.06942600
C	3.08438200	-1.48871300	-1.02952400	H	-2.86331000	-4.96084300	-0.44081400
C	2.35668000	-1.31759800	-2.20446700	C	-7.19081000	-3.77353800	0.24743300
C	0.93707800	-1.49947500	-2.26345800	H	-8.07876800	-3.66814800	-0.38370600
H	2.65285300	-2.20449800	-0.33201500	H	-6.55020000	-4.54389900	-0.20287000
H	0.44849300	-1.24890500	-3.20208700	Pd	1.22829700	-0.02713300	-0.81976300
H	0.51014200	-2.35478900	-1.74216200	C	-1.05097600	-0.08260800	3.75713200
F	2.93568600	-0.70028500	-3.27043100	H	-0.31509100	-0.83497700	4.06166200
C	-6.64875300	-1.42527100	-0.53674800	H	-1.66404300	-0.48076400	2.94607900
C	-6.43599200	-2.47459200	0.37025700	H	-1.70521200	0.12955500	4.60995700
C	-5.47793600	-2.30693000	1.38270400	C	-0.37007900	1.19857900	3.32907100
C	-4.73107300	-1.13724300	1.47967100	H	-1.09878700	1.93367200	2.98102300
C	-4.94817600	-0.12341300	0.54499100	H	0.22872200	1.62131400	4.14111800
C	-5.91249700	-0.24557700	-0.45666600	O	0.50942100	0.86593900	2.21042000
H	-7.39695800	-1.53480200	-1.31721500	C	1.29916300	1.77538400	1.65954800
H	-5.30890100	-3.10746500	2.09796300	O	1.91820800	1.47302900	0.63388700
H	-3.98614900	-1.01338800	2.25700200	C	1.42939400	3.13884700	2.27420600

H	0.45324800	3.63754700	2.27214100	C	-3.31345800	3.77699000	-0.90121600
H	1.77304600	3.07333600	3.31214200	C	-1.10723300	2.71697800	-0.79035000
H	2.13576500	3.72739500	1.68878800	C	-2.66729100	5.01631400	-0.93964900
TS20				H	-4.39283500	3.70665100	-0.93019900
C	9.34731400	-1.70016000	0.31630200	C	-0.47615600	3.96494500	-0.84536500
C	8.79431200	-0.46193600	0.06242500	C	-1.26645700	5.11211900	-0.91540000
C	7.41062100	-0.32980000	-0.22360000	H	-3.26610700	5.92086100	-1.00196000
C	6.58475300	-1.50224000	-0.24583300	H	0.60894700	4.02542800	-0.83470500
C	7.18598100	-2.76508300	0.02135900	H	-0.79513500	6.09040600	-0.95794400
C	8.53342200	-2.86125400	0.29485700	C	-0.57135800	1.36294100	-0.73870600
H	7.41409700	1.82156200	-0.47513800	C	-1.64587300	0.50631700	-0.81050100
H	10.40834100	-1.79071200	0.53354200	C	-1.62968900	-0.93705300	-1.06799800
H	9.41313200	0.43268800	0.07724900	C	-0.76865000	-1.78958200	-0.35448400
C	6.79734600	0.92548100	-0.49262100	C	-2.42353900	-1.48585500	-2.09380700
C	5.20525300	-1.36811900	-0.53444200	C	-0.70642300	-3.15175700	-0.65586100
H	6.56158900	-3.65572000	0.00488200	H	-0.17248500	-1.37576800	0.45297800
H	8.97924700	-3.83207400	0.49607700	C	-2.36691700	-2.84648900	-2.38482600
C	4.61377300	-0.13356000	-0.80019500	H	-3.08661100	-0.83509600	-2.65444100
C	5.45633500	1.02765200	-0.77020600	C	-1.50803200	-3.68704100	-1.66703900
H	4.59189900	-2.26728300	-0.54675900	H	-0.04087400	-3.79604100	-0.08683500
H	5.02773400	2.00115800	-0.96821900	H	-2.99144200	-3.25263400	-3.17614000
C	3.18439500	-0.10247700	-1.08538800	H	-1.46614500	-4.74885700	-1.89492900
C	2.39233300	0.93909200	-1.52257500	C	-6.01395000	-4.66459500	-1.12047000
C	0.96926700	0.89935600	-1.89969900	H	-6.89774000	-4.62321400	-1.76468200
H	2.67926700	-1.06555200	-1.06568200	H	-5.21565500	-5.17112800	-1.67961300
H	0.73039000	1.70165100	-2.59535900	Pd	1.17602900	0.99673900	0.30260700
H	0.63517500	-0.07567000	-2.24663600	C	-1.24939300	-2.65558100	3.20475600
F	2.96996000	2.17015300	-1.73993800	H	-0.24335600	-3.03421500	3.41498100
C	-5.99951500	-2.14386300	-1.38560300	H	-1.45306100	-2.77766100	2.13764100
C	-5.56328900	-3.28877100	-0.70117500	H	-1.97094600	-3.25715600	3.76901800
C	-4.66678900	-3.13399400	0.36822200	C	-1.37612100	-1.20560100	3.62384600
C	-4.19438400	-1.87779500	0.73347400	H	-2.36438100	-0.80069100	3.39265100
C	-4.62872400	-0.76179300	0.01682700	H	-1.17868700	-1.09102900	4.69417700
C	-5.54034200	-0.87664500	-1.03404600	O	-0.38270500	-0.44890800	2.87216800
H	-6.70418100	-2.24598600	-2.20646800	C	-0.21386200	0.85576000	3.07773800
H	-4.32504200	-4.00991000	0.91315100	O	0.61219400	1.45535200	2.38635900
H	-3.49085200	-1.76442100	1.54841700	C	-1.02533300	1.56585000	4.12295800
H	-5.87881800	0.00380600	-1.57035200	H	-2.08447800	1.52226300	3.84621200
O	-5.13299900	1.80793100	0.32634300	H	-0.90943300	1.10122700	5.10762200
O	-3.29291000	0.75724100	1.72883100	H	-0.70779800	2.60784500	4.16908600
H	-6.24670500	-5.29066700	-0.25170800	INT29			
S	-4.02548700	0.85346500	0.45336000	C	9.17811200	-1.54070500	-0.19307400
N	-2.89174500	1.25175600	-0.83859000	C	8.50829500	-0.34615600	-0.02759500
C	-2.51443900	2.63690200	-0.82898600	C	7.10649600	-0.26485100	-0.23638800

C	6.38829300	-1.44426400	-0.62151700	H	0.95309600	3.88456000	-1.80822600
C	7.10797400	-2.66101500	-0.78288200	H	-0.08148900	6.07213700	-1.20792400
C	8.46990900	-2.70815700	-0.57434500	C	-0.49734800	1.36687800	-1.50854800
H	6.91066800	1.84365700	0.22260300	C	-1.59786100	0.62987300	-1.17882700
H	10.25174800	-1.59149700	-0.03182600	C	-1.80717300	-0.81782900	-1.39004000
H	9.04672600	0.55259400	0.26521800	C	-1.05697200	-1.75686300	-0.66720000
C	6.37492500	0.94533300	-0.07655800	C	-2.71429000	-1.26700300	-2.36390500
C	4.98813800	-1.35980700	-0.83244900	C	-1.21132700	-3.12307900	-0.91643200
H	6.56335300	-3.55614400	-1.07531000	H	-0.36137900	-1.40595400	0.09076800
H	9.00764800	-3.64418100	-0.70210600	C	-2.87332000	-2.63069200	-2.60370800
C	4.28653300	-0.17115100	-0.67709700	H	-3.29642500	-0.54192500	-2.92422400
C	5.01816500	0.99597200	-0.28484100	C	-2.12120400	-3.56280800	-1.88090600
H	4.45449900	-2.26243100	-1.12469300	H	-0.62401600	-3.84160200	-0.35071200
H	4.48634500	1.92814300	-0.14254600	H	-3.58154500	-2.96631900	-3.35639000
C	2.82892900	-0.17869000	-0.91588200	H	-2.24383700	-4.62591900	-2.07079500
C	1.98868800	0.91619500	-1.21607300	C	-6.97718500	-3.56491500	-1.44386400
C	0.76688100	0.82223300	-2.11491500	H	-7.87587700	-3.21185100	-1.95934800
H	2.44261300	-1.14345000	-1.24513600	H	-6.38600300	-4.14519100	-2.16522000
H	1.00438200	1.35907000	-3.04524300	Pd	1.65207300	0.42396300	0.76081200
H	0.61477100	-0.22827500	-2.37505200	C	-1.43372200	-3.13632100	2.89536200
F	2.56512700	2.18267800	-1.33295900	H	-0.46530300	-3.63861700	2.99287800
C	-6.32165500	-1.11753200	-1.39574000	H	-1.66887400	-3.03091200	1.83277200
C	-6.16113400	-2.42074100	-0.89871600	H	-2.19948100	-3.76566400	3.36271900
C	-5.19802400	-2.64893500	0.09653900	C	-1.41388700	-1.78515300	3.57781500
C	-4.39890200	-1.61533600	0.57566500	H	-2.36484700	-1.26296300	3.45227000
C	-4.57216800	-0.33585700	0.04652400	H	-1.18813700	-1.88031800	4.64501600
C	-5.53623600	-0.06767300	-0.92721600	O	-0.36303000	-0.99947000	2.94327700
H	-7.06935300	-0.92355000	-2.15990400	C	-0.17039900	0.27371900	3.26571400
H	-5.06414000	-3.65196000	0.49275500	O	0.68973600	0.91204800	2.65224200
H	-3.64197300	-1.79789000	1.32903400	C	-0.96596200	0.90276200	4.37240100
H	-5.66298100	0.93662300	-1.31859800	H	-2.02282300	0.93497300	4.09107200
O	-4.46927100	2.13559100	0.97406000	H	-0.87505600	0.32495500	5.29809400
O	-2.68974400	0.48574600	1.71355600	H	-0.60526800	1.91867300	4.53506400
H	-7.28133100	-4.25320600	-0.64742700	INT30			
S	-3.58706200	1.00505000	0.67018600	C	6.97842200	-2.51010000	0.98675600
N	-2.63898500	1.49732100	-0.70469900	C	5.91225500	-3.38091400	0.89882500
C	-2.10908700	2.82331100	-0.71480100	C	4.59923400	-2.95145700	1.22411100
C	-2.70557000	4.04121000	-0.38133400	C	4.39766400	-1.60012100	1.65685600
C	-0.79344500	2.75570700	-1.22736400	C	5.51780800	-0.72737800	1.74154200
C	-1.94867600	5.19998900	-0.56258900	C	6.77854300	-1.17108100	1.40892200
H	-3.71583000	4.08842900	0.00068500	H	3.61015200	-4.83179900	0.80174600
C	-0.05643100	3.93335500	-1.41591100	H	7.97883500	-2.84674000	0.72743400
C	-0.64061400	5.15000500	-1.07386600	H	6.06256000	-4.40687700	0.57046400
H	-2.38949600	6.16019400	-0.30878600	C	3.46381400	-3.80239600	1.12118600

C	3.08599800	-1.16099700	1.95334000	C	1.06752100	-4.41653800	-1.72348400
H	5.35552400	0.30124800	2.05122200	C	-1.49345800	-3.64463800	-2.53908800
H	7.62578800	-0.49274800	1.46249800	H	-0.71674500	-1.62785000	-2.53398200
C	1.98051800	-1.99372600	1.81059000	C	0.06881700	-5.37439100	-1.88983700
C	2.19825700	-3.34650400	1.39612000	H	2.06332300	-4.70768700	-1.40521400
H	2.94720700	-0.12866600	2.25925400	C	-1.21353200	-4.99334300	-2.29868900
H	1.35495300	-4.01321600	1.28153300	H	-2.48854400	-3.34281800	-2.85252700
C	0.66698100	-1.41790000	2.06900100	H	0.29261900	-6.42148600	-1.70315600
C	-0.57624000	-2.00773100	2.04312300	H	-1.98830300	-5.74369700	-2.43288400
C	-1.81113100	-1.28203200	2.16756500	C	0.95062600	7.25048800	-2.53455800
H	0.66556900	-0.39377000	2.43356300	H	-0.10931400	7.40059900	-2.77482000
H	-2.71516800	-1.88830800	2.18493100	H	1.32089800	8.15794800	-2.04743000
H	-1.82267500	-0.45822600	2.88233400	F	-0.15449200	0.41814600	-1.23935600
F	-0.70150100	-3.31811500	1.68945500	H	1.26827300	0.68405300	-0.57737500
Pd	-1.19357800	-0.44745700	0.37891600	P	-3.34116400	0.23065000	-0.06679600
C	1.77539500	6.12300100	-0.41728600	C	-4.48457900	-1.19000600	-0.33217900
C	1.14009700	6.03386900	-1.66303800	C	-3.91922600	-2.47499800	-0.39819000
C	0.68579400	4.77647100	-2.09812300	C	-5.87545000	-1.06084200	-0.50964300
C	0.85511300	3.63859700	-1.31657600	C	-4.71466900	-3.59805800	-0.63348800
C	1.49089600	3.76250400	-0.07600200	H	-2.84803400	-2.59512400	-0.27375800
C	1.95544300	4.99326500	0.38348500	C	-6.66968100	-2.18549100	-0.73957200
H	2.13813800	7.08622000	-0.06809800	H	-6.35144600	-0.08891500	-0.46645800
H	0.19699800	4.68917700	-3.06543200	C	-6.09275500	-3.45664000	-0.80317800
H	0.50742700	2.66869000	-1.65841100	H	-4.25089000	-4.57926300	-0.68520400
H	2.45702100	5.06472700	1.34305200	H	-7.74167200	-2.06484400	-0.87047500
O	2.73701800	2.54259100	1.92564700	H	-6.71450500	-4.32925400	-0.98459400
O	0.32774800	1.93236200	1.45769300	C	-3.95616100	1.20232200	1.37320600
H	1.48221500	7.13600400	-3.48780200	C	-3.07367700	2.16592600	1.90106400
S	1.66004000	2.30691900	0.95166700	C	-5.19543900	1.00587100	1.99960500
N	2.10704700	1.08841600	-0.08573100	C	-3.44481300	2.93974200	2.99968400
C	3.38027600	0.96813500	-0.68281800	H	-2.08503600	2.29114300	1.47005500
C	4.39971700	1.92100900	-0.53830800	C	-5.55830400	1.77724900	3.10820700
C	3.64508300	-0.20744900	-1.43867100	H	-5.88012400	0.24389800	1.64715500
C	5.65639500	1.71182500	-1.10471700	C	-4.69097500	2.75073800	3.60511200
H	4.22596000	2.82442300	0.03087400	H	-2.75161300	3.67948300	3.39142000
C	4.92331200	-0.39367800	-1.99814000	H	-6.52122900	1.60925800	3.58342700
C	5.92909400	0.55189000	-1.83209000	H	-4.97601400	3.34811400	4.46704000
H	6.42605300	2.46701900	-0.96965000	C	-3.50591500	1.36305100	-1.58589500
H	5.11029800	-1.30563600	-2.55696200	C	-2.61842600	2.59904300	-1.34743800
H	6.91158500	0.38578700	-2.26382600	H	-2.54712500	3.16784300	-2.28382900
C	2.65063000	-1.20908400	-1.61955400	H	-3.04222000	3.26419200	-0.58821300
C	1.80405800	-2.06612200	-1.78036400	H	-1.60926200	2.31462900	-1.04583600
C	0.79106600	-3.05392000	-1.95700400	C	-2.97530600	0.56805000	-2.79352200
C	-0.50471600	-2.67717600	-2.36647300	H	-1.91557800	0.33482400	-2.66627800

H	-3.53395400	-0.36286800	-2.94702500	H	4.89404000	6.75958600	-2.79824100
H	-3.08886600	1.17736800	-3.69990300	S	1.25501300	2.63643700	0.77713600
C	-4.95214300	1.81634500	-1.84289600	N	1.16796600	1.37526900	-0.32443700
H	-4.94280700	2.58717900	-2.62461200	C	2.34902700	0.67681000	-0.69109700
H	-5.58119600	0.99695000	-2.20077300	C	3.65380400	1.04340300	-0.31344900
H	-5.41452300	2.25472400	-0.95072000	C	2.19923300	-0.47878900	-1.50963000
TS21				C	4.76363000	0.32030900	-0.74537700
C	7.35641500	-4.60920500	0.62143100	H	3.81825300	1.89185400	0.33462600
C	6.06207800	-4.96958000	0.30858000	C	3.33519100	-1.19757700	-1.92969200
C	4.97209500	-4.12808700	0.65289700	C	4.61463300	-0.80448800	-1.55857100
C	5.23323100	-2.89530800	1.33584500	H	5.75332000	0.63758000	-0.42774500
C	6.57897100	-2.55214300	1.64520900	H	3.18640800	-2.08269400	-2.54035700
C	7.61654800	-3.38888600	1.29524900	H	5.47891100	-1.37873000	-1.87768400
H	3.41795000	-5.38322900	-0.18521700	C	0.91659300	-0.96038400	-1.89866700
H	8.18390200	-5.25983800	0.35104000	C	-0.14056700	-1.43330800	-2.27638700
H	5.85927600	-5.90373800	-0.21042600	C	-1.37357600	-1.94458500	-2.78325500
C	3.62279300	-4.45080600	0.33606600	C	-2.08021500	-1.22845800	-3.76966700
C	4.14752100	-2.04684000	1.66106100	C	-1.89228200	-3.16696100	-2.31440500
H	6.77401300	-1.61375500	2.15936500	C	-3.27914100	-1.72876300	-4.27420400
H	8.64106800	-3.11589700	1.53423100	H	-1.68119900	-0.28393900	-4.12581600
C	2.83330400	-2.37005000	1.34002900	C	-3.08896800	-3.66056600	-2.82843000
C	2.58821700	-3.61033200	0.66565300	H	-1.35683700	-3.70887300	-1.54122600
H	4.35875100	-1.10338200	2.15832600	C	-3.78625100	-2.94450400	-3.80596300
H	1.57497600	-3.88018200	0.39971000	H	-3.81860200	-1.16726800	-5.03228600
C	1.79565700	-1.40222200	1.66723700	H	-3.48728100	-4.59792800	-2.45281000
C	0.45191800	-1.49636800	1.56450100	H	-4.72318700	-3.33125800	-4.19770200
C	-0.51889400	-0.45591700	1.86254900	C	4.19803400	7.16739100	-2.05285300
H	2.14144000	-0.44113400	2.03784800	H	3.50077100	7.82254200	-2.58743700
H	-1.40196600	-0.83159300	2.37779900	H	4.78018200	7.77933300	-1.35622900
H	-0.08020500	0.38129600	2.40874400	F	-0.55228600	1.83378700	-1.99739700
F	-0.12190800	-2.65937600	1.11344800	H	0.29917700	1.70847700	-1.35583500
Pd	-0.95137300	0.36738600	0.02543700	P	-3.20724600	0.29357200	0.40298700
C	3.85162900	5.64415000	-0.05664100	C	-4.02167600	-1.34356300	0.13780500
C	3.46867000	6.05558900	-1.34015400	C	-3.39714000	-2.44983200	0.74408800
C	2.39975400	5.39169400	-1.96609700	C	-5.22148500	-1.55869200	-0.55760200
C	1.73136600	4.34581400	-1.33706500	C	-3.97345600	-3.71778600	0.69055100
C	2.14458400	3.95101300	-0.06024200	H	-2.44695200	-2.33194000	1.24852000
C	3.19676600	4.59432300	0.58930900	C	-5.79104600	-2.83363000	-0.62149800
H	4.67300000	6.14865600	0.44577100	H	-5.73050300	-0.74821300	-1.05980000
H	2.08747700	5.69977900	-2.96084700	C	-5.17845300	-3.91467700	0.01164800
H	0.90984400	3.83978700	-1.83427200	H	-3.47122700	-4.55337800	1.17075800
H	3.49944100	4.27357200	1.58074900	H	-6.71939700	-2.97361000	-1.16872100
O	2.01641500	2.24057800	1.97950200	H	-5.62743100	-4.90321300	-0.03390000
O	-0.13280100	3.10294300	0.95935500	C	-3.64118100	0.70217300	2.14403200

C	-2.84276500	1.63145600	2.83389400	H	-2.17492600	1.94910200	-1.41797100
C	-4.76109800	0.14960900	2.78390500	H	0.79401700	0.29129900	-2.76561700
C	-3.17115100	2.00879500	4.13662700	H	0.18533900	1.86062300	-2.10748800
H	-1.96306400	2.05071100	2.35272900	F	-1.26747900	-1.07177500	-2.38471400
C	-5.08020300	0.52458200	4.09095100	Pd	1.00414500	0.43341400	-0.17054700
H	-5.38509900	-0.57247600	2.26599700	C	5.57797200	1.71249200	0.68423900
C	-4.28843300	1.45533100	4.76826000	C	5.95919000	0.99444400	-0.45851800
H	-2.54702100	2.72841900	4.65988900	C	5.12508400	1.03793100	-1.58667100
H	-5.94811900	0.08829000	4.57835500	C	3.93400600	1.75898700	-1.57213800
H	-4.53787500	1.74391000	5.78593200	C	3.57086500	2.45034900	-0.41208100
C	-4.05888200	1.66413400	-0.61431200	C	4.39511800	2.45026600	0.71386700
C	-3.29011600	2.97549800	-0.33832900	H	6.21906800	1.70162800	1.56186500
H	-3.74254400	3.77078100	-0.94574500	H	5.41204200	0.49923000	-2.48631600
H	-3.36541100	3.27869400	0.71052700	H	3.29427900	1.79782900	-2.44648400
H	-2.23265500	2.90501900	-0.60066600	H	4.11550800	3.01070600	1.59720400
C	-3.93334000	1.32074500	-2.11025600	O	2.36995700	4.69337900	0.35619300
H	-2.88392800	1.24349300	-2.40737400	O	1.75254300	3.66758900	-1.87294100
H	-4.43120400	0.38658700	-2.38163800	H	6.98099200	-0.88958400	-0.25901800
H	-4.38978700	2.12790300	-2.69828100	S	2.10424100	3.48387400	-0.44583400
C	-5.52718200	1.88306500	-0.20072600	N	0.94834000	2.53424200	0.35658600
H	-5.93792400	2.70161600	-0.80601400	C	-0.35798700	3.09781600	0.45966600
H	-6.16561700	1.01074900	-0.35592200	C	-0.82245500	4.17560200	-0.31934300
H	-5.60741600	2.17511400	0.85111100	C	-1.27594000	2.50821200	1.37973500
INT31				C	-2.12220100	4.66374700	-0.18875800
C	-8.67578200	0.09093900	-0.48118600	H	-0.17182100	4.63590900	-1.04977000
C	-7.73737000	-0.82681700	-0.90558000	C	-2.58936200	3.00684900	1.48056800
C	-6.38990600	-0.43730700	-1.12273400	C	-3.01740500	4.08292100	0.71105900
C	-6.01445600	0.92799400	-0.89663900	H	-2.43290100	5.50076900	-0.80828500
C	-7.00599900	1.85038800	-0.45897300	H	-3.26620600	2.53018500	2.18321500
C	-8.30596000	1.44135900	-0.25547900	H	-4.03203600	4.45742300	0.80976800
H	-5.66332400	-2.38638900	-1.72853500	C	-0.91341900	1.41857600	2.22338900
H	-9.70482800	-0.21797500	-0.31757700	C	-0.68843200	0.52308700	3.01667500
H	-8.01801200	-1.86322700	-1.07932900	C	-0.35016600	-0.50299200	3.94612700
C	-5.38673100	-1.34865200	-1.55623600	C	0.84224000	-0.40839500	4.69312500
C	-4.66994800	1.31559700	-1.11024700	C	-1.18154000	-1.62780400	4.11473600
H	-6.71805100	2.88496700	-0.28663900	C	1.19299100	-1.42428600	5.57947300
H	-9.05508800	2.15363700	0.08005300	H	1.48606700	0.45176800	4.54430500
C	-3.69448500	0.41221100	-1.52601900	C	-0.81898300	-2.64024100	5.00128800
C	-4.08805900	-0.94794000	-1.75264400	H	-2.09708800	-1.70482700	3.53830500
H	-4.39388000	2.35108000	-0.93088500	C	0.36772300	-2.54319100	5.73459100
H	-3.34972600	-1.66948200	-2.07302300	H	2.11644900	-1.34575700	6.14697900
C	-2.33149100	0.90375000	-1.66809100	H	-1.46300100	-3.50788900	5.11712700
C	-1.20360600	0.24793900	-2.02548100	H	0.64833900	-3.33567100	6.42319700
C	0.14973200	0.77514400	-2.03011800	C	7.21653100	0.16253600	-0.46936100

H	7.71035700	0.19529500	-1.44685500
H	7.92965800	0.49869800	0.29021700
P	1.19588300	-1.85336800	-0.46246200
C	-0.32044600	-2.77106700	0.02718100
C	-1.40118200	-2.01903400	0.51520100
C	-0.45119700	-4.17034600	-0.04501200
C	-2.58457500	-2.64331500	0.91290500
H	-1.31892500	-0.93944400	0.58113700
C	-1.63377800	-4.79281900	0.35797400
H	0.35803000	-4.78239500	-0.42511700
C	-2.70375900	-4.03184000	0.83639900
H	-3.41208300	-2.03917700	1.27290400
H	-1.71823700	-5.87426700	0.29284500
H	-3.62521600	-4.51916800	1.14361100
C	1.64329900	-2.35601000	-2.17313900
C	2.66798900	-1.62376700	-2.80109800
C	0.99058900	-3.36047600	-2.90234200
C	3.05971500	-1.91945000	-4.10635400
H	3.14300800	-0.80230000	-2.27562700
C	1.37894500	-3.64880300	-4.21323600
H	0.16261000	-3.90786600	-2.46861400
C	2.41830700	-2.93825800	-4.81609100
H	3.85429200	-1.34299800	-4.57289600
H	0.85964300	-4.42847500	-4.76411400
H	2.71564000	-3.16471100	-5.83640100
C	2.59365000	-2.47809500	0.67456800
C	3.87552700	-1.68588200	0.35769800
H	4.64328700	-1.95219800	1.09548400
H	4.27271900	-1.92521900	-0.63307700
H	3.71870800	-0.60441700	0.41802100
C	2.15975500	-2.16951800	2.11792000
H	2.03190700	-1.09503200	2.28048900
H	1.22479500	-2.66930400	2.38980600
H	2.93841600	-2.51576200	2.80931600
C	2.86917900	-3.98053400	0.50822700
H	3.76273200	-4.24207300	1.09014600
H	2.04609000	-4.59306500	0.88595600
H	3.06082400	-4.25100800	-0.53641900
F	2.19495500	1.62605600	2.47470600
H	1.65737500	2.03125400	1.74923800

TS22

C	-7.62084500	4.43822800	0.62818700
C	-7.68101100	3.13663000	0.17525400
C	-6.54631500	2.52213400	-0.41614500
C	-5.33241800	3.27544000	-0.54039800
C	-5.30303800	4.61652000	-0.06485700
C	-6.42071300	5.18412000	0.50712800
H	-7.47780100	0.60459600	-0.79887200
H	-8.49478600	4.89836800	1.08152200
H	-8.59989100	2.56200500	0.26700500
C	-6.55850100	1.17909500	-0.88607600
C	-4.19886100	2.65872400	-1.12170000
H	-4.38002500	5.18442800	-0.15781000
H	-6.38702700	6.20816700	0.86941300
C	-4.21822200	1.33571600	-1.55431900
C	-5.43937500	0.59905600	-1.43018600
H	-3.28006400	3.23447900	-1.20337100
H	-5.47804400	-0.42862900	-1.76645200
C	-2.98351300	0.77705100	-2.08420600
C	-2.63958300	-0.51256700	-2.30071500
C	-1.34829400	-0.99681900	-2.75577100
H	-2.18715900	1.48840100	-2.28685100
H	-1.40488200	-1.96143700	-3.26567900
H	-0.80825800	-0.25256800	-3.34212000
F	-3.52545100	-1.51329100	-2.02173900
C	7.88790300	2.25893400	0.30411200
C	7.51911000	3.41820800	-0.38857000
C	6.15053800	3.71947200	-0.50770600
C	5.18057000	2.88760600	0.04202400
C	5.57530800	1.73216700	0.72662400
C	6.92460700	1.41327500	0.86145500
H	8.94122600	2.01076300	0.41066300
H	5.84644900	4.61862800	-1.03891900
H	4.12639600	3.12941000	-0.05625500
H	7.21384600	0.51766100	1.40092600
O	5.00943000	-0.46461700	2.08430800
O	3.41850100	1.49217500	2.23657200
H	8.52543600	4.25550000	-2.10698400
S	4.30380100	0.65250300	1.40628700
N	3.43177500	0.17561100	0.12344100
C	1.45723000	0.59685700	-0.82977400
C	0.75824000	1.65485000	-0.16887700
C	0.55562500	1.63113300	1.22599400
C	0.19446300	2.69558500	-0.93790200
C	-0.21629700	2.61972500	1.82994600
H	1.02163400	0.84909300	1.81162900
C	-0.58684100	3.67164400	-0.32285300
H	0.36566300	2.71552700	-2.00998500

C	-0.79872400	3.63317900	1.05935800	H	-2.23234100	-6.20930400	0.87354300
H	-0.37046800	2.59646500	2.90501500	H	-1.34095000	-5.09723300	1.92551200
H	-1.02443600	4.46643600	-0.92066700	H	-3.05310900	-4.81241000	1.57999100
C	3.90016300	-0.70277700	-0.82404200	C	-2.75826500	-4.46406200	-1.21795300
C	5.14006300	-1.38369600	-0.86172900	H	-2.44567200	-3.92790600	-2.11941400
C	2.98098100	-0.95789800	-1.90138800	H	-2.89060800	-5.52132600	-1.48064600
C	5.44334600	-2.24657400	-1.91281700	H	-3.73125400	-4.06858600	-0.91559500
H	5.85301800	-1.24430800	-0.05865000	C	-0.36249900	-4.92495900	-0.63577100
C	3.30065400	-1.84528900	-2.93545000	H	-0.51160100	-5.97648100	-0.91180400
C	4.53657900	-2.48740000	-2.95512100	H	-0.01303000	-4.38782800	-1.52532500
H	6.40905200	-2.74734200	-1.91455400	H	0.42746100	-4.88913800	0.12147200
H	2.57097400	-2.01471200	-3.72358000	INT32			
H	4.79266200	-3.16580300	-3.76393100	C	8.48564200	-2.13619500	0.79752400
C	1.72612400	-0.26216700	-1.74411700	C	7.93539800	-1.46202900	-0.27256600
H	-1.40897000	4.39558400	1.53593000	C	6.55102900	-1.57517600	-0.56639600
C	8.55448400	4.32269100	-1.01125800	C	5.72737600	-2.40287800	0.26425100
H	8.37451400	5.37248500	-0.74967300	C	6.32556200	-3.08895700	1.35814000
H	9.56682700	4.05923800	-0.68808300	C	7.67222400	-2.95739900	1.61948800
Pd	-0.05837800	-1.29083600	-1.17537800	H	6.55119800	-0.23564600	-2.26642400
P	-1.37877200	-2.53734800	0.27769700	H	9.54603200	-2.04090000	1.01569800
C	-2.85281100	-1.66642400	0.93884500	H	8.55452400	-0.82925200	-0.90455200
C	-4.10282400	-2.24011200	1.21619100	C	5.93586200	-0.87776600	-1.64131300
C	-2.66430100	-0.29583100	1.19930400	C	4.34377000	-2.50232100	-0.02300300
C	-5.13069100	-1.46233000	1.75541400	H	5.69914500	-3.71715400	1.98758900
H	-4.29371700	-3.28733700	1.01936600	H	8.11788600	-3.48381800	2.45947100
C	-3.68801800	0.47375500	1.74755400	C	3.75383800	-1.80851900	-1.07366100
H	-1.71028500	0.17329400	0.97839500	C	4.58799800	-0.97586200	-1.88448500
C	-4.92686800	-0.10803900	2.02657000	H	3.72980400	-3.14120400	0.60765800
H	-6.09362800	-1.92158600	1.96225100	H	4.15202300	-0.40964100	-2.69559900
H	-3.52051500	1.52996600	1.93570500	C	2.30993400	-1.96391300	-1.27577200
H	-5.73149100	0.49389400	2.43909000	C	1.55805000	-1.65337500	-2.41210200
C	-0.19921400	-2.49601300	1.69822800	C	0.14668400	-1.75659600	-2.47621200
C	-0.62998500	-2.30732500	3.02199300	H	1.82779500	-2.67983800	-0.61332400
C	1.18432100	-2.52098400	1.43066600	H	-0.34220500	-1.40673000	-3.38077600
C	0.30138900	-2.13240800	4.04664600	H	-0.33567100	-2.59030900	-1.97203700
H	-1.69046900	-2.27987800	3.25194200	F	2.15233600	-0.97687100	-3.43546300
C	2.11326000	-2.32133800	2.45387900	C	-7.28970500	-1.92267500	0.00266700
H	1.55042600	-2.67685400	0.41783200	C	-6.88351700	-2.79226700	1.02598800
C	1.67065600	-2.12264800	3.76323800	C	-5.80948300	-2.41290800	1.84710400
H	-0.04518400	-1.98785100	5.06654000	C	-5.13790000	-1.21187900	1.64286000
H	3.17257300	-2.27950600	2.22151900	C	-5.54998100	-0.38166100	0.59866000
H	2.39124700	-1.95121500	4.55804100	C	-6.63030300	-0.71580900	-0.21904900
C	-1.69742000	-4.35850100	-0.10619900	H	-8.12922200	-2.19557000	-0.63104700
C	-2.10923100	-5.15340600	1.14691800	H	-5.48920600	-3.07231400	2.64923900

H	-4.30176100	-0.92563200	2.27033700	C	-0.05581400	-0.13458000	3.04486600
H	-6.94553900	-0.04808700	-1.01375900	H	-0.66302700	-0.59649000	2.26244300
O	-5.67258700	2.13088700	-0.18496700	H	-0.08201600	-0.79163200	3.92368200
O	-3.89071800	1.46934100	1.50208700	H	-0.52779600	0.81107100	3.32449200
H	-8.53969700	-4.16017700	0.74499500	C	0.60883100	2.54387700	1.30503700
S	-4.69541900	1.15186700	0.30924900	C	-0.79158600	2.59510000	1.40266700
N	-3.61882400	0.82328300	-1.04047300	C	1.34612100	3.71506800	1.54707900
C	-2.98462800	2.01526800	-1.52117900	C	-1.44138900	3.78786400	1.71931200
C	-3.55046300	3.21829200	-1.94330700	H	-1.38710000	1.71070200	1.21965300
C	-1.59058700	1.79252200	-1.55094400	C	0.69307900	4.90988000	1.85852500
C	-2.68550000	4.20911400	-2.41624100	H	2.42957300	3.70293000	1.49142000
H	-4.62004500	3.37850500	-1.90976400	C	-0.70111200	4.95085100	1.94180400
C	-0.74629900	2.78951900	-2.05723700	H	-2.52577700	3.79553200	1.77405900
C	-1.29839700	3.99707200	-2.47919300	H	1.27791500	5.80850700	2.03783300
H	-3.10116400	5.15383500	-2.75637400	H	-1.20629600	5.88395800	2.17772500
H	0.32270300	2.60981400	-2.11585600	C	3.12723900	1.42566100	0.45160500
H	-0.65253500	4.78091100	-2.86644700	C	4.30755800	1.05832900	1.11402400
C	-1.31162400	0.45664200	-1.04489900	C	3.23432200	2.22808000	-0.70168500
C	-2.52960400	-0.11633700	-0.78265000	C	5.54978800	1.51655500	0.66570200
C	-2.83145300	-1.53945500	-0.56210700	H	4.28522800	0.41127200	1.97978800
C	-2.07096400	-2.32329100	0.32278000	C	4.47295800	2.68748200	-1.14557900
C	-3.84630600	-2.17205200	-1.30412600	H	2.33791800	2.51304600	-1.24418100
C	-2.31864400	-3.68864100	0.46844900	C	5.63788200	2.33953400	-0.45596900
H	-1.28161100	-1.85363800	0.89773200	H	6.44914700	1.21220900	1.19338000
C	-4.09760900	-3.53461200	-1.15518100	H	4.52601100	3.31512100	-2.03126100
H	-4.43847500	-1.58271300	-1.99642600	H	6.60547400	2.69402700	-0.80073500
C	-3.33643100	-4.30200900	-0.26701300	TS23			
H	-1.72085700	-4.27101300	1.16560700	C	8.26259500	-2.09982600	0.42726700
H	-4.88981600	-3.99942900	-1.73632100	C	7.77081200	-1.41011300	-0.66130500
H	-3.53542000	-5.36402700	-0.15021000	C	6.40734000	-1.52614000	-1.03854700
C	-7.55552100	-4.12706300	1.22295100	C	5.54260300	-2.38047800	-0.27888600
H	-6.94393300	-4.92690500	0.78362400	C	6.08161700	-3.08405300	0.83482500
H	-7.67791000	-4.36083500	2.28647700	C	7.40794500	-2.94376500	1.18230500
Pd	0.53843000	-0.37451000	-0.87348900	H	6.50223100	-0.16437700	-2.71920200
P	1.40916900	0.92616100	0.91746600	H	9.30664000	-1.99915900	0.71171600
C	1.41455100	0.05613800	2.61596900	H	8.42050100	-0.75924300	-1.24226600
C	2.11518300	0.88613700	3.70788900	C	5.85082700	-0.80703500	-2.13132700
H	1.66392300	1.87927100	3.80156500	C	4.17552700	-2.46646300	-0.63409500
H	1.99704400	0.37360600	4.67163400	H	5.42472700	-3.72932100	1.41402000
H	3.18487800	1.01822500	3.53478900	H	7.80593200	-3.48183000	2.03880600
C	2.05866200	-1.33423400	2.46235200	C	3.63401400	-1.72378500	-1.67966400
H	3.09216400	-1.29242800	2.11204000	C	4.51610300	-0.89392400	-2.44326200
H	2.05509100	-1.84282200	3.43525700	H	3.52312900	-3.09781300	-0.03365800
H	1.49184200	-1.95330200	1.75800800	H	4.12349700	-0.32314100	-3.27418400

C	2.18756000	-1.78913500	-1.88379900
C	1.37066900	-0.97453600	-2.62887000
C	-0.09950900	-0.94304000	-2.63770900
H	1.66936700	-2.59327000	-1.36577500
H	-0.47674700	-0.47988900	-3.54651500
H	-0.55658500	-1.90894400	-2.43475400
F	1.92912300	0.02165400	-3.39031700
C	-6.93563300	-2.13579700	0.53211800
C	-6.29839500	-2.80490500	1.58763200
C	-5.13867700	-2.23987700	2.14338100
C	-4.60862700	-1.05363100	1.64787300
C	-5.24923200	-0.43057700	0.57392800
C	-6.41851600	-0.94953100	0.01651200
H	-7.84328700	-2.55201100	0.10349800
H	-4.64091500	-2.74112600	2.96908900
H	-3.71190300	-0.62091000	2.07727000
H	-6.90979700	-0.43792500	-0.80406600
O	-5.67232600	1.85223400	-0.68021500
O	-3.71959400	1.69116700	0.94108300
H	-7.85952500	-4.29131100	1.80383900
S	-4.57623600	1.07611500	-0.08544800
N	-3.56089800	0.58755400	-1.45533700
C	-2.95564800	1.74493700	-2.05212200
C	-3.55176900	2.91143400	-2.53091600
C	-1.56262900	1.54496200	-2.11402400
C	-2.71454500	3.87967900	-3.09279500
H	-4.62206100	3.06109300	-2.47114200
C	-0.74013200	2.51727500	-2.69435700
C	-1.32595100	3.68659500	-3.17804400
H	-3.15378700	4.79482900	-3.48035900
H	0.33271600	2.35517000	-2.75246600
H	-0.70434700	4.45576900	-3.62854900
C	-1.25812200	0.24394300	-1.53265000
C	-2.46357000	-0.32218400	-1.17174700
C	-2.71625400	-1.72005900	-0.81592000
C	-1.82597800	-2.42164000	0.01971900
C	-3.81423300	-2.41824700	-1.35509400
C	-2.03175800	-3.76855200	0.31622400
H	-0.97946800	-1.89036000	0.44451600
C	-4.02282200	-3.76117000	-1.04984400
H	-4.50376400	-1.89585800	-2.00999000
C	-3.13482000	-4.44483900	-0.21160600
H	-1.33514700	-4.28552100	0.97191600
H	-4.88132900	-4.27802200	-1.47064500
H	-3.30191900	-5.49232500	0.02489100
C	-6.81848100	-4.12417800	2.09782400
H	-6.21912100	-4.94909000	1.68919200
H	-6.75148400	-4.18579600	3.18976200
Pd	0.62730500	-0.06788800	-0.63503700
P	1.24941400	0.95899000	1.32054000
C	0.85777100	-0.00254000	2.91906900
C	1.50632100	0.62482600	4.16337300
H	1.16318200	1.65393800	4.31339300
H	1.22291700	0.04677100	5.05323800
H	2.59884900	0.63598100	4.10827200
C	1.29127200	-1.47284100	2.74763000
H	2.37301700	-1.59564000	2.64998200
H	0.97232000	-2.04799600	3.62704000
H	0.82661600	-1.92180700	1.86274400
C	-0.67791100	0.02630000	3.07929200
H	-1.18571600	-0.38259900	2.19939700
H	-0.95661700	-0.58711900	3.94620900
H	-1.05658600	1.03854300	3.24956000
C	0.54474600	2.63166200	1.63728900
C	-0.74709200	2.89467400	1.15659900
C	1.22429300	3.63268300	2.35164600
C	-1.35341900	4.13074600	1.38728600
H	-1.28583800	2.13308800	0.60585100
C	0.62054500	4.87211700	2.57288200
H	2.22801300	3.45045600	2.72452400
C	-0.66848800	5.12369300	2.09136000
H	-2.35642000	4.30777700	1.00986400
H	1.15738100	5.64181900	3.12173200
H	-1.13418300	6.09060100	2.26454100
C	3.06792200	1.28303100	1.20157000
C	4.06668000	0.49450700	1.79375500
C	3.46547200	2.28998100	0.29832300
C	5.41671800	0.70612400	1.49858600
H	3.81076700	-0.30061300	2.48134900
C	4.81203900	2.50685600	0.01333700
H	2.71315500	2.90501400	-0.18892600
C	5.79548900	1.71062400	0.60941800
H	6.16843500	0.06777300	1.95444000
H	5.09237300	3.29151000	-0.68474400
H	6.84482300	1.86531300	0.37398500
INT33			
C	7.91378300	-2.74773300	0.30525000
C	7.34385900	-2.06465600	-0.74974200

C	5.93929600	-2.08650900	-0.95424500	H	-2.91431200	3.86976500	-4.24635000
C	5.11325100	-2.83202500	-0.04992600	H	-0.50637000	0.31205400	-4.62094300
C	5.73218200	-3.53077800	1.02422200	H	-1.21263400	2.54714500	-5.47178800
C	7.09880400	-3.48742100	1.19900700	C	-1.63781000	-0.83128100	-2.18809000
H	5.92650400	-0.80435900	-2.70000600	C	-2.45140600	-0.80005500	-1.08985900
H	8.98983900	-2.72178600	0.45508000	C	-2.61034100	-1.84925800	-0.05483700
H	7.96385100	-1.49507200	-1.43853600	C	-1.84863700	-1.81164400	1.12174000
C	5.30718500	-1.37596600	-2.01255100	C	-3.49138100	-2.91975500	-0.26906700
C	3.70923900	-2.83202800	-0.24179000	C	-1.97882400	-2.81928100	2.07845600
H	5.10557300	-4.09703700	1.70979600	H	-1.15543300	-0.99274100	1.27202800
H	7.55851000	-4.02164400	2.02647800	C	-3.62128500	-3.92698800	0.68843200
C	3.10398500	-2.11238500	-1.26603600	H	-4.08360900	-2.94961600	-1.17884300
C	3.94301000	-1.38194100	-2.16682900	C	-2.86844400	-3.87616000	1.86541100
H	3.08989700	-3.38583800	0.46115300	H	-1.38618800	-2.77645300	2.98863700
H	3.48947700	-0.81023300	-2.96545300	H	-4.31271600	-4.74766100	0.51751800
C	1.63318800	-2.11068800	-1.33436500	H	-2.97368300	-4.65870900	2.61235900
C	0.77810200	-1.52070300	-2.26120300	C	-8.08068800	-3.17875800	1.62769000
C	-0.65946200	-1.93012300	-2.50896000	H	-7.69689000	-4.16074100	1.31887400
H	1.14716400	-2.83013400	-0.67671900	H	-8.29069300	-3.23295300	2.70106600
H	-0.74957400	-2.24095800	-3.55887100	Pd	0.96534500	-0.15287000	-0.56469400
H	-0.88287100	-2.80284600	-1.88955000	P	1.52349700	1.42469800	1.05810700
F	1.30803300	-0.87788200	-3.37481700	C	1.38804000	0.83868600	2.88467200
C	-7.08339000	-1.45243700	0.06805200	C	2.35774000	1.55938400	3.83673200
C	-7.07487600	-2.10002600	1.31512300	H	2.18446400	2.63857700	3.87905800
C	-6.08967100	-1.74906400	2.24924700	H	2.22081400	1.16659100	4.85350400
C	-5.12385400	-0.78993900	1.95261600	H	3.40223100	1.39591700	3.55287900
C	-5.15328700	-0.17639200	0.70090700	C	1.72277100	-0.66720700	2.89367500
C	-6.13130900	-0.48795300	-0.24730600	H	2.73663000	-0.86447600	2.52774100
H	-7.84516800	-1.70885400	-0.66336500	H	1.66095500	-1.04629900	3.92310600
H	-6.06979000	-2.24064600	3.21807300	H	1.02544500	-1.23932200	2.27288500
H	-4.34695700	-0.53984400	2.66549100	C	-0.06399300	1.04058700	3.35383400
H	-6.14099500	0.00266500	-1.21576400	H	-0.79330500	0.64438400	2.64104800
O	-4.61412200	2.29068000	-0.12585000	H	-0.21048600	0.52188000	4.31106400
O	-2.95431500	1.12474100	1.39678900	H	-0.29955100	2.09783200	3.50740100
H	-9.02454300	-3.01492300	1.09705400	C	0.55279400	2.98971500	0.92390500
S	-3.93992000	1.06613500	0.31402300	C	-0.32556400	3.09863000	-0.16816600
N	-3.19523600	0.41395600	-1.09764600	C	0.61487100	4.05666800	1.83876900
C	-2.79160900	1.17463900	-2.21971600	C	-1.11029000	4.24005100	-0.34753000
C	-3.20254400	2.42639300	-2.69105300	H	-0.40525000	2.27971900	-0.88016000
C	-1.82751500	0.40142600	-2.91485100	C	-0.17438800	5.19442400	1.66401800
C	-2.61466800	2.89743600	-3.86477100	H	1.28136300	4.00804200	2.69240200
H	-3.94134900	3.01258500	-2.16355900	C	-1.03853700	5.28934100	0.56968100
C	-1.25483300	0.89682100	-4.09663800	H	-1.78133400	4.29664200	-1.19922400
C	-1.64989400	2.14642700	-4.56133500	H	-0.11369300	6.00631300	2.38426500

H	-1.65417900	6.17507900	0.43600700	H	4.43045600	-3.46819800	-0.63864300
C	3.29756700	1.92927100	0.89758000	C	3.65565300	-2.21158800	1.71826000
C	4.24771500	0.90417500	0.72821300	H	4.35749300	-3.04236000	1.87710800
C	3.74689300	3.25792500	0.94458200	H	4.25261200	-1.29813700	1.65957000
C	5.60958600	1.19841000	0.65094100	H	3.02220900	-2.13954800	2.60818200
H	3.92073900	-0.12719500	0.63754900	C	0.56921700	5.15766500	-0.66893500
C	5.10972700	3.55225900	0.84599300	C	-0.39135300	4.48967900	-1.39831900
H	3.03919800	4.07286400	1.05067000	C	-1.05170400	3.35274000	-0.86027300
C	6.04554000	2.52493500	0.71029800	C	-0.72556000	2.92255000	0.46664600
H	6.32498100	0.39028600	0.52664700	C	0.27733900	3.62590600	1.18913100
H	5.43710400	4.58851200	0.87848600	C	0.91357400	4.71437900	0.63304700
H	7.10531600	2.75604800	0.63905300	H	-2.25604700	2.91465700	-2.60797100
INT38				H	1.07449200	6.02121300	-1.09389000
P	1.46775200	-1.18276600	0.03711100	H	-0.64853000	4.81694300	-2.40347000
C	2.35303500	0.35420400	-0.53899400	C	-2.01959200	2.61060800	-1.59077500
C	1.66628200	1.13844300	-1.48328500	C	-1.41246200	1.81095200	1.01968900
C	3.62350300	0.79067400	-0.12463500	H	0.53586000	3.28304200	2.18772700
C	2.22814700	2.30669500	-1.99982200	H	1.68328400	5.23976800	1.19265400
H	0.68083300	0.81977300	-1.81285600	C	-2.36580300	1.11408500	0.30058600
C	4.18881600	1.95992100	-0.64063200	C	-2.65052400	1.52184900	-1.03556300
H	4.18973400	0.22498400	0.60392000	H	-1.16523200	1.50014900	2.03080400
C	3.49371000	2.72197900	-1.58167000	H	-3.37942400	0.97177300	-1.61990000
H	1.66980100	2.89434000	-2.72179300	C	-3.05847500	-0.03018900	0.95336900
H	5.17506100	2.27177000	-0.30482700	C	-4.46900600	-0.42426700	0.67887000
H	3.93331600	3.63161100	-1.98334200	C	-3.42834900	-1.33596000	0.18545100
C	0.89344000	-0.70732800	1.74175700	H	-2.75316200	-0.20515700	1.98091400
C	-0.15959000	-1.45087700	2.30100400	H	-3.26597100	-2.26996500	0.71496900
C	1.45137200	0.33355300	2.50061800	H	-3.21285300	-1.36124100	-0.87903400
C	-0.63189800	-1.17249900	3.58576500	F	-5.25789800	-0.79500700	1.72777600
H	-0.62826000	-2.23241900	1.70884200	F	-5.22488100	0.29051100	-0.20074700
C	0.97151700	0.62249100	3.78092000	Pd	-0.11104300	-1.87740900	-1.36892500
H	2.25281500	0.93781800	2.08874500	Cl	-1.78101000	-2.61970000	-2.93968900
C	-0.07022300	-0.13049100	4.32973100	TS27			
H	-1.44946400	-1.75919200	3.99806400	P	0.58656900	1.54974500	-0.14549000
H	1.41184800	1.43897900	4.34857300	C	-1.10659900	1.72431600	-0.89858900
H	-0.44509900	0.09638100	5.32462100	C	-1.50138900	0.70278100	-1.77887000
C	2.82653300	-2.48853200	0.45037700	C	-2.01441900	2.77341500	-0.65907800
C	2.08309600	-3.82307800	0.66888900	C	-2.75450600	0.72230600	-2.39562900
H	2.81238300	-4.61679500	0.88498000	H	-0.81859100	-0.12175200	-1.96644500
H	1.39255300	-3.76647200	1.51884400	C	-3.26746300	2.79600100	-1.27520100
H	1.50478100	-4.11253200	-0.21455400	H	-1.75972400	3.57281800	0.02638700
C	3.74410500	-2.62120900	-0.77724500	C	-3.64246100	1.76921200	-2.14552200
H	3.16083400	-2.80488100	-1.68762700	H	-3.03820500	-0.08994600	-3.05906700
H	4.34874600	-1.72280700	-0.93904900	H	-3.95244700	3.61509700	-1.06919800

H	-4.62104000	1.78317700	-2.61895800	C	2.65756000	-2.45796200	-0.09718100
C	0.26685200	1.65439600	1.68891700	H	1.37469900	-1.39785100	1.72053200
C	1.35657800	1.36157000	2.53406600	H	3.58417200	-1.93118000	0.11753900
C	-0.98400200	1.87050100	2.29150100	H	2.52390600	-2.83423900	-1.10696100
C	1.21225900	1.32693300	3.92132800	F	2.83041000	-3.41097000	2.12980000
H	2.32124400	1.12377000	2.09375100	F	1.58440000	-4.49792100	0.65313300
C	-1.13502700	1.81818200	3.68132900	Pd	1.72262000	-0.32626700	-0.71842900
H	-1.86147700	2.04923800	1.68182300	Cl	3.11527200	-0.63553700	-2.92826500
C	-0.03836700	1.55583800	4.50395900	INT39			
H	2.07383200	1.10285900	4.54582600	P	1.03697900	1.21783400	-0.20842900
H	-2.11806100	1.97999700	4.11784300	C	-0.54397900	1.66026800	-1.06007300
H	-0.15763600	1.51452100	5.58363400	C	-1.10911200	0.67200900	-1.88398600
C	1.46645600	3.21500500	-0.54557800	C	-1.21115800	2.89480800	-0.95285100
C	2.90687600	3.11519000	-0.00749900	C	-2.31227800	0.89577600	-2.55593900
H	3.48662600	3.98087000	-0.35717700	H	-0.60911500	-0.28635300	-1.98575200
H	2.93299600	3.12426600	1.08783800	C	-2.41482000	3.11877800	-1.62379500
H	3.40719200	2.20552800	-0.35814400	H	-0.80407900	3.68872300	-0.33842200
C	1.51162700	3.31660100	-2.08153400	C	-2.97278800	2.11765400	-2.42268000
H	1.99585400	2.43838100	-2.52463600	H	-2.73625200	0.10707900	-3.17077900
H	0.50653400	3.40408300	-2.51068900	H	-2.91740200	4.07695300	-1.51797600
H	2.08139800	4.20860000	-2.37741300	H	-3.91587000	2.28906800	-2.93505000
C	0.81093200	4.47322200	0.04690200	C	0.75866900	1.52686700	1.59593100
H	1.47381200	5.33737500	-0.10295700	C	1.71791500	0.98876900	2.47415000
H	-0.13812400	4.71324700	-0.44003300	C	-0.33545400	2.21044600	2.14845200
H	0.63429700	4.37510200	1.12452200	C	1.60397400	1.15573600	3.85509400
C	-5.20361100	-1.61801300	-0.28057700	H	2.54392400	0.40700000	2.07448400
C	-4.23264700	-2.33922000	-0.94354300	C	-0.45688200	2.36717500	3.53218700
C	-2.88545100	-2.32709100	-0.49574200	H	-1.11801800	2.60108300	1.50953600
C	-2.54305100	-1.56107200	0.66720800	C	0.51452200	1.84771700	4.39032100
C	-3.56867200	-0.83135100	1.33138600	H	2.35829800	0.72910500	4.51127900
C	-4.86575400	-0.85548000	0.86666200	H	-1.31803800	2.89320000	3.93704000
H	-2.09665400	-3.61374700	-2.05127500	H	0.41713600	1.96928100	5.46604500
H	-6.23062700	-1.62837500	-0.63653000	C	2.28481900	2.58907900	-0.69355500
H	-4.48424800	-2.92117500	-1.82779500	C	3.67656600	2.10861300	-0.23666100
C	-1.84763800	-3.02883400	-1.16855100	H	4.43400700	2.83311300	-0.56668800
C	-1.19603200	-1.53159300	1.10503000	H	3.74354300	2.04087900	0.85517100
H	-3.30379100	-0.24214400	2.20612200	H	3.92514400	1.13351600	-0.66537300
H	-5.63740200	-0.28555800	1.37827800	C	2.26008800	2.71856700	-2.22750600
C	-0.19126800	-2.19331700	0.41434000	H	2.46474800	1.75843200	-2.71072300
C	-0.54582800	-2.96772200	-0.73203800	H	1.29473000	3.09382300	-2.58529000
H	-0.94611300	-0.93225700	1.97536900	H	3.03457100	3.43154900	-2.54263100
H	0.22769200	-3.49994100	-1.27469300	C	1.99836800	3.95714200	-0.05136700
C	1.20804300	-2.09450900	0.90335400	H	2.81104800	4.64977600	-0.31104800
C	2.09498900	-3.27005400	0.98027100	H	1.06938700	4.40280500	-0.41803200

H	1.94716400	3.89972000	1.04111500	H	2.51785900	-0.20154800	-1.99809800
C	-5.76369900	-0.22060700	-0.21691800	H	1.98620800	2.45477100	1.32343700
C	-4.99628200	-1.21729500	-0.78498900	C	0.92977900	1.76268100	-1.07085300
C	-3.67469200	-1.46487600	-0.33213400	C	0.58100700	3.14868700	-0.92924500
C	-3.14056300	-0.67092200	0.73516200	C	-0.68202000	3.47384600	-1.48707100
C	-3.95916800	0.34439200	1.30441400	H	0.73764000	1.37544500	-2.07353400
C	-5.23724400	0.56735400	0.83758700	H	-1.13640200	4.42865000	-1.23338700
H	-3.23540100	-3.08601900	-1.70228000	H	-0.88032600	3.11363000	-2.49814200
H	-6.77297000	-0.03542000	-0.57594700	F	1.52968000	4.08857000	-0.66860900
H	-5.39313400	-1.82368400	-1.59690800	F	0.12996000	3.25280500	1.01189700
C	-2.83682600	-2.46404500	-0.90310700	P	-1.33706300	-0.57406800	0.33330500
C	-1.81131400	-0.89909800	1.16986800	C	-2.82687900	-1.63343100	0.02065000
H	-3.55049600	0.95055600	2.11006800	C	-4.08849100	-1.03673200	-0.12473300
H	-5.84762500	1.35273700	1.27697800	C	-2.73279800	-3.03623500	-0.03211000
C	-0.98223800	-1.83944400	0.57017100	C	-5.22792800	-1.82408200	-0.31568300
C	-1.54505700	-2.64515300	-0.47247200	H	-4.17438700	0.04466500	-0.09794800
H	-1.42021800	-0.28266400	1.97391300	C	-3.87166300	-3.81927100	-0.22485600
H	-0.93337600	-3.40970900	-0.93790100	H	-1.76802100	-3.52192900	0.07668400
C	0.44201200	-1.92082400	0.97133200	C	-5.12441900	-3.21514300	-0.36746900
C	1.19801300	-3.22111600	0.85083400	H	-6.19637700	-1.34325500	-0.43006500
C	1.86236700	-3.16584300	-0.48329400	H	-3.77902500	-4.90190600	-0.26386000
H	0.62757600	-1.43547100	1.93139500	H	-6.01084800	-3.82569500	-0.52072800
H	2.89070000	-3.53734600	-0.49763000	C	-0.04033900	-1.65678600	-0.41820700
H	1.26385300	-3.60363300	-1.28681900	C	0.96349500	-2.36561900	0.25470600
F	2.16217900	-3.26468900	1.86220700	C	-0.11209300	-1.76876300	-1.82025700
F	0.40805600	-4.36959000	1.08365300	C	1.85000200	-3.18764100	-0.44934000
Pd	1.64712200	-1.09101800	-0.55580700	H	1.07907000	-2.28280500	1.32750700
Cl	3.12995400	-0.83834500	-2.55094000	C	0.77000600	-2.58853800	-2.52170800
TS28				H	-0.87108200	-1.20891000	-2.36228200
C	6.30793600	-1.45620300	0.78751100	C	1.75321800	-3.30899900	-1.83487600
C	5.60633200	-0.45222300	1.42252400	H	2.62734200	-3.71953000	0.09222600
C	4.44969300	0.11743700	0.82708000	H	0.69116600	-2.66347600	-3.60336200
C	4.01291100	-0.36806900	-0.44935600	H	2.44421700	-3.94827000	-2.37806300
C	4.76186600	-1.40001100	-1.08072700	C	-1.20481800	-0.58301300	2.23233700
C	5.88166400	-1.93268900	-0.47812700	C	-1.28890300	-1.98204300	2.86673300
H	4.02172700	1.52854700	2.41540100	H	-1.22467400	-1.88145600	3.95865100
H	7.19143300	-1.88443700	1.25428800	H	-2.24020800	-2.47150800	2.63454000
H	5.93064200	-0.08159200	2.39277600	H	-0.48342800	-2.65009400	2.55131500
C	3.69691600	1.15473400	1.44631300	C	0.09636200	0.14006100	2.62788100
C	2.84835300	0.18797400	-1.03822200	H	0.11613500	1.15985500	2.23084300
H	4.42835300	-1.76696700	-2.04814200	H	0.15536100	0.19843700	3.72369700
H	6.44283800	-2.72210100	-0.97205800	H	0.99358400	-0.37525900	2.27465600
C	2.12456700	1.19590100	-0.41877400	C	-2.40037800	0.25420500	2.73587900
C	2.57706000	1.67928200	0.84990700	H	-2.33570000	0.34274700	3.82871900

H	-2.39920300	1.26175600	2.30900000	C	-0.22117900	1.98297300	-1.48901900
H	-3.36047900	-0.21697500	2.49605600	C	-2.31618800	2.78078200	0.15783400
Pd	-1.22818100	1.61977500	-0.51723200	H	-1.32294600	1.71355700	1.71880500
Cl	-3.56179700	2.39954700	-0.28035700	C	-1.25986800	2.75438000	-2.00837500
INT40				H	0.59060600	1.67621400	-2.14347600
C	-6.35160900	0.93657700	0.72693000	C	-2.30886300	3.16780300	-1.18143300
C	-5.43800700	0.13361300	1.37778500	H	-3.14160700	3.06609300	0.80426300
C	-4.27889400	-0.34295300	0.70863600	H	-1.24772800	3.03332600	-3.05908000
C	-4.07010900	0.02524200	-0.66060300	H	-3.12139900	3.76741900	-1.58262200
C	-5.03307800	0.84861900	-1.30600200	C	1.41075600	0.71538900	2.32221600
C	-6.14795000	1.29576700	-0.62953600	C	1.37113800	2.15497100	2.86392700
H	-3.45677900	-1.43019000	2.39235400	H	1.43491800	2.11724300	3.95983500
H	-7.23242100	1.29730200	1.25218500	H	2.22005100	2.74658800	2.50673700
H	-5.59103900	-0.14374700	2.41859200	H	0.45206900	2.68825900	2.60558300
C	-3.30131100	-1.15472400	1.35100800	C	0.31698900	-0.15857600	2.97022900
C	-2.88888200	-0.41025600	-1.31528000	H	0.33685300	-1.18701700	2.58260100
H	-4.86745600	1.13011800	-2.34352500	H	0.49648800	-0.18635000	4.05474100
H	-6.87426300	1.92892700	-1.13297200	H	-0.69037100	0.24213200	2.82260100
C	-1.94867400	-1.18900800	-0.66523500	C	2.78345300	0.09822600	2.66225100
C	-2.16904100	-1.57381800	0.69417800	H	2.90827200	0.09923100	3.75346800
H	-2.71972400	-0.09866700	-2.34352700	H	2.86000700	-0.93288000	2.30799800
H	-1.39379900	-2.16483000	1.19088800	H	3.61143800	0.67212600	2.23033400
C	-0.70693000	-1.58216900	-1.36916000	Pd	1.25146900	-1.60559500	-0.39666800
C	-0.26657200	-2.94113800	-1.39621000	Cl	3.61890500	-2.24906500	-0.02708100
C	0.99172000	-3.29933100	-1.85504000	HF			
H	-0.47536100	-1.00611100	-2.26487800	F	0.00000000	0.00000000	0.09397100
H	1.36692400	-4.29499700	-1.63916500	H	0.00000000	0.00000000	-0.84573600
H	1.45027700	-2.75375500	-2.67453700	[Pd(II)(allyl)Cl]			
F	-0.97515900	-3.85691000	-0.71097100	Pd	-0.01231600	-0.26390300	-0.03879100
F	0.33091800	-2.90767200	1.60811300	Cl	-2.32469000	0.15301500	0.02282900
P	1.25055400	0.60613100	0.42502800	C	1.96162300	0.48890800	-0.39486300
C	2.61846100	1.69541000	-0.19922900	H	2.23067800	0.58188300	-1.44492600
C	3.77740700	1.13054700	-0.75001800	C	2.11135100	-0.72872500	0.28260500
C	2.51929100	3.09804400	-0.13068700	H	2.12456300	-0.76842000	1.37121400
C	4.81747100	1.94538100	-1.20803800	C	1.13323600	1.46918900	0.23369600
H	3.86909600	0.05186700	-0.81115500	H	0.79946600	2.33280300	-0.33764000
C	3.55837600	3.90907500	-0.58749200	H	2.52751700	-1.59005400	-0.23559000
H	1.62245700	3.56167300	0.26716200	H	1.16679300	1.60584600	1.31463300
C	4.71334600	3.33446600	-1.12718700	Pd-^{t}BuPPh$_2$			
H	5.70763400	1.48684900	-1.63167000	P	-0.01947600	-0.29244300	0.13780300
H	3.46296000	4.99031300	-0.52601100	C	1.55900200	0.64153800	-0.15360200
H	5.52152100	3.96684100	-1.48623800	C	2.54220900	0.01864100	-0.94138600
C	-0.19982800	1.61306400	-0.13037500	C	1.85404600	1.90314300	0.39716900
C	-1.27571800	2.00550900	0.67861300	C	3.77859900	0.62755400	-1.16902200

H	2.33082700	-0.95575500	-1.37591400
C	3.08833800	2.51411200	0.16793000
H	1.12139300	2.42338300	1.00174800
C	4.05588200	1.87774900	-0.61364400
H	4.52191600	0.12353700	-1.78127700
H	3.29175800	3.48955300	0.60217700
H	5.01652700	2.35478100	-0.78947300
C	-1.39088800	0.90373600	-0.23273300
C	-2.70930300	0.41275200	-0.15167800
C	-1.20667600	2.23162700	-0.65042800
C	-3.80223300	1.23539000	-0.42204800
H	-2.88109200	-0.62924800	0.10094400
C	-2.30269500	3.05139800	-0.93705800
H	-0.20995400	2.63717100	-0.77422800
C	-3.60349100	2.56323000	-0.81180500
H	-4.80912300	0.83336100	-0.34348900
H	-2.13209000	4.07491100	-1.26131600
H	-4.45369300	3.20341200	-1.03184100
C	-0.06927000	-0.52362800	2.04790900
C	-1.32042100	-1.34506800	2.41290100
H	-1.27233800	-1.61591900	3.47615700
H	-2.24168300	-0.77324800	2.26322100
H	-1.38721200	-2.27002800	1.82836900
C	1.18859700	-1.32705800	2.42688000
H	1.21738600	-2.29277200	1.90791200
H	2.10898700	-0.78287200	2.18772000
H	1.18543800	-1.52152800	3.50766100
C	-0.10172500	0.79728900	2.83560400
H	-0.28591900	0.57877800	3.89603100
H	0.84931600	1.33244200	2.77857800
H	-0.90054900	1.46393800	2.49097600
Pd	-0.22038200	-2.19090600	-0.99958500
C	-2.98698400	-1.98587400	0.00050700
Pd-EtOAc			
H	-2.52333500	-2.42376100	0.89058700
H	-2.52389300	-2.42446400	-0.88950300
H	-4.05237900	-2.24158500	0.00093400
C	-2.83211400	-0.47941200	-0.00019600
H	-3.28445000	-0.03271900	-0.89169400
H	-3.28373100	-0.03187800	0.89122600
O	-1.40247500	-0.20013900	-0.00095400
C	-0.93990000	1.04891800	-0.00010400
O	0.28029700	1.22457400	0.00058500
C	-1.89499500	2.20971200	0.00005400
H	-2.54223300	2.17900300	-0.88359800
H	-2.54029900	2.18005100	0.88519000
H	-1.32370900	3.13838100	-0.00099500
Pd	1.80381300	-0.28909900	-0.00001600