

Supporting Information

Catalytic Synthesis of 9-*cis*-Retinoids: Mechanistic Insights

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I. HPLC analysis

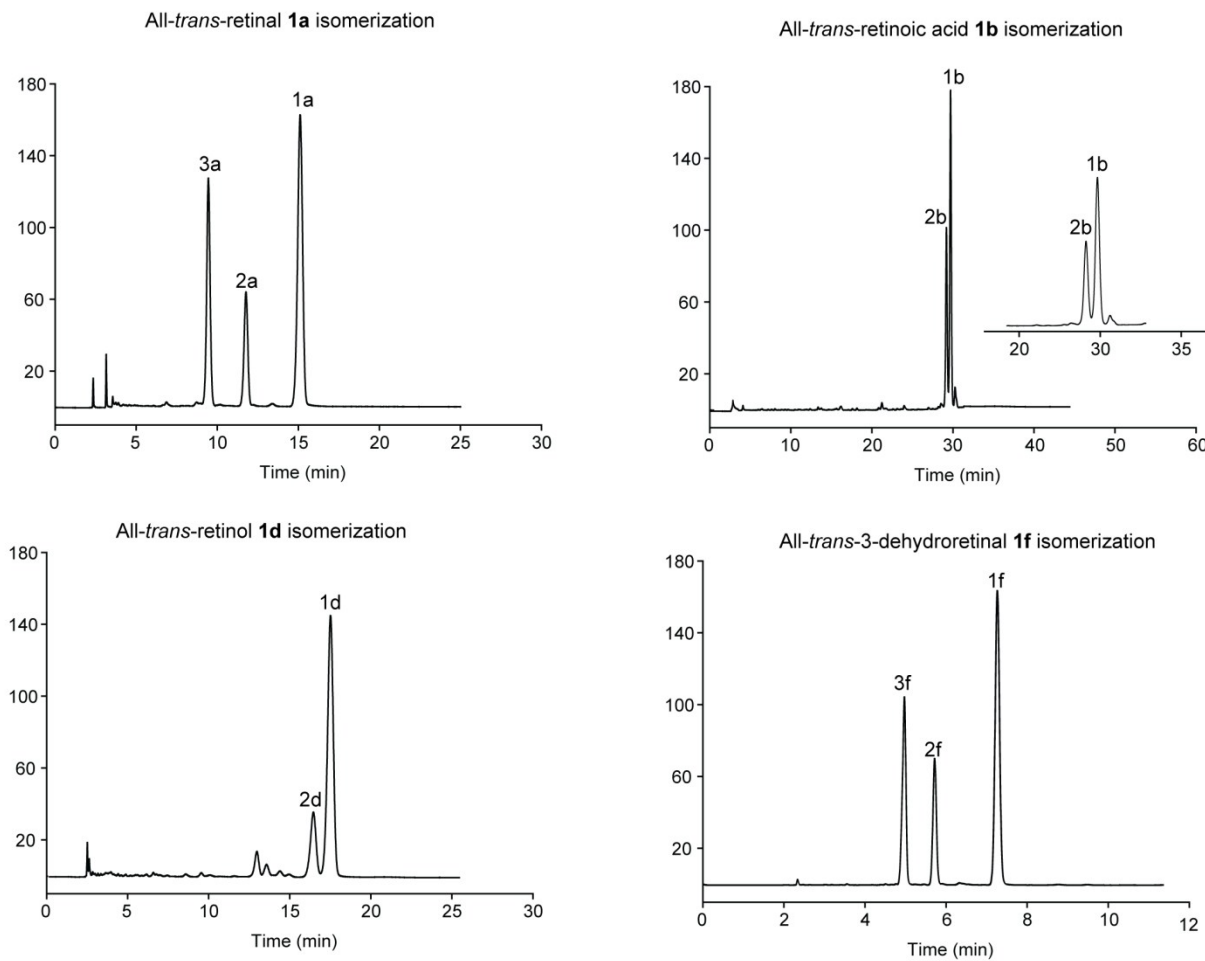


Figure S1. Representative HPLC chromatograms of a mixture of all-*trans*-retinal **1a**, all-*trans*-retinoic acid **1b**, all-*trans*-retinol **1d** and all-*trans*-3-dehydroretinal **1f**, obtained following traditional heat treatment.

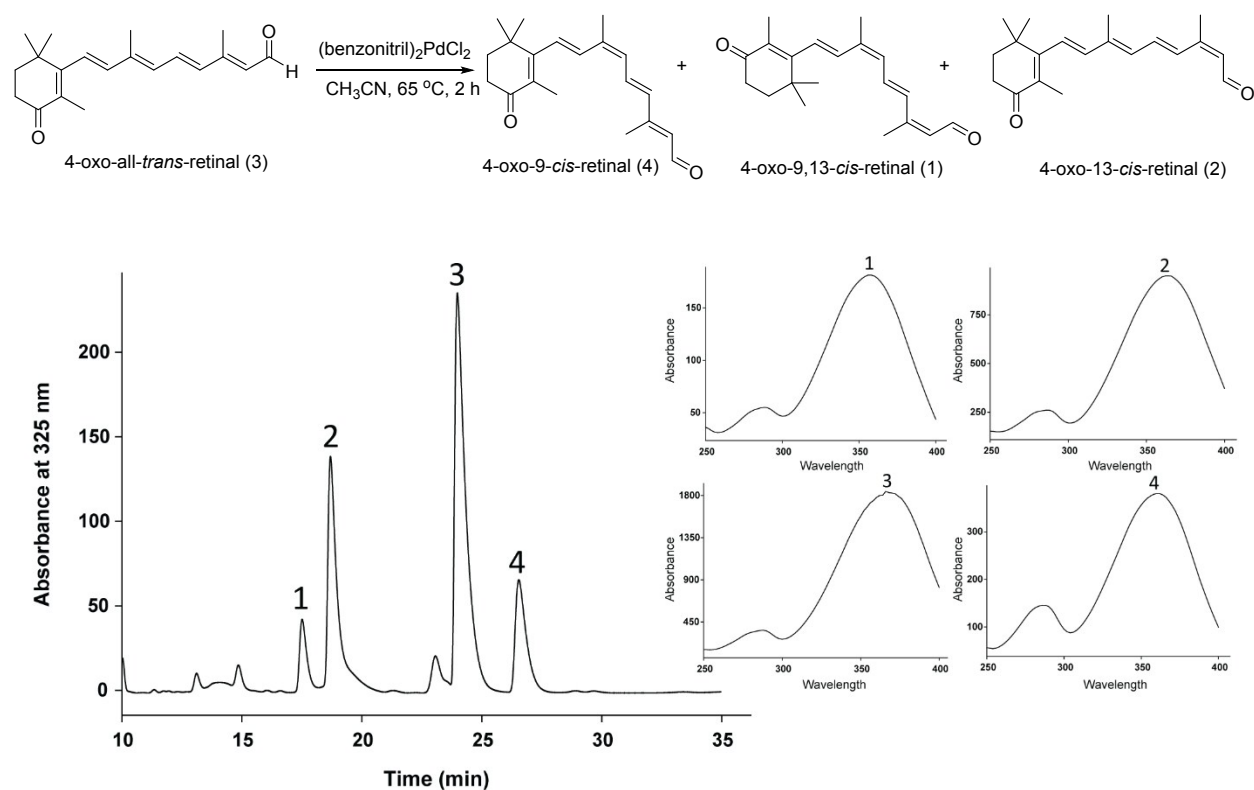
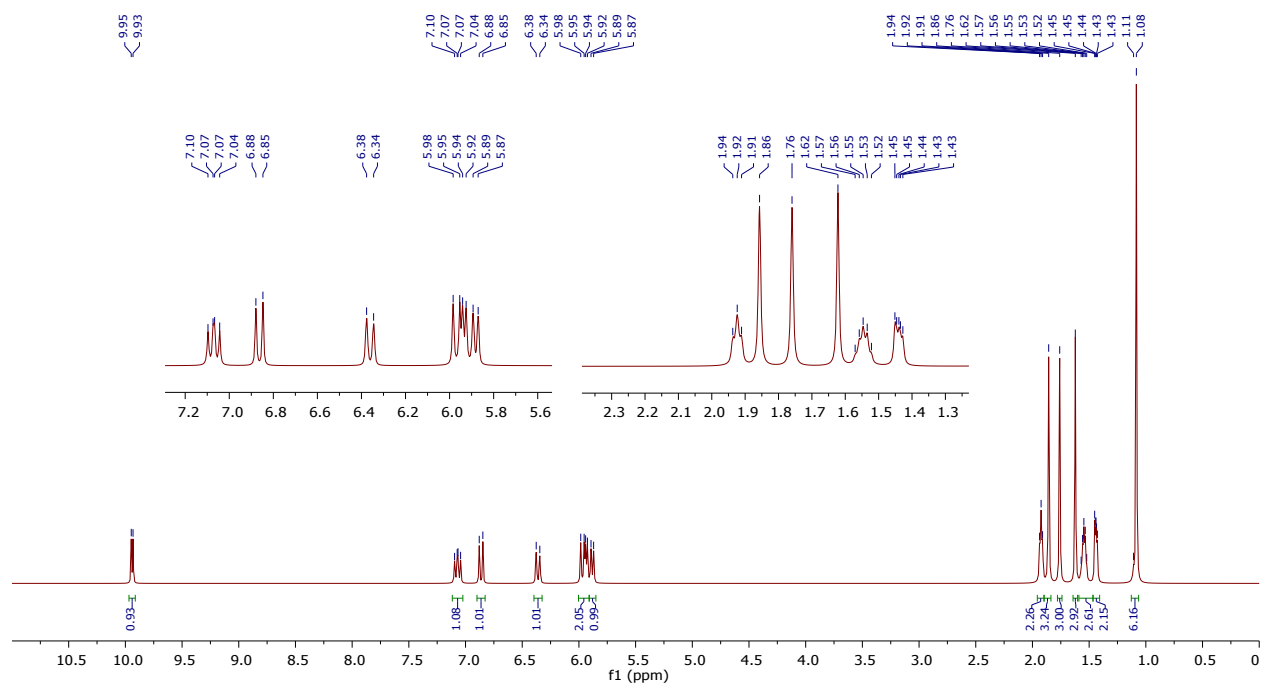


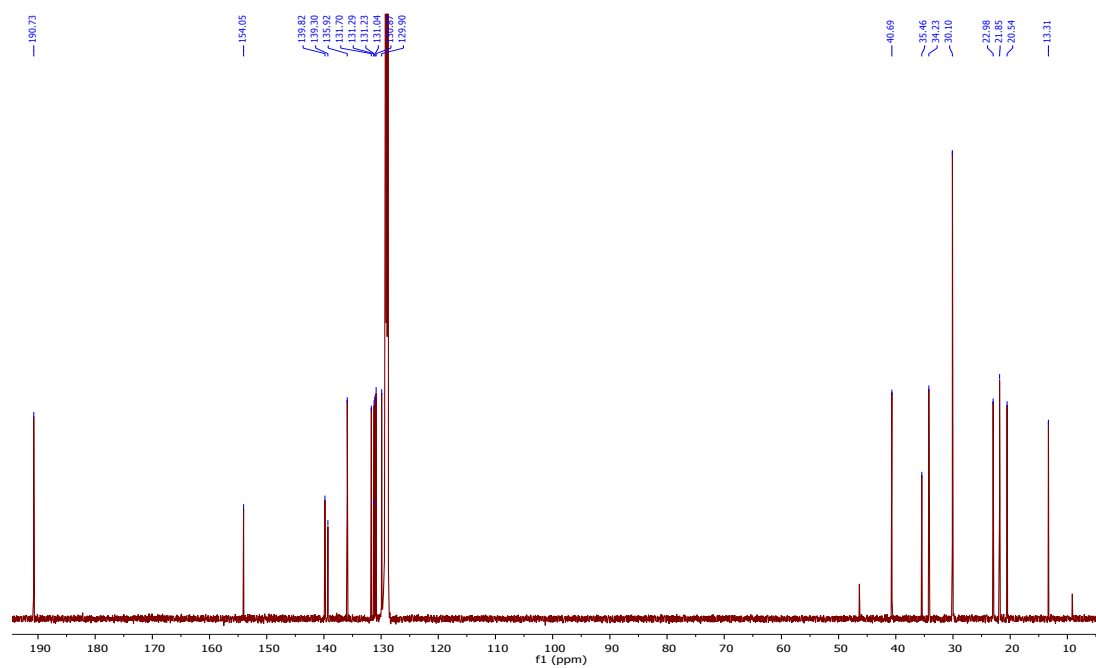
Figure S2. Representative HPLC chromatograms of a mixture of 4-keto-retinal isomers obtained following traditional heat treatment.

II. NMR spectra

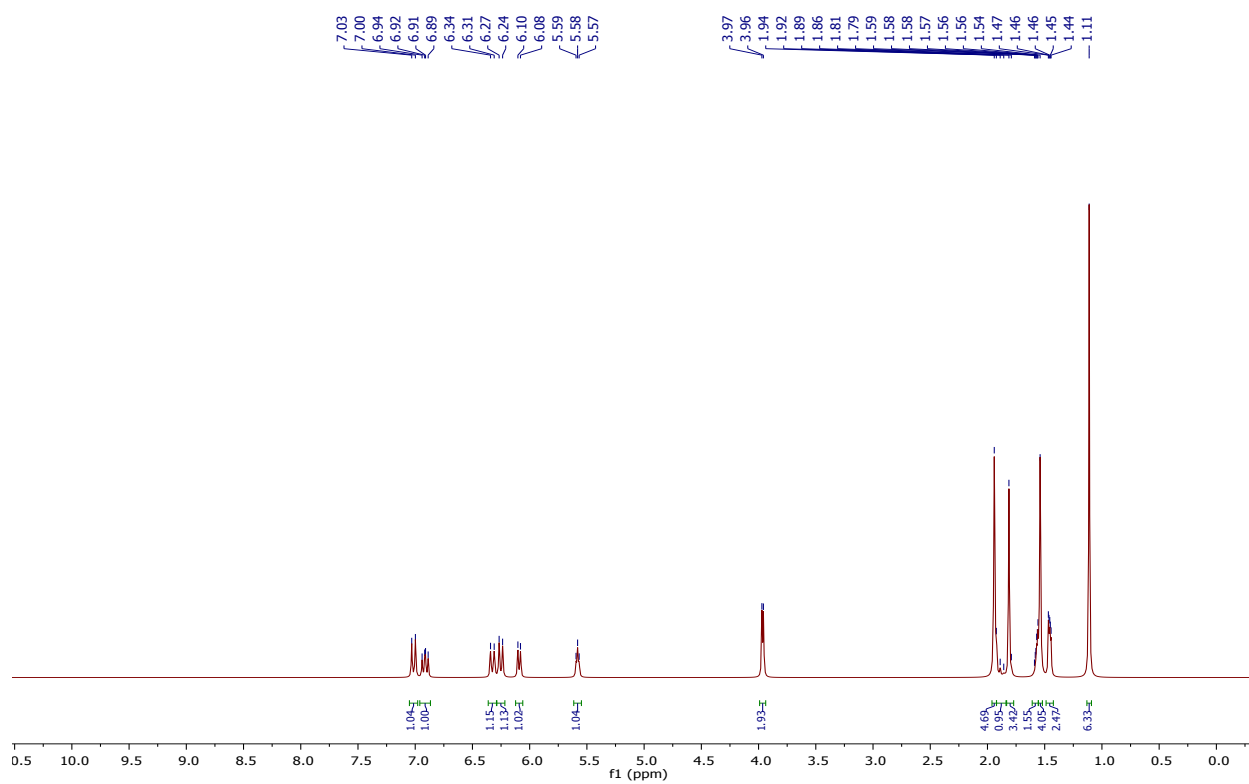
9-*cis*-retinal **2a**- ¹H-NMR



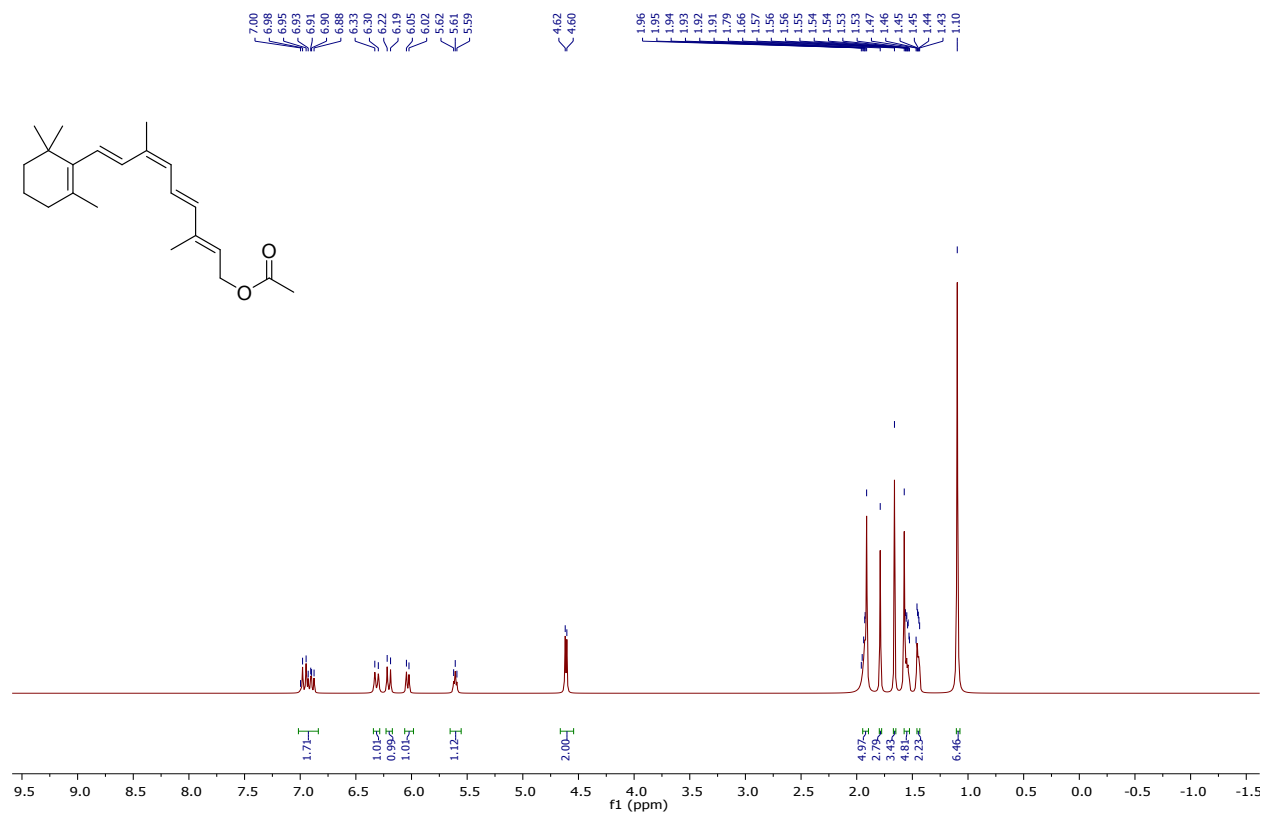
9-*cis*-retinal **2a**- ¹³C-NMR



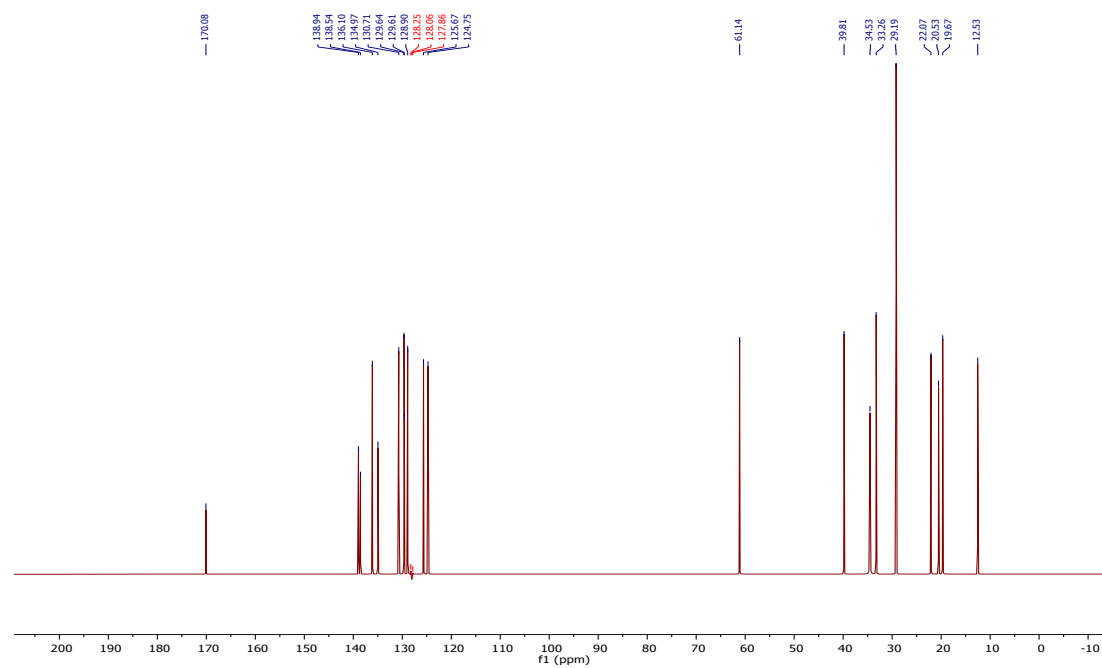
9-*cis*-retinol **2b**- ¹H-NMR



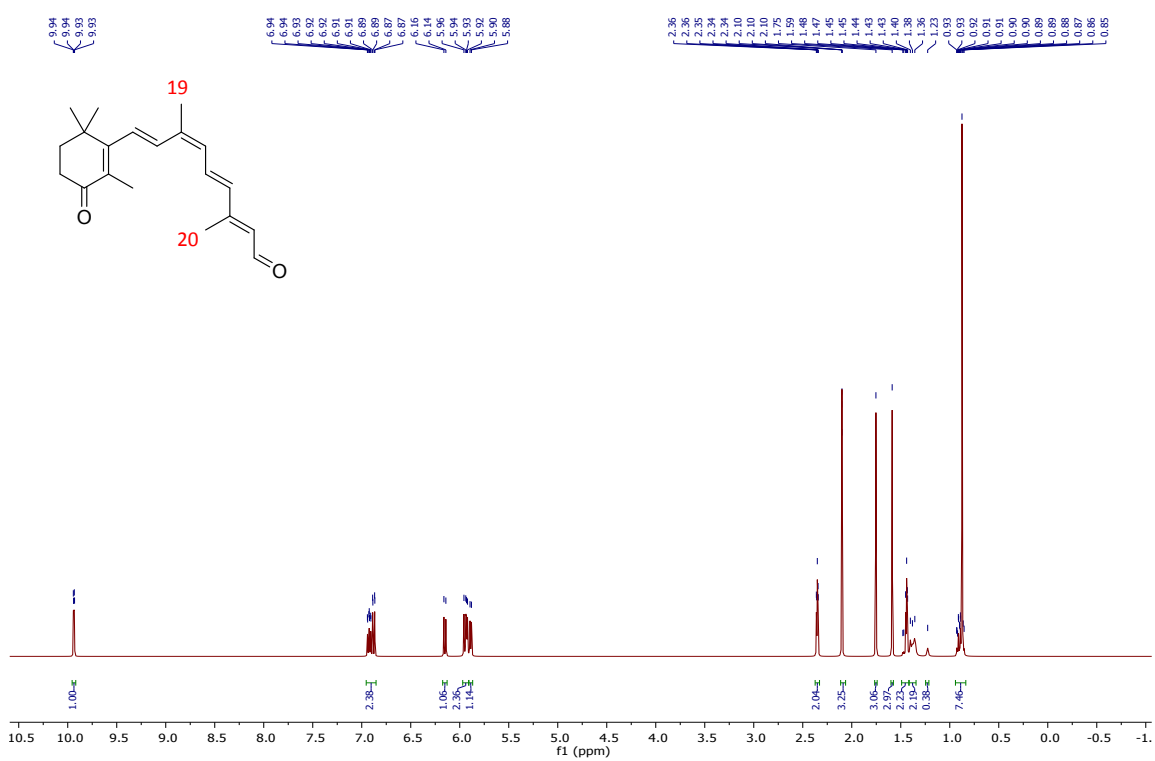
9-*cis*-retinyl acetate **2c**- ¹H-NMR



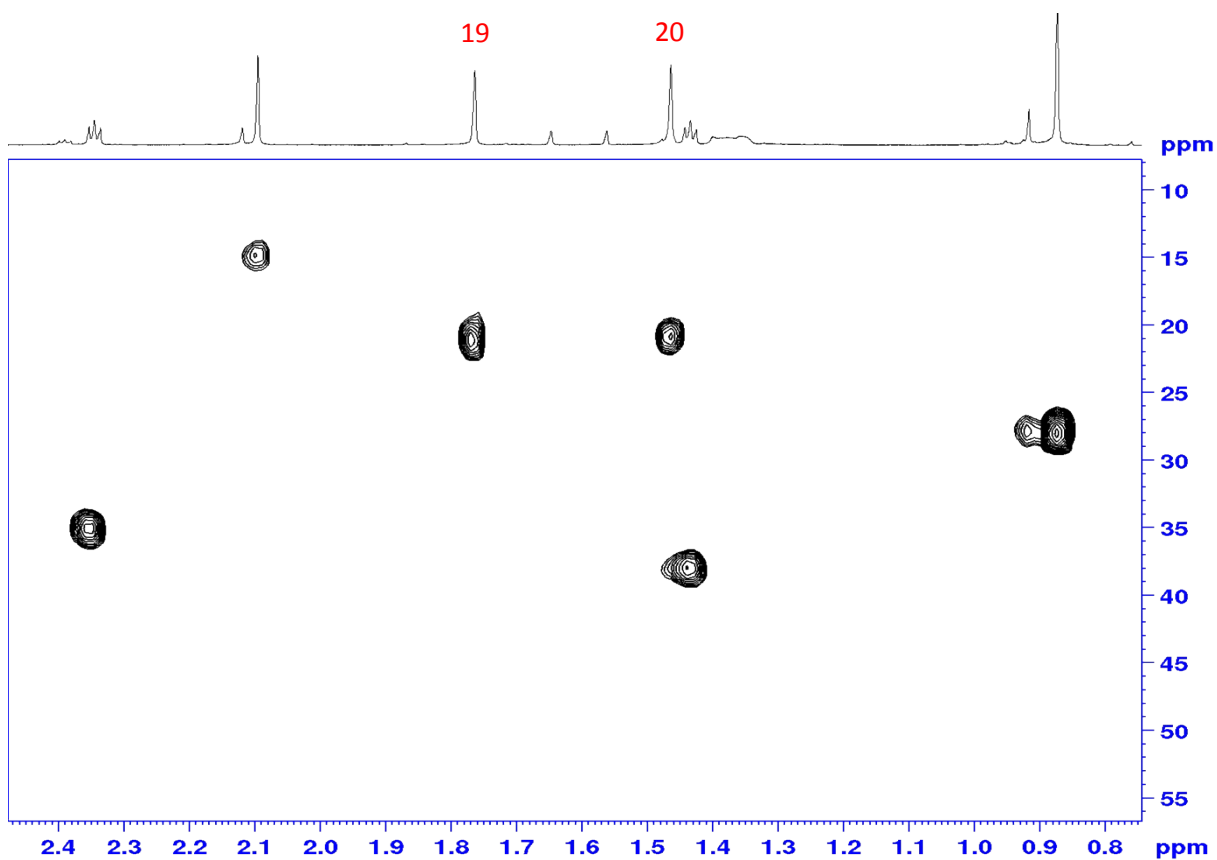
9-*cis*-retinyl acetate **2c**- ¹³C-NMR



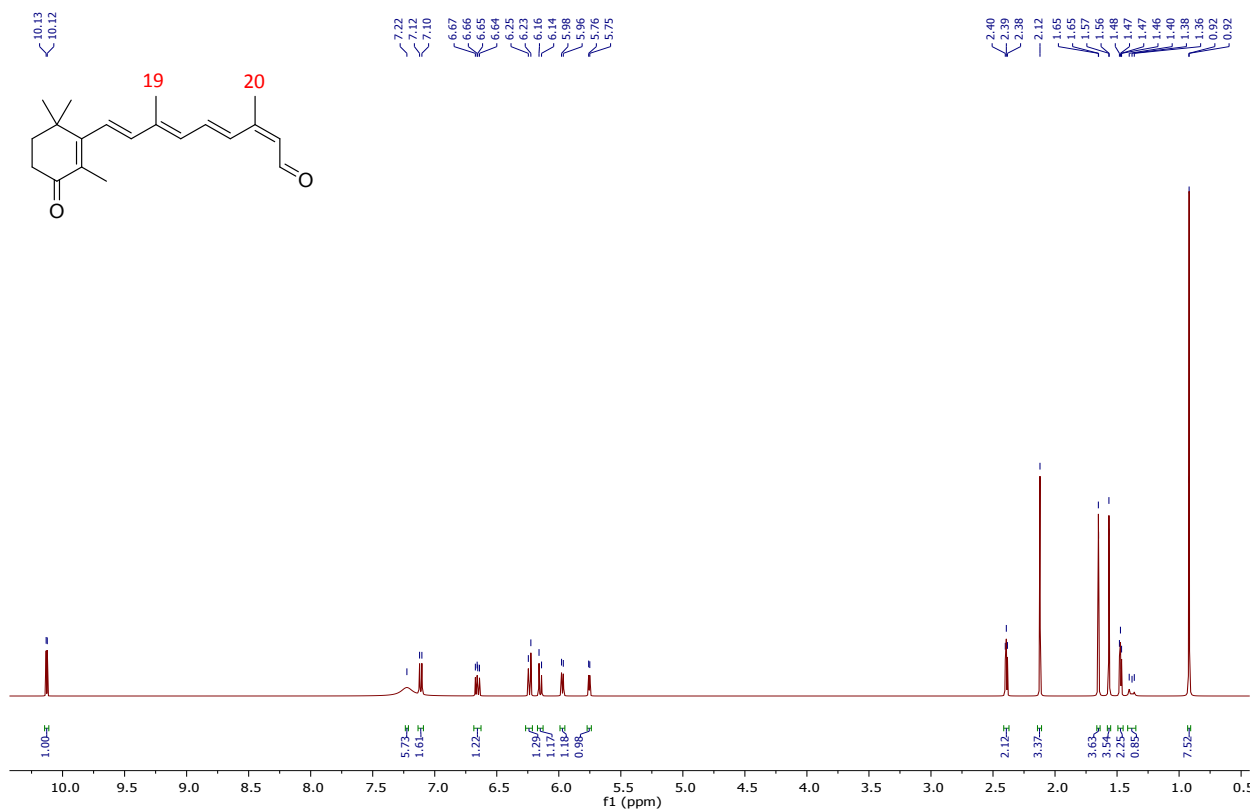
4-keto-9-*cis*-retinal -1H-NMR



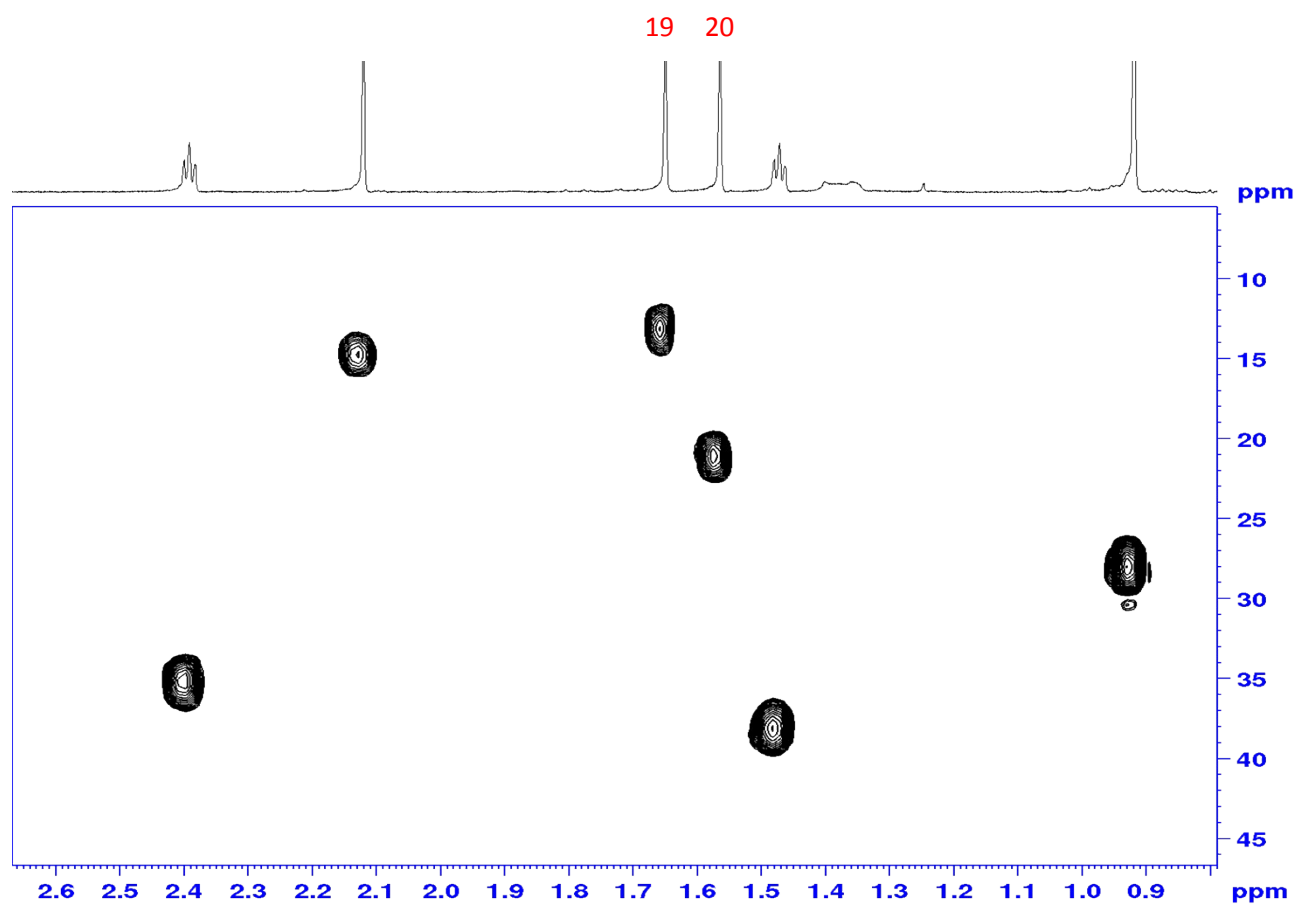
4-keto-9,13-*dicis*-retinal -HSQC



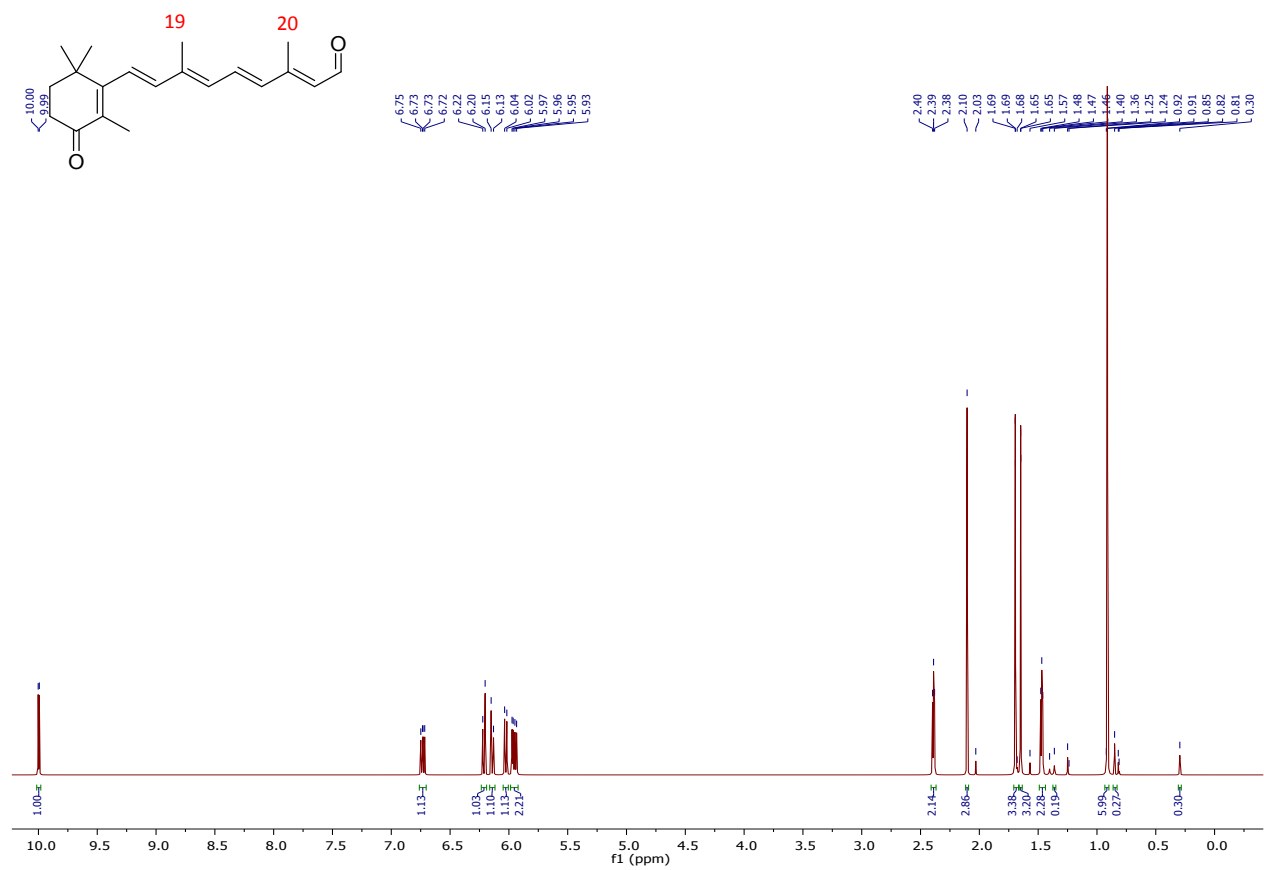
4-keto-13-*cis*-retinal -1H-NMR



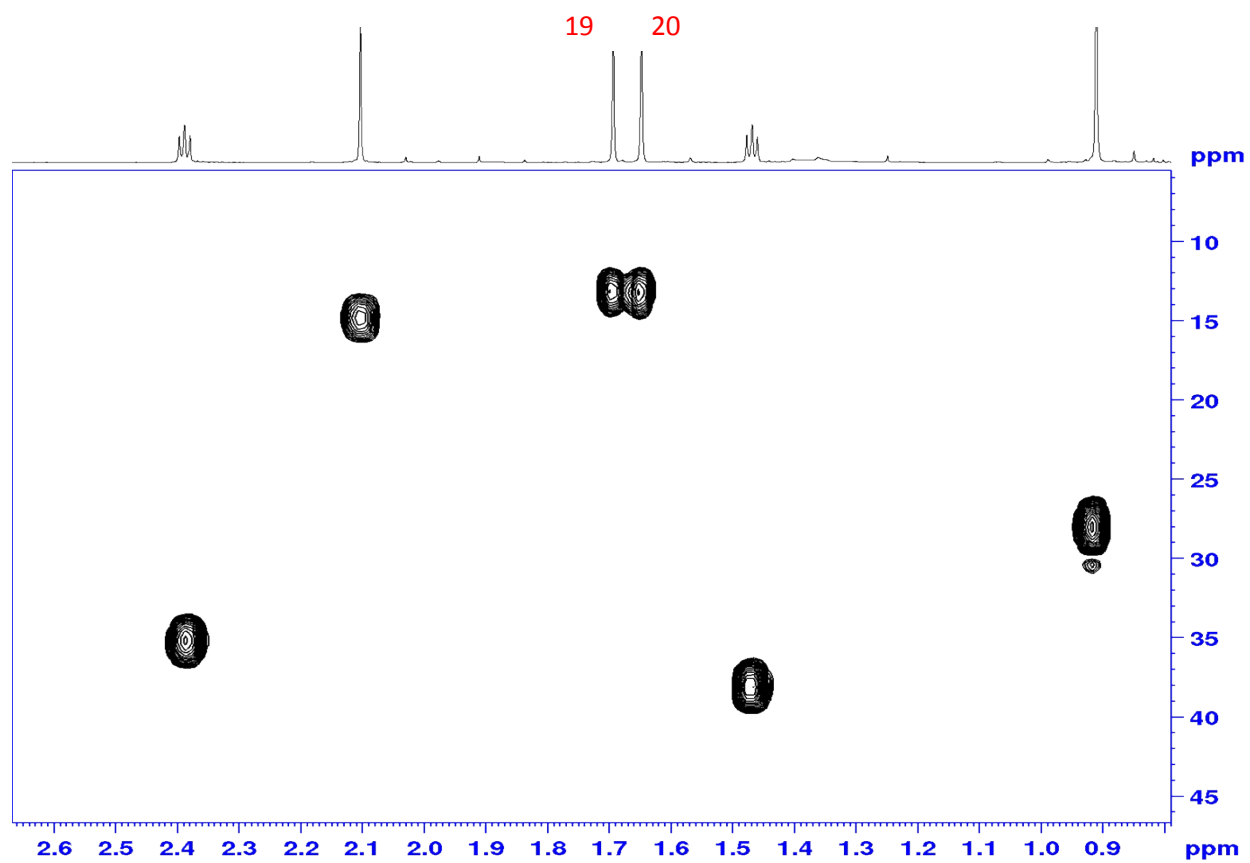
4-keto-13-*cis*-retinal -HSQC



4-keto-all-*trans*-retinal - ¹H-NMR

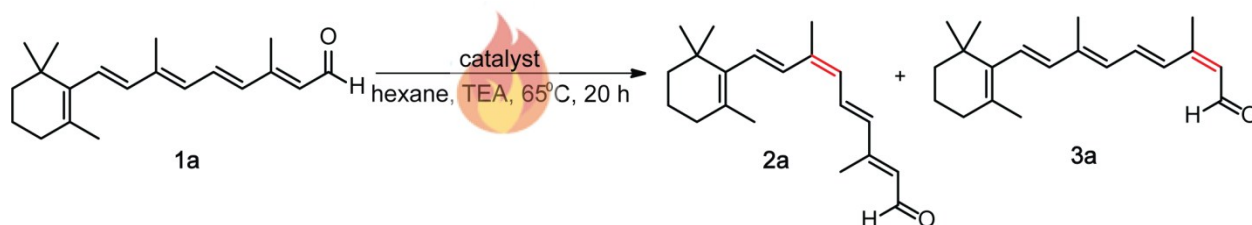


4-keto-all-*trans*-retinal -HSQC



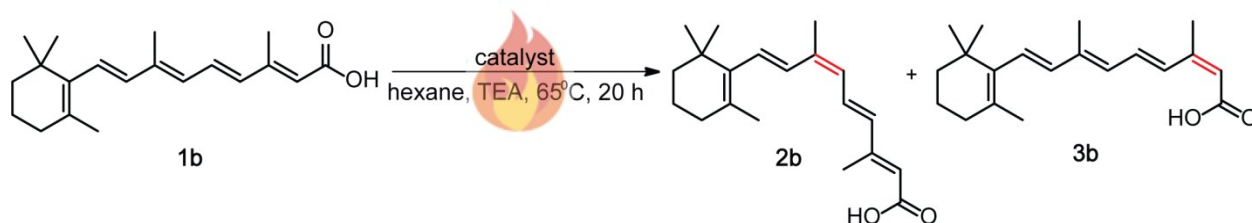
III. Extended results

Table S1. all-*trans*-retinal **1a** isomerization. Reactions were performed with 0.1 mmol **1a**, 2 mol % catalysts and 0.2 μ mol TEA at 65 °C for 20 h in C₆H₁₄ under N₂. Each yield is averaged from $n \geq 2$ reactions, as determined by normal phase HPLC.



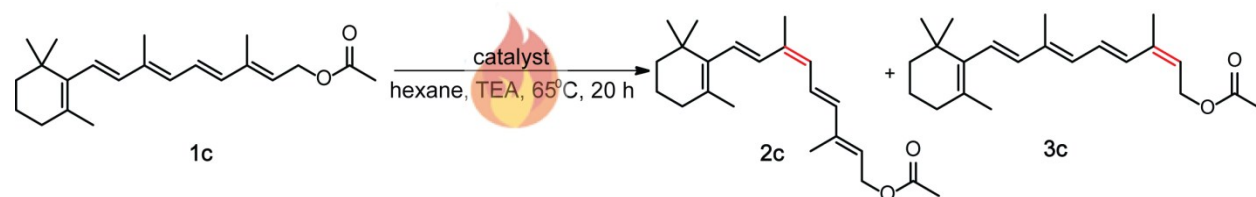
Entry	Catalyst (No)	9- <i>cis</i> - 2a (%)	13- <i>cis</i> - 3a (%)	all- <i>trans</i> - 1a (%)
1	Pd (I)	15.3	23.8	60.9
2	Pd (II)	15.8	20.4	63.8
3	Pd (III)	14.5	23.7	61.8
4	Pd (IV)	15.3	22.7	62.0
5	Pd (V)	14.9	23.6	61.5
6	Pd (VI)	7.1	13.9	79.4
7	Pd (VII)	15.1	18.3	66.5
8	Pd (VIII)	6.4	7.1	86.5
9	Pd (IX)	5.8	10.7	83.5
10	Pd (X)	6.2	8.0	85.8
11	Pd (XI)	5.6	9.4	85.0
12	Pt (XII)	2.1	4.1	93.4
13	Pt (XIII)	4.9	7.1	88.1
14	Pt (XIV)	2.9	3.7	93.0
15	Pt (XV)	0.7	2.3	96.3
16	Ru (XVI)	4.3	5.0	90.3
17	Ru (XVII)	trace	5.4	90.2
18	Ir (XVIII)	5.4	8.4	86.2
19	Au (XIX)	7.2	5.8	87.0
20	Rh (XX)	5.3	8.3	86.4

Table S2. all-*trans*-retinoic acid **1b** isomerization. Reactions were performed with 0.1 mmol **1b**, 2 mol % catalysts and 0.2 μmol TEA at 65 °C for 24 h in C₆H₁₄ under N₂. Each yield is averaged from n ≥ 2 reactions, as determined by reverse phase HPLC.



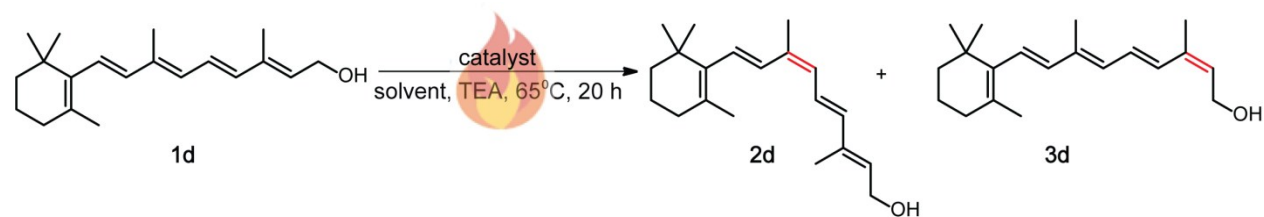
Entry	Catalyst (No)	9- <i>cis</i> - 2b (%)	13- <i>cis</i> - 3b (%)	all- <i>trans</i> - 1b (%)
1	Pd (I)	26.1	trace	73.2
2	Pd (II)	4.7	trace	35.0
3	Pd (III)	34.0	trace	59.3
4	Pd (IV)	15.2	trace	63.9
5	Pd (V)	25.2	1.7	72.8
6	Pd (VI)	trace	trace	100.0
7	Pd (VII)	32.1	trace	67.9
8	Pd (VII)	trace	9.8	90.2
9	Pd (IX)	trace	trace	100.0
10	Pd (X)	trace	trace	100.0
11	Pd (XI)	trace	trace	100.0
12	Pt (XIII)	trace	7.2	92.8
13	Pt (XIV)	trace	6.8	89.8
14	Pt (XV)	trace	15.8	84.5
15	Pt (XVI)	trace	1.9	98.0
16	Ru (XVII)	trace	trace	100.0
17	Ru (XVIII)	trace	3.0	97.0
18	Ir (XIX)	8.0	30.9	61.1
19	Au (XII)	trace	trace	100.0
20	Rh (XX)	14.6	43.9	41.5

Table S3. all-*trans*-retinyl acetate **1c** isomerization. Reactions were performed with 0.1 mmol **1c**, 2 mol % catalysts and 0.2 μ mol TEA at 65 °C for 20 h in C₆H₁₄ under N₂. Each yield is averaged from n $\geq$ 2 reactions, as determined by normal phase HPLC.



Entry	Catalyst (No)	9- <i>cis</i> - 2c (%)	13- <i>cis</i> - 3c (%)	all- <i>trans</i> - 1c (%)
1	Pd (I)	16.6	4.2	77.7
2	Pd (II)	19.3	2.2	77.7
3	Pd (III)	20.3	2.4	75.1
4	Pd (IV)	19.6	2.7	76.6
5	Pd (V)	15.4	2.7	81.6
6	Pd (VI)	trace	4.0	91.1
7	Pd (VII)	19.8	2.3	75.2
8	Pd (VII)	2.1	3.5	94.3
9	Pd (IX)	4.2	2.9	91.9
10	Pd (X)	3.9	2.6	92.8
11	Pd (XI)	1.1	6.2	92.2
12	Pt (XIII)	trace	3.0	96.8
13	Pt (XIV)	trace	3.0	97.0
14	Pt (XV)	trace	3.7	95.1
15	Pt (XVI)	trace	3.2	96.2
16	Ru (XVII)	trace	3.8	94.2
17	Ru (XVIII)	trace	3.0	97.0
18	Ir (XIX)	trace	3.2	95.7
19	Au (XII)	trace	3.0	94.3
20	Rh (XX)	1.1	3.8	92.8

Table S4. all-*trans*-retinol **1d** isomerization. Reactions were performed with 0.1 mmol **1d**, 2 mol % catalysts and 0.2 μ mol TEA at 65 °C for 24 h in C₆H₁₄ under N₂. Each yield is averaged from n $\geq$ 2 reactions, as determined by normal phase HPLC.



Entry	Catalyst (No)	9- <i>cis</i> - 2d (%)	13- <i>cis</i> - 3d (%)	all- <i>trans</i> - 1d (%)
1	Pd (I)	trace	trace	trace
2	Pd (II)	18.0	1.1	78.8
3	Pd (III)	trace	trace	trace
4	Pd (IV)	18.6	1.1	77.7
5	Pd (V)	trace	trace	trace
6	Pd (VI)	trace	trace	trace
7	Pd (VII)	13.7	1.9	82.9
8	Pd (VII)	16.3	4.7	65.9
9	Pd (IX)	10.9	6.5	41.7
10	Pd (X)	trace	trace	trace
11	Pd (XI)	trace	trace	trace
12	Pt (XIII)	2.6	1.6	92.6
13	Pt (XIV)	2.7	10.0	78.4
14	Pt (XV)	trace	trace	trace
15	Pt (XVI)	3.7	2.0	90.6
16	Ru (XVII)	trace	3.0	93.1
17	Ru (XVIII)	5.4	18.8	63.3
18	Ir (XIX)	trace	trace	trace
19	Au (XII)	trace	1.1	96.5
20	Rh (XX)	3.4	6.5	72.9

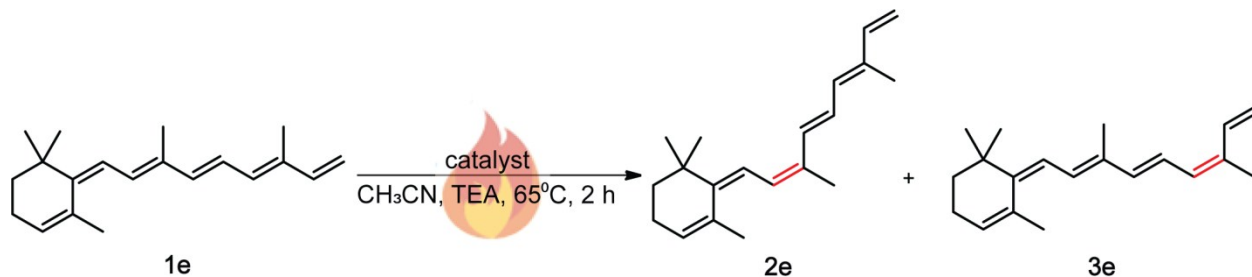
IV. Optimization conditions for retinoid isomerization reactions following conventional heat treatment

Table S5. Optimization of retinoid isomerizations with selected catalysts in several solvents and different periods of time.

Entry	Sub	Cat (No)	Solvent; time (h)	9- <i>cis</i> (%)	13- <i>cis</i> (%)	all- <i>trans</i> (%)	Entry	Sub	Cat (No)	Solvent; time (h)	9- <i>cis</i> (%)	13- <i>cis</i> (%)	all- <i>trans</i> (%)
1	1a	Pd (I)	C ₆ H ₁₄ ; 20	15.3	28.3	51.8	23	1b	Pd (I)	CH ₃ CN; 2	24.3	1.3	56.2
2	1a	Pd (I)	Acetone; 1	12.2	28.1	59.7	24	1b	Pd (XI)	Acetone; 2	14.6	32.9	52.5
3	1a	Pd (I)	Acetone; 3	2.7	23.1	74.2	25	1b	Pd (XI)	CH ₃ CN; 2	14.8	40.1	41.0
4	1a	Pd (I)	CH ₃ CN; 2	16.1	21.7	54.1	26	1b	Pd (XI)	CH ₃ CN; 24	12.3	33.7	54.0
5	1a	Pd (V)	Acetone; 1	16.6	23.4	54.1	27	1b	Pd (XI)	DCM; 24	13.8	32.0	54.2
6	1a	Pd (V)	Acetone; 3	15.9	28.6	55.5	28	1c	Pd (I)	C ₆ H ₁₄ ; 20	16.6	4.2	77.7
7	1a	Pd (V)	CH ₃ CN; 2	18.1	27.8	53.9	29	1c	Pd (I)	Acetone; 2	13.1	6.0	80.9
8	1a	Pd (IV)	Acetone; 1	12.6	25.3	58.7	30	1c	Pd (I)	CH ₃ CN; 2	19.6	2.3	78.2
9	1a	Pd (IV)	Acetone; 3	16.8	28.0	55.2	31	1c	Pd (V)	THF; 24	18.7	8.1	71.4

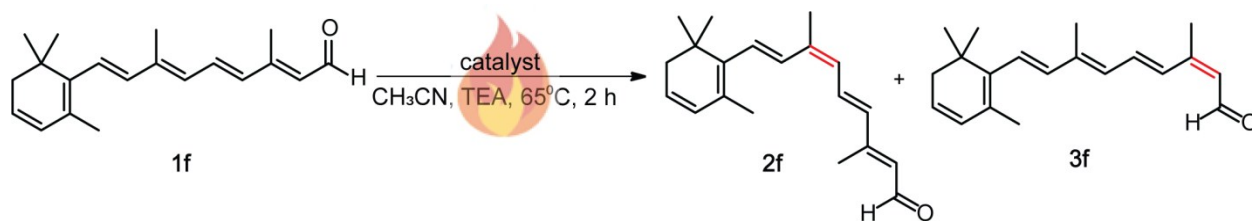
10	1a	Pd (IV)	CH ₃ CN; 2	17.5	27.3	56.0	32	1c	Pd (V)	CH ₃ CN; 2	19.6	6.0	72.4
11	1a	Au (XII)	Acetone; 1	trace	trace	100	33	1c	Pd (IV)	THF; 24	19.0	2.6	78.4
12	1a	Au (XII)	Acetone; 3	trace	trace	100	34	1c	Pd (IV)	CH ₃ CN; 2	20.1	2.7	76.0
13	1a	Au (XII)	CH ₃ CN; 2	3.1	8.3	87.5	35	1c	Pd (IV)	DCM; 2	18.9	2.1	77.6
14	1a	Ru (XVII)	Acetone; 3	trace	trace	100	36	1c	Pd (IV)	Acetone; 24	19.5	2.6	77.8
15	1a	Ru (XVIII)	CH ₃ CN; 2	4.2	5.0	88.3	37	1d	Pd (IV)	THF; 24	18.8	trace	trace
16	1b	Pd (VIII)	Acetone; 24	2.9	14.7	35.3	38	1d	Pd (IV)	Acetone; 24	trace	trace	trace
17	1b	Pd (VIII)	DCM; 24	trace	trace	trace	39	1d	Pd (IV)	DCM; 24	trace	trace	trace
18	1b	Pd (VIII)	CH ₃ CN; 2	8.3	30.8	61.1	40	1d	Pd (IV)	CH ₃ CN; 2	18.9	2.1	77.6
19	1b	Pd (VIII)	EtOH; 24	4.6	21.4	52.7	41	1d	Pd (I)	C ₆ H ₁₄ ; 20	trace	trace	trace
20	1b	Pd (I)	C ₆ H ₁₄ ; 20	26.1	trace	73.2	42	1f	Pd (I)	CH ₃ CN; 2	18.1	27.7	54.2
21	1b	Pd (I)	Acetone; 2	9.6	5.1	66.3	43	1g	Pd (I)	CH ₃ CN; 2	16.3	11.7	53.8
22	1c	Pd (V)	DCM; 24	19.5	6.0	72.4	44						

1 Table S6. all-*trans*-anhydroretinol **1e** isomerization. Reactions were performed with 0.1 mmol **1f**,
 2 2 mol % catalysts and 0.2 μmol TEA at 65 °C for 2 h in CH₃CN under N₂. Each yield is
 3 averaged from n ≥ 2 reactions, as determined by reverse phase HPLC. **1e** was obtained as a
 4 mixture of all-*trans*, 8-*cis* and 12-*cis*. The reaction was conducted on a small set of catalysts due
 5 to limitations in product separation.



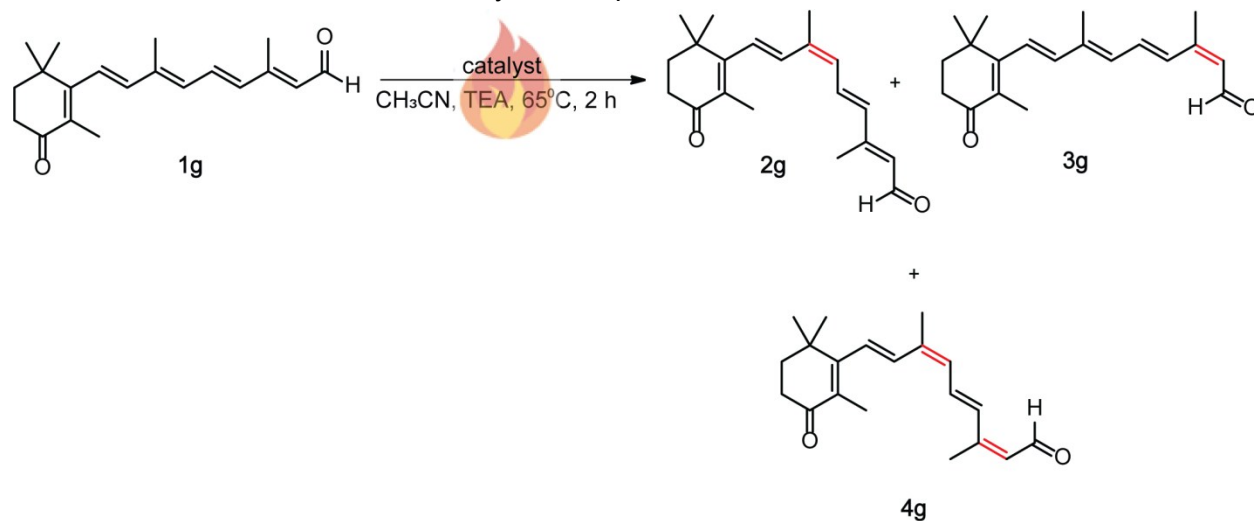
Entry	Catalyst (No)	8- <i>cis</i> - 2e (%)	12- <i>cis</i> - 3e (%)	all- <i>trans</i> - 1e (%)
1	Pd (I)	10.6	2.1	75.5
2	Pd (XVI)	trace	3.7	76.1
3	Pd (IX)	trace	4.5	73.2
4	Pt (XIII)	trace	trace	98.6
5	Ru (XVIII)	trace	trace	99.0
6	Ir (XIX)	trace	5.7	96.8
7	Au(XII)	trace	3.1	95.0

Table S7. all-*trans*-3-dehydro retinal **1f** isomerization. Reactions were performed with 0.1 mmol **1f**, 2 mol % catalysts and 0.2 μ mol TEA at 65 °C for 2 h in CH₃CN under N₂. Each yield is averaged from n $\geq$ 2 reactions, as determined by normal phase HPLC.



Entry	Catalyst (No)	9- <i>cis</i> - 2f (%)	13- <i>cis</i> - 3f (%)	all- <i>trans</i> - 1f (%)
1	Pd (I)	18.1	27.7	54.2
2	Pd (II)	18.8	24.4	56.8
3	Pd (III)	17.6	27.8	54.6
4	Pd (IV)	17.8	26.5	55.7
5	Pd (V)	17.9	27.6	54.5
6	Pd (VI)	trace	trace	91.1
7	Pd (VII)	16.8	27.6	55.6
8	Pd (VII)	17.5	27.4	55.1
9	Pd (IX)	18.2	27.8	53.9
10	Pd (X)	18.4	26.8	54.7
11	Pd (XI)	trace	trace	89.9
12	Pt (XIII)	1.2	3.6	95.2
13	Pt (XIV)	1.2	5.6	95.1
14	Pt (XV)	3.1	8.3	88.5
15	Pt (XVI)	3	9	88.1
16	Ru (XVII)	3.8	8	88.2
17	Ru (XVIII)	trace	trace	96.5
18	Ir (XIX)	16.8	27.6	55.6
19	Au (XII)	3	9	88.1
20	Rh (XX)	9.8	11.92	54.6

33 Table S8. all-*trans*-4-ketoretinal **1g** isomerization. Reactions were performed with 0.1 mmol **1g**,
 34 2 mol % catalysts and 0.2 μ mol TEA at 65 °C for 2 h in CH₃CN under N₂. Each yield is averaged
 35 from n $\geq$ 2 reactions, as determined by normal phase HPLC.



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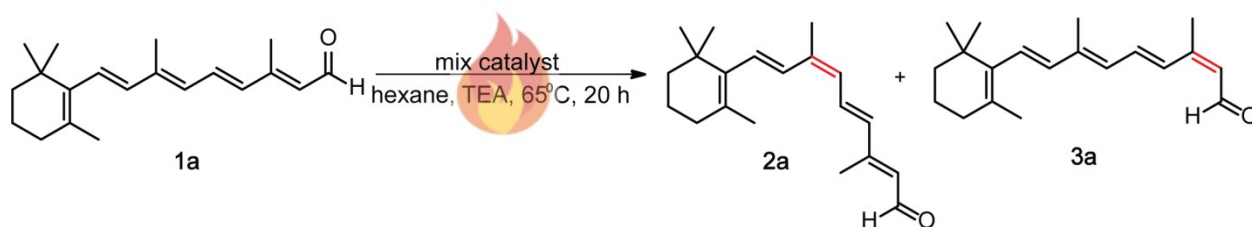
Entry	Catalyst (No)	9,13- <i>dicis</i> - 4g (%)	9- <i>cis</i> - 2g (%)	13- <i>cis</i> - 3g (%)	all- <i>trans</i> - 1g (%)
1	Pd (I)	4.3	16.5	11.6	67.6
2	Pd (II)	5	18.7	14.2	62.1
3	Pd (III)	4.2	17.2	12.3	66.3
4	Pd (IV)	4.4	16.6	15.4	63.6
5	Pd (V)	4.8	21.5	13.0	57.2
6	Pd (VI)	4.1	16.0	10.4	69.5
7	Pd (VII)	4.5	18.1	12.9	64.5
8	Pd (VII)	3.8	16.5	13.7	66.0
9	Pd (IX)	3.1	16.3	14.3	64.3
10	Pd (X)	3.6	17.3	15.7	62.3
11	Pd (XI)	4.7	19.8	12.8	61.2
12	Pt (XIII)	5.0	15.4	13.1	64.1
13	Pt (XIV)	3.1	16.2	13.9	62.8
14	Pt (XV)	4.9	15.8	14.1	62.2
15	Pt (XVI)	4.3	16.0	14.2	65.0
16	Ru (XVII)	3.3	14.7	10.1	67.3
17	Ru (XVIII)	5.1	14.5	11.4	66.9
18	Ir (XIX)	2.3	12.8	9.4	73.1
19	Au (XII)	2.8	12.3	8.2	76.0
20	Rh (XX)	trace	10.5	trace	89.5

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Table S9. Synergetic catalysis effect on Z-isomerization of all-*trans*-retinal **1a**. Reactions were carried out with all-*trans*-retinal (0.1 mmol), catalyst (2 mol %) and TEA (0.2 μmol) at 65 °C under N₂. The yield was determined by HPLC.

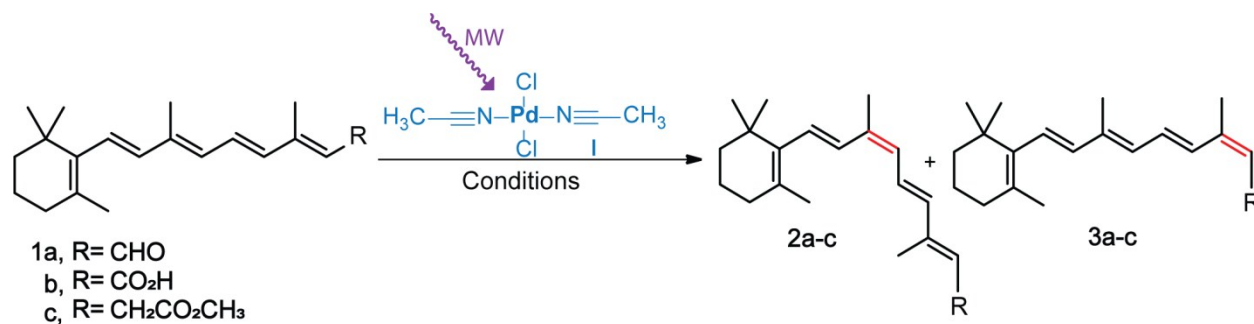


Entry	Catalyst (group/ No)	Conversion (%)	Product (3a:2a)	Ratio range
1	IV, II	41	13- <i>cis</i> : 9- <i>cis</i>	1.1: 1
2	IV, VIII	49	13- <i>cis</i> : 9- <i>cis</i>	1.8: 1
3	IV, XVIII	44	13- <i>cis</i> : 9- <i>cis</i>	1.9: 1

Table S10. all-*trans*-retinoids isomerization in the absence of catalysts. Reactions were performed with 0.1 mmol **1a** for 2 h in CH₃CN under N₂. Each yield is averaged from n ≥ 2 reactions, as determined by HPLC.

Entry	Retinoids	9- <i>cis</i> (%)	13- <i>cis</i> (%)	all- <i>trans</i> (%)
1	1a	trace	7.6	92.4
2	1b	trace	trace	100.0
3	1c	trace	1.5	98.5
4	1d	1.2	2.6	95.8
5	1e	trace	trace	99.0
6	1f	trace	8.6	91.4
7	1g	trace	5.4	94.6

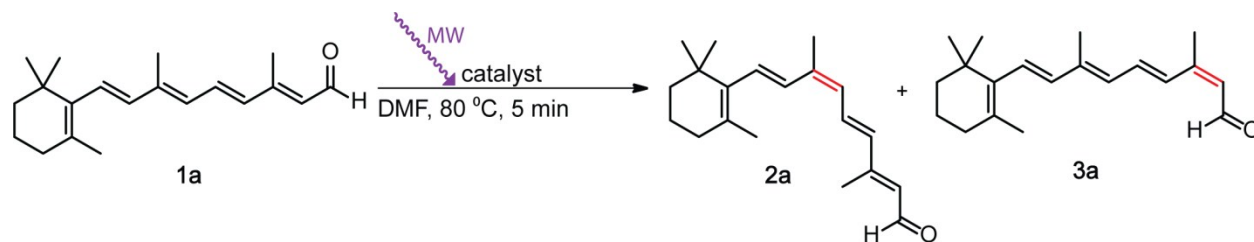
56 Table S11. Optimization of reaction conditions by microwave irradiation. Reaction conditions:
 57 all-*trans*-retinoid (0.1 mmol) and catalyst **I** (2 mol %) under N₂ as determined by HPLC. Each
 58 yield was averaged from n ≥ 2 reactions. nd = not detected. No reaction occurred without a
 59 catalyst for all substrates. Microwave irradiation is indicated by .



Entry	Sub	Solvent	Time (min)	Temp (°C)	Product (3:2)	Ratio
1	1a	CH ₃ CN	5	80	13- <i>cis</i> : 9- <i>cis</i>	1.6:1
2	1a	CH ₃ CN	10	60	13- <i>cis</i> : 9- <i>cis</i>	3.43:1
3	1a	CH ₃ CN	15	70	13- <i>cis</i> : 9- <i>cis</i>	1.7:1
4	1a	DMF	5	100	13- <i>cis</i> : 9- <i>cis</i>	1.5:1
5	1a	DMF	5	150	13- <i>cis</i> : 9- <i>cis</i>	1.6:1
6	1a	DMF	10	100	13- <i>cis</i> : 9- <i>cis</i>	1.5:1
7	1a	DMF	5	80	13-<i>cis</i>: 9-<i>cis</i>	0.67:1
8	1b	CH ₃ CN	5	80	13- <i>cis</i> : 9- <i>cis</i>	1.27:1
9	1b	CH ₃ CN	10	60	13- <i>cis</i> : 9- <i>cis</i>	1.5:1
10	1b	CH ₃ CN	15	70	13- <i>cis</i> : 9- <i>cis</i>	1.4:1
11	1b	DMF	5	80	13- <i>cis</i> : 9- <i>cis</i>	0.09:1
12	1b	DMF	5	150	13- <i>cis</i> : 9- <i>cis</i>	1.16:1
13	1b	DMF	10	100	13-<i>cis</i>: 9-<i>cis</i>	0.08:1
14	1b	DMF	5	80	13- <i>cis</i> : 9- <i>cis</i>	0.1:1
15	1c	CH ₃ CN	5	80	13- <i>cis</i> : 9- <i>cis</i>	0.6:1
16	1c	CH ₃ CN	10	60	13- <i>cis</i> : 9- <i>cis</i>	0.4:1
17	1c	CH ₃ CN	15	70	13- <i>cis</i> : 9- <i>cis</i>	0.3:1
18	1c	DMF	5	100	13- <i>cis</i> : 9- <i>cis</i>	0.7:1
19	1c	DMF	5	150	13- <i>cis</i> : 9- <i>cis</i>	nd
20	1c	DMF	10	100	13- <i>cis</i> : 9- <i>cis</i>	1.3:1

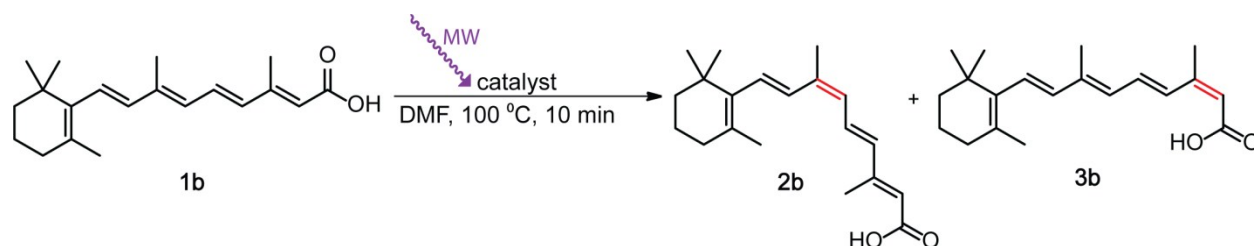
21	1c	DMF	15	150	13- <i>cis</i> : 9- <i>cis</i>	nd
22	1c	DMF	15	80	13-<i>cis</i>: 9-<i>cis</i>	0.2:1
23	1c	DMF	20	70	13- <i>cis</i> : 9- <i>cis</i>	0.6:1
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Table S12. all-*trans*-retinal **1a** isomerization. Reaction conditions: all-*trans*-retinoid (0.1 mmol) and catalyst **I** (2 mol %) under N₂ as determined by HPLC. Each yield was averaged from n ≥ 2 reactions. nd = not detected. No reaction occurred without a catalyst for all substrates. Microwave irradiation is indicated by .



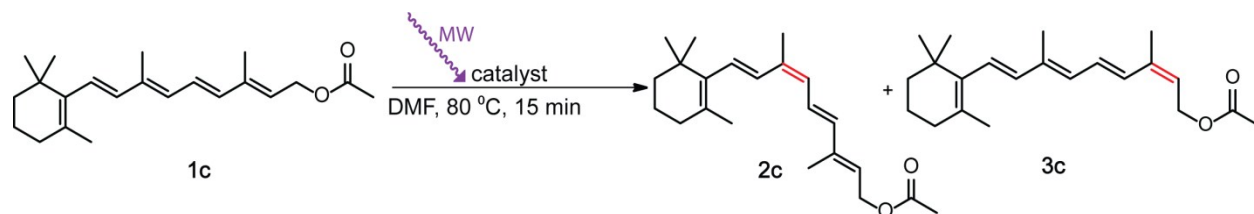
Entry	Catalyst (No)	9- <i>cis</i> - 2a (%)	13- <i>cis</i> - 3a (%)	all- <i>trans</i> - 1a (%)
1	Pd (I)	15.2	10.9	72.0
2	Pd (V)	16.2	10.9	72.9
3	Pd (XI)	0.7	3.4	98.6
4	Pt (XV)	trace	1.4	98.6
5	Ru (XVII)	trace	trace	99.0
6	Ir (XIX)	trace	trace	99.0

Table S13. all-*trans*-retinoic acid **1b** isomerization. Reaction conditions: all-*trans*-retinoid (0.1 mmol) and catalyst **I** (2 mol %) under N₂ as determined by HPLC. Each yield was averaged from n ≥ 2 reactions. nd = not detected. No reaction occurred without a catalyst for all substrates. Microwave irradiation is indicated by .



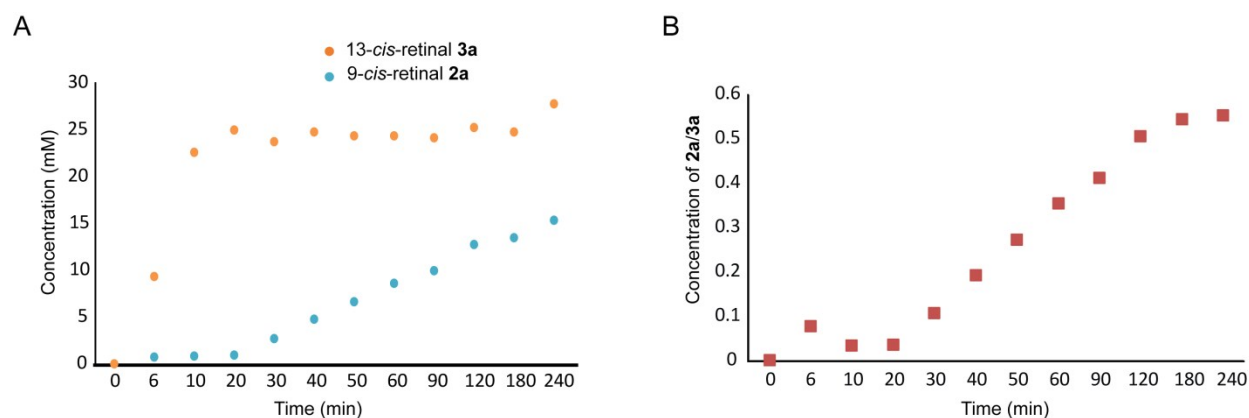
Entry	Catalyst (No)	9- <i>cis</i> - 2b (%)	13- <i>cis</i> - 3b (%)	all- <i>trans</i> - 1b (%)
1	Pd (I)	22.9	1.6	75.5
2	Pd (V)	22.2	1.7	76.1
3	Pd (XI)	trace	trace	98.6
4	Pt (XV)	trace	trace	98.6
5	Ru (XVII)	trace	trace	99.0
6	Ir (XIX)	4.3	trace	95.7
7	Au (XII)	trace	trace	99.0
8	Rh (XX)	trace	trace	99.0

Table S14. *all-trans*-retinyl acetate **1c** isomerization. Reaction conditions: *all-trans*-retinoid (0.1 mmol) and catalyst **I** (2 mol %) under N₂ as determined by HPLC. Each yield was averaged from n ≥ 2 reactions. nd = not detected. No reaction occurred without a catalyst for all substrates. Microwave irradiation is indicated by .

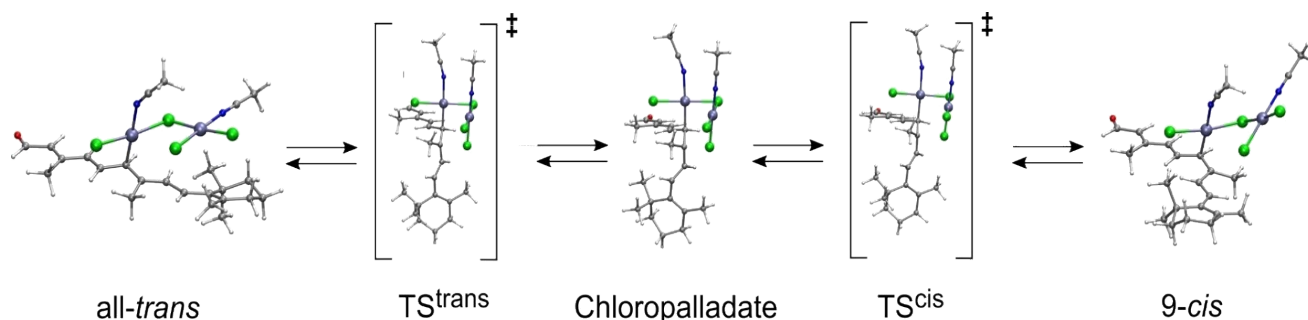


Entry	Catalyst (No)	9- <i>cis</i> - 2c (%)	13- <i>cis</i> - 3c (%)	<i>all-trans</i> - 1c (%)
1	Pd (I)	16.4	8.1	73.4
2	Pd (V)	18.9	3.3	76.9
3	Pd (XI)	1.7	2.2	98.6
3	Pt (XV)	1.1	2.2	96.7
4	Ru (XVII)	1.1	2.6	96.3
5	Ir (XIX)	0.9	2.1	96.9

Figure S3. Reaction of *all-trans*-retinal **1a** (0.1 mmol) with catalyst **I** monitored over time (4 h). A) concentration distribution of the resulting **2a** and **3a** *cis* isomers. B) Concentration ratio of **2a** and **3a** over time.

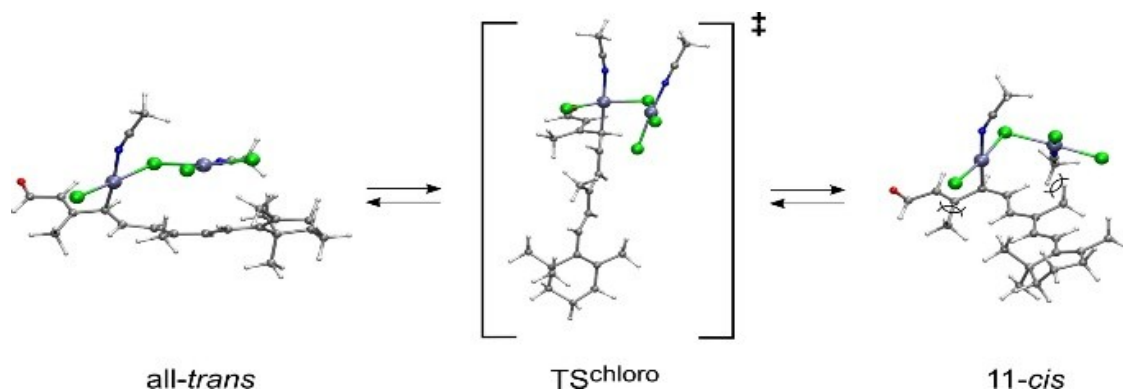


V. Computational Study



	all- <i>trans</i>	TS ^{trans}	Chloropalladate	TS ^{cis}	9- <i>cis</i>
$r(\text{CC})$ [Å]	1.44	1.48	1.53	1.51	1.44
$r(\text{C}\cdots\text{Cl})$ [Å]	3.75	2.38	2.06	2.26	3.68
$d(\text{CCCC})$ [°]	155	71	60	61	22

Figure S4. Structures of intermediates for all-*trans*-retinal to 9-*cis*-retinal isomerization. The 13-*trans*-to-*cis* isomerization has similar outcomes. Key geometric parameters are given in the Table.



	all- <i>trans</i>	TS ^{chloro}	11- <i>cis</i>
$r(\text{CC})$ [Å]	1.43	1.49	1.43
$r(\text{C}\cdots\text{Cl})$ [Å]	4.73	2.22	4.22
$d(\text{CCCC})$ [°]	155	64	17

Figure S5. Structures of intermediates for all-*trans*-retinal to 11-*cis*-retinal isomerization. Key geometric parameters are given in the Table.

Table S15. Absolute DLPNO-CCSD(T)/CBS energies for all calculated species along with free energy corrections obtained at the BP86+D3/def2-TZVP level of theory. The number of imaginary frequencies is reported in the last column. The energies of all-*trans*-retinal bound to Pd catalyst via C₉, C₁₁ and C₁₃ were set to zero (marked in bold) in Scheme 2 of the main manuscript and all energies reported therein are relative to these baseline energies. All values are provided in atomic units.

	DLPNO-CCSD(T)/CBS	G _{corr}	G	Imaginary freq.
Isolated molecules				
<i>all-trans</i>	-852.88459576	0.36653369141902	-852.51806206858	0
9- <i>cis</i>	-852.884656865	0.36649614530200	-852.51816071970	0
11- <i>cis</i>	-852.877275579	0.36713085225904	-852.51014472674	0
13- <i>cis</i>	-852.883544402	0.36635142197497	-852.51719298002	0
PdCl ₂ (ACN) ₂	-1312.374452507	0.05437355354002	-1312.3200789535	0
Pd ₂ Cl ₄ (ACN) ₂	-2359.58080515	0.04884400810033	-2359.5319611419	0
trans-PtCl ₂ (ACN) ₂	-1303.693344038	0.05448677048980	-1303.6388572675	0
cis-PtCl ₂ (ACN) ₂	-1303.68349973	0.05450281514004	-1303.6289969149	0
Pt ₂ Cl ₄ (ACN) ₂	-2342.200310627	0.04990015413978	-2342.1504104729	0
PdCl ₂ (PPh ₃) ₂	-3116.95708727405	0.4719724804900	-3116.4851147936	0
Pd ₂ Cl ₄ (PPh ₃) ₂	-4164.19143321695	0.47179482757019	-4163.7196383894	0
ACN	-132.574844488	0.02072925029498	-132.55411523771	0
Complexes retinal + catalyst monomer (Ior XV)				
1 PdCl₂(ACN)₂				
9- <i>trans</i>	-2032.689098845	0.402238471	-2032.286860375	0
9-TS	-2032.613191662	0.400022496	-2032.213169166	1
9- <i>cis</i>	-2032.688168688	0.403426832	-2032.284741856	0
11- <i>trans</i>	-2032.691802396	0.403924556	-2032.287877841	0

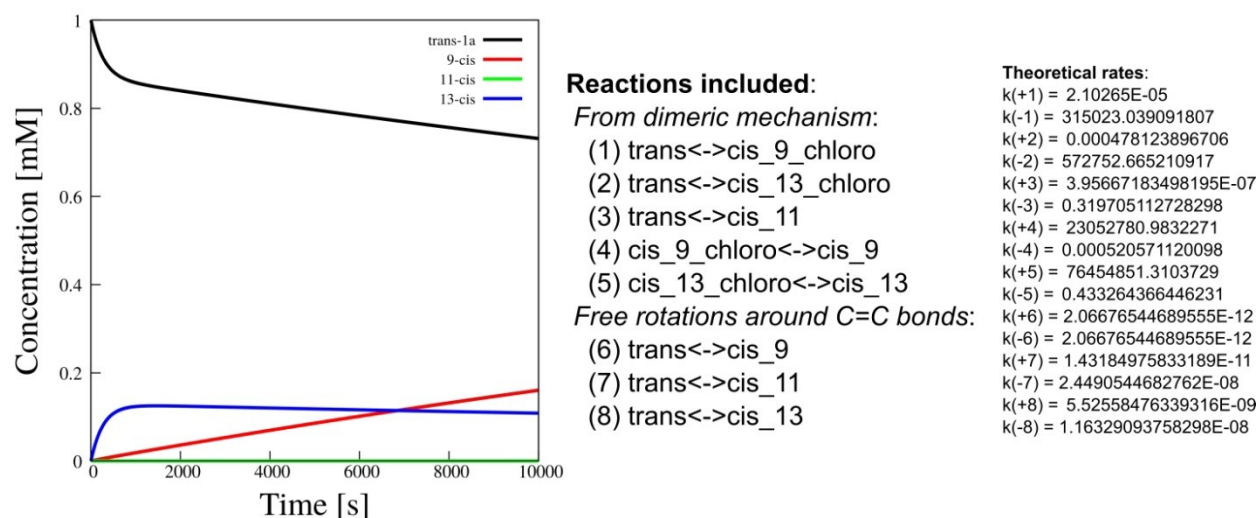
11-TS	-2032.609340749	0.399855039	-2032.209485710	1
11-cis	-2032.687932086	0.402417874	-2032.285514212	0
13-trans	-2032.680517878	0.401828619	-2032.278689259	0
13-TS	-2032.623937534	0.397023620	-2032.226913914	1
13-cis	-2032.681031588	0.402451466	-2032.278580122	0
xv PtCl₂(ACN)₂				
9-trans	-2024.008400770	0.403417254	-2023.604983517	0
9-TS	-2023.931396586	0.398403778	-2023.532992808	1
9-cis	-2024.005816390	0.403871053	-2023.601945337	0
11-trans	-2024.009682233	0.402641598	-2023.607040634	0
11-TS	-2023.922825135	0.398755566	-2023.524069569	1
11-cis	-2024.005240862	0.402534967	-2023.602705895	0
13-trans	-2024.002360855	0.403488366	-2023.598872489	0
13-TS	-2023.932532178	0.400119955	-2023.532412223	1
13-cis	-2023.999675399	0.402318151	-2023.597357248	0
Complexes retinal + catalyst dimer I				
9-all-trans	-3212.485866344	0.443317986469992	-3212.04254835753	0
11-all-trans	-3212.489647297	0.442887144670294	-3212.04676015233	0
13-all-trans	-3212.485403371	0.445545994500208	-3212.0398573765	0
9-cis	-3212.486622539	0.44291421762	-3212.04370832138	0
11-cis	-3212.47874682	0.446545545379649	-3212.03220127462	0
13-cis	-3212.480692377	0.442884914929891	-3212.03780746207	0
9-TS-trans	-3212.447447726	0.440696278290034	-3212.00675144771	1
13-TS-trans	-3212.447719676	0.440315430809733	-3212.00740424519	1

9-TS- <i>cis</i>	-3212.452879939	0.441533710970361	-3212.01134622803	1
13-TS- <i>cis</i>	-3212.453181847	0.440539444839942	-3212.01264240216	1
11-TS-chloropalladate	-3212.446606063	0.439895171589797	-3212.00671089141	1
9-chloropalladate	-3212.458753475	0.441282896219946	-3212.01747057878	0
13-chloropalladate	-3212.458388604	0.440905074920011	-3212.01748352908	0

158

159 Figure S6. Results of the kinetic simulations of the *E/Z* isomerization of all-*trans*-**1a** catalyzed by
160 complex **I** (left panel). Initial concentration of the substrate was set to 1 mM. Reactions included
161 in the kinetic scheme are given in the middle (we accounted only for reactions for which Gibbs
162 free energy barriers were calculated at the DLPNO-CCSD(T)/CBS level). Theoretical rates for
163 the elementary steps were calculated using text-book Eyring equation $k = (k_B T/h) \exp(-dG_{act}/RT)$
164 where k_B , h and R are the Boltzmann, Planck's and gas constants, respectively. T denotes
165 reaction temperature (338 K) and dG_{act} is the activation free energy for a given step. All
166 simulations were performed with the program Tenua (Tenua 2.1 by D. Wachsstock available
167 from <http://bililite.com/tenua>; accessed 15.05.2019).

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171 **Coordinates of all the calculated structures**

172 **Retinal 1a isomers**

173 **all-trans**

174 C	1.79525905993918	2.62082152371687	0.88179948881828
175 C	0.45266946971734	2.33691131840265	1.08828550610539
176 H	2.51901527141678	1.85629126634412	1.21697090786777
177 C	2.35599119687795	3.78994593879444	0.27993026547455
178 H	1.66533731276614	4.58041319788284	-0.05565289350613
179 C	3.70910409560993	3.97827064117392	0.09679771975701

180	H	4.39296960675528	3.17879891747468	0.43204230803456
181	C	4.33153701561883	5.13761515774839	-0.50372654304938
182	C	5.70909377749818	5.15709290821525	-0.62077852176396
183	H	6.28428000665867	4.28901278887142	-0.25466816806476
184	C	6.53406200222153	6.21819910670180	-1.18966637932211
185	O	7.76003013127377	6.16271280711250	-1.26561445694116
186	H	5.98342668557749	7.12962082804379	-1.57305246024213
187	C	3.44583621082082	6.26962583523687	-0.97272049194132
188	H	2.72297662673580	5.91249670235972	-1.73571516194912
189	H	2.84936242597893	6.67251867869379	-0.12801573946817
190	H	4.01591947107875	7.10618657351803	-1.41291889198592
191	C	-0.65239459246264	3.27834210727613	0.67672533223805
192	H	-1.32887328794138	2.79460294315664	-0.05970879065772
193	H	-1.27881756878955	3.55977519166813	1.54879879851653
194	H	-0.27244465732946	4.20923317925683	0.22075250599708
195	C	0.10957467191874	1.08013771735542	1.71883336121219
196	H	0.97016499626465	0.45153556527165	1.98995317346147
197	C	-1.17391314811941	0.64958835503894	1.96096164248054
198	H	-1.96476045488311	1.33438998509162	1.62181405312009
199	C	-3.02763933949338	-0.83678551210321	2.47306446888818
200	C	-3.65206314925818	-2.14508980273677	2.89775653779002
201	C	-2.64506601367770	-3.26795134932113	3.13227026599027
202	C	-1.47762603613487	-2.71671745079168	3.94242418530949
203	C	-0.69777680248901	-1.59976955663907	3.20163850463495
204	C	-1.66827157744173	-0.59054521885001	2.54481409991071
205	H	-4.41005087354317	-2.43742682404952	2.13605114946118
206	H	-4.24736768321380	-1.96302709191463	3.82639527592563
207	H	-3.12664000632300	-4.11992770996566	3.65499080094754
208	H	-2.28543491393423	-3.66116007446653	2.15780122979880
209	H	-0.76171535836459	-3.51839117570942	4.22013802717129
210	H	-1.87258080236833	-2.30538488135938	4.89759440988261
211	C	-4.03168175134912	0.15280837294558	1.92129248134163
212	H	-5.05036637547585	-0.09277999833981	2.28303623401140
213	H	-3.82318944053750	1.20143681392765	2.20932339744302
214	H	-4.07109516779800	0.11840251348423	0.80931624702361
215	C	0.21007062885941	-2.25545873566714	2.13276431825957
216	H	0.76308489640199	-1.51039222475931	1.53112108458193
217	H	0.95582741096699	-2.92039691089538	2.61700817176496
218	H	-0.38207411518996	-2.86702460175996	1.42249632502343
219	C	0.16669234244724	-0.89871785077190	4.27814454161289
220	H	0.76668677129898	-1.65552311378839	4.82658126484843
221	H	0.86820400523161	-0.15114789996534	3.86677867576803
222	H	-0.47828169581699	-0.37848027890968	5.01565770741879
223				
224	9-cis			
225	C	1.88393814903650	2.91669999927618	1.47946211404557
226	C	0.56580451402901	2.47900922513569	1.46812236712397
227	H	2.08805969607581	3.90890276139498	1.04097901673871
228	C	3.02002085150051	2.22030122501035	2.00357552178418
229	H	2.85526285014512	1.22600804305507	2.44817902748091
230	C	4.30207774802056	2.72081131774738	1.98549968243984
231	H	4.46597229119263	3.71862878817032	1.54270414232035
232	C	5.47682954082412	2.05148071919144	2.50258635960511
233	C	6.69553966990434	2.69707867430342	2.41521930616453
234	H	6.73281900493981	3.69910948425486	1.95530062284935
235	C	7.98999697253157	2.20234256366169	2.87409424835582
236	O	9.03877621000458	2.83535228298393	2.76639403949035
237	H	7.99319763986031	1.17668186406410	3.35065006194680
238	C	5.31050220809726	0.67806406542625	3.11213573098603
239	H	4.60283816582359	0.71335516313113	3.96651602726312
240	H	4.88417188121884	-0.02815747085040	2.36964270863549
241	H	6.26185591455126	0.25426675511616	3.47584310506975
242	C	-0.49614337536260	3.36796112368345	0.86738886226698
243	H	-1.01789942256650	2.86352147102139	0.02640512563236
244	H	-1.27563147681972	3.62686728090892	1.61486118294460
245	H	-0.06405878236956	4.31107092088721	0.48335615657196
246	C	0.18210262685180	1.19870088304271	2.02292567761770
247	H	0.99492210612116	0.59478925126696	2.44334267755707
248	C	-1.09996186436383	0.70561554412026	2.03655439358385
249	H	-1.85721710600338	1.34669279810036	1.56315521013680
250	C	-2.91051937171372	-0.91073447701474	2.20612651075330
251	C	-3.51699135522292	-2.25347545898510	2.53982751907519
252	C	-2.51054919406514	-3.28732298864482	3.03544651813036

253	C	-1.57617104765176	-2.62207766008098	4.03942931512883
254	C	-0.72799251119385	-1.48516401633119	3.41171362912284
255	C	-1.61483156206682	-0.56143179602112	2.54145911720359
256	H	-4.06450930635032	-2.62467059785174	1.64364811342190
257	H	-4.31489943463826	-2.09344554890203	3.30546995830541
258	H	-3.03281318545477	-4.15493160364876	3.48875077958849
259	H	-1.92746032911930	-3.68520663563187	2.17781738889886
260	H	-0.88815796257565	-3.36187044730821	4.50093036705260
261	H	-2.18459883291982	-2.19992287794018	4.87030900792476
262	C	-3.85081178345420	-0.01482720127457	1.42880811050335
263	H	-4.90367541962136	-0.29961720579413	1.63113291177662
264	H	-3.74641798424130	1.06055013889742	1.67226044877338
265	H	-3.69687348664538	-0.12034657345198	0.33117564652548
266	C	0.39791005815706	-2.12157093579879	2.55939659094340
267	H	1.02133751077361	-1.36467611899210	2.04749441794503
268	H	1.06568566007870	-2.73534000348453	3.20021028919136
269	H	-0.01803868383306	-2.78008213856103	1.77094501489081
270	C	-0.11608819305186	-0.69982790754239	4.59810432605652
271	H	0.38004683467116	-1.40710597256170	5.29561168227284
272	H	0.63595492174778	0.04867601044883	4.29073555890837
273	H	-0.90778935485198	-0.16511771762807	5.16186540899551

274

275 11-cis

276	C	1.49052928498927	5.11166191717647	0.67057609338908
277	C	0.28102296902581	4.94946946157904	1.33584713914165
278	H	1.62117723871761	6.07600485727013	0.16147904599914
279	C	2.55126116496534	4.15348755740576	0.59002385453694
280	H	2.37174638064427	3.20276401470493	1.12004603785111
281	C	3.77729544103032	4.21425576105714	-0.04880121524624
282	H	4.40359690509630	3.31289705164348	0.06278708806714
283	C	4.40291058058005	5.24750989916318	-0.85121059324976
284	C	5.66580094855057	4.97697966435956	-1.34973893827726
285	H	6.12972606993593	4.00348766790407	-1.11532516567615
286	C	6.50017362975204	5.84240563927035	-2.17731653579173
287	O	7.61797002486607	5.52604044802159	-2.58128676124673
288	H	6.06815735555131	6.85212752821842	-2.44486512243888
289	C	3.69434569426819	6.55322175424895	-1.12390028600854
290	H	2.72680009503568	6.37365378050613	-1.63585532610498
291	H	3.46868778308885	7.08137891046018	-0.17486603236844
292	H	4.29132284660423	7.23381613249700	-1.75622523015993
293	C	-0.08672172462514	3.69969281732389	2.09548221330128
294	H	-0.30900362953954	3.93492302954281	3.15745890895024
295	H	-1.00341212966032	3.23851537395798	1.67187477349339
296	H	0.71154283081268	2.93614998540245	2.08263801211704
297	C	-0.67098369005879	6.03855326317775	1.27842986675634
298	H	-0.3324734083031	6.91443087754708	0.70641257717355
299	C	-1.90646559197869	6.03733456720706	1.88075743123758
300	H	-2.13616294365303	5.13911992223009	2.47240289191641
301	C	-3.99200421297115	6.89033270738691	2.79482816245278
302	C	-5.07518549962101	7.92305684737989	2.99789127615328
303	C	-4.79315513575490	9.26853650977277	2.33519915787324
304	C	-4.24714073638112	9.02281689851846	0.93312475307500
305	C	-2.89600434781297	8.26062084582470	0.93420119811156
306	C	-2.95395775890523	7.04913695264667	1.89479744103565
307	H	-5.24853103693719	8.04276259189283	4.09123212183215
308	H	-6.03282897790026	7.49776004273509	2.61002740137082
309	H	-5.71388914816723	9.88657797285631	2.30235310925307
310	H	-4.05422604150409	9.83991505429312	2.93847217475299
311	H	-4.11382325438398	9.97573005619054	0.37796010180807
312	H	-4.99167490179855	8.42753079412466	0.35844012847840
313	C	-4.13630499669725	5.68948291274272	3.70436001129482
314	H	-5.18173634452337	5.59867602448325	4.06083030539325
315	H	-3.86905092135751	4.73142710617732	3.21777333633541
316	H	-3.49802097018222	5.78537418494953	4.61036843029444
317	C	-1.77391921621779	9.23752530615468	1.36349262659992
318	H	-0.78289346835466	8.74904910650463	1.40615794525635
319	H	-1.70426661060378	10.08541882043377	0.65025126539896
320	H	-1.97051022093333	9.65365697816968	2.37209714044771
321	C	-2.66989011432686	7.79383435901696	-0.52460744987457
322	H	-2.77066747332431	8.65940948994660	-1.21155624341129
323	H	-1.67510822710583	7.34504111740008	-0.69620985177930
324	H	-3.43000388540408	7.03996862552337	-0.81342795351494

325

326	13-cis			
327	C	1.37526119768514	7.76072498762426	-0.33802832661236
328	C	0.14990419472427	7.98415536722028	0.27356823734548
329	H	1.76078566613438	8.56993985197090	-0.98410782884993
330	C	2.20208858179018	6.59859988184446	-0.22959184337243
331	H	1.84408008354512	5.77008908089955	0.40165025671279
332	C	3.41369006104879	6.46177161570891	-0.87178233497618
333	H	3.75436376351752	7.30212758124021	-1.49678214199204
334	C	4.27318848625013	5.29997932318026	-0.78932640910900
335	C	5.48066836087995	5.21330278938056	-1.46098975513448
336	H	6.08771716444466	4.29802125530459	-1.35586648027403
337	C	6.08212539905817	6.22343401194093	-2.32940389938043
338	O	7.16281978463173	6.07620522007400	-2.89570338234530
339	H	5.49725358419239	7.18165769290083	-2.46761282293704
340	C	3.83096163001040	4.13530538504366	0.06759851193411
341	H	3.70260994291741	4.44312682191114	1.12687685777268
342	H	2.85118065877835	3.73764689756509	-0.27101073918480
343	H	4.56680296075317	3.30965243536270	0.03617820983718
344	C	-0.49864878186605	6.97629264568708	1.19010688544352
345	H	-0.63340951308735	7.39793573225186	2.20869559696254
346	H	-1.50850573736514	6.69885809033701	0.82283579590406
347	H	0.09023412232023	6.04761949852099	1.28822287539397
348	C	-0.52371015242691	9.23888118434807	0.01649839025274
349	H	0.01294008192489	9.92125185520096	-0.65805633844950
350	C	-1.72974283023958	9.60964278840821	0.56181915408146
351	H	-2.17136174477681	8.88098658621886	1.25783740924487
352	C	-3.57773143253722	11.03220942149997	1.25460342426348
353	C	-4.36695323494762	12.31983542652096	1.30199085708650
354	C	-3.71132201350265	13.48048075146322	0.55791994766433
355	C	-3.20784189553922	12.97524777451097	-0.78950252500231
356	C	-2.10775643683842	11.88970301693565	-0.65528539220340
357	C	-2.50039433436444	10.83697362492428	0.40879248065024
358	H	-4.55352466856096	12.57985597728168	2.36861476606956
359	H	-5.38368661405646	12.12091518503169	0.88341981897840
360	H	-4.42984981205074	14.31610751352099	0.42820263439308
361	H	-2.86599516954870	13.88244179708412	1.15709362754011
362	H	-2.80692997165937	13.80466463521482	-1.40977276938194
363	H	-4.06673645451334	12.54840353233184	-1.35406752095248
364	C	-4.05972469293830	10.00413740959539	2.25521999614252
365	H	-5.12042691873871	10.19269917608978	2.51783521889508
366	H	-3.98917951823400	8.96170290628295	1.89003765161292
367	H	-3.48290955071045	10.05995169147191	3.20532504524619
368	C	-0.77516050141563	12.57985339838654	-0.27057471583693
369	H	0.05054472538767	11.85735104228226	-0.13001557680184
370	H	-0.47220196942009	13.29612040326242	-1.06260540133882
371	H	-0.87748370308471	13.14221744305538	0.67901156733311
372	C	-1.98287133327250	11.23296035251932	-2.05252550945404
373	H	-1.83152574408293	12.02015937935044	-2.82046154267003
374	H	-1.14119447312232	10.52115752331998	-2.13221470744438
375	H	-2.91109232909394	10.68180950791799	-2.30895875405725

376

377 **Catalysts structures (monomeric and dimeric) and labile ligands**

378	PdCl₂(ACN)₂ 1			
379	Pd	1.66644753426362	0.63746731898125	-0.91322008430209
380	Cl	2.55006215723261	-0.83289369462513	0.66982555591406
381	Cl	0.78310084617721	2.10878692823027	-2.49508081567017
382	C	4.53612910201644	1.39368663447016	-1.83576786885220
383	N	3.46342907171979	1.11090396434907	-1.48350666449572
384	C	5.87203203211007	1.75223297396562	-2.27694314268443
385	H	6.30174775124200	0.93477478962975	-2.89056463574728
386	H	6.52891194145986	1.92256744614721	-1.40076777584607
387	H	5.83467723378289	2.67749210577192	-2.88608755657470
388	C	-1.20079053318673	-0.13206567390513	0.00666915035328
389	N	-0.13023717831300	0.16036987514273	-0.34436468263275
390	C	-2.53454635002627	-0.49995621017890	0.44692112890011
391	H	-3.14365774450063	0.41038129338375	0.61619472272580
392	H	-2.47552802555965	-1.07508492745317	1.39265244997460
393	H	-3.03136040641820	-1.12373950690940	-0.32352805006246

394

395 **Pd₂Cl₄(ACN)₂**

396	Pd	1.94605023118089	1.51276676476480	-0.45468472918362
397	Pd	-0.99283642734277	2.28081573872782	-1.45592430672021
398	Cl	2.66616757139337	-0.23815318637421	0.84250968242514
399	Cl	1.08121833522943	3.32296848784450	-1.78358076118644
400	Cl	-0.10304343341249	1.62576780170784	0.68211196144488
401	Cl	-1.72855143716763	2.92877523019878	-3.53177171116242
402	C	4.61879555900790	1.35494297558056	-2.03375334569661
403	N	3.61400948624979	1.43578167941296	-1.44887104165380
404	C	5.87384564270798	1.24355292758611	-2.75517544742302
405	H	5.79778512269341	0.45820084372039	-3.53423724108411
406	H	6.68830291847622	0.97425613287257	-2.05320558003289
407	H	6.12338924828869	2.20802398142296	-3.24108750618782
408	C	-3.70101788585749	0.82220861615309	-1.00830169393192
409	N	-2.68675537665843	1.37677268388752	-1.15623547078966
410	C	-4.96688919224357	0.13410494192578	-0.82992045528417
411	H	-5.78341854626989	0.87038933276975	-0.69082163423618
412	H	-4.92100120485991	-0.52452563903320	0.06066994696871
413	H	-5.19103600041551	-0.48390659616805	-1.72271956726586

414

415 **PtCl₂(ACN)₂**

416	Pt	1.66885211784125	0.63167305171186	-0.91043405413343
417	Cl	2.56081798275630	-0.97780553863286	0.56349131137765
418	Cl	0.77677497575956	2.24178734677189	-2.38365751554053
419	C	4.52585785727623	1.37488497109633	-1.84698575736085
420	N	3.45186319668699	1.09498779556134	-1.49103888411985
421	C	5.85943572556521	1.73148287098632	-2.29478694362048
422	H	6.27669951904718	0.92609088780643	-2.93297346419058
423	H	6.52844861113992	1.87788654996370	-1.42310006743073
424	H	5.82301447898810	2.67145674231641	-2.88153667888921
425	C	-1.18821003434692	-0.11732696790807	0.02135484745701
426	N	-0.11434032996762	0.16703893706334	-0.33136643843184
427	C	-2.52418812711280	-0.47414492246204	0.46179381853530
428	H	-3.10023671048286	0.43956715624982	0.71128191693465
429	H	-2.46722616857071	-1.11951227915780	1.36149087418049
430	H	-3.05714609457984	-1.02314260136666	-0.34109996476759

431

432 **Pt₂Cl₄(ACN)₂**

433	Pt	2.04787728235454	1.18787507680027	-0.56055765556953
434	Pt	-1.05308712092879	2.16481942445081	-1.37942721692325
435	Cl	2.81620285700040	-0.69109114997926	0.53872824292614
436	Cl	1.08736641850678	3.12862294351741	-1.65969883428332
437	Cl	-0.04298511518506	1.07020740942322	0.53888045239884
438	Cl	-1.86851707342159	3.24981827448960	-3.24733082252043
439	C	4.74083563607232	1.36304962684853	-2.05184056876689
440	N	3.71620268049215	1.32006827741681	-1.49343800346389
441	C	6.01272975929702	1.41325560891492	-2.74998212246577
442	H	6.37659268997943	0.38500414622797	-2.94801740592243
443	H	6.76781639107720	1.94706521659234	-2.13782395995294
444	H	5.89772278604825	1.94267227207685	-3.71706035677714
445	C	-3.82105946496126	0.86552514928907	-0.98261629250101
446	N	-2.76572476960866	1.34810187902806	-1.11248890267651
447	C	-5.13432183405658	0.26876511547074	-0.81918639413927
448	H	-5.87881858250884	0.82703889634053	-1.42140548660786
449	H	-5.44133252446075	0.29900876860034	0.24592926579572
450	H	-5.12248540469655	-0.78706421850825	-1.15766283955048

451

452 **PdCl₂(PPh₃)₂**

453	Pd	1.90480844978600	1.22918450093786	-0.87058839776648
454	Cl	2.09349205116253	-0.31589000313914	0.85777833234463
455	Cl	1.81113597791841	2.81271670852718	-2.60977929668292
456	P	0.51946652599429	2.61482148226449	0.36893909333275
457	P	3.75679174034955	0.33910480452865	-1.93063117302632
458	C	3.77520749881070	0.09834021787455	-3.74759964256386
459	C	4.97752687129408	-0.25830143790048	-4.39559782919236
460	C	2.58009006168865	0.19637061184385	-4.48629240171965
461	C	4.98398303581015	-0.49994647168979	-5.77699742979102
462	C	2.59178563441650	-0.05594197132217	-5.86764587226596
463	C	3.79026433432768	-0.40084235586220	-6.51398415979749
464	H	5.90766315860210	-0.35763933241973	-3.81487237021383
465	H	1.65359883409963	0.49577544392994	-3.97593235789688
466	H	5.92361315233470	-0.77697176313112	-6.27890654040649

467	H	1.65633857969749	0.02289823349938	-6.44244469428325
468	H	3.79528556930971	-0.59920469206695	-7.59691907168515
469	C	4.50829683341017	-1.21881966231771	-1.32694985954280
470	C	3.67129588522119	-2.34838958107610	-1.21355639755011
471	C	5.88215970284165	-1.32977585676854	-1.03678333687856
472	C	4.21137192644949	-3.58228903020383	-0.82580718271493
473	C	6.41600409647276	-2.56765990585409	-0.64067528523748
474	C	5.58313600615564	-3.69350792520578	-0.53646978660065
475	H	2.59467935288958	-2.24928317190160	-1.41527982929236
476	H	6.53369540536977	-0.44692116475752	-1.11462656658174
477	H	3.55468690354364	-4.46067923701914	-0.73315242494616
478	H	7.48909248071487	-2.64944266613639	-0.40912884692676
479	H	6.00253381158353	-4.66124492153152	-0.22121312472284
480	C	4.96712940133173	1.65331999965600	-1.53658116255675
481	C	5.30238873972648	1.84072603089296	-0.17571108682616
482	C	5.40844829907364	2.57587326435779	-2.50398981326122
483	C	6.10231123436203	2.92705851872695	0.20273213144517
484	C	6.20415863823743	3.66680204999731	-2.11466702887454
485	C	6.55537929229040	3.84157818400249	-0.76590258400106
486	H	4.90948670935239	1.14564270788956	0.58329632644037
487	H	5.11315227296621	2.45090518907461	-3.55563708557713
488	H	6.35823457483633	3.07112728339098	1.26320457464471
489	H	6.54639986245762	4.38772950560742	-2.87255403123677
490	H	7.17788074950281	4.69847863406710	-0.46457354491221
491	C	0.79249098020051	3.44142189833786	-0.60597109586943
492	C	-1.43951531550984	2.69588106651387	-1.61308160210294
493	C	-1.19589596475609	4.76318824147170	-0.33901900209683
494	C	-2.49844121768215	3.26575704688493	-2.33409321729068
495	C	-2.25081266651563	5.33240787827452	-1.07071482493708
496	C	-2.90479567262228	4.58440219441033	-2.06416942791495
497	H	-1.09716363808777	1.67304241158629	-1.83274446168852
498	H	-0.68106410838551	5.34922384615705	0.43707797933635
499	H	-3.00108278915000	2.68202239535929	-3.12021732100049
500	H	-2.56190907156657	6.36752225120839	-0.86349193105265
501	H	-3.73119429935121	5.03380992437732	-2.63589415814838
502	C	-0.37501701209698	1.93115619440533	1.81356863811008
503	C	-1.78116877407052	1.83440472452447	1.82899919957335
504	C	0.37205685100996	1.45014954428268	2.91267009497154
505	C	-2.43497103128038	1.27011961148723	2.93690287915045
506	C	-0.28850847310741	0.89805500446333	4.01882019763874
507	C	-1.69139756560876	0.80370904206894	4.03300069127548
508	H	-2.36780652277723	2.20739533244064	0.97680038792911
509	H	1.46908320348401	1.50597929039045	2.89381313067778
510	H	-3.53379246846199	1.19959747641593	2.94218593471341
511	H	0.29853747164960	0.52758683318003	4.87310890349980
512	H	-2.20521022611749	0.36422825862401	4.90206686709398
513	C	1.55388933865101	3.96149986186004	1.07467228017987
514	C	1.21201685444759	4.58077848547938	2.29657563519113
515	C	2.69982908621062	4.38931309837028	0.37007089817224
516	C	2.01224496304732	5.61446433571442	2.80849739837306
517	C	3.49329562588097	5.42262237417960	0.88906959802083
518	C	3.15457268851816	6.03539670187371	2.10694179441987
519	H	0.32323049402474	4.24644966391358	2.85236646540921
520	H	2.95998589542334	3.91790963877887	-0.58983011324070
521	H	1.74227702345179	6.08960056893016	3.76376081727247
522	H	4.38907977331399	5.74057869405641	0.33506399910367
523	H	3.78320842984370	6.84289453621361	2.51330755755451
524				
525	Pd₂Cl₄(PPh₃)₂			
526	Pd	1.53683568984597	0.58974217640657	-2.73073402020439
527	Pd	-0.58207114628384	2.60489143712948	-2.65367401145823
528	Cl	1.76040972183513	-1.38322016435824	-1.55113007503147
529	Cl	1.61743419514805	2.77888964268324	-3.72004302676862
530	Cl	0.71446081931028	1.84751401735356	-0.77829966118090
531	Cl	-1.77305435082083	3.13489607525965	-4.56082586537364
532	P	-2.42086629934418	1.84418176641911	-1.65563201764727
533	P	2.03566822712305	-0.53107523853819	-4.60404374549104
534	C	-2.15652707681506	0.04308560161362	-1.67818180252998
535	C	-2.07991393378448	-0.58315913554205	-2.94405895404675
536	C	-1.87537692389641	-0.68594528737788	-0.50780679237475
537	C	-1.77501573957243	-1.94653345352529	-3.02438991010294
538	C	-1.55168523122994	-2.04767832773261	-0.60257958628847
539	C	-1.50944139855285	-2.67826678399779	-1.85472815556889
540	H	-2.24376017100572	0.00874857406485	-3.85829434688832

541	H	-1.88283357668048	-0.18360112703227	0.46999081410955
542	H	-1.71551920127768	-2.43631938156284	-4.00588215963738
543	H	-1.30810977443955	-2.61192454156269	0.30949313593320
544	H	-1.23695843230959	-3.74135323943031	-1.92781743632977
545	C	-4.05835746639842	2.15274991849818	-2.40808898218564
546	C	-4.43886786294142	3.49238842764680	-2.63406864019194
547	C	-4.95550776019127	1.10526530447931	-2.69118611896033
548	C	-5.71458138577286	3.77801832714432	-3.13563188529718
549	C	-6.23257029719540	1.40020824672301	-3.19833036352291
550	C	-6.61236104076535	2.73293402701984	-3.42077444201715
551	H	-3.72789031016497	4.30532735881173	-2.42470010088109
552	H	-4.65665556623787	0.06143507766331	-2.51536196775042
553	H	-6.00794357958051	4.82291827611665	-3.31790736762513
554	H	-6.93248546662379	0.58047141451204	-3.42085616102003
555	H	-7.61160102202389	2.96124304060690	-3.82159631087175
556	C	-2.68296694236864	2.37256436092917	0.07679947925164
557	C	-3.76530814941099	1.82584936936314	0.80049334584388
558	C	-1.86496724086121	3.35472997660678	0.66668700763561
559	C	-4.00811977555888	2.24503840508349	2.11591542515213
560	C	-2.12045436679121	3.77728190996484	1.98113802387904
561	C	-3.18618687894038	3.22164391510162	2.70700865622926
562	H	-4.42050327582356	1.07638408046998	0.32977080553037
563	H	-1.02714827152116	3.78075340849991	0.09525989370212
564	H	-4.84828553259797	1.81283428938414	2.68034526265513
565	H	-1.47940429982064	4.54546234599024	2.43937052606683
566	H	-3.38310312005978	3.55419497093162	3.73740094616474
567	C	1.85300430405440	0.49828042918470	-6.10447525771070
568	C	2.87049833728112	0.58121955008034	-7.07476401460737
569	C	0.65206486982774	1.21955243920900	-6.27574438261482
570	C	2.67407185321284	1.36923195324392	-8.22109584011482
571	C	0.46240508920196	1.99995299948359	-7.42276450564882
572	C	1.47181794391091	2.07411265080296	-8.39851776960813
573	H	3.81609832345424	0.03821958948834	-6.93341954797554
574	H	-0.12975977476513	1.21013313450236	-5.50090522952484
575	H	3.47211972331333	1.43694963069626	-8.97685152815546
576	H	-0.47112194691562	2.57263343788711	-7.52679005606220
577	H	1.32714340487555	2.69596795147545	-9.29548669967773
578	C	1.03978646649412	-2.03055529507834	-4.98093637057605
579	C	1.22145088368674	-3.19825009319965	-4.20607019062239
580	C	0.12056052042942	-2.04099284288975	-6.05051514566448
581	C	0.48916672010943	-4.35602346056152	-4.50316843795945
582	C	-0.61567564216626	-3.20290663363340	-6.33546385609637
583	C	-0.43396120621833	-4.36239403931739	-5.56380919138511
584	H	1.92124728361844	-3.18188322286384	-3.35947424491360
585	H	-0.01697866769037	-1.14351572158167	-6.66958352531359
586	H	0.64080028690087	-5.26215211883423	-3.89687421603898
587	H	-1.33099354918481	-3.19949114568942	-7.17208821952455
588	H	-1.00902417561743	-5.27299004765337	-5.79098027241275
589	C	3.76855374764228	-1.10838770732060	-4.59158113424521
590	C	4.70647537264220	-0.40416130132178	-3.81004678450093
591	C	4.18335803671983	-2.20276910585733	-5.37851694716860
592	C	6.05461712289443	-0.79146876133672	-3.81993702665793
593	C	5.53322003111878	-2.58745363762415	-5.37976795936162
594	C	6.46832623741573	-1.88339858187930	-4.60193274993346
595	H	4.36699606546839	0.43750929622085	-3.18509138273489
596	H	3.44956265077519	-2.75547789628112	-5.98389389764695
597	H	6.78316235241981	-0.24291805698801	-3.20439910217011
598	H	5.85549144517545	-3.44652831866314	-5.98795016691798
599	H	7.52483260031547	-2.19277946151707	-4.59975046736166

ACN

601	C	-1.48024146029218	-0.16076550656092	0.06585695827409
602	N	-0.47908787542501	0.11200858122096	-0.47683779463074
603	C	-2.72713076308486	-0.51024256037803	0.74084869062426
604	H	-3.35055546192378	0.39306658571146	0.89596279674507
605	H	-2.51622705271691	-0.96467025471045	1.72943968972708
606	H	-3.30411513555726	-1.23693083728301	0.13408140926025

PPh₃

607	P	2.60407466187921	-0.89481285564782	-5.00065388134421
608	C	2.37792119282937	0.42608546344932	-6.27884934940362
609	C	3.42160252971759	0.93509949298472	-7.07965575315942
610	C	1.07430344115574	0.94749188240075	-6.44027700634562

614	C	3.16382628203933	1.94074422999379	-8.02650883940949
615	C	0.81586967094789	1.94041606023586	-7.39704584333671
616	C	1.86207584126884	2.44279098037970	-8.19085141764980
617	H	4.44117041884073	0.53930348060905	-6.96216124464544
618	H	0.25550325295826	0.56534720774269	-5.80932464770750
619	H	3.98805033547039	2.33213845687251	-8.64268221784386
620	H	-0.20565861081530	2.33324942044258	-7.51629913504784
621	H	1.66217644691243	3.23072128601502	-8.93351205918807
622	C	2.11297361414124	-2.40177389937156	-5.95879347774677
623	C	2.00496385374478	-3.61363689876181	-5.23973856967205
624	C	1.83527982274181	-2.40059591741708	-7.34190247124607
625	C	1.64678822605305	-4.80229844027187	-5.89330584221699
626	C	1.46219252246697	-3.58938963377876	-7.99178917343968
627	C	1.37043866261748	-4.79214028014476	-7.27200665615589
628	H	2.20955635944931	-3.62177366060170	-4.15650519199213
629	H	1.91357962642856	-1.46318634421704	-7.91274517542110
630	H	1.57161550504881	-5.74045044003420	-5.32163457931626
631	H	1.24333487321823	-3.57435994353962	-9.07077208910319
632	H	1.07759533654882	-5.72208355986666	-7.78303244160363
633	C	4.44808466879126	-1.06650929038464	-4.99201009822470
634	C	5.17060475306033	-0.19142245794401	-4.15011399758501
635	C	5.15536641453841	-2.00984153003603	-5.76652694797646
636	C	6.57187961043385	-0.24404332532730	-4.09927580316565
637	C	6.55772365253631	-2.07083317026324	-5.70381669624981
638	C	7.26918505606166	-1.18761446088392	-4.87435132254863
639	H	4.62381923607836	0.53913221022400	-3.53157392246080
640	H	4.60328475488829	-2.69885341155153	-6.42361594195211
641	H	7.12314038423043	0.44787836137534	-3.44351382843020
642	H	7.09907553272815	-2.81340806320218	-6.31078543740240
643	H	8.36851811598941	-1.23802808247959	-4.82648551300886

Monomer mechanism (catalysts I and XV)

646	pd_monomer_9-trans-initial			
647	Pd	1.00955630380667	0.90499070482364	-0.31455693990091
648	Cl	1.45402390096353	-1.04001859938959	0.93629005042008
649	Cl	0.77168438075630	2.76767576307060	-1.74953250918386
650	C	1.28001580821944	2.33863402526738	1.29481040738557
651	C	-0.05239053955687	1.90278084224374	1.60440854459545
652	H	1.36415599716462	3.27118939436723	0.71110176913629
653	C	2.48896848765069	1.89379188850364	1.95967287488316
654	H	2.42384625874152	0.98345570145482	2.57151218264227
655	C	3.70233443629425	2.50411781116155	1.78168600334221
656	H	3.75475340469688	3.40655547306472	1.14870573263136
657	C	4.95485781186600	2.02345453637771	2.33633024752544
658	C	6.10131265416979	2.74577213074346	2.07953402137156
659	H	6.02619649941583	3.66700701474420	1.47633762825209
660	C	7.45760017718745	2.43051161339330	2.52374856306795
661	O	8.43669734950947	3.12543574489310	2.26348279122371
662	H	7.57564059417352	1.48835069073572	3.13783619797766
663	C	4.92605566715367	0.74722061685224	3.14364206180139
664	H	4.29517683880001	0.87606743647312	4.04791455385985
665	H	4.46667173473098	-0.07072415437749	2.55019622005628
666	H	5.92729748390086	0.42153566296690	3.47321892315167
667	C	-0.32207790387770	0.95846908944756	2.74731879273555
668	H	-0.49554926434409	1.56022890833213	3.66626800264275
669	H	-1.22068722708755	0.34172788824482	2.56351956248679
670	H	0.51674300010294	0.26466655731827	2.92315388352114
671	C	-1.15634686833364	2.58459268696977	0.96089237985192
672	H	-0.86617404289267	3.25488425285884	0.14207867462331
673	C	-2.47355685961457	2.43266607673425	1.32067568348100
674	H	-2.66349986592033	1.77298200013297	2.17996822108107
675	C	1.14127688949365	-0.92088051598848	-2.90923370008473
676	N	1.05935256664733	-0.26477434420125	-1.95052624766499
677	C	1.24752197258537	-1.74148692028615	-4.10292051181461
678	H	0.24171047972833	-2.07652077821814	-4.42505704678193
679	H	1.87277892984927	-2.63285882648097	-3.89685750208396
680	H	1.70955410647291	-1.15816716395425	-4.92433734358313
681	C	-4.80753425226795	3.08383114607822	1.51812954649154
682	C	-6.07122071509033	3.78635186402381	1.08218817576420
683	C	-5.90792972889108	4.67369069114278	-0.14873955727402
684	C	-5.05797835812804	3.93338309442260	-1.17585217316823
685	C	-3.61595647675982	3.65201532903685	-0.67944941673738

686	C	-3.65581925838579	3.05715141695123	0.74964298995894
687	H	-6.47448987951817	4.36002636740429	1.94712221721614
688	H	-6.84050184957950	2.99977931105028	0.88707859002324
689	H	-6.90024308861612	4.94139417174841	-0.56600006617697
690	H	-5.42076379451753	5.63109861940811	0.13356936333578
691	H	-4.99566280037130	4.49651948167028	-2.13046485536846
692	H	-5.54859278450111	2.96310939447288	-1.41569298257370
693	C	-4.92473592634565	2.46791147256593	2.89288167060995
694	H	-4.29481844264157	1.57113906162610	3.04299694940735
695	H	-4.64277624463513	3.20112471436891	3.68083976617963
696	H	-5.97584667423194	2.17754381194569	3.09489644600833
697	C	-2.80952284799592	4.97498592270717	-0.71511990736414
698	H	-1.74034857170252	4.82720704544882	-0.47800622306515
699	H	-2.85643441017659	5.41523167710189	-1.73314968576367
700	H	-3.21149032933961	5.71908875826233	0.00135997548103
701	C	-2.99831581429586	2.63686897960100	-1.67176774797988
702	H	-3.14026687771293	3.00834257981876	-2.70851004071238
703	H	-1.91224607013510	2.48175348912411	-1.53451534670048
704	H	-3.50658996661434	1.65378439174008	-1.59271386024104
705				
706	pd_monomer_9-ts			
707	Pd	1.44827074845956	2.49386898802312	-0.91224863393554
708	Cl	2.12581208995367	0.27017572922236	-0.87108956576442
709	Cl	0.59585839139686	4.69746463987139	-1.00777813517786
710	C	1.35217340772782	2.48296479495352	1.26469732970489
711	C	0.13880562536298	3.00058913822672	1.83417892929043
712	H	1.83712012318297	3.32497642703008	0.60660553244296
713	C	2.37665953469513	1.87518048548973	2.07641557916976
714	H	2.05108059960862	1.46837704158583	3.04782075501474
715	C	3.68363993785397	1.69617281490743	1.68776031221462
716	H	3.98923812852985	2.07984338831108	0.70082267003171
717	C	4.69915674897566	1.00686771538164	2.45107849916643
718	C	5.97378089741270	0.93936348092941	1.92145930601349
719	H	6.16445484415123	1.40258527018901	0.93873172096406
720	C	7.14391839791273	0.30491721231169	2.52175253124078
721	O	8.25447910319725	0.28699894294715	1.99436094591454
722	H	6.98640644567255	-0.18839378610107	3.52676404798137
723	C	4.31564521010741	0.39168055915413	3.77689076547358
724	H	3.88218342239105	1.15789002273223	4.45262351879965
725	H	3.53791352158585	-0.38623419598906	3.62770412539971
726	H	5.16991727725655	-0.07478014795176	4.29738541705025
727	C	0.14099327344903	3.43236142718203	3.28092481924463
728	H	1.14538841902945	3.76483683025503	3.602408014445138
729	H	-0.56516920530022	4.27265776626316	3.43525627218442
730	H	-0.18241285787792	2.61031290655759	3.95738375897918
731	C	-1.08697436108718	2.75237533294468	1.15933200201222
732	H	-0.96502060926325	2.35200816899399	0.14614780469515
733	C	-2.35515520862113	2.96602868382557	1.66776209519705
734	H	-2.40675670434426	3.39569991976973	2.67825513195676
735	C	1.49292084235594	2.33175175581252	-4.08262271718707
736	N	1.48512742114013	2.43125607561586	-2.92214463246966
737	C	1.50864667241764	2.19964613488225	-5.52908577992663
738	H	0.47761478186142	2.26590069011605	-5.92966808192455
739	H	1.94208223731022	1.22034612571988	-5.81486270660091
740	H	2.11850161052334	3.00777766515042	-5.98009775050248
741	C	-4.77591891778753	3.11740641590481	1.69455259413985
742	C	-6.13819411203963	3.12519122363795	1.04767499158556
743	C	-6.10725323497784	2.95118847952708	-0.46724259485026
744	C	-5.15123908670432	1.81315116311549	-0.80476690849504
745	C	-3.68190240426404	2.11139978127633	-0.40077632063484
746	C	-3.62483346199194	2.72504860312900	1.02099316068737
747	H	-6.66191128651104	4.06434623108813	1.34015417052546
748	H	-6.74640485284534	2.31276888587652	1.51643384732202
749	H	-7.12656976283456	2.74842085473099	-0.85548792455835
750	H	-5.76862518389201	3.89355528311508	-0.94810413716200
751	H	-5.17176981559311	1.57487833255159	-1.88868378258015
752	H	-5.49116441896220	0.89466675840443	-0.27554293465721
753	C	-4.79555240752410	3.62194982131249	3.11768018662854
754	H	-3.99446267897272	3.20775629511289	3.75668754772933
755	H	-4.71271629792630	4.73164968361630	3.14674251650733
756	H	-5.76617429209910	3.37066614687812	3.59295368761218
757	C	-3.07032907678659	3.08533175859530	-1.43975306333366
758	H	-2.04062828674979	3.40849376951231	-1.19603350625708
759	H	-3.04353877527121	2.59887610211900	-2.43686039433583

760	H	-3.68141618918461	4.00481712693762	-1.52553512325560
761	C	-2.94978631759283	0.74407614998921	-0.44453528114062
762	H	-3.17291426435408	0.24237503440591	-1.40968649356123
763	H	-1.85006459566341	0.81471462059522	-0.36354921989968
764	H	-3.30751504649951	0.08046947425505	0.36976710087918

765
766 **pd_monomer_9-cis-final**

767	Pd	1.61668925908240	1.38130015112732	-0.88017660924650
768	Cl	2.22843365067868	-0.71998506957614	0.05814534770457
769	Cl	1.26297178921569	3.39719721667352	-2.01148589691630
770	C	1.72659699871338	2.52123009427740	0.96244755749184
771	C	0.36504660394337	2.06951465898873	1.04576164075863
772	H	1.86703400331134	3.54814085092709	0.58529452969309
773	C	2.85984336085750	1.94380737831771	1.66226037484035
774	H	2.72334246255373	0.95585352472136	2.12182615893834
775	C	4.09086023471774	2.53869752825995	1.71132447336491
776	H	4.22788810328777	3.52387771958883	1.23386243234228
777	C	5.26390221649070	1.93678050465116	2.32054905356425
778	C	6.44374970361147	2.65026146183862	2.31502257381159
779	H	6.45649620581559	3.65516267272588	1.86025006156200
780	C	7.73072508969847	2.22163647720321	2.86020938897625
781	O	8.74526112578544	2.91423881656292	2.83163083123258
782	H	7.75711566505145	1.19255509994495	3.32751143885800
783	C	5.12057546013711	0.55058777391409	2.90265645750690
784	H	4.41854775349413	0.56295394388429	3.76317823542394
785	H	4.68666730404317	-0.13655234471400	2.14684460116194
786	H	6.07853411212117	0.13054426293966	3.25319485349830
787	C	-0.72827808919957	3.02007906378232	0.61450138244076
788	H	-1.54028477207026	2.49601858418396	0.07407981163735
789	H	-1.17444639006977	3.49116726231038	1.51678292172493
790	H	-0.33294666619589	3.80651951199070	-0.05202174711779
791	C	0.01325281192362	0.87116813071133	1.77767769857526
792	H	0.84380374606566	0.22237442574060	2.07074854539310
793	C	-1.27945492770167	0.52914297395532	2.09285849762499
794	H	-2.05614104707729	1.19880872272189	1.70007583922401
795	C	2.07097908118076	0.00930475835447	-3.71214675851635
796	N	1.85763500058940	0.49119346059966	-2.67362888123911
797	C	2.34017101235510	-0.59253390072151	-5.00623349015776
798	H	1.43178046474686	-1.10249402078181	-5.38500208213786
799	H	3.15661860742024	-1.33679880768576	-4.91487503240310
800	H	2.64114517555777	0.18802640165623	-5.73301737281307
801	C	-3.16015915833773	-0.78493931196670	2.87865331842318
802	C	-3.81570154950330	-1.99359527012117	3.50205090588132
803	C	-2.85166268814619	-3.12836894303534	3.83582592189270
804	C	-1.60967643293315	-2.53928150930975	4.49386387540114
805	C	-0.82282970903268	-1.58420239684103	3.55755522163484
806	C	-1.78664610079107	-0.60306104496610	2.84929018548521
807	H	-4.63132622565032	-2.33935607829479	2.82706900954294
808	H	-4.34628161783022	-1.65369518235771	4.42504889678420
809	H	-3.34171595109792	-3.87293049261246	4.49674894994741
810	H	-2.57156363071078	-3.66982875392588	2.90696529595959
811	H	-0.91892143011838	-3.33695344365810	4.83920566301679
812	H	-1.91892262200206	-1.97766750288314	5.40411242273520
813	C	-4.15828957102987	0.16970978208769	2.26226411815854
814	H	-5.13465170882447	0.08500146472979	2.78050198459543
815	H	-3.85289389476568	1.23231782039613	2.30058038775206
816	H	-4.34551822172447	-0.08443438246205	1.19474116831995
817	C	-0.05314718797327	-2.42384733812423	2.50922488914127
818	H	0.50556215230099	-1.80710473186411	1.77934339519817
819	H	0.67730941935082	-3.08746107186959	3.01792662721760
820	H	-0.74633638552501	-3.06425215442260	1.92725775473467
821	C	0.17198548740218	-0.82715086760272	4.47193307588179
822	H	0.73185653904216	-1.55957940614286	5.09024297666959
823	H	0.91755307269645	-0.22800073947596	3.91901881673032
824	H	-0.36733269493115	-0.14447673435170	5.16068830209375

825
826 **pd_monomer_11-trans-initial**

827	Pd	3.33301608881701	0.57735943058388	0.09094493982322
828	Cl	3.24729340180431	-1.06507270472262	1.78870077616015
829	Cl	3.36075521335437	2.05985219586891	-1.73236606881040
830	C	1.28375746005773	2.43621693420551	1.06732944702113
831	C	0.01257713210196	1.98355165306478	1.39004869189839
832	H	1.38284595690996	3.20048263825036	0.27856472278979

833	C	2.49824572816947	1.94347708720853	1.65379586119982
834	H	2.40921751897341	1.30108786112732	2.54236972781409
835	C	3.80071190678405	2.36369619345419	1.27133368036308
836	H	3.87402061113146	3.11883913858652	0.47183369704809
837	C	5.03321976295516	2.15242927701608	2.04482819290907
838	C	6.19674064510528	2.63265183276213	1.48777048717528
839	H	6.15606387892928	3.10752821080154	0.49342988623294
840	C	7.53517135062066	2.56187284190419	2.07710956851300
841	O	8.54071616234886	3.00201185981885	1.52740176152702
842	H	7.60704849576622	2.07218445986730	3.09280270211697
843	C	4.94209302493937	1.46454165690879	3.37841710832435
844	H	4.25958760500476	2.02534572468485	4.05187340448859
845	H	4.50553186467477	0.45102568143311	3.24094007099417
846	H	5.92080338080695	1.36307517746173	3.87708799391987
847	C	-0.20463667795989	0.85187263022005	2.36528676069115
848	H	-0.48821391096633	1.23396691290938	3.36960294289120
849	H	-1.03087681843314	0.19532332957667	2.02784990010499
850	H	0.69328575312214	0.21335816115696	2.47096491650920
851	C	-1.11146450656188	2.63141715224720	0.75241779990730
852	H	-0.83802288933667	3.43171600622794	0.04960969297499
853	C	-2.43221695165627	2.33756533552268	0.99608459823854
854	H	-2.60220440016368	1.54559192965340	1.74031877695845
855	C	3.40017256843402	-1.81869567218208	-1.99783930710193
856	N	3.34553637768939	-0.94350014036247	-1.23177456865141
857	C	3.47789197857173	-2.91623435683585	-2.94551124494005
858	H	3.10365533530966	-2.59286359037985	-3.93708294274768
859	H	2.86728889242739	-3.76947880373460	-2.58829729920333
860	H	4.52964186925821	-3.24933243180176	-3.04918516577361
861	C	-4.85002681831478	2.57124090029063	1.05238339569231
862	C	-6.16489553387188	3.23396843625117	0.71550640204017
863	C	-6.02508827302977	4.52504610322067	-0.08582425263920
864	C	-5.01234829377850	4.29784321673423	-1.20215091098915
865	C	-3.58913041649092	3.97629136795376	-0.67590241401426
866	C	-3.64853807480077	2.93965946430502	0.47102286470724
867	H	-6.72483622921396	3.40462915217648	1.66303336145409
868	H	-6.78940848892549	2.49866783235343	0.15192423862993
869	H	-7.00757640648903	4.83778121259202	-0.49509911417406
870	H	-5.68837686010558	5.34774171827649	0.58106126821699
871	H	-4.94642483745548	5.17831770048667	-1.87611926129377
872	H	-5.36163284316392	3.44888188217723	-1.83172155427887
873	C	-4.98252913883953	1.50554670907378	2.11771828503836
874	H	-4.27586899585244	0.66250736068600	1.99958941186619
875	H	-4.82568033501544	1.92935857266105	3.13476327384264
876	H	-6.00778397988551	1.08248702831993	2.10871007268661
877	C	-2.93525374140316	5.29137285797311	-0.18097346716242
878	H	-1.91913852237194	5.13122416912029	0.22403274808027
879	H	-2.85609063647071	6.01926513247863	-1.01544747580018
880	H	-3.53624454827442	5.75511356340691	0.62632472230335
881	C	-2.80489418941861	3.41335245555494	-1.88784739531895
882	H	-2.89776142051167	4.11210476748423	-2.74577521956125
883	H	-1.72762898352000	3.26906289338503	-1.69190965945010
884	H	-3.22158324178620	2.43420689053467	-2.20087983124235

pd_monomer_11-ts				
886	Pd	3.92886669325444	2.04068651608574	-0.78669531830031
887	Cl	4.50802574310250	-0.21133587547890	-0.89922706226789
888	Cl	3.18048393859173	4.27332661777802	-0.72616946089968
889	C	1.27232180807084	2.28781466167473	1.34903009877922
890	C	0.05143632117469	2.59304675760515	1.96880184335559
891	H	1.23321830742541	1.95842859641079	0.29750703583411
892	C	2.54899010754066	2.35710508187083	1.93250484320371
893	H	2.56121578633846	2.47928196092052	3.03352847200391
894	C	3.75655074105552	1.85697951427371	1.36629285777792
895	H	4.31939851673515	2.72036832242967	0.80835532322549
896	C	4.73985843852458	1.12733342768442	2.16599650209991
897	C	6.05298675435443	1.06664968434987	1.75004748443368
898	H	6.35106754911694	1.60770720930356	0.83672967113036
899	C	7.13272100293727	0.31362035785492	2.38106062991244
900	O	8.30169521471861	0.35449267729494	2.00476900732276
901	H	6.84345967604481	-0.33536157849506	3.26133419905666
902	C	4.22478511258734	0.42940503867905	3.40072427284364
903	H	3.93897735968087	1.16866033333853	4.17950258878538
904	H	3.31149026626948	-0.15100330687921	3.15635983796990
905	H	4.96856948310986	-0.25139488900037	3.85127774090174

907	C	-0.03308344031867	3.12525905391266	3.37530392824359
908	H	0.93778376340180	3.08723294128531	3.90106403237849
909	H	-0.35803720882791	4.18721314216392	3.36710752461693
910	H	-0.77377139607957	2.56161522393128	3.97823131715676
911	C	-1.14578250733267	2.38524055119422	1.20371388586598
912	H	-0.98291522623472	2.00268273149068	0.18709657761269
913	C	-2.42073039202201	2.67411772028754	1.64945297053401
914	H	-2.47394408302687	3.09061248524457	2.66471293105109
915	C	4.16046820008148	2.08706164699971	-3.94909878396091
916	N	4.05408581866813	2.12040861921111	-2.78972643329894
917	C	4.30441743154083	2.03436317643937	-5.39358614318039
918	H	5.02882615039610	2.80184513587981	-5.73236634007589
919	H	3.32878342040714	2.22419257507241	-5.88371831329843
920	H	4.67136769033533	1.03421812807241	-5.69957810814315
921	C	-4.80085727125947	3.13856620282193	1.60530393031543
922	C	-6.15146911383245	3.26498658588915	0.94477295902535
923	C	-6.13914257313694	3.00038848282262	-0.55750127075473
924	C	-5.30517720717637	1.75307895377900	-0.82710369239126
925	C	-3.81678781650627	1.92103835499725	-0.42293516424757
926	C	-3.69892490197897	2.58286926596336	0.97051082624410
927	H	-6.56079376613956	4.27478436803309	1.17556714052355
928	H	-6.85197164031094	2.55959158870679	1.45535747099613
929	H	-7.17350549951418	2.88111795492527	-0.93994134673813
930	H	-5.70604243064428	3.87357254659454	-1.09039103490476
931	H	-5.34635503599948	1.46245894588280	-1.89774449195235
932	H	-5.73820239969081	0.90363730904096	-0.25343857652109
933	C	-4.76708964511640	3.72040967705026	3.00051058007995
934	H	-4.09896590413790	3.17808916904463	3.69596043843716
935	H	-4.43771426140470	4.78299298307755	2.98291538659104
936	H	-5.78400240399596	3.71349893974039	3.44229795772064
937	C	-3.10561161703185	2.78487549318186	-1.49350392822636
938	H	-2.04749389926780	2.98589750872705	-1.24416830778021
939	H	-3.13194455294688	2.27213291121779	-2.47726327486194
940	H	-3.60250839400722	3.76857450530985	-1.60764922490689
941	C	-3.21763700922914	0.49323470910882	-0.39868864457469
942	H	-3.42478056135540	-0.01373509350263	-1.36429480804388
943	H	-2.12410126759976	0.47480072663209	-0.24360567516276
944	H	-3.68199486933925	-0.11020132793035	0.40777413846320
945				
946	pd_monomer_11-cis-final			
947	Pd	3.32829341143804	-0.11409291771986	1.08930654883129
948	Cl	4.94761934140169	-0.27614122729073	2.79234072212172
949	Cl	1.70789965750088	-0.09589320481559	-0.60208864256512
950	C	2.57351382435361	2.05092040244819	3.07600526600173
951	C	1.44123373644988	1.97799810893967	3.87576131914182
952	H	3.53807638707870	2.13228370858654	3.59191776914550
953	C	2.57262872666862	1.92936736759737	1.64696084258252
954	H	1.58603238438292	1.87347133676710	1.16039610227121
955	C	3.64531550603082	2.01143743357058	0.70786659428394
956	H	3.30502663006955	2.00801223787222	-0.34176635071620
957	C	5.03394596358073	2.48052839891397	0.85853631232839
958	C	5.79848622218484	2.45593921530029	-0.28529858433798
959	H	5.35493131391382	2.06795645742699	-1.21790019414867
960	C	7.19607215190082	2.87250557232490	-0.41195361399310
961	O	7.82665347596439	2.81259598832815	-1.46364377102482
962	H	7.69028193944355	3.26113492003253	0.52687382420875
963	C	5.52783543797602	2.98922008999243	2.18402962064087
964	H	4.81614588197377	3.72877512530385	2.60440745156118
965	H	5.58921365159523	2.13194726641756	2.88707084504122
966	H	6.52314897995096	3.46090168938135	2.11259990492154
967	C	0.05505432577341	1.75865242736354	3.32578469179552
968	H	-0.41265310828853	0.87421673026665	3.80601131332857
969	H	-0.60342832677946	2.62747631436557	3.53888144288427
970	H	0.04837146210596	1.57769873367406	2.23609016706861
971	C	1.63372883090227	2.09446736137304	5.30417718612221
972	H	2.68006084887670	2.22205554449299	5.61441409002492
973	C	0.63153420409451	2.02863501945380	6.24183045462478
974	H	-0.37719512058347	1.86690917543389	5.83605243218661
975	C	3.34204655398628	-3.29608279743235	1.00193152744787
976	N	3.30457533502057	-2.13396651598385	1.06611455125425
977	C	3.39086141382680	-4.74503433357773	0.91544838175446
978	H	2.95363939365196	-5.08315717339708	-0.04514810400431
979	H	2.81809122466698	-5.19676222048611	1.74981928615568
980	H	4.44145676671948	-5.09207521729036	0.97583659781514

981	C	-0.45976407476018	1.79680739612050	8.40185806211012
982	C	-0.48683436842762	1.63751029276628	9.90348793118851
983	C	0.89380461773657	1.51071385880513	10.53934548435476
984	C	1.80488624878165	2.57551685482490	9.94015392834760
985	C	2.02984479069338	2.39337304117822	8.41575151540112
986	C	0.69799537961796	2.07539757715479	7.69506901356246
987	H	-1.12820907170090	0.76135317978842	10.15183765993980
988	H	-1.03078733134177	2.51272899284562	10.33652373249298
989	H	0.82650946776642	1.61507867110995	11.64172492220553
990	H	1.30681229564501	0.49695601972171	10.34357015871974
991	H	2.79607069993779	2.58902413813723	10.43988446485912
992	H	1.34985140073776	3.57550915639904	10.12121072463974
993	C	-1.81150854481372	1.57535930541984	7.76120674854715
994	H	-1.97500762015129	2.16716756174300	6.84141358077982
995	H	-1.96241899283285	0.50411362308558	7.50079924124121
996	H	-2.61814844159062	1.84032054822167	8.47478721164560
997	C	3.04957577685387	1.24681521252356	8.20255502035791
998	H	3.25080091691097	1.04405429303838	7.13460864736161
999	H	4.01457584364123	1.49954305649652	8.68895730847291
1000	H	2.68278438902486	0.29949830964710	8.64587718085552
1001	C	2.61662947983507	3.73466265683673	7.90953352832440
1002	H	3.50314562032809	4.00632953479154	8.51915248966548
1003	H	2.93656810007724	3.70673885657032	6.85257786804471
1004	H	1.86992725219881	4.54817471214038	8.01246484012774
1005				
1006	pd_monomer_13-trans-initial			
1007	Pd	6.43630697925436	1.04012832274585	0.27438146398473
1008	Cl	7.42263377965204	-0.63303550362830	1.59511806200608
1009	Cl	5.63912161536944	2.69596541313884	-1.18782637853342
1010	C	1.40512918860433	2.37819560005076	1.30140193926534
1011	C	0.07986851071450	2.06612640156084	1.59103953976935
1012	H	1.57997920806273	3.11692392469301	0.49917612228456
1013	C	2.56943662391571	1.85765979620258	1.93274278059583
1014	H	2.44190851861192	1.10111615201614	2.72407090188907
1015	C	3.84691024131534	2.27279762046119	1.60304416947333
1016	H	3.96693465652666	3.01068642582922	0.79196418897577
1017	C	5.06231747422691	1.80938725352222	2.21747240974788
1018	C	6.28970792612049	2.46564093840233	1.85772321681032
1019	H	6.20281584442270	3.40330091352518	1.28160221810454
1020	C	7.54412790530129	2.40173750305621	2.66380643579501
1021	O	8.41626968540162	3.25244756073823	2.56706462710140
1022	H	7.64766706291493	1.53418288172130	3.37027097812272
1023	C	5.01597915919570	0.80920690946338	3.34268252086715
1024	H	4.97511150418659	1.35373245098637	4.31094912360106
1025	H	4.12779667655670	0.15409631965782	3.28082370228539
1026	H	5.91228569232067	0.16098591095072	3.33651500451538
1027	C	-0.30877354775438	1.08274470543525	2.66613873007814
1028	H	-0.90499178110582	1.58073489205985	3.45976982558530
1029	H	-0.94415867327707	0.27336441450764	2.25022861872734
1030	H	0.56488607743316	0.611777818479986	3.14888420991923
1031	C	-0.95205357318602	2.72949552234384	0.82981544897222
1032	H	-0.58390088410827	3.41666870325231	0.05430306047954
1033	C	-2.30390569542496	2.57497875710284	1.03809155499954
1034	H	-2.57430159887408	1.89683823615803	1.86093203665016
1035	C	6.71028149845556	-0.93519387874525	-2.19753852369263
1036	N	6.64382616750647	-0.19584062284327	-1.30001233022078
1037	C	6.80692272337920	-1.83516227521655	-3.33389495982984
1038	H	5.80437686344140	-2.22679840523505	-3.59666614323999
1039	H	7.47242703169634	-2.68744227843386	-3.09175176639279
1040	H	7.21835345300524	-1.29476124168564	-4.20980645239034
1041	C	-4.68912959932598	3.03480881450054	0.95456392312488
1042	C	-5.92189247074428	3.75990999622019	0.46896979036855
1043	C	-5.63283489764867	4.90490034980859	-0.49723583384691
1044	C	-4.61028871626917	4.42974022815370	-1.52315902948779
1045	C	-3.24248826169418	4.06468393954483	-0.88961104243392
1046	C	-3.43837183923609	3.20809591949664	0.38399498715397
1047	H	-6.49316051495824	4.11502788829229	1.35640067730281
1048	H	-6.59450647816678	3.00941555914615	-0.01461901389855
1049	H	-6.56722489729752	5.24420903312825	-0.98921995749350
1050	H	-5.23868947761937	5.78000517449846	0.06270208986896
1051	H	-4.44035252427077	5.19304020158725	-2.31146151749234
1052	H	-5.01744794991670	3.53217364192597	-2.04041148873432
1053	C	4.95994802947212	2.14983845475074	2.15069309669484
1054	H	-4.32967814737095	1.24180383514156	2.19236439850779

1055	H	-4.80684895277675	2.70498613391686	3.10304371946661
1056	H	-6.01781881913261	1.81820560200936	2.14777297057582
1057	C	-2.48906898613918	5.37576967441788	-0.55158458019572
1058	H	-1.51679956576047	5.19238417489957	-0.05804614304230
1059	H	-2.29436349453459	5.95549580604381	-1.47772783403374
1060	H	-3.08316442627244	6.01284081456927	0.13392816309749
1061	C	-2.47094562573766	3.26710923243073	-1.96979420838534
1062	H	-2.45252176269791	3.84784917357331	-2.91502957422713
1063	H	-1.42480819870425	3.04653619616576	-1.69347214971917
1064	H	-2.97381767811479	2.30017164718443	-2.17434277947757
1065				

pd_monomer_13-ts

1066	Pd	6.37481468736306	1.28340912625535	-0.12300625683883
1067	Cl	6.47507328170980	-1.03722916203849	-0.33873463395751
1068	Cl	6.05809143269430	3.61254913029277	0.11315871912893
1069	C	1.38827135679210	2.08849690996382	1.65166990389140
1070	C	0.08888564723811	2.33165115122727	2.09717351643182
1071	H	1.54182047683711	2.05782236426368	0.55848904230421
1072	C	2.54361533924161	1.88613271114329	2.44925869213839
1073	H	2.43336814929288	1.91562529117780	3.54585422323185
1074	C	3.79787521310436	1.63030884999368	1.90943189628146
1075	H	3.90419295751840	1.61993919285810	0.81138458872010
1076	C	4.97779123814558	1.34810876011359	2.65345215731712
1077	C	6.16504095712354	0.93515583624884	1.98120077663017
1078	H	6.71947287854464	1.87012889922656	1.55907704579985
1079	C	7.17518189011487	0.05856656990587	2.62884896919208
1080	O	8.36531598909123	0.04099692619891	2.35788190575527
1081	H	6.75299176188816	-0.64433522367704	3.40917985086583
1082	C	4.89499053717427	1.19749896833011	4.15685815273492
1083	H	5.89055722826978	1.24418151334972	4.63368920554327
1084	H	4.27590111986837	2.00278344058616	4.59986958811476
1085	H	4.42304024110714	0.23090554016635	4.43950632654136
1086	C	-0.26946897726951	2.39187841838037	3.56058553715846
1087	H	-0.67388012853269	3.39080246978018	3.82656294820645
1088	H	-1.05824095843371	1.65013911357941	3.80416197585096
1089	H	0.59267180996126	2.19363016121574	4.22108225581115
1090	C	-0.93720296500807	2.53664829569418	1.10578303301601
1091	H	-0.59085738056450	2.48337553810145	0.06361801738937
1092	C	-2.25855515351100	2.80375515405530	1.39077576771444
1093	H	-2.49832793774578	2.86985620378909	2.46182830160482
1094	C	6.73009403986543	1.47638439547986	-3.26231431233235
1095	N	6.57936783139573	1.45813386684154	-2.10714785182030
1096	C	6.92783296685202	1.48572378136541	-4.70153572748369
1097	H	6.14366242936746	2.09384917454433	-5.19490072698866
1098	H	6.88268123824255	0.45104236983125	-5.09609951257285
1099	H	7.91941069065474	1.91669852726336	-4.94628028807086
1100	C	-4.56652910689707	3.49611038044622	1.09276365482565
1101	C	-5.75742442470653	3.95888095580344	0.28895191287059
1102	C	-5.46309372744758	4.18923751188152	-1.18994754682445
1103	C	-4.63599050893808	3.01983565308090	-1.71048599515690
1104	C	-3.25055785401334	2.90455424387872	-1.02243525452253
1105	C	-3.38366066289212	3.06638801193920	0.51032246388638
1106	H	-6.16832572351290	4.87686355069177	0.76684087878820
1107	H	-6.56751929454046	3.19808835420384	0.40633370855213
1108	H	-6.40656668275957	4.29938890815121	-1.76204289168403
1109	H	-4.90474133264047	5.14141453408606	-1.31821274266977
1110	H	-4.47774271539553	3.09047578415480	-2.80711896529237
1111	H	-5.20192559987827	2.07715381719131	-1.53444641638804
1112	C	-4.78877438311827	3.59597698216842	2.58481016943016
1113	H	-4.26419379738471	2.81899073948520	3.17218710258453
1114	H	-4.45956828989170	4.58533810636195	2.97384104122850
1115	H	-5.87017511972384	3.51254780051887	2.81561383951880
1116	C	-2.31573088622985	3.99681212502559	-1.99886618270118
1117	H	-1.31394909824475	3.98758346670387	-1.13164255898967
1118	H	-2.18235324893288	3.84999511095262	-2.69109569321314
1119	H	-2.73761897153528	5.00959139533469	-1.43871798557444
1120	C	-2.71714720317829	1.49565394101610	-1.38299933059027
1121	H	-2.75866525952861	1.35530365314273	-2.48299515547008
1122	H	-1.67419660268642	1.32087652711594	-1.06500313181875
1123	H	-3.34390439431689	0.71001318115734	-0.91478300809876
1124				
1125				

pd_monomer_13-cis-final

1126	Pd	6.04085993407688	1.42190839729974	-0.01223721441198
1127				

1128	CI	7.30624325969731	-0.40360191106221	0.78345552657564
1129	CI	4.93818373367339	3.20743464012305	-1.04168106544412
1130	C	4.72084029806404	-0.37630110990797	4.78579924276738
1131	C	3.75900899208801	-0.85995522801648	5.66738232931433
1132	H	5.67216432607157	-0.93382194673551	4.72943557389389
1133	C	4.61543720045261	0.76166975079401	3.93574809218410
1134	H	3.67991418142832	1.34263165193661	3.95448124151160
1135	C	5.63672404738299	1.16143170081101	3.09379220083076
1136	H	6.54326372899542	0.53985367235456	3.05086055597111
1137	C	5.58092807230689	2.31027122987030	2.22706823009296
1138	C	6.73163444762432	2.76331057547906	1.49303388522115
1139	H	6.64273472343873	3.74843625097057	1.00404477158707
1140	C	8.15199459895238	2.42325122619695	1.82137116536181
1141	O	9.08433252679232	3.08267945034285	1.39036510253146
1142	H	8.31997841964222	1.55263012249842	2.51050912037317
1143	C	4.35039378709618	3.18517384499182	2.23529303159769
1144	H	3.41935117322537	2.58931775842075	2.17532676106221
1145	H	4.32446658743877	3.76171455988862	3.18533274998157
1146	H	4.35962165454074	3.88467908032291	1.38069129624471
1147	C	2.41370221292802	-0.20182338241164	5.84337665302246
1148	H	1.59257210610412	-0.91408597700935	5.61827953043259
1149	H	2.27107956316797	0.13141903057852	6.89243941879592
1150	H	2.28214360177186	0.67827628917297	5.19026556993207
1151	C	4.07953366022226	-2.03801564009432	6.43872768507805
1152	H	5.08159421896197	-2.45157269651651	6.25742383798425
1153	C	3.22833482598653	-2.64853019337786	7.33129217761695
1154	H	2.23345505371414	-2.18819182437956	7.41861819064690
1155	C	5.30400187899410	-0.38732645996000	-2.51753610243695
1156	N	5.52159634281486	0.26112498015067	-1.57485664422900
1157	C	5.03736731325937	-1.19029404436135	-3.69862991208951
1158	H	3.96263192700180	-1.45532329275913	-3.74654679743648
1159	H	5.63561555355238	-2.12228359830859	-3.66860840393346
1160	H	5.30561291879872	-0.62028598378340	-4.61098658124705
1161	C	2.30605992296304	-4.35955877325857	8.79115307508112
1162	C	2.33182189335027	-5.66807894679256	9.54469603705222
1163	C	3.58241799371324	-6.50670447756078	9.29586355494145
1164	C	4.80362165510028	-5.59772659414024	9.36672796127270
1165	C	4.80867672341601	-4.50145621597109	8.26901818995410
1166	C	3.41560642835752	-3.83850495991646	8.14712859264721
1167	H	1.40800688512053	-6.23691074430910	9.29383101662308
1168	H	2.23082791487405	-5.44131514354466	10.63451916773530
1169	H	3.65356085647924	-7.32983194201413	10.03630795735670
1170	H	3.51922268184015	-6.98939950981328	8.29714779838525
1171	H	5.74599293035455	-6.17962504455719	9.28525809517724
1172	H	4.82376614737422	-5.10610969502461	10.36485325003173
1173	C	0.93980033878248	-3.70964938152316	8.77886234478773
1174	H	0.97123661373967	-2.60306704862239	8.79080039525255
1175	H	0.35553922103414	-4.01502776541652	7.88187535253673
1176	H	0.35251731927505	-4.03434997648996	9.66247902666106
1177	C	5.22121303210250	-5.15180452961930	6.92489277673261
1178	H	5.19757218216306	-4.43859352737801	6.07950445237833
1179	H	6.25141467718731	-5.55835889686470	6.99675450043301
1180	H	4.54201987612053	-5.98641263226662	6.66082149210187
1181	C	5.86765124936336	-3.46011459752817	8.70932647683910
1182	H	6.83017308346099	-3.97261616144109	8.91418836029730
1183	H	6.06077617597326	-2.67644793229731	7.95463571347942
1184	H	5.54732832758798	-2.95378542716965	9.64284019285892
1185				
1186	pt_monomer_9-trans-initial			
1187	Pt	0.96044568136993	0.71003526190395	-0.32597962075974
1188	CI	1.44080017344092	-1.13588677501562	1.08334182297578
1189	CI	0.73203693146409	2.44196241364007	-1.92970618065288
1190	C	1.30951542554970	2.27829093916830	1.12631156222455
1191	C	-0.03072551574701	1.85665689579442	1.44550768618854
1192	H	1.39821350990581	3.18146777277776	0.49705563605336
1193	C	2.50961789314960	1.90355974698169	1.85815538424474
1194	H	2.44112080476165	1.03341252554392	2.52618603942700
1195	C	3.71442972454597	2.52380667570251	1.67539364092815
1196	H	3.77079482535111	3.38062525630422	0.98165718752243
1197	C	4.95756803278478	2.11335417045229	2.30569707932717
1198	C	6.09770777872495	2.83857342764248	2.03273944434638
1199	H	6.02637029554151	3.70843129782124	1.35679171433394
1200	C	7.44336126612350	2.58863262403016	2.54559106063661
1201	O	8.41826677358521	3.27987211266619	2.26172196789083

1202	H	7.55714146005359	1.70280294318020	3.23976117582530
1203	C	4.92598977460010	0.90178349078909	3.20688836981243
1204	H	4.25782473516240	1.08248603872281	4.07484061748494
1205	H	4.50874445107670	0.02906662677768	2.66246413594684
1206	H	5.92093499311078	0.62623937968903	3.59601405424944
1207	C	-0.31699861394598	1.00677397374028	2.66015843752668
1208	H	-0.55788227655056	1.68509862360454	3.50677454489548
1209	H	-1.18242227901144	0.33935195164566	2.49317012541116
1210	H	0.53410189945181	0.36519821620433	2.93791954274873
1211	C	-1.13853668453872	2.55315606230967	0.80275982949606
1212	H	-0.84780084697078	3.22090915857450	-0.01806477207268
1213	C	-2.44980204914451	2.40819627086110	1.17662440566748
1214	H	-2.62951913930657	1.72193366862532	2.01608807975211
1215	C	1.09863391074670	-1.32378269847666	-2.74042909848484
1216	N	1.01234287615836	-0.58779948939259	-1.84078933143549
1217	C	1.20291868613025	-2.23877598397491	-3.86228969684845
1218	H	0.70434193457375	-1.80723433370869	-4.75294442057896
1219	H	0.72025036875396	-3.20435070982264	-3.61088341225611
1220	H	2.26856198856062	-2.42553260007413	-4.10241808955372
1221	C	-4.81057352799923	2.92343360010996	1.40101356447863
1222	C	-6.08480827005902	3.66272885169246	1.06891275488792
1223	C	-5.91129224811803	4.77656262911095	0.04025149304492
1224	C	-5.03189914291701	4.26680280058848	-1.09524220148216
1225	C	-3.59818140322709	3.89346535050436	-0.63636604674883
1226	C	-3.64539663638283	3.06390558749099	0.66731947448951
1227	H	-6.52014783697804	4.05401954945886	2.01611201363265
1228	H	-6.83277625310888	2.91477479974999	0.70852147932687
1229	H	-6.89806942267449	5.11471064691517	-0.33687064197556
1230	H	-5.44126662267989	5.66091948385844	0.52112712357179
1231	H	-4.95392129430098	5.01400152092964	-1.91333033135144
1232	H	-5.50872813229822	3.36496585725555	-1.53995765456893
1233	C	-4.93297629301847	2.05964640811321	2.63803955365044
1234	H	-4.35701773821659	1.11627550558936	2.58579099960440
1235	H	-4.59023521807970	2.60397121106953	3.54556087497206
1236	H	-5.99346340236730	1.79004212573030	2.81217008662500
1237	C	-2.79071135869334	5.19770814530709	-0.42065518611033
1238	H	-1.76549899619549	5.00374597946676	-0.05619625035365
1239	H	-2.70706919253971	5.75647382411067	-1.37578643095194
1240	H	-3.28488274345051	5.85618170369971	0.32225591250334
1241	C	-2.97660631851751	3.06331887237554	-1.78646445527182
1242	H	-3.12725038771090	3.60111498969271	-2.74639145251874
1243	H	-1.89124446315817	2.88180531110595	-1.68471018635569
1244	H	-3.47891588677077	2.07777631138615	-1.86920741537175
1245				

1246 pt_monomer_9-ts

1247	Pt	1.47410435695552	2.31359577719154	-0.99416569460729
1248	Cl	2.30069415985953	0.12503279731612	-0.90654269339697
1249	Cl	0.49505693506636	4.47289330027109	-1.18912274363103
1250	C	1.33875586128503	2.36750575988750	1.14153552755977
1251	C	0.15371518549943	2.93006626068062	1.73474752180839
1252	H	1.86247051076427	3.22907826390661	0.49845932400255
1253	C	2.37432436479045	1.79858175502432	1.98538511016040
1254	H	2.04210114489610	1.41261931122604	2.96291286681331
1255	C	3.69325399856272	1.64737461040382	1.63481543349163
1256	H	4.01979592148295	2.02518068586775	0.65241814651157
1257	C	4.70649912045815	1.00160976038537	2.44113721338898
1258	C	5.99717064145933	0.96286907903299	1.95061728862836
1259	H	6.20321971442244	1.41523104022788	0.96594421701390
1260	C	7.16703022366009	0.37371582927263	2.59575260698952
1261	O	8.29350416336349	0.38206305753985	2.10304513248022
1262	H	6.99360517816174	-0.10924873847955	3.60325700445402
1263	C	4.30152332453980	0.39929399563857	3.76626079608356
1264	H	3.83584981774106	1.16736780113475	4.41819315263143
1265	H	3.54268517231957	-0.39570005101859	3.61044207222681
1266	H	5.15122829825150	-0.04188511297067	4.31559592569494
1267	C	0.21266480660964	3.40111304100285	3.16711858210982
1268	H	-0.49070386718362	4.24079736257980	3.33349777205003
1269	H	-0.07504456712626	2.59463846068349	3.87770864902865
1270	H	1.22906819064087	3.74335071228515	3.43788801618689
1271	C	-1.10110088251932	2.72156246741660	1.09801121824271
1272	H	-1.02456258147234	2.29226340923317	0.09297431106334
1273	C	-2.34168813939165	3.00120037793630	1.64109925253935
1274	H	-2.34128249313776	3.45686085329675	2.64147517743452
1275	C	1.59261800996022	2.06748173915973	-4.14520710375231

1276	N	1.55831107879204	2.19906993072124	-2.98714858148655
1277	C	1.64847639372138	1.89839241718457	-5.58610357315277
1278	H	1.39050561770544	2.84944097348816	-6.09359021345604
1279	H	0.93230579599123	1.11514105226706	-5.90661204395467
1280	H	2.66921547726377	1.59333558273523	-5.89249876871003
1281	C	-4.74947293895687	3.26016242122258	1.75792378223912
1282	C	-6.13639448953350	3.31416427611388	1.16844039081997
1283	C	-6.17721134904380	3.10552593254510	-0.34187378991991
1284	C	-5.28386269482565	1.92144773447350	-0.69251072799941
1285	C	-3.78836581462169	2.16772574731286	-0.35688547562290
1286	C	-3.64562337762058	2.80333283667454	1.04809849411274
1287	H	-6.60500156151334	4.28198667756598	1.46026730206877
1288	H	-6.75942945645973	2.54076107201475	1.68153444308497
1289	H	-7.21958231633305	2.93793758412025	-0.68272503768082
1290	H	-5.81892555751017	4.02099640868172	-0.85877394992818
1291	H	-5.36020755573979	1.66353220703912	-1.76945885642074
1292	H	-5.63804888505922	1.02886925572728	-0.12955961718097
1293	C	-4.68206233779326	3.79748341769203	3.16839670681644
1294	H	-3.90783789800432	3.31765163112483	3.79540376394950
1295	H	-4.48500565323711	4.89300284336934	3.16863574461133
1296	H	-5.65843035592479	3.65651457449605	3.67570554440562
1297	C	-3.18175303882655	3.10022425992957	-1.43553924699991
1298	H	-2.12752912329552	3.37521137773316	-1.24121463562434
1299	H	-3.22427532027404	2.60405855790027	-2.42754548844182
1300	H	-3.75167607858474	4.04721530292265	-1.50351325660330
1301	C	-3.10945104372194	0.77411738385342	-0.40754818807131
1302	H	-3.39581360696018	0.26240558425237	-1.35045727563656
1303	H	-2.00544026349309	0.81190640578162	-0.38073567129438
1304	H	-3.44855421606010	0.13853894492427	0.43664014286890
1305				

1306 pt_monomer_9-cis-final

1307	Pt	1.57026882262484	1.35461030187913	-0.93019649104636
1308	Cl	2.20674178162796	-0.75168788244723	0.00267582561026
1309	Cl	1.21369949543877	3.38689294310491	-2.06532309280235
1310	C	1.75757104675094	2.48971702682480	0.90167015891306
1311	C	0.39149852025399	2.03071064922503	0.97106718937005
1312	H	1.89265312668368	3.52870366323419	0.55412949640183
1313	C	2.88055686734325	1.92478338318951	1.63882959029273
1314	H	2.74446034426930	0.92859966876123	2.08106855852048
1315	C	4.09746507021326	2.53704206066292	1.73209494974629
1316	H	4.23513454023336	3.52739855351087	1.26551392979628
1317	C	5.25930960849198	1.95187509588420	2.38136209582511
1318	C	6.42799860339857	2.68131108042830	2.41534357225545
1319	H	6.44257176406603	3.68582272935491	1.95968552961812
1320	C	7.70149579040430	2.27111789494393	3.00508356477778
1321	O	8.70779578189716	2.97600366350072	3.00709428476199
1322	H	7.72501728148734	1.24436395480331	3.47784982656793
1323	C	5.11534119409884	0.56440494058137	2.96030554709228
1324	H	4.36851663922313	0.56405000872124	3.78238607300322
1325	H	4.73680540963611	-0.13429034362631	2.18555964248096
1326	H	6.06227674757347	0.16470695715663	3.36141018643741
1327	C	-0.70735066119904	2.99445837467815	0.57812905164178
1328	H	-1.52707004006728	2.48192982823119	0.03874865837977
1329	H	-1.13476642967835	3.44474703706841	1.49936419306242
1330	H	-0.32274981119816	3.79501031595923	-0.07672858010341
1331	C	0.03393997193312	0.84272267339876	1.73154593548551
1332	H	0.86255355759454	0.19315644327713	2.02722054749096
1333	C	-1.25512411015759	0.51551128766428	2.06184233171382
1334	H	-2.03138131136342	1.18453021777170	1.66757630611479
1335	C	1.98708414845584	0.00680980822219	-3.75965249540718
1336	N	1.78555458212411	0.47677648781731	-2.71215113475310
1337	C	2.23633818612552	-0.58237374190128	-5.06243245921525
1338	H	1.29036040950801	-0.65092117887254	-5.63651852459062
1339	H	2.66032202841628	-1.59946869573893	-4.94387425716993
1340	H	2.95369251983033	0.04430375562283	-5.63009671084612
1341	C	-3.13706766142640	-0.78016926920908	2.88243675039531
1342	C	-3.79372044998226	-1.97968387561785	3.52407126969036
1343	C	-2.83238834416249	-3.11807711107870	3.85335423720665
1344	C	-1.57989660347150	-2.53219260790766	4.49394153342396
1345	C	-0.79865016170271	-1.58633550134437	3.54364270694824
1346	C	-1.76456180608799	-0.60675386465836	2.83652258547856
1347	H	-4.61903236237617	-2.32600993692981	2.86132435550618
1348	H	-4.31050565492413	-1.63086086495751	4.45142885208501
1349	H	-3.31855940784090	-3.85604216826053	4.52459156818594

1350	H	-2.56612005631078	-3.66693558966921	2.92454109697160
1351	H	-0.88968034640774	-3.33179577423138	4.83632718556371
1352	H	-1.87639587674581	-1.96410262462875	5.40447071358226
1353	C	-4.13819388664585	0.17286995047603	2.26824534671680
1354	H	-5.10074798676880	0.11623222860940	2.81583189244611
1355	H	-3.81798417696411	1.23173189043760	2.26828502860224
1356	H	-4.35969673366753	-0.10795432666910	1.21404780416627
1357	C	-0.04163613468132	-2.43768628284990	2.49534888578304
1358	H	0.50498277862070	-1.82930271767508	1.74983702103691
1359	H	0.69668250349004	-3.09428990211323	3.00198186499721
1360	H	-0.74197706248322	-3.08562016516030	1.93042504419649
1361	C	0.20699013630081	-0.82660906930037	4.44389707496797
1362	H	0.77015875761079	-1.55675051740813	5.06195905286495
1363	H	0.94872965281981	-0.23252721097232	3.88051020294845
1364	H	-0.32450559223258	-0.13784265177345	5.13261462680984

1365

1366 pt_monomer_11-trans-initial

1367	Pt	3.33397832133151	0.52404091116405	0.07433012659413
1368	Cl	3.25749199892592	-1.11762124989334	1.78955986533519
1369	Cl	3.34704834420085	2.00947900815975	-1.76182868209223
1370	C	1.26793912993771	2.40518620030848	1.04531340447006
1371	C	-0.00345316325596	1.96390673844749	1.36798061646442
1372	H	1.37319449312872	3.17853080001339	0.26630517622607
1373	C	2.48624681147731	1.88481415147316	1.61621538804302
1374	H	2.39205798037280	1.25565705879298	2.51453677385326
1375	C	3.79592161792650	2.30941619614864	1.24583576082546
1376	H	3.87054113866504	3.08531208988022	0.46510765178477
1377	C	5.01925039343063	2.12819673075808	2.05144726759530
1378	C	6.18257969630682	2.63128696542998	1.52004709626516
1379	H	6.15472638607541	3.10405890741778	0.52422203669282
1380	C	7.50834642632013	2.59086556296332	2.14042633501504
1381	O	8.51786386105493	3.04824447430878	1.61280057299300
1382	H	7.56561428774227	2.10807694506323	3.16030632958659
1383	C	4.91185088393392	1.43953786731699	3.38275185459644
1384	H	4.19570254652931	1.98070193531982	4.03708588837125
1385	H	4.50671999926591	0.41408974160122	3.23715612603506
1386	H	5.87959074022310	1.36614117528728	3.90763384235051
1387	C	-0.23396323306090	0.82498401050822	2.33203156942060
1388	H	-0.55788381602320	1.19693639671796	3.32760167461513
1389	H	-1.03870427690548	0.15877114233548	1.96154993417949
1390	H	0.66773243707039	0.19807832395911	2.46498625360274
1391	C	-1.12585166547387	2.62822329831467	0.73947627578641
1392	H	-0.84742866304062	3.42360796827512	0.03305525831850
1393	C	-2.44686926374265	2.35310160269901	0.99568008269879
1394	H	-2.62115194091578	1.56760453862556	1.74606213960877
1395	C	3.48901628196541	-1.85957895271077	-1.99529260956999
1396	N	3.39849279925687	-0.98513013358701	-1.23031130419774
1397	C	3.60648132626051	-2.94833373859166	-2.94741542192963
1398	H	2.80850838187472	-2.87462406826963	-3.71356424608598
1399	H	3.51832751712017	-3.92119810462858	-2.42404482632981
1400	H	4.59199724945361	-2.90173802200393	-3.45301445590620
1401	C	-4.86097708933182	2.62384038496642	1.07409047261953
1402	C	-6.17045109282794	3.30005282494986	0.74191076464897
1403	C	-6.02048467642672	4.57733938754124	-0.07919023983287
1404	C	-5.02223677763770	4.32033392239163	-1.20213728487861
1405	C	-3.59848107599145	3.98639765030904	-0.68526499831979
1406	C	-3.66106270056979	2.96800768322466	0.47718220935087
1407	H	-6.71715566066187	3.49318681248840	1.69282673232276
1408	H	-6.81246966675656	2.56655214501676	0.19563210751256
1409	H	-7.00250664638430	4.89840962822419	-0.48322415237511
1410	H	-5.66577225973972	5.40482013704631	0.57272022470425
1411	H	-4.95132517490315	5.19010421527468	-1.88950634337540
1412	H	-5.38965814765163	3.46710999122511	-1.81568488774751
1413	C	-4.99437113693369	1.57278864155012	2.15446186042051
1414	H	-4.31786634925682	0.70718349326662	2.02169659101627
1415	H	-4.79157034629944	1.99874185213863	3.16235714435139
1416	H	-6.03138256305749	1.18136738850183	2.18138731012674
1417	C	-2.91942938442921	5.29943458448033	-0.22064819428519
1418	H	-1.90197404352423	5.13078155279872	0.17749318102767
1419	H	-2.83715031940267	6.01021976375222	-1.06946733529415
1420	H	-3.50497734692156	5.78812587245979	0.58347021756200
1421	C	-2.83527936921589	3.39104577088969	-1.89516771051657
1422	H	-2.92264570547871	4.07756630974794	-2.76334921301665
1423	H	-1.75951834986061	3.22962499233155	-1.70447636137797

1424 H -3.27265614416890 2.41487352381937 -2.18806484986008
1425

1426 **pt_monomer_11-ts**

1427 Pt 4.02152398720480 1.85355809858141 -0.80264056625360
1428 Cl 2.43320863977285 0.13137299237426 -1.01854058926923
1429 Cl 5.64192356692794 3.60397355094746 -0.63184901878373
1430 C 1.23628696911838 2.33474800929757 1.30908158665199
1431 C 0.03901520086475 2.72815258970371 1.92275007461728
1432 H 1.17737774314873 1.93920182801037 0.28156484755204
1433 C 2.51337478634658 2.31683778965792 1.89999749457022
1434 H 2.54451294158842 2.45885967023405 2.99731488840365
1435 C 3.68517351186431 1.74419208563612 1.32357043161062
1436 H 4.21384712996806 2.67353296537160 0.79240423765946
1437 C 4.65719256183654 1.01494116992031 2.14710149588572
1438 C 5.95281898620943 0.83270465197926 1.70962554994421
1439 H 6.27127136493619 1.31009129401150 0.76838926068296
1440 C 6.99040654951860 0.05204351587441 2.37913065248013
1441 O 8.14866013390865 -0.02692760993416 1.97653054262218
1442 H 6.67928944381320 -0.50403638651285 3.31409826295091
1443 C 4.13495806992973 0.44323323688139 3.44488578302505
1444 H 3.94518146834145 1.25396766035989 4.18132336213297
1445 H 3.16683791762289 -0.07145738082161 3.27587361458882
1446 H 4.83758964918838 -0.26742981353978 3.91478025350317
1447 C -0.01476772320721 3.32030403220071 3.30706997674593
1448 H 0.97431604750897 3.33795620872332 3.79888089136398
1449 H -0.37910072596891 4.36841261498995 3.26715696086731
1450 H -0.71582566417927 2.75889368413768 3.95871092188530
1451 C -1.17171108142814 2.52128361341940 1.17699195254809
1452 H -1.02547941314044 2.09231907612695 0.17664824015933
1453 C -2.43664894293766 2.84039879032822 1.62825160825343
1454 H -2.47443607586235 3.29277469357520 2.62897191409929
1455 C 4.42533038568105 1.72364454082782 -3.92136285391454
1456 N 4.27672786474558 1.81013123247419 -2.76776442490088
1457 C 4.61401229707364 1.60630282989268 -5.35620327160909
1458 H 4.18496655691851 2.48729387427244 -5.87473692318797
1459 H 4.11109864705347 0.69177411843076 -5.72992766958961
1460 H 5.69457666040652 1.54280928211715 -5.59446029332196
1461 C -4.81888126012867 3.30021537289151 1.60161194452696
1462 C -6.17725079681473 3.40691177696454 0.95339806069860
1463 C -6.17954298661206 3.10499580160368 -0.54175759606223
1464 C -5.35093213274301 1.84908332529439 -0.78664041141236
1465 C -3.85806954530119 2.02431434847569 -0.40223485203118
1466 C -3.72413116428332 2.72836818455995 0.96929315004981
1467 H -6.58721006600240 4.42101152069592 1.16380930424881
1468 H -6.87040113586880 2.71245661488777 1.48832971732864
1469 H -7.21762142616765 2.97929905842375 -0.91198347999564
1470 H -5.74842740173911 3.96328319115978 -1.10006539847934
1471 H -5.40320158138847 1.53013595809496 -1.84868946770724
1472 H -5.77991642377592 1.01584720687449 -0.18657154744001
1473 C -4.77128010398517 3.91815982629440 2.98091633246328
1474 H -4.08407840326702 3.40398852848452 3.67900185973795
1475 H -4.46012572664820 4.98528831296524 2.93124892153052
1476 H -5.78115825813698 3.90655953123804 3.43879077039241
1477 C -3.15534388513392 2.85305379260136 -1.50553798127102
1478 H -2.09507024973686 3.05965710535412 -1.27064102203337
1479 H -3.18845060323960 2.30885077013006 -2.47198864260336
1480 H -3.65303124711099 3.83295918533422 -1.64776121974212
1481 C -3.26354756789752 0.59504278595289 -0.34152411073523
1482 H -3.49392494804847 0.05742624856399 -1.28499599372485
1483 H -2.16689418321422 0.57406663335660 -0.21061515605936
1484 H -3.71450535752921 0.02170141024879 0.49406862434694
1485

1486 **pt_monomer_11-cis-final**

1487 Pt 3.32497209452357 -0.14570027098195 1.09417780452487
1488 Cl 4.94298510124674 -0.30729297649000 2.82030563097419
1489 Cl 1.70778765928198 -0.11684445578165 -0.62040399855604
1490 C 2.56664968551153 2.01881117994871 3.08627737545651
1491 C 1.43456627058581 1.96873329936126 3.88242043274072
1492 H 3.53252698306123 2.08459879642387 3.60217934932139
1493 C 2.56843538069693 1.88224103046062 1.65226132355479
1494 H 1.57949386478364 1.86594272473629 1.16646868465039
1495 C 3.64467387832465 1.97140224986327 0.70936905901226
1496 H 3.29759194224117 2.01750928342472 -0.33775856923109

1497	C	5.03371423623834	2.45716314341059	0.86271347200463
1498	C	5.79923378304006	2.43865918151960	-0.27824331624372
1499	H	5.36058255297356	2.04621715463528	-1.21120267324269
1500	C	7.19376359839056	2.86667691934836	-0.40183626256259
1501	O	7.82890485139218	2.80989526243237	-1.45076501124034
1502	H	7.68138580938110	3.26131961920817	0.53816360181950
1503	C	5.51996106326187	2.96500693756661	2.19054035536950
1504	H	4.79980768177491	3.69464998631745	2.61378385498975
1505	H	5.58896474375056	2.10702178021096	2.89210576482963
1506	H	6.51063881662120	3.44702408364166	2.12276277668170
1507	C	0.04509221710375	1.76928222192366	3.33268100622126
1508	H	-0.43383167643764	0.88998407358147	3.81118575807090
1509	H	-0.60191536611762	2.64599617963892	3.54867933463703
1510	H	0.03510711251916	1.59183237305333	2.24246597377116
1511	C	1.62559960111201	2.08979747525461	5.31268635612216
1512	H	2.67329699573311	2.20491948049898	5.62348365786775
1513	C	0.62243265679096	2.04016731954028	6.24862620360863
1514	H	-0.38810796827905	1.89001787034437	5.84282355022737
1515	C	3.39086533932528	-3.30418782172913	0.95452684419050
1516	N	3.33626367776289	-2.14313011369686	1.04085025202783
1517	C	3.46364360495896	-4.74931311381651	0.84257242303803
1518	H	2.67004847513251	-5.12009553046432	0.16341361527941
1519	H	3.33498124640250	-5.21669847083018	1.83924327609475
1520	H	4.45180849820876	-5.04597056989587	0.43665266086926
1521	C	-0.47115040743784	1.82366040702503	8.41029022388013
1522	C	-0.50064925619265	1.66986110841277	9.91278071924948
1523	C	0.87878746728309	1.53488020938757	10.54970234335481
1524	C	1.79869221843006	2.58972012810262	9.94621882883722
1525	C	2.02269484301095	2.39923033826471	8.42273286378804
1526	C	0.68831450008212	2.08992243858517	7.70294832184184
1527	H	-1.14785275070666	0.79869843145527	10.16375818436441
1528	H	-1.03839211282783	2.55013230551909	10.34333065736060
1529	H	0.81219082812338	1.64457984766786	11.65166929223406
1530	H	1.28383276933670	0.51701867423759	10.35840908467121
1531	H	2.78975994765802	2.59773407492546	10.44647072346338
1532	H	1.35134383422088	3.59399220908036	10.12262734208064
1533	C	-1.82431839406638	1.61064817768858	7.76910114497122
1534	H	-1.98379152591314	2.20573332272860	6.85058389934113
1535	H	-1.98162503666790	0.54103982138830	7.50568100712268
1536	H	-2.62983668878205	1.87903504111764	8.48273537372247
1537	C	3.03299269995975	1.24329737087664	8.21508357565230
1538	H	3.23444037740844	1.03566530032211	7.14813840693895
1539	H	3.99919820447869	1.48922944111553	8.70267519373245
1540	H	2.65677434940392	0.30067162220632	8.66041828592801
1541	C	2.62110128230607	3.73315634162225	7.91092291845783
1542	H	3.51101589998998	3.99932475002015	8.51808090221091
1543	H	2.93847391420986	3.69824939108541	6.85340298488472
1544	H	1.88168088739537	4.55353081150604	8.01204440303210

1546 pt_monomer_13-trans-initial

1547	Pt	6.26724747405804	0.91081152977170	0.31403398340151
1548	Cl	7.15665054893695	-0.82174816618527	1.65645897915453
1549	Cl	5.60702698049964	2.58695968850347	-1.22103457753101
1550	C	1.40279874188681	2.39311684077287	1.29551979721720
1551	C	0.08172804160777	2.08905605815755	1.59859889184071
1552	H	1.57282316178861	3.12717646745481	0.48781034261997
1553	C	2.57642245222729	1.86627773846145	1.91281082523472
1554	H	2.45576470243256	1.10939743817401	2.70485237563710
1555	C	3.84640855370117	2.26899034703506	1.56007838955166
1556	H	3.96097816490736	3.00576780196073	0.74823806362344
1557	C	5.07440333218535	1.77742529270643	2.15251136148999
1558	C	6.31088575251163	2.43545599050453	1.80321846681300
1559	H	6.23070030051318	3.38426111477726	1.24336899920958
1560	C	7.56832549696747	2.36105539424705	2.60799206806399
1561	O	8.38816549236573	3.26579443787132	2.60185692443749
1562	H	7.73135143502527	1.42079306258816	3.20201280197730
1563	C	4.97678462627847	0.83296732573296	3.32809463259633
1564	H	4.61205801026858	1.40980644904109	4.20540368013719
1565	H	4.25798940934164	0.01620966784267	3.12967167371645
1566	H	5.94109328952169	0.36246754874508	3.57551599393226
1567	C	-0.30265806848813	1.11283265173070	2.68191635341488
1568	H	-0.90314148818745	1.61395585479711	3.47037819478562
1569	H	-0.93291463698415	0.29612456253510	2.27206423739559
1570	H	0.57336044211745	0.65122092534987	3.16975532829412

1571	C	-0.95642754935282	2.75020280077294	0.83980447786638
1572	H	-0.59105352831820	3.43252724089057	0.05858044596894
1573	C	-2.30626592212588	2.59637524849386	1.05279075732558
1574	H	-2.57423646026014	1.92274803524760	1.88012058752703
1575	C	6.70572383220237	-0.99295151107492	-2.16922500696213
1576	N	6.47957902894895	-0.32826725150142	-1.23864653219770
1577	C	6.99282746567551	-1.81739399893356	-3.32875409480308
1578	H	6.06261890355837	-2.29156094959778	-3.70091987183644
1579	H	7.71906444513776	-2.61075283563343	-3.06104463333121
1580	H	7.42186665084641	-1.19312236583221	-4.13833994455081
1581	C	-4.69441244281616	3.05089794398144	0.96723394216492
1582	C	-5.92931572754940	3.77192058547718	0.47913287874666
1583	C	-5.64061332317290	4.91621406334735	-0.48804277277284
1584	C	-4.61849225322881	4.43985198850682	-1.51384056756982
1585	C	-3.25032152438705	4.07627006178177	-0.88010192847319
1586	C	-3.44451282304949	3.22468757355794	0.39729389325097
1587	H	-6.50175535775162	4.12835597691987	1.36530494650106
1588	H	-6.60080335949170	3.02056597803933	-0.00465253698139
1589	H	-6.57502444076697	5.25576004397852	-0.98012034950076
1590	H	-5.24559135619699	5.79148380714911	0.07097383803493
1591	H	-4.44901065595940	5.20204143542681	-2.30350141574033
1592	H	-5.02608454278716	3.54151873323017	-2.02935143708936
1593	C	-4.96449016577281	2.16899710748200	2.16594916762785
1594	H	-4.32615003922747	1.26710660756676	2.21594541180939
1595	H	-4.82351377613549	2.72958435439979	3.11706805069097
1596	H	-6.01929804572781	1.82716327393920	2.15725354881265
1597	C	-2.49596843289703	5.38855536205119	-0.54846928318298
1598	H	-1.52447361963224	5.20693615499499	-0.05275850821809
1599	H	-2.30015282361699	5.96335302335885	-1.47755526400994
1600	H	-3.09063170402746	6.02941157199700	0.13304776666672
1601	C	-2.48057830250077	3.27446727881954	-1.95843299141982
1602	H	-2.46322458341544	3.85128118880535	-2.90623604182598
1603	H	-1.43429370662905	3.05441624882650	-1.68222890042681
1604	H	-2.98411107505503	2.30686820095513	-2.15817041911507
1605				

1606 pt_monomer_13-ts

1607	Pt	6.842340	1.552814	0.142848
1608	Cl	5.507472	-0.280184	-0.458084
1609	Cl	8.109549	3.460141	0.275428
1610	C	1.686400	1.982166	1.669884
1611	C	0.359120	2.298662	2.016515
1612	H	1.863107	1.757765	0.605669
1613	C	2.807652	1.958495	2.511508
1614	H	2.691578	2.226234	3.574952
1615	C	4.092249	1.658916	2.015073
1616	H	4.177245	1.376929	0.953338
1617	C	5.281360	1.716548	2.740472
1618	C	6.603404	1.466443	2.128937
1619	H	7.379085	2.094545	2.611436
1620	C	7.062468	-0.016692	2.360531
1621	O	8.069791	-0.290429	2.978251
1622	H	6.364000	-0.782187	1.930013
1623	C	5.344048	2.061271	4.204363
1624	H	5.704299	3.105821	4.328876
1625	H	4.372229	1.967106	4.722968
1626	H	6.084638	1.416015	4.721378
1627	C	-0.062730	2.584847	3.433953
1628	H	-0.534868	3.585732	3.513673
1629	H	-0.817052	1.845235	3.775591
1630	H	0.781220	2.550668	4.145546
1631	C	-0.588473	2.341058	0.943831
1632	H	-0.163276	2.166814	-0.054532
1633	C	-1.934356	2.618046	1.111610
1634	H	-2.251855	2.801475	2.148627
1635	C	2.671249	2.193142	-2.053286
1636	N	1.551293	2.144927	-1.712666
1637	C	4.070590	2.225111	-2.446593
1638	H	4.589029	3.072591	-1.953756
1639	H	4.165443	2.326737	-3.545614
1640	H	4.563939	1.286293	-2.105948
1641	C	-4.221590	3.201263	0.579421
1642	C	-5.348826	3.568126	-0.351343
1643	C	-4.947830	3.675812	-1.818679
1644	C	-4.054254	2.490747	-2.166081

1645	C	-2.720802	2.481305	-1.373183
1646	C	-2.981969	2.757440	0.126699
1647	H	-5.813656	4.510068	0.019162
1648	H	-6.149793	2.798446	-0.225470
1649	H	-5.849039	3.705034	-2.463643
1650	H	-4.405597	4.629839	-1.992282
1651	H	-3.812982	2.470388	-3.249004
1652	H	-4.608287	1.548829	-1.950410
1653	C	-4.573261	3.406916	2.033984
1654	H	-4.063975	2.713062	2.727811
1655	H	-4.329948	4.443717	2.356674
1656	H	-5.665499	3.282898	2.180491
1657	C	-1.777636	3.561789	-1.957710
1658	H	-0.780564	3.552292	-1.483123
1659	H	-1.621180	3.376552	-3.040354
1660	H	-2.205657	4.578049	-1.841466
1661	C	-2.107509	1.074703	-1.584580
1662	H	-2.129575	0.828587	-2.665949
1663	H	-1.053420	1.000706	-1.266648
1664	H	-2.694213	0.302067	-1.04787
1665				
1666	pt_monomer_13-cis-final			
1667	Pt	5.99063395674227	1.40904822935397	0.00744942702136
1668	Cl	7.22280063656795	-0.46161724135028	0.80579069016148
1669	Cl	4.92726713807616	3.22574808625887	-1.05243161786370
1670	C	4.73268255383172	-0.37623499259557	4.79199212520814
1671	C	3.76890622510577	-0.86177026315868	5.66712303421569
1672	H	5.69172837183524	-0.92169428837162	4.75317677641856
1673	C	4.62008025706512	0.74711801749621	3.91943378929951
1674	H	3.67204928864503	1.30720548122237	3.91115369625163
1675	C	5.64408399118984	1.14896440210572	3.08761182019762
1676	H	6.56515228143827	0.54918750348911	3.07737761611747
1677	C	5.57597544383999	2.27711789060433	2.18457516456906
1678	C	6.73701493722019	2.76088636087660	1.47188732553135
1679	H	6.64461566113928	3.76548303174715	1.02290404255040
1680	C	8.15736256283680	2.44512368823087	1.83201862501870
1681	O	9.07778817283341	3.17365247218096	1.50116066888393
1682	H	8.33393672163559	1.50943932485707	2.42781070453691
1683	C	4.33759693776483	3.14381337971761	2.20176696404223
1684	H	3.41336892335988	2.54030598945051	2.12106009756429
1685	H	4.30307586030880	3.69699505907715	3.16465895073349
1686	H	4.34515915528886	3.86200217062420	1.36377334739813
1687	C	2.41486722364990	-0.21685470425799	5.82571338319239
1688	H	1.60328082750889	-0.93679153014560	5.59033396611324
1689	H	2.25562286388361	0.11437730291313	6.87306132367168
1690	H	2.28353862232545	0.66275312579185	5.17175434691194
1691	C	4.09201878108393	-2.03328138507634	6.45013224528853
1692	H	5.09811282021589	-2.44080744960561	6.27818740806077
1693	C	3.23857386891983	-2.64556030676982	7.33804981900451
1694	H	2.24101336619739	-2.18978401215053	7.41814738945441
1695	C	5.28185851583330	-0.35658631355427	-2.51411302991438
1696	N	5.48414954388004	0.27292934065251	-1.55374866710613
1697	C	5.03067844997023	-1.14475668203021	-3.70697226905902
1698	H	3.94286555442479	-1.31656385097860	-3.83096406897513
1699	H	5.54273170873504	-2.12422402959153	-3.62874841945612
1700	H	5.41151414622848	-0.61129964963898	-4.60104480744516
1701	C	2.31353711795741	-4.35548405431238	8.79801176063214
1702	C	2.33486157202211	-5.66571898006998	9.54922457104312
1703	C	3.58384120798590	-6.50647584416452	9.29925044561875
1704	C	4.80705034147658	-5.60049083879736	9.37313197504306
1705	C	4.81566782886051	-4.50131846785858	8.27828868192665
1706	C	3.42408416115215	-3.83578492499114	8.15573568175161
1707	H	1.41049662780395	-6.23224740521592	9.29448945205646
1708	H	2.23240156418492	-5.44292365548360	10.63982927215798
1709	H	3.65288608548490	-7.33187057270504	10.03743254382941
1710	H	3.52009827756890	-6.98619517881805	8.29911779812743
1711	H	5.74819989391400	-6.18434049146575	9.29121062821586
1712	H	4.82733625919494	-5.11137091713499	10.37244545142826
1713	C	0.94908182806384	-3.70041398623366	8.78474605839004
1714	H	0.98645651739277	-2.59440230226003	8.82009761616464
1715	H	0.37225114449515	-3.98314467167300	7.87554363105714
1716	C	0.35131492869104	-0.40400031712378	9.65548097202574
1717	C	5.22852382765246	-5.14905606355432	6.93305916045187
1718	H	5.20825280847979	-4.43279788264685	6.09035479771542

1719	H	6.25716624785518	-5.55933811513900	7.00489168953794
1720	H	4.54694485206618	-5.98072408434615	6.66584407812322
1721	C	5.87627783946962	-3.46362365945870	8.72277678915838
1722	H	6.83738051951383	-3.97868710661849	8.92740620551470
1723	H	6.07171199145909	-2.67794596542213	7.97091636703197
1724	H	5.55621221767301	-2.95961767188107	9.65744950540034

1725
1726

1727 Dimer mechanism

1728 C⁹-C¹⁰ *trans*-to-*cis*

1729

1730 all-*trans*-catalyst complex

1731	Pd	1.111867000	0.427530000	-0.142282000
1732	Pd	-2.258300000	0.945544000	-1.981601000
1733	Cl	2.165932000	-0.987707000	1.394571000
1734	Cl	0.038069000	1.680397000	-1.905344000
1735	Cl	-4.451062000	0.251434000	-2.254402000
1736	Cl	-2.036996000	-0.515857000	-0.207682000
1737	C	1.489219000	2.219133000	1.038124000
1738	C	0.152406000	1.989261000	1.529067000
1739	H	1.566867000	2.982241000	0.242043000
1740	C	2.712164000	1.999139000	1.788399000
1741	H	2.648140000	1.369513000	2.685401000
1742	C	3.921724000	2.512542000	1.406055000
1743	H	3.970728000	3.135801000	0.496047000
1744	C	5.177588000	2.262410000	2.089354000
1745	C	6.319500000	2.860032000	1.598192000
1746	H	6.241583000	3.511205000	0.710290000
1747	C	7.675232000	2.731901000	2.128732000
1748	O	8.650324000	3.304232000	1.647799000
1749	H	7.795817000	2.063605000	3.033057000
1750	C	5.158072000	1.338219000	3.282959000
1751	H	4.546521000	1.773660000	4.101315000
1752	H	4.683777000	0.373670000	3.005212000
1753	H	6.164471000	1.131365000	3.684146000
1754	C	-0.126588000	1.138906000	2.739207000
1755	H	-0.354139000	1.793134000	3.607728000
1756	H	-1.010079000	0.496741000	2.556470000
1757	H	0.716091000	0.468666000	2.982210000
1758	C	-0.899636000	2.748883000	0.913885000
1759	H	-0.572596000	3.481412000	0.171565000
1760	C	-2.244735000	2.510433000	1.111003000
1761	H	-2.464508000	1.668057000	1.779870000
1762	C	0.209841000	-1.899873000	-2.027587000
1763	N	0.893528000	-1.179313000	-1.416174000
1764	C	-0.720977000	-2.734858000	-2.761789000
1765	H	-1.646070000	-2.144534000	-2.929866000
1766	H	-0.978655000	-3.630412000	-2.163588000
1767	H	-0.293629000	-3.049596000	-3.733494000
1768	C	-2.717721000	2.911270000	-4.371784000
1769	N	-2.512749000	2.169305000	-3.495339000
1770	C	-2.989467000	3.851853000	-5.443818000
1771	H	-3.404387000	4.790225000	-5.024000000
1772	H	-3.725745000	3.420911000	-6.151958000
1773	H	-2.057067000	4.088014000	-5.994434000
1774	C	-4.603780000	2.386506000	0.652100000
1775	C	-5.875918000	2.762421000	-0.053715000
1776	C	-5.924296000	4.170119000	-0.639660000
1777	C	-4.573775000	4.515737000	-1.254689000
1778	C	-3.402201000	4.458216000	-0.241914000
1779	C	-3.412623000	3.096260000	0.498063000
1780	H	-6.738251000	2.568737000	0.620249000
1781	H	-5.965958000	2.001408000	-0.868474000
1782	H	-6.730727000	4.238578000	-1.399406000
1783	H	-6.181026000	4.906618000	0.151348000
1784	H	-4.596719000	5.531742000	-1.704125000
1785	H	-4.354524000	3.796604000	-2.073896000
1786	C	-4.697386000	1.079673000	1.394171000
1787	H	-4.153627000	0.287803000	0.831529000
1788	H	-4.248603000	1.123498000	2.406933000
1789	H	-5.751189000	0.762211000	1.502261000

1790	C	-3.556715000	5.563429000	0.831724000
1791	H	-2.715240000	5.520665000	1.553354000
1792	H	-3.556663000	6.570406000	0.362415000
1793	H	-4.494760000	5.448442000	1.409058000
1794	C	-2.121174000	4.759854000	-1.053380000
1795	H	-2.333661000	5.588976000	-1.759671000
1796	H	-1.286222000	5.105023000	-0.415254000
1797	H	-1.777395000	3.887945000	-1.639592000
1798	TS-trans			
1799	Pd	1.643116000	0.671474000	-0.780651000
1800	Pd	-0.772158000	1.713177000	-2.275260000
1801	Cl	1.531007000	-0.671536000	1.170317000
1802	Cl	1.558919000	1.990211000	-2.814974000
1803	Cl	-2.972975000	1.366416000	-1.678735000
1804	Cl	-0.733204000	3.650095000	-1.006348000
1805	C	1.703500000	2.440604000	0.274524000
1806	C	0.437791000	2.926418000	0.940227000
1807	H	2.034663000	3.187092000	-0.474288000
1808	C	2.777255000	2.147371000	1.243540000
1809	H	2.482368000	1.594444000	2.146632000
1810	C	4.096565000	2.455624000	1.038202000
1811	H	4.377518000	3.002323000	0.121158000
1812	C	5.176352000	2.056887000	1.919901000
1813	C	6.467323000	2.422254000	1.591406000
1814	H	6.636735000	3.002176000	0.667774000
1815	C	7.681287000	2.124508000	2.343355000
1816	O	8.807511000	2.478626000	1.997414000
1817	H	7.542649000	1.533353000	3.298156000
1818	C	4.823081000	1.245549000	3.144361000
1819	H	4.161701000	1.829694000	3.818684000
1820	H	4.253910000	0.339349000	2.849473000
1821	H	5.708804000	0.932040000	3.723213000
1822	C	-0.546634000	1.942883000	1.473324000
1823	H	-1.421475000	2.412400000	1.955892000
1824	H	-0.893242000	1.271192000	0.665246000
1825	H	-0.009099000	1.272709000	2.181841000
1826	C	0.560915000	4.258974000	1.496386000
1827	H	1.364963000	4.877997000	1.071094000
1828	C	-0.171023000	4.742177000	2.548696000
1829	H	-0.884350000	4.048945000	3.028941000
1830	C	2.111495000	-2.218689000	-2.118774000
1831	N	1.851255000	-1.124876000	-1.804397000
1832	C	2.480053000	-3.586166000	-2.450155000
1833	H	1.577363000	-4.208663000	-2.610998000
1834	H	3.058470000	-4.023198000	-1.610533000
1835	H	3.105251000	-3.611952000	-3.365093000
1836	C	-0.889293000	-0.899350000	-3.961494000
1837	N	-0.837671000	0.088322000	-3.346667000
1838	C	-0.961083000	-2.133253000	-4.723162000
1839	H	-1.687417000	-2.027457000	-5.554050000
1840	H	-1.291639000	-2.964516000	-4.068311000
1841	H	0.031924000	-2.378522000	-5.149212000
1842	C	0.132442000	7.206941000	2.446792000
1843	C	0.269056000	8.558473000	3.113241000
1844	C	-0.137374000	8.591343000	4.587818000
1845	C	0.405404000	7.358716000	5.305312000
1846	C	-0.144615000	6.038420000	4.718433000
1847	C	-0.031567000	6.050227000	3.175845000
1848	H	-0.304252000	9.309465000	2.527841000
1849	H	1.335994000	8.871289000	3.004850000
1850	H	0.232281000	9.521414000	5.066488000
1851	H	-1.245706000	8.620927000	4.667951000
1852	H	0.171661000	7.391745000	6.391093000
1853	H	1.515443000	7.349586000	5.221862000
1854	C	0.181175000	7.260770000	0.940280000
1855	H	1.229433000	7.364550000	0.580204000
1856	H	-0.252244000	6.371553000	0.448430000
1857	H	-0.357035000	8.159643000	0.573716000
1858	C	-1.624267000	5.846531000	5.126139000
1859	H	-2.046625000	4.911977000	4.705106000
1860	H	-1.716280000	5.783183000	6.230951000
1861	H	-2.258647000	6.682933000	4.770950000
1862	C	0.696292000	4.876681000	5.296088000
1863	H	0.697170000	4.919980000	6.405340000

1864	H	0.300004000	3.883853000	5.001881000
1865	H	1.747749000	4.935581000	4.948749000

1866 Chloropalladate

1867	Pd	1.580315000	0.741225000	-0.989617000
1868	Pd	-0.881566000	1.642519000	-2.468696000
1869	Cl	1.553780000	-0.507632000	1.015669000
1870	Cl	1.420102000	1.968378000	-3.071978000
1871	Cl	-3.074012000	1.278620000	-1.854172000
1872	Cl	-0.833264000	3.583105000	-1.156032000
1873	C	1.551486000	2.549556000	0.000234000
1874	C	0.198973000	3.024459000	0.534103000
1875	H	1.911523000	3.259357000	-0.771182000
1876	C	2.551463000	2.393647000	1.071684000
1877	H	2.214422000	1.884332000	1.985432000
1878	C	3.858574000	2.782395000	0.963214000
1879	H	4.185649000	3.297549000	0.042933000
1880	C	4.876150000	2.529855000	1.967309000
1881	C	6.149694000	3.018300000	1.754227000
1882	H	6.354999000	3.583066000	0.828261000
1883	C	7.301692000	2.878694000	2.638823000
1884	O	8.413400000	3.346280000	2.397376000
1885	H	7.125386000	2.303085000	3.596804000
1886	C	4.479857000	1.727661000	3.184083000
1887	H	3.708640000	2.269852000	3.769428000
1888	H	4.023899000	0.765485000	2.871579000
1889	H	5.328987000	1.514334000	3.856404000
1890	C	-0.705861000	2.009534000	1.182745000
1891	H	-1.645102000	2.467231000	1.543036000
1892	H	-0.940573000	1.192946000	0.476318000
1893	H	-0.161007000	1.535204000	2.024866000
1894	C	0.356293000	4.338612000	1.201016000
1895	H	0.973133000	5.075780000	0.662356000
1896	C	-0.050193000	4.603250000	2.468683000
1897	H	-0.563394000	3.798968000	3.025797000
1898	C	2.052538000	-2.241252000	-2.099684000
1899	N	1.810767000	-1.112381000	-1.924065000
1900	C	2.378746000	-3.652230000	-2.231045000
1901	H	1.527065000	-4.219078000	-2.657308000
1902	H	2.607737000	-4.063540000	-1.226889000
1903	H	3.264396000	-3.789399000	-2.883106000
1904	C	-0.981621000	-0.950353000	-4.172875000
1905	N	-0.946278000	0.040062000	-3.562025000
1906	C	-1.031212000	-2.186415000	-4.932236000
1907	H	-1.693455000	-2.066926000	-5.812995000
1908	H	-1.429297000	-3.004332000	-4.298457000
1909	H	-0.016459000	-2.458289000	-5.284132000
1910	C	0.018474000	7.078426000	2.749266000
1911	C	0.360436000	8.320516000	3.545523000
1912	C	0.659210000	8.060273000	5.023371000
1913	C	1.557039000	6.832256000	5.163245000
1914	C	0.895000000	5.547883000	4.613849000
1915	C	0.268342000	5.820547000	3.228193000
1916	H	-0.462565000	9.060858000	3.434150000
1917	H	1.242048000	8.802175000	3.057779000
1918	H	1.136430000	8.950904000	5.482245000
1919	H	-0.292010000	7.901023000	5.576185000
1920	H	1.845226000	6.663829000	6.222541000
1921	H	2.503634000	7.011791000	4.606202000
1922	C	-0.615664000	7.360803000	1.410290000
1923	H	0.124754000	7.810433000	0.711283000
1924	H	-1.034875000	6.461347000	0.924921000
1925	H	-1.427874000	8.111337000	1.521401000
1926	C	-0.197314000	5.047456000	5.588290000
1927	H	-0.699443000	4.137108000	5.203218000
1928	H	0.248425000	4.787659000	6.570642000
1929	H	-0.980250000	5.814002000	5.752572000
1930	C	1.987664000	4.461384000	4.479206000
1931	H	2.516444000	4.324528000	5.445689000
1932	H	1.561122000	3.480217000	4.187858000
1933	H	2.735025000	4.738865000	3.708815000

1934 TS-cis

1935	Pd	1.584201000	0.758160000	-0.956718000
1936	Pd	-0.679281000	1.882169000	-2.638428000

1937	Cl	1.285863000	-0.698521000	0.876785000
1938	Cl	1.689851000	2.207629000	-2.897338000
1939	Cl	-2.938271000	1.518044000	-2.344844000
1940	Cl	-0.791060000	3.721431000	-1.220751000
1941	C	1.435501000	2.441981000	0.217466000
1942	C	0.059025000	2.865944000	0.694760000
1943	H	1.857423000	3.238610000	-0.428107000
1944	C	2.343268000	2.156320000	1.346325000
1945	H	1.932489000	1.542118000	2.161179000
1946	C	3.653544000	2.549813000	1.391677000
1947	H	4.055007000	3.156922000	0.561266000
1948	C	4.583355000	2.186132000	2.444386000
1949	C	5.879146000	2.657588000	2.372000000
1950	H	6.167581000	3.292191000	1.515964000
1951	C	6.957363000	2.413260000	3.324359000
1952	O	8.093601000	2.868672000	3.204837000
1953	H	6.698027000	1.764572000	4.214112000
1954	C	4.076810000	1.298174000	3.556897000
1955	H	3.255509000	1.801308000	4.109355000
1956	H	3.649028000	0.365149000	3.135101000
1957	H	4.861869000	1.028939000	4.284263000
1958	C	-0.964652000	1.822012000	1.012215000
1959	H	-1.936012000	2.254017000	1.310619000
1960	H	-1.114672000	1.148638000	0.148243000
1961	H	-0.557584000	1.174695000	1.820821000
1962	C	0.097018000	4.110087000	1.458049000
1963	H	0.904689000	4.807794000	1.189356000
1964	C	-0.710593000	4.395353000	2.521196000
1965	H	-1.427488000	3.618290000	2.840036000
1966	C	2.370113000	-1.979002000	-2.467078000
1967	N	1.998754000	-0.943776000	-2.075166000
1968	C	2.858776000	-3.279969000	-2.897102000
1969	H	2.104766000	-4.063775000	-2.682030000
1970	H	3.787246000	-3.528722000	-2.345013000
1971	H	3.084885000	-3.279784000	-3.981706000
1972	C	-0.586573000	-0.649096000	-4.438201000
1973	N	-0.613202000	0.323911000	-3.799134000
1974	C	-0.556536000	-1.866890000	-5.227385000
1975	H	-1.432066000	-1.901792000	-5.906891000
1976	H	-0.593072000	-2.750868000	-4.559659000
1977	H	0.368552000	-1.907306000	-5.836716000
1978	C	-0.542099000	6.855810000	2.841387000
1979	C	-0.488620000	8.081579000	3.728356000
1980	C	-0.923286000	7.837304000	5.174903000
1981	C	-0.300433000	6.542512000	5.691271000
1982	C	-0.745167000	5.303886000	4.879847000
1983	C	-0.642957000	5.588582000	3.363341000
1984	H	-1.094013000	8.891086000	3.265286000
1985	H	0.560465000	8.463588000	3.707222000
1986	H	-0.633381000	8.697003000	5.813960000
1987	H	-2.032087000	7.773554000	5.224532000
1988	H	-0.547392000	6.376766000	6.761826000
1989	H	0.807915000	6.627180000	5.633060000
1990	C	-0.489425000	7.163480000	1.365660000
1991	H	-0.813450000	6.323068000	0.725540000
1992	H	-1.127384000	8.042764000	1.136496000
1993	H	0.542159000	7.444323000	1.056586000
1994	C	-2.200902000	4.922498000	5.240269000
1995	H	-2.548222000	4.040218000	4.665612000
1996	H	-2.275821000	4.666256000	6.317714000
1997	H	-2.905203000	5.751850000	5.030812000
1998	C	0.190217000	4.129477000	5.250591000
1999	H	0.187640000	3.969361000	6.348999000
2000	H	-0.123641000	3.178891000	4.774188000
2001	H	1.233349000	4.336822000	4.935572000
2002	9-cis-catalyst complex			
2003	Pd	1.722123000	1.292004000	-0.631272000
2004	Pd	-0.918963000	1.982858000	-3.142212000
2005	Cl	2.793928000	-0.532885000	0.414657000
2006	Cl	0.862409000	3.095717000	-1.950999000
2007	Cl	-2.446889000	0.808657000	-4.423702000
2008	Cl	-1.562215000	0.789156000	-1.275712000
2009	C	2.019952000	2.605024000	1.088995000
2010	C	0.640563000	2.233296000	1.299244000

2011	H	2.170933000	3.598599000	0.632092000
2012	C	3.152567000	2.113109000	1.852925000
2013	H	3.003582000	1.209231000	2.457793000
2014	C	4.381568000	2.713177000	1.829392000
2015	H	4.517738000	3.620366000	1.215821000
2016	C	5.553094000	2.217256000	2.529002000
2017	C	6.724794000	2.938326000	2.434997000
2018	H	6.730700000	3.872441000	1.847516000
2019	C	8.011839000	2.607194000	3.043248000
2020	O	9.016411000	3.305436000	2.929151000
2021	H	8.048643000	1.650247000	3.644389000
2022	C	5.418952000	0.924875000	3.298017000
2023	H	4.693959000	1.043704000	4.130537000
2024	H	5.019031000	0.130815000	2.633988000
2025	H	6.374192000	0.577052000	3.726791000
2026	C	-0.427133000	3.242868000	0.953675000
2027	H	-1.210559000	2.798088000	0.306329000
2028	H	-0.902518000	3.586835000	1.896100000
2029	H	-0.005885000	4.117521000	0.431087000
2030	C	0.269031000	1.015991000	1.969955000
2031	H	1.084641000	0.346099000	2.266190000
2032	C	-1.049513000	0.625952000	2.088004000
2033	H	-1.779052000	1.325965000	1.661984000
2034	C	1.071035000	-0.589746000	-3.096683000
2035	N	1.559029000	0.071463000	-2.268726000
2036	C	0.379951000	-1.373322000	-4.100101000
2037	H	-0.576840000	-0.850116000	-4.346051000
2038	H	0.151718000	-2.380140000	-3.698967000
2039	H	0.995930000	-1.471969000	-5.015200000
2040	C	-0.124848000	3.583781000	-5.712772000
2041	N	-0.403814000	2.994005000	-4.745708000
2042	C	0.210567000	4.315452000	-6.922230000
2043	H	-0.267037000	5.315339000	-6.909423000
2044	H	-0.151262000	3.761649000	-7.811603000
2045	H	1.308450000	4.445888000	-7.001506000
2046	C	-2.960929000	-0.825113000	2.277588000
2047	C	-3.664115000	-2.118763000	2.597995000
2048	C	-2.752849000	-3.248797000	3.071351000
2049	C	-1.704992000	-2.686407000	4.025493000
2050	C	-0.780500000	-1.637987000	3.355920000
2051	C	-1.625175000	-0.600702000	2.586543000
2052	H	-4.260141000	-2.421356000	1.707470000
2053	H	-4.433922000	-1.888724000	3.374926000
2054	H	-3.350903000	-4.045324000	3.560294000
2055	H	-2.257818000	-3.722744000	2.198003000
2056	H	-1.071891000	-3.496208000	4.444507000
2057	H	-2.220796000	-2.211475000	4.890320000
2058	C	-3.829803000	0.176213000	1.551867000
2059	H	-4.894755000	-0.124345000	1.599582000
2060	H	-3.751766000	1.200763000	1.967911000
2061	H	-3.547719000	0.246249000	0.476917000
2062	C	0.189888000	-2.354245000	2.386904000
2063	H	0.897523000	-1.664867000	1.888821000
2064	H	0.787969000	-3.109329000	2.939612000
2065	H	-0.361625000	-2.876409000	1.580428000
2066	C	0.013832000	-0.963223000	4.498691000
2067	H	0.512680000	-1.741344000	5.113672000
2068	H	0.798159000	-0.273181000	4.138309000
2069	H	-0.662360000	-0.386534000	5.163216000
2070				

C¹¹-C¹² *trans*-to-*cis*

2071				
2072				
2073				
2074	Pd	3.124266000	0.425262000	0.540635000
2075	Pd	-0.061589000	1.330698000	-1.841218000
2076	Cl	3.718386000	-0.806716000	2.426631000
2077	Cl	2.342688000	1.498867000	-1.469701000
2078	Cl	-2.245403000	1.174382000	-2.601740000
2079	Cl	-0.455993000	-0.468165000	-0.450381000
2080	C	1.449855000	2.807709000	1.447433000
2081	C	0.163418000	2.388700000	1.767376000
2082	H	1.547530000	3.562616000	0.648869000
2083	C	2.657887000	2.205946000	1.909118000

2084	H	2.664290000	1.691002000	2.882858000
2085	C	3.893860000	2.352107000	1.211692000
2086	H	3.850192000	2.924741000	0.268820000
2087	C	5.246095000	2.241438000	1.782492000
2088	C	6.298420000	2.435834000	0.917813000
2089	H	6.088309000	2.625492000	-0.148976000
2090	C	7.723258000	2.408599000	1.253667000
2091	O	8.613887000	2.590179000	0.428810000
2092	H	7.977113000	2.208413000	2.336272000
2093	C	5.385870000	1.984685000	3.256242000
2094	H	4.833024000	2.755723000	3.832859000
2095	H	4.928792000	1.000745000	3.494871000
2096	H	6.436259000	1.976880000	3.593807000
2097	C	-0.081731000	1.198556000	2.648825000
2098	H	-0.984746000	1.328555000	3.275392000
2099	H	-0.240695000	0.316803000	1.987877000
2100	H	0.780458000	0.961975000	3.298668000
2101	C	-0.927259000	3.025519000	1.076102000
2102	H	-0.685067000	3.978734000	0.587514000
2103	C	-2.161915000	2.441553000	0.907704000
2104	H	-2.264262000	1.445525000	1.358400000
2105	C	2.161373000	-2.154272000	-1.013888000
2106	N	2.701711000	-1.321898000	-0.405036000
2107	C	1.419153000	-3.139733000	-1.774390000
2108	H	0.369996000	-2.778746000	-1.825159000
2109	H	1.452673000	-4.127811000	-1.274961000
2110	H	1.830911000	-3.229219000	-2.798719000
2111	C	0.221797000	3.834244000	-3.692676000
2112	N	0.167549000	2.887997000	-3.013290000
2113	C	0.253799000	5.017427000	-4.533550000
2114	H	-0.536518000	5.725508000	-4.211251000
2115	H	0.073846000	4.739314000	-5.591697000
2116	H	1.239543000	5.518817000	-4.457869000
2117	C	-4.367737000	1.972764000	0.068815000
2118	C	-5.732137000	2.354676000	-0.438977000
2119	C	-5.983845000	3.858838000	-0.417130000
2120	C	-4.801618000	4.546837000	-1.089277000
2121	C	-3.455841000	4.336611000	-0.342334000
2122	C	-3.342762000	2.895329000	0.206940000
2123	H	-6.493662000	1.799484000	0.153340000
2124	H	-5.837828000	1.960166000	-1.478906000
2125	H	-6.933514000	4.105776000	-0.935042000
2126	H	-6.095683000	4.208215000	0.632648000
2127	H	-4.972164000	5.638519000	-1.201729000
2128	H	-4.703559000	4.135881000	-2.117851000
2129	C	-4.218531000	0.508711000	0.405788000
2130	H	-3.209936000	0.114705000	0.180535000
2131	H	-4.451815000	0.315054000	1.477482000
2132	H	-4.944673000	-0.085415000	-0.183825000
2133	C	-3.351182000	5.354917000	0.815879000
2134	H	-2.419383000	5.222134000	1.398649000
2135	H	-3.363737000	6.392733000	0.421200000
2136	H	-4.198625000	5.247608000	1.523743000
2137	C	-2.357032000	4.609862000	-1.400755000
2138	H	-2.564541000	5.583074000	-1.896375000
2139	H	-1.337423000	4.664722000	-0.979119000
2140	H	-2.366258000	3.803571000	-2.160535000
2141				
2142	TS_{chloro}			
2143	Pd	1.864499000	0.574247000	-0.760426000
2144	Pd	-0.525914000	1.537018000	-2.255930000
2145	Cl	1.237941000	-0.595778000	1.185581000
2146	Cl	1.820091000	1.930479000	-2.775345000
2147	Cl	-2.757323000	1.090161000	-1.876212000
2148	Cl	-0.591341000	3.056805000	-0.479997000
2149	C	2.130723000	2.332819000	0.281116000
2150	C	0.916412000	2.652963000	1.091988000
2151	H	2.273946000	3.087696000	-0.515947000
2152	C	-0.028061000	4.041084000	2.921120000
2153	H	0.390908000	1.773702000	1.499410000
2154	C	0.854424000	3.860712000	1.863534000
2155	H	1.543704000	4.678831000	1.595077000
2156	C	3.417785000	2.114593000	1.003463000
2157	C	4.580324000	2.350471000	0.298841000

2158	H	4.509814000	2.704781000	-0.743280000
2159	C	5.943176000	2.156461000	0.781979000
2160	O	6.947180000	2.395659000	0.112680000
2161	H	6.045176000	1.764392000	1.837712000
2162	C	3.379074000	1.661863000	2.437182000
2163	H	2.902459000	2.443674000	3.066725000
2164	H	2.741621000	0.755109000	2.506931000
2165	H	4.378750000	1.443259000	2.849588000
2166	C	-1.025932000	2.964361000	3.268722000
2167	H	-1.714274000	2.795062000	2.414952000
2168	H	-0.520357000	1.996064000	3.458415000
2169	H	-1.636283000	3.211411000	4.154898000
2170	C	0.036327000	5.285446000	3.655057000
2171	H	0.786713000	6.006379000	3.293875000
2172	C	-0.701343000	5.606642000	4.765125000
2173	H	-1.366022000	4.823177000	5.170134000
2174	C	1.338426000	-2.286138000	-2.119067000
2175	N	1.626091000	-1.209949000	-1.771598000
2176	C	0.969318000	-3.636511000	-2.510797000
2177	H	-0.117326000	-3.683010000	-2.726125000
2178	H	1.191862000	-4.338477000	-1.681582000
2179	H	1.533413000	-3.958204000	-3.408616000
2180	C	-0.598251000	-0.301951000	-4.761715000
2181	N	-0.573225000	0.361866000	-3.804458000
2182	C	-0.640327000	-1.120065000	-5.961289000
2183	H	-1.088032000	-0.545482000	-6.797230000
2184	H	-1.252941000	-2.027279000	-5.788864000
2185	H	0.384670000	-1.424837000	-6.251482000
2186	C	-0.572373000	8.089578000	4.966270000
2187	C	-0.532379000	9.355555000	5.796552000
2188	C	-0.973179000	9.177531000	7.250374000
2189	C	-0.345455000	7.912532000	7.828835000
2190	C	-0.772769000	6.633771000	7.071621000
2191	C	-0.652807000	6.842281000	5.541760000
2192	H	-1.140959000	10.138169000	5.293001000
2193	H	0.513654000	9.745728000	5.763407000
2194	H	-0.691532000	10.067908000	7.850027000
2195	H	-2.081762000	9.109718000	7.297888000
2196	H	-0.600298000	7.793269000	8.903679000
2197	H	0.762801000	8.002896000	7.776502000
2198	C	-0.529102000	8.334535000	3.478264000
2199	H	0.507491000	8.553476000	3.136685000
2200	H	-0.901798000	7.480400000	2.883409000
2201	H	-1.131354000	9.230709000	3.220157000
2202	C	-2.232960000	6.265093000	7.427560000
2203	H	-2.566540000	5.353605000	6.891759000
2204	H	-2.326065000	6.063163000	8.515161000
2205	H	-2.936853000	7.079021000	7.163097000
2206	C	0.160026000	5.485951000	7.522130000
2207	H	0.134184000	5.383510000	8.627300000
2208	H	-0.136144000	4.508677000	7.090535000
2209	H	1.208806000	5.683490000	7.219919000
2210				

11-cis-catalyst complex

2211				
2212	Pd	3.811033720	-0.334535652	0.667149165
2213	Pd	0.066666595	-0.088231940	0.138049664
2214	Cl	5.362884251	-0.771866903	2.380212729
2215	Cl	2.166467504	-0.133359332	-1.058220341
2216	Cl	-2.030507064	0.064703361	1.127057542
2217	Cl	0.378760954	-2.101291558	1.212205345
2218	C	2.854672536	2.174237591	2.959398404
2219	C	1.777867699	1.737393828	3.761982212
2220	H	3.789922479	2.442336079	3.471734259
2221	C	2.934277572	1.805617466	1.604885187
2222	H	2.043765204	1.302834646	1.188256982
2223	C	4.074112117	1.817478562	0.721487203
2224	H	3.802672755	2.041023335	-0.324691184
2225	C	5.456788175	2.228347935	1.037295277
2226	C	6.371932060	2.147830066	0.012956246
2227	H	6.050199163	1.746437270	-0.963627372
2228	C	7.782749675	2.526549687	0.068418743
2229	O	8.549884464	2.430941017	-0.886187535
2230	H	8.153942742	2.925629848	1.058718992
2231	C	5.777796831	2.759675597	2.406487008

2232	H	4.987710671	3.457622335	2.750386528
2233	H	5.807723348	1.910376596	3.119766282
2234	H	6.752039910	3.278228849	2.440451239
2235	C	0.804645327	0.698686741	3.291360043
2236	H	0.932823517	-0.273800182	3.816319575
2237	H	-0.232429436	1.034958510	3.498322366
2238	H	0.886742637	0.521470425	2.203820848
2239	C	1.812577643	2.179017783	5.117315427
2240	H	2.787347696	2.537082280	5.471799469
2241	C	0.817361038	1.822839818	6.012755550
2242	H	0.141567527	1.027949447	5.669113898
2243	C	3.205096769	-3.426296676	0.415889531
2244	N	3.607326553	-2.336198325	0.483331048
2245	C	2.621354623	-4.751207942	0.341092941
2246	H	1.518907862	-4.623148292	0.319418944
2247	H	2.904324489	-5.346613040	1.231725130
2248	H	2.956155021	-5.278780318	-0.574162707
2249	C	-0.437044847	2.688025737	-1.225485934
2250	N	-0.244522483	1.654373829	-0.719664419
2251	C	-0.685177597	3.971403163	-1.859113106
2252	H	-0.499320021	4.796932072	-1.142842465
2253	H	-1.737841351	4.027576460	-2.201635636
2254	H	-0.017481209	4.100166487	-2.734187350
2255	C	-0.435462520	1.658014561	8.055994737
2256	C	-0.585811823	1.690675787	9.553676395
2257	C	0.662726649	2.123796364	10.318153507
2258	C	1.314985884	3.291963737	9.585582933
2259	C	1.804140123	2.907667937	8.165801328
2260	C	0.683565438	2.168210226	7.403571153
2261	H	-0.936207634	0.684865596	9.878899930
2262	H	-1.441483719	2.370515848	9.787640575
2263	H	0.401163944	2.399782499	11.360437988
2264	H	1.373164217	1.272461836	10.388155709
2265	H	2.177274659	3.695746027	10.156598445
2266	H	0.576796427	4.121513252	9.501329438
2267	C	-1.565301553	0.955251221	7.352662294
2268	H	-1.866085817	1.441544186	6.405715627
2269	H	-1.269441270	-0.090001307	7.103056776
2270	H	-2.456987610	0.900496907	8.007813139
2271	C	3.053584913	1.999047137	8.297739553
2272	H	3.542147579	1.770204428	7.333677239
2273	H	3.812969273	2.486097034	8.944255174
2274	H	2.782182204	1.021909341	8.741424459
2275	C	2.174219614	4.230304096	7.455109451
2276	H	2.920009577	4.786681063	8.060030463
2277	H	2.612498543	4.077339221	6.452622225
2278	H	1.280481321	4.876482074	7.337116965
2279				

2280 **C¹³-C¹⁴ *trans*-to-*cis***

2281

2282 **all-*trans*-catalyst complex**

2283	Pd	5.738207000	0.948741000	0.086475000
2284	Pd	1.969420000	1.361726000	-0.717229000
2285	Cl	7.297277000	-0.528139000	0.949349000
2286	Cl	4.124240000	2.415584000	-0.938057000
2287	Cl	-0.095005000	0.289769000	-0.786367000
2288	Cl	2.625549000	-0.063765000	0.976152000
2289	C	1.711661000	3.313696000	2.130959000
2290	C	0.438031000	2.740361000	2.165503000
2291	H	1.837066000	4.227531000	1.525096000
2292	C	2.890003000	2.686724000	2.600599000
2293	H	2.788596000	1.780707000	3.214401000
2294	C	4.152247000	3.042098000	2.142432000
2295	H	4.222971000	3.899757000	1.454837000
2296	C	5.317906000	2.235813000	2.273910000
2297	C	6.417516000	2.509425000	1.377919000
2298	H	6.303697000	3.410564000	0.746063000
2299	C	7.857124000	2.299266000	1.743638000
2300	O	8.756918000	2.908454000	1.188904000
2301	H	8.059970000	1.595196000	2.595176000
2302	C	5.390290000	1.150233000	3.315209000
2303	H	5.395343000	1.596575000	4.332178000

2304	H	4.499875000	0.494347000	3.237860000
2305	H	6.276206000	0.505930000	3.178523000
2306	C	0.161034000	1.447034000	2.878896000
2307	H	-0.841874000	1.456129000	3.348598000
2308	H	0.200490000	0.612610000	2.144165000
2309	H	0.907084000	1.229300000	3.662424000
2310	C	-0.584114000	3.334993000	1.344466000
2311	H	-0.341566000	4.319197000	0.919949000
2312	C	-1.737832000	2.667617000	0.999016000
2313	H	-1.841832000	1.677371000	1.458528000
2314	C	4.175456000	-1.178942000	-1.626176000
2315	N	5.007047000	-0.494250000	-1.178963000
2316	C	3.068568000	-1.981743000	-2.111035000
2317	H	2.122658000	-1.466271000	-1.832602000
2318	H	3.085059000	-2.978247000	-1.628500000
2319	H	3.117563000	-2.103821000	-3.210759000
2320	C	1.117600000	3.225746000	-3.079491000
2321	N	1.407236000	2.536364000	-2.184277000
2322	C	0.762029000	4.084933000	-4.194940000
2323	H	0.753825000	5.145505000	-3.872196000
2324	H	-0.247071000	3.821867000	-4.569190000
2325	H	1.495053000	3.966513000	-5.018518000
2326	C	-3.869294000	2.105606000	0.014459000
2327	C	-5.164619000	2.420011000	-0.689098000
2328	C	-5.349350000	3.902848000	-0.997802000
2329	C	-4.059968000	4.430581000	-1.616670000
2330	C	-2.849628000	4.359733000	-0.647930000
2331	C	-2.838559000	3.025194000	0.128456000
2332	H	-6.001384000	2.025285000	-0.068974000
2333	H	-5.209107000	1.819915000	-1.630172000
2334	H	-6.212309000	4.056623000	-1.677781000
2335	H	-5.581953000	4.455816000	-0.061900000
2336	H	-4.172900000	5.479490000	-1.962333000
2337	H	-3.832063000	3.824113000	-2.522010000
2338	C	-3.802296000	0.711949000	0.597566000
2339	H	-2.809274000	0.241007000	0.453854000
2340	H	-4.024753000	0.710886000	1.687844000
2341	H	-4.559017000	0.059760000	0.118643000
2342	C	-2.911303000	5.561891000	0.322119000
2343	H	-2.098505000	5.541436000	1.072528000
2344	H	-2.834549000	6.516584000	-0.239862000
2345	H	-3.868566000	5.572966000	0.880943000
2346	C	-1.586257000	4.444878000	-1.538448000
2347	H	-1.676012000	5.308212000	-2.231982000
2348	H	-0.650629000	4.567500000	-0.964838000
2349	H	-1.485465000	3.515565000	-2.134358000
2350				
2351	TS-trans			
2352	Pd	1.696517	0.682871	-1.309126
2353	Pd	-1.356545	0.918815	-1.702695
2354	Cl	2.736837	-0.700535	0.256535
2355	Cl	0.450555	2.028497	-2.865541
2356	Cl	-3.079147	-0.182920	-0.638511
2357	Cl	-1.258562	2.434914	0.029225
2358	C	1.835326	2.372756	-0.128925
2359	C	0.906278	2.541719	1.014621
2360	H	1.709806	3.210629	-0.841052
2361	C	-0.118853	6.088565	4.408384
2362	H	-0.007061	3.513994	3.395031
2363	C	0.313375	5.648756	3.162939
2364	H	0.702458	6.412818	2.467630
2365	C	0.326999	4.300826	2.700608
2366	C	0.762696	3.913795	1.450429
2367	H	1.058313	4.687533	0.721938
2368	C	3.310253	2.330351	0.258039
2369	O	4.169909	2.932979	-0.360238
2370	H	3.555460	1.691269	1.148881
2371	C	-0.711825	5.163501	5.440541
2372	H	-0.102793	5.162218	6.368770
2373	H	-1.729617	5.500030	5.726450
2374	H	-0.794116	4.121321	5.086693
2375	C	0.676917	1.403261	1.960802
2376	H	-0.119944	1.613332	2.695787
2377	H	0.434160	0.482089	1.402422

2378	H	1.627061	1.197039	2.501871
2379	C	0.017723	7.494462	4.723853
2380	H	0.493636	8.114211	3.947954
2381	C	-0.335335	8.069079	5.918517
2382	H	-0.725448	7.391440	6.697173
2383	C	1.842367	-1.954184	-3.115368
2384	N	1.676208	-0.948332	-2.548714
2385	C	2.091128	-3.220694	-3.784428
2386	H	1.162778	-3.824170	-3.838055
2387	H	2.849253	-3.795009	-3.213873
2388	H	2.472553	-3.051497	-4.811196
2389	C	-1.663919	-1.087135	-4.068310
2390	N	-1.519202	-0.345816	-3.180964
2391	C	-1.861617	-2.000882	-5.180126
2392	H	-2.898268	-1.910829	-5.563284
2393	H	-1.698520	-3.048267	-4.854797
2394	H	-1.157706	-1.763703	-6.002938
2395	C	-0.377954	10.536410	5.512467
2396	C	-0.190220	11.963229	5.983834
2397	C	-0.155968	12.132635	7.502989
2398	C	0.713373	11.044710	8.124783
2399	C	0.185396	9.619623	7.840528
2400	C	-0.173467	9.458117	6.341866
2401	H	-0.983213	12.599931	5.534585
2402	H	0.761394	12.343790	5.538134
2403	H	0.223428	13.140608	7.769978
2404	H	-1.188734	12.073167	7.908494
2405	H	0.801909	11.180710	9.223926
2406	H	1.744929	11.128933	7.716012
2407	C	-0.807823	10.421218	4.071333
2408	H	0.057180	10.538944	3.380168
2409	H	-1.288835	9.452930	3.839079
2410	H	-1.516412	11.237111	3.816739
2411	C	-1.072101	9.337894	8.696779
2412	H	-1.479878	8.325005	8.501530
2413	H	-0.826665	9.393642	9.778017
2414	H	-1.881705	10.064389	8.484544
2415	C	1.299244	8.623275	8.236017
2416	H	1.604772	8.792745	9.289750
2417	H	0.973852	7.567856	8.149382
2418	H	2.193865	8.752994	7.593556
2419				

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2420				
2421	Pd	1.75400818708753	0.52560108949756	-1.17086126581191
2422	Pd	-0.89775924015415	1.56771457600069	-2.17844324230859
2423	Cl	2.06016805828787	-0.97023793289723	0.59592914123358
2424	Cl	1.31123584550926	2.02795821199292	-3.01230864355697
2425	Cl	-2.99438413960151	1.08791877282266	-1.34720177371100
2426	Cl	-0.64335742698871	3.26233454262058	-0.59475163948447
2427	C	1.89780631029304	2.17239523789919	0.06363989694337
2428	C	0.65439275352606	2.56372035551806	0.84119151027597
2429	H	2.17584496888238	2.97540542883597	-0.64456861272690
2430	C	3.07740678416429	6.67093705821573	2.43159259691891
2431	H	2.66519825225794	4.42283072835500	0.91077470429499
2432	C	1.97590391621406	5.83068564650120	2.40820125400792
2433	H	1.11970688526040	6.09696598669512	3.05297766190293
2434	C	1.84556255501210	4.65182659178023	1.60778988335208
2435	C	0.78063010180673	3.78879594552706	1.65950222417226
2436	H	-0.05435995026685	3.99904569939483	2.35129874860469
2437	C	3.09894342110747	1.89539098953692	0.93697069469953
2438	O	4.21257437542952	2.33914126897846	0.68678997179458
2439	H	2.91678856579959	1.25141347219570	1.83853983167124
2440	C	3.32965016499164	6.39646305856357	1.63657992064947
2441	H	4.45634029547544	7.14521731216210	0.82603219275193
2442	H	5.22473030287865	6.47472563715328	2.28608643067652
2443	H	4.34032196089394	5.39087958140991	1.18057337060644
2444	C	-0.13842225628731	1.45799866113422	1.50172530352268
2445	H	-1.02947451585323	1.85578628437005	2.02308387913314
2446	H	-0.44219717638976	0.68937085536256	0.76831111240295
2447	H	0.52549555457318	0.95555912696174	2.23674585005025
2448	C	3.01087692416249	7.86615921830144	3.25073794719946
2449	H	2.07134736808794	8.01250958109275	3.80902076176043
2450	C	3.98148225207924	8.82902956640605	3.32470841121009
2451	H	4.86348426335624	8.70245941329164	2.671638164449216

2452	C	1.89935568098683	-2.22396690207945	-2.81598838079373
2453	N	1.75918159809583	-1.14724083631518	-2.38750985097245
2454	C	2.12114148389477	-3.58181611452153	-3.28658244791357
2455	H	1.15747328432486	-4.09601511183507	-3.47425012135358
2456	H	2.67430395867983	-4.14911689783283	-2.51018750562773
2457	H	2.71832835528228	-3.58024488623826	-4.22028367122288
2458	C	-1.27110080694919	-0.65250060327426	-4.32499842047088
2459	N	-1.13371161131850	0.18604905950559	-3.52876294147316
2460	C	-1.44339012720204	-1.69717809552641	-5.31865837732105
2461	H	-2.16833867080798	-1.37236893187702	-6.09198459000282
2462	H	-1.82829531299335	-2.61946587954247	-4.83933583463611
2463	H	-0.47536036849657	-1.91913763228164	-5.81030147190166
2464	C	3.50182435483969	10.13559511272465	5.39868341799616
2465	C	3.47764024733872	11.43503045421827	6.17802985157628
2466	C	4.35186957320649	12.53965228158750	5.58465356973734
2467	C	4.13780416187493	12.60898761324198	4.07553882373603
2468	C	4.52854667681528	11.29757431204267	3.35546678350068
2469	C	3.95110063636309	10.06987828991505	4.10205666600092
2470	H	3.76365241637324	11.23046565131902	7.23265161853338
2471	H	2.41681341028463	11.78113936398283	6.23438753359288
2472	H	4.12020934071047	13.51415773901163	6.06249597099821
2473	H	5.42031298794445	12.32979500743167	5.80812294276070
2474	H	4.70958691866280	13.44917408629002	3.62646351644905
2475	C	3.06370108485341	12.81829231870068	3.87474992664533
2476	C	3.00151620516836	8.94494251216545	6.17866633818596
2477	H	1.88935804486310	8.93052446428227	6.22974762565638
2478	H	3.32645821451627	7.97994434355912	5.74834926784845
2479	H	3.35669351930805	8.99925469676440	7.22931709926626
2480	C	6.06912729121674	11.17451073522463	3.27874188443261
2481	H	6.38038219857332	10.22919330156004	2.78941023747434
2482	H	6.49533004970511	12.00944602571103	2.68387666162305
2483	H	6.53233200690750	11.19263382677417	4.28491278787963
2484	C	3.95655659184221	11.35866814653464	1.92080145739861
2485	H	4.31121581071993	12.27728739343400	1.40813338366181
2486	H	4.26707950678141	10.48994326492040	1.30700955412508
2487	H	2.84760944903853	11.37635052874233	1.93731145188284
2488				

2489 TS-cis

2490	Pd	1.79018774422095	0.28197256973409	-1.06789297355372
2491	Pd	-0.47053610901261	2.08969658584918	-2.20294598795136
2492	Cl	1.67588288250703	-1.35970609990997	0.58800942049839
2493	Cl	1.86302244108583	2.00217771321804	-2.76228313243153
2494	Cl	-2.70833778534899	2.08646339726375	-1.64460554673356
2495	Cl	-0.03759469796180	3.61545896396465	-0.50331947602175
2496	C	2.08301100216244	1.74477700782938	0.33595771958183
2497	C	0.86565235310530	2.24729967825964	1.08364085866779
2498	H	2.50096884917010	2.56853529132059	-0.27474215681255
2499	C	3.70731366640401	5.48497656430024	3.63087229418246
2500	H	3.07770998121442	3.74172965850051	1.60601002697886
2501	C	2.50950507056112	4.82107654917911	3.39460319323410
2502	H	1.67081027746759	5.02826243604580	4.08297850988938
2503	C	2.26872165389124	3.90083581250802	2.33464792819601
2504	C	1.09602201513480	3.19495694513076	2.16012015653779
2505	H	0.25687238805699	3.36827820894629	2.85629288980590
2506	C	3.22186744819389	1.27904159050350	1.22220365387533
2507	O	4.37805929112999	1.64596593417120	1.06179224778669
2508	H	2.94478812398270	0.55517917286615	2.03537037167949
2509	C	4.94247262115215	5.25672077766790	2.79689032771248
2510	H	5.17168721303938	6.15165977137129	2.18014538681031
2511	H	5.82293686477625	5.08140630807289	3.44768820707232
2512	H	4.85499165925537	4.38575675858499	2.12324419714791
2513	C	-0.29458861662740	1.31641544980892	1.29702578495333
2514	H	-1.12972617707583	1.80598361516473	1.83238159113501
2515	H	-0.66137866356191	0.88422961030314	0.34822858433261
2516	H	0.09014772660228	0.45717638130886	1.89199523865615
2517	C	3.75187643979416	6.43581379361496	4.72121445810260
2518	H	2.81438309940400	6.55747355800059	5.28826735717287
2519	C	4.82880761572851	7.21701593164488	5.05193697920900
2520	H	5.71935581388011	7.14784766198013	4.40275604152198
2521	C	1.62720570338814	-2.26356691561138	-3.02044407825161
2522	N	1.61917450128255	-1.24220474713764	-2.45509732916877
2523	C	1.68790654664919	-3.56037739614063	-3.67600527304709
2524	H	0.70094995162427	-3.84006003331657	-4.09528828709935
2525	H	1.98348707063773	-4.33125501050450	-2.93583808314317

2526	H	2.43544558788711	-3.54674392498202	-4.49451796836778
2527	C	-1.12667606001703	0.02283364617742	-4.43374630866054
2528	N	-0.85985573359370	0.80999941302950	-3.61783201256873
2529	C	-1.45916981063177	-0.96411393246068	-5.44548236779724
2530	H	-2.02696812840560	-0.49007232953967	-6.27148723108018
2531	H	-2.08230760685866	-1.76736761078375	-5.00283290085848
2532	H	-0.53440229971628	-1.40937226022505	-5.86334514856552
2533	C	4.39862598115077	7.99932436299156	7.38285870542413
2534	C	4.48483873726646	9.04775400293006	8.47301595210858
2535	C	5.49546327892781	10.16223215819449	8.20396724222963
2536	C	5.37705490871537	10.62718486373527	6.75609128982752
2537	C	5.67316130637876	9.49985825486390	5.74005465542255
2538	C	4.90746387640895	8.21007290175305	6.12285607359718
2539	H	4.70044978803416	8.54564619261175	9.44113536655202
2540	H	3.46476321778524	9.48417745701011	8.60339512649718
2541	H	5.33455562385741	11.00669077195743	8.90522700037784
2542	H	6.52376454693562	9.78831074757237	8.39955687057022
2543	H	6.05748726018945	11.48110420029311	6.55117856703704
2544	H	4.34311371232310	10.99916658658073	6.57935001822414
2545	C	3.72079176032447	6.72363083581804	7.81769238899849
2546	H	2.61428944545934	6.84272033314453	7.84583201963389
2547	H	3.94581432219778	5.86676834287830	7.15638640272032
2548	H	4.02784809145371	6.46193293628607	8.85197323827101
2549	C	7.19115206134801	9.20307532055311	5.70063730905719
2550	H	7.43160121266300	8.39838725909557	4.97616851510440
2551	H	7.75493808134958	10.10752329966117	5.38916537364563
2552	H	7.57119298412772	8.88196450513239	6.69029194377699
2553	C	5.21890512650349	9.99623791473688	4.34800232749295
2554	H	5.70380921415479	10.96624043872425	4.11265993346574
2555	H	5.48275963064442	9.28637863847480	3.53916677369078
2556	H	4.12039050522264	10.14465631629187	4.32020361564697

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2557	Pd	6.111767000	1.188870000	0.319207000
2558	Pd	2.464844000	1.123597000	-0.530195000
2559	Cl	7.852443000	-0.159210000	1.099832000
2560	Cl	4.411323000	2.536922000	-0.693844000
2561	Cl	0.691177000	-0.366455000	-0.539107000
2562	Cl	2.895519000	0.590882000	1.671107000
2563	C	5.142542000	0.051231000	4.952327000
2564	C	4.065487000	-0.577530000	5.577952000
2565	H	6.133913000	-0.423401000	5.052891000
2566	C	5.060439000	1.196490000	4.121875000
2567	H	4.089170000	1.703872000	4.039278000
2568	C	6.099923000	1.637706000	3.314570000
2569	H	7.036652000	1.058798000	3.301873000
2570	C	5.926821000	2.658901000	2.328600000
2571	C	6.917907000	2.900705000	1.303875000
2572	H	6.707293000	3.744648000	0.622520000
2573	C	8.396785000	2.745261000	1.513139000
2574	O	9.209160000	3.289824000	0.784756000
2575	H	8.717018000	2.160218000	2.417206000
2576	C	4.695074000	3.524880000	2.366149000
2577	H	3.781217000	2.902754000	2.258022000
2578	H	4.645572000	4.049692000	3.342735000
2579	H	4.698844000	4.271257000	1.553909000
2580	C	2.649036000	-0.081005000	5.438089000
2581	H	2.057354000	-0.781480000	4.811443000
2582	H	2.148389000	-0.014916000	6.424847000
2583	H	2.587049000	0.905778000	4.949472000
2584	C	4.329471000	-1.781162000	6.327069000
2585	H	5.387938000	-2.073690000	6.383969000
2586	C	3.353986000	-2.564810000	6.903484000
2587	H	2.324451000	-2.214089000	6.742414000
2588	C	4.557040000	-1.341731000	-0.792024000
2589	N	5.283125000	-0.464885000	-0.538297000
2590	C	3.589030000	-2.382703000	-1.070608000
2591	H	2.568276000	-1.953400000	-0.916172000
2592	H	3.738709000	-3.234765000	-0.378975000
2593	H	3.686489000	-2.736554000	-2.115758000
2594	C	1.806366000	1.838437000	-3.505352000
2595	N	2.063276000	1.571144000	-2.399262000
2596	C	1.478992000	2.169268000	-4.881601000
2597	H	0.856789000	3.086431000	-4.916898000
2598	H	0.913632000	1.337490000	-5.348568000
2599	H			

2600	H	2.405296000	2.344486000	-5.464476000
2601	C	2.281115000	-4.512636000	7.873430000
2602	C	2.254441000	-5.889655000	8.490939000
2603	C	3.621074000	-6.563442000	8.584037000
2604	C	4.638487000	-5.544592000	9.084961000
2605	C	4.825408000	-4.347582000	8.116747000
2606	C	3.455111000	-3.813892000	7.638217000
2607	H	1.533070000	-6.515656000	7.918968000
2608	H	1.798567000	-5.799849000	9.507417000
2609	H	3.574362000	-7.445680000	9.254601000
2610	H	3.921178000	-6.945676000	7.584861000
2611	H	5.629553000	-6.014559000	9.258342000
2612	H	4.300160000	-5.157698000	10.071549000
2613	C	0.907948000	-4.000505000	7.498293000
2614	H	0.778652000	-2.914085000	7.667452000
2615	H	0.683623000	-4.195570000	6.426489000
2616	H	0.129036000	-4.523236000	8.087549000
2617	C	5.679546000	-4.811846000	6.911565000
2618	H	5.841706000	-4.009691000	6.167241000
2619	H	6.675780000	-5.155794000	7.258899000
2620	H	5.193873000	-5.653237000	6.378283000
2621	C	5.579507000	-3.260169000	8.919713000
2622	H	6.501058000	-3.694156000	9.358890000
2623	H	5.880012000	-2.389379000	8.310038000
2624	H	4.951181000	-2.883540000	9.752511000
2625				