Supplementary Material for:

Single-factor analysis of Ni-B-AC-catalyzed β-pinene hydrogenation: based on hierarchical analysis

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Criteria for Hierarchical Analysis data:
Single-factor investigation of the preparation of Ni-B-AC catalysts

Reaction Time	**2h**	**3h**	**5h**	**4.5h**	**4h**
2h	-	22.78%	46.12%	38.16%	63.25%
3h	-	-	1.24%	15.38%	40.47%
5h	-	-	-	14.14%	39.23%
4.5h	-	-	-	-	25.09%
4h	-	-	-	-	-
AC/Ni	**1:4**	**1:7**	**1:5**	**1:8**	**1:6**
1:4	-	71.42%	12.28%	44.93%	47.35%
1:7	-	-	59.14%	26.49%	24.07%
1:5	-	-	-	32.65%	35.07%
1:8	-	-	-	-	2.42%
1:6	-	-	-	-	-
pH	**pH=11**	**pH=9**	**pH=12**	**pH=13**	**pH=14**
pH=11	-	12.94%	13.56%	26.51%	3.02%
pH=9	-	-	26.50%	39.45%	9.92%
pH=12	-	-	-	12.95%	16.58%
pH=13	-	-	-	-	29.53%
pH=14	-	-	-	-	-
Rates of Drops	**45drops/ min**	**30drops/ min**	**60drops/ min**	**50drops/ min**	**70drops/ min**
45drops/min	-	12.03%	5.93%	20.32%	33.16%
30drops/min	-	-	17.96%	32.35%	21.13%
60drops/min	-	-	-	14.39%	39.09%
50drops/min	-	-	-	-	53.48%
70drops/min	-	-	-	-	-
Ni/B	**1:3**	**1:4**	**1:5**	**1:6**	**1:7**
1:3	-	8.61%	16.85%	30.63%	34.10%
1:4	-	-	25.46%	39.24%	42.71%
1:5	-	-	-	13.78%	17.25%
1:6	-	-	-	-	3.47%
1:7	-	-	-	-	-

β-pinene hydrogenation process Single-factor examination:

Stir	**600r/min**	**700r/min**	**750r/min**	**800r/min**	**850r/min**
600r/min	-	17.40%	43.10%	40.57%	6.58%
700r/min	-	-	25.70%	23.17%	10.82%
750r/min	-	-	-	2.53%	36.52%
800r/min	-	-	-	-	33.99%
850r/min	-	-	-	-	-
Pressure	**2MPa**	**2.5MPa**	**3.0MPa**	**4.0MPa**	**5.0MPa**
2MPa	-	1.25%	2.81%	2.23%	8.34%
2.5MPa	-	-	1.56%	3.48%	9.59%
3.0MPa	-	-	-	5.04%	11.15%
4.0MPa	-	-	-	-	6.11%
5.0MPa	-	-	-	-	-
wt%	**3wt%**	**4wt%**	**5wt%**	**6wt%**	**7wt%**
3wt%	-	5.13%	5.76%	5.16%	1.15%
4wt%	-	-	0.63%	0.03%	3.98%
5wt%	-	-	-	0.60%	4.61%
6wt%	-	-	-	-	4.01%
7wt%	-	-	-	-	-
Reaction Temperature	**100℃**	**110℃**	**140℃**	**130℃**	**120℃**
100℃	-	4.26%	11.16%	5.55%	7.73%
110℃	-	-	15.42%	1.29%	3.15%
140℃	-	-	-	16.71%	18.57%
130℃	-	-	-	-	1.86%

Criteria for Gaussian 16:

Partial citation of references 54:

54. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 16 Rev. C.01*, Wallingford, CT, 2016.

Atoms Coordinates：

NiB_2

Symbolic Z-matrix:
Charge=0 Multiplicity=1

B	-0.23754	0.19435	0.000
B	0.30346	1.72035	0.074
Ni	-1.32254	1.49135	-1.074
H	-0.09854	-1.09665	0.376
H	1.21146	2.59835	0.555

Ni_2B_2
Symbolic Z-matrix:
Charge=0 Multiplicity=1

B	0.10797	0.04319	0.000
B	1.62497	-0.76981	-0.256
Ni	0.32797	-1.70781	0.955
Ni	0.07897	-1.45281	-1.338

Ni_3B_2
Symbolic Z-matrix:
Charge=0 Multiplicity=1

B	-0.15116	0.08638	0.000
B	0.07384	-1.84862	0.000
Ni	-2.14116	-1.12562	0.000
Ni	-0.47816	-0.93262	-1.478
Ni	-0.47816	-0.93262	1.478

Ni_4B_2
Symbolic Z-matrix:
Charge=0 Multiplicity=1

Ni	0.15116	0.06478	0.000
Ni	2.68416	-0.35522	-0.06
Ni	-0.26984	-2.46922	-0.06
Ni	2.26316	-2.88922	-0.12
B	1.18916	-1.38622	-1.016
B	1.22516	-1.43822	0.896