absToolkit

———*an open-source frequencies searcher, also a small subroutine of SIMUPKGS distributed independently*

For reporting issue or uploading datasets, contact me via:
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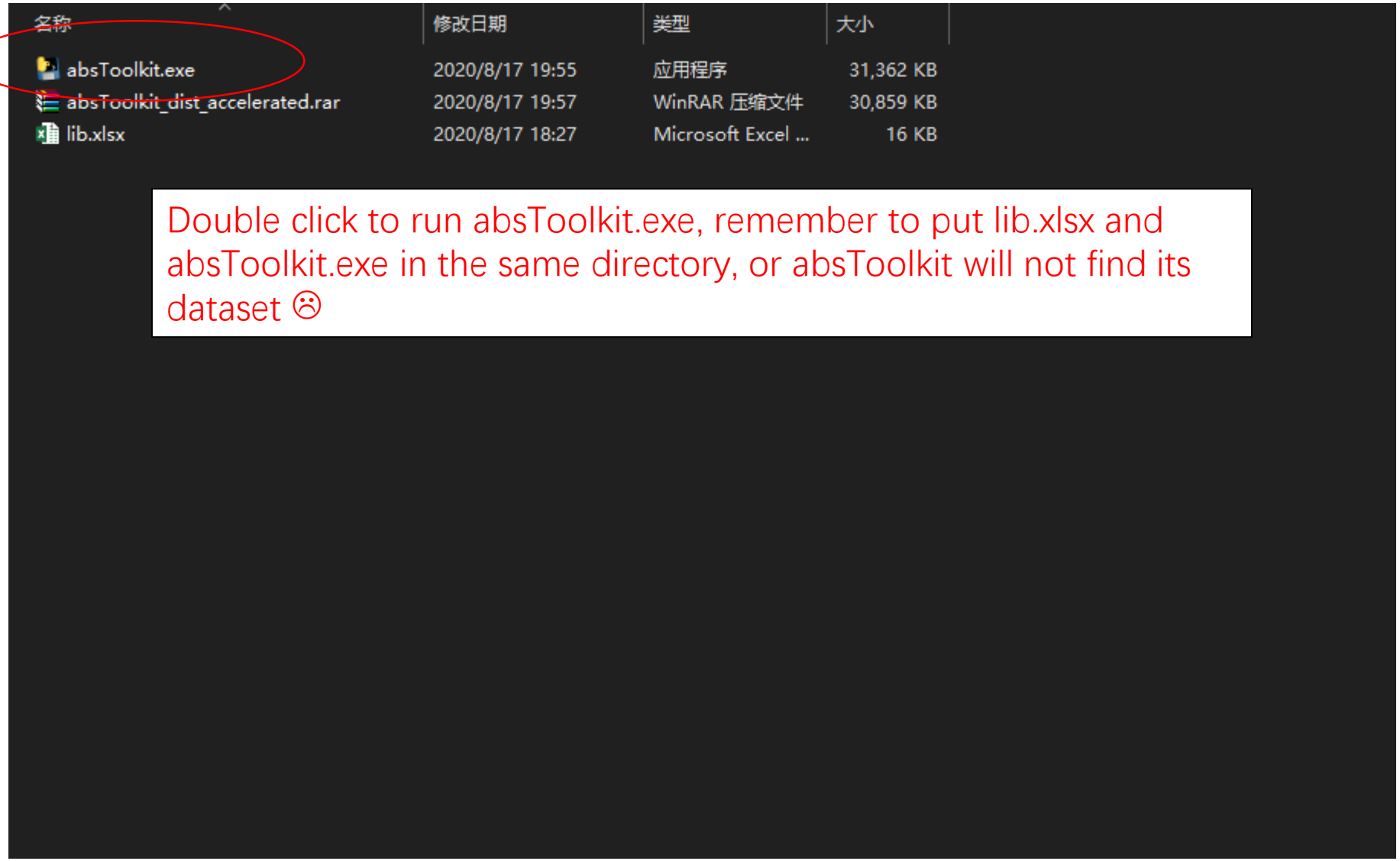
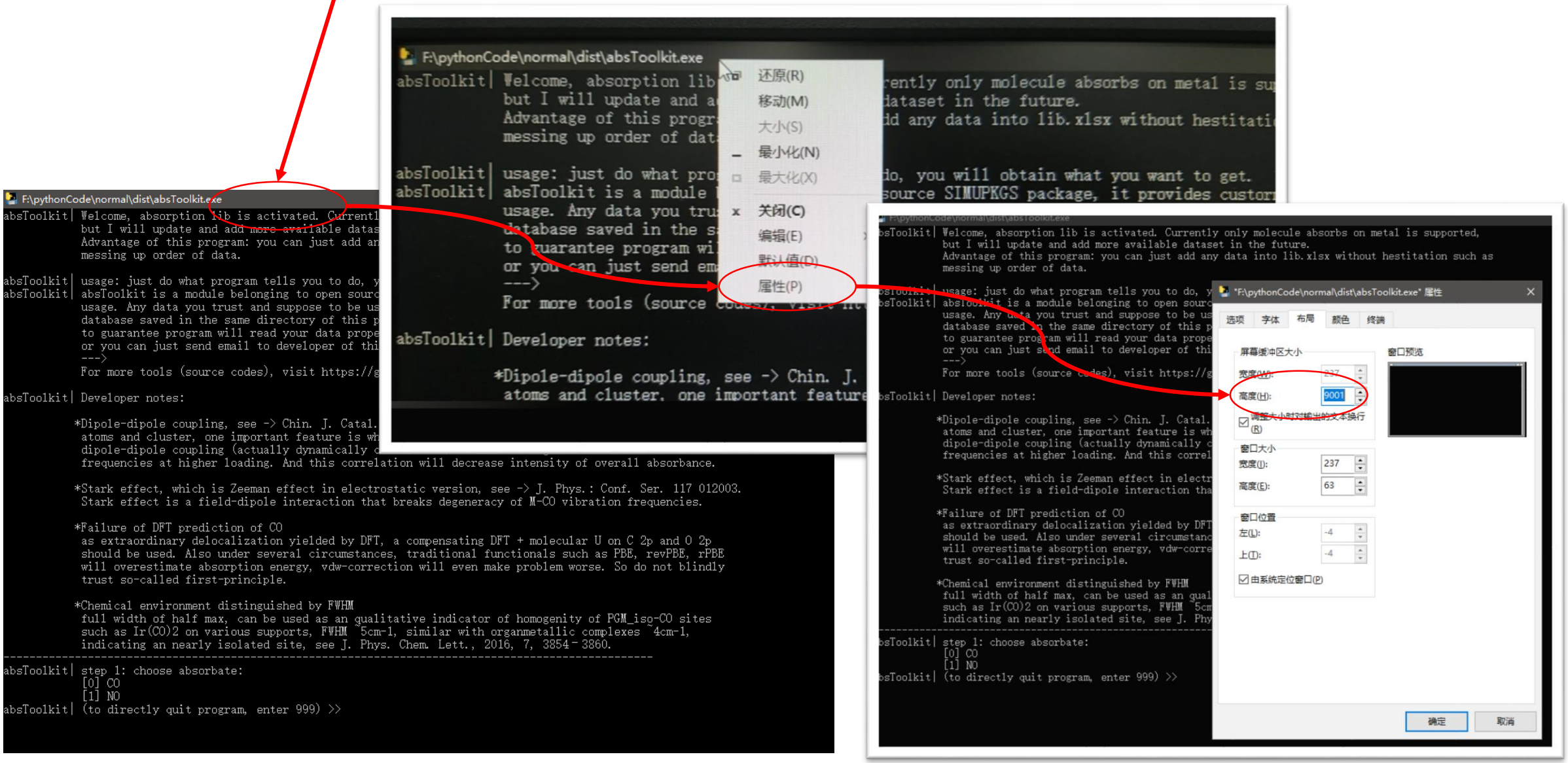

名称
修改日期
类型
大小
absToolkit.exe
2020/8/17 19:55
应用程序
31,362 KB
absToolkit_dist_accelerated.rar
2020/8/17 19:57
WinRAR 压缩文件
30,859 KB
lib.xlsx
2020/8/17 18:27
Microsoft Excel ...
16 KB
Double click to run absToolkit.exe, remember to put lib.xlsx and absToolkit.exe in the same directory, or absToolkit will not find its dataset ☹

To get a not bad program using experience, maximize this window size. If you find trouble when want to maximize it, **right click on the header** of this window and, click setting to change something in it.



To choose CO absorption, press 0 and ENTER

```
          will overestimate absorption energy, vdw-correction will even make problem worse. So do not blindly
          trust so-called first-principle.

         *Chemical environment distinguished by FWHM
          full width of half max, can be used as an qualitative indicator of homogenity of PGM_iso-CO sites
          such as Ir(CO)2 on various supports, FWHM ~5cm-1, similar with organmetallic complexes ~4cm-1,
          indicating an nearly isolated site, see J. Phys. Chem. Lett., 2016, 7, 3854-3860.
-------------------------------------------------------------------------------------------
absToolkit| step 1: choose absorbate:
          [0] CO
          [1] NO
absToolkit| (to directly quit program, enter 999) >> 0
```

For instance, if you want to look up CO frequencies of moiety CO-Au/support, type-in Au and ENTER

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-------------------------------------------------------------------------------------------
absToolkit| step 1: choose absorbate:
          [0] CO
          [1] NO
absToolkit| (to directly quit program, enter 999) >> 0
absToolkit| for molecule you choose, there are 37 lines of data available.
-------------------------------------------------------------------------------------------
absToolkit| step 2: type-in element symbol of your metal, currently supported metals: ['Rh', 'Pt', 'Au']
absToolkit| (to directly quit program, enter 999) >> Au
```

Enter frequency you measured in experiment, e.g., 2100, then ENTER

```
-------------------------------------------------------------------------------------------
absToolkit| step 2: type-in element symbol of your metal, currently supported metals: ['Rh', 'Pt', 'Au']
absToolkit| (to directly quit program, enter 999) >> Au
-------------------------------------------------------------------------------------------
absToolkit| step 3: type-in frequence in cm-1 you want to look up.
absToolkit| >> 2100
```

Just ENTER, under most common circumstances, this function is not needed.

```
absToolkit| step 3: type-in frequence in cm-1 you want to look up.
absToolkit| >> 2100
------------------------------------------------------------------------------------------------
absToolkit| step 4: (press Enter directly or choose 'normal mode' if you dont know what this step means)
            [1] normal mode (0)
            [2] very tight (0.0001)
            [3] tight (0.001)
            [4] default (0.01)
            [5] loose (0.1)
            [6] very loose (0.3)
            [7] awfully loose (0.5)
            [8] Do you feel lucky? (1.0)
            ----->>> I just salute to Gaussian software :)
absToolkit| >> _
```

```
            [5] loose (0.1)
            [6] very loose (0.3)
            [7] awfully loose (0.5)
            [8] Do you feel lucky? (1.0)
            ----->>> I just salute to Gaussian software :)
absToolkit| >>
----------------------------------------SEARCH RESULT----------------------------------------------
   active metal support frequencey domain  mode description                       reference                       reference.1
11          Au     TiO2              2100  CO on anionic Au  J. Phys. Chem. C 2011, 115, 22400-22408  J. Am. Chem. Soc. 2006, 128, 6341
---------------------------------------------------------------------------------------------------
absToolkit| thank you, absorption toolkit will quit. Results above only the first two reference is listed.
            If you need more reference to cite, search the number emerges at head of line, it is the line number
            of datafile lib.xlsx.

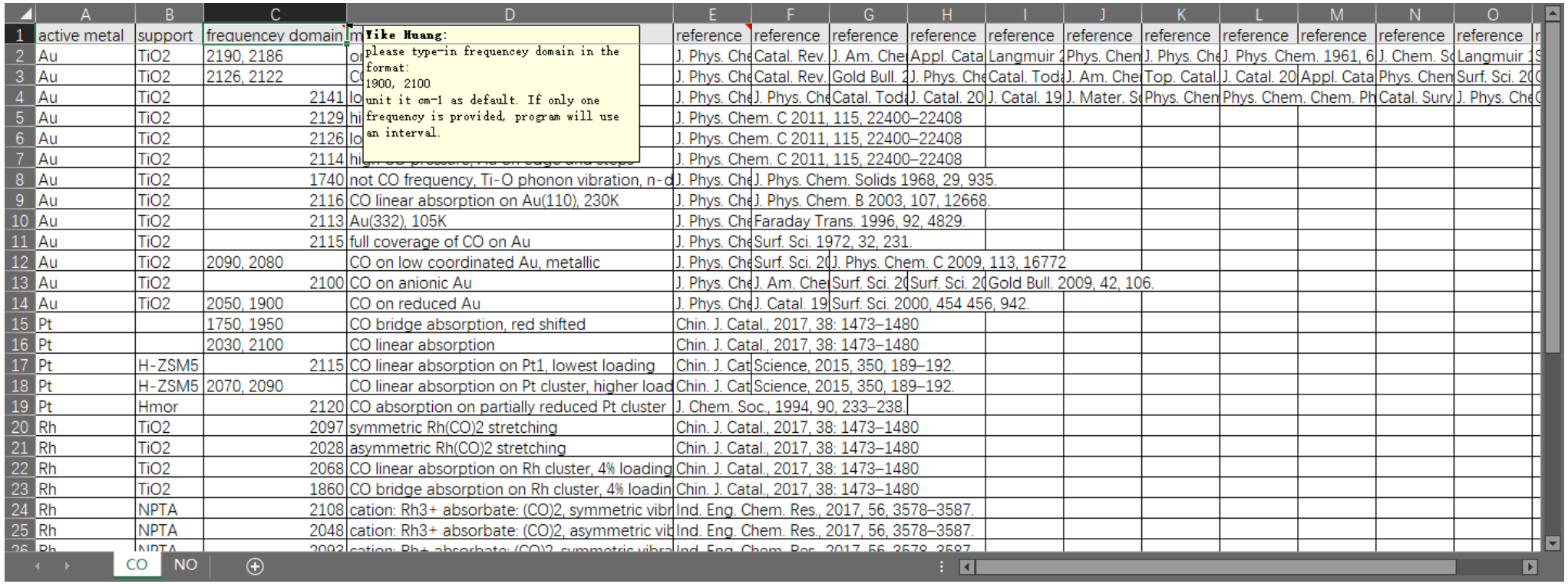
            If you want to have contribution on this program,
            -> send your customized lib.xlsx to me ykhuang@dicp.ac.cn
            -> make comments and report issues at https://github.com/kirk0830/SIMUPKGS

absToolkit| press ENTER to quit. >> _
```

Finally we obtain relating data (if exists), "**mode description**" is a short description of vibration, also there are **two references provided** explicitly. For more information, please read instructions of absToolkit.

Data extension: in lib.xlsx, you can add more data once you see in paper, for your future use. To properly type-in new data, just follow format of present data. Also it is highly recommended to share your customized data with other absToolkit users. An updated version of lib.xlsx is welcome if sent to ykhuang@dicp.ac.cn. Once there is any updated version of lib.xlsx, I will update it at https://github.com/kirk0830/SIMUPKGS. ***WARNING***: in the third column, Chinese comma (‘，’) is strictly illegal! Use English comma and a blank (‘, ’).

If one frequency is provided, program absToolkit will search around ±5cm-1, if two frequencies are provided, and normal mode is used in step 4., absToolkit will search directly in interval of them two.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	active metal	support	frequencey domain	m	reference	reference	reference	reference	reference	reference	reference	reference	reference	reference	reference
2	Au	TiO2	2190, 2186	o	J. Phys. Che	Catal. Rev.	J. Am. Che	Appl. Cata	Langmuir 2	Phys. Chem	J. Phys. Che	J. Phys. Chem. 1961, 6	J. Chem. Sc	Langmuir 19	
3	Au	TiO2	2126, 2122	C	J. Phys. Che	Catal. Rev.	Gold Bull. 2	J. Phys. Che	Catal. Toda	J. Am. Che	Top. Catal.	J. Catal. 20	Appl. Cata	Phys. Chem	Surf. Sci. 20
4	Au	TiO2	2141	lo	J. Phys. Che	J. Phys. Che	Catal. Toda	J. Catal. 20	J. Catal. 19	J. Mater. Sc	Phys. Chem	Phys. Chem. Chem. Ph	Catal. Surv	J. Phys. Che	
5	Au	TiO2	2129	hi	J. Phys. Chem. C 2011, 115, 22400–22408										
6	Au	TiO2	2126	lo	J. Phys. Chem. C 2011, 115, 22400–22408										
7	Au	TiO2	2114	hi	J. Phys. Chem. C 2011, 115, 22400–22408										
8	Au	TiO2	1740	not CO frequency, Ti-O phonon vibration, n-d	J. Phys. Che	J. Phys. Chem. Solids 1968, 29, 935.									
9	Au	TiO2	2116	CO linear absorption on Au(110), 230K	J. Phys. Che	J. Phys. Chem. B 2003, 107, 12668.									
10	Au	TiO2	2113	Au(332), 105K	J. Phys. Che	Faraday Trans. 1996, 92, 4829.									
11	Au	TiO2	2115	full coverage of CO on Au	J. Phys. Che	Surf. Sci. 1972, 32, 231.									
12	Au	TiO2	2090, 2080	CO on low coordinated Au, metallic	J. Phys. Che	Surf. Sci. 20	J. Phys. Chem. C 2009, 113, 16772								
13	Au	TiO2	2100	CO on anionic Au	J. Phys. Che	J. Am. Che	Surf. Sci. 20	Surf. Sci. 20	Gold Bull. 2009, 42, 106.						
14	Au	TiO2	2050, 1900	CO on reduced Au	J. Phys. Che	J. Catal. 19	Surf. Sci. 2000, 454 456, 942.								
15	Pt		1750, 1950	CO bridge absorption, red shifted	Chin. J. Catal., 2017, 38: 1473–1480										
16	Pt		2030, 2100	CO linear absorption	Chin. J. Catal., 2017, 38: 1473–1480										
17	Pt	H-ZSM5	2115	CO linear absorption on Pt1, lowest loading	Chin. J. Cat	Science, 2015, 350, 189–192.									
18	Pt	H-ZSM5	2070, 2090	CO linear absorption on Pt cluster, higher load	Chin. J. Cat	Science, 2015, 350, 189–192.									
19	Pt	Hmor	2120	CO absorption on partially reduced Pt cluster	J. Chem. Soc., 1994, 90, 233–238.										
20	Rh	TiO2	2097	symmetric Rh(CO)2 stretching	Chin. J. Catal., 2017, 38: 1473–1480										
21	Rh	TiO2	2028	asymmetric Rh(CO)2 stretching	Chin. J. Catal., 2017, 38: 1473–1480										
22	Rh	TiO2	2068	CO linear absorption on Rh cluster, 4% loading	Chin. J. Catal., 2017, 38: 1473–1480										
23	Rh	TiO2	1860	CO bridge absorption on Rh cluster, 4% loadin	Chin. J. Catal., 2017, 38: 1473–1480										
24	Rh	NPTA	2108	cation: Rh3+ absorbate: (CO)2, symmetric vibr	Ind. Eng. Chem. Res., 2017, 56, 3578–3587.										
25	Rh	NPTA	2048	cation: Rh3+ absorbate: (CO)2, asymmetric vib	Ind. Eng. Chem. Res., 2017, 56, 3578–3587.										