

# Eh-pH図アトラス

## 熱力学データベースの相互比較

地質調査総合センター研究資料集 No.419

独立行政法人 産業技術総合研究所  
深部地質環境研究センター  
竹野 直人

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## 1 はじめに

この研究資料は、熱力学データベース間のデータの相互比較を実用的で便利な Eh-pH 図を用いて示すことを試みたものである。Eh-pH 図は、Eh, pH をそれぞれ縦軸、横軸にとり、化学組成を与えた水溶液の溶存卓越化学種と固相種の変化を、Eh および pH の関数として図示するものである。固相の出現する条件は、溶解度と関係し、溶存卓越化学種は、吸着やコロイドなどの物質表面の現象の理解に基本的な情報となるので、Eh-pH 図は、地下水中の放射性核種などの溶質の移動にとって本質的なデータを提供する。

Eh-pH 図を集成したものとして、材料の腐食・不動態などの耐性を論じた Pourbaix (1966)<sup>1</sup>、放射性廃棄物の地層処分での地球化学を論じた Brookins (1988) がよく知られているが、その後も熱力学データは増大し、さまざまな評価を経た複数の熱力学データセットがデータベースとして供給されるようになってきている。これには、計算機の性能の向上と利用の普及にともなって、さまざまな地球化学コードを用いた複雑な化学平衡計算が行なわれるようになり、熱力学データが実用上からも重要になったこともあずかっている。

地球化学コードの中には、簡便に Eh-pH 図を作成するものもある。そこで、この機能を利用して熱力学データベース間のデータを比較する素材として Eh-pH 図を利用すれば、データベースの現状 (state-of-the-arts) とそれらの差異を視覚的に把握しやすくするとともに、実用上も便利ではないかと考え、この資料をまとめた。

基本的にこの資料では、データからの作図結果をありのままに、すなわち”as is”で提示することにして、判断は利用者にゆだねた。データベース利用の際の参考となれば幸である。なお、Eh-pH 図によって示される内容は、熱力学データベースの一面にすぎないこと、かつデータベースはたえず更新されるのが常であり、この資料もデータベースのある時期のスナップショットであることに留意いただきたい。

## 2 データベースについて

比較に使用した熱力学データベースは下に示す 7 つである。1 は無機化学工学向けの汎用データベース、2 と 3 は地球化学向けの汎用データベースである。4 と 5 は放射性廃棄物の地層処分向けのデータベースであるが、汎用といっても差し支えないほどデータが網羅されている。一方、6 と 7 は放射性元素を主としていて、他の元素についてはデータが十分ではない。したがって本資料では、6 と 7 については放射性元素に限定して図を載せた。

1. GTT-Technologies 製ソフトウェア FactSage 5.2 (FACTSAGE と略称, Bale et al., 2002) に添付される FACT データベース (FACT と略称)。
2. Johnson et al. (1992) の SUPCRT92 に Everette Shock によりインターネット上で公開された 98 アップデートを適用したもの (SUPCRT と略称)。
3. イリノイ大学 C.M.Bethke の Geochemist's Workbench Release 4.0 (GWB と略称) に therm.dat として標準的に添付される Laurence Livermore National Lab. Data 0.3245r46 (LLNL と略称)。
4. 核燃料サイクル機構によって、インターネット上で公開されている、JNC-TDB 011213g0 および 011213g2 (JNC-TDB と略称)。
5. NEA Computer Program Services にて配布されている ZZ-HATCHES-15 (HATCHES と略称)。
6. OECD/NEA の Chemical Thermodynamics の第 1-4 巻のデータベース (Grenthe et al., 1992; Silva et al., 1995; Rard et al., 1999; Lemire et al., 2001, 一括して OECD-NEA と略称)。

<sup>1</sup>本資料の表題にあるアトラスという語はこの種の図表集の嚆矢ともいえる Pourbaix (1966) にならったものである。

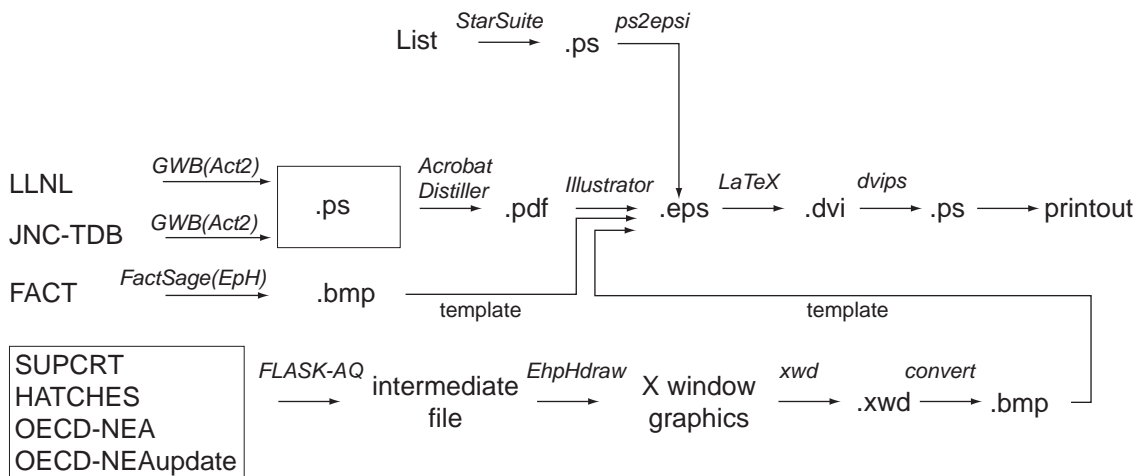


図 1: 本報告の作成フロー図  
 斜体はソフトウェア名．ドット名は拡張子の意味するファイルを示す．

7. OECD/NEA の Chemical Thermodynamics の第 5 巻 (Guillaumont et al., 2003, OECD-NEAupdate と略称)．これは Chemical Thermodynamics 第 1-4 巻のデータを改訂したものである．

### 3 作成法

この Eh-pH 図集で扱う系は，地下水中の化学反応を扱う上で最も基本的と考えられる X-H-O 系とした．X には元素名が入る．放射性廃棄物の地層処分で重要な役割を果たす天然バリアの地球化学的ふるまいを理解するために作図対象とする元素種を放射性元素に限定せず，データベースで利用できる全元素とした．ただし，OECD-NEA データベースのみ先に記した理由で特定の放射性元素のみ示した．全濃度は， $10^{-10}$  mole/kg とした．これは希薄溶液として，活動度係数を 1 と置くためと，できるだけひろい Eh-pH 領域で沈殿固相の影響を受けずに溶存卓越種を比較するためである．温度，圧力はそれぞれ 298.15K， $10^5$  Pa である．

データのコンバージョンにともなう，誤りの発生を防ぐため，商用ソフトウェア同梱のデータベースおよび特定ソフトウェア向けのフォーマットで提供されるデータベースでは，それぞれ同梱ソフト，対象ソフトウェアを使用して作図した．これに該当するのは，FACTSAGE に同梱される FACT と GWB に同梱される LLNL と GWB フォーマットの JNC-TDB である．これに該当しない，SUPCRT，HATCHES，OECD-NEA，OECD-NEAupdate は深部地質環境研究センターのインハウスソフトウェアである FLASK-AQ フォーマットのファイルを作成して，FLASK-AQ とそのコンパニオンソフトウェア EhpHdraw を用いて作図した．

Eh-pH 図の作図については，化学熱力学に詳しい地球化学の教科書 (例えば Garrels and Christ (1965) など) を参照されたい．商用ソフトウェアである FACTSAGE と GWB の Eh-pH 図の作図アルゴリズムは特に文書化されていない．FLASK-AQ は Eh -0.8 から 1.2 まで，および pH 0 から 14 までの領域をそれぞれ 0.005 および 0.04 に分割した計 140000 グリッドの Eh-pH 値に対して，溶存卓越種または沈殿固相を化学平衡計算により求めて Eh-pH 図を作成する．この方法は Anderko et al. (1997) を先例とするものと思われる．この方法では原理的に図中の領域の境界線の位置の精度が刻みに依存するので，今回の場合 Eh で  $\pm 0.0025$ ，pH で  $\pm 0.02$  の誤差を含む．次にデータから作図までの詳細をデータベースごとに記す．なお"/" の前にデータベース略称を"/" の後に使用ソフトウェア略称を示した (図 1)．

### 3.1 FACT/FACTSAGE

FACTSAGE の  $E_pH$  を用いて作成した Eh-pH 図を bmp ファイルで保存し、これを Adobe Illustrator (以下 Illustrator) のテンプレートとして、製図したのち、共通の縦・横の辺長になるように拡大・縮小した。

### 3.2 SUPCRT/FLASK-AQ

FLASK-AQ 用のデータを作成したのち、FLASK-AQ により中間ファイルを作成し、EhpHdraw を用いて、Eh-pH 図を作成する。この Eh-pH 図のウィンドウイメージを xwd を用いて取得したのち、ImageMagic の convert を用いて bmp ファイルとした。これを Illustrator のテンプレートとして、製図したのち、共通の縦・横の辺長になるように拡大・縮小した。膨大な数の有機化学種は全て、C, H, O の反応で表現したので常温の水の安定領域ではほとんどが分解してしまっている。

### 3.3 LLNL/GWB

GWB の Act2 を用いて作成した Eh-pH 図をポストスクリプトファイルで保存し、Adobe Acrobat Distiller (以下 Acrobat Distiller) を用いて pdf ファイル (ポータブルドキュメントファイル) に変換して、Illustrator で開き、共通の縦・横の辺長になるように拡大・縮小した。こうしたのは、GWB で eps ファイルで保存した Eh-pH 図を直接 Illustrator で開けなかったためである。

### 3.4 JNC-TDB/GWB

GWB の Act2 を用いて作成した Eh-pH 図をポストスクリプトファイルで保存し、Acrobat Distiller を用いて pdf ファイルに変換して、Illustrator で開き、共通の縦・横の辺長になるように拡大・縮小した。このようにしたのは、GWB で eps ファイルで保存した Eh-pH 図を直接 Illustrator で開けなかったためである。図は 011213g0 を用いて作成したが、その後、S と U のデータを修正した 011213g2 が公開されたので、S と U の図をこれを用いて入れ換えた。その他の図は 011213g0 と 011213g2 の間で相違が無いことを目視により確認したので、そのままとした。

### 3.5 HATCHES/FLASK-AQ

HATCHES に添付される複数の EQ3/6 用データファイルを 1 つのファイルにつなげたのち、aux 種でありながら、キーワードが basis となっているものを aux に直して、インハウスソフトウェア tdbconvert を用いて FLASK-AQ 用ファイルを作成した。FLASK-AQ により Eh-pH 計算結果を収めた中間ファイルを作成し、EhpHdraw を用いて、Eh-pH 図を作成した。この Eh-pH 図のウィンドウイメージを xwd を用いて取得したのち、ImageMagic の convert を用いて bmp ファイルとした。これを Illustrator のテンプレートとして、製図したのち、共通の縦・横の辺長になるように拡大・縮小した。有機化学種は基を basis 種としているので、SUPCRT/FLASK-AQ とは取り扱い方が異なることに注意してほしい。しかし X-H-O 系では成分として扱われていないので、結果的に図にはあらわれず、違いがほとんどない。

### 3.6 OECD/NEA

OECD-NEA の Chemical Thermodynamics の第 1 巻から第 4 巻までの熱力学データの表のうちギブス自由生成エネルギーが掲載されている表のデータを PC 上のスプレッドシートに入力し、テキストファイルに保存したのち当センター作成のソフトを用いて FLASK-AQ 用のファイルを作成した。FLASK-AQ

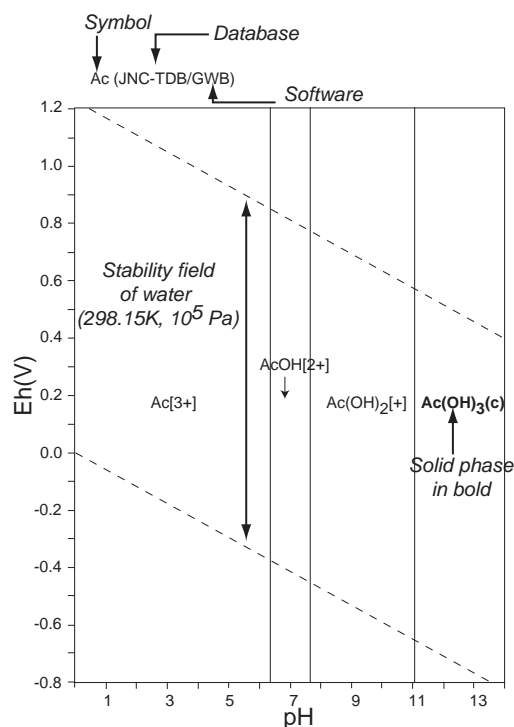


図 2: Eh-pH ダイアグラムの凡例

により Eh-pH 計算結果を収めた中間ファイルを作成し，EhpHdraw を用いて，Eh-pH 図を作成した．この Eh-pH 図のウィンドウイメージを xwd を用いて取得したのち，ImageMagic の convert を用いて bmp ファイルとした．これを Illustrator のテンプレートとして，製図したのち，共通の縦・横の辺長になるように拡大・縮小した．

### 3.7 OECD-NEAupdate

OECD-NEA の Chemical Thermodynamics の第 5 巻を用いた以外は，上記 OECD/NEA と同じ手順である．

## 4 図表の説明

図表は，元素記号のアルファベット順に並べ，各元素ごとに表，図の順に並べてある．表にはデータベース名を，図には”/”の前にデータベース名を”/”の後に使用ソフトウェア名をいずれも略称で記した(図 2)．表で空欄および図で NODATA と記したものには，その元素のデータが全く無い場合と固相やガスのデータはあっても，溶存化学種のデータが無い場合の両方が含まれる．図および表に用いた化学式の表示は原則として出典のデータベースそのまま，すなわち”as is”である．特に水和にかかわる表示を統一していないことに注意されたい．ただし，電荷の表示法は [] 使用に統一した．固相の表示法も統一せず，”as is”である．固相にかかわる次の用法はデータベースに依存する．am は非晶質，c または cr は結晶質，s または無指定は区別が明示されていないことを示し，鉱物名を示したものもある．FACT では，同質多形固相を s1, s2, s3 等のように区別して表示しているが，これもそのままである．表も図も固相名はボールド体になっている．図を左上から右下に横切る 2 本の平行な破線の間が 298.15K 10<sup>5</sup> Pa での水の安定領域である．表は，計算で考慮することのできた化学種をデータベースごとに示した．図の中に表示されていない化学種があるときは，それが，実際に安定でないことを意味する場合とデー

表 1: 使用ソフトウェア一覧

Software	Version	OS	Description
Acrobat Distiller	4.0	Windows 2000 Professional	conversion from PS to pdf
convert	5.3.8	Linux (SuSE 7.3)	conversion from xwd to bmp
EhpHdraw	1.0	Linux (SuSE 7.3)	X window software for Eh-pH drawing
FactSage	5.2	Windows 2000 Server	Eh-pH calculation and drawing
FLASK-AQ	1.1	Linux (SuSE 7.3)	Eh-pH calculation
GWB	4.0	Windows 2000 Server	Eh-pH calculation and drawing
Illustrator	8.0	Windows 2000 Professional	final drawing of Eh-pH diagrams
Intel C++ compiler	7.0	Linux (SuSE 7.3)	compiling FLASK-AQ and EhpHdraw
pdvips	5.92b p1.6	Linux (Fedra CORE 2)	conversion from dvi to PS and printing
pLaTeX	tetex 2.0.2	Linux (Fedra CORE 2)	document processing of this report
ps2epsi	5.2.1	Linux (Fedra CORE 2)	conversion from PS to epsi
StarSuite	6.0	Linux (RedHat 9.0)	writing tables of species
tdbconvert	1.0	Linux (RedHat 9.0)	database file convert
xwd	X11R6.5	Linux (SuSE 7.3)	X window dump software

データベースにデータが収録されていないことに起因する場合がありますので、図と表をかならず対応して見る  
ことが大切である。

## 5 信頼性と精度について

最終的な図の精度は次の3つに依存する。1) データベースのデータの精度、2) 計算ソフトの精度、3) 製図の精度。データベースの精度については、OECD-NEAのChemical Thermodynamicsのシリーズを除くと記載されていない。計算ソフトの精度については、FLASK-AQについて示したが、商用ソフトウェアは記載されていない。製図の精度は、FLASK-AQのEh-pHグリッド間隔未満であることを目視で確認した。したがって、データベースおよび商用ソフトウェアに起因する誤差を別にして、誤差は最大でEhが $\pm 0.0025$ およびpHが $\pm 0.02$ と考えてよい。

## 6 使用ソフトウェアとその実行環境

作図に使用したソフトウェアは、商用ソフトウェアであるGTT-Technologies製FactSage 5.2、イリノイ大学C.M.BethkeのGeochemist's Workbench 4.0および深部地質環境研究センター作成のインハウスソフトウェアFLASK-AQ 1.1である。FactSage 5.2とGeochemist's Workbench 4.0はDell PowerEdge 2600 (Xeon 2.4GHz x2 SMP, 4GB メモリー) 上のMicrosoft Windows 2000 Serverにて使用した。Flask-AQ 1.1はHIT製PC (Pentium4 2.8GHz, 1GB メモリー) 上のSuSE Linux 7.3 (kernel 2.4.20)にてIntel C++ 7.0 コンパイラでコンパイルした実行可能ソフトをPlatform製バッチスケジューリングソフトウェアLSF 4.2環境下でバッチ実行した。FLASK-AQ 1.1は中間ファイルを生成するのみなので、Eh-pH図を得るために深部地質環境研究センター作成のインハウスソフトウェアEhpHdrawを使用した。ZZ-HATCHES-15データからFLASK-AQ 1.1用フォーマットへの変換には、深部地質環境研究センターが日本sgiに依頼して作成したインハウスソフトウェアtdbconvertを使用した。これらのインハウスソフトウェアはいずれ公開する予定である。

EhpHdrawの描くEh-pH図のスナップショットを得るのにX Window dumpソフトウェアxwdを使用した。xwdからbmpフォーマットへのコンバージョンにImageMagicのconvertを使用した。この過

程では, IA32PC (インテルの Pentium 等の 32 ビットアーキテクチャを持った CPU を使用した PC) 上の Red Hat Linux ver.9 または Fedra Core 2 を実行環境とした .

ポストスクリプトファイルから pdf へのコンバージョンには, Adobe Acrobat Distiller 4.0 を使用し, 図のサイズおよび形式を揃えた最終出力図作成には, Adobe Illustrator 8.0 を使用した . この過程では, IA32PC 上の Microsoft Windows 2000 Professional を実行環境とした .

化学種リストの作成には Sun StarSuite 6.0 を使用し, ポストスクリプトファイルにしたのち, ps2epsi により eps ファイルとした . 最終的な資料の作成には ASCII pLaTeX を使用し, pdvips を使用してレーザープリンタに出力した . この実行環境は IA32PC 上の Fedra Core 2 である (表 1) .

なお, 特に断わらないが, ソフトウェア名, フォーマット名等の固有名詞には, 登録商標または商標が含まれており, その所有者に所有権が属す .

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表 2: List of Ac species

FACT	SUPCRT	LLNL	JNC-TDB
			Ac[3+], AcOH[2+], Ac(OH) <sub>2</sub> [+], Ac(OH) <sub>3</sub> (aq), <b>Ac(OH)<sub>3</sub>(am)</b> , <b>Ac(OH)<sub>3</sub>(c)</b>

HATCHES			
Ac[3+], AcOH[2+], <b>Ac(OH)<sub>3</sub></b>			

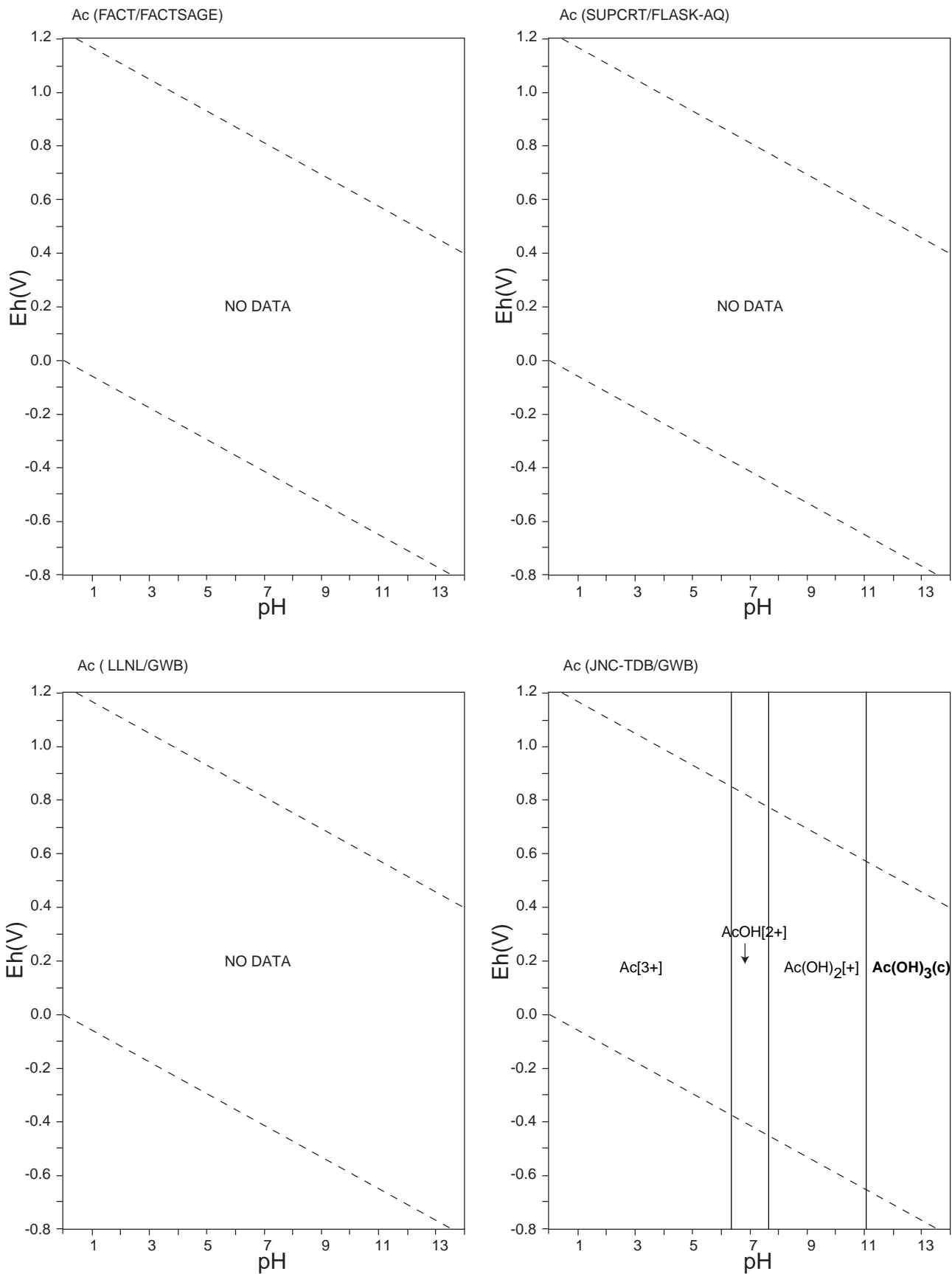


Figure 3: Eh-pH diagrams of the system Ac-O-H (1).  $\sum \text{Ac} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

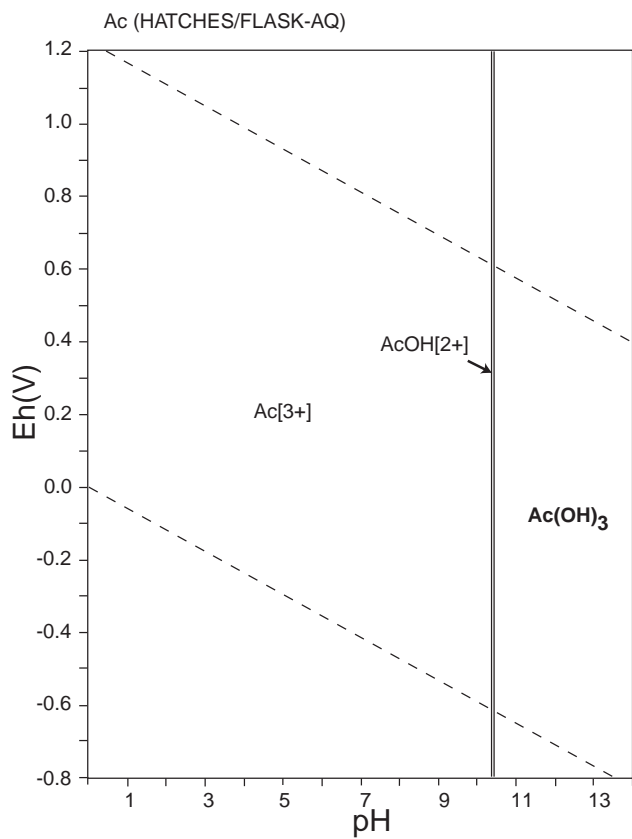


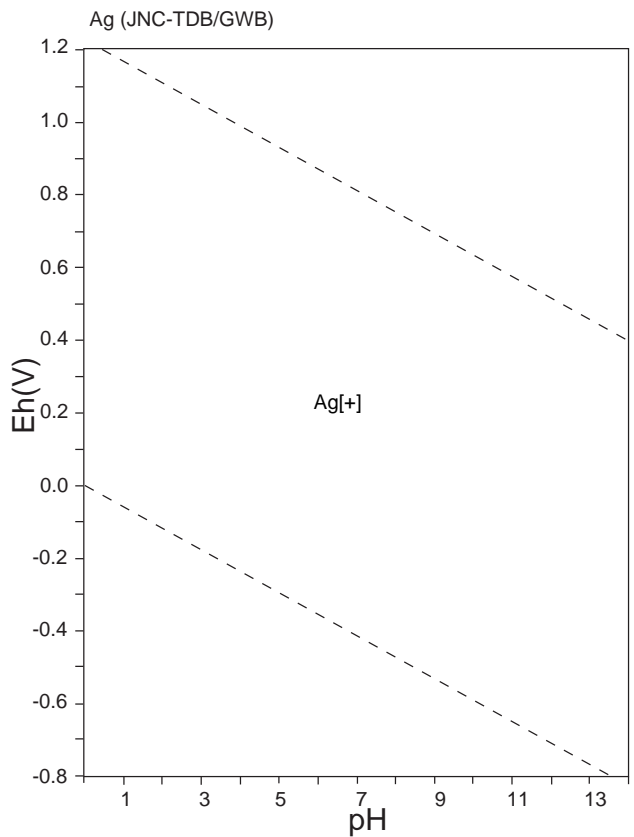
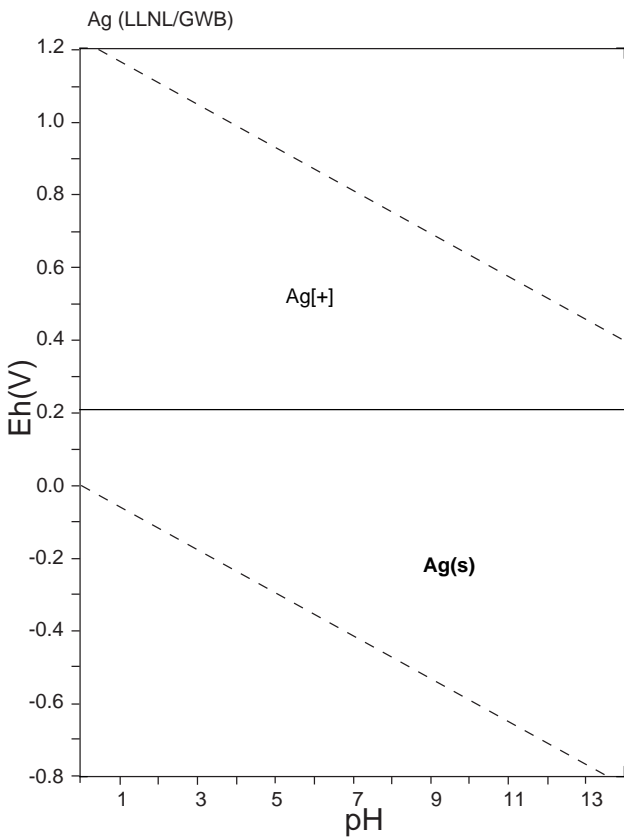
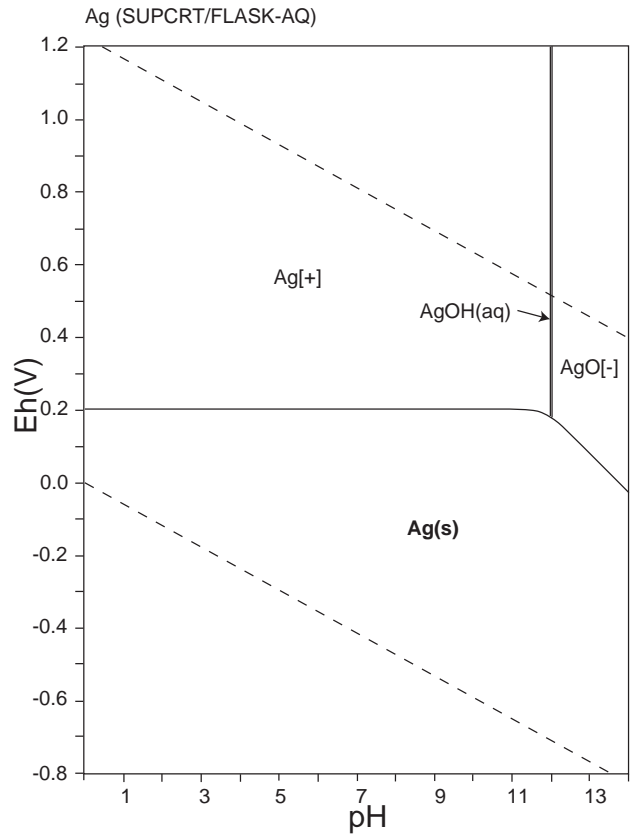
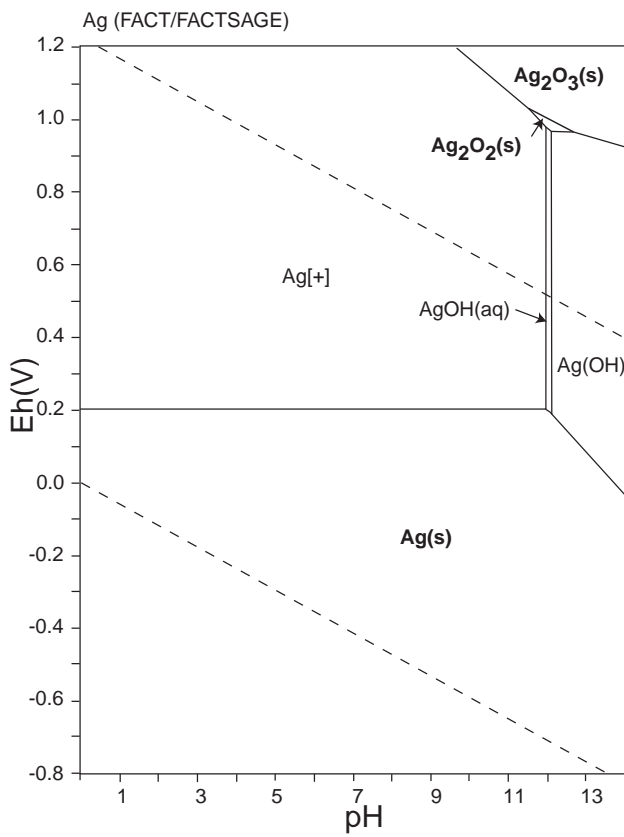
图 4: Eh-pH diagrams of the system Ac-O-H (2).  $\sum Ac = 10^{-10}$ , 298.15K,  $10^5$  Pa.



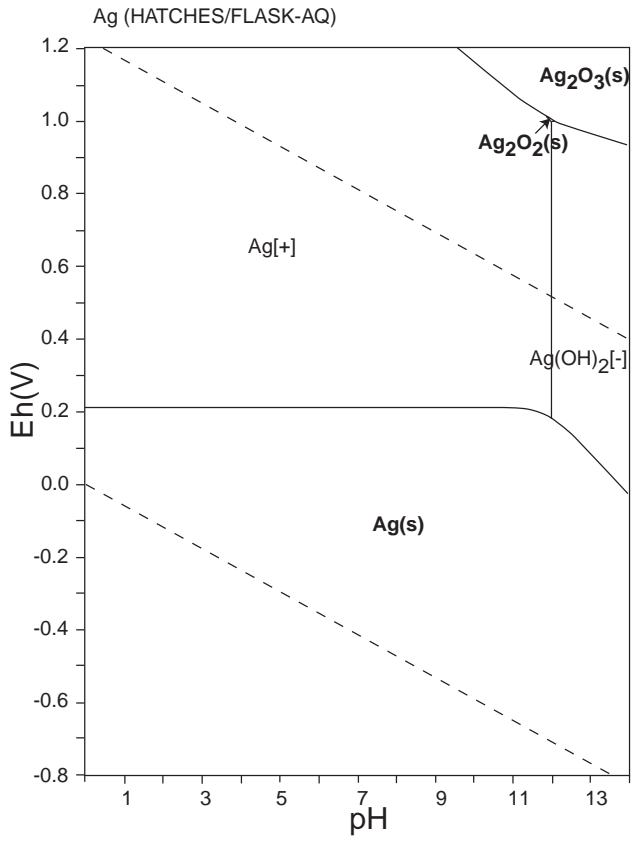
表 3: List of Ag species

FACT	SUPCRT	LLNL	JNC-TDB
Ag[+], AgOH(aq), Ag(OH) <sub>2</sub> [-], <b>Ag<sub>2</sub>O(s)</b> , <b>Ag<sub>2</sub>O<sub>2</sub>(s)</b> , <b>Ag<sub>2</sub>O<sub>3</sub>(s)</b> , <b>Ag(Native silver)</b>	Ag[2+], Ag[+], AgOH(aq), AgO[-], <b>Ag(Native silver)</b>	Ag[+], <b>Silver</b>	Ag[+]

HATCHES			
Ag[+], Ag(OH) <sub>2</sub> [-], AgOH(aq), <b>Ag</b> , <b>Ag<sub>2</sub>O</b> , <b>Ag<sub>2</sub>O<sub>2</sub></b> , <b>Ag<sub>2</sub>O<sub>3</sub></b>			



☒ 5: Eh-pH diagrams of the system Ag-O-H (1).  $\sum \text{Ag} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 6: Eh-pH diagrams of the system Ag-O-H (2).  $\sum \text{Ag} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





表 4: List of Al species

FACT	SUPCRT	LLNL	JNC-TDB
$\text{Al}[3+]$ , $\text{AlO}_2[-]$ , $\text{AlOH}[2+]$ , <b>Al(s)</b> , $\text{AlH}_3(\text{s})$ , $\text{Al}_2\text{O}_3(\text{s})$ , $\text{Al}_2\text{O}_3(\text{s}2)$ , $\text{Al}_2\text{O}_3(\text{s}3)$ , $\text{Al}_2\text{O}_3(\text{s}4)$ , $\text{Al}(\text{OH})_3(\text{s})$ , $\text{Al}_2\text{O}_3(\text{H}_2\text{O})(\text{s})$ , $\text{Al}_2\text{O}_3(\text{H}_2\text{O})(\text{s}2)$ , $\text{Al}_2\text{O}_3(\text{H}_2\text{O})_3(\text{s})$	$\text{AlO}[+]$ , $\text{HAlO}_2(\text{aq})$ , $\text{Al}[3+]$ , $\text{AlO}_2[-]$ , $\text{AlOH}[2+]$ , $\text{Al}_2\text{O}_3(\text{Corundum})$ , $\text{AlO}(\text{OH})(\text{Diaspore})$ , $\text{AlO}(\text{OH})(\text{Boehmite})$ , $\text{Al}(\text{OH})_3(\text{Gibbsite})$ , $\text{AlO}[+]$ , $\text{HAlO}_2(\text{aq})$	$\text{Al}[3+]$ , $\text{Al}(\text{OH})_2[+]$ , $\text{Al}(\text{OH})_3(\text{aq})$ , $\text{Al}(\text{OH})_4[-]$ , $\text{Al}_{13}\text{O}_4(\text{OH})_{24}[7+]$ , $\text{Al}_2(\text{OH})_2[4+]$ , $\text{Al}_3(\text{OH})_4[5+]$ , $\text{AlOH}[2+]$ , <b>Boehmite</b> , <b>Corundum</b> , <b>Diaspore</b> , <b>Gibbsite</b>	$\text{Al}[3+]$ , $\text{AlOH}[2+]$ , $\text{Al}(\text{OH})_2[+]$ , $\text{Al}(\text{OH})_3(\text{aq})$ , $\text{Al}(\text{OH})_4[-]$ , <b>Gibbsite</b>

HATCHES			
$\text{Al}[3+]$ , $\text{Al}(\text{OH})[2+]$ , $\text{Al}(\text{OH})_2[+]$ , $\text{Al}(\text{OH})_3(\text{aq})$ , $\text{Al}(\text{OH})_4[-]$ , <b>Boehmite</b> , <b>Corundum</b> , <b>Diaspore</b> , <b>Gibbsite</b>			

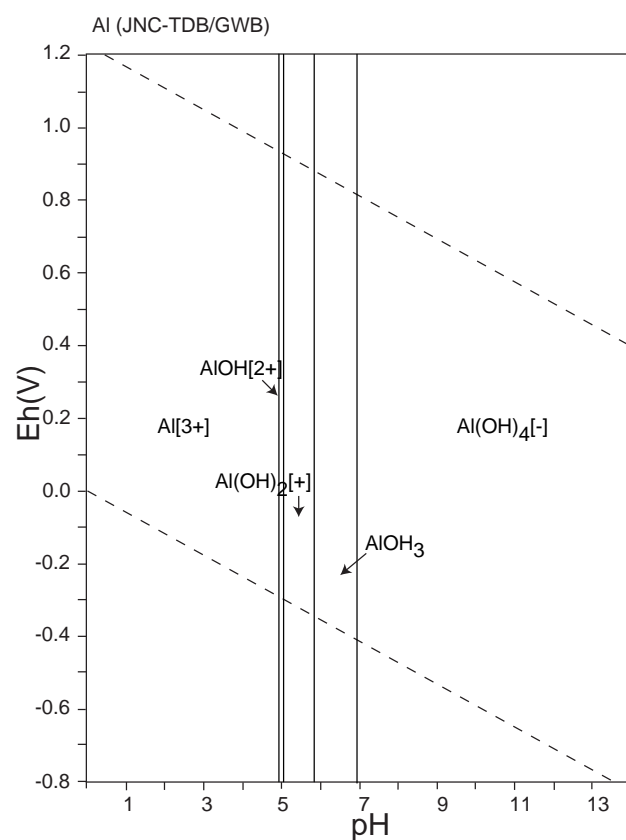
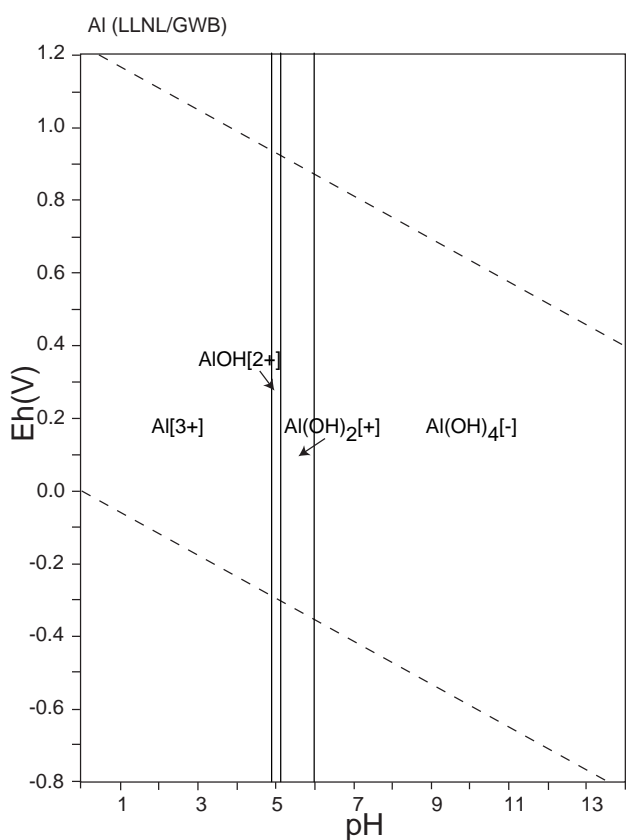
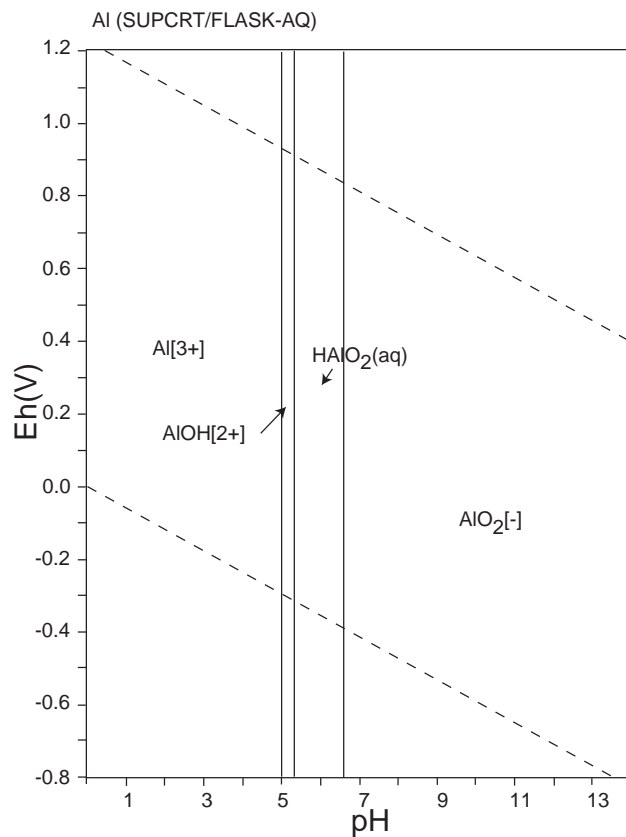
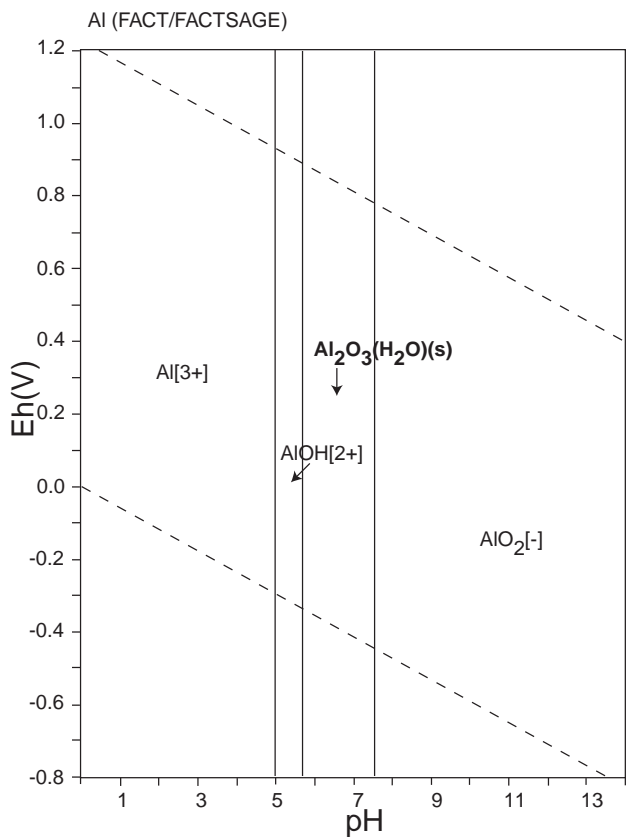


Figure 7: Eh-pH diagrams of the system Al-O-H (1).  $\sum \text{Al} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

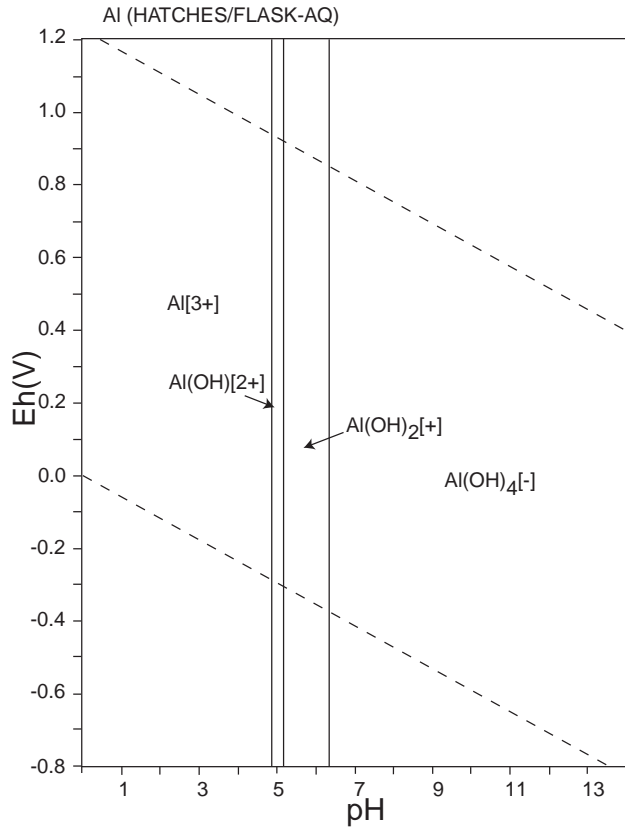


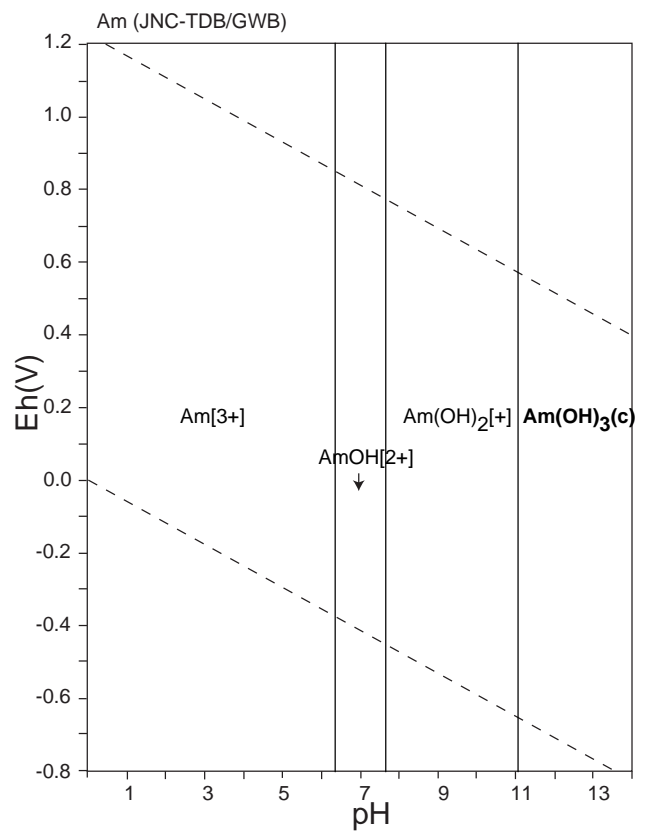
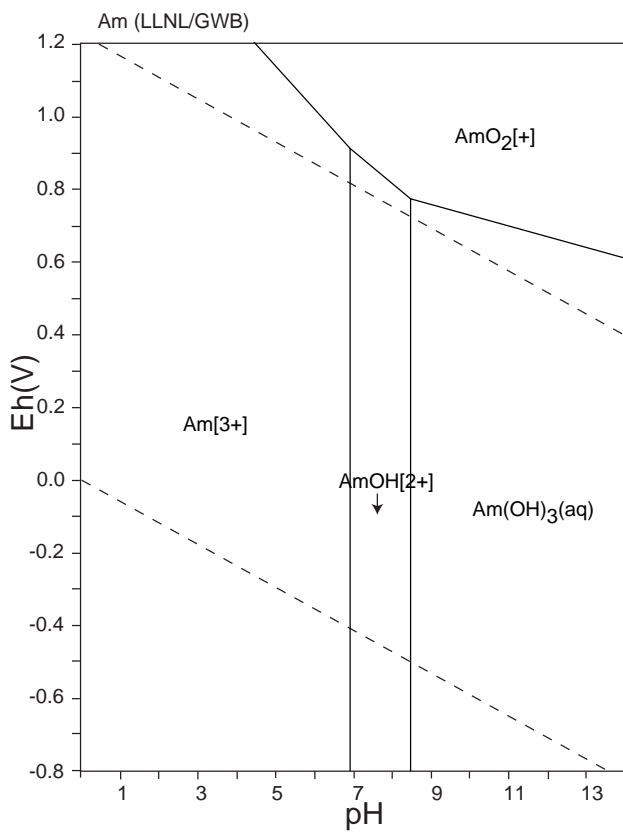
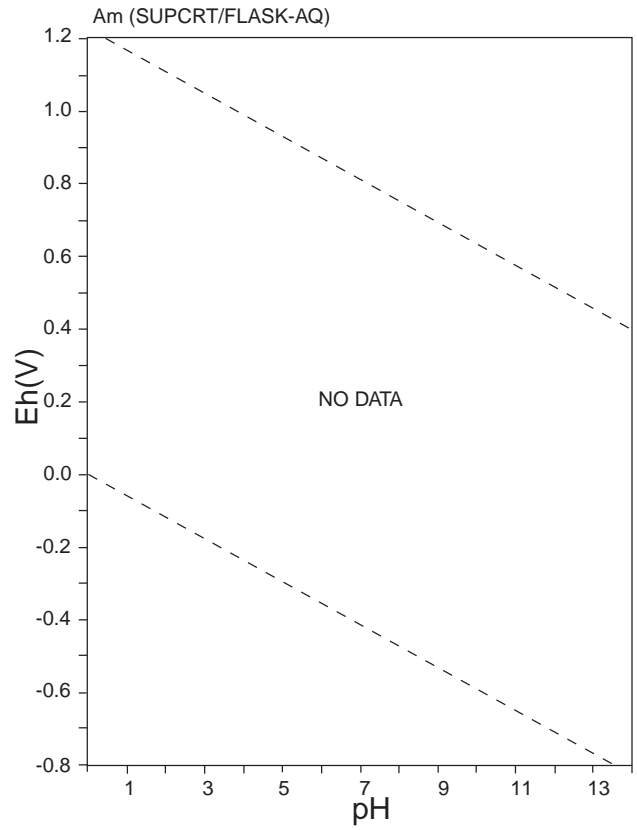
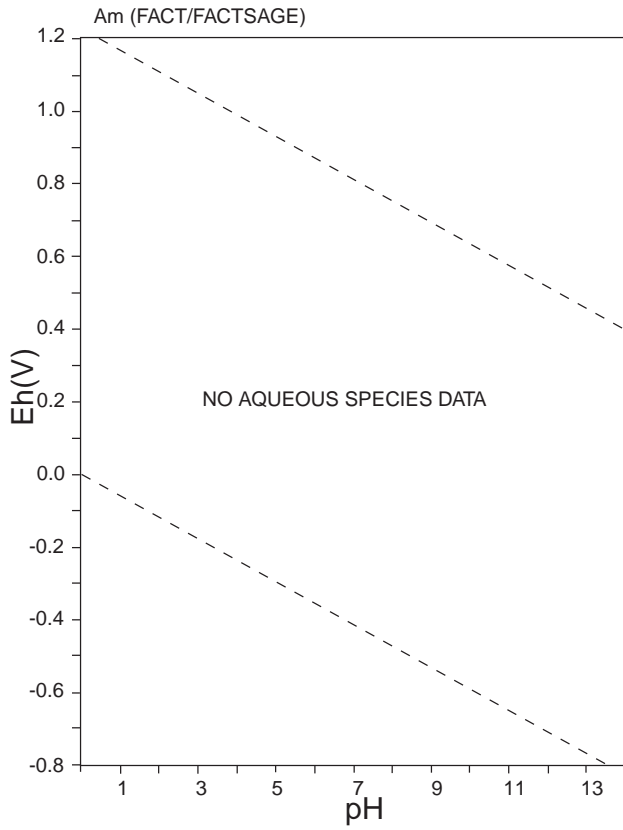
图 8: Eh-pH diagrams of the system Al-O-H (2).  $\sum \text{Al} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



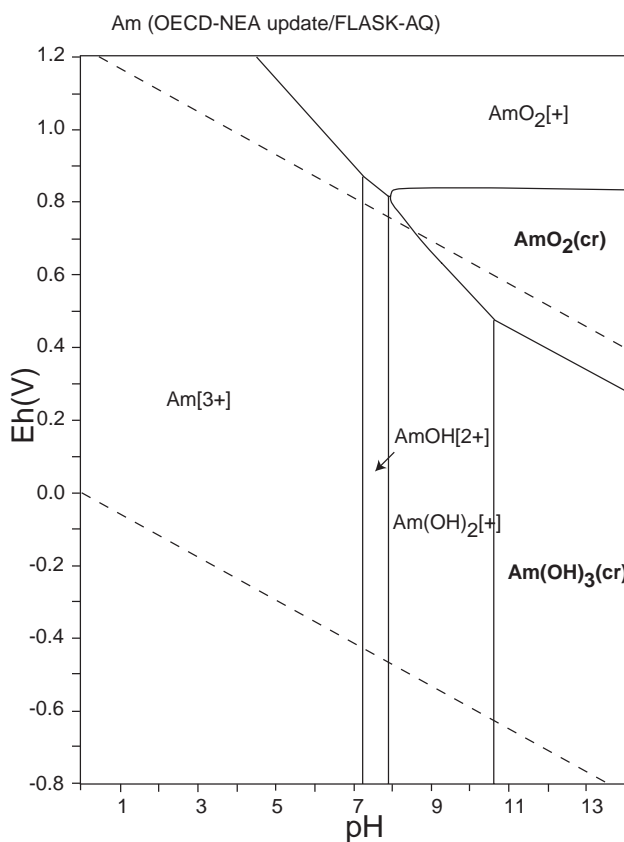
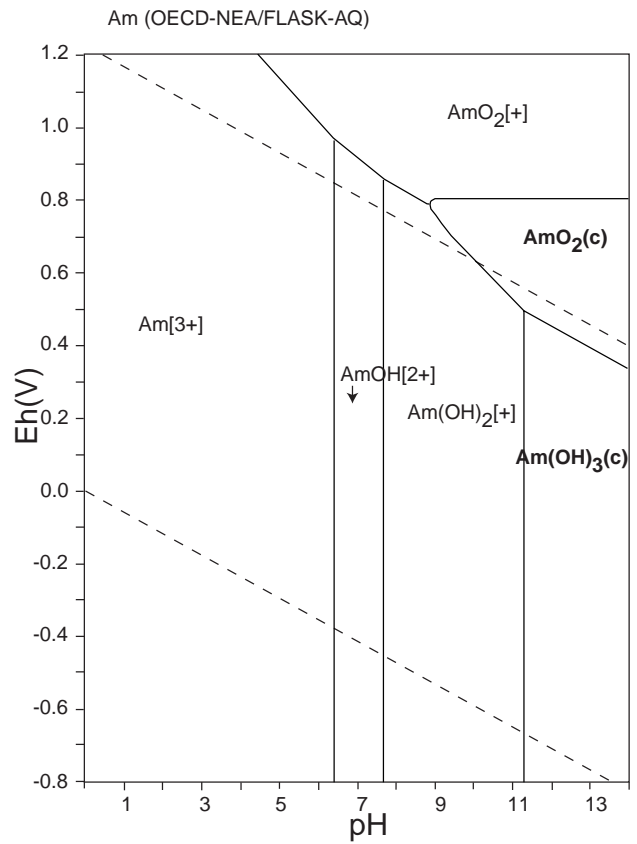
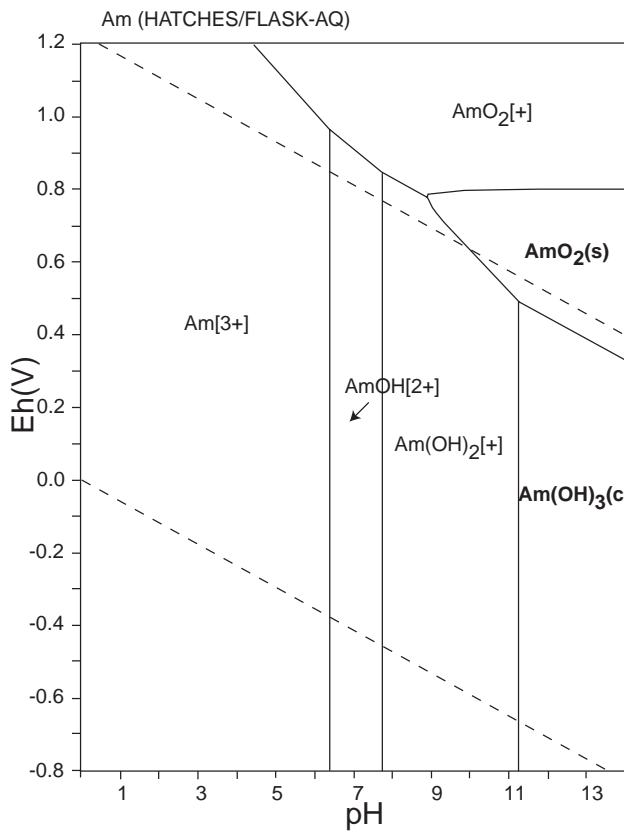
表 5: List of Am species

FACT	SUPCRT	LLNL	JNC-TDB
<b>Am(s), Am(s2), Am(s3), AmO<sub>2</sub>(s), Am<sub>2</sub>O<sub>3</sub>(s)</b>		Am[3+], Am[4+], AmO <sub>2</sub> [+], AmO <sub>2</sub> [2+], Am(OH) <sub>2</sub> [+], Am(OH) <sub>3</sub> (aq), AmOH[2+], <b>Am(OH)<sub>3</sub>(am), Am(OH)<sub>3</sub>(c)</b>	Am[3+], AmOH[2+], Am(OH) <sub>2</sub> [+], Am(OH) <sub>3</sub> (aq), <b>Am(OH)<sub>3</sub>(am), Am(OH)<sub>3</sub>(c)</b>

HATCHES	OECD-NEA	OECD-NEA update	
Am[3+], Am[4+], AmO <sub>2</sub> [+], AmO <sub>2</sub> [2+], Am(OH) <sub>2</sub> [+], Am(OH) <sub>3</sub> (aq), AmOH[2+], <b>Am, Am(OH)<sub>3</sub>, Am<sub>2</sub>O<sub>3</sub>, AmH<sub>2</sub>, AmO<sub>2</sub>, Am(OH)<sub>3</sub>(cr)</b>	Am[4+], Am[2+], Am[3+], AmO <sub>2</sub> [+], AmO <sub>2</sub> [2+], AmOH[2+], Am(OH) <sub>2</sub> [+], Am(OH) <sub>3</sub> (aq), <b>Am(c), AmO<sub>2</sub>(c), Am<sub>2</sub>O<sub>3</sub>(c), AmH<sub>2</sub>(c), Am(OH)<sub>3</sub>(am), Am(OH)<sub>3</sub>(c)</b>	Am[4+], Am[2+], Am[3+], AmO <sub>2</sub> [+], AmO <sub>2</sub> [2+], AmOH[2+], Am(OH) <sub>2</sub> [+], Am(OH) <sub>3</sub> (aq), <b>Am(cr), AmO<sub>2</sub>(cr), Am<sub>2</sub>O<sub>3</sub>(cr), AmH<sub>2</sub>(cr), Am(OH)<sub>3</sub>(cr)</b>	



☒ 9: Eh-pH diagrams of the system Am-O-H (1).  $\sum \text{Am} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 10: Eh-pH diagrams of the system Am-O-H (2).  $\sum \text{Am} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





表 6: List of As species

FACT	SUPCRT	LLNL	JNC-TDB
$\text{AsO}_2[-]$ , $\text{AsO}_4[3-]$ , $\text{HAsO}_2(\text{aq})$ , $\text{H}_2\text{AsO}_3[-]$ , $\text{H}_2\text{AsO}_4[2-]$ , $\text{H}_2\text{AsO}_4[-]$ , $\text{H}_3\text{AsO}_4(\text{aq})$ , $\text{AsO}[+]$ , <b>As(s)</b> , <b>As<sub>2</sub>O<sub>3</sub>(s)</b> , <b>As<sub>2</sub>O<sub>3</sub>(s2)</b> , <b>As<sub>2</sub>O<sub>5</sub>(s)</b> ,	$\text{AsO}_2[-]$ , $\text{AsO}_4[3-]$ , $\text{HAsO}_2(\text{aq})$ , $\text{H}_2\text{AsO}_3[-]$ , $\text{HAsO}_4[2-]$ , $\text{H}_2\text{AsO}_4[-]$ , $\text{H}_3\text{AsO}_4(\text{aq})$	$\text{As}(\text{OH})_4[-]$ , $\text{AsH}_3(\text{aq})$ , $\text{AsO}_4[3-]$ , $\text{As}(\text{OH})_3(\text{aq})$ , $\text{AsO}_2\text{OH}[2-]$ , $\text{H}_2\text{AsO}_4[-]$ , $\text{H}_3\text{AsO}_4(\text{aq})$ , $\text{HAsO}_4[2-]$ <b>Arsenolite</b> , <b>As<sub>2</sub>O<sub>5</sub>(c)</b> , <b>Claudetite</b>	

HATCHES			
$\text{As}(\text{OH})_4[-]$ , $\text{H}_2\text{AsO}_4[-]$ , $\text{As}(\text{OH})_3(\text{aq})$ , $\text{AsO}[+]$ , $\text{AsO}_4[3-]$ , $\text{H}_3\text{AsO}_4(\text{aq})$ , $\text{HAsO}_2(\text{aq})$ , $\text{HAsO}_4[2-]$ , <b>Arsenolite</b> , <b>As<sub>2</sub>O<sub>5</sub>(c)</b> , <b>As<sub>4</sub>O<sub>6</sub></b> , <b>Claudetite</b>			

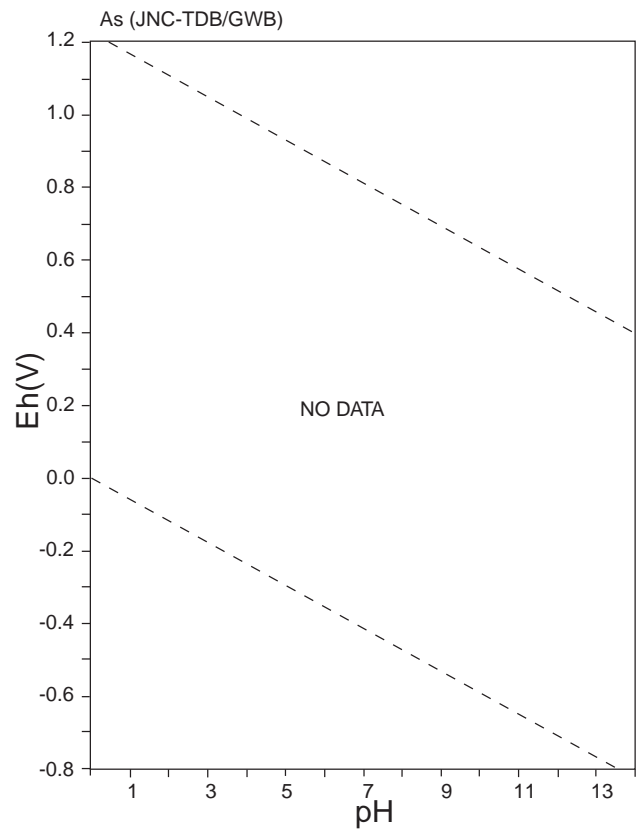
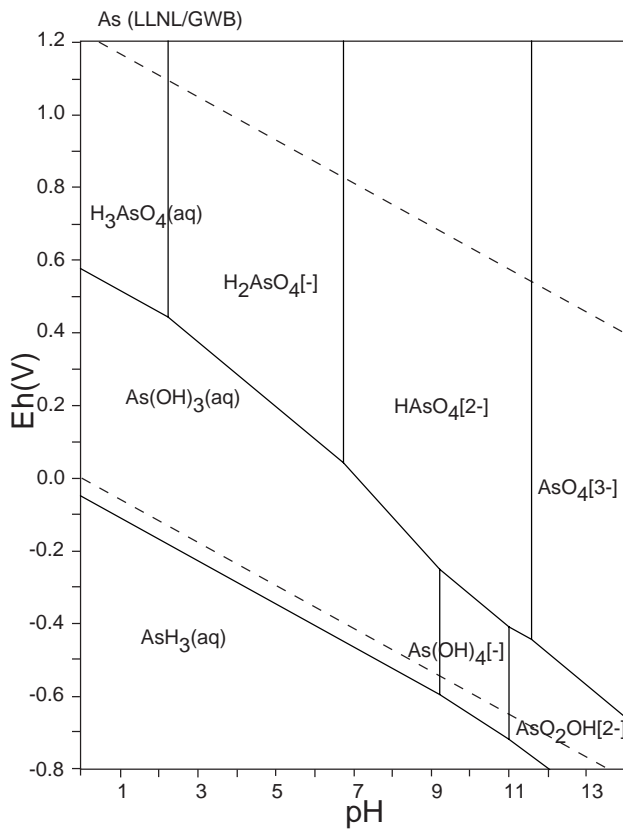
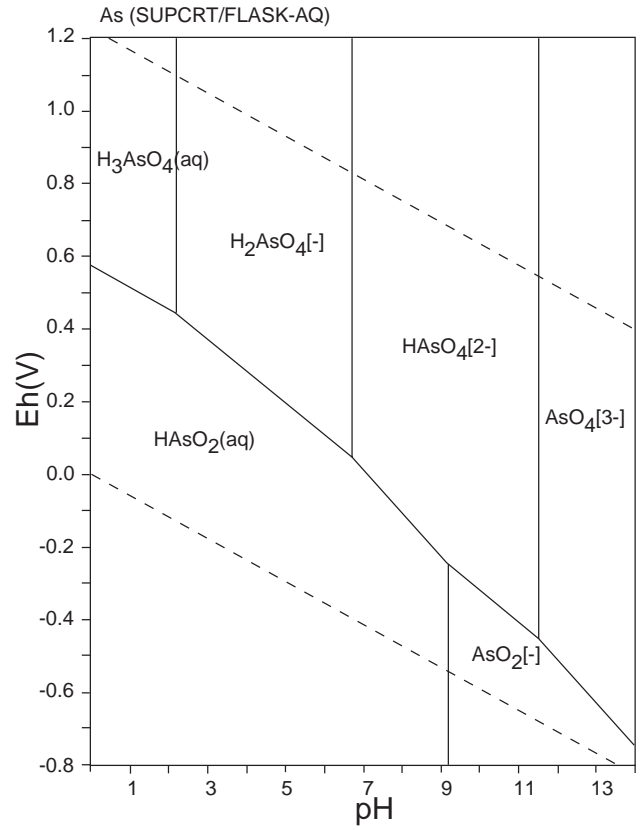
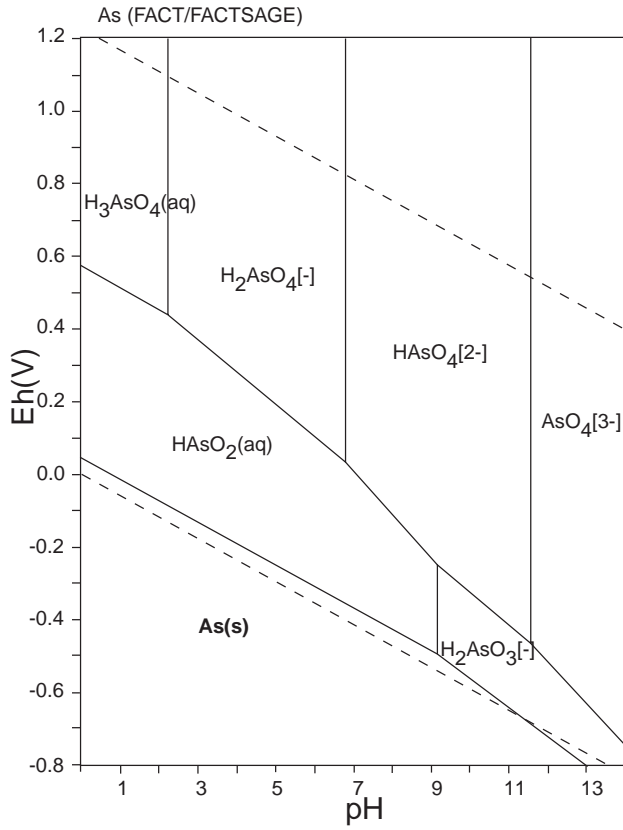


Figure 11: Eh-pH diagrams of the system As-O-H (1).  $\sum \text{As} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

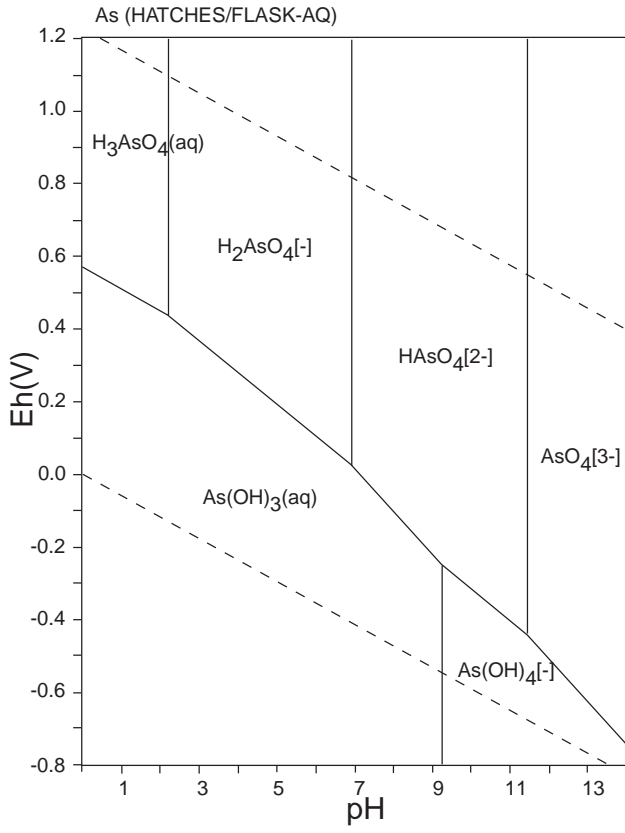
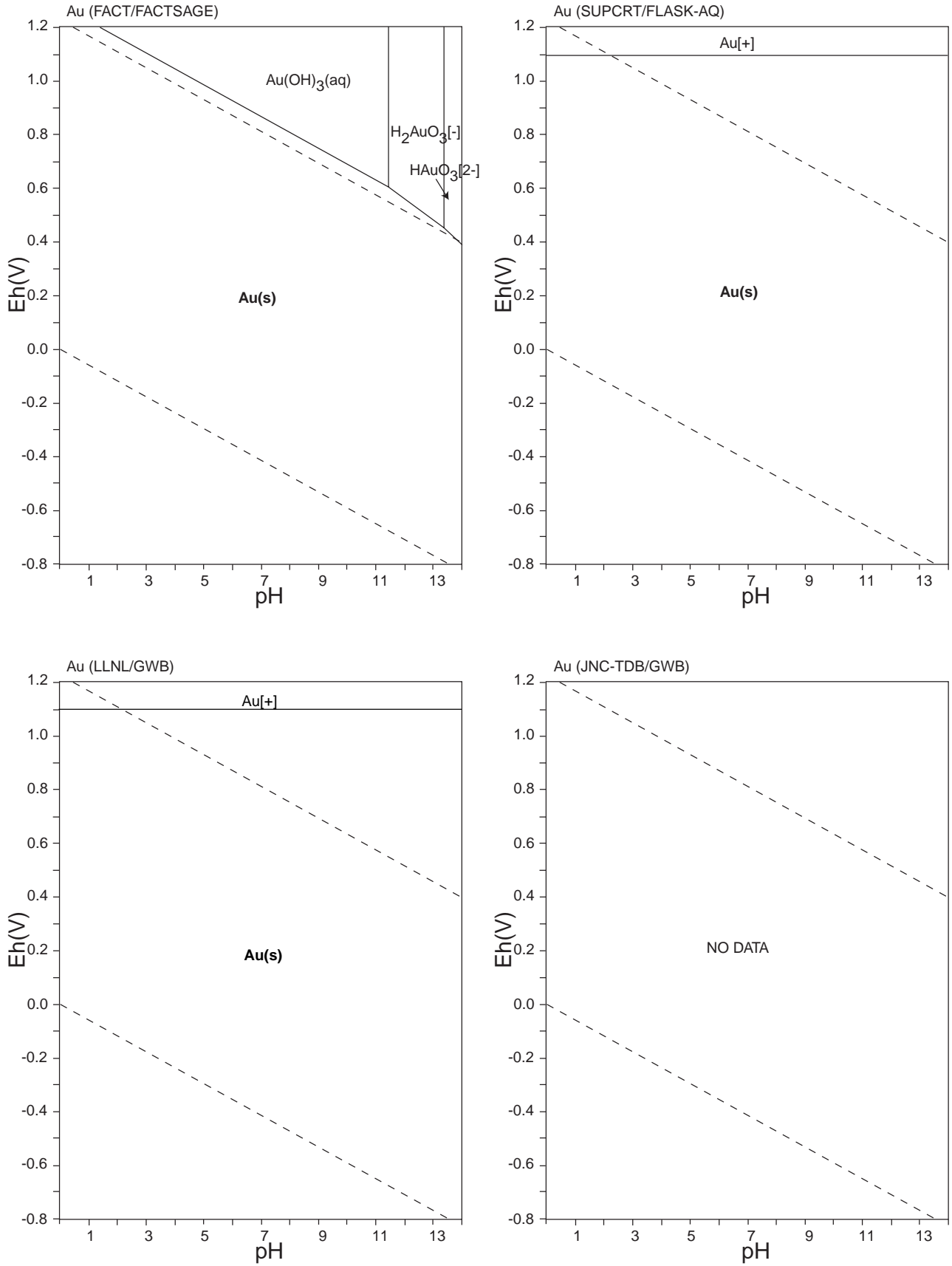


图 12: Eh-pH diagrams of the system As-O-H (2).  $\sum \text{As} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 7: List of Au species

FACT	SUPCRT	LLNL	JNC-TDB
$\text{AuO}_3[3-]$ , $\text{HAuO}_3[2-]$ , $\text{H}_2\text{AuO}_3[-]$ , $\text{Au}(\text{OH})_3(\text{aq})$ , $\text{Au}_2\text{O}_3(\text{s})$ , $\text{Au}(\text{OH})_3(\text{s})$ , $\text{Au}(\text{s})$	$\text{Au}[3+]$ , $\text{Au}[+]$ , $\text{Au}(\text{Native gold})$	$\text{Au}[+]$ , $\text{Au}[3+]$ , <b>Gold</b>	



☒ 13: Eh-pH diagrams of the system Au-O-H.  $\Sigma \text{Au} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 8: List of B species

FACT	SUPCRT	LLNL	JNC-TDB
$\text{BH}_4^-$ , $\text{BO}_2^-$ , $\text{B}_4\text{O}_7^{2-}$ , $\text{H}_2\text{BO}_3^-$ , $\text{H}_3\text{BO}_3(\text{aq})$ , $\text{H}_2\text{BO}_3(\text{H}_2\text{O}_2)^-$ , $\text{HB}_4\text{O}_7^-$ , $\text{H}_2\text{B}_4\text{O}_7(\text{aq})$ , $\text{H}_5(\text{BO}_3)_2(\text{H}_2\text{O}_2)_2^-$ , <b>B(s)</b> , <b>B<sub>10</sub>H<sub>14</sub>(s)</b> , <b>B<sub>2</sub>O<sub>3</sub>(s)</b> , <b>HBO<sub>2</sub>(s)</b> , <b>HBO<sub>2</sub>(s2)</b> , <b>HBO<sub>2</sub>(s3)</b> , <b>H<sub>3</sub>BO<sub>3</sub>(s)</b> , <b>B<sub>3</sub>H<sub>3</sub>O<sub>3</sub>(s)</b> , <b>B<sub>2</sub>(OH)<sub>4</sub>(s)</b>	$\text{BO}_2^-$ , $\text{B}(\text{OH})_3(\text{aq})$	$\text{B}(\text{OH})_3(\text{aq})$ , $\text{B}(\text{OH})_4^-$ , $\text{B}_2\text{O}(\text{OH})_5^-$ , $\text{B}_3\text{O}_3(\text{OH})_4^-$ , $\text{B}_4\text{O}_5(\text{OH})_4^{2-}$ , $\text{BH}_4^-$ , <b>B(OH)<sub>3</sub>(c, Boric acid)</b>	$\text{B}(\text{OH})_3(\text{aq})$ , $\text{H}_2\text{BO}_3^-$ , <b>B(c)</b> , <b>B<sub>2</sub>O<sub>3</sub>(c)</b> , <b>B(OH)<sub>3</sub>(c)</b> , B(g)

HATCHES			
$\text{B}(\text{OH})_3(\text{aq})$ , $\text{B}_4\text{O}_7^{2-}$ , $\text{BH}_4^-$ , $\text{H}_2\text{B}_4\text{O}_7(\text{aq})$ , $\text{H}_2\text{BO}_3^-$ , $\text{HB}_4\text{O}_7^-$ , <b>B<sub>2</sub>O<sub>3</sub></b> , <b>Boric Acid</b> , <b>H<sub>3</sub>BO<sub>3</sub>(c)</b> , <b>HBO<sub>2</sub></b>			

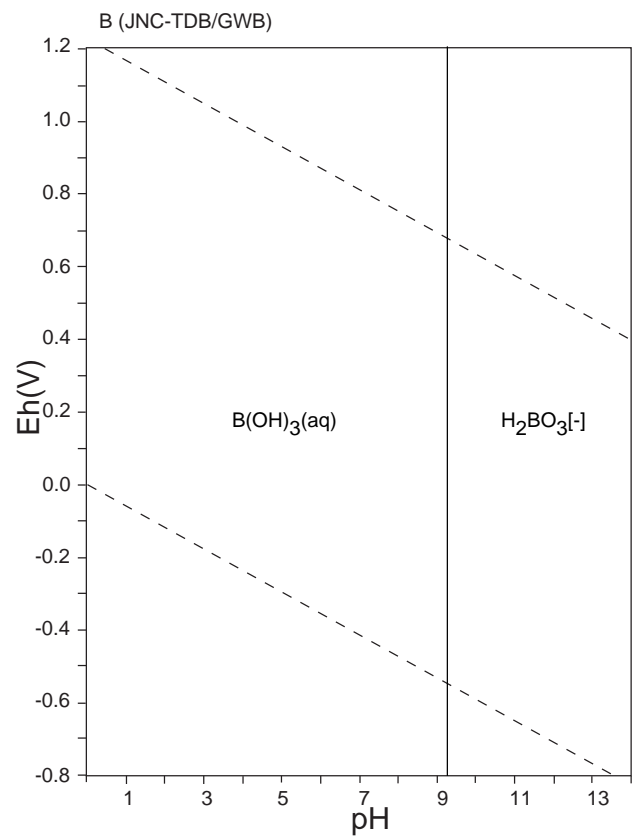
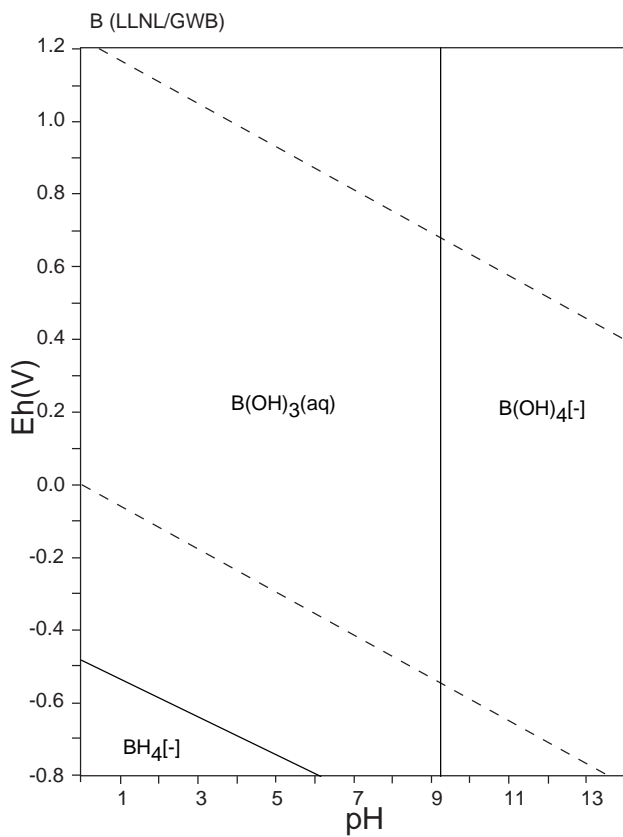
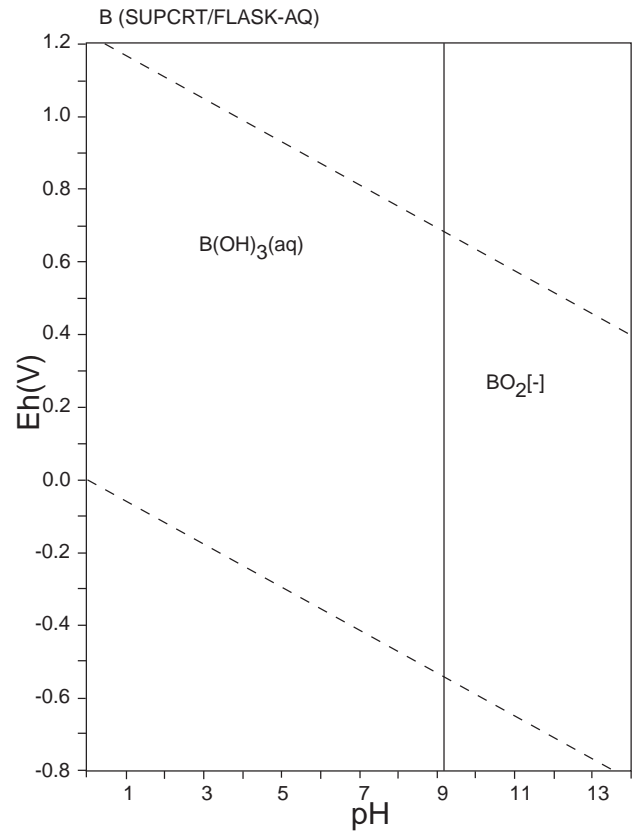
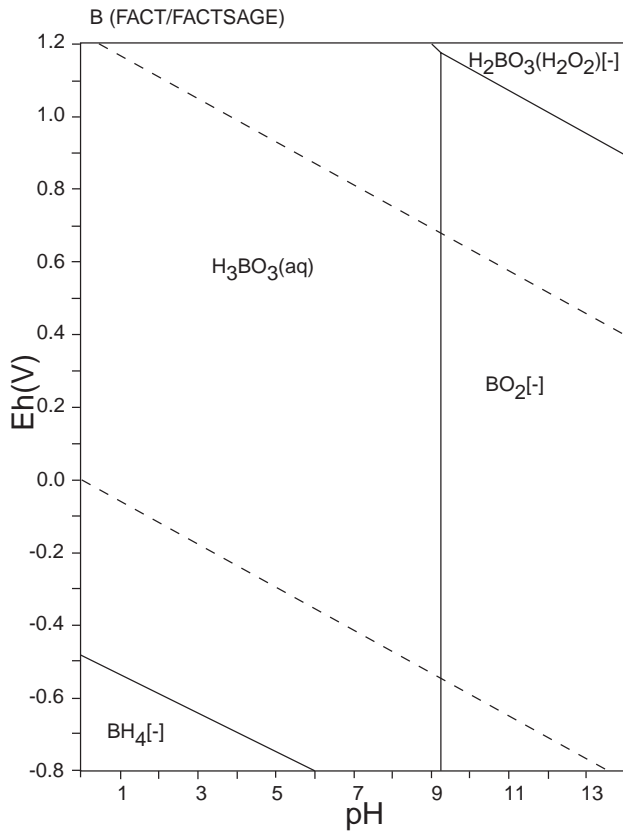
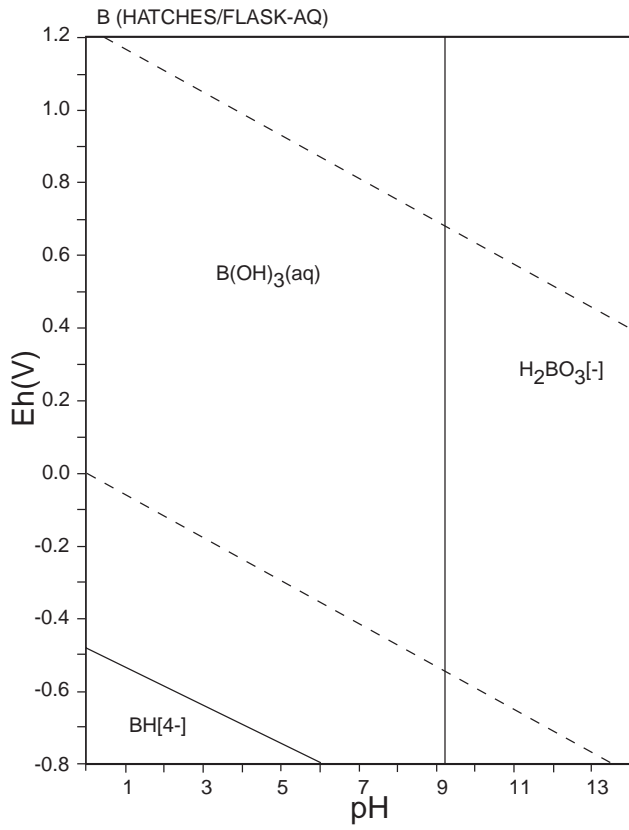


图 14: Eh-pH diagrams of the system B-O-H (1).  $\sum \text{B} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





☒ 15: Eh-pH diagrams of the system B-O-H (2).  $\sum B = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 9: List of Ba species

FACT	SUPCRT	LLNL	JNC-TDB
$\text{Ba}[2+]$ , $\text{BaOH}[+]$ , $\text{Ba}(\text{s})$ , $\text{BaH}_2(\text{s})$ , $\text{BaO}(\text{s})$ , $\text{BaO}_2(\text{s})$ , $\text{Ba}(\text{OH})_2(\text{s})$ , $\text{Ba}(\text{OH})_2(\text{H}_2\text{O})_8(\text{s})$	$\text{Ba}[2+]$ , $\text{BaOH}[+]$	$\text{Ba}[2+]$ , $\text{BaOH}[+]$ , $\text{Ba}(\text{OH})_2 \cdot 8\text{H}_2\text{O}(\text{c})$ , $\text{BaO}(\text{c})$	$\text{Ba}[2+]$ , $\text{BaOH}[+]$ , $\text{Ba}(\text{c})$ , $\text{BaO}(\text{c})$

HATCHES			
$\text{Ba}[2+]$ , $\text{Ba}(\text{OH})[+]$ , $\text{Ba}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$ , $\text{BaO}(\text{c})$			

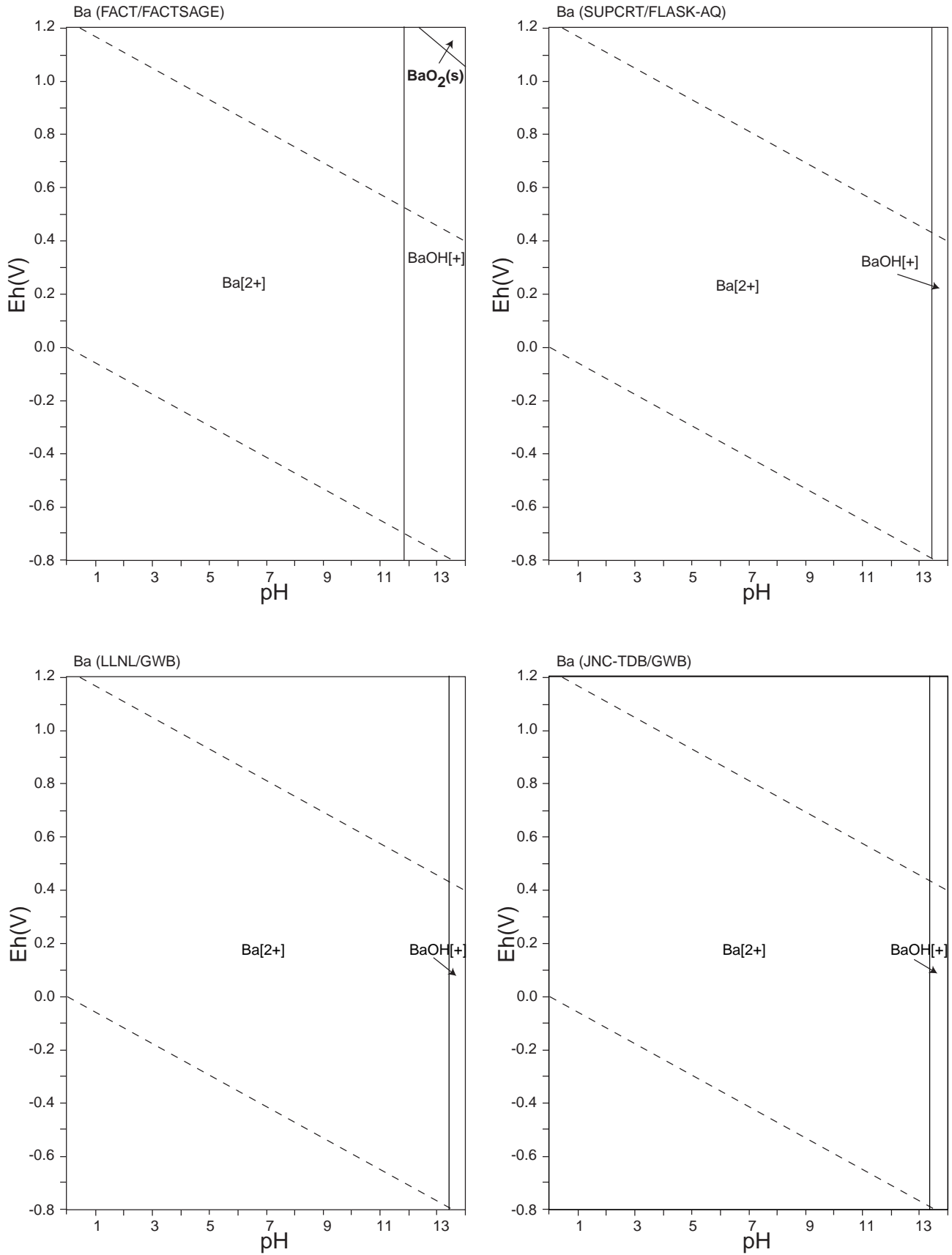
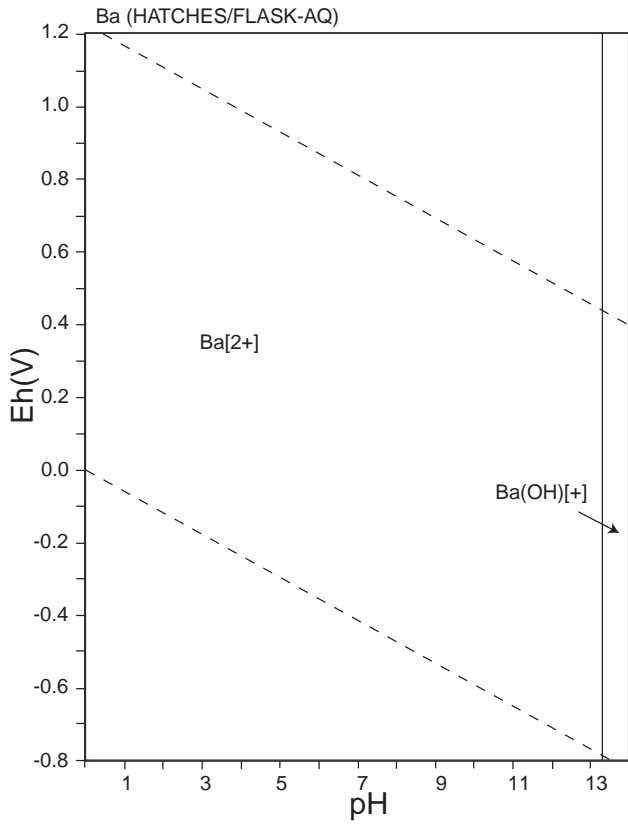


Figure 16: Eh-pH diagrams of the system Ba-O-H (1).  $\Sigma \text{Ba} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



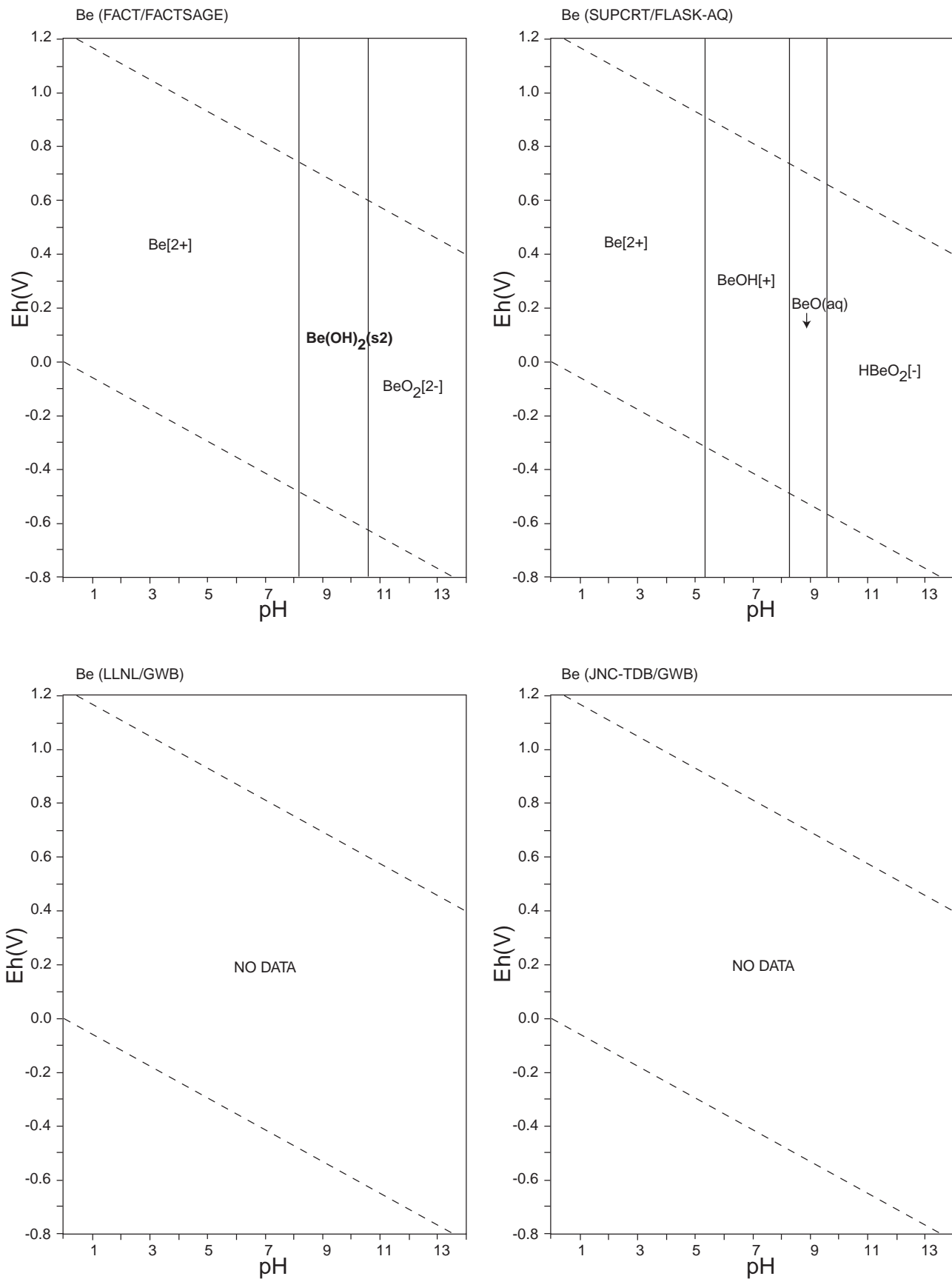
☒ 17: Eh-pH diagrams of the system Ba-O-H (2).  $\sum \text{Ba} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 10: List of Be species

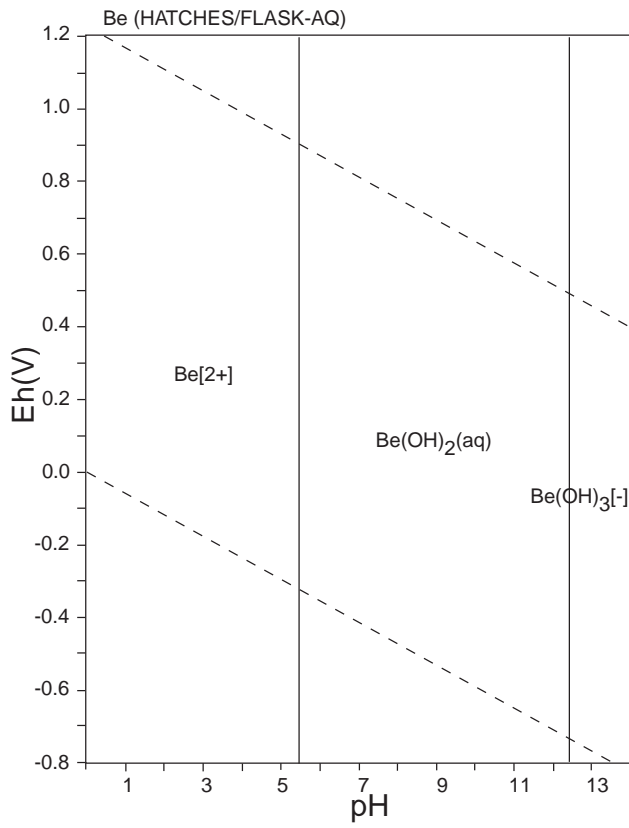
FACT	SUPCRT	LLNL	JNC-TDB
$\text{Be}[2+]$ , $\text{BeO}_2[2-]$ , $\text{Be}_3(\text{OH})_3[3+]$ , $\text{Be}(\text{s})$ , $\text{Be}(\text{s}2)$ , $\text{BeO}(\text{s})$ , $\text{BeO}(\text{s}2)$ , $\text{Be}(\text{OH})_2(\text{s})$ , $\text{Be}(\text{OH})_2(\text{s}2)$	$\text{Be}[2+]$ , $\text{BeO}_2[2-]$ , $\text{BeOH}[+]$ , $\text{BeO}(\text{aq})$ , $\text{HBeO}_2[-]$		

HATCHES			
$\text{Be}[2+]$ , $\text{BeOH}[+]$ , $\text{Be}(\text{OH})_2(\text{aq})$ , $\text{Be}(\text{OH})_3[-]$ , $\text{Be}(\text{OH})_4[2-]$ , $\text{Be}_2(\text{OH})[3+]$ , $\text{Be}_3(\text{OH})_3[3+]$ , $\text{Be}_5(\text{OH})_6[4+]$ , $\text{Be}_6(\text{OH})_8[4+]$ , $\text{Be}(\text{OH})_2(\text{alpha})$ , $\text{Be}(\text{OH})_2(\text{beta})$			



☒ 18: Eh-pH diagrams of the system Be-O-H (1).  $\sum \text{Be} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





☒ 19: Eh-pH diagrams of the system Be-O-H (2).  $\sum \text{Be} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 11: List of Bi species

FACT	SUPCRT	LLNL	JNC-TDB
Bi[3+], BiO[+], BiOH[2+], Bi <sub>6</sub> O <sub>6</sub> [6+], Bi <sub>6</sub> O <sub>6</sub> (OH) <sub>3</sub> [3+], Bi <sub>9</sub> (OH) <sub>20</sub> [7+], Bi <sub>9</sub> (OH) <sub>21</sub> [6+], Bi <sub>9</sub> (OH) <sub>22</sub> [5+], <b>Bi(s), Bi<sub>2</sub>O<sub>3</sub>(s),</b> <b>Bi<sub>2</sub>O<sub>3</sub>(s2), BiOOH(s)</b>	Bi[3+], BiO[+], BiOH[2+], HBiO <sub>2</sub> (aq), BiO <sub>2</sub> [-]		Bi[3+], BiOH[2+], Bi(OH) <sub>2</sub> [+], Bi(OH) <sub>3</sub> (aq), Bi(OH) <sub>4</sub> [-], Bi <sub>6</sub> (OH) <sub>12</sub> [6+], Bi <sub>9</sub> (OH) <sub>20</sub> [7+], Bi <sub>9</sub> (OH) <sub>21</sub> [6+], Bi <sub>9</sub> (OH) <sub>22</sub> [5+], Bi <sub>3</sub> (OH) <sub>4</sub> [5+] <b>Bi(c), Bi<sub>2</sub>O<sub>3</sub>(s)</b>

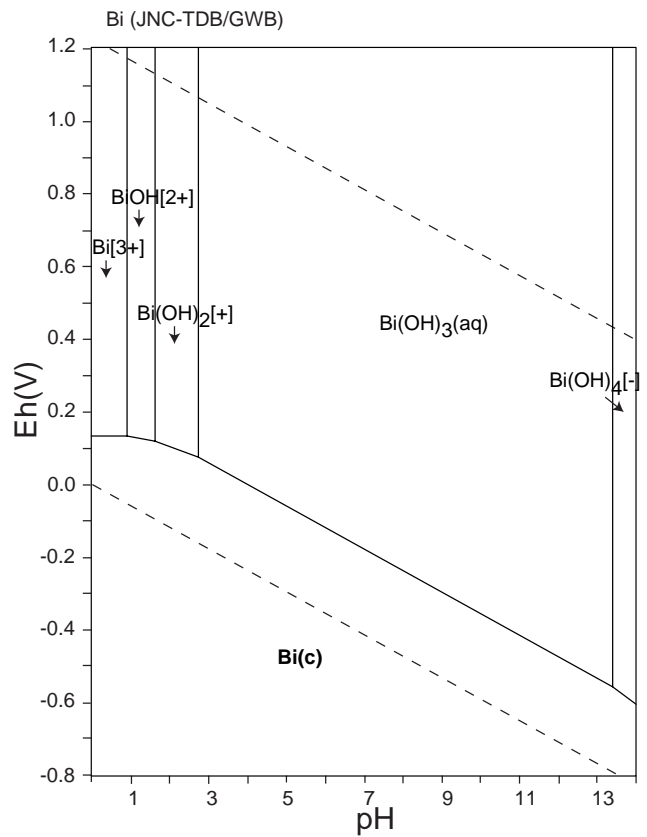
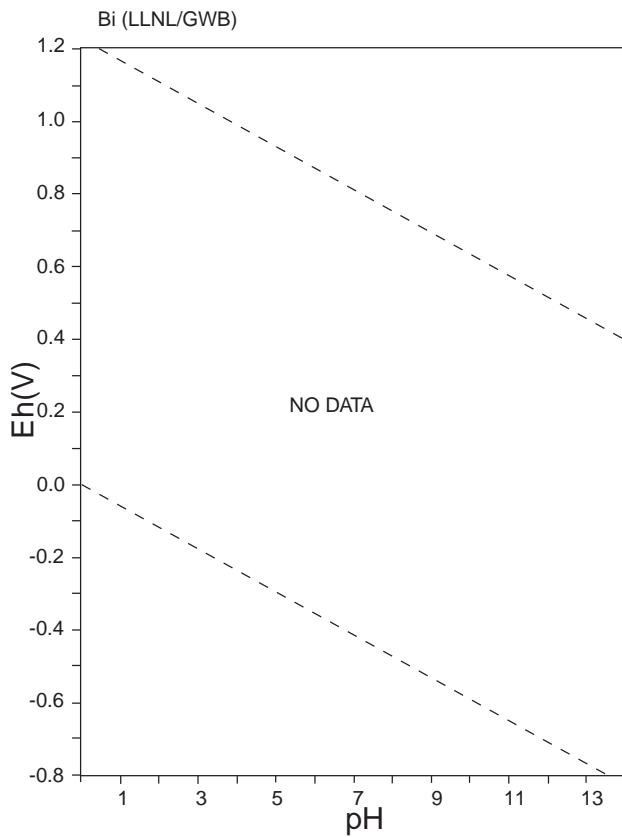
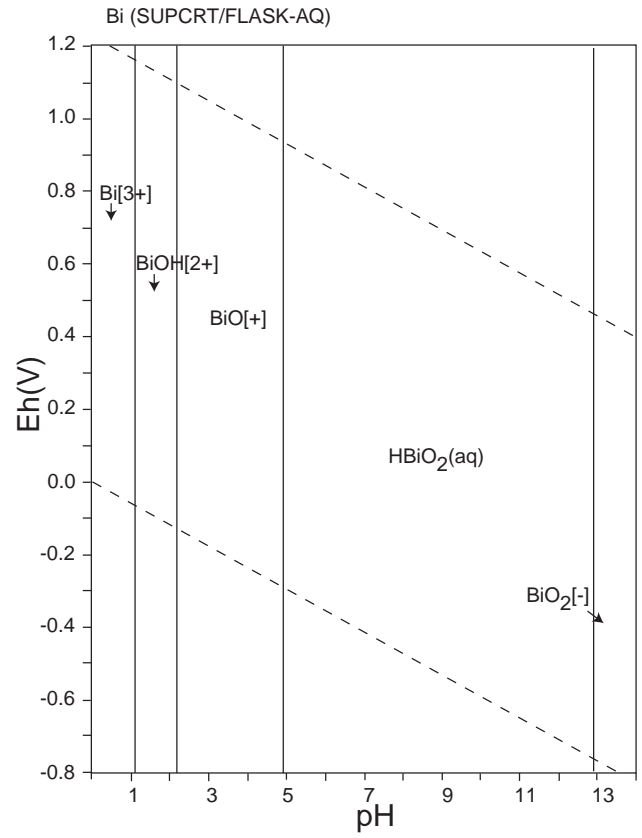
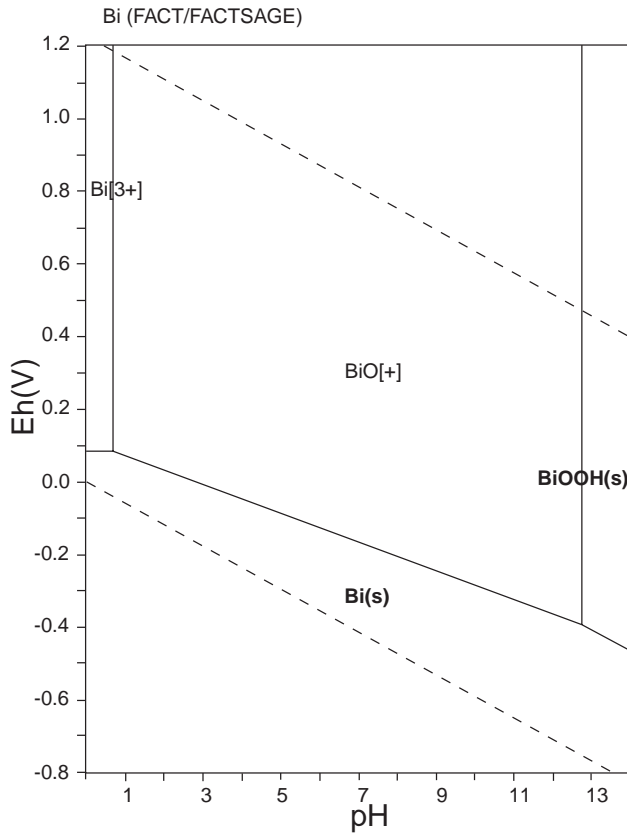
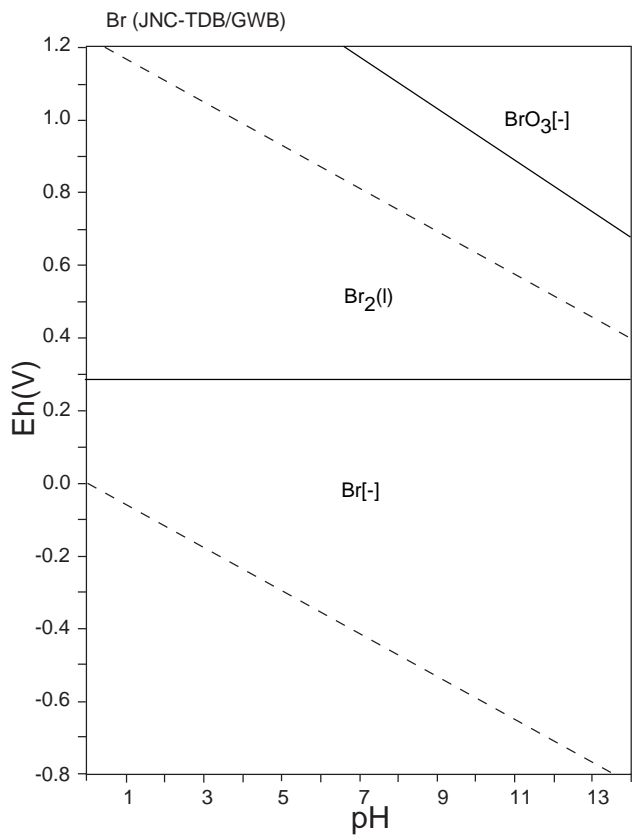
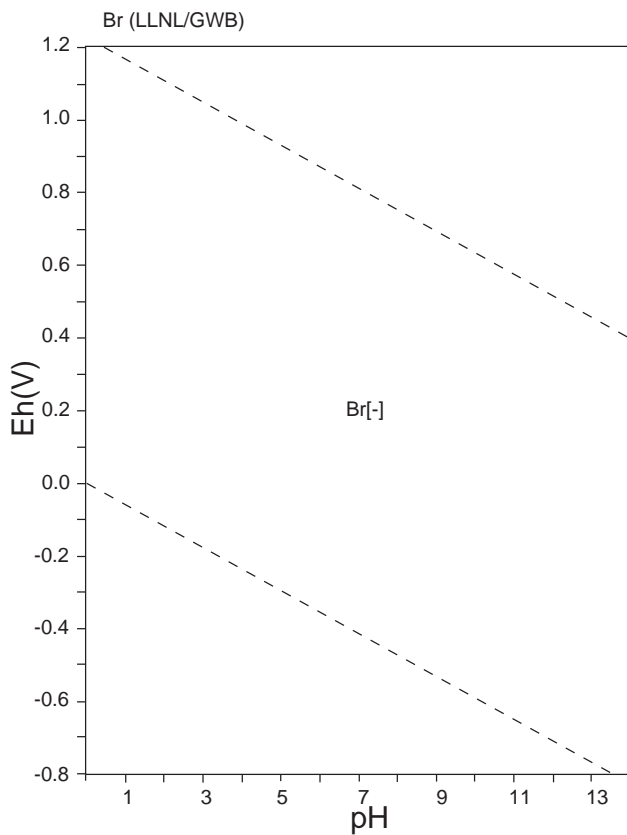
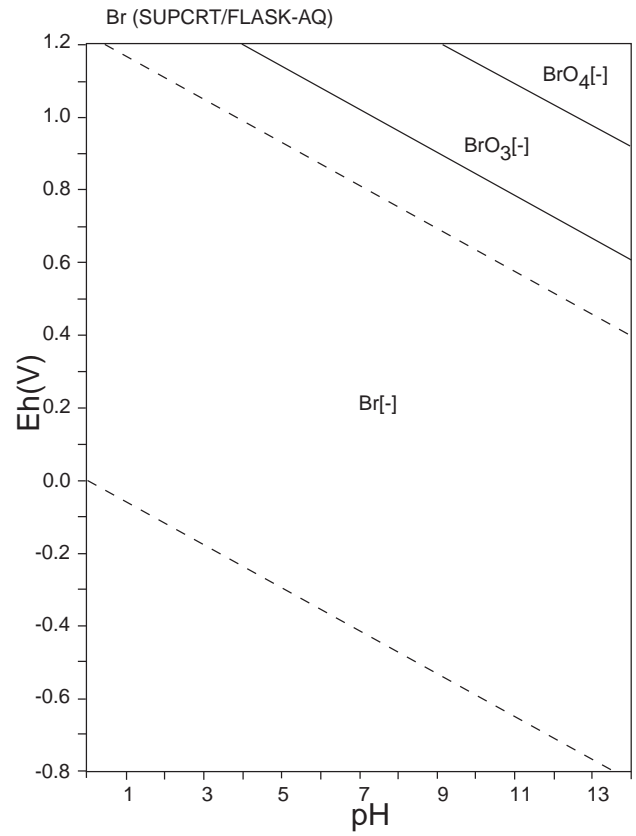
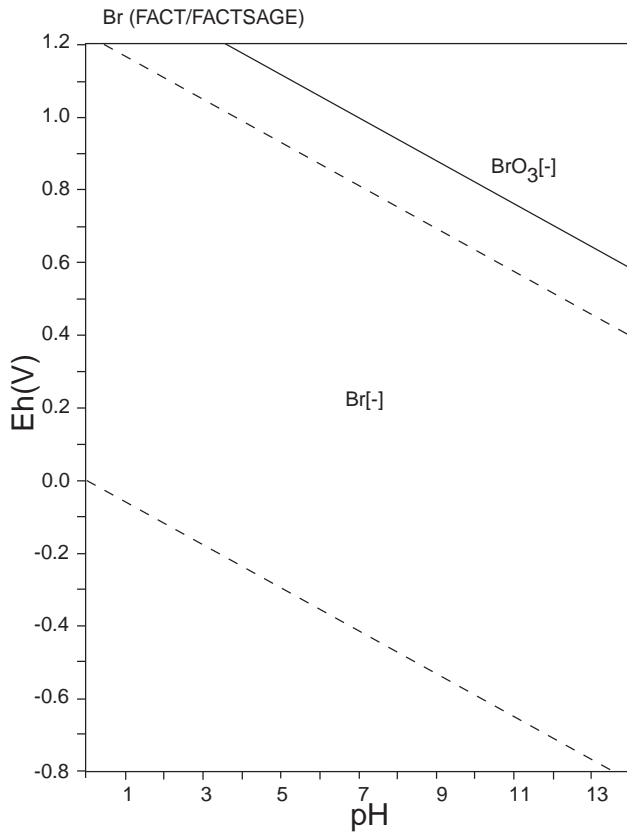


Figure 20: Eh-pH diagrams of the system Bi-O-H.  $\sum \text{Bi} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 12: List of Br species

FACT	SUPCRT	LLNL	JNC-TDB
Br[-], Br <sub>2</sub> (aq), Br <sub>3</sub> [-], Br <sub>5</sub> [-], BrO[-], BrO <sub>3</sub> [-], HBrO(aq)	Br[-], Br <sub>3</sub> [-], BrO[-], BrO <sub>3</sub> [-], HBrO(aq), BrO <sub>4</sub> [-]	Br[-]	Br[-], Br <sub>2</sub> (aq), Br <sub>2</sub> (l), BrO[-], BrO <sub>3</sub> [-], HBrO(aq), Br(g), Br <sub>2</sub> (g), HBr(g)



☒ 21: Eh-pH diagrams of the system Br-O-H.  $\sum \text{Br} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 13: List of C species (1)

FACT	SUPCRT	LLNL	JNC-TDB
<p>CH<sub>4</sub>(aq), C<sub>2</sub>H<sub>2</sub>(aq), C<sub>2</sub>H<sub>4</sub>(aq), C<sub>2</sub>H<sub>6</sub>(aq), CO(aq), CO<sub>2</sub>(aq), CO<sub>3</sub>[2-], C<sub>2</sub>O<sub>4</sub>[2-], CH<sub>3</sub>OH(aq), C<sub>2</sub>H<sub>5</sub>O[-], CH<sub>3</sub>CH<sub>2</sub>OH(aq), HCOO[-], HCOOH(aq), CH<sub>3</sub>COO[-], CH<sub>3</sub>COOH(aq), HCO<sub>3</sub>[-], HC<sub>2</sub>O<sub>4</sub>[-], <b>C(s)</b>, <b>C(s2)</b></p>	<p>CH<sub>4</sub>(aq,Methan), C<sub>2</sub>H<sub>2</sub>(aq,Ethyne), C<sub>2</sub>H<sub>4</sub>(aq,Ethylene), C<sub>2</sub>H<sub>6</sub>(aq,Ethane), CO(aq), CO<sub>2</sub>(aq), CO<sub>3</sub>[2-], C<sub>2</sub>O<sub>4</sub>[2-] (Oxalate), CH<sub>3</sub>OH(aq,Methanol), C<sub>2</sub>H<sub>5</sub>OH(aq,Ethanol), HCO<sub>2</sub>[-](Formate), H<sub>2</sub>CO<sub>2</sub>(aq, Formic-acid), C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>[-] (Acetate), C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>(aq,Acetic-acid), HCO<sub>3</sub>[-], C<sub>2</sub>HO<sub>4</sub>[-] (H-Oxalate), C<sub>4</sub>H<sub>9</sub>OH (aq,1-Butanol), C<sub>4</sub>H<sub>8</sub>(aq,1-Butene), C<sub>4</sub>H<sub>6</sub>(aq,1-Butyne), C<sub>7</sub>H<sub>15</sub>OH (aq,1-Heptanol), C<sub>7</sub>H<sub>14</sub>(aq,1-Heptene), C<sub>7</sub>H<sub>12</sub>(aq,1-Heptyne), C<sub>6</sub>H<sub>13</sub>OH(aq,1-Hexanol), C<sub>6</sub>H<sub>12</sub>(aq,1-Hexene), C<sub>6</sub>H<sub>10</sub>(aq,1-Hexyne), C<sub>8</sub>H<sub>17</sub>OH(aq,1-Octanol), C<sub>8</sub>H<sub>16</sub>(aq,1-Octene), C<sub>8</sub>H<sub>14</sub>(aq,1-Octyne), C<sub>5</sub>H<sub>11</sub>OH(aq,1-Pentanol), C<sub>5</sub>H<sub>10</sub>(aq,1-Pentene), C<sub>5</sub>H<sub>8</sub>(aq,1-Pentyne), C<sub>3</sub>H<sub>7</sub>OH(aq,1-Propanol), C<sub>3</sub>H<sub>6</sub>(aq,1-Propene), C<sub>3</sub>H<sub>4</sub>(aq,1-Propyne), C<sub>4</sub>H<sub>8</sub>O(aq,2-Butanone), C<sub>7</sub>H<sub>14</sub>O(aq,2-Heptanone), C<sub>6</sub>H<sub>12</sub>O(aq,2-Hexanone), C<sub>4</sub>H<sub>7</sub>O<sub>3</sub>[-] (2-Hydroxybutanoate), C<sub>4</sub>H<sub>9</sub>O<sub>3</sub>(aq,2-Hydroxybutanoic), C<sub>10</sub>H<sub>19</sub>O<sub>3</sub>[-] (2-Hydroxydecanoate), C<sub>10</sub>H<sub>20</sub>O<sub>3</sub>(aq,2-Hydroxydecanoic), C<sub>7</sub>H<sub>13</sub>O<sub>3</sub>[-] (2-Hydroxyheptanoate), C<sub>7</sub>H<sub>14</sub>O<sub>3</sub>(aq,2-Hydroxyheptanoic), C<sub>6</sub>H<sub>11</sub>O<sub>3</sub>[-] (2-Hydroxyhexanoate), C<sub>6</sub>H<sub>12</sub>O<sub>3</sub>(aq,2-Hydroxyhexanoic), C<sub>9</sub>H<sub>17</sub>O<sub>3</sub>[-] (2-Hydroxynonanoate), C<sub>9</sub>H<sub>18</sub>O<sub>3</sub>(aq,2-Hydroxynonanoic),</p>	<p>HCO<sub>3</sub>[-], (O-phth)[2-], CH<sub>3</sub>COO[-], CH<sub>4</sub>(aq), CO<sub>2</sub>(aq), CO<sub>3</sub>[2-], H(O-phth)[-], H<sub>2</sub>(O-phth), HCH<sub>3</sub>COO, <b>Graphite</b>, <b>O-phth acid(c)</b>, CH<sub>4</sub>(g), CO<sub>2</sub>(g)</p>	<p>CO<sub>3</sub>[2-], CH<sub>4</sub>(aq), HCO<sub>3</sub>[-], CO<sub>2</sub>(aq), <b>C(c)</b>, CH<sub>4</sub>(g), C(g), CO(g), CO<sub>2</sub>(g)</p>

表 14: List of C species (2)

C (CONTINUED)

FACT	SUPCRT	LLNL	JNC-TDB
	<p> <math>C_8H_{15}O_3[-]</math> (2-Hydroxyoctanoate),  <math>C_8H_{16}O_3(aq, 2-</math>Hydroxyoctanoic),  <math>C_5H_9O_3[-]</math> (2-Hydroxypentanoate),  <math>C_5H_{10}O_3(aq, 2-</math>Hydroxypentanoic),  <math>C_8H_{16}O(aq, 2-</math>Octanone),  <math>C_5H_{10}O(aq, 2-</math>Pentanone), <math>C_3H_6O(aq, Acetone)</math>,  <math>C_6H_8O_4[2-]</math> (Adipate), <math>C_6H_{10}O_4(aq, Adipic-acid)</math>,  <math>C_9H_{16}O_4(aq, Azelaic-acid)</math>,  <math>C_9H_{14}O_4[2-]</math> (Azelate), <math>C_6H_6(aq, Benzene)</math>, <math>C_7H_5O_2[-]</math> (Benzoate),  <math>C_7H_5O_2(aq, Benzoic-acid)</math>, <math>C_4H_{10}(aq, Butane)</math>, <math>C_4H_8O_2(aq, Butanoic-acid)</math>,  <math>C_6H_4OHCH_3(aq, o-</math>Cresol),  <math>C_6H_4OHCH_3(aq, m-</math>Cresol),  <math>C_6H_4OHCH_3(aq, p-</math>Cresol), <math>C_{10}H_{19}O_2[-]</math> (Decanoate),  <math>C_{10}H_{20}O_2(aq, Decanoic-acid)</math>,  <math>C_6H_3OHCH_3CH_3(aq, 2-3DMP)</math>,  <math>C_6H_3OHCH_3CH_3(aq, 2-4DMP)</math>,  <math>C_6H_3OHCH_3CH_3(aq, 2-5DMP)</math>,  <math>C_6H_3OHCH_3CH_3(aq, 2-6DMP)</math>,  <math>C_6H_3OHCH_3CH_3(aq, 3-4DMP)</math>,  <math>C_6H_3OHCH_3CH_3(aq, 3-5DMP)</math>,  <math>C_{12}H_{23}O_2[-]</math> (Dodecanoate),  <math>C_{12}H_{24}O_2(aq, Dodecanoic-acid)</math>,  <math>CH_3COOCH_2CH_3(aq, Ethylacetate)</math>,  <math>C_6H_5C_2H_5(aq, Ethylbenzene)</math>,  <math>C_5H_6O_4[2-]</math> (Glutarate), <math>C_5H_8O_4(aq, Glutaric-acid)</math>,  <math>C_2H_3O_3[-]</math> (Glycolate), <math>C_2H_4O_3(aq, Glycolic-acid)</math>,  <math>C_6H_9O_4[-]</math> (H-Adipate), <math>C_9H_{15}O_4[-]</math> (H-Azelate),                 </p>		

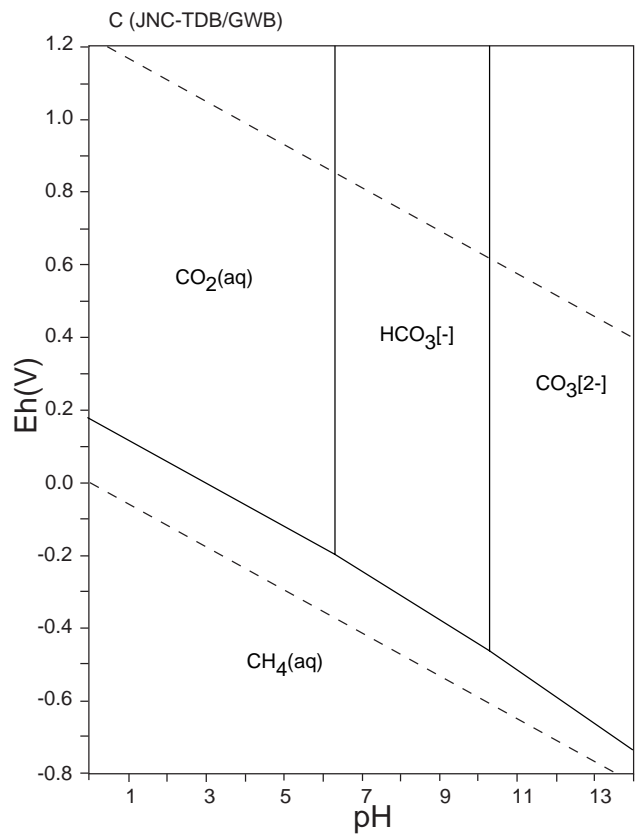
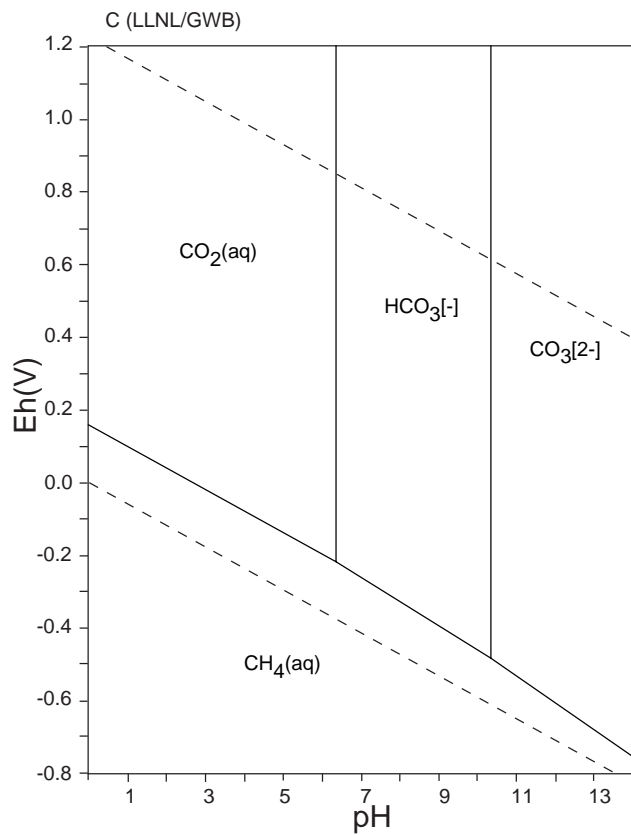
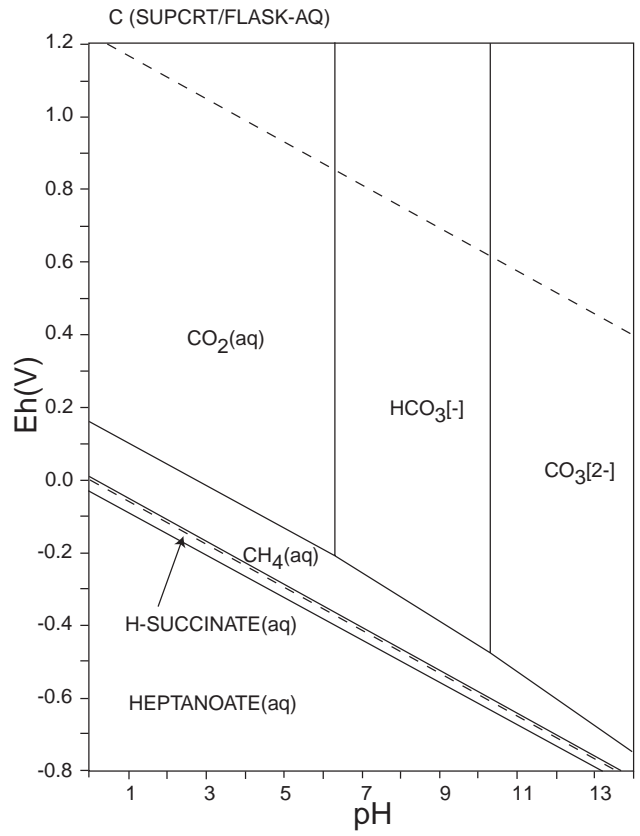
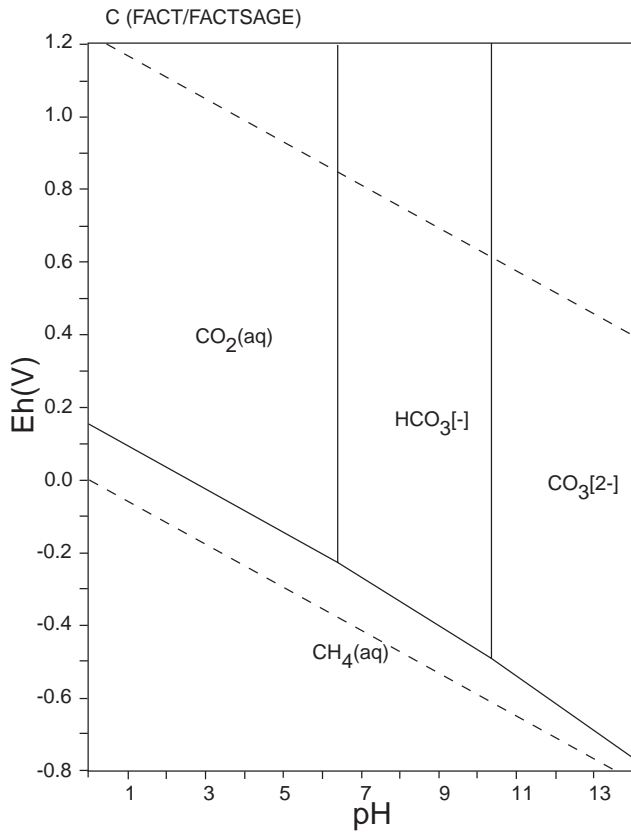
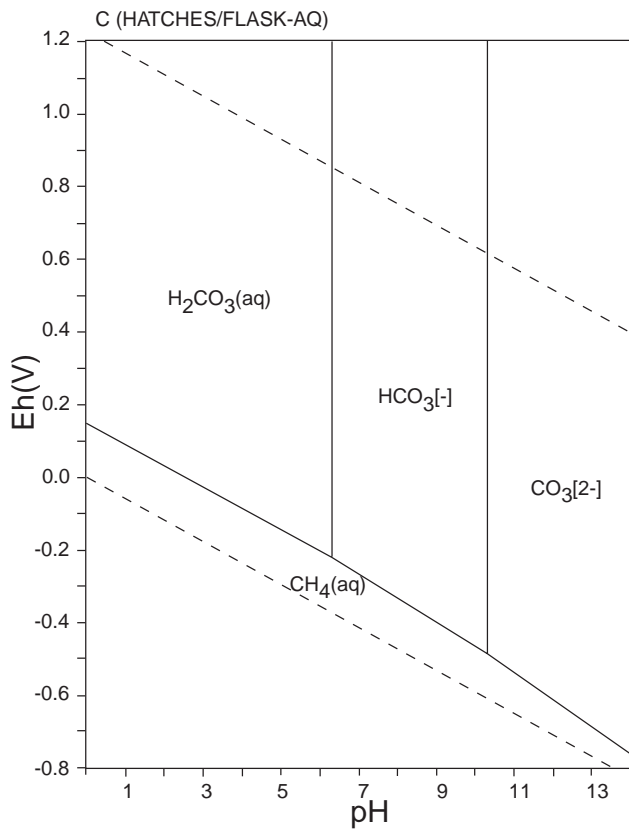


Figure 22: Eh-pH diagrams of the system C-O-H (1).  $\sum C = 10^{-10}$ , 298.15K,  $10^5$  Pa.





☒ 23: Eh-pH diagrams of the system C-O-H (2).  $\sum C = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 15: List of Ca species

FACT	SUPCRT	LLNL	JNC-TDB
Ca[2+], CaOH[+], Ca(s), Ca(s2), CaH <sub>2</sub> (s), CaO <sub>2</sub> (s), Ca(OH) <sub>2</sub> (s), CaO(s)	Ca[2+], CaOH[+], CaO(Lime)	Ca[2+], CaOH[+], Ca(OH) <sub>2</sub> (c), Lime, Portlandite	Ca[2+], CaOH[+], CaO(s, Lime_qu), Ca(c), CaO(c), Ca(g)

HATCHES			
Ca[2+], Ca(OH)[+], Ca(OH) <sub>2</sub> , CaO			

Remarks

JNC-TDB: Detailed description of Lime\_qu is not given, it may be lime quenched?

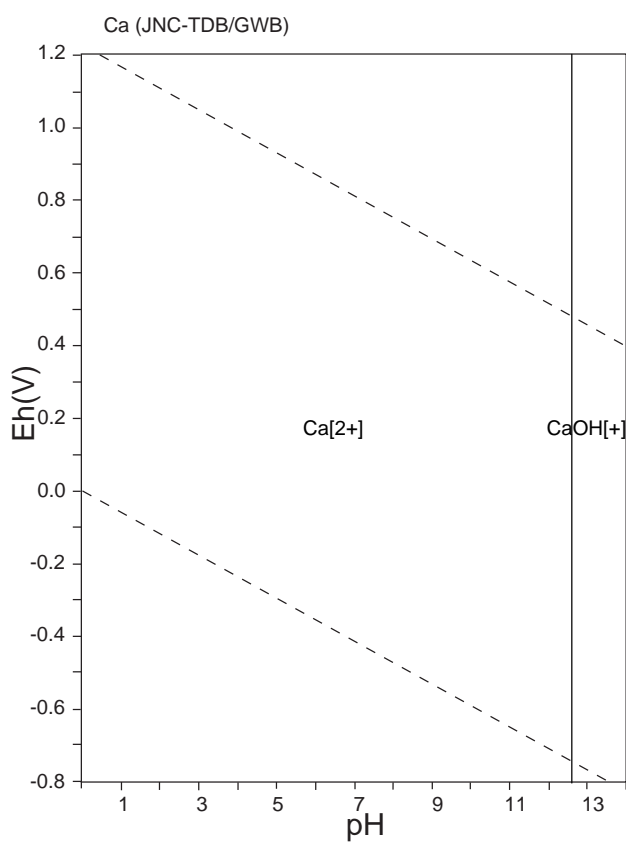
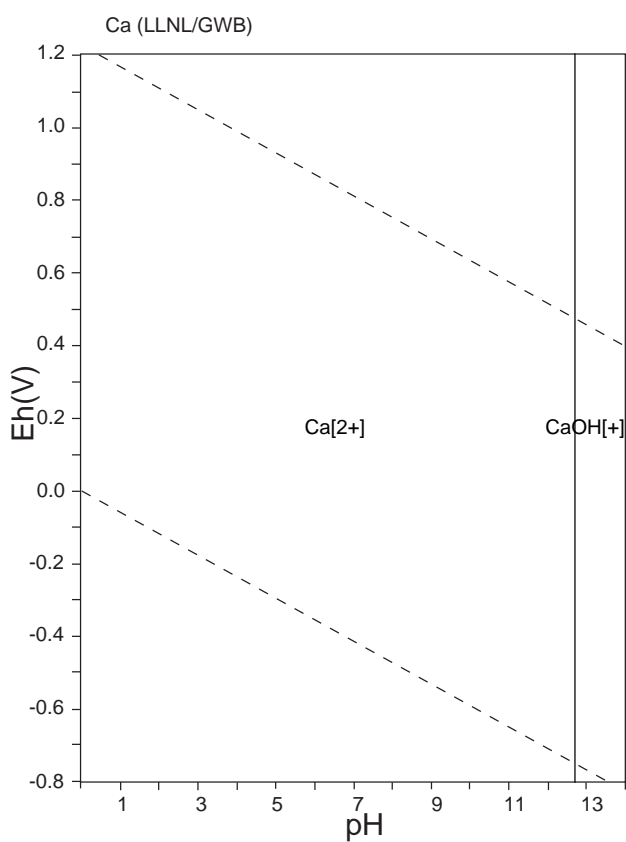
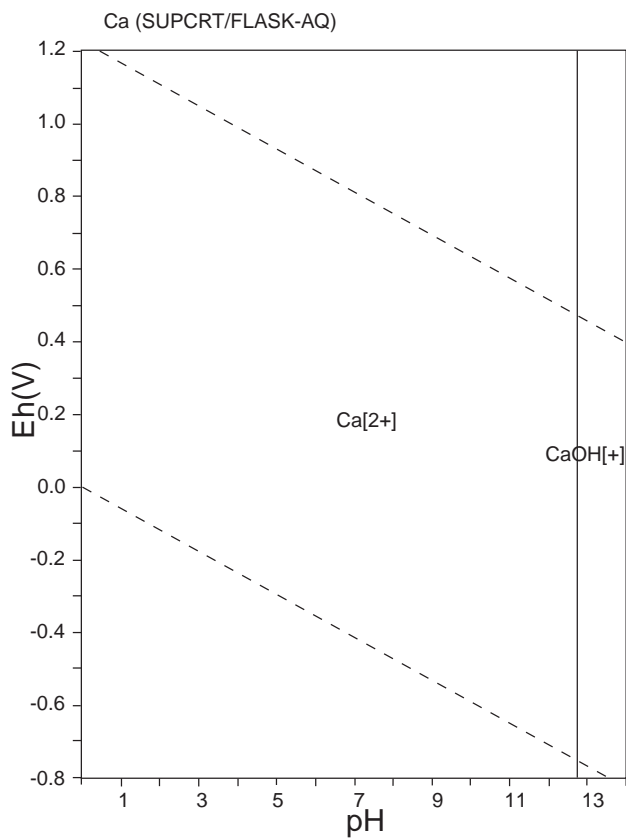
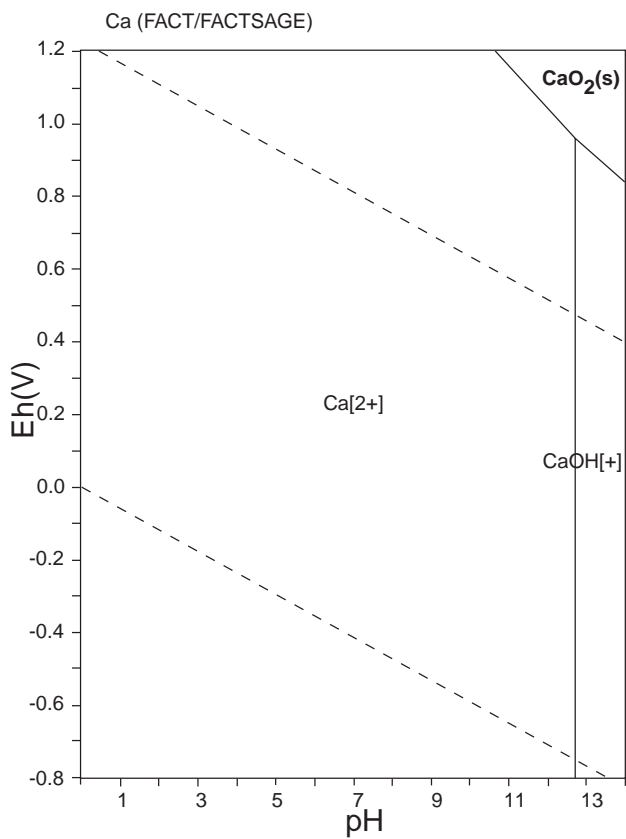


Figure 24: Eh-pH diagrams of the system Ca-O-H (1).  $\sum \text{Ca} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

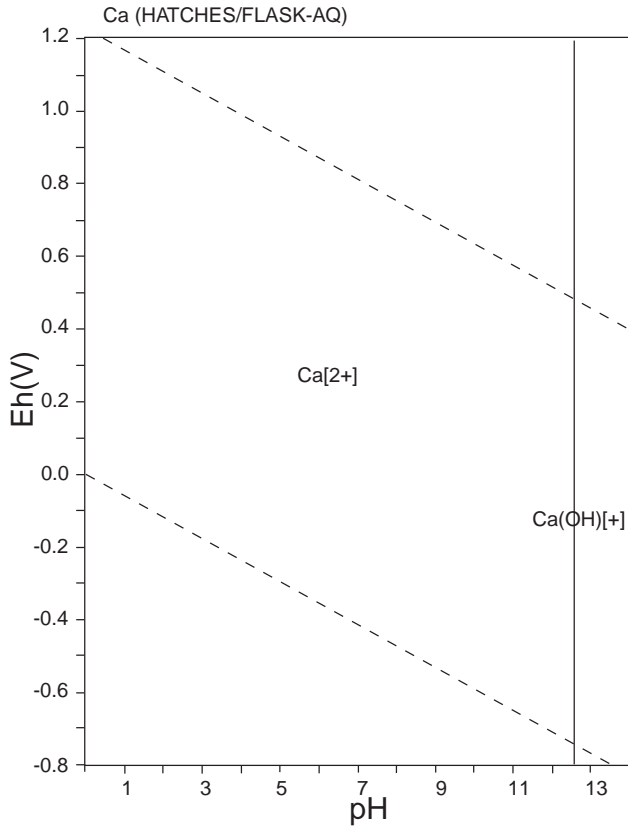


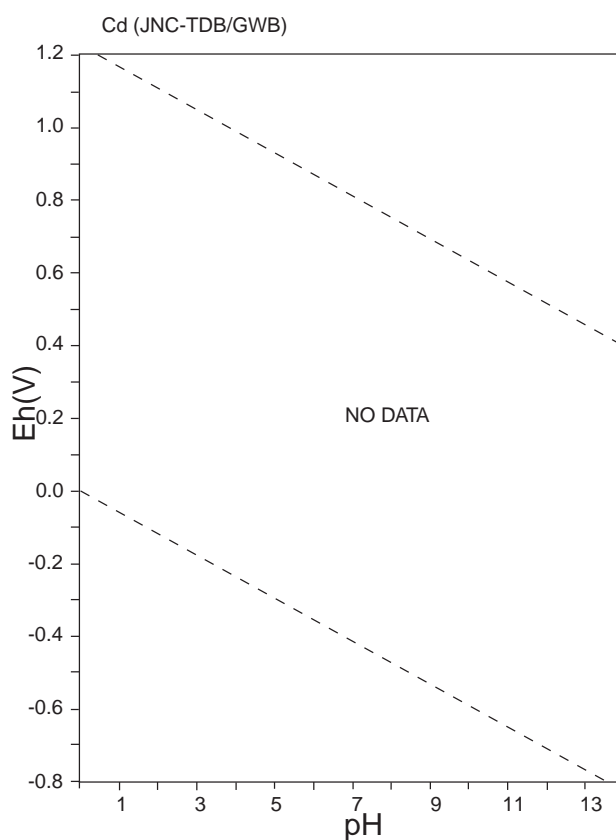
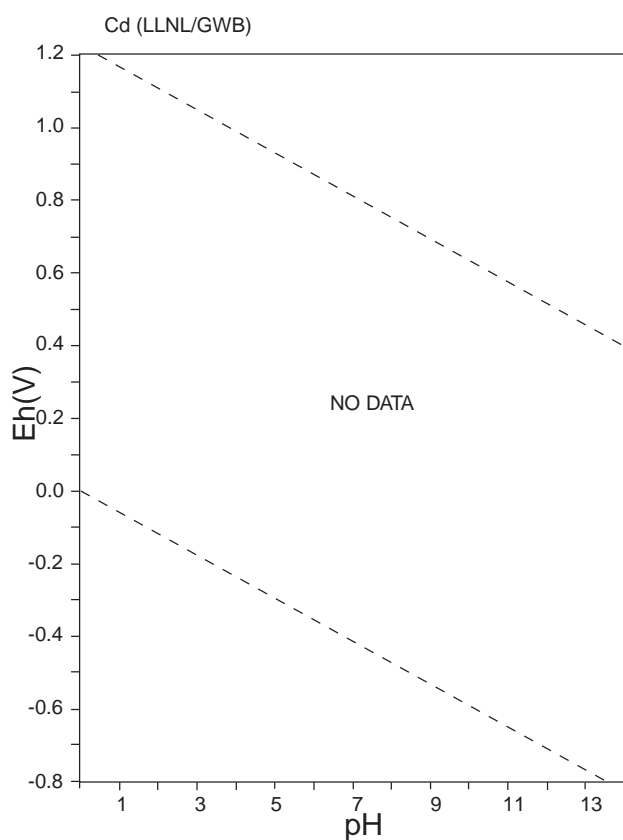
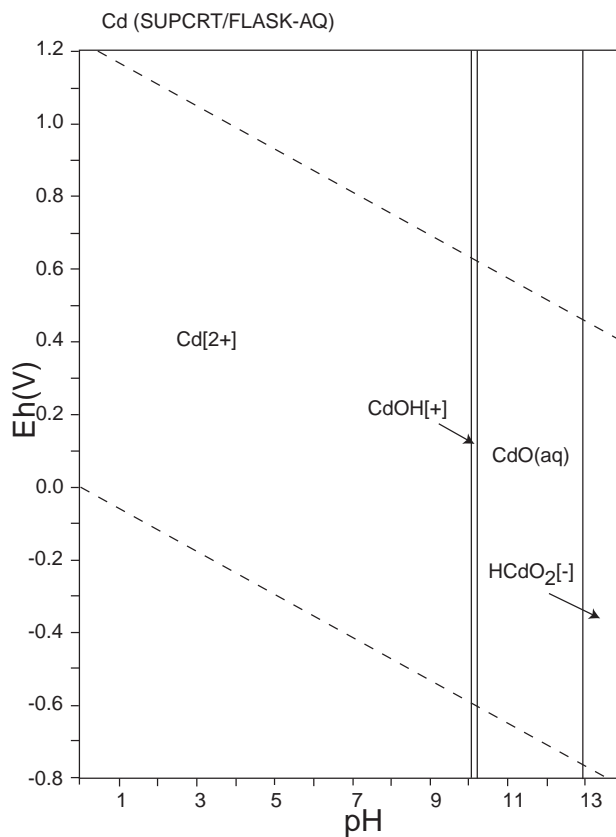
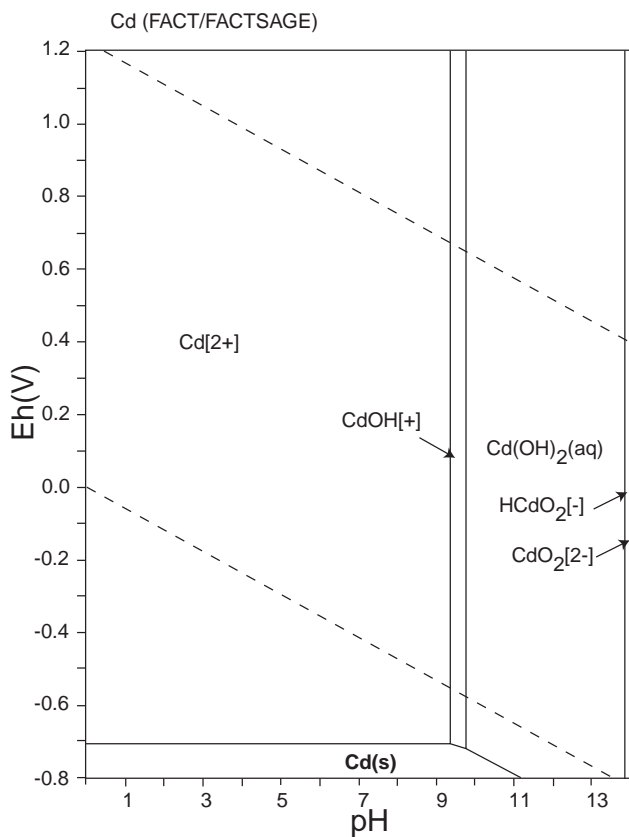
图 25: Eh-pH diagrams of the system Ca-O-H (2).  $\sum \text{Ca} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 16: List of Cd species

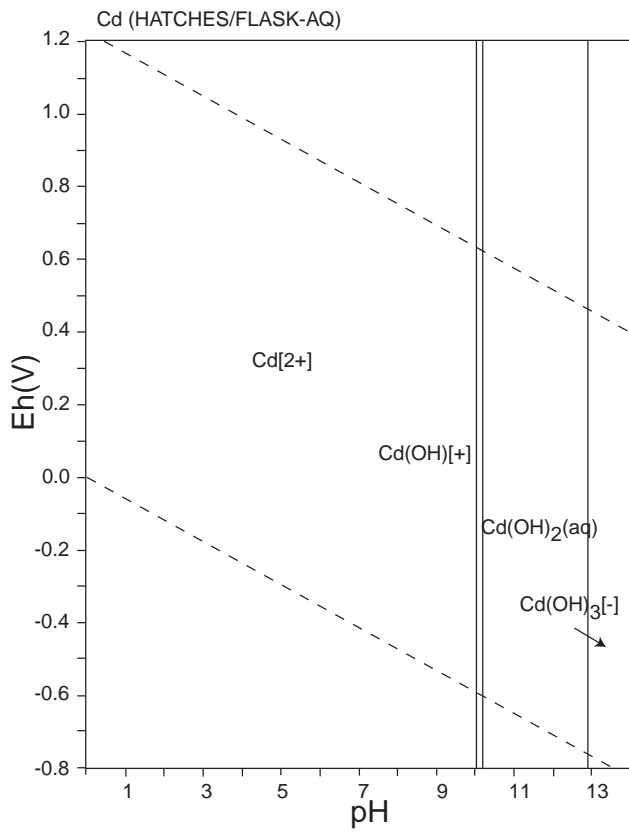
FACT	SUPCRT	LLNL	JNC-TDB
Cd[2+], CdO <sub>2</sub> [2-], CdOH[+], HCdO <sub>2</sub> [-], Cd(OH) <sub>2</sub> (aq), <b>Cd(s)</b> , <b>cdO(s)</b> , <b>cd(OH)<sub>2</sub>(s)</b>	Cd[2+], CdO <sub>2</sub> [2-], CdOH[+], HCdO <sub>2</sub> [-], CdO(aq)		

HATCHES			
Cd[2+], Cd(OH) <sub>2</sub> (aq), Cd(OH) <sub>3</sub> [-], Cd(OH) <sub>4</sub> [2-], Cd <sub>2</sub> OH[3+], Cd <sub>4</sub> (OH) <sub>4</sub> [4+], CdOH[+], <b>cd(OH)<sub>2</sub></b>			



☒ 26: Eh-pH diagrams of the system Cd-O-H (1).  $\sum \text{Cd} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





☒ 27: Eh-pH diagrams of the system Cd-O-H (2).  $\sum \text{Cd} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 17: List of Ce species

FACT	SUPCRT	LLNL	JNC-TDB
Ce[3+], Ce[4+], <b>Ce(s)</b> , <b>Ce(s2)</b> , <b>CeH<sub>2</sub>(s)</b> , <b>CeO<sub>2</sub>(s)</b> , <b>Ce<sub>2</sub>O<sub>3</sub>(s)</b> , <b>Ce<sub>6</sub>O<sub>11</sub>(s)</b> , <b>Ce<sub>18</sub>O<sub>31</sub>(s)</b>	Ce[3+], Ce[4+], Ce[2+], CeOH[2+], CeO[+], CeO <sub>2</sub> H (aq), CeO <sub>2</sub> [-]		

HATCHES			
Ce[3+], Ce <sub>2</sub> (OH) <sub>2</sub> [4+], Ce <sub>3</sub> (OH) <sub>5</sub> [4+], CeOH[2+], <b>Ce(OH)<sub>3</sub></b> , <b>Ce<sub>2</sub>O<sub>3</sub></b>			

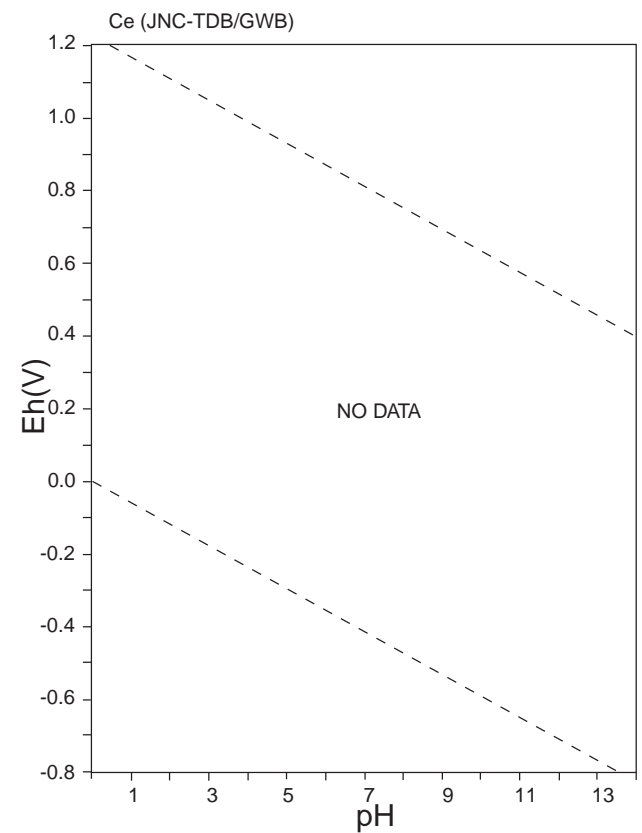
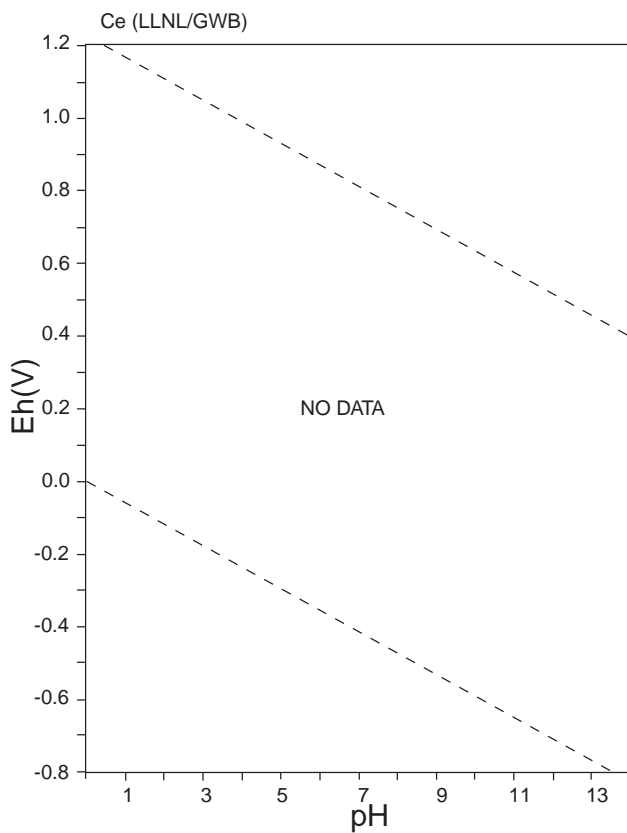
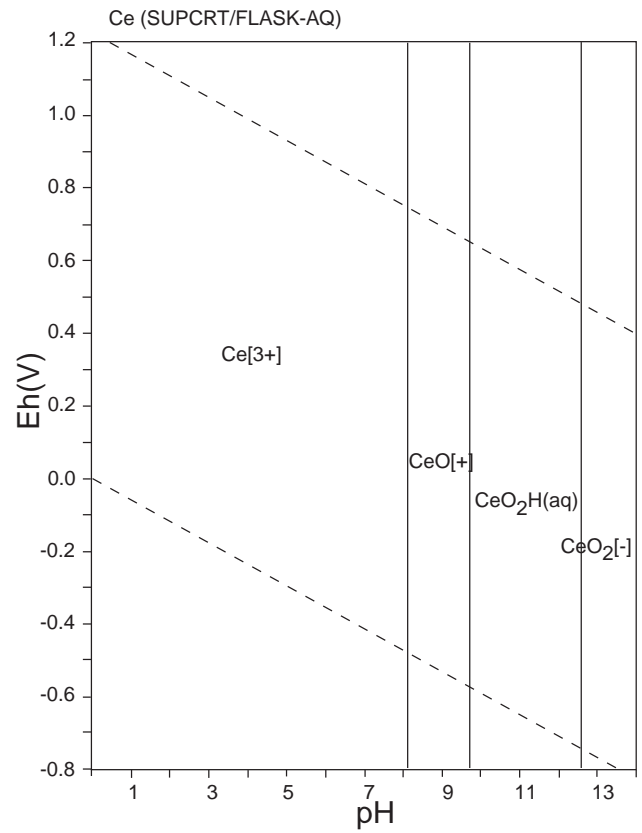
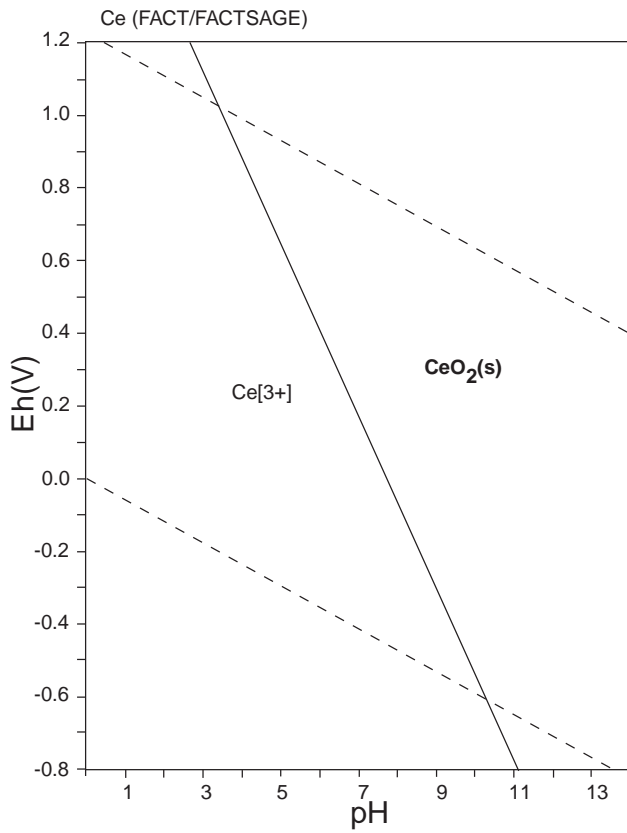
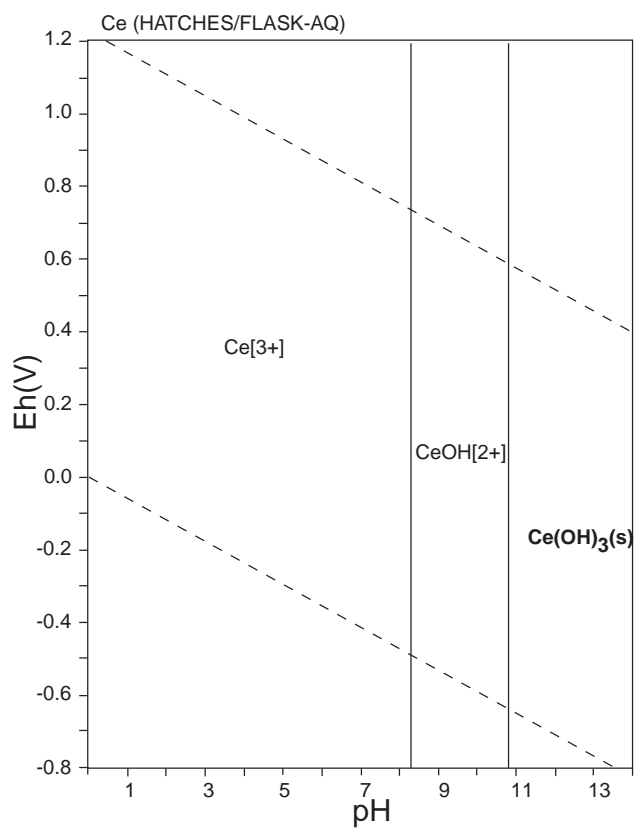


图 28: Eh-pH diagrams of the system Ce-O-H (1).  $\sum \text{Ce} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 29: Eh-pH diagrams of the system Ce-O-H (2).  $\sum \text{Ce} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 18: List of Cl species

FACT	SUPCRT	LLNL	JNC-TDB
Cl <sub>2</sub> (aq), Cl <sub>3</sub> [-], ClO <sub>2</sub> (aq), Cl[-], ClO[-], ClO <sub>2</sub> [-], ClO <sub>3</sub> [-], ClO <sub>4</sub> [-], HOCl(aq), HClO <sub>2</sub> (aq)	Cl[-], ClO[-], ClO <sub>2</sub> [-], ClO <sub>3</sub> [-], ClO <sub>4</sub> [-], HClO(aq), HClO <sub>2</sub> (aq), HCl(aq)	Cl[-], ClO <sub>4</sub> [-], HCl(aq)	Cl[-], ClO[-], ClO <sub>2</sub> [-], ClO <sub>3</sub> [-], ClO <sub>4</sub> [-], HClO(aq), HClO <sub>2</sub> (aq), Cl(g), Cl <sub>2</sub> (g), HCl(g)

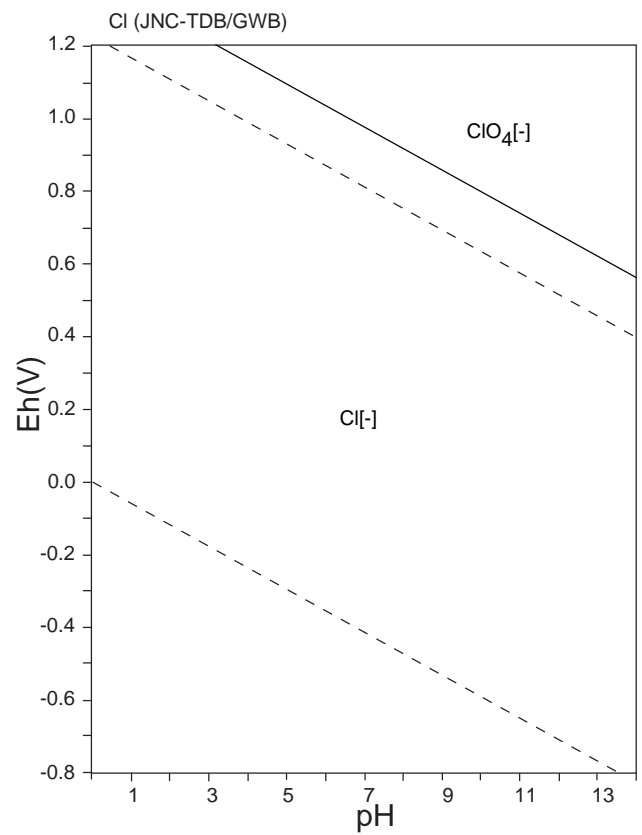
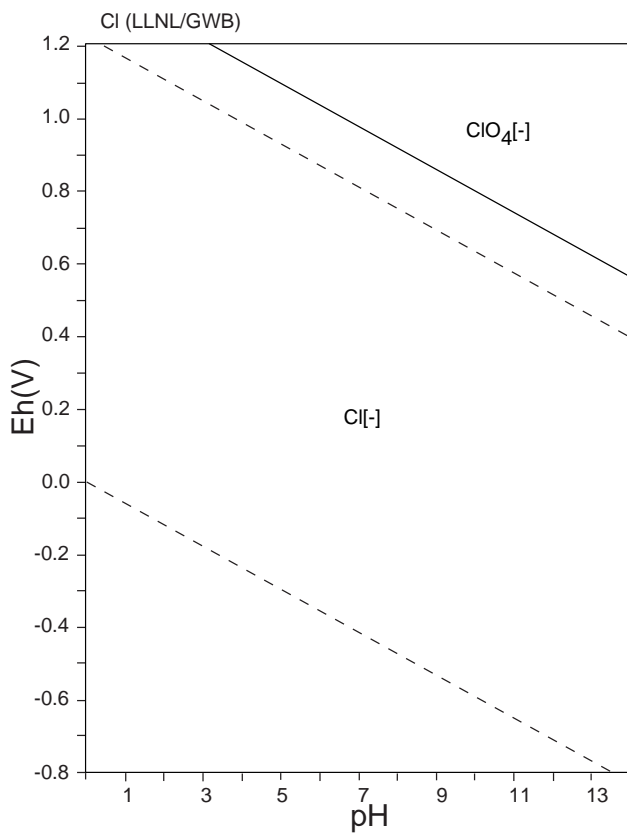
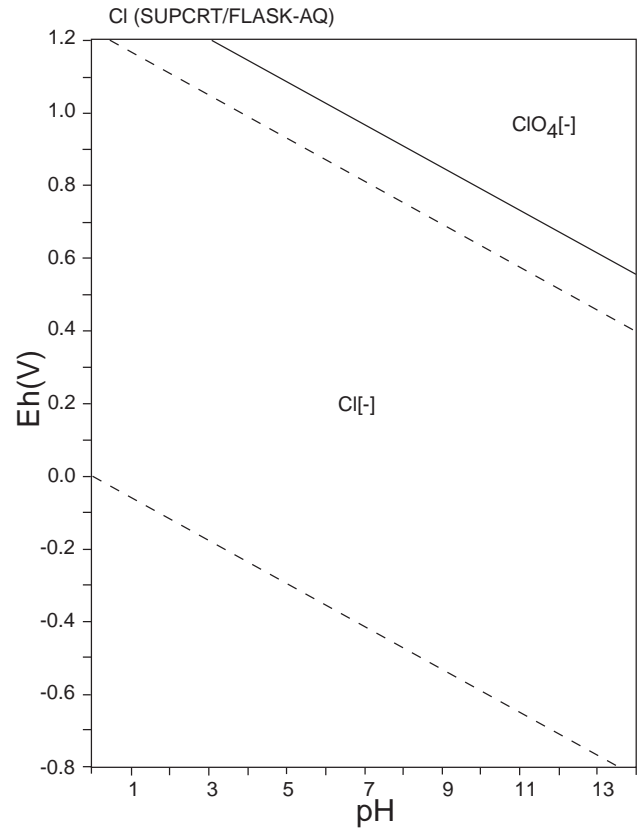
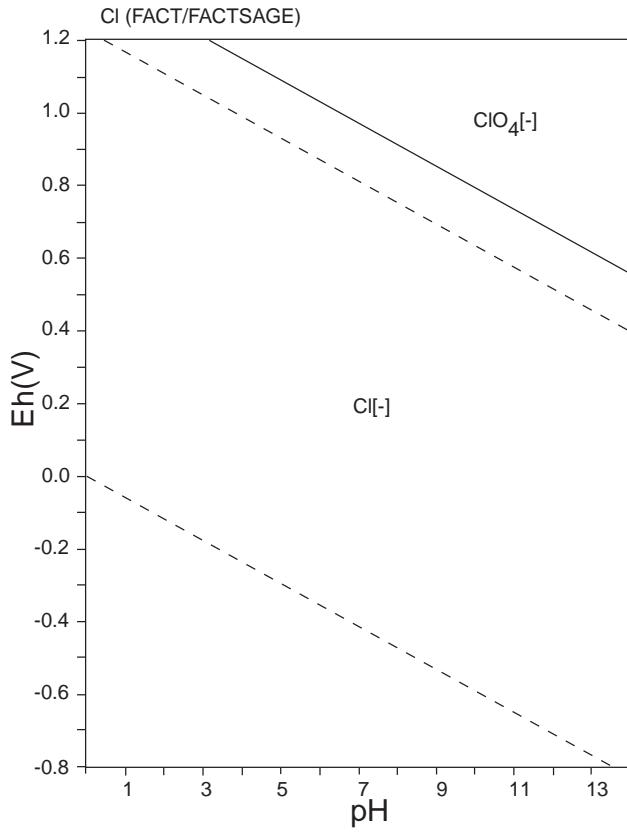


图 30: Eh-pH diagrams of the system Cl-O-H.  $\sum \text{Cl} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

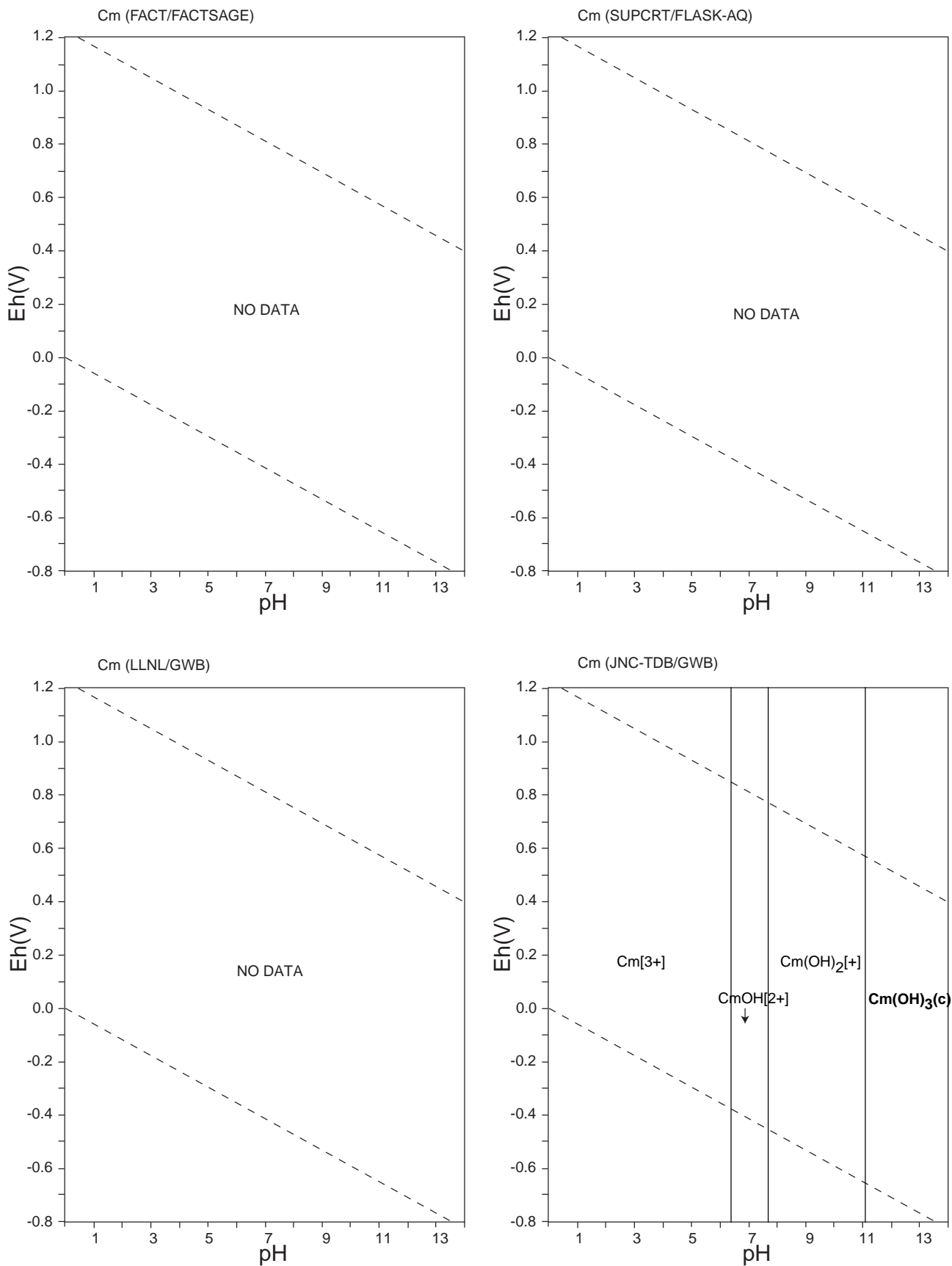




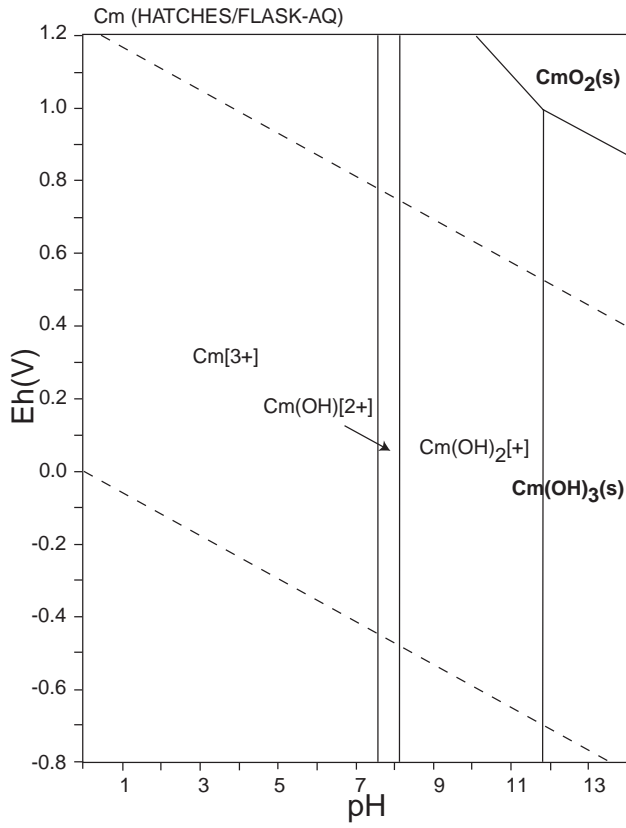
表 19: List of Cm species

FACT	SUPCRT	LLNL	JNC-TDB
			Cm[3+], CmOH[2+], Cm(OH) <sub>2</sub> [+], Cm(OH) <sub>3</sub> (aq), <b>Cm(OH)<sub>3</sub>(am)</b> , <b>Cm(OH)<sub>3</sub>(c)</b>

HATCHES			
Cm[3+], Cm[4+], Cm(OH)[2+], Cm(OH) <sub>2</sub> [+], <b>Cm(OH)<sub>3</sub>, Cm<sub>2</sub>O<sub>3</sub>, CmO<sub>2</sub></b>			



☒ 31: Eh-pH diagrams of the system Cm-O-H (1).  $\sum C_m = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 32: Eh-pH diagrams of the system Cm-O-H (2).  $\sum \text{Cm} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 20: List of Co species

FACT	SUPCRT	LLNL	JNC-TDB
Co[2+], Co[3+], HCoO <sub>2</sub> [-], Co(OH) <sub>2</sub> (aq), <b>Co(s)</b> , <b>Co(s2)</b> , <b>CoO(s)</b> , <b>Co<sub>3</sub>O<sub>4</sub>(s)</b> , <b>Co(OH)<sub>2</sub>(s)</b>	Co[2+], Co[3+], HCoO <sub>2</sub> [-], CoO(aq), CoOH[+], CoO <sub>2</sub> [2-], CoOH[2+]	Co[2+], Co[3+], Co(OH) <sub>2</sub> (aq), Co(OH) <sub>3</sub> [-], Co(OH) <sub>4</sub> [2-], Co <sub>2</sub> (OH) <sub>3</sub> [+], Co <sub>4</sub> (OH) <sub>4</sub> [4+], CoOH[+], HCoO <sub>2</sub> [-], <b>Co(OH)<sub>2</sub>(s,pink)</b> , <b>Co<sub>3</sub>O<sub>4</sub></b> , <b>CoO</b>	Co[2+], <b>CoO(s)</b> , <b>COBALTO2</b>

HATCHES			
Co[2+], Co[3+], Co(OH) <sub>2</sub> (aq), Co(OH) <sub>3</sub> [-], Co(OH) <sub>4</sub> [2-], Co <sub>2</sub> OH[3+], Co <sub>4</sub> (OH) <sub>4</sub> [4+], CoOH[+], <b>Co(OH)<sub>2</sub></b> , <b>Co<sub>3</sub>O<sub>4</sub></b> , <b>CoO</b>			

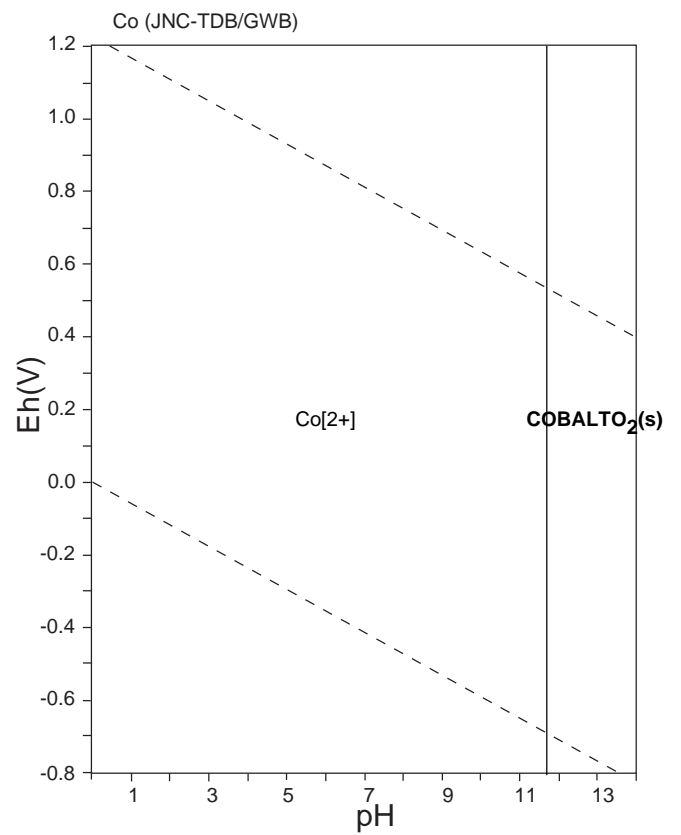
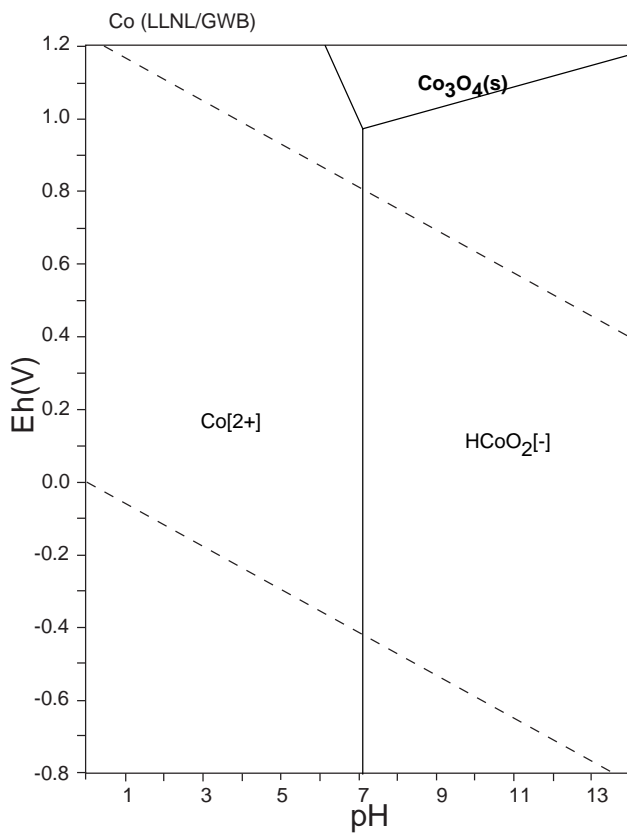
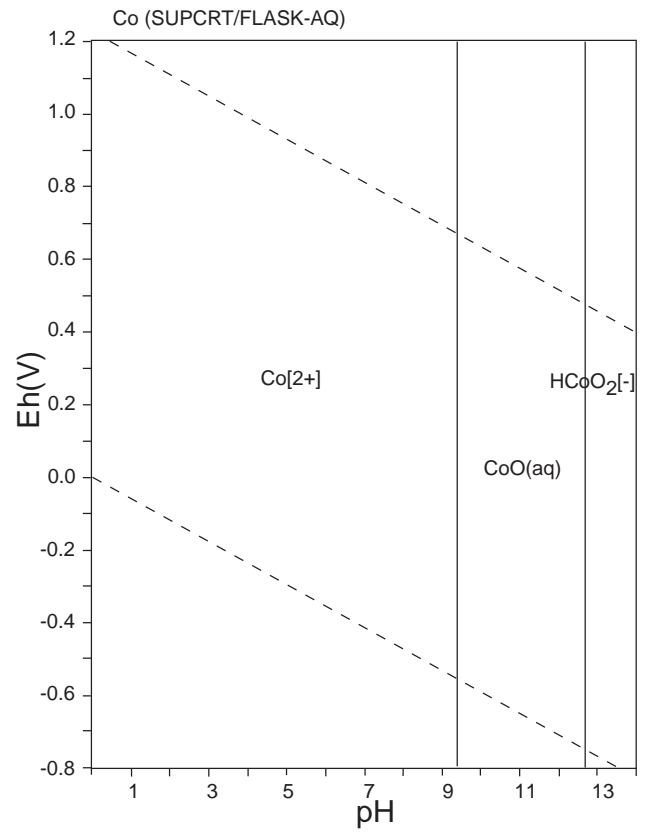
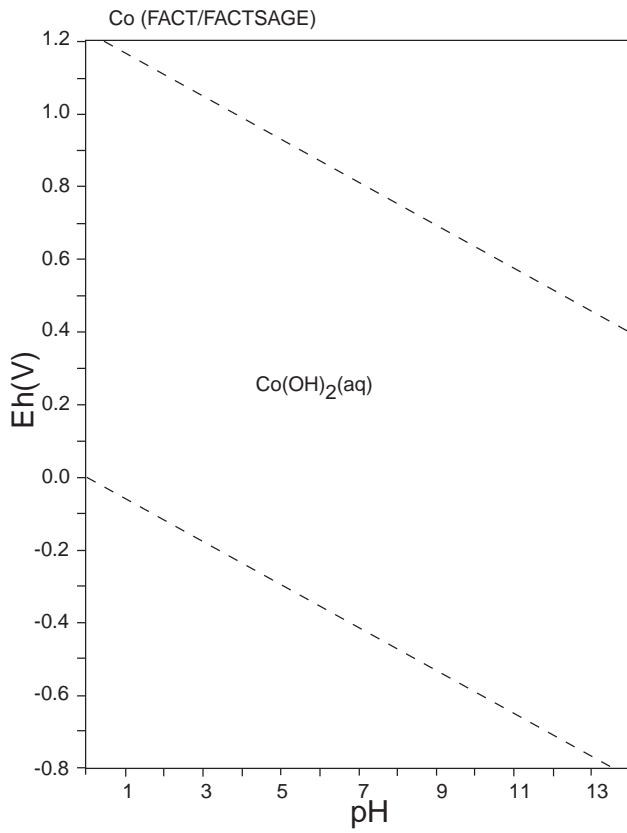


图 33: Eh-pH diagrams of the system Co-O-H (1).  $\sum \text{Co} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

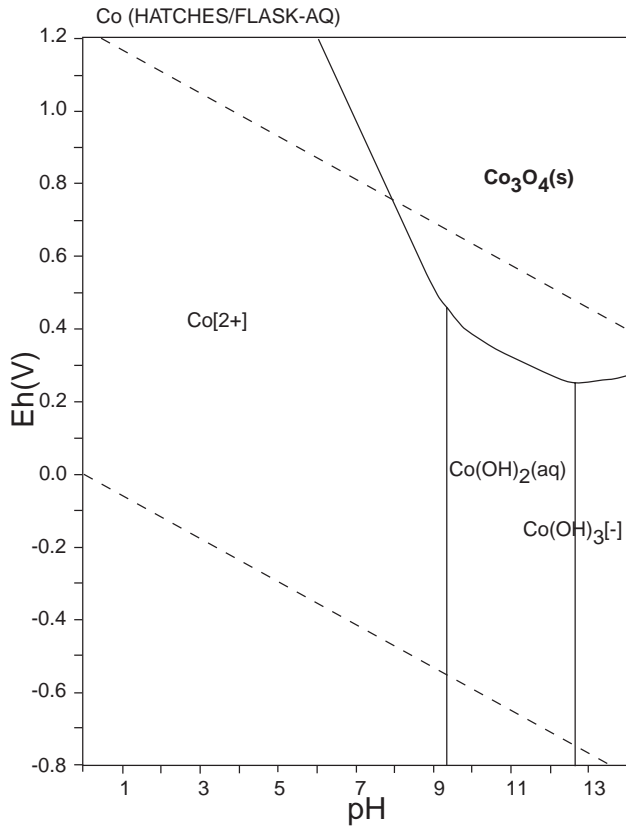


图 34: Eh-pH diagrams of the system Co-O-H (2).  $\sum \text{Co} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





表 21: List of Cr species

FACT	SUPCRT	LLNL	JNC-TDB
Cr[2+], Cr[3+], CrO <sub>4</sub> [2-], Cr <sub>2</sub> O <sub>7</sub> [2-], CrOH[2+], HCrO <sub>4</sub> [-], <b>Cr(s), CrO<sub>2</sub>(s),</b> <b>CrO<sub>3</sub>(s), Cr<sub>2</sub>O<sub>3</sub>(s),</b> <b>Cr<sub>3</sub>O<sub>4</sub>(s), Cr<sub>5</sub>O<sub>12</sub>(s),</b> <b>Cr<sub>8</sub>O<sub>21</sub>(s)</b>	Cr[2+], Cr[3+], CrO <sub>4</sub> [2-], Cr <sub>2</sub> O <sub>7</sub> [2-], CrOH[2+], HCrO <sub>4</sub> [-], HCrO <sub>2</sub> (aq), CrO <sub>2</sub> [-], CrO[+]	Cr[3+], Cr[2+], CrO <sub>4</sub> [2-], CrO <sub>4</sub> [3-], Cr(OH) <sub>2</sub> [+], Cr(OH) <sub>3</sub> (aq), Cr(OH) <sub>4</sub> [-], Cr <sub>2</sub> (OH) <sub>2</sub> [4+], Cr <sub>2</sub> O <sub>7</sub> [2-], Cr <sub>3</sub> (OH) <sub>4</sub> [5+], CrOH[2+], H <sub>2</sub> CrO <sub>4</sub> (aq), HCrO <sub>4</sub> [-], <b>Cr<sub>2</sub>O<sub>3</sub>(s),</b> <b>CrO<sub>2</sub>(s), CrO<sub>3</sub>(s)</b>	

HATCHES			
Cr[3+], Cr[2+], CrO <sub>4</sub> [2-], Cr(OH) <sub>2</sub> [+], Cr(OH) <sub>3</sub> (aq), Cr(OH) <sub>4</sub> [-], Cr <sub>2</sub> (OH) <sub>2</sub> [4+], Cr <sub>2</sub> O <sub>7</sub> [2-], Cr <sub>3</sub> (OH) <sub>4</sub> [4+], CrOH[2+], H <sub>2</sub> CrO <sub>4</sub> (aq), HCrO <sub>4</sub> [-], <b>Cr(OH)<sub>3</sub>, Cr<sub>2</sub>O<sub>3</sub>,</b> <b>CrO<sub>2</sub></b>			

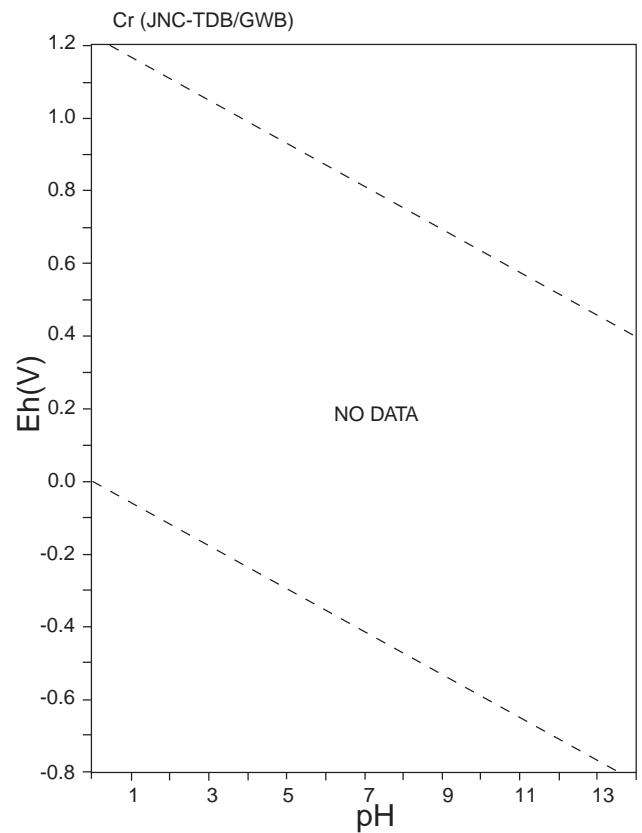
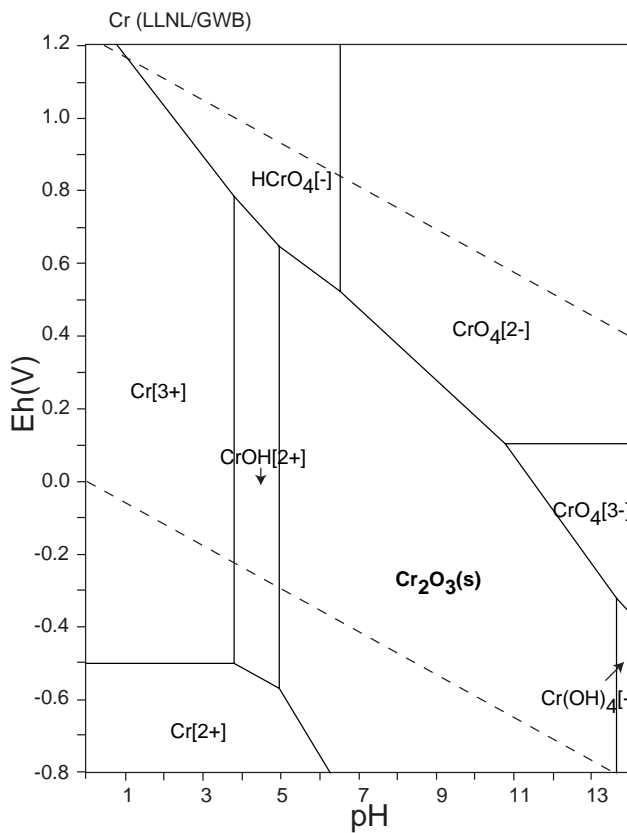
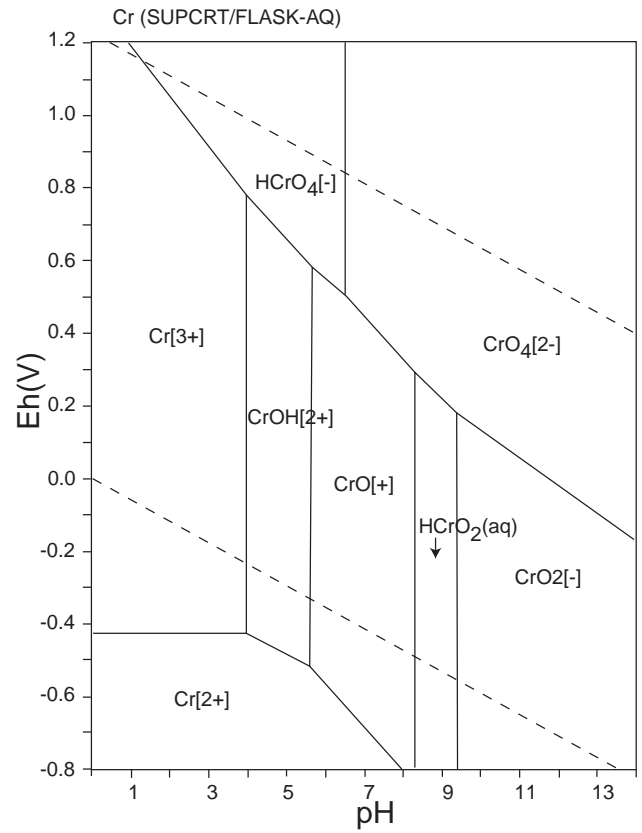
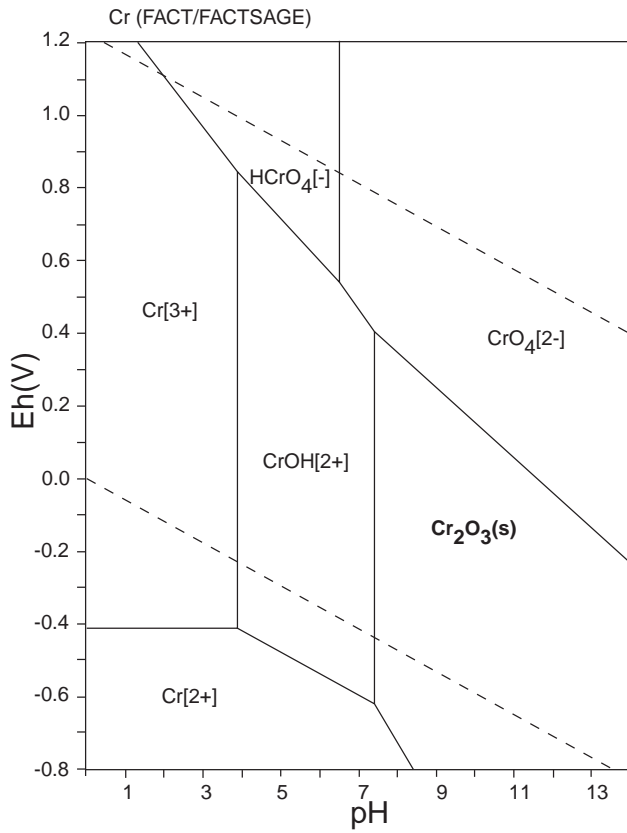
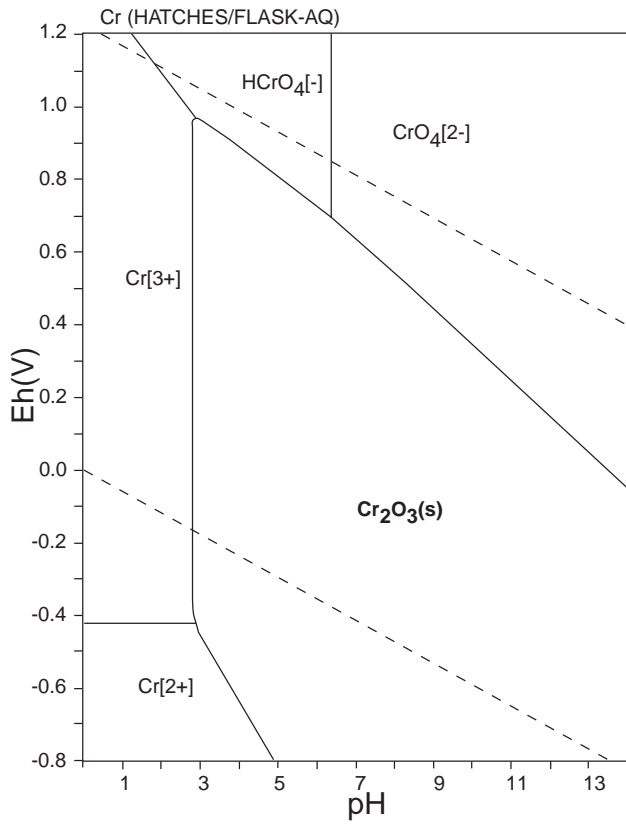


图 35: Eh-pH diagrams of the system Cr-O-H (1).  $\sum \text{Cr} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



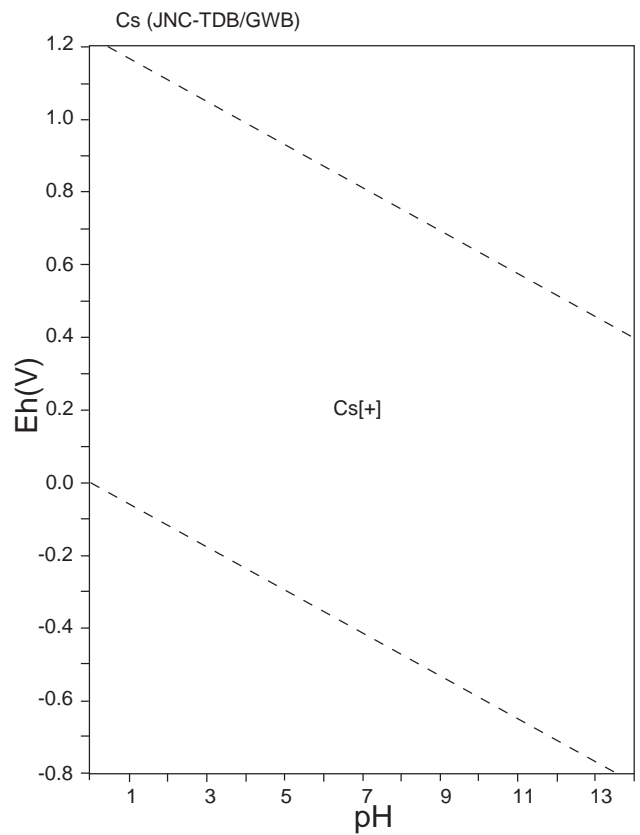
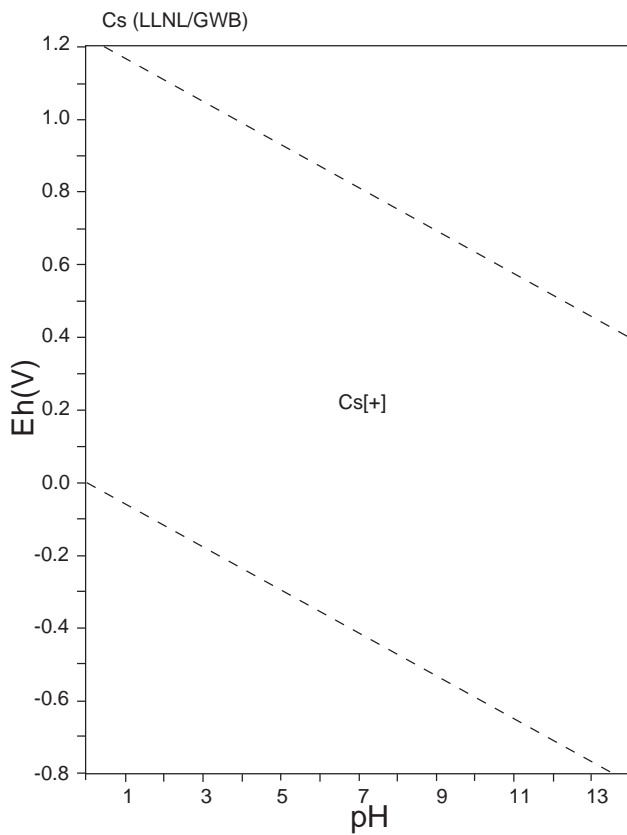
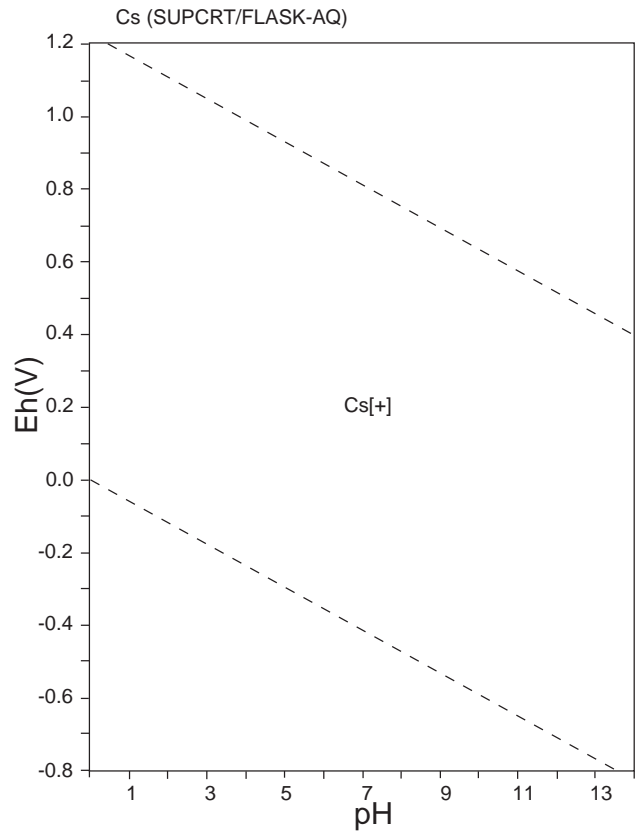
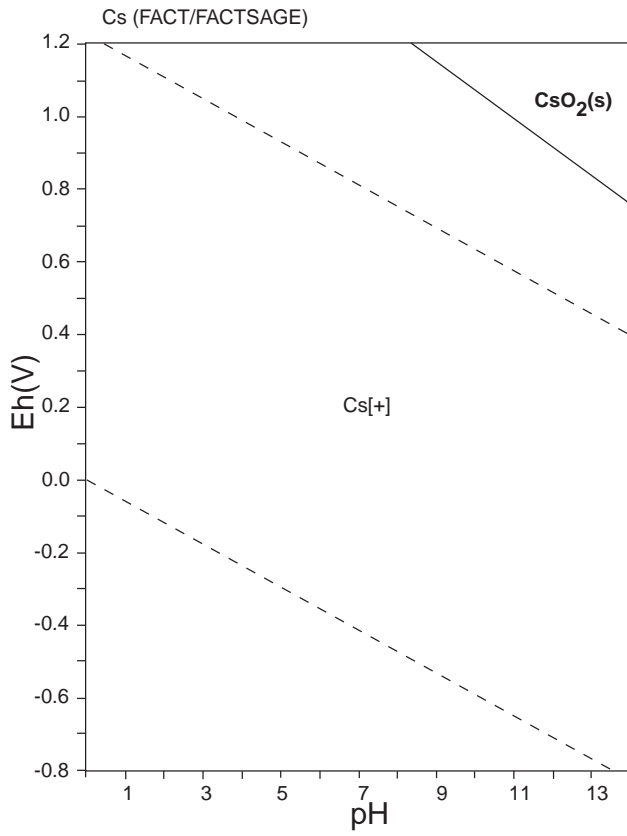
☒ 36: Eh-pH diagrams of the system Cr-O-H (2).  $\sum \text{Cr} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



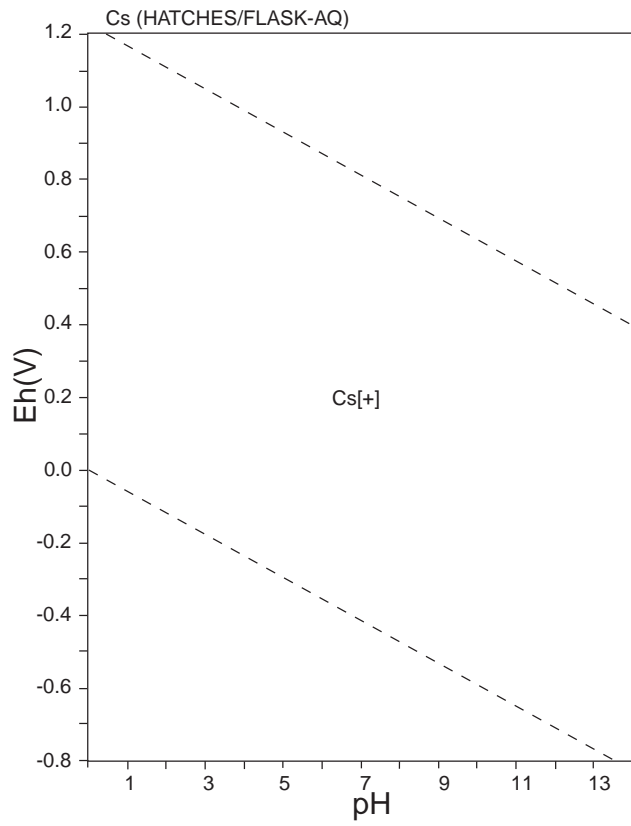
表 22: List of Cs species

FACT	SUPCRT	LLNL	JNC-TDB
Cs[+], Cs(s), CsO <sub>2</sub> (s), Cs <sub>2</sub> O(s), Cs <sub>2</sub> O <sub>3</sub> (s), CsOH(s), CsOH(s2), CsOH(s3)	Cs[+], CsOH(aq)	Cs[+]	Cs[+], Cs(c), Cs <sub>2</sub> O(s), CsOH(s), Cs(g)

HATCHES			
Cs[+], CsO, CsOH			



☒ 37: Eh-pH diagrams of the system Cs-O-H (1).  $\sum Cs = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 38: Eh-pH diagrams of the system Cs-O-H (2).  $\sum Cs = 10^{-10}$ , 298.15K,  $10^5$  Pa.

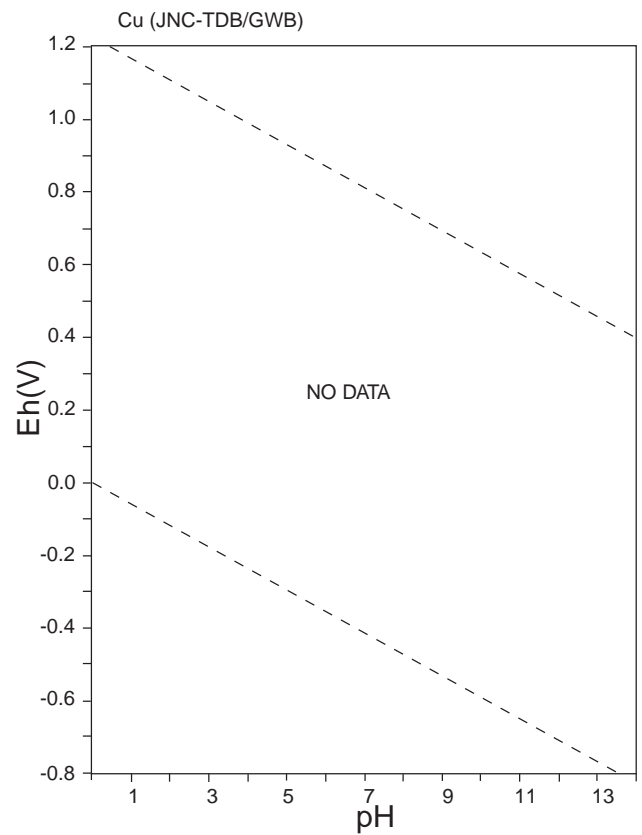
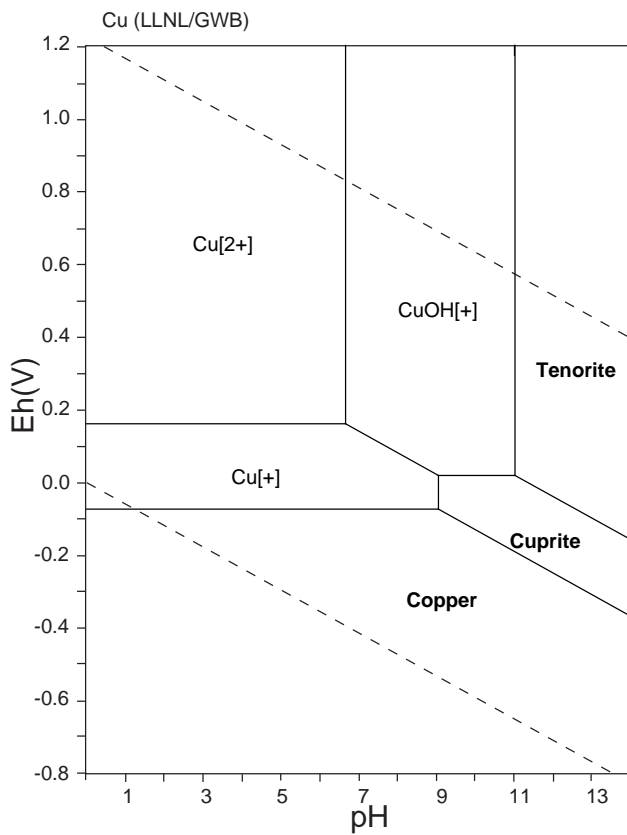
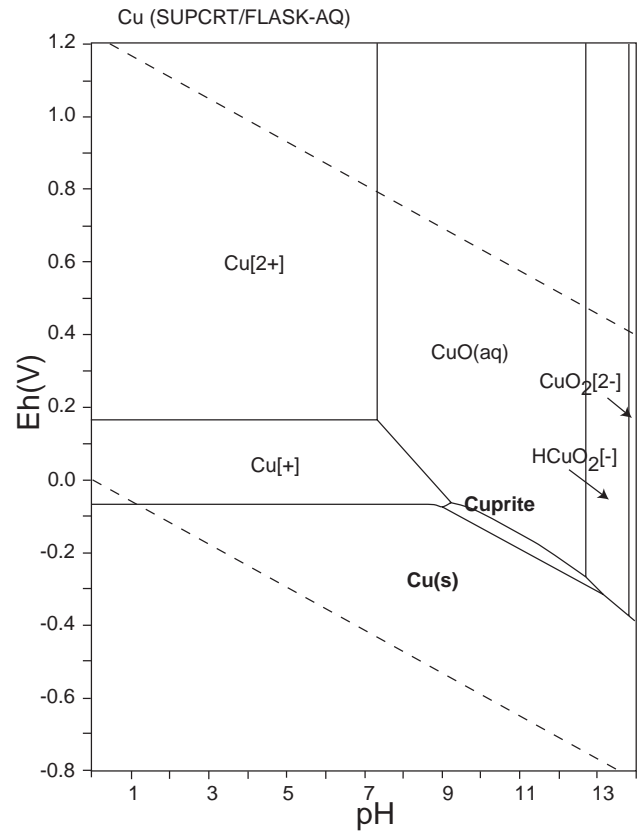
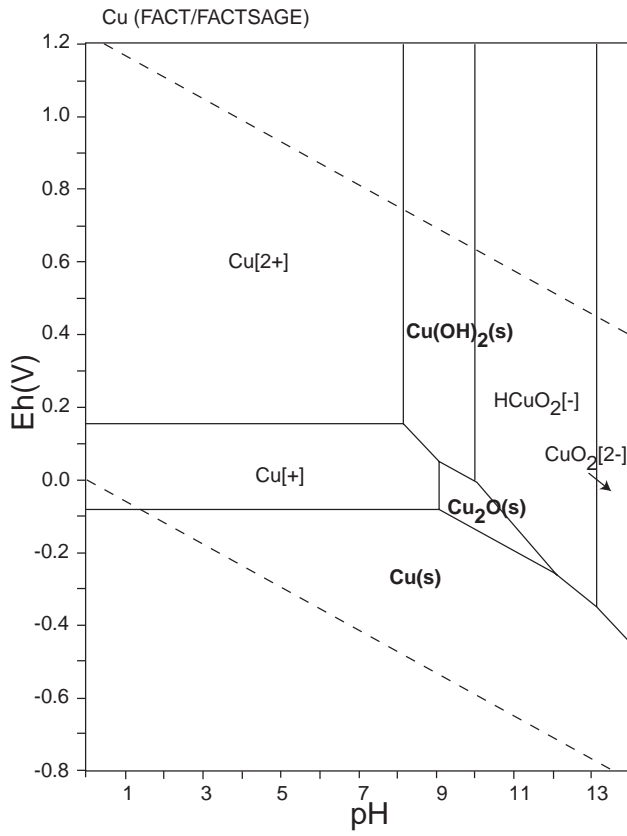




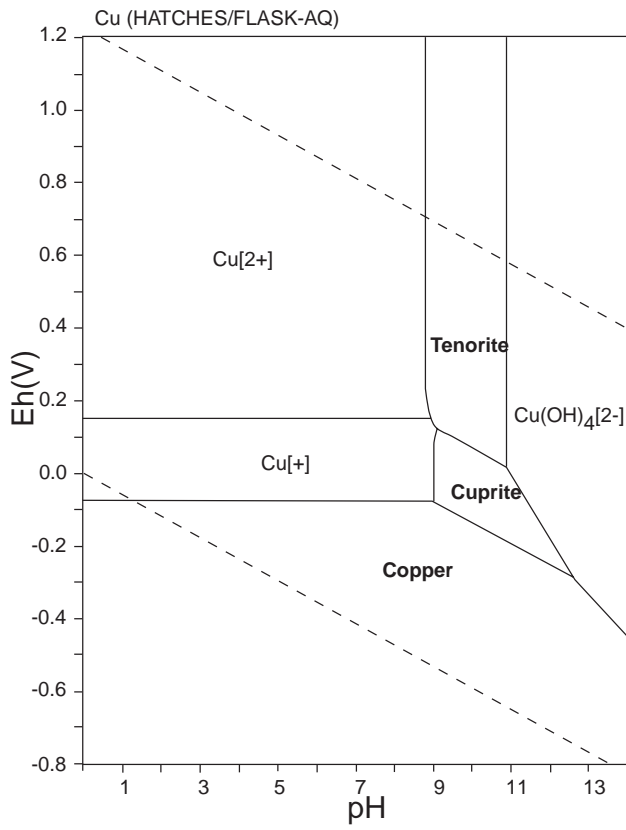
表 23: List of Cu species

FACT	SUPCRT	LLNL	JNC-TDB
Cu[+], Cu[2+], CuO <sub>2</sub> [2-], HCuO <sub>2</sub> [-], Cu(OH) <sub>2</sub> (s), Cu (s), CuO(s), Cu <sub>2</sub> O(s)	Cu[+], Cu[2+], CuO <sub>2</sub> [2-], HCuO <sub>2</sub> [-], CuOH[+], CuO(aq), Cu(Native Copper), CuO(Tenorite), Cu <sub>2</sub> O (Cuprite)	Cu[+], Cu[2+], CuOH[+], <b>Copper,</b> <b>Cuprite, Tenorite</b>	

HATCHES			
Cu[2+], Cu[+], Cu(OH) <sub>4</sub> [2-], Cu <sub>2</sub> (OH) <sub>2</sub> [2+], <b>Copper, Cuprite,</b> <b>Tenorite</b>			



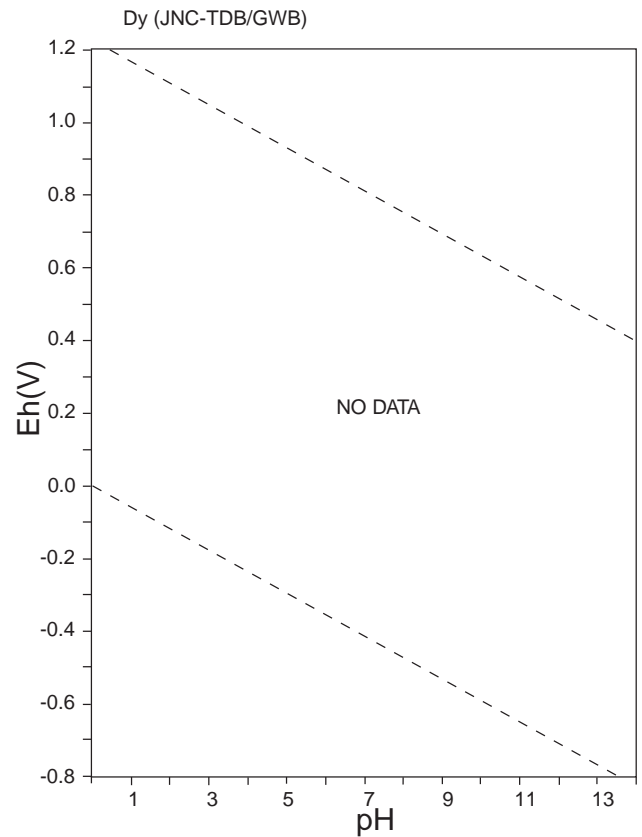
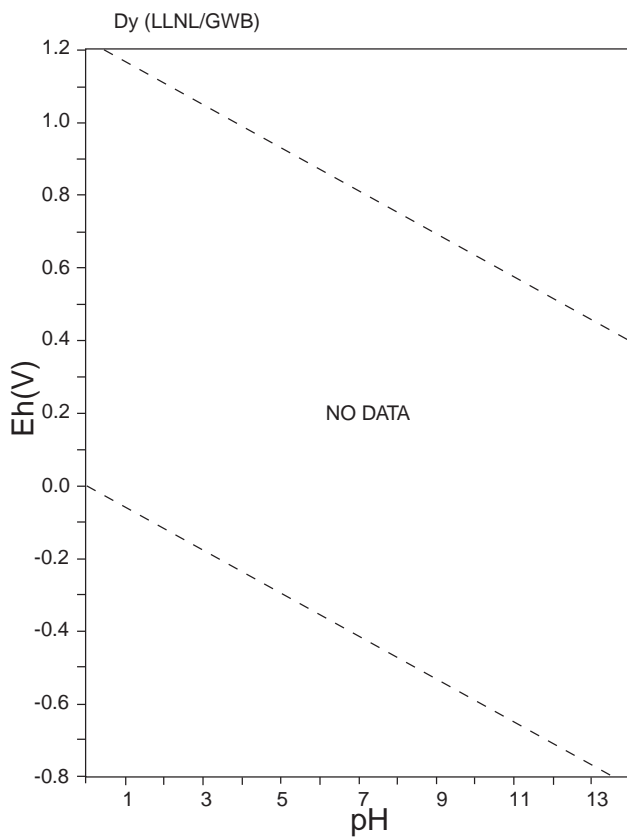
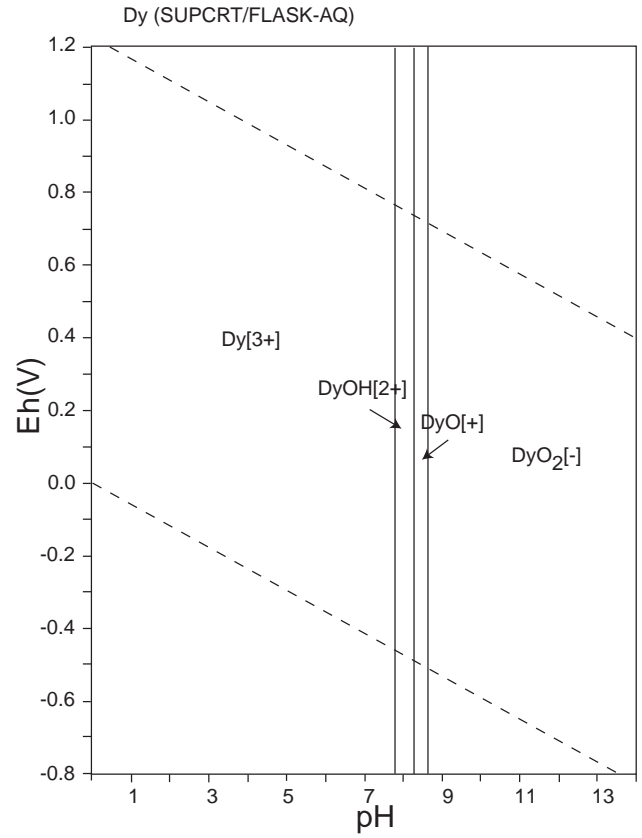
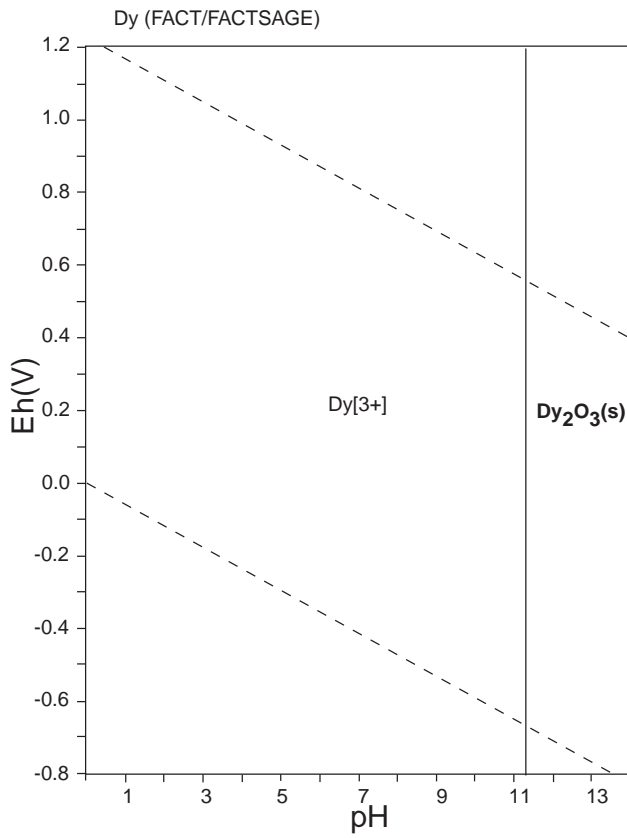
☒ 39: Eh-pH diagrams of the system Cu-O-H (1).  $\sum \text{Cu} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 40: Eh-pH diagrams of the system Cu-O-H (2).  $\sum \text{Cu} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 24: List of Dy species

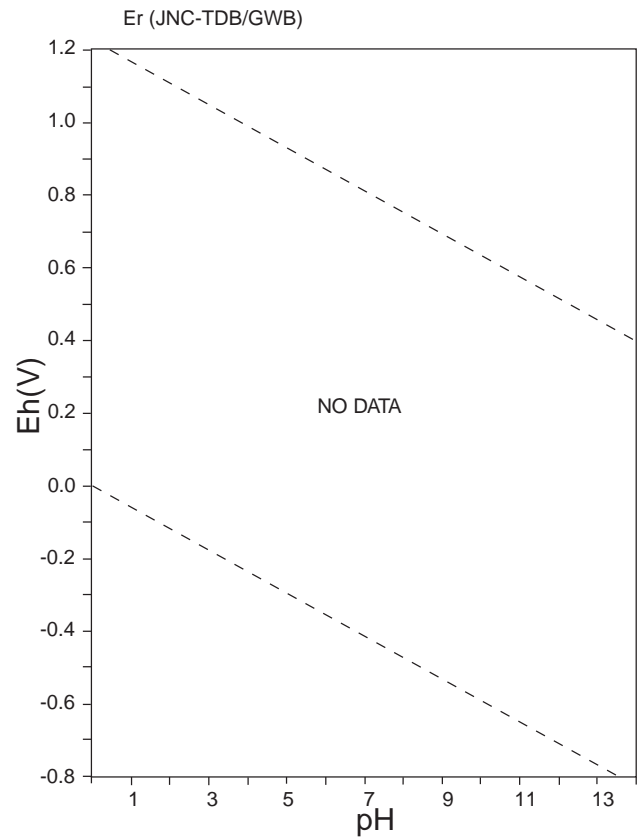
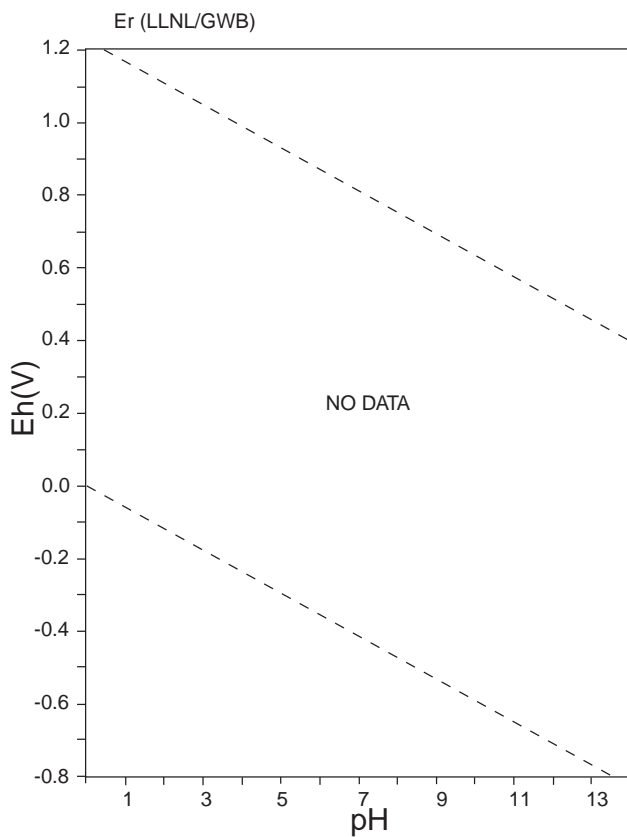
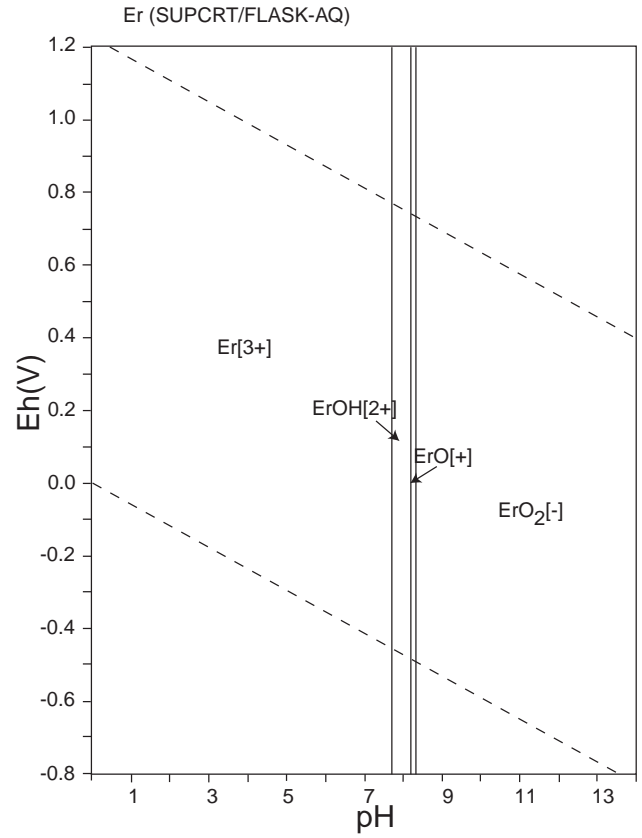
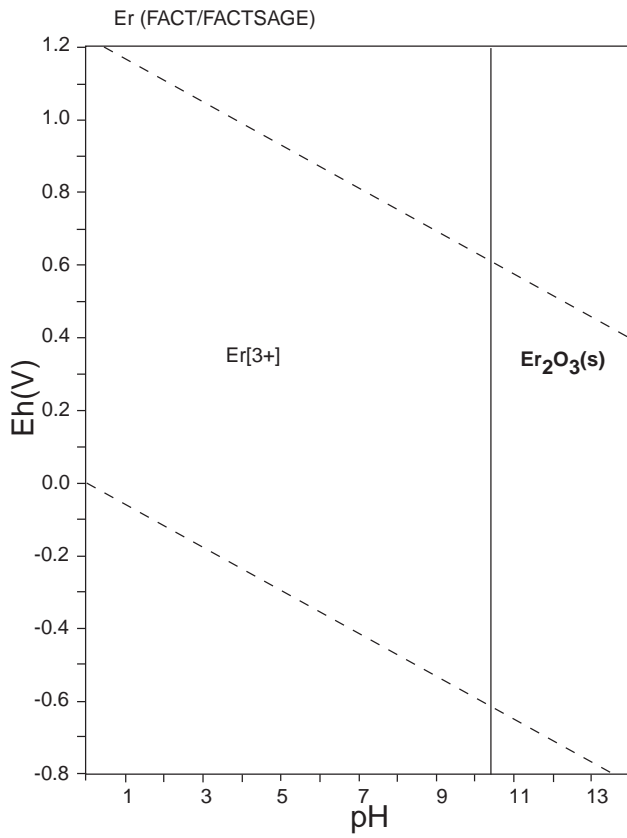
FACT	SUPCRT	LLNL	JNC-TDB
$\text{Dy}^{3+}$ , $\text{Dy}(\text{s})$ , $\text{Dy}(\text{s}_2)$ , $\text{Dy}_2\text{O}_3(\text{s})$	$\text{Dy}^{3+}$ , $\text{Dy}^{2+}$ , $\text{Dy}^{4+}$ , $\text{DyOH}^{2+}$ , $\text{DyO}^{+}$ , $\text{DyO}_2\text{H}(\text{aq})$ , $\text{DyO}_2^{-}$		



☒ 41: Eh-pH diagrams of the system Dy-O-H.  $\sum \text{Dy} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 25: List of Er species

FACT	SUPCRT	LLNL	JNC-TDB
Er[3+], <b>Er(s)</b> , <b>Er<sub>2</sub>O<sub>3</sub>(s)</b> , <b>Er<sub>2</sub>O<sub>3</sub>(s2)</b>	Er[3+], Er[2+], Er[4+], ErOH[2+], ErO[+], ErO <sub>2</sub> H(aq), ErO <sub>2</sub> [-]		



☒ 42: Eh-pH diagrams of the system Er-O-H.  $\sum \text{Er} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





表 26: List of Eu species

FACT	SUPCRT	LLNL	JNC-TDB
Eu[2+], Eu[3+], <b>Eu(s), EuH<sub>2</sub>(s),</b> <b>EuO(s), Eu<sub>2</sub>O<sub>3</sub>(s),</b> <b>Eu<sub>2</sub>O<sub>3</sub>(s2), Eu<sub>3</sub>O<sub>4</sub>(s),</b> <b>Eu<sub>3</sub>H<sub>3</sub>(s)</b>	Eu[2+], Eu[3+], Eu[4+], EuOH[2+], EuO[+], EuO <sub>2</sub> H(aq), EuO <sub>2</sub> [-]	Eu[3+], Eu[2+], Eu(OH) <sub>2</sub> [+], EuOH[2+], <b>Eu(s),</b> <b>Eu(OH)<sub>3</sub>(s),</b> <b>Eu<sub>2</sub>O<sub>3</sub>(cubic),</b> <b>Eu<sub>2</sub>O<sub>3</sub>(monoclinic),</b> <b>Eu<sub>3</sub>O<sub>4</sub>(s), EuO(s)</b>	

HATCHES			
Eu[3+], Eu(OH)[2+], <b>Eu, Eu(OH)<sub>3</sub>,</b> <b>Eu<sub>2</sub>O<sub>3</sub>(cubic),</b> <b>Eu<sub>2</sub>O<sub>3</sub>(monoclinic),</b> <b>Eu<sub>3</sub>O<sub>4</sub>, EuO</b>			

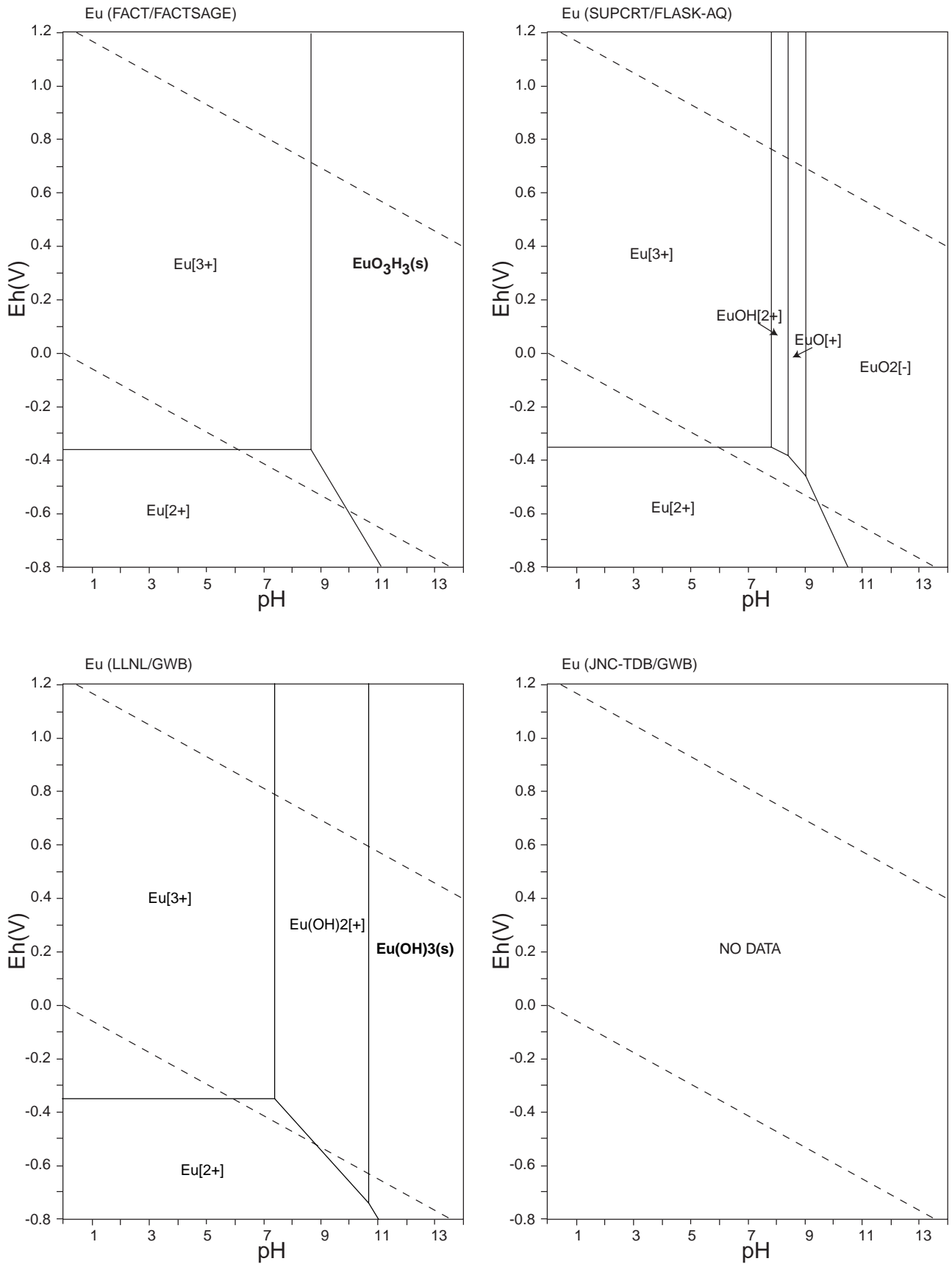


图 43: Eh-pH diagrams of the system Eu-O-H (1).  $\sum \text{Eu} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

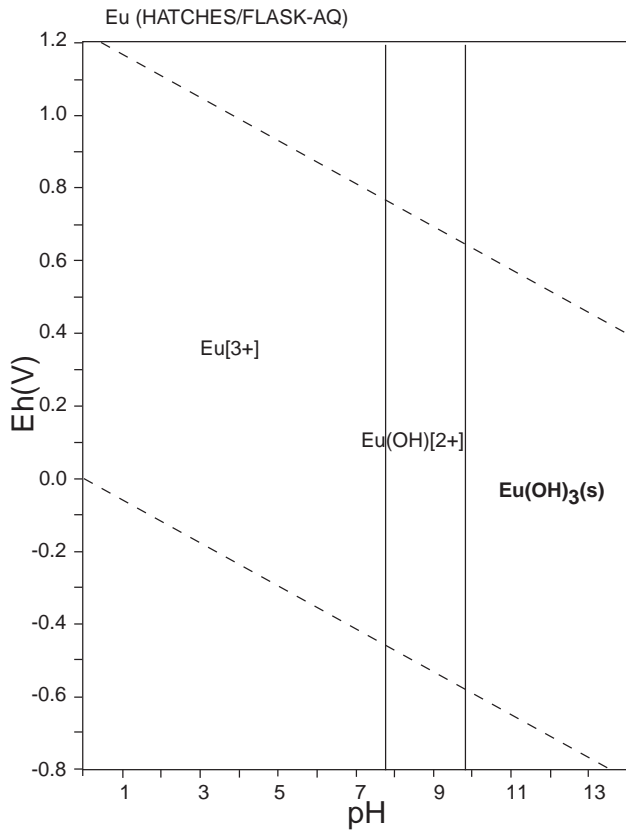


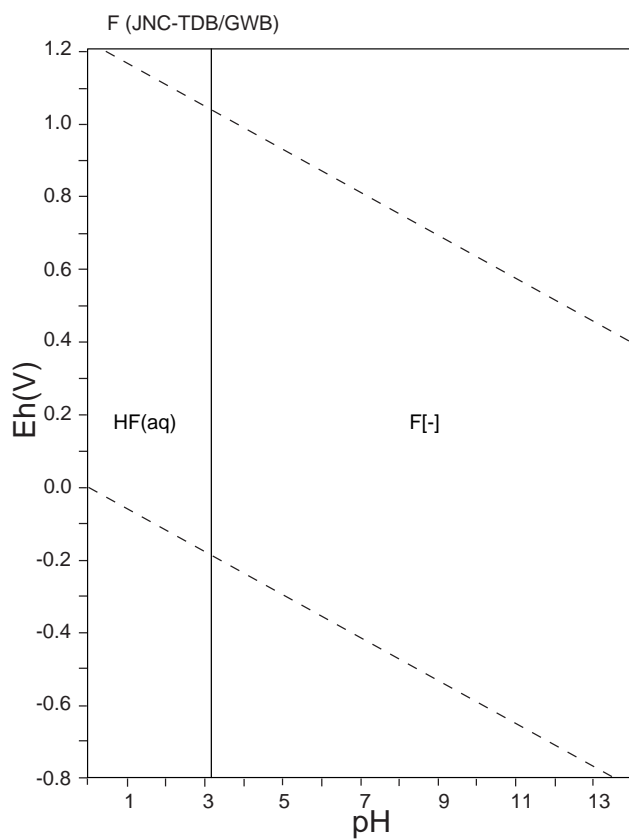
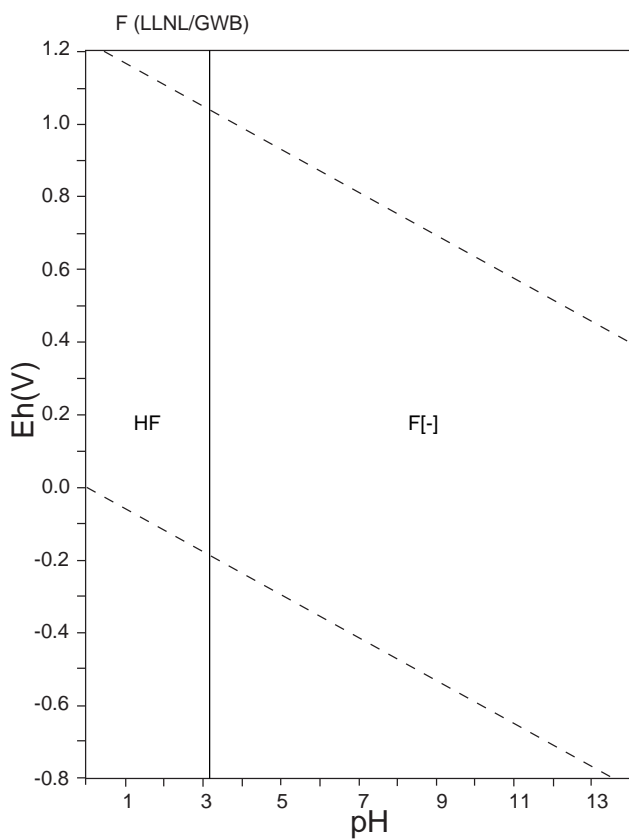
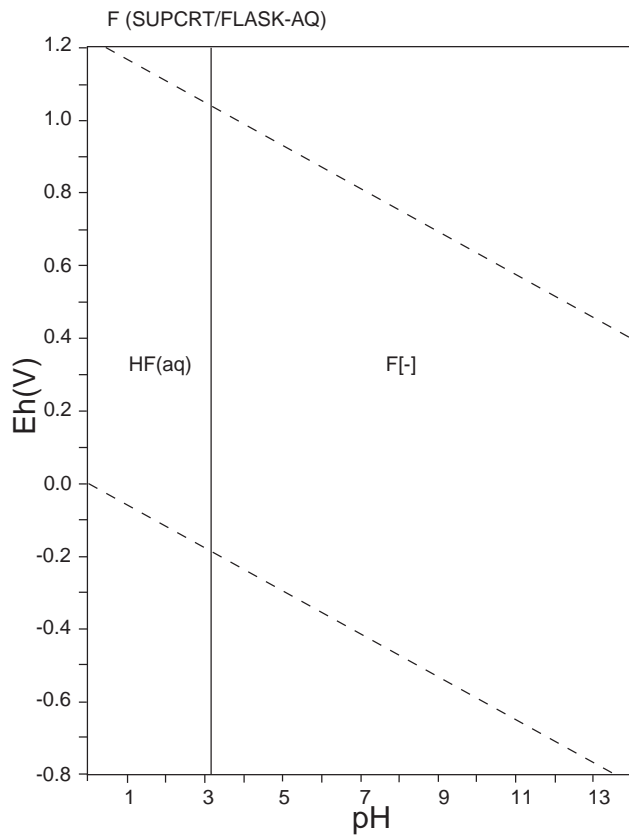
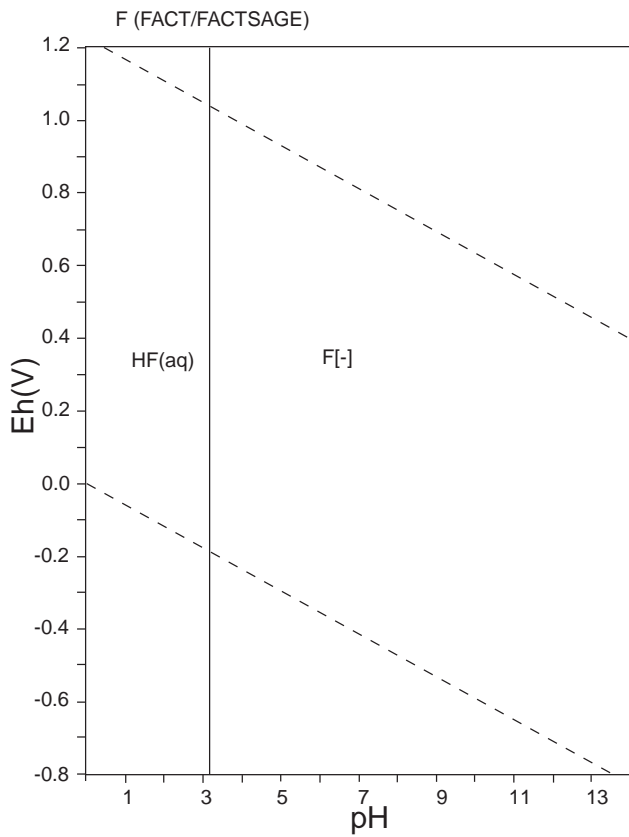
图 44: Eh-pH diagrams of the system Eu-O-H (2).  $\sum \text{Eu} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



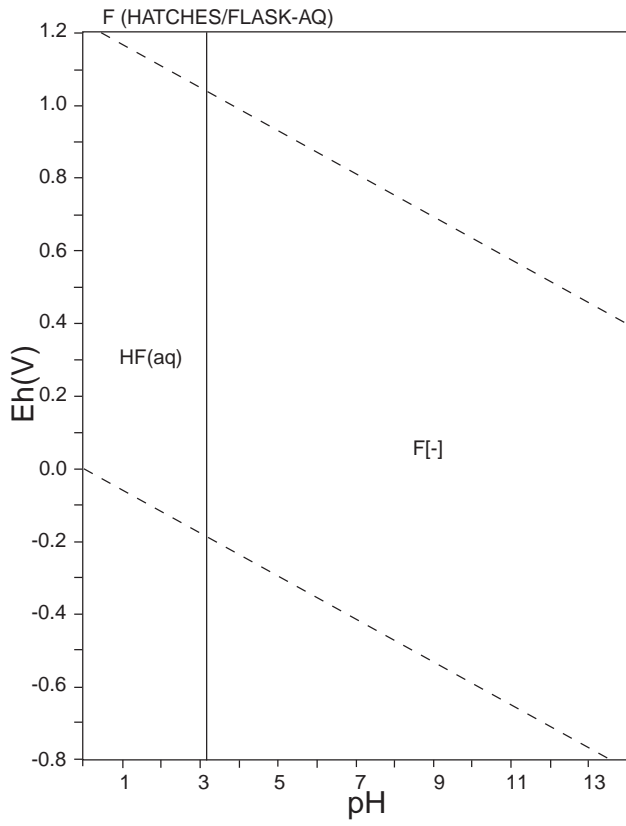
表 27: List of F species

FACT	SUPCRT	LLNL	JNC-TDB
F[-], HF(aq), HF <sub>2</sub> [-]	F[-], HF(aq), HF <sub>2</sub> [-]	F[-], H <sub>2</sub> F <sub>2</sub> , HF, HF <sub>2</sub> [-]	F-, HF(aq), HF <sub>2</sub> [-], F(g), F <sub>2</sub> (g), HF(g)

HATCHES			
F[-], HF(aq), HF <sub>2</sub> [-]			



☒ 45: Eh-pH diagrams of the system F-O-H (1).  $\sum F = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 46: Eh-pH diagrams of the system F-O-H (2).  $\sum F = 10^{-10}$ , 298.15K,  $10^5$  Pa.

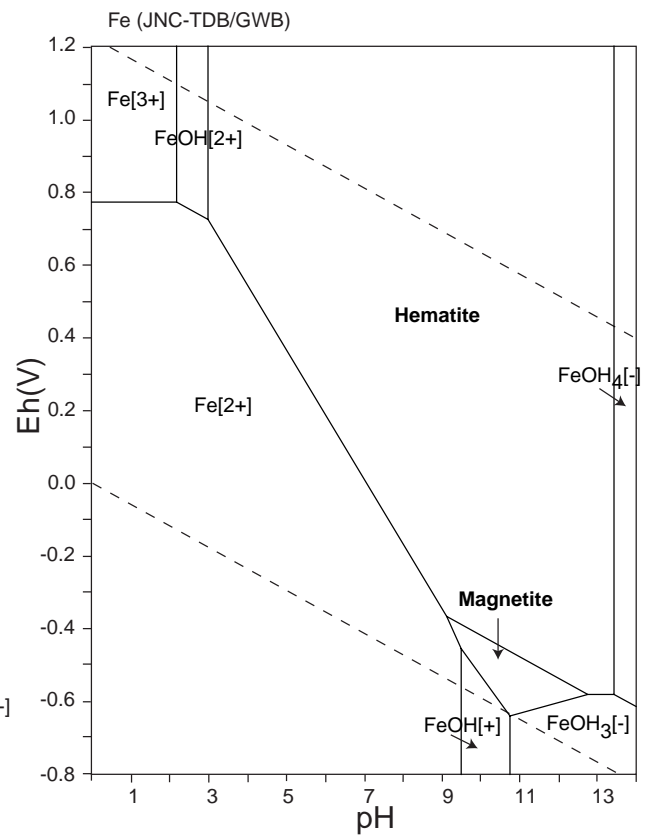
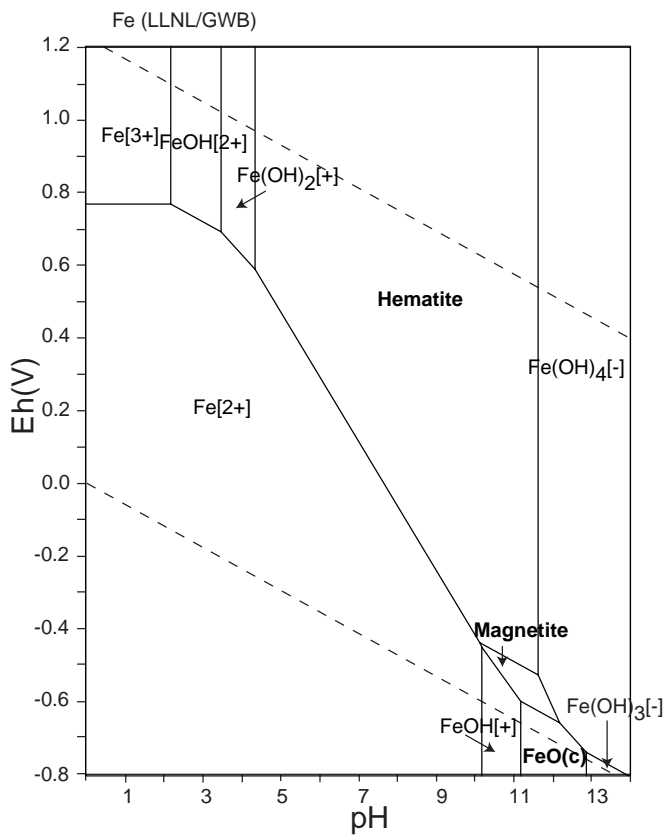
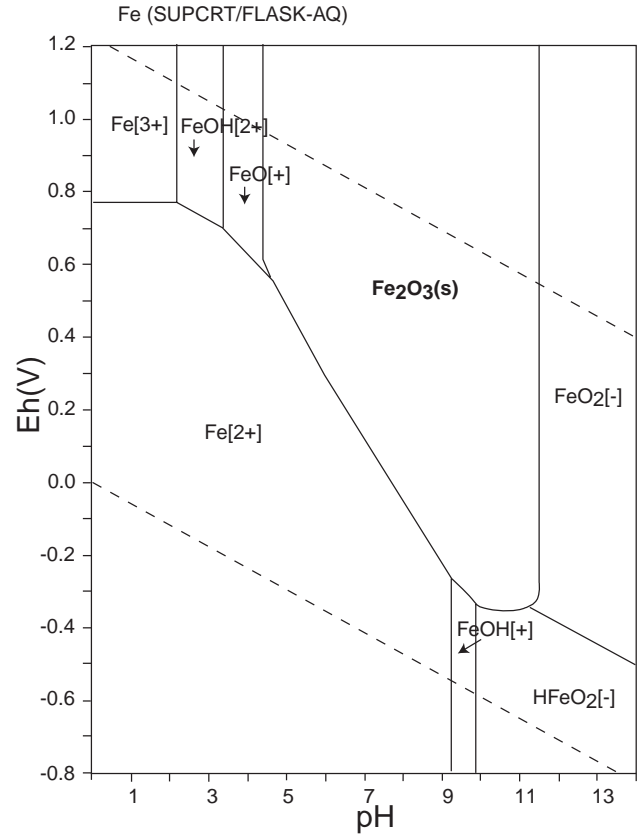
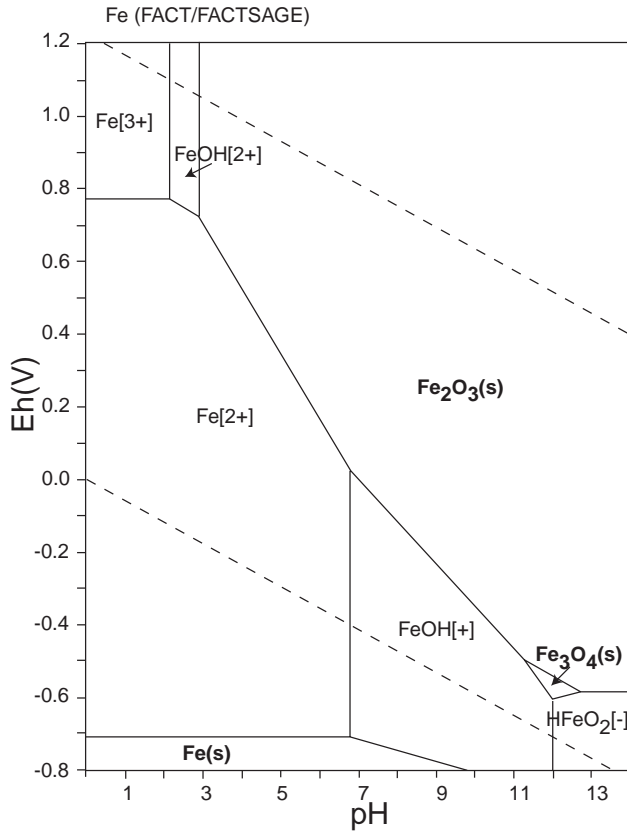




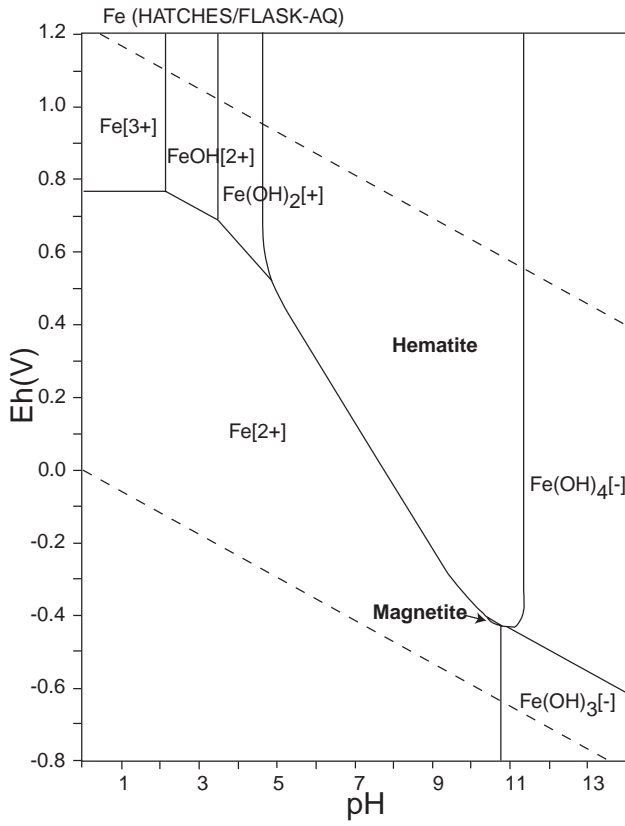
表 28: List of Fe species

FACT	SUPCRT	LLNL	JNC-TDB
Fe[2+], Fe[3+], FeOH[+], FeOH[2+], HFeO <sub>2</sub> [-], Fe(OH) <sub>2</sub> [+], FeO <sub>2</sub> [2-], Fe(OH) <sub>3</sub> (aq), Fe <sub>2</sub> (OH) <sub>2</sub> [4+], <b>Fe(s), Fe(s2),</b> <b>Fe<sub>2</sub>O<sub>3</sub>(s2),</b> <b>Fe<sub>2</sub>O<sub>3</sub>(s3),</b> <b>Fe<sub>3</sub>O<sub>4</sub>(s2),</b> <b>Fe<sub>3</sub>O<sub>4</sub>(s3),</b> <b>Fe<sub>3</sub>O<sub>4</sub>(s4),</b> <b>Fe(OH)<sub>2</sub>(s),</b> <b>Fe(OH)<sub>3</sub>(s),</b> <b>Fe<sub>2</sub>O<sub>3</sub>(H<sub>2</sub>O)(s), FeO</b> <b>(s), Fe<sub>2</sub>O<sub>3</sub>(s),</b> <b>Fe<sub>3</sub>O<sub>4</sub>(s)</b>	HFeO <sub>2</sub> (aq), FeO <sub>2</sub> [-], FeO(aq), Fe[2+], Fe[3+], FeOH[+], FeOH[2+], HFeO <sub>2</sub> [-], FeO[+], <b>FeO</b> <b>(Ferrous-oxide),</b> <b>Fe<sub>2</sub>O<sub>3</sub>(Hematite),</b> <b>Fe<sub>3</sub>O<sub>4</sub>(Magnetite)</b>	Fe[2+], Fe[3+], Fe(OH) <sub>2</sub> (aq), Fe(OH) <sub>2</sub> [+], Fe(OH) <sub>3</sub> (aq), Fe(OH) <sub>3</sub> [-], Fe(OH) <sub>4</sub> [-], Fe <sub>2</sub> (OH) <sub>2</sub> [4+], Fe <sub>3</sub> (OH) <sub>4</sub> [5+], FeOH[+], FeOH[2+], <b>Fe(OH)<sub>2</sub>(ppd),</b> <b>Fe(OH)<sub>3</sub>(ppd),</b> <b>FeO(c)</b> Goethite, Hematite, Magnetite, Wustite	Fe[2+], Fe[3+], FeOH[2+], Fe(OH) <sub>2</sub> [+], Fe(OH) <sub>3</sub> (aq), FeOH <sub>4</sub> [-], Fe <sub>2</sub> (OH) <sub>2</sub> [4+], Fe <sub>3</sub> (OH) <sub>4</sub> [5+], FeOH[+], Fe(OH) <sub>2</sub> (aq), Fe(OH) <sub>3</sub> [-], <b>Fe(OH)<sub>3</sub>(a)</b> Hematite, Magnetite, Goethite

HATCHES			
Fe[2+], Fe[3+], Fe(OH)[+], Fe(OH) <sub>2</sub> (aq), Fe(OH) <sub>2</sub> [+], Fe(OH) <sub>3</sub> (aq), Fe(OH) <sub>3</sub> [-], Fe(OH) <sub>4</sub> [-], Fe(OH) <sub>4</sub> [2-], Fe <sub>2</sub> (OH) <sub>2</sub> [4+], Fe <sub>3</sub> (OH) <sub>4</sub> [5+], FeOH[2+], <b>Fe(OH)<sub>2</sub>,</b> <b>Fe(OH)<sub>3</sub>, FeO(c),</b> Goethite, Hematite, Magnetite, Wustite			



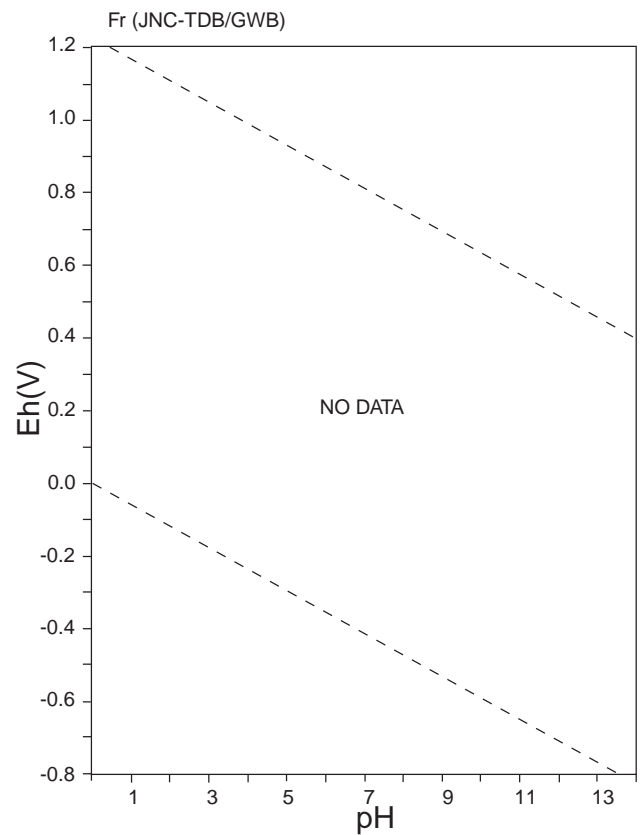
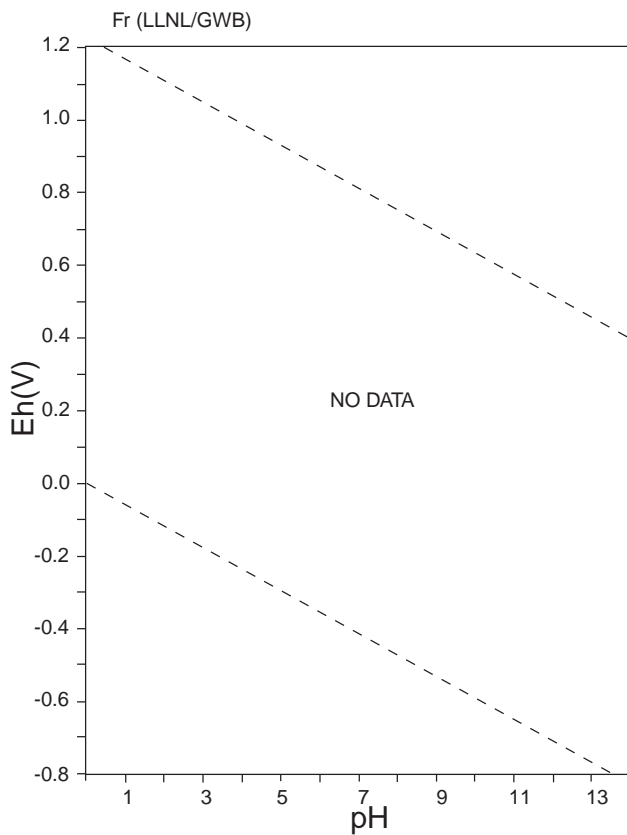
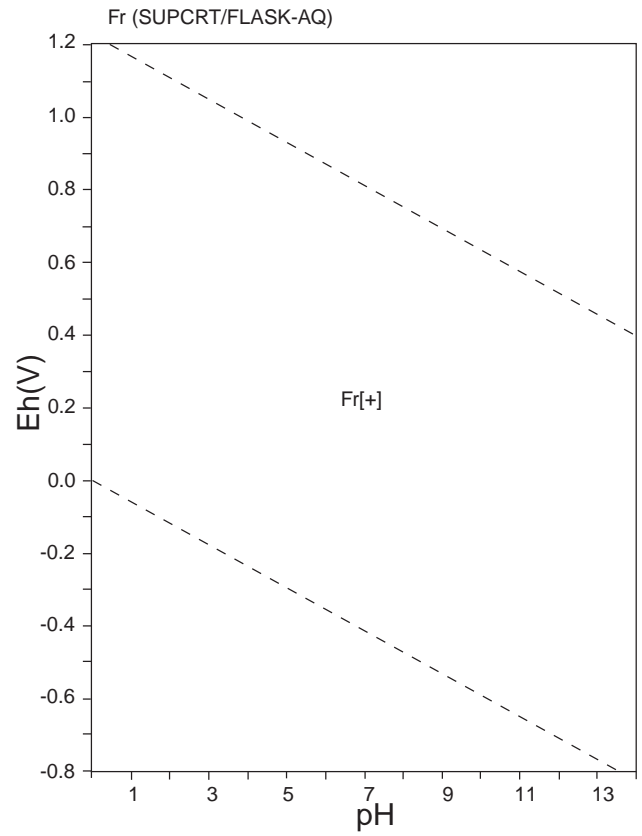
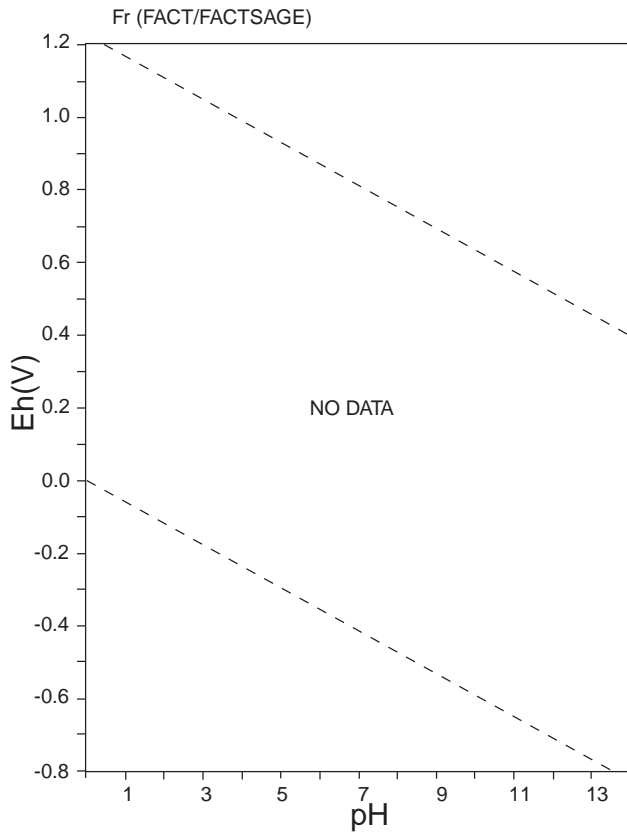
☒ 47: Eh-pH diagrams of the system Fe-O-H (1).  $\Sigma \text{Fe} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 48: Eh-pH diagrams of the system Fe-O-H (2).  $\sum \text{Fe} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 29: List of Fr species

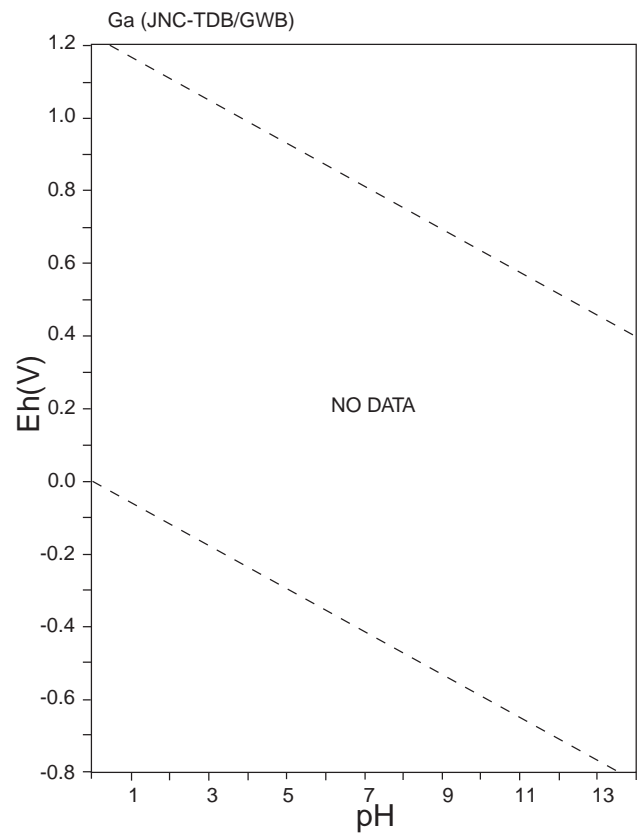
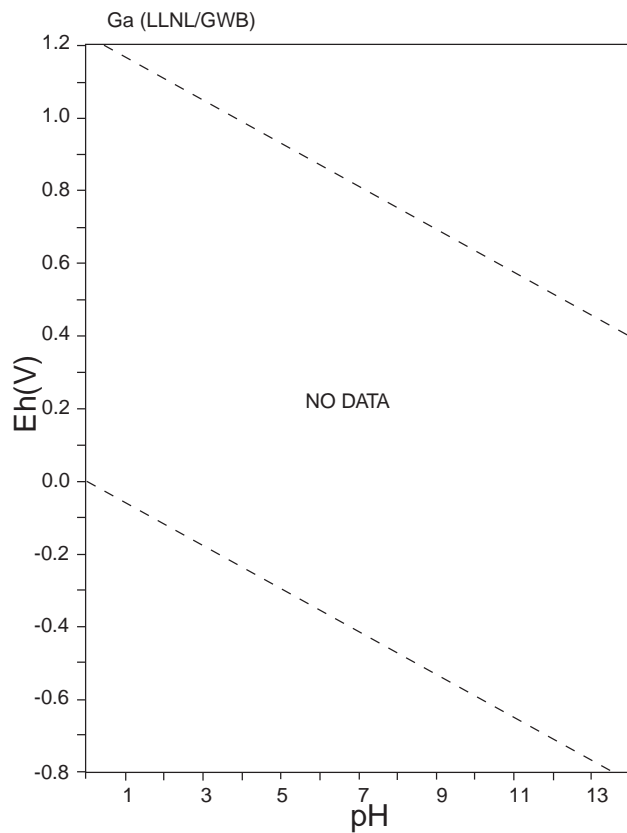
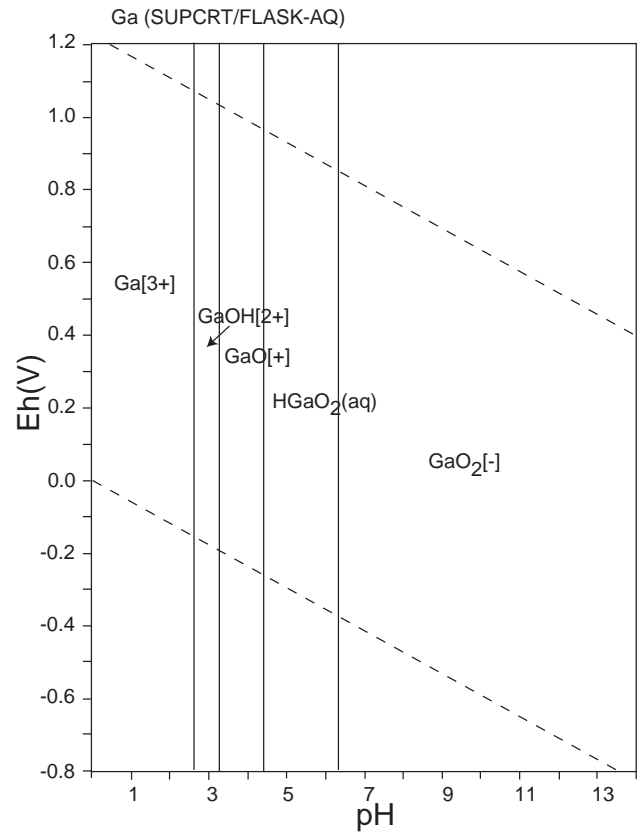
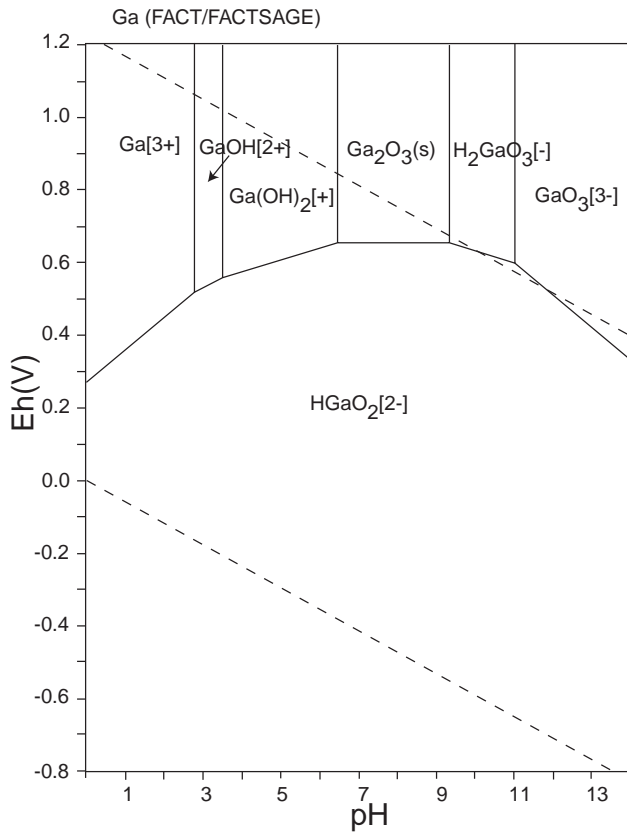
FACT	SUPCRT	LLNL	JNC-TDB
	Fr [ + ]		



☒ 49: Eh-pH diagrams of the system Fr-O-H.  $\sum \text{Fr} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 30: List of Ga species

FACT	SUPCRT	LLNL	JNC-TDB
Ga[3+], GaOH[2+], Ga(OH) <sub>2</sub> [+], H <sub>2</sub> GaO <sub>3</sub> [-], Ga[2+], GaO <sub>3</sub> [3-], HGaO <sub>2</sub> [2-], <b>Ga(s)</b> , <b>Ga<sub>2</sub>O<sub>3</sub>(s)</b> , <b>Ga(OH)<sub>3</sub>(s)</b>	Ga[3+], GaOH[2+], GaO[+], GaO <sub>2</sub> [-], HGaO <sub>2</sub> (aq)		

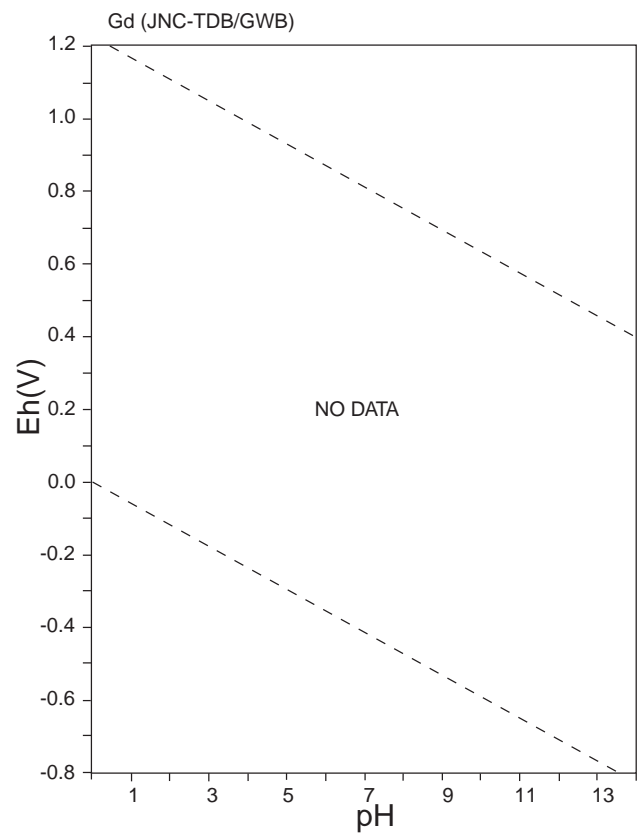
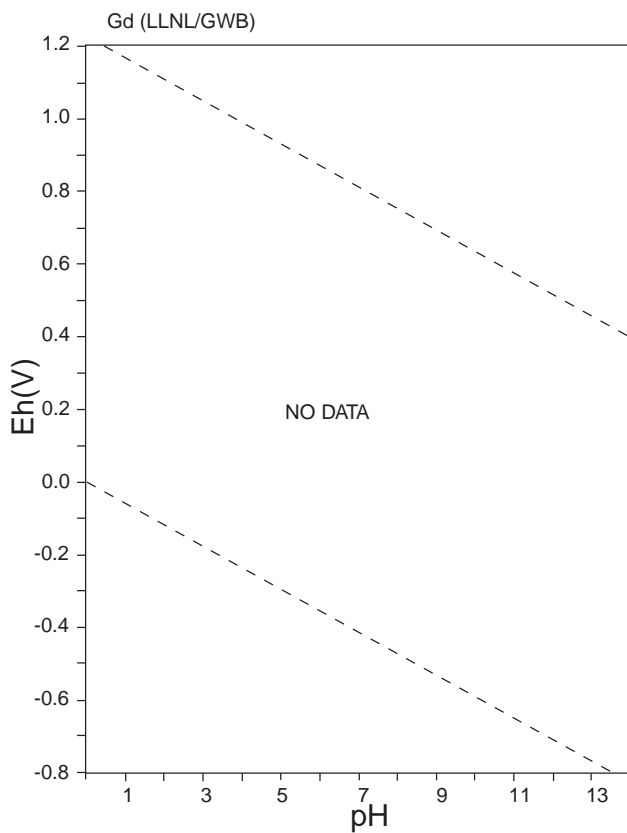
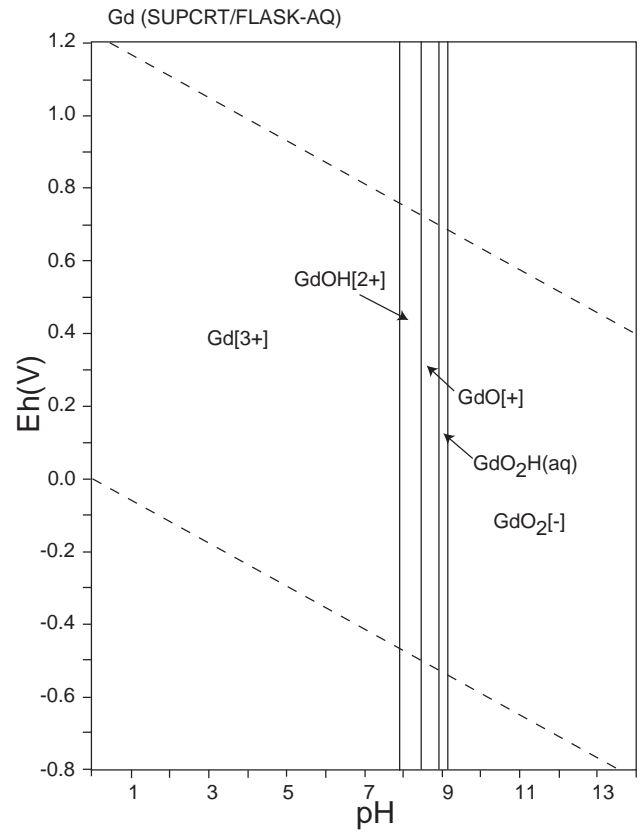
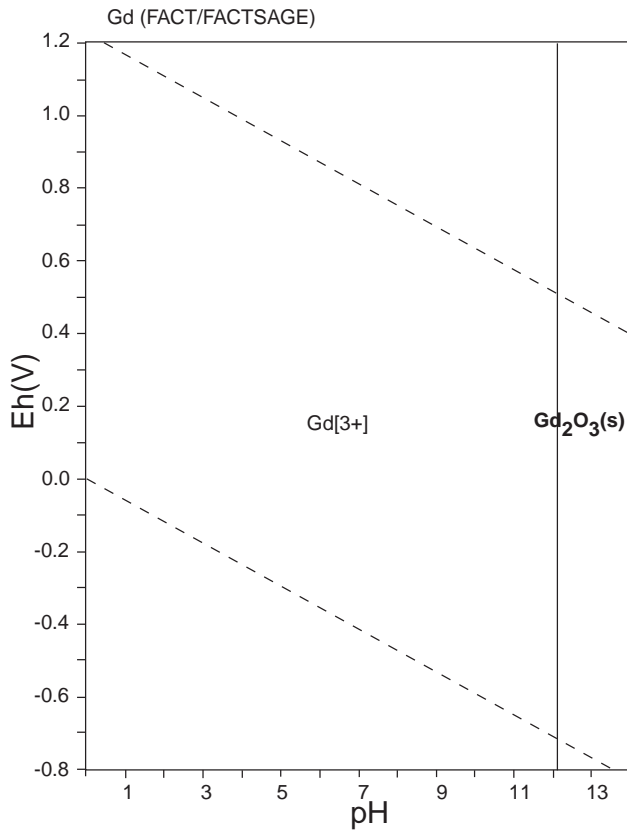


☒ 50: Eh-pH diagrams of the system Ga-O-H.  $\sum \text{Ga} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 31: List of Gd species

FACT	SUPCRT	LLNL	JNC-TDB
Gd[3+], <b>Gd(s)</b> , <b>Gd(s2)</b> , <b>Gd<sub>2</sub>O<sub>3</sub>(s)</b>	Gd[3+], Gd[4+], Gd[2+], GdOH[2+], GdO[+], GdO <sub>2</sub> H(aq), GdO <sub>2</sub> [-]		

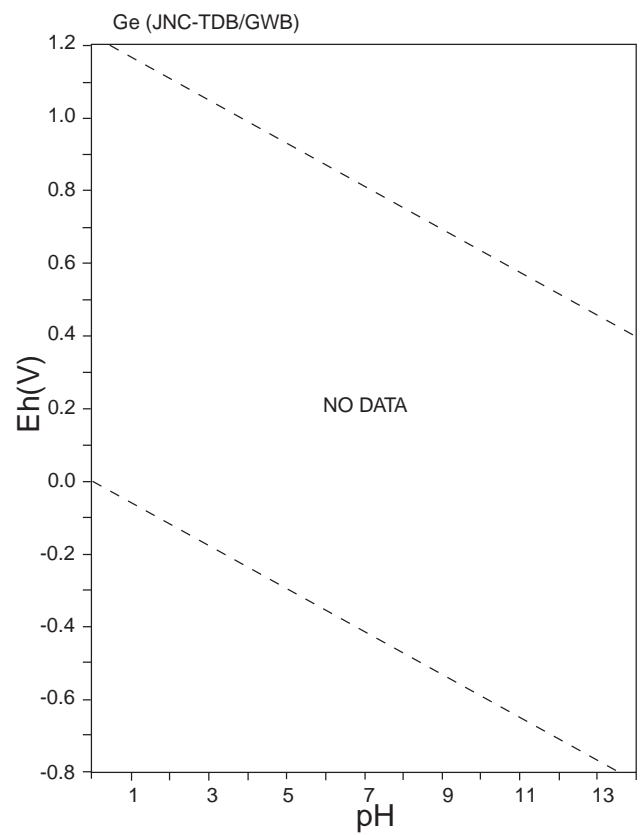
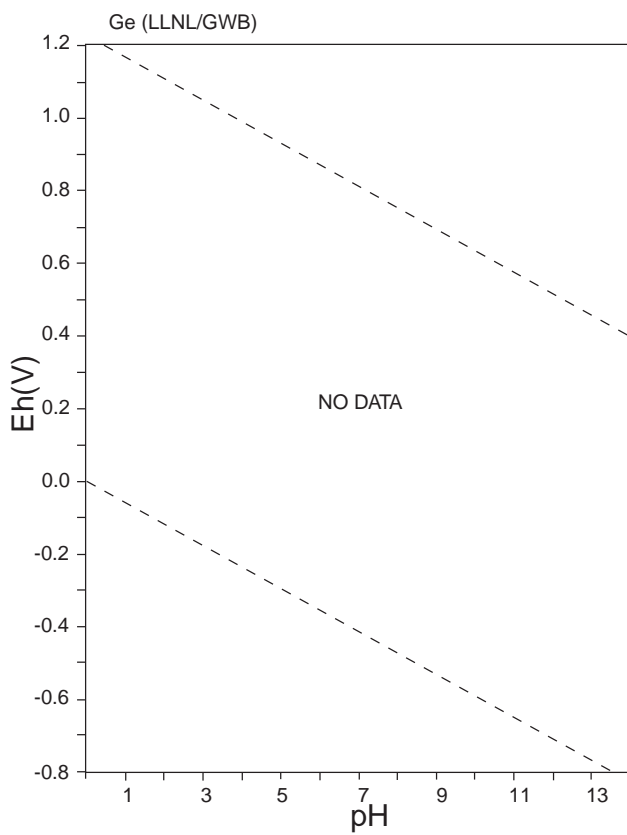
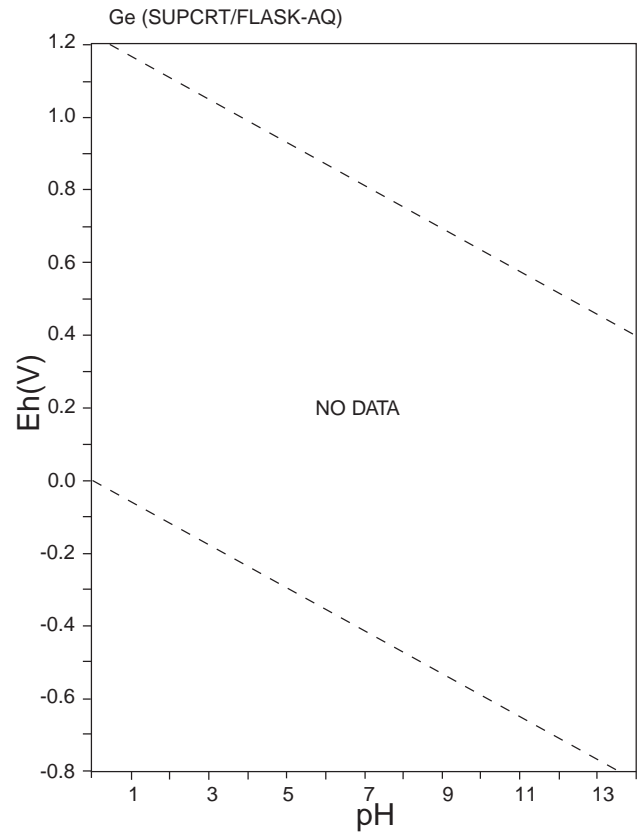
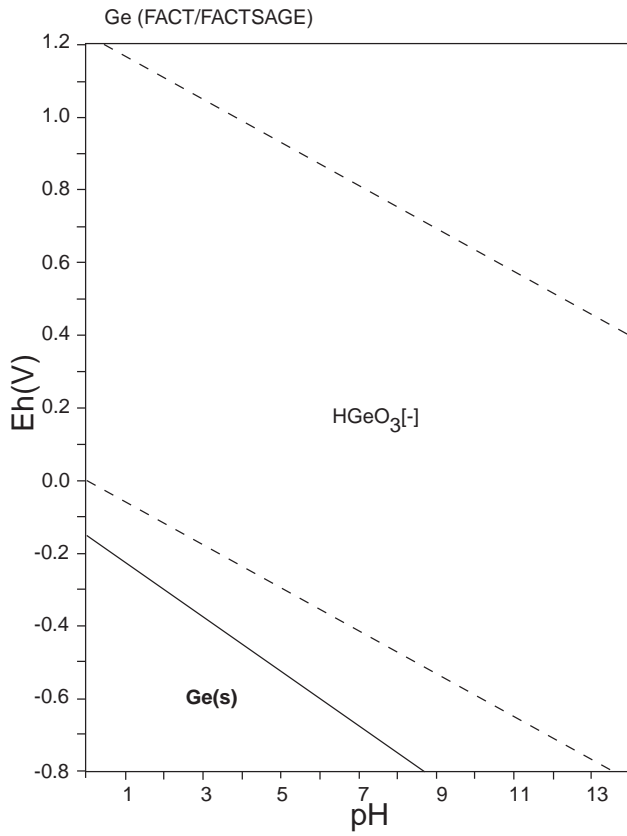




☒ 51: Eh-pH diagrams of the system Gd-O-H.  $\sum Gd = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 32: List of Ge species

FACT	SUPCRT	LLNL	JNC-TDB
$\text{HGeO}_3[-]$ , $\text{Ge}(\mathbf{s})$ , $\text{GeO}(\mathbf{s})$ , $\text{GeO}(\mathbf{s}2)$ , $\text{GeO}_2(\mathbf{s})$ , $\text{GeO}_2(\mathbf{s}2)$			



☒ 52: Eh-pH diagrams of the system Ge-O-H.  $\sum \text{Ge} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 33: List of Hf species

FACT	SUPCRT	LLNL	JNC-TDB
<b>Hf(s), Hf(s2), HfO<sub>2</sub>(s), HfO<sub>2</sub>(s2)</b>	Hf[4+], HfOH[3+], HfO[2+], HHfO <sub>2</sub> [+], HfO <sub>2</sub> (aq), HHfO <sub>3</sub> [-]		

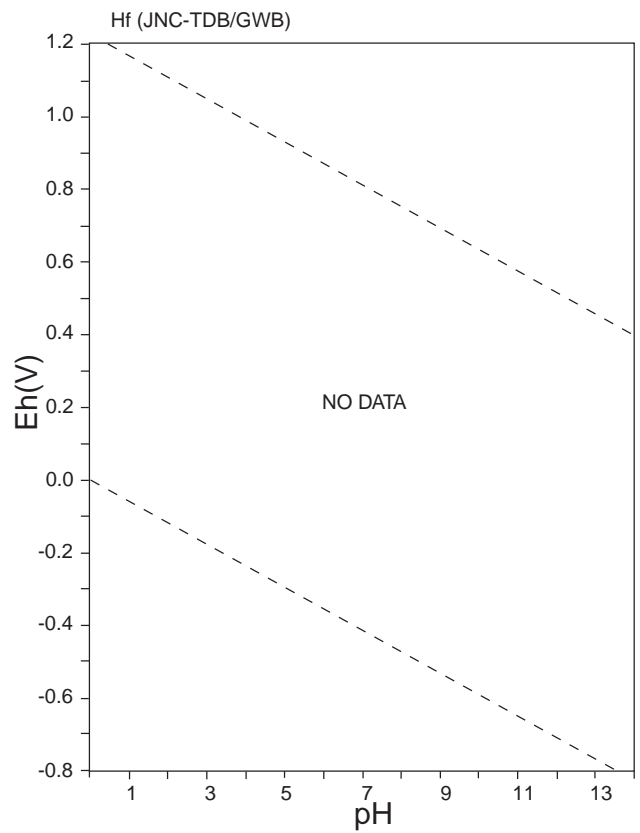
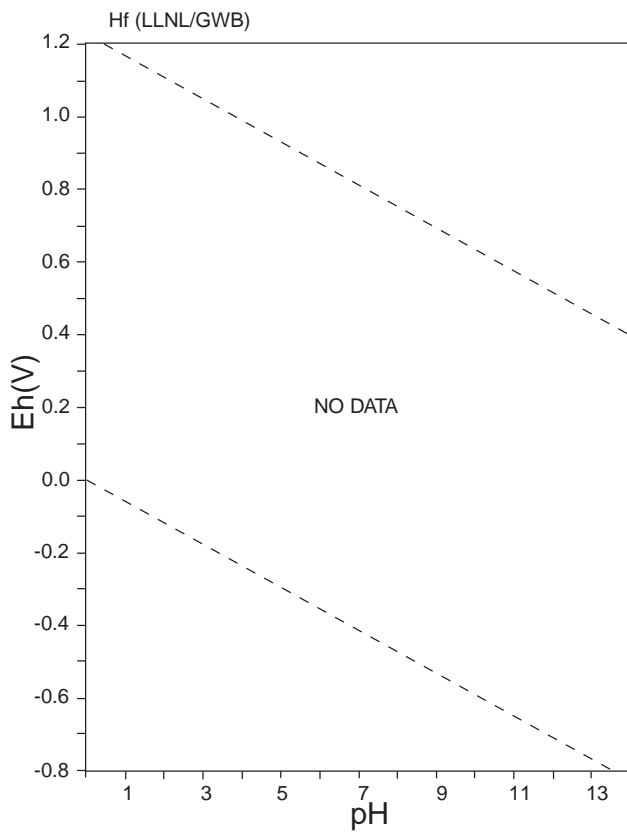
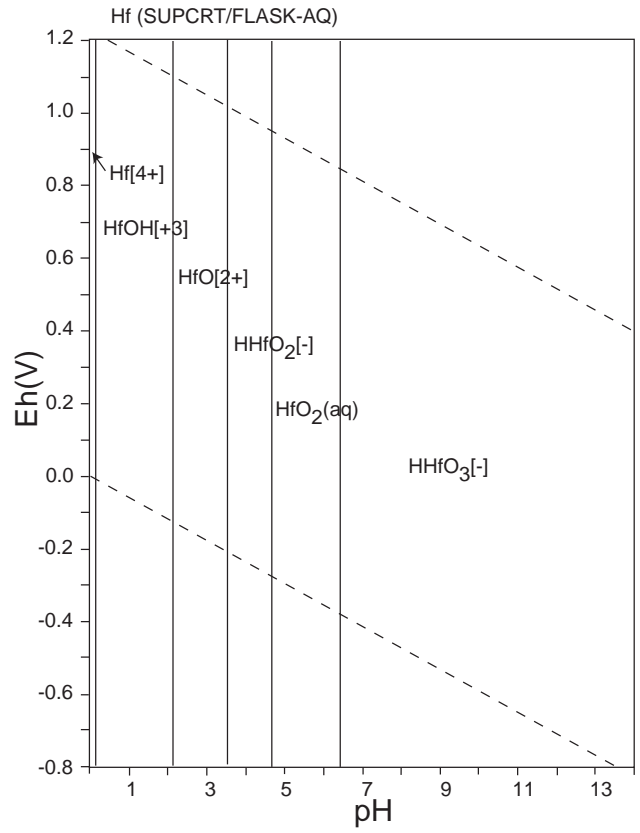
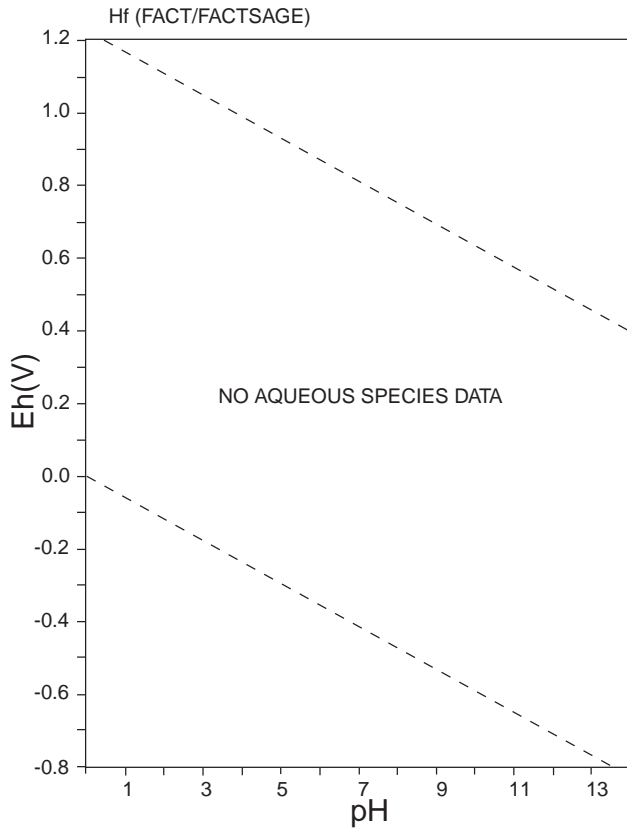


Figure 53: Eh-pH diagrams of the system Hf-O-H.  $\sum \text{Hf} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 34: List of Hg species

FACT	SUPCRT	LLNL	JNC-TDB
Hg[2+], Hg <sub>2</sub> [2+], HgOH[+], HHgO <sub>2</sub> [-], Hg(OH) <sub>2</sub> , Hg(aq), <b>HgO(s)</b>	Hg[2+], Hg <sub>2</sub> [2+], HgOH[+], HHgO <sub>2</sub> [-], HgO(aq), <b>Hg(Quicksilver)</b>	Hg[2+], Hg <sub>2</sub> [2+], <b>Quicksilver</b>	

HATCHES			
Hg[2+], Hg(OH) <sub>2</sub> (aq), Hg(OH) <sub>3</sub> [-], Hg <sub>2</sub> OH[3+], Hg <sub>3</sub> (OH) <sub>3</sub> [3+], HgOH[+], <b>HgO</b> , <b>Quicksilver</b>			

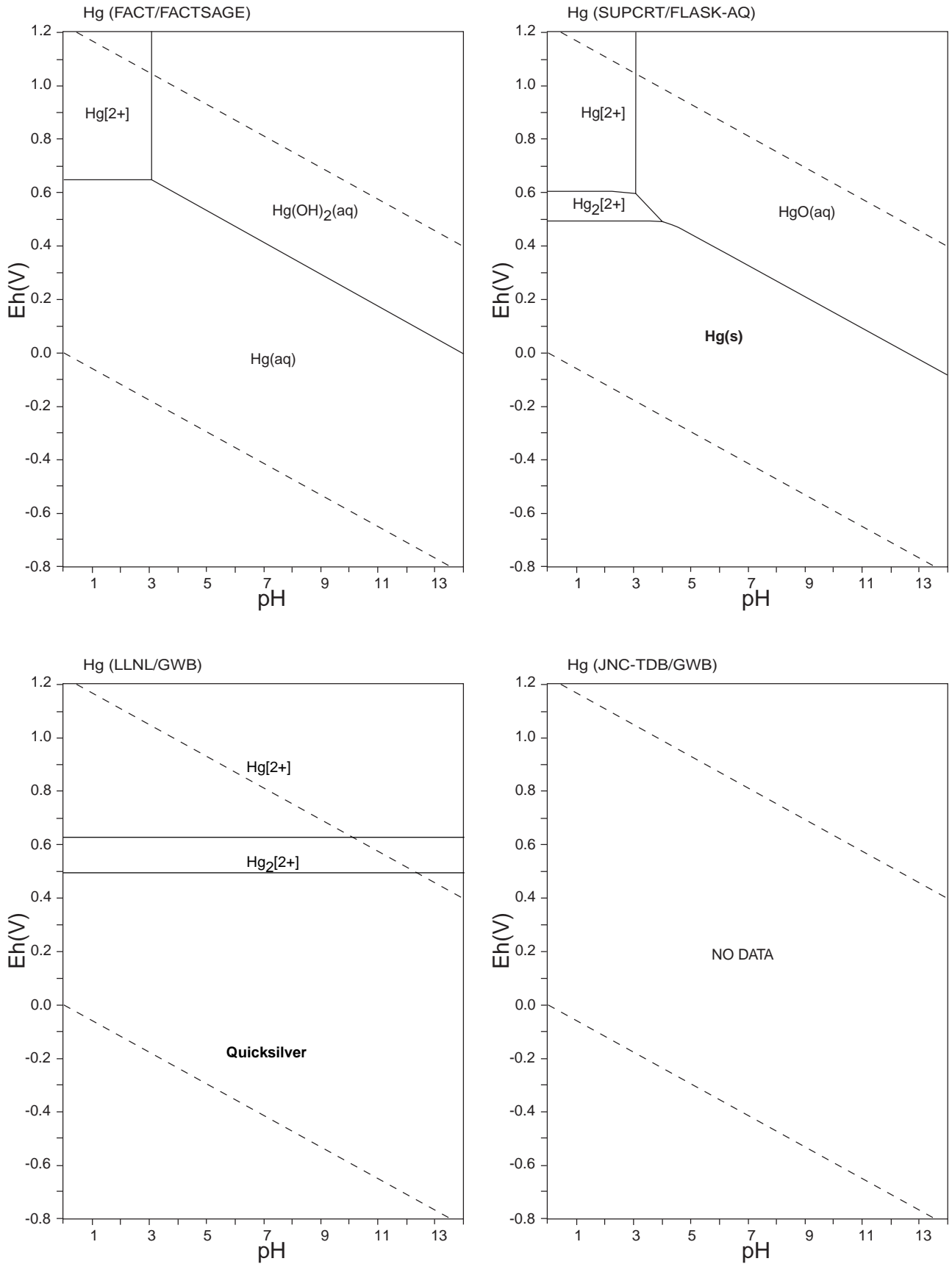
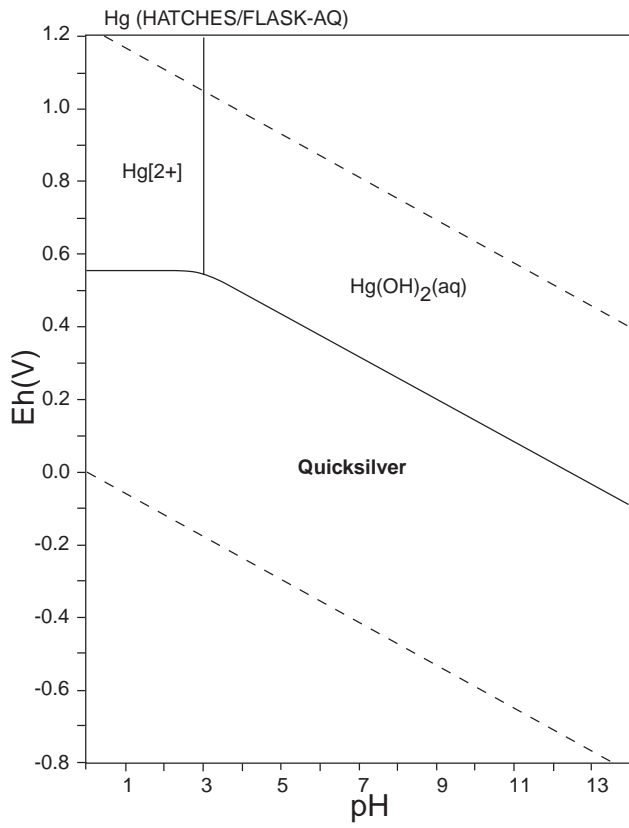


图 54: Eh-pH diagrams of the system Hg-O-H (1).  $\sum \text{Hg} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

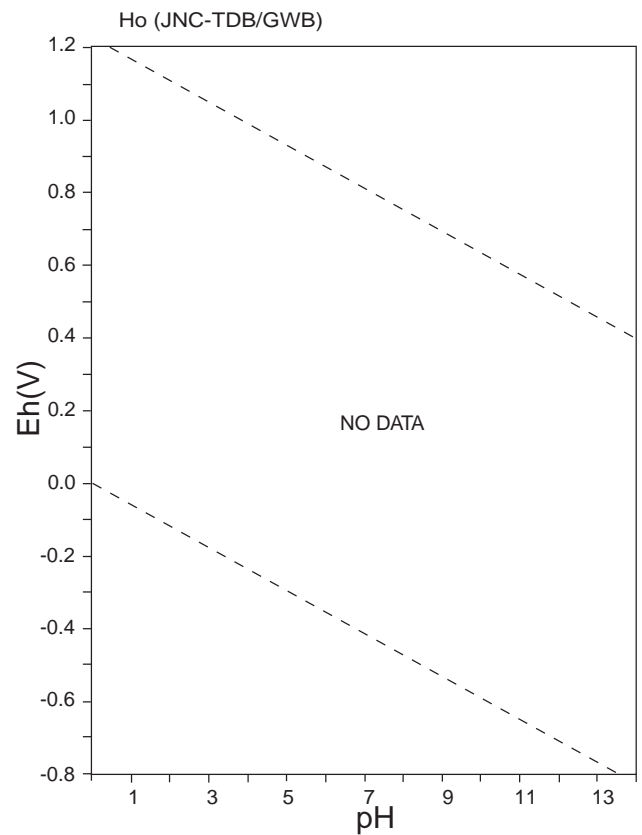
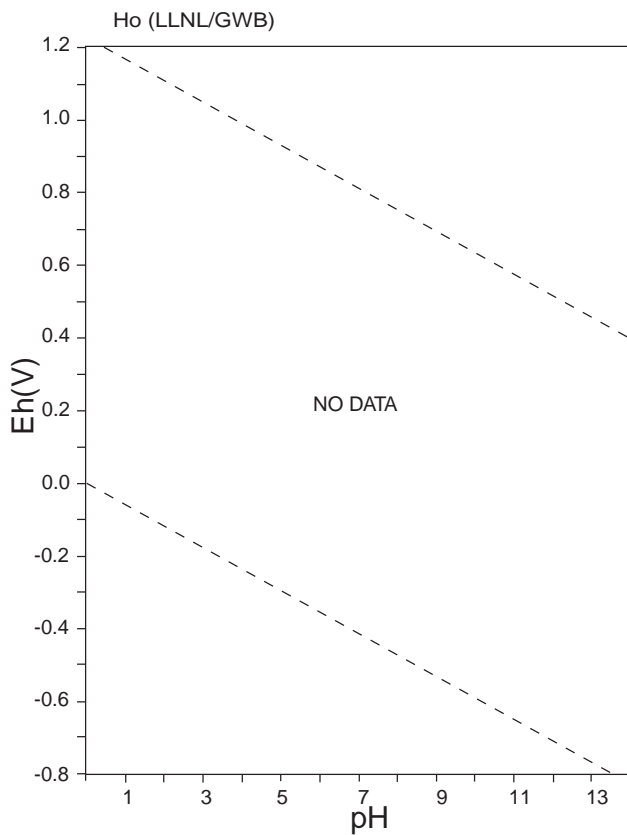
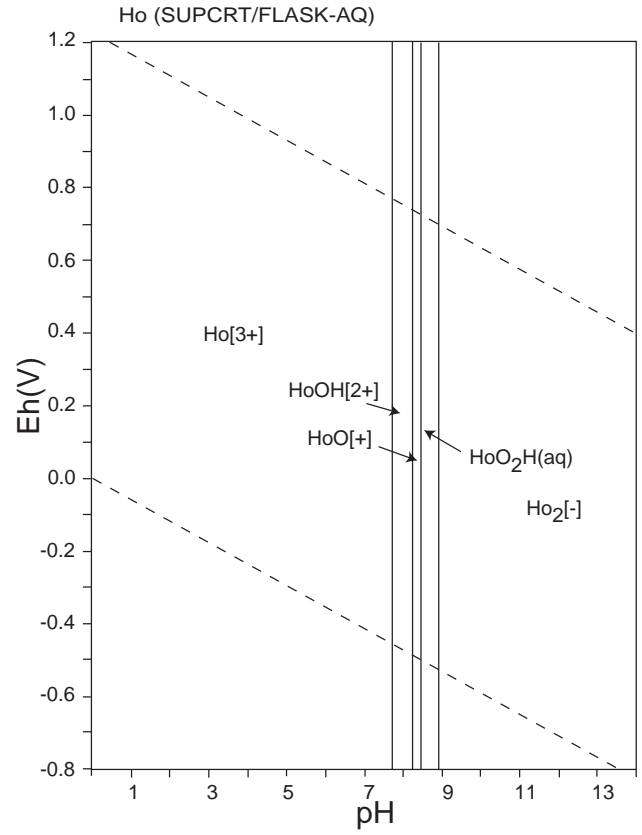
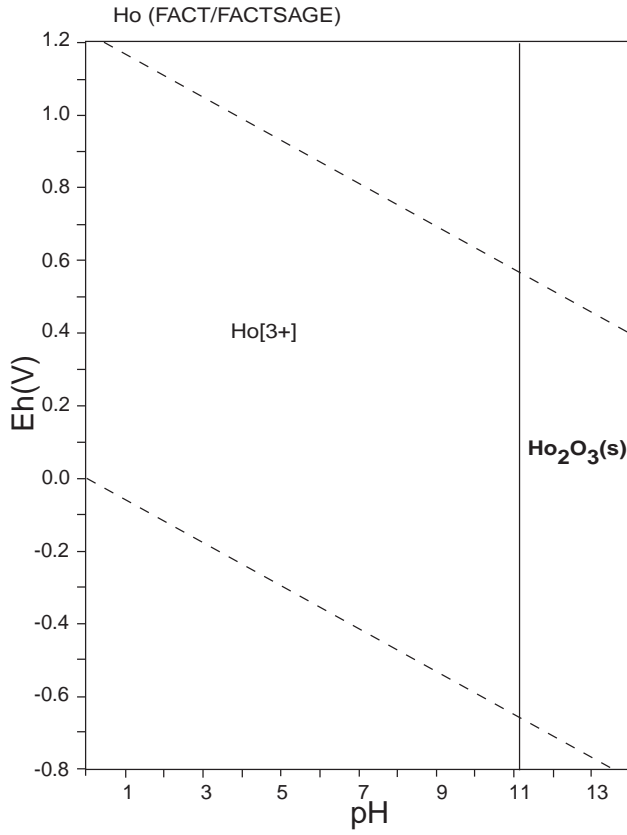




☒ 55: Eh-pH diagrams of the system Hg-O-H (2).  $\sum \text{Hg} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 35: List of Ho species

FACT	SUPCRT	LLNL	JNC-TDB
Ho[3+], <b>Ho(s)</b> , <b>Ho(s2)</b> , <b>Ho<sub>2</sub>O<sub>3</sub>(s)</b> , <b>Ho<sub>2</sub>O<sub>3</sub>(s2)</b>	Ho[3+], Ho[4+], Ho[2+], HoOH[2+], HoO[+], HoO <sub>2</sub> H(aq), HoO <sub>2</sub> [-]		



☒ 56: Eh-pH diagrams of the system Ho-O-H.  $\sum \text{Ho} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 36: List of I species

FACT	SUPCRT	LLNL	JNC-TDB
I[-], I <sub>3</sub> [-], IO[-], IO <sub>3</sub> [-], HIO(aq), HIO <sub>3</sub> (aq), I <sub>2</sub> (aq), H <sub>2</sub> OI[+], I <sub>2</sub> OH[-], <b>I<sub>2</sub>(s)</b>	I[-], I <sub>3</sub> [-], IO[-], IO <sub>3</sub> [-], HIO(aq), HIO <sub>3</sub> (aq), IO <sub>4</sub> [-]	I[-]	I[-], IO <sub>3</sub> [-], HIO <sub>3</sub> (aq), I <sub>3</sub> [-], IO[-], IO <sub>4</sub> [-], I <sub>2</sub> O[2-], HIO(aq), I <sub>2</sub> OH[-], I <sub>2</sub> (aq), HI(aq), H <sub>2</sub> OI[-], <b>I<sub>2</sub>(s), I<sub>2</sub>(c)</b> , I(g), I <sub>2</sub> (g), HI(g)

HATCHES			
I[-], IO <sub>3</sub> [-], H <sub>2</sub> IO[+], HI(aq), HIO(aq), HIO <sub>3</sub> (aq), I <sub>2</sub> (aq), I <sub>2</sub> O[2-], I <sub>2</sub> OH[-], I <sub>3</sub> [-], IO[-], IO <sub>4</sub> [-], <b>I<sub>2</sub></b>			

Remarks

JNC-TDB: I<sub>2</sub>(s) is originally given as I<sub>2</sub> in the database file, but its detailed description is not given. Then (s) is appended to I<sub>2</sub> to avoid confusion with I<sub>2</sub>(c).

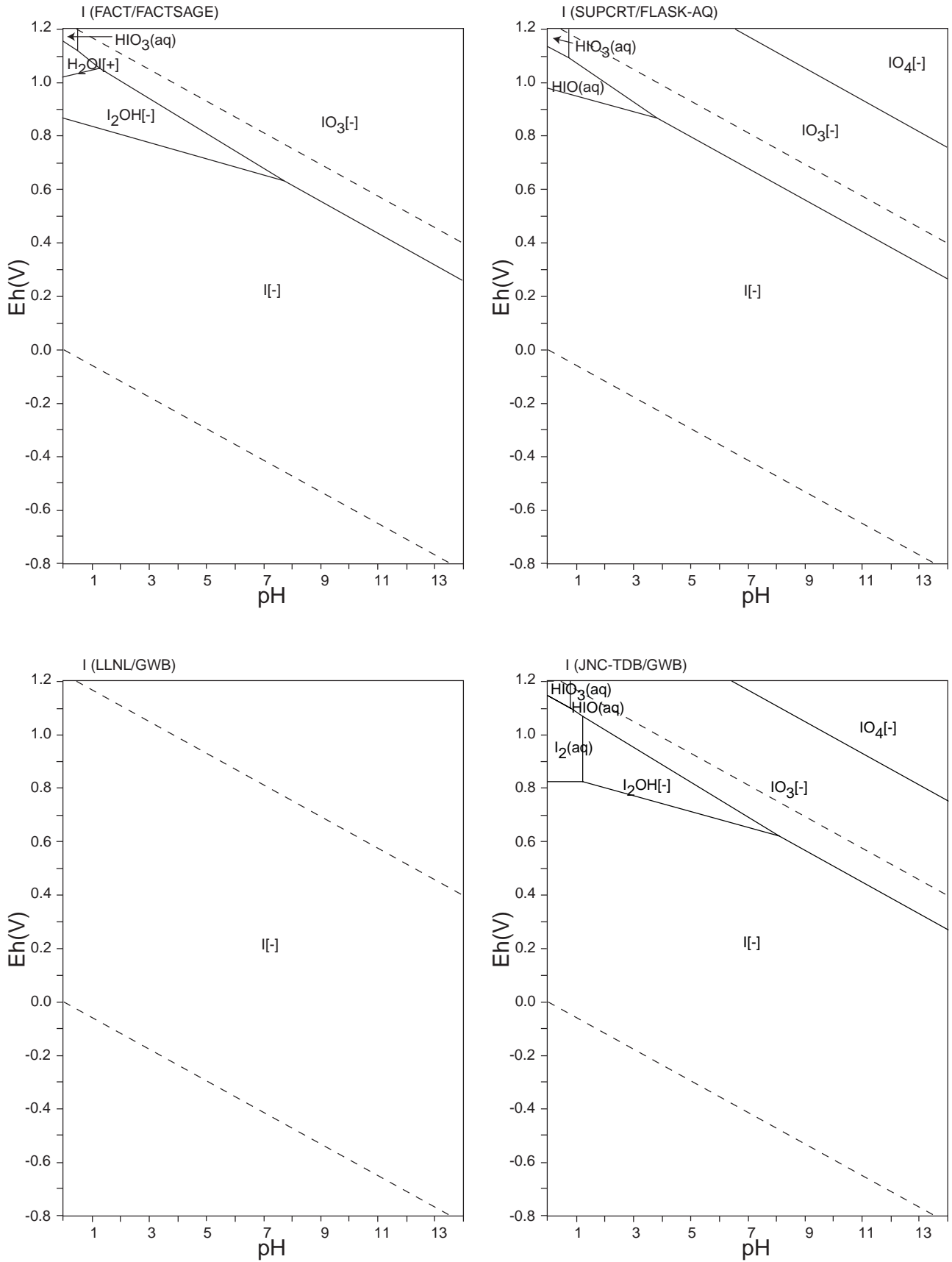
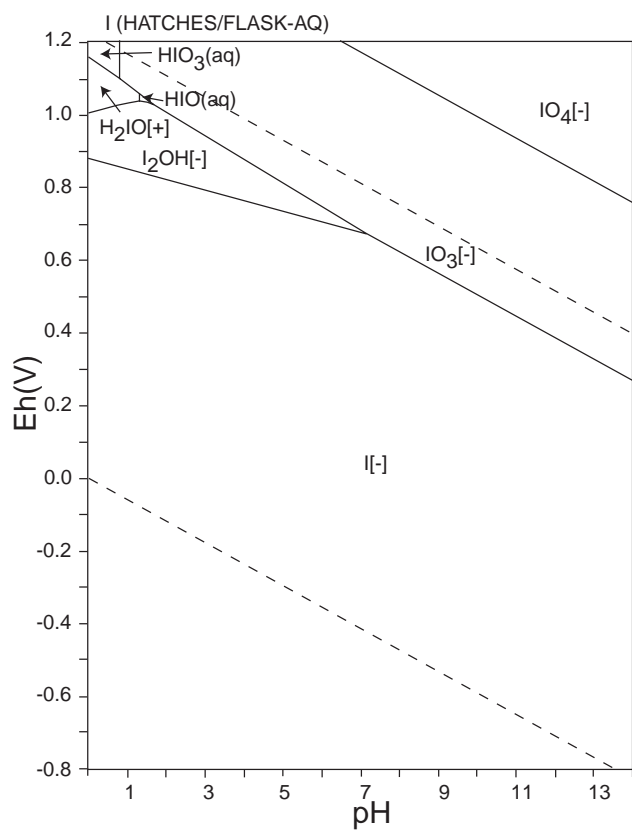


图 57: Eh-pH diagrams of the system I-O-H (1).  $\sum \text{I} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 58: Eh-pH diagrams of the system I-O-H (2).  $\sum I = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 37: List of In species

FACT	SUPCRT	LLNL	JNC-TDB
In[3+], InOH[2+], In(OH) <sub>2</sub> [+], In[+], In[2+], <b>In(s)</b> , <b>In<sub>2</sub>O<sub>3</sub>(s)</b> , <b>In<sub>2</sub>O<sub>3</sub>(s2)</b>	In[3+], InOH[2+], InO[+], HInO <sub>2</sub> (aq), InO <sub>2</sub> [-]		



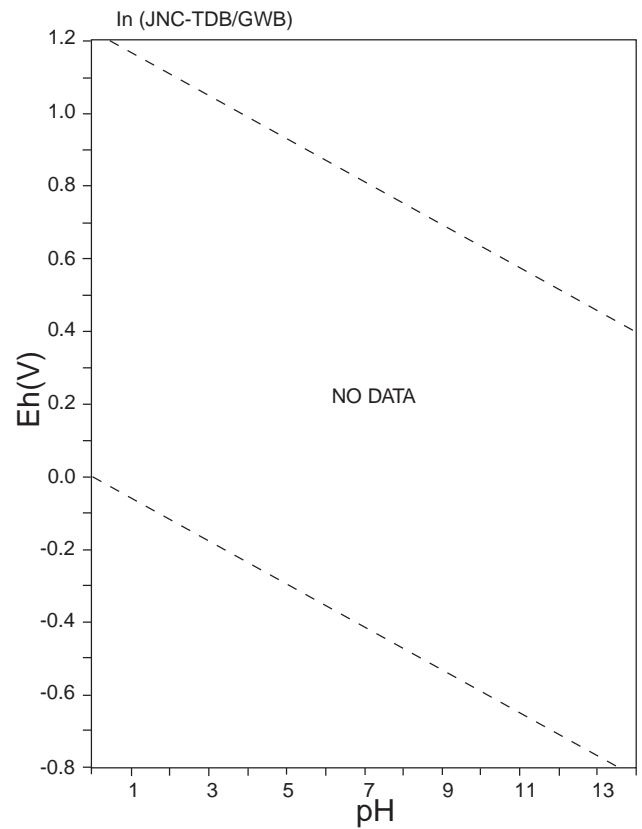
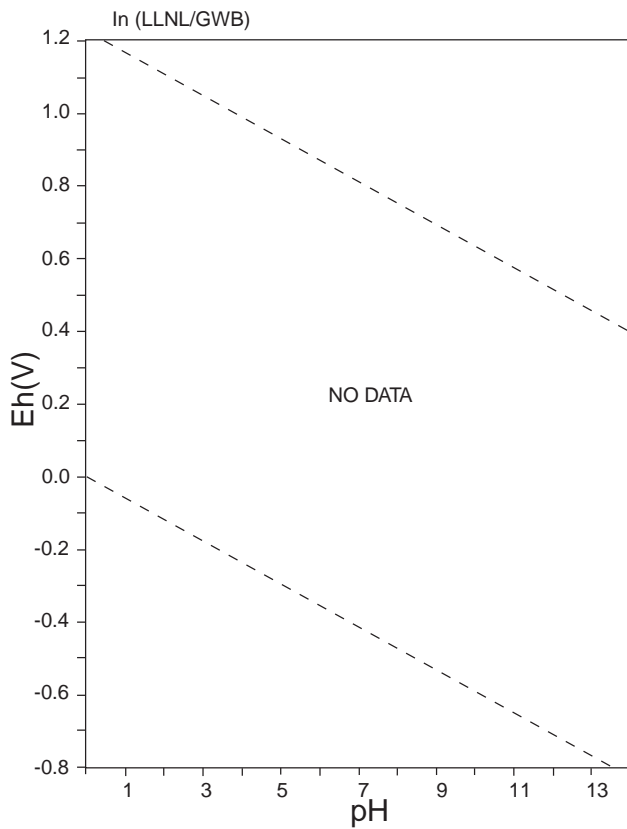
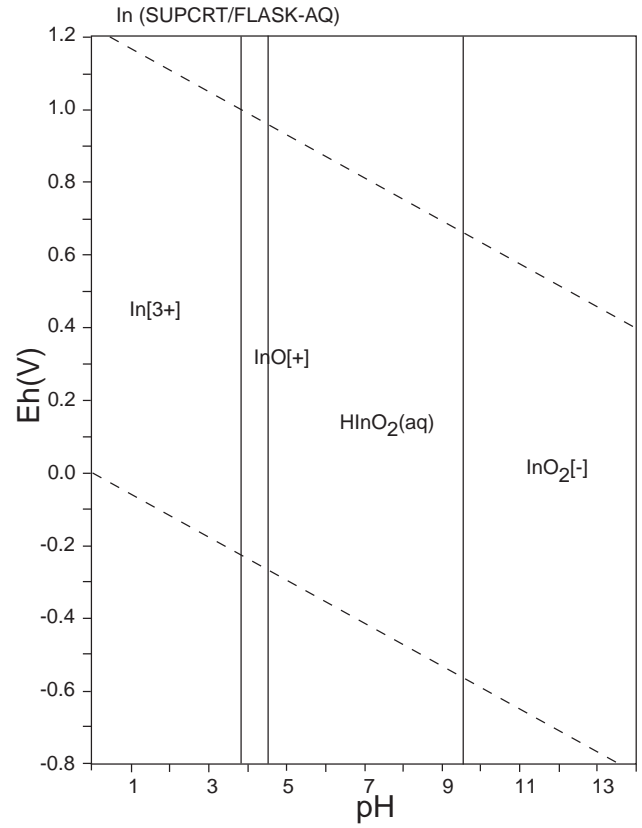
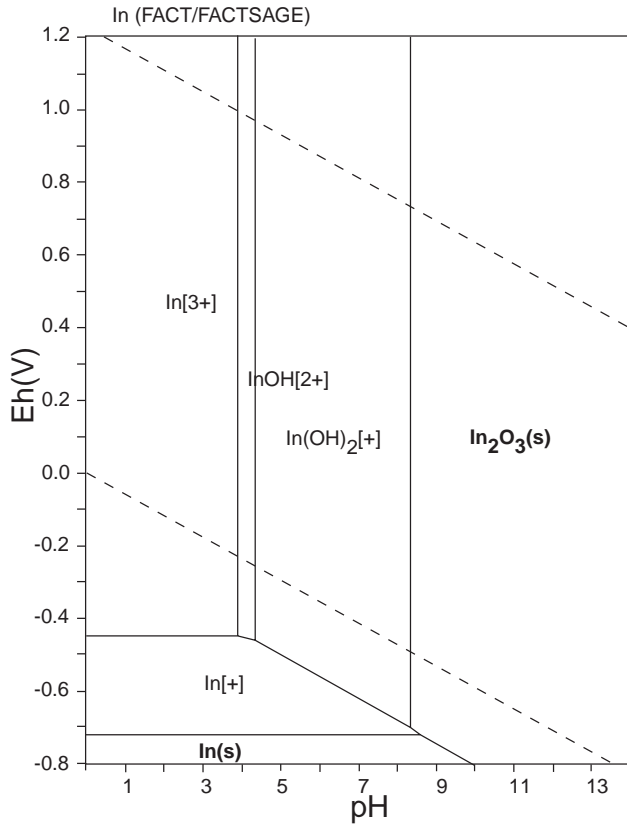


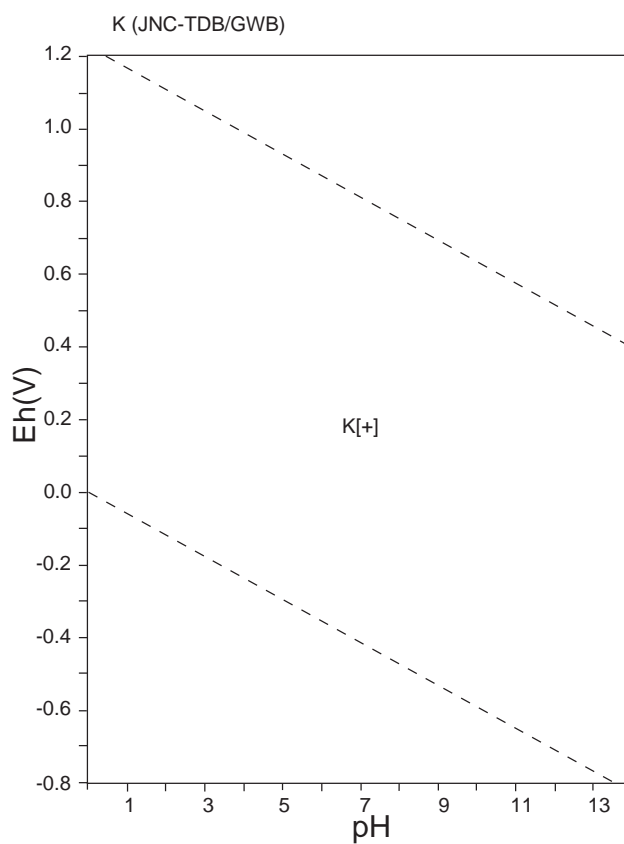
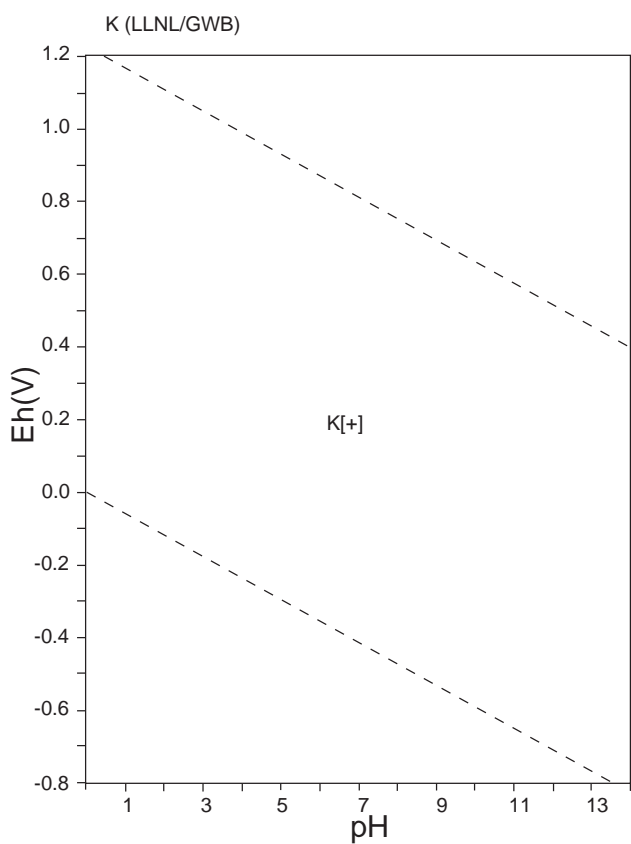
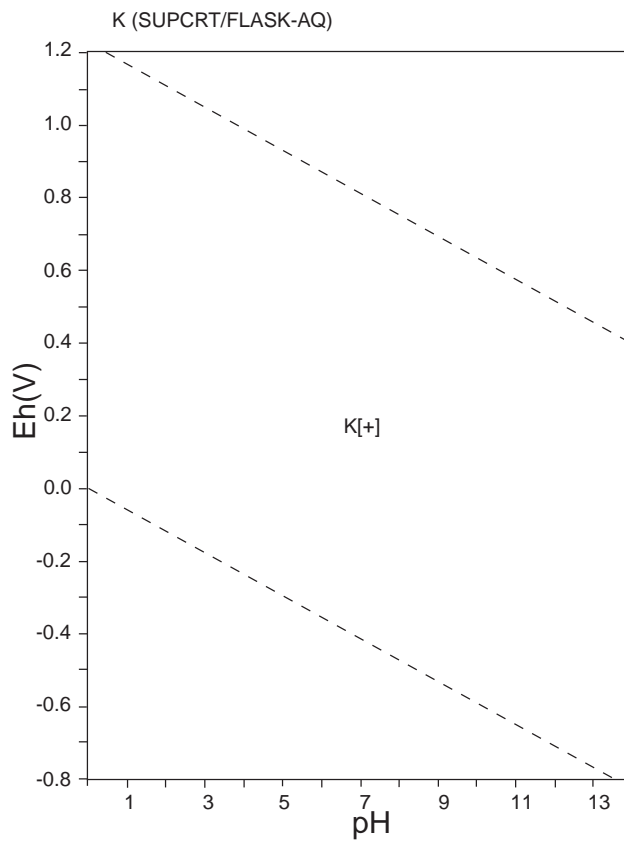
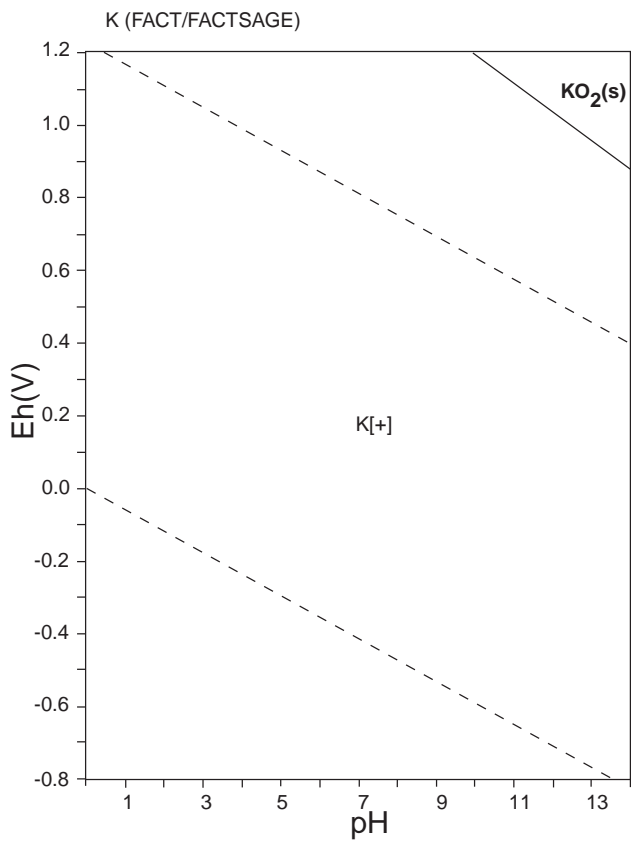
图 59: Eh-pH diagrams of the system In-O-H.  $\sum \text{In} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



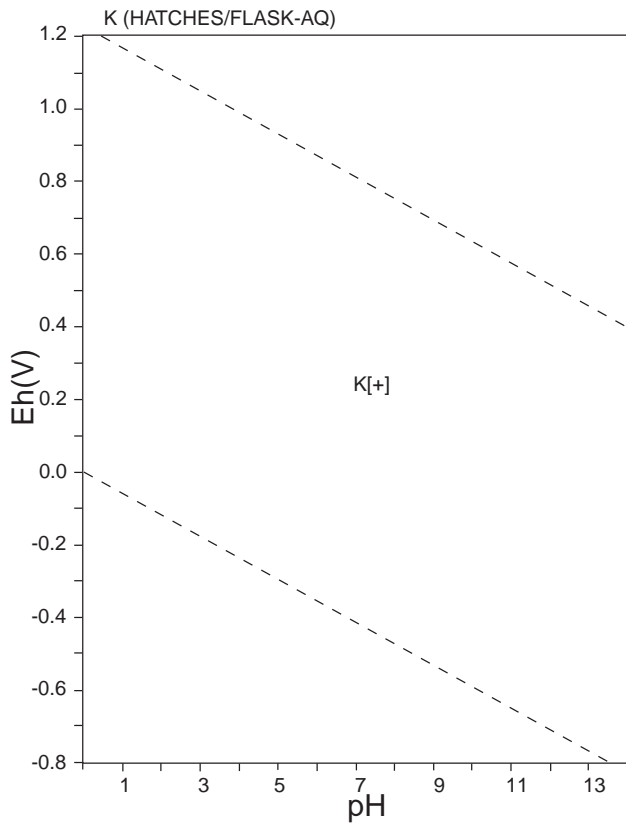
表 38: List of K species

FACT	SUPCRT	LLNL	JNC-TDB
K[+], <b>K(s)</b> , <b>KH(s)</b> , <b>KO<sub>2</sub>(s)</b> , <b>K<sub>2</sub>O(s)</b> , <b>K<sub>2</sub>O<sub>2</sub>(s)</b> , <b>KOH(s)</b> , <b>KOH(s2)</b>	K[+], KOH(aq), <b>K<sub>2</sub>O</b> <b>(Potassium-oxide)</b>	K[+], KOH(aq)	K[+], <b>K(c)</b> , K(g)

HATCHES			
K[+], <b>KOH</b>			



☒ 60: Eh-pH diagrams of the system K-O-H (1).  $\sum K = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 61: Eh-pH diagrams of the system K-O-H (2).  $\sum K = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 39: List of La species

FACT	SUPCRT	LLNL	JNC-TDB
La[3+], <b>La(s)</b> , <b>La(s2)</b> , <b>La(s3)</b> , <b>LaH<sub>2</sub>(s)</b> , <b>La<sub>2</sub>O<sub>3</sub>(s)</b>	La[3+], La[2+], LaOH[2+], LaO[+], LaO <sub>2</sub> H(aq), LaO <sub>2</sub> [-]		

HATCHES			
La[3+], La <sub>2</sub> OH[5+], La <sub>5</sub> (OH) <sub>9</sub> [6+], LaOH[2+], <b>La(OH)<sub>3</sub></b>			

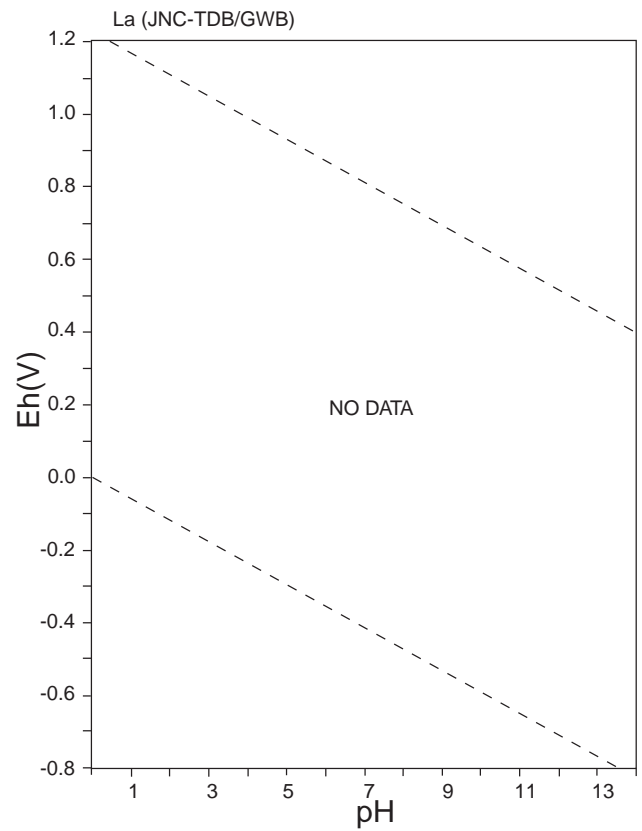
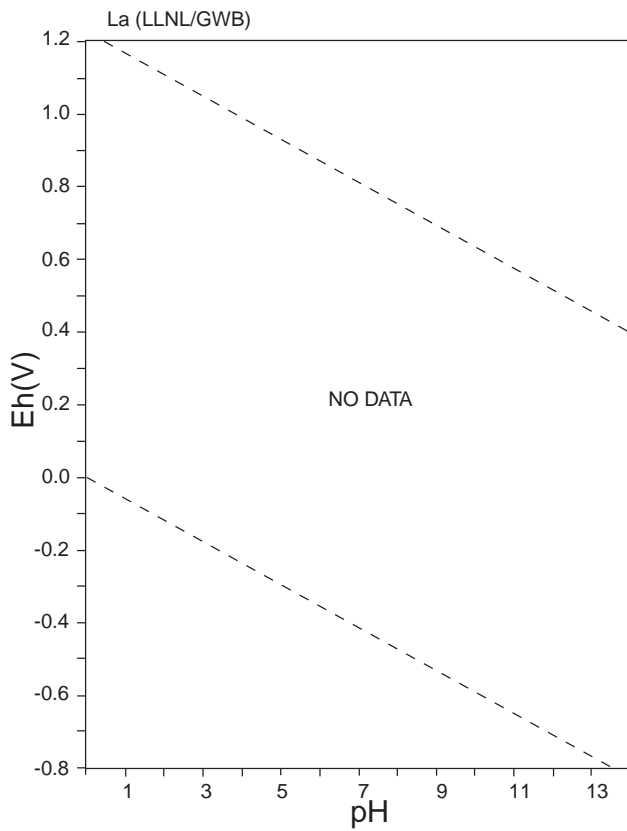
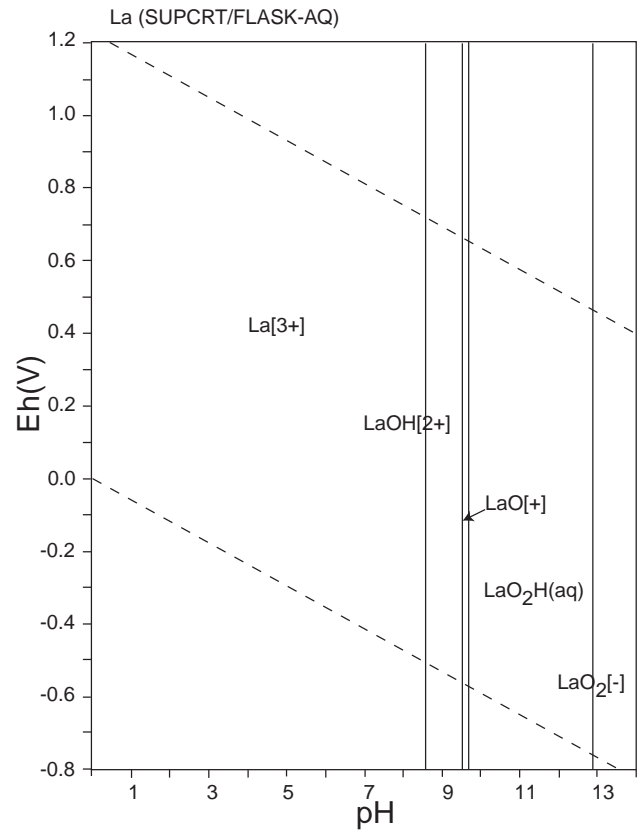
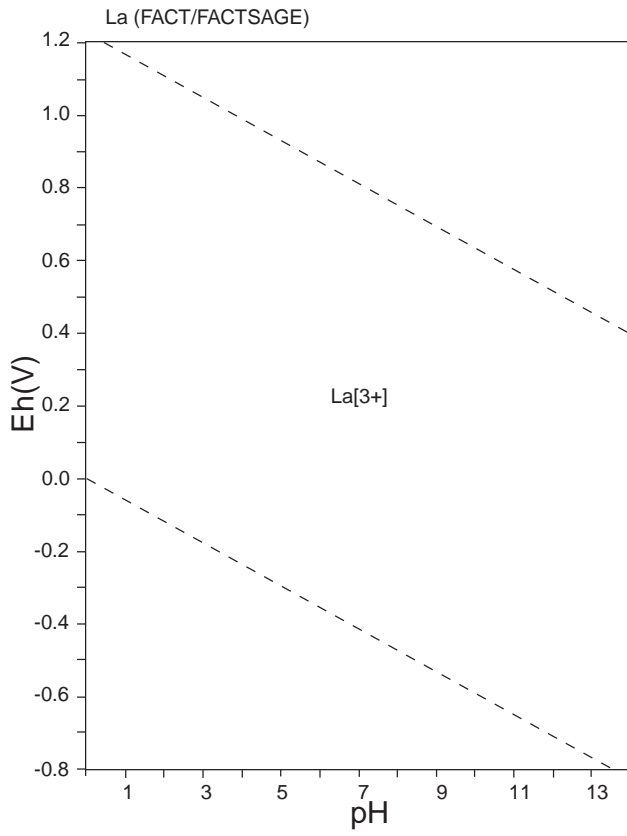
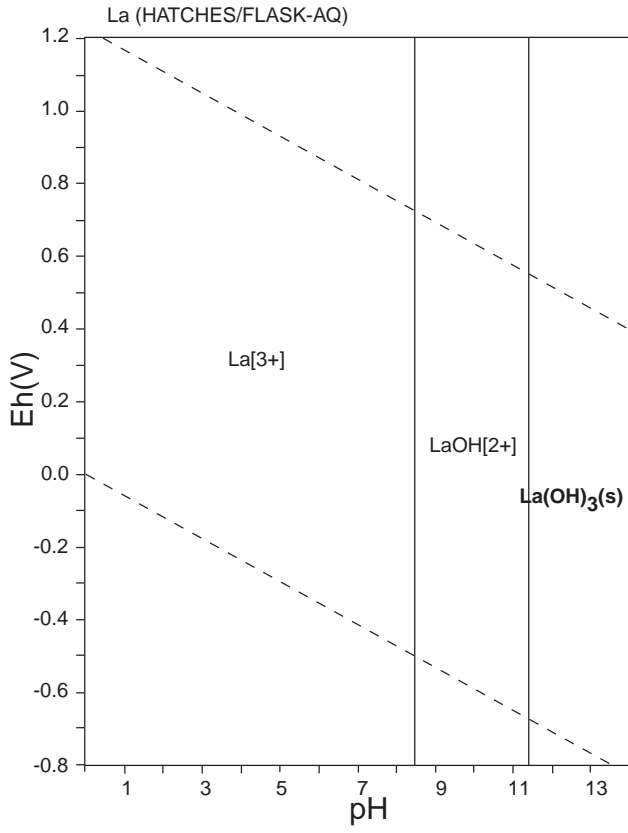


Figure 62: Eh-pH diagrams of the system La-O-H (1).  $\sum \text{La} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





☒ 63: Eh-pH diagrams of the system La-O-H (2).  $\sum \text{La} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 40: List of Li species

FACT	SUPCRT	LLNL	JNC-TDB
Li[+], LiOH(aq), Li(s), LiH(s), Li <sub>2</sub> O(s), Li <sub>2</sub> O <sub>2</sub> (s), LiOH(s)	Li[+], LiOH(aq)	Li[+], LiOH(aq)	Li[+]

HATCHES			
Li[+]			

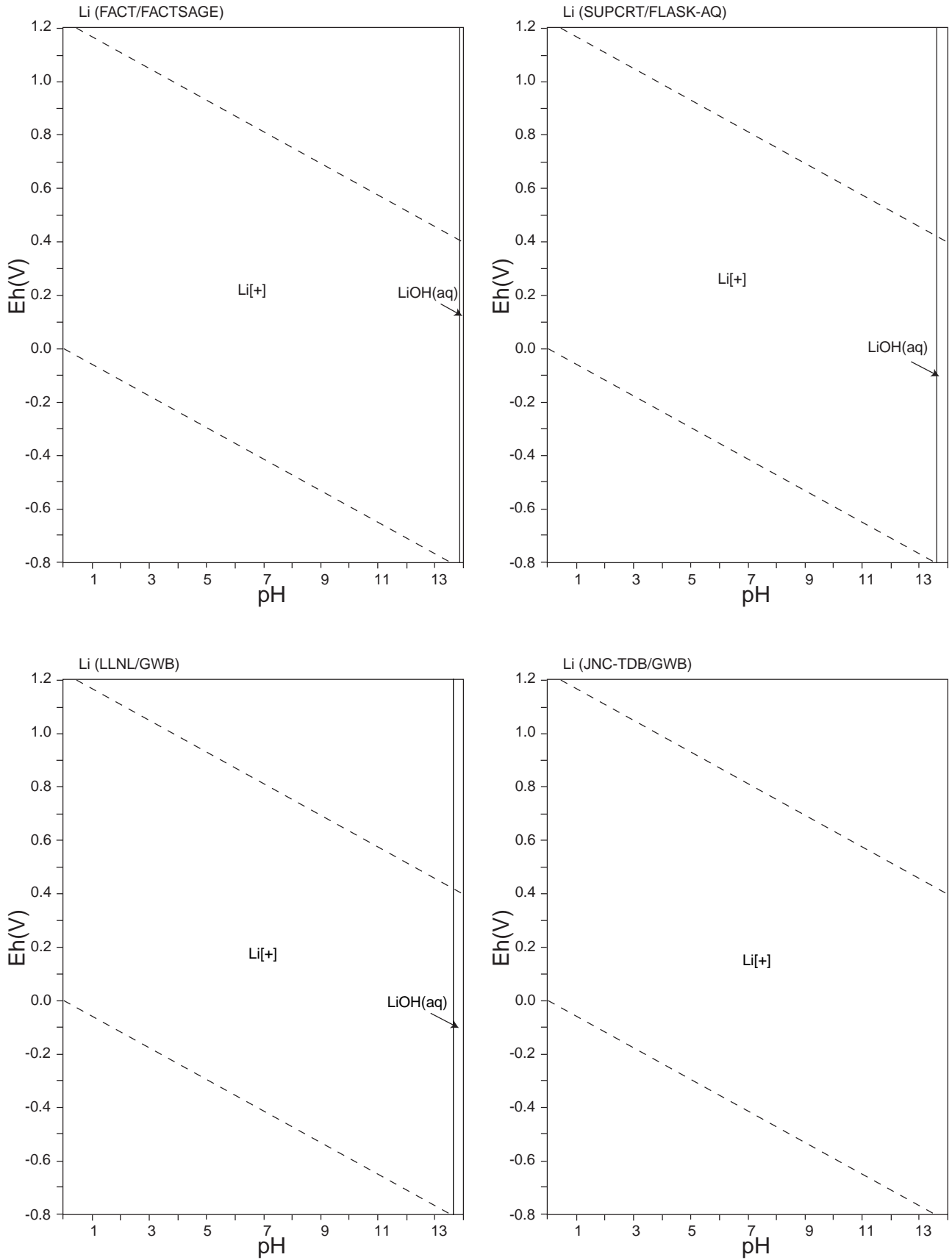


图 64: Eh-pH diagrams of the system Li-O-H (1).  $\sum \text{Li} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

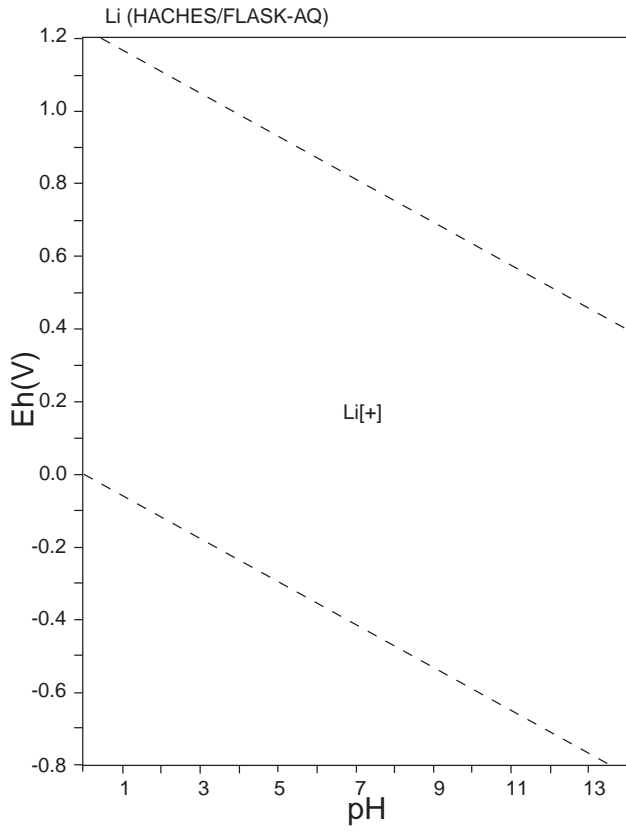
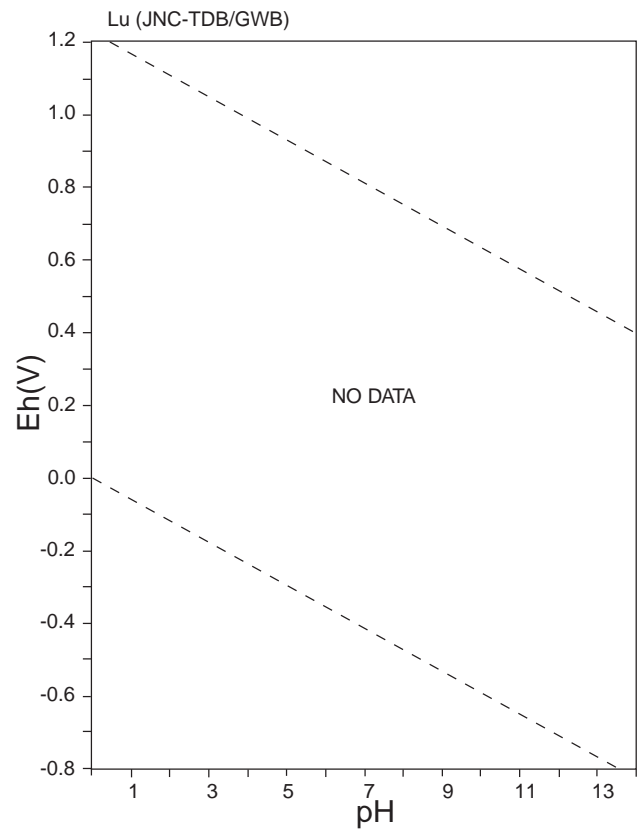
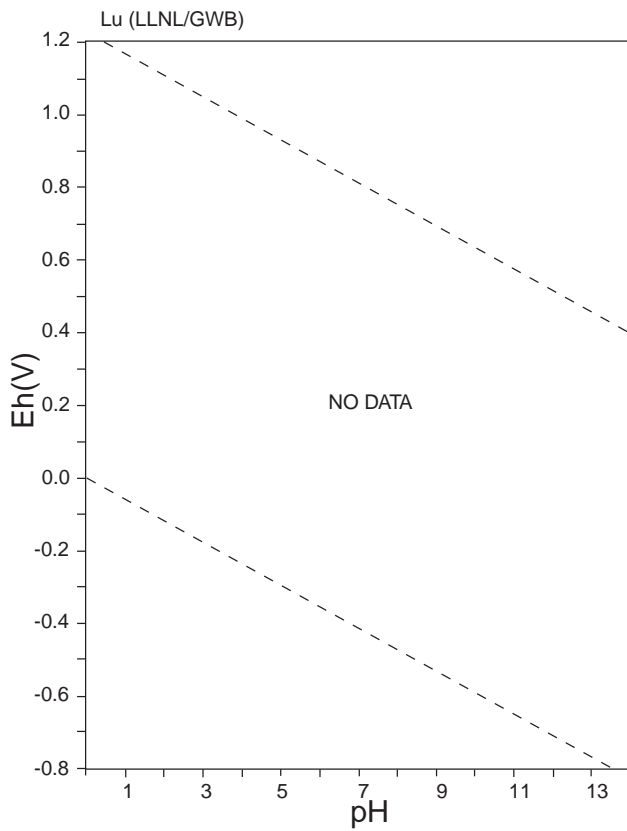
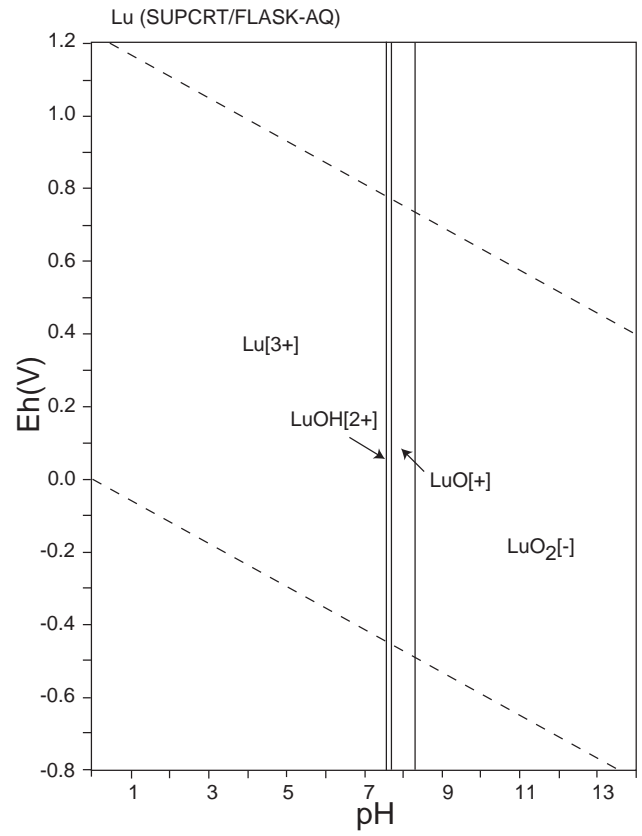
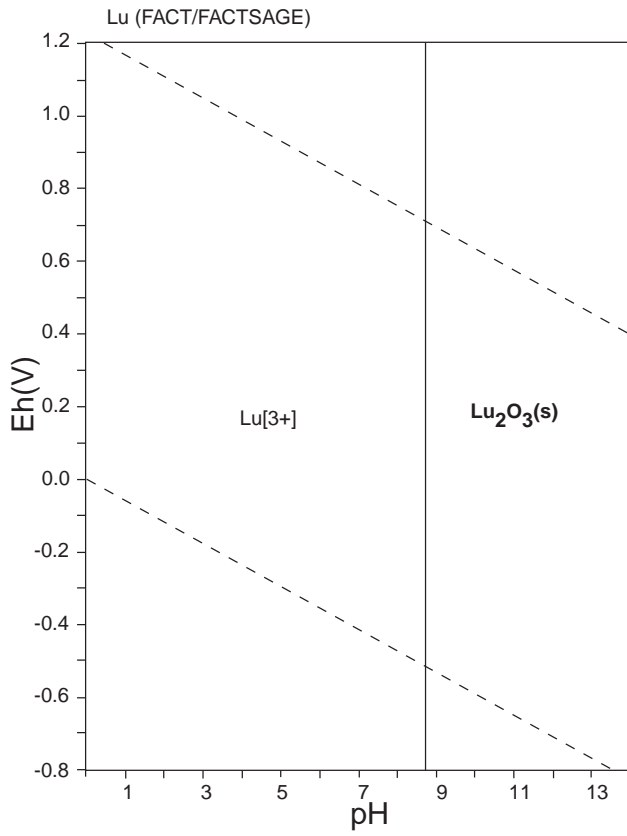


图 65: Eh-pH diagrams of the system Li-O-H (2).  $\sum \text{Li} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 41: List of Lu species

FACT	SUPCRT	LLNL	JNC-TDB
Lu[3+], Lu(s), Lu <sub>2</sub> O <sub>3</sub> (s)	Lu[3+], Lu[4+], LuOH[2+], LuO[+], LuO <sub>2</sub> H(aq), LuO <sub>2</sub> [-]		



☒ 66: Eh-pH diagrams of the system Lu-O-H.  $\sum \text{Lu} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





表 42: List of Mg species

FACT	SUPCRT	LLNL	JNC-TDB
Mg[2+], MgOH[+], <b>Mg(s), MgH<sub>2</sub>(s), MgO(s), Mg(OH)<sub>2</sub>(s)</b>	Mg[2+], MgOH[+], <b>MgO(Periclase), Mg(OH)<sub>2</sub>(Brucite)</b>	Mg[2+], Mg <sub>2</sub> OH[3+], Mg <sub>4</sub> (OH) <sub>4</sub> [4+], MgOH[+], <b>Brucite</b>	Mg[2+], MgOH[+], <b>Periclase</b>

HATCHES			
Mg[2+], MgOH[+], <b>Mg(OH)<sub>2</sub></b>			

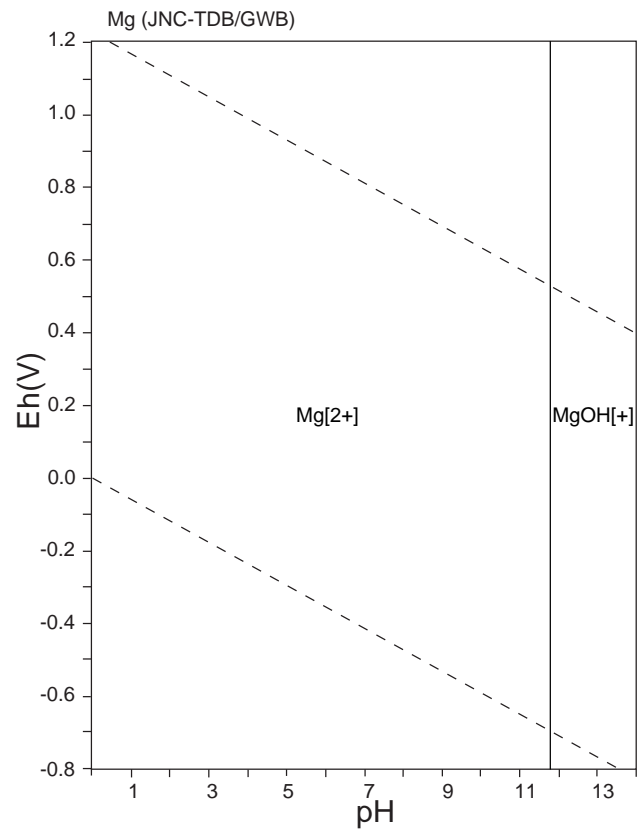
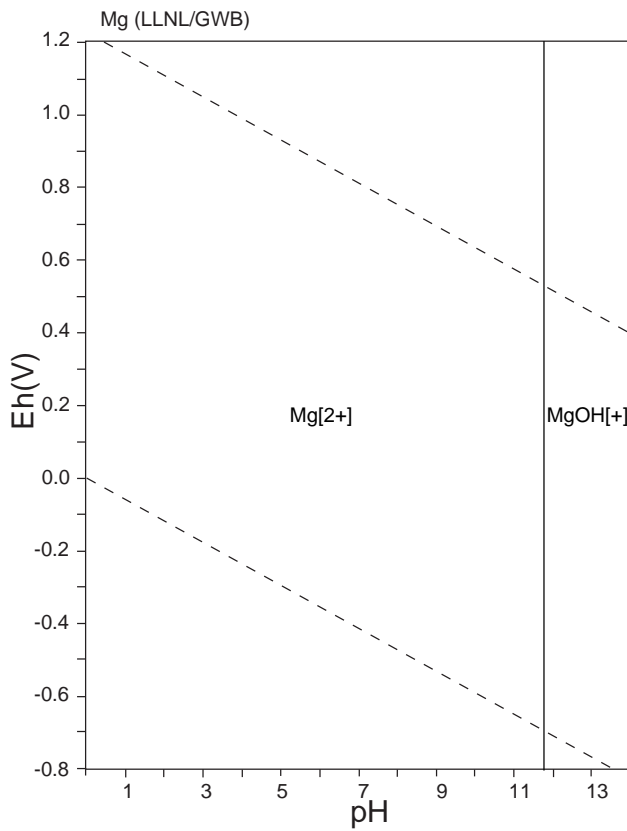
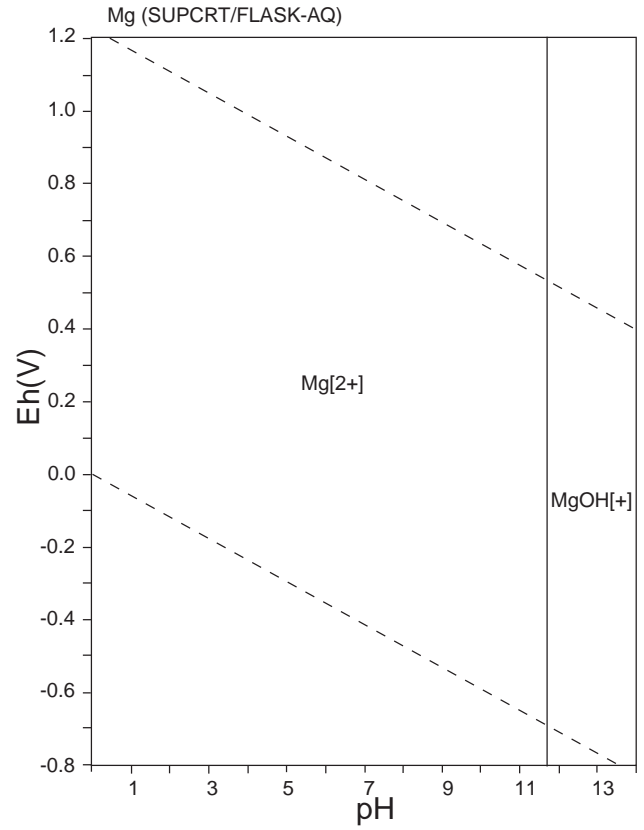
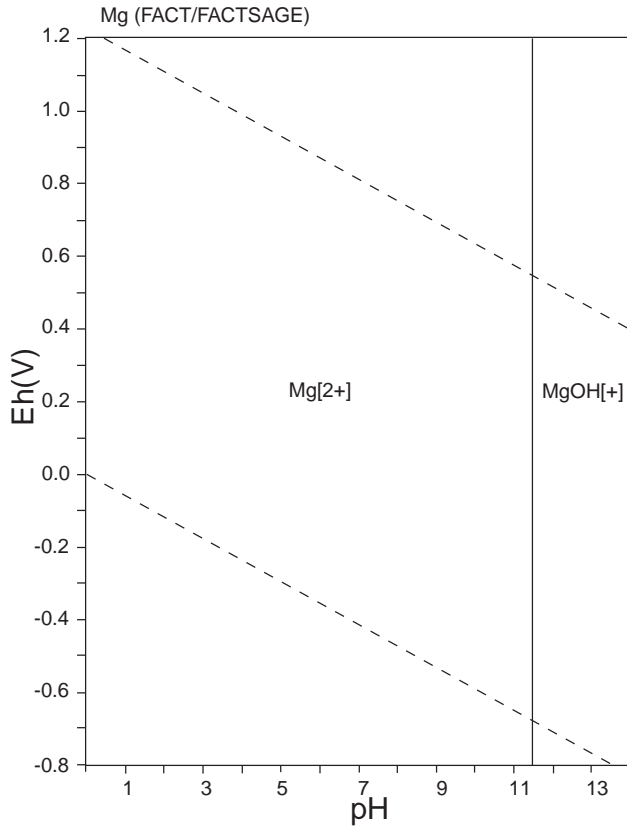


Figure 67: Eh-pH diagrams of the system Mg-O-H (1).  $\sum \text{Mg} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

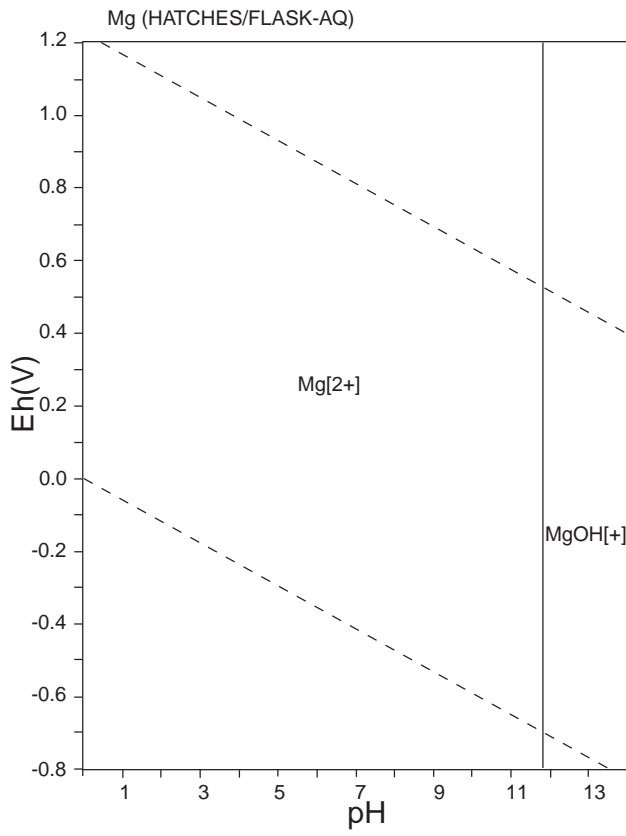


图 68: Eh-pH diagrams of the system Mg-O-H (2).  $\sum \text{Mg} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 43: List of Mn species

FACT	SUPCRT	LLNL	JNC-TDB
Mn[2+], Mn[3+], MnO <sub>4</sub> [2-], MnO <sub>4</sub> [-], MnOH[+], Mn(OH) <sub>3</sub> [-], <b>Mn(s), Mn(s2), Mn(s3), Mn(s4), MnO<sub>2</sub>(s), Mn<sub>2</sub>O<sub>3</sub>(s), Mn<sub>3</sub>O<sub>4</sub>(s), Mn<sub>3</sub>O<sub>4</sub>(s2), MnO(s)</b>	Mn[2+], Mn[3+], MnO <sub>4</sub> [2-], MnO <sub>4</sub> [-], MnOH[+], HMnO <sub>2</sub> [-], MnO(aq), MnO <sub>2</sub> [2-], <b>MnO(Manganosite)</b>	Mn[2+], MnO <sub>4</sub> [-], MnO <sub>4</sub> [2-], Mn(OH) <sub>2</sub> (aq), Mn(OH) <sub>3</sub> [-], Mn(OH) <sub>4</sub> [2-], Mn <sub>2</sub> (OH) <sub>3</sub> [+], Mn <sub>2</sub> OH[3+], MnOH[+], <b>Birnessite, Bixbyite, Hausmannite, Manganite, Manganosite, Mn(OH)<sub>2</sub>(am), Mn(OH)<sub>3</sub>(c), Pyrolusite, Todorokite</b>	Mn[2+], Mn[3+], MnO <sub>4</sub> [2-], MnO <sub>4</sub> [-], MnOH[+], Mn(OH) <sub>3</sub> [-], <b>Birnesite, Manganite, Pyrolusite</b>

HATCHES			
Mn[2+], Mn[3+], MnO <sub>4</sub> [2-], Mn(OH) <sub>2</sub> (aq), Mn(OH) <sub>3</sub> [-], Mn(OH) <sub>4</sub> [2-], Mn <sub>2</sub> (OH) <sub>3</sub> [+], Mn <sub>2</sub> OH[3+], MnO <sub>4</sub> [-], MnOH[+], MnOH[2+], <b>Birnessite, Bixbyite, Hausmannite, Manganite, Manganosite, Mn(OH)<sub>2</sub>, Mn(OH)<sub>3</sub>, Mn(OH)<sub>3</sub>(c), Mn<sub>3</sub>O<sub>4</sub>, MnOOH, Pyrolusite, Todorokite</b>			

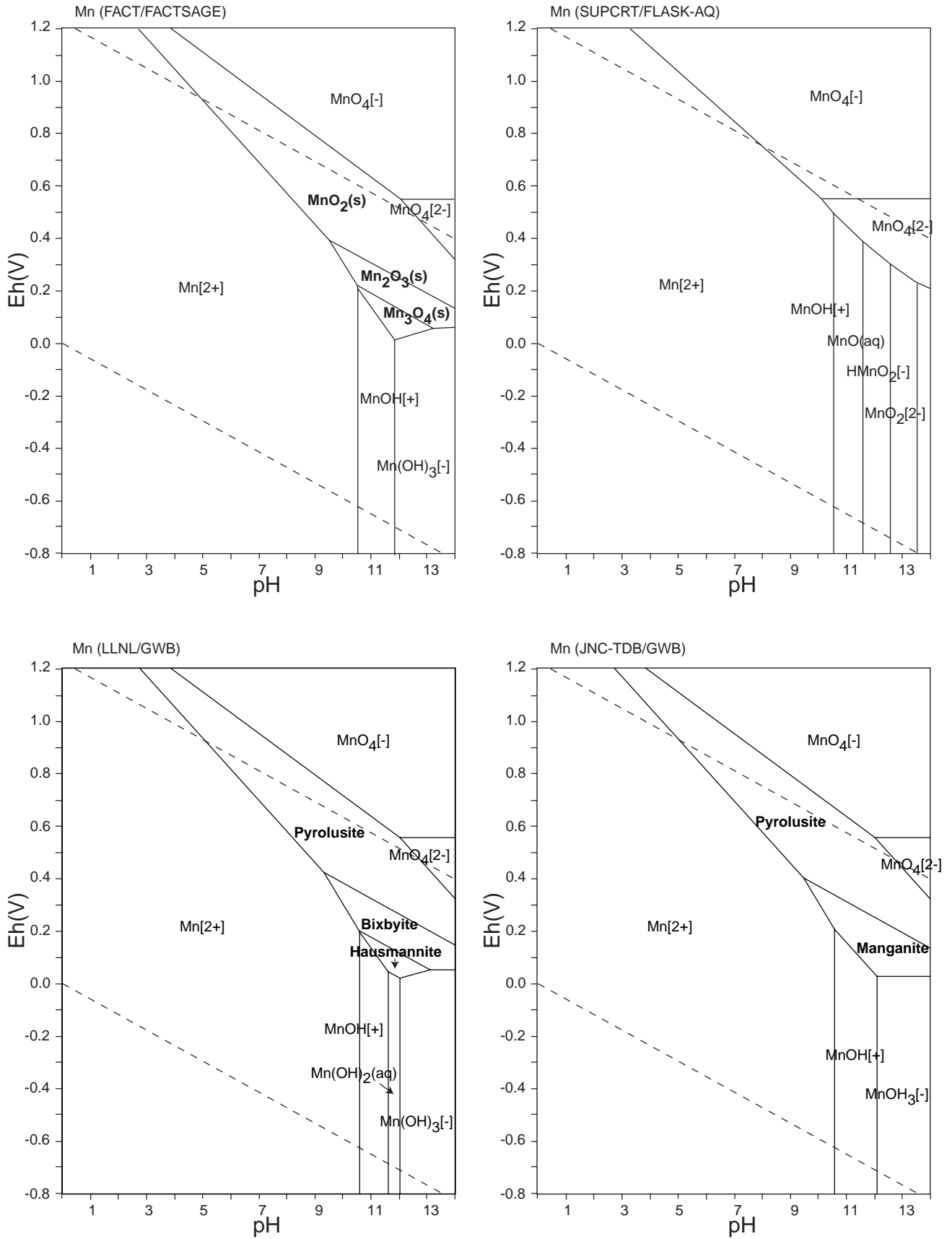


图 69: Eh-pH diagrams of the system Mn-O-H (1).  $\sum \text{Mn} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

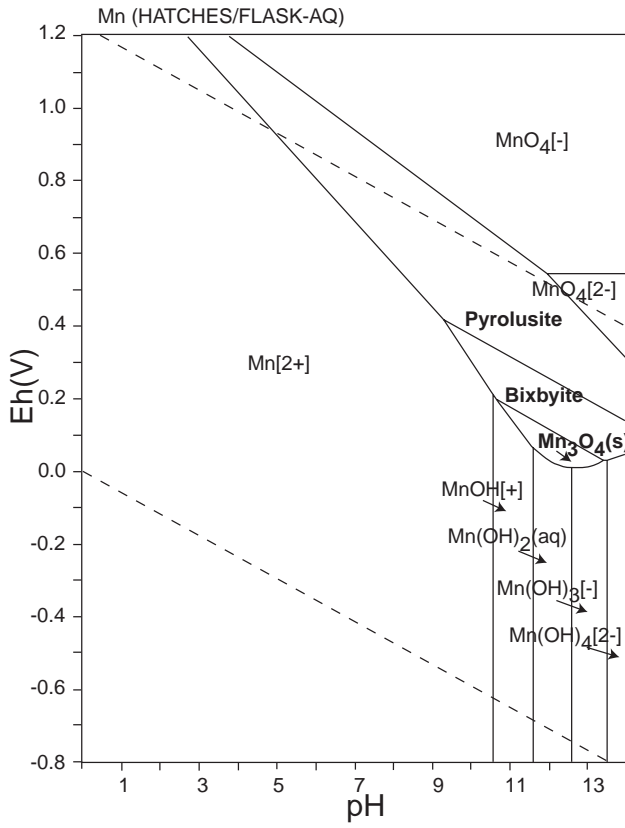


图 70: Eh-pH diagrams of the system Mn-O-H (2).  $\sum Mn = 10^{-10}$ , 298.15K,  $10^5$  Pa.

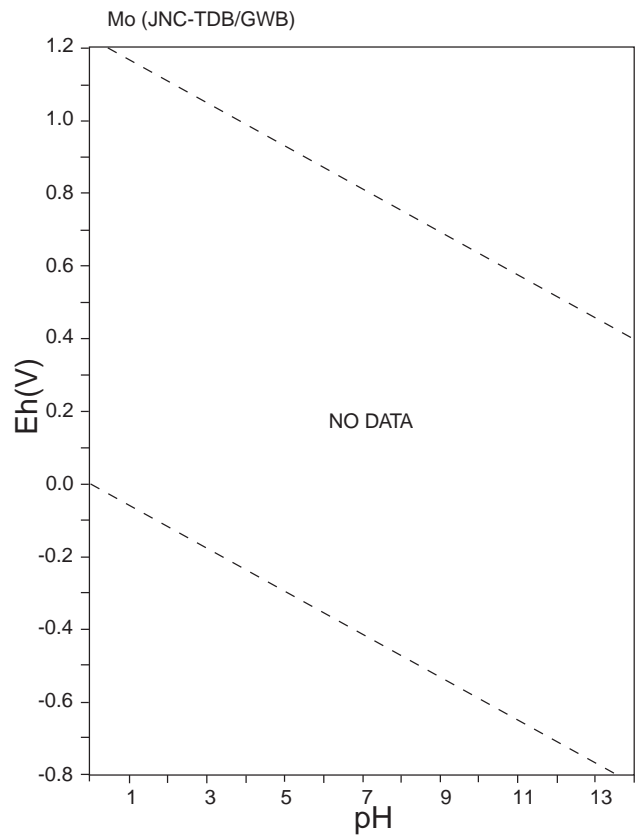
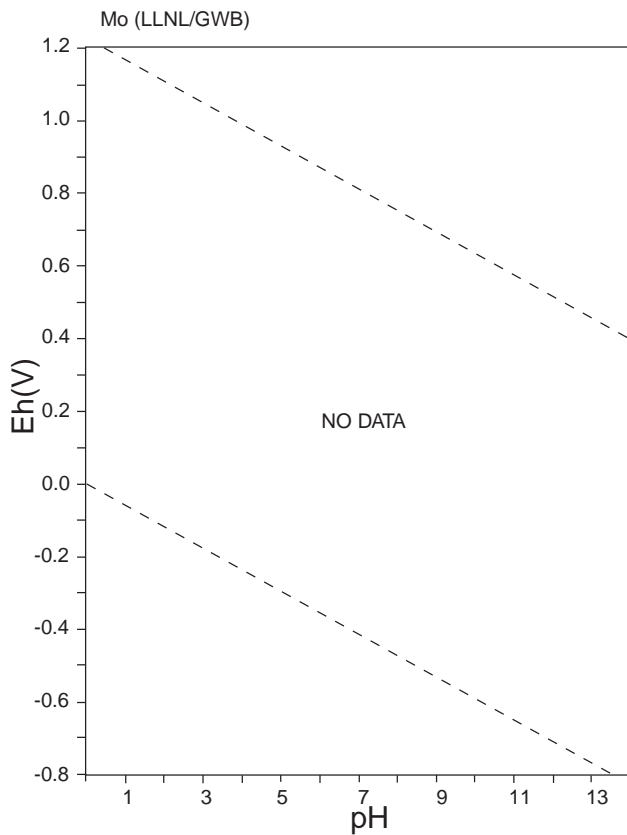
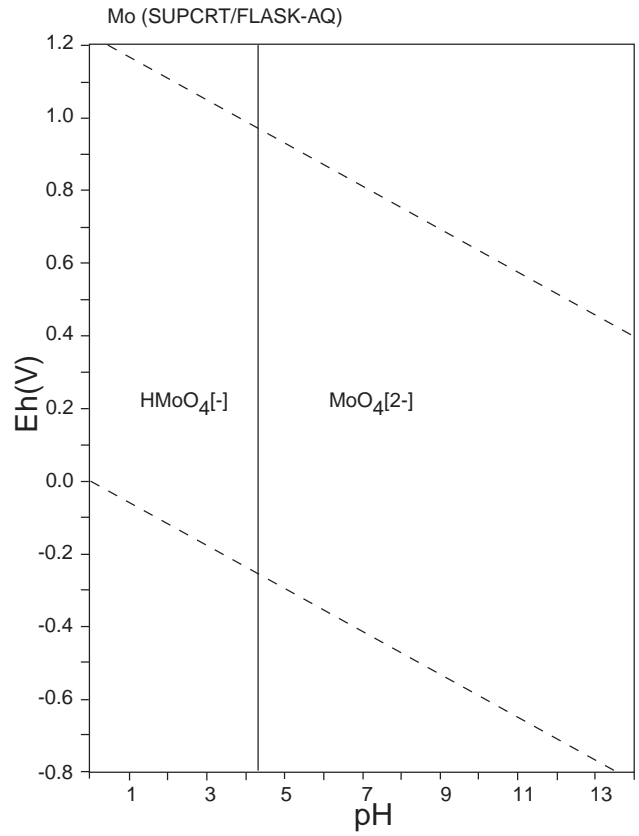
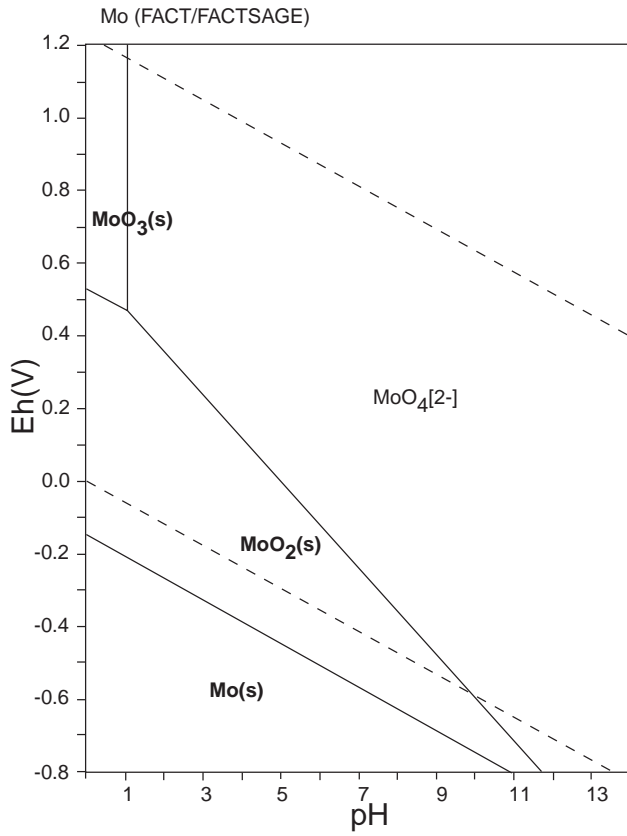




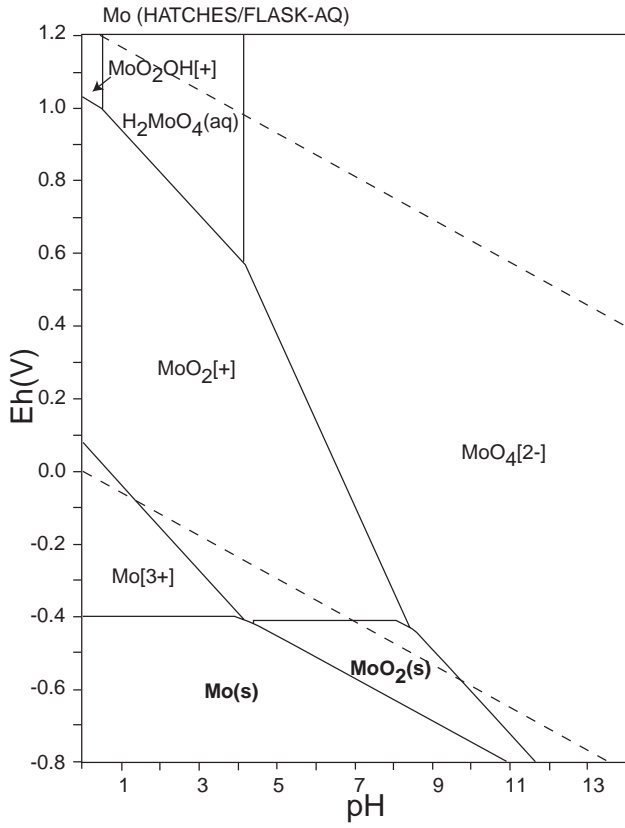
表 44: List of Mo species

FACT	SUPCRT	LLNL	JNC-TDB
MoO <sub>4</sub> [2-], Mo(s), MoO <sub>2</sub> (s), MoO <sub>3</sub> (s)	MoO <sub>4</sub> [2-], HMoO <sub>4</sub> [-]		

HATCHES			
MoO <sub>4</sub> [2-], Mo[3+], MoO <sub>2</sub> [+], H <sub>2</sub> MoO <sub>4</sub> (aq), HMoO <sub>4</sub> [-], Mo <sub>7</sub> O <sub>21</sub> (OH) <sub>3</sub> [3-], Mo <sub>7</sub> O <sub>22</sub> (OH) <sub>2</sub> [4-], Mo <sub>7</sub> O <sub>23</sub> OH[5-], Mo <sub>7</sub> O <sub>24</sub> [6-], MoO[3+], MoO <sub>2</sub> [2+], MoO <sub>2</sub> OH[+], H <sub>2</sub> MoO <sub>4</sub> , Mo, MoO <sub>2</sub> , MoO <sub>3</sub>			



☒ 71: Eh-pH diagrams of the system Mo-O-H (1).  $\sum \text{Mo} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



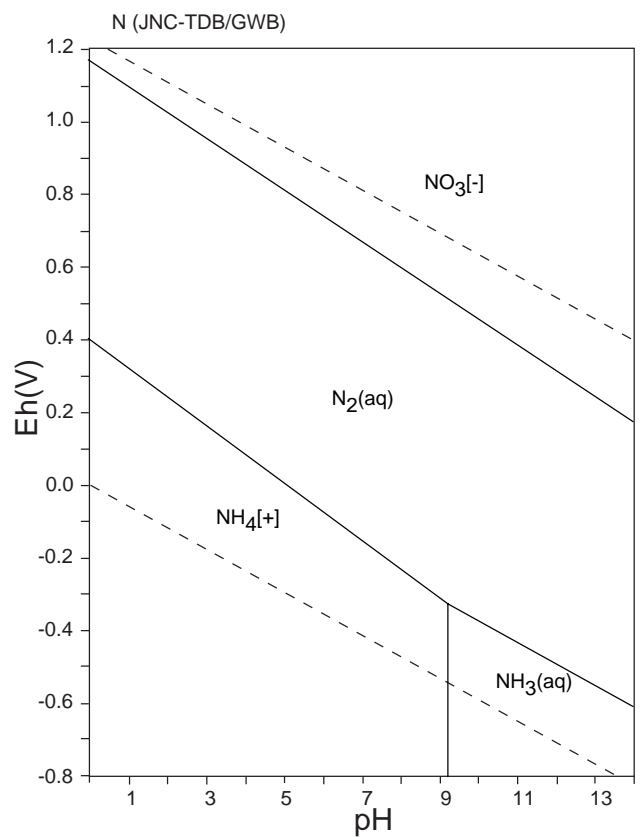
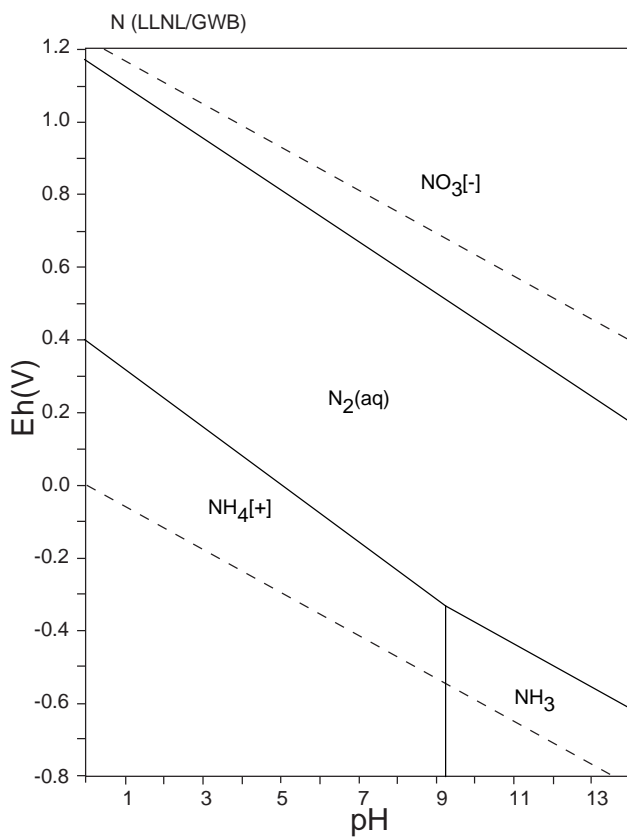
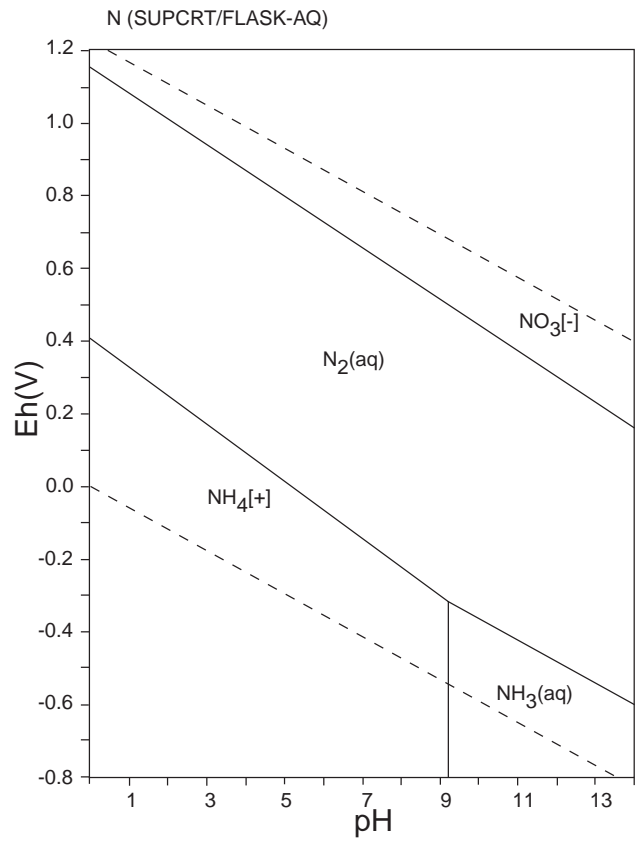
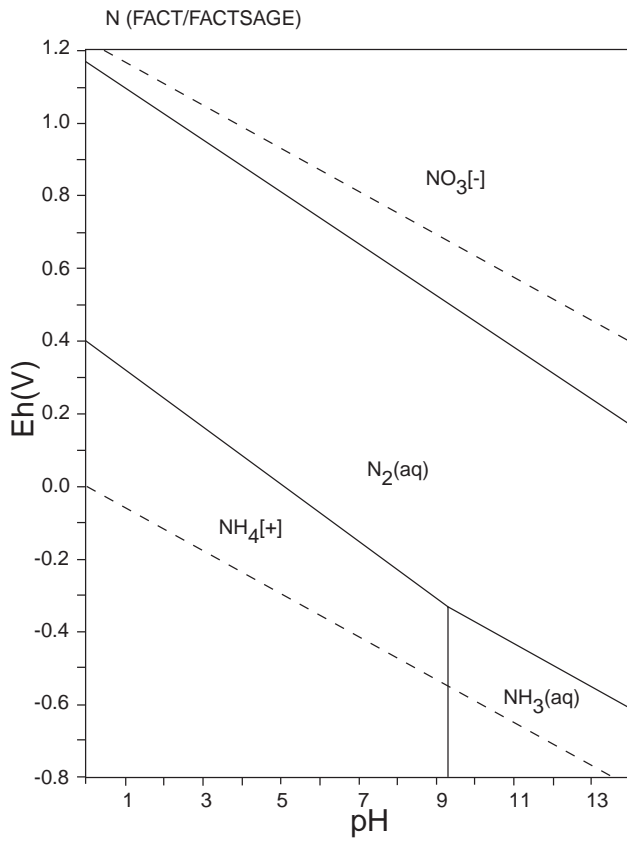
☒ 72: Eh-pH diagrams of the system Mo-O-H (2).  $\sum \text{Mo} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



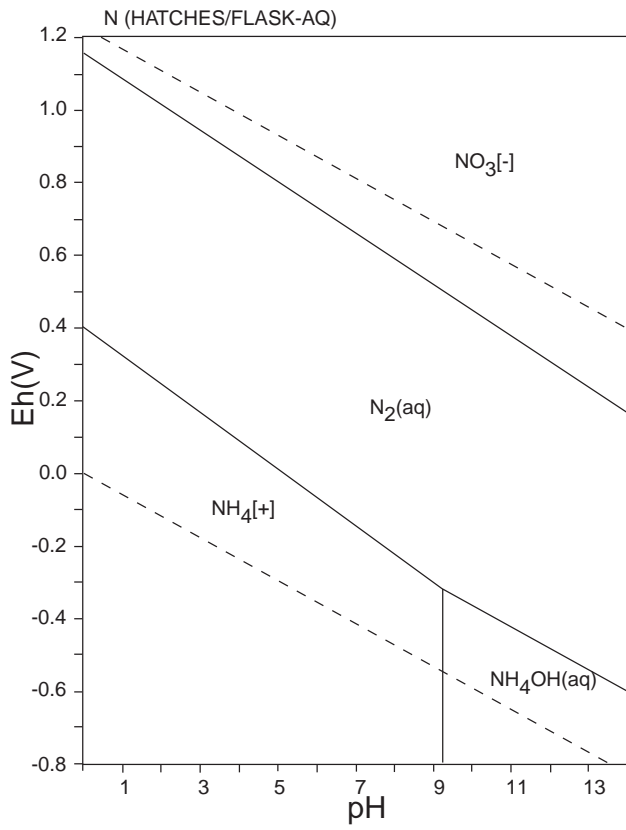
表 45: List of N species

FACT	SUPCRT	LLNL	JNC-TDB
$N_2(aq)$ , $NH_3(aq)$ , $NH_4[+]$ , $N_2H_5[+]$ , $ONO[-]$ , $N_2O_2[2-]$ , $NO_3[-]$ , $HONO(aq)$ , $N_3[-]$ , $N_2H_4(aq)$ , $HN_3(aq)$ , <b><math>NH_4N_3(s)</math></b> , <b><math>N_2O_4(s)</math></b> , <b><math>N_2O_5(s)</math></b> , <b><math>NH_4NO_3(s)</math></b>	$N_2(aq)$ , $NH_3(aq)$ , $NH_4[+]$ , $N_2H_5[+]$ , $NO_2[-]$ , $N_2O_2[2-]$ , $NO_3[-]$ , $HNO_2(aq)$ , $HNO_3(aq)$ , $H_2N_2O_2(aq)$ , $HN_2O_2[-]$ , $N_2H_6[2+]$	$NO_3[-]$ , $N_2(aq)$ , $NH_4[+]$ , $NO_2[-]$ , $HNO_2(aq)$ , $NH_3(aq)$ , $N_2(g)$	$NO_3[-]$ , $NH_3(aq)$ , $NH_4[+]$ , $NO_2[-]$ , $N_2(aq)$ , $N(g)$ , $N_2(g)$ , $NH_3(g)$

HATCHES			
$NO_3[-]$ , $N_2(aq)$ , $NH_4[+]$ , $NO_2[-]$ , $HNO_3(aq)$ , $NH_3(aq)$ , $NH_4NO_3(aq)$ , $NH_4OH(aq)$			



73: Eh-pH diagrams of the system N-O-H (1).  $\sum \text{N} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 74: Eh-pH diagrams of the system N-O-H (2).  $\sum N = 10^{-10}$ , 298.15K,  $10^5$  Pa.





表 46: List of Na species

FACT	SUPCRT	LLNL	JNC-TDB
Na[+], <b>Na(s)</b> , <b>NaH(s)</b> , <b>NaO<sub>2</sub>(s)</b> , <b>Na<sub>2</sub>O(s2)</b> , <b>Na<sub>2</sub>O(s3)</b> , <b>Na<sub>2</sub>O<sub>2</sub>(s)</b> , <b>Na<sub>2</sub>O<sub>2</sub>(s2)</b> , <b>NaOH(s)</b> , <b>NaOH(s2)</b> , <b>Na<sub>2</sub>O(s)</b>	Na[+], NaOH(aq), <b>Na<sub>2</sub>O(Sodium-oxide)</b>	Na[+], NaOH(aq)	Na+, <b>Na(c)</b> , Na(g)

HATCHES			
Na[+]			

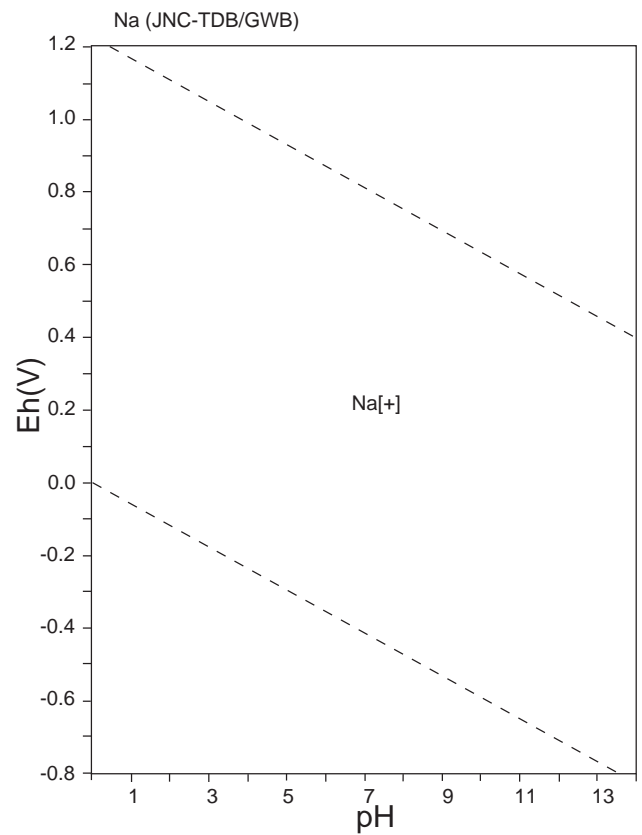
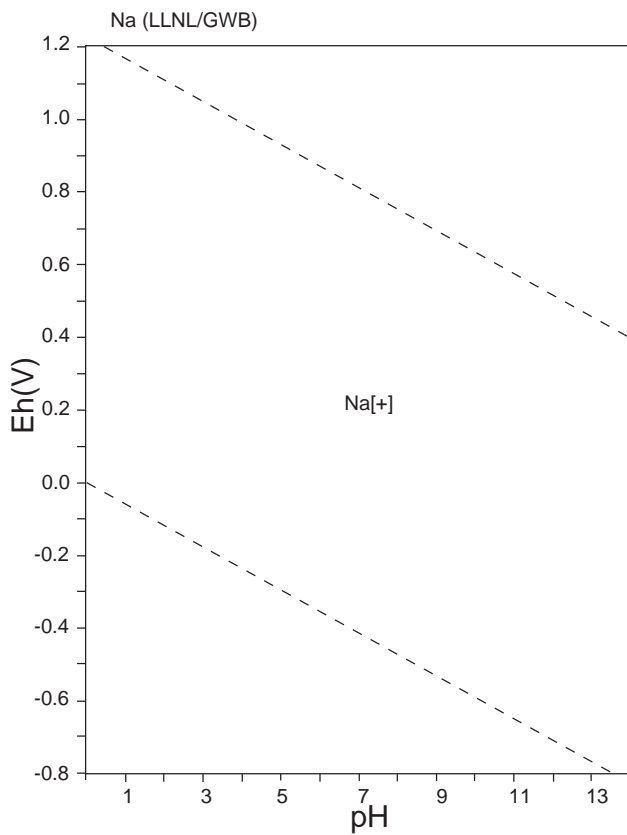
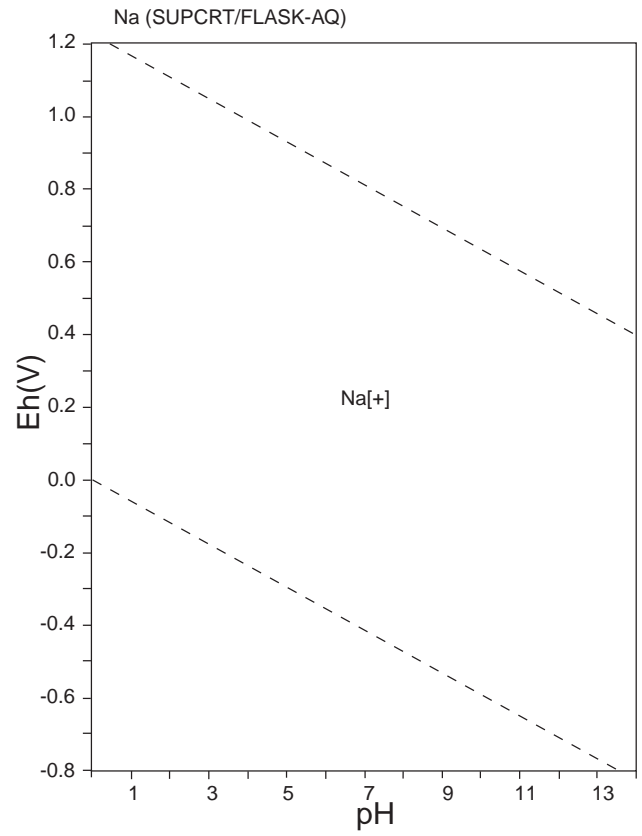
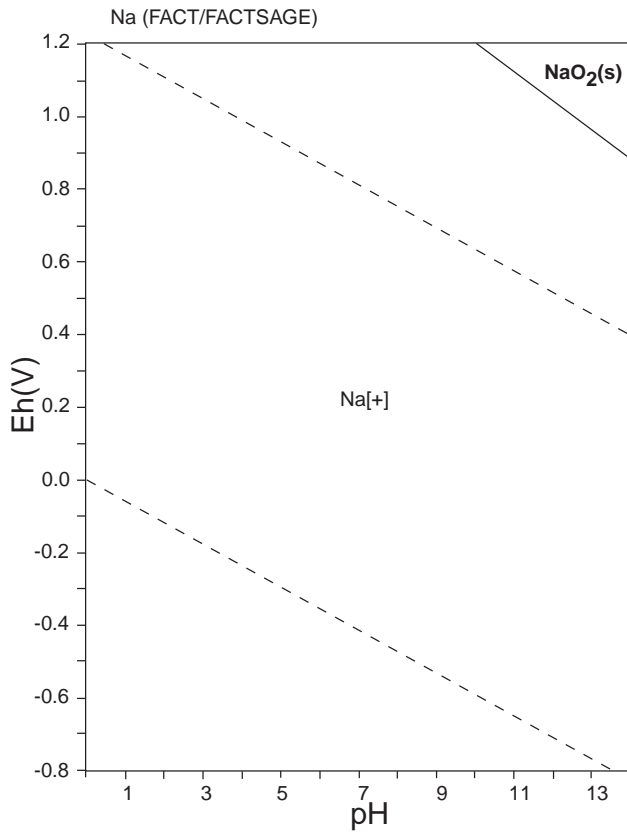


Figure 75: Eh-pH diagrams of the system Na-O-H (1).  $\sum \text{Na} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

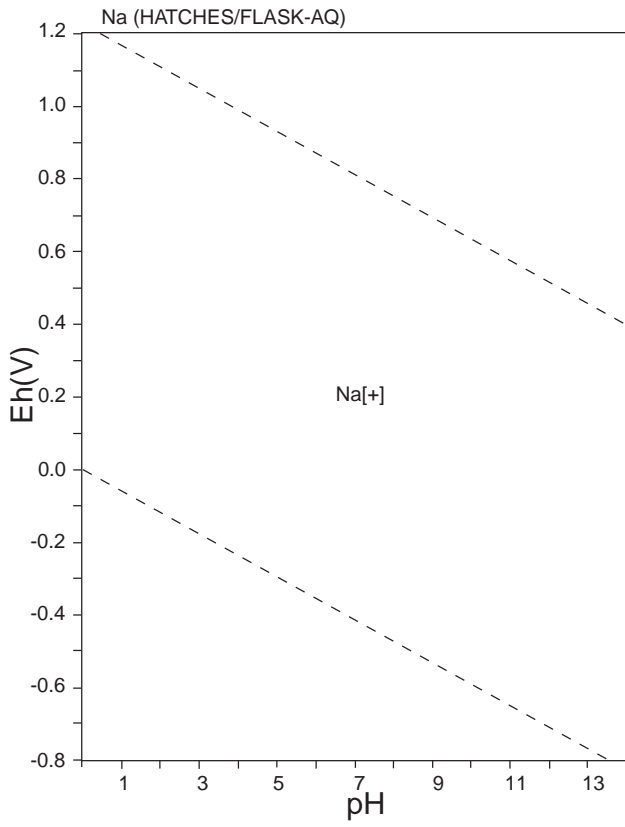


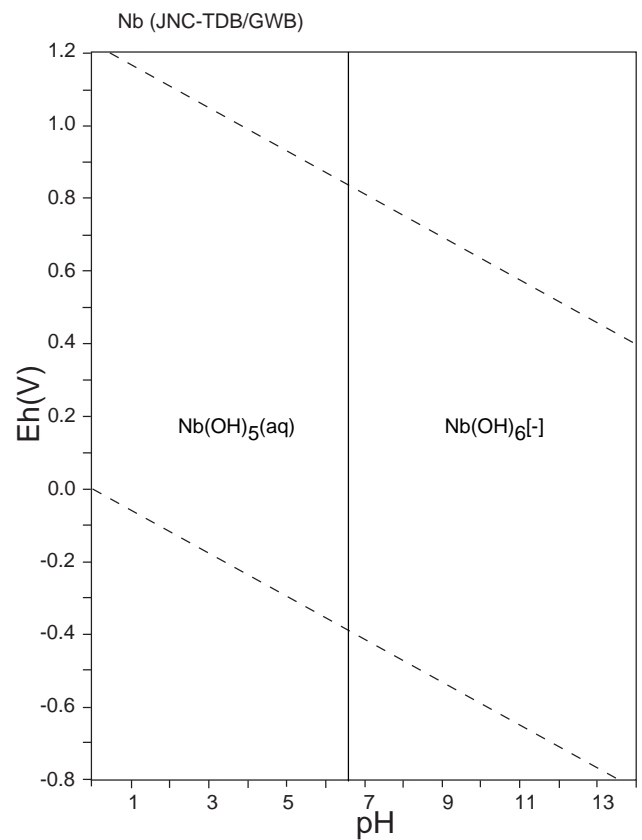
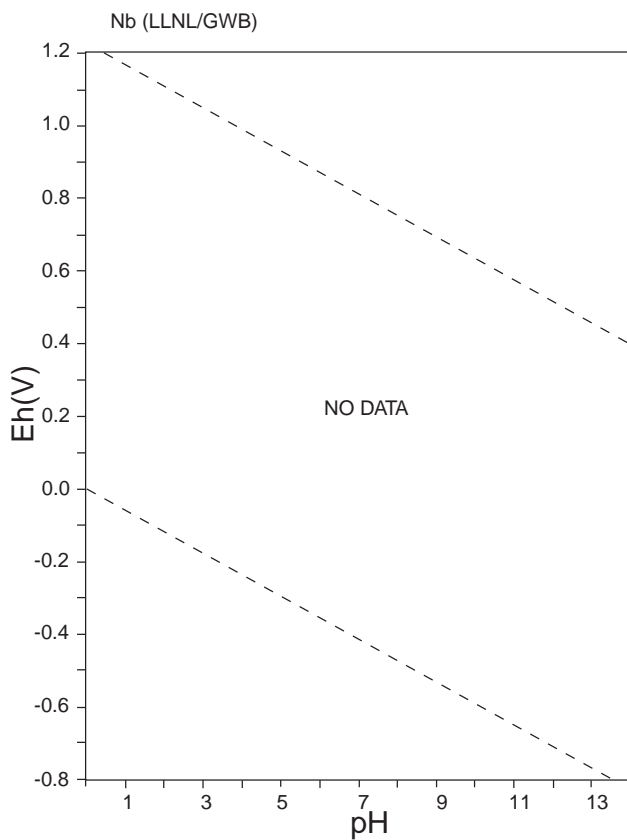
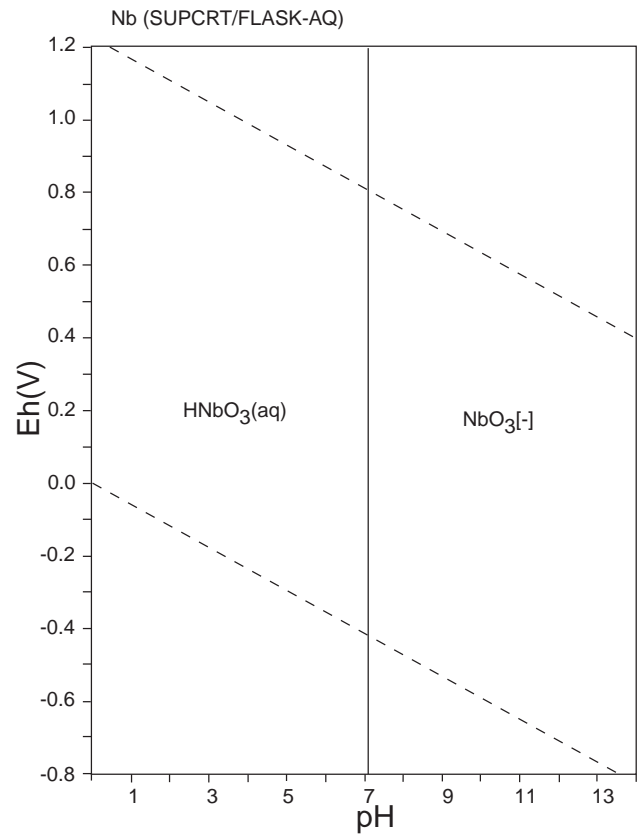
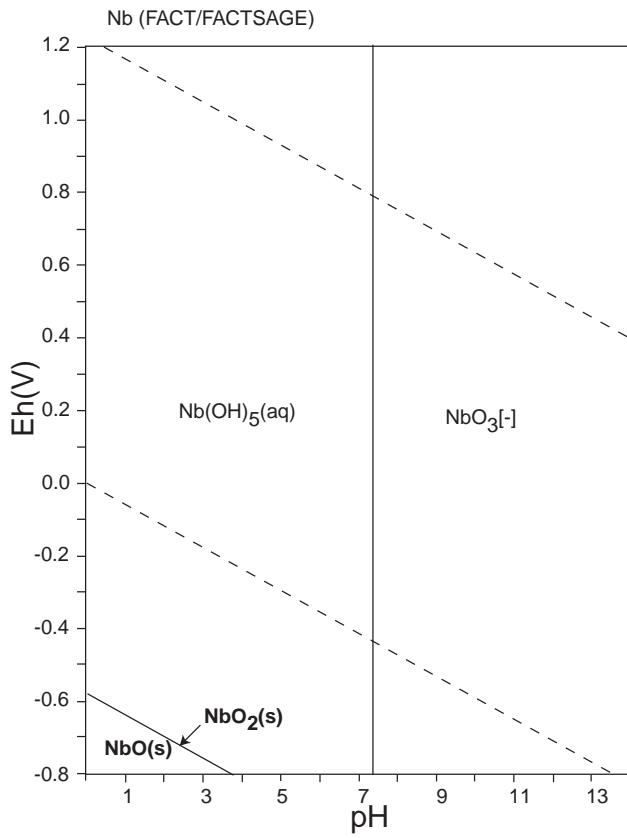
图 76: Eh-pH diagrams of the system Na-O-H (2).  $\sum \text{Na} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



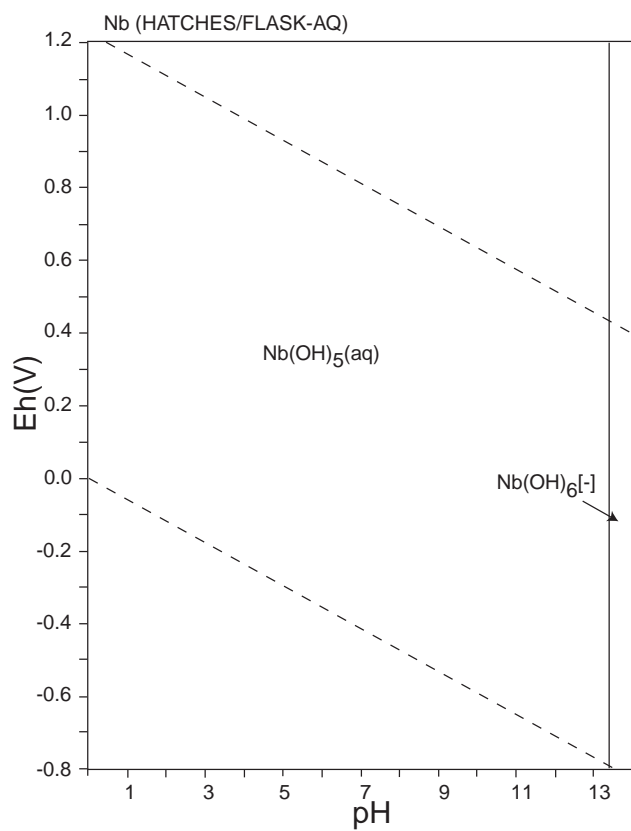
表 47: List of Nb species

FACT	SUPCRT	LLNL	JNC-TDB
$\text{NbO}_3[-]$ , $\text{Nb}(\text{OH})_5(\text{aq})$ , $\text{Nb}(\text{OH})_4[+]$ , <b>Nb(s)</b> , <b>NbO(s)</b> , <b>NbO<sub>2</sub>(s)</b> , <b>NbO<sub>2</sub>(s2)</b> , <b>NbO<sub>2</sub>(s3)</b> , <b>Nb<sub>2</sub>O<sub>5</sub>(s)</b>	$\text{NbO}_3[-]$ , $\text{HNbO}_3(\text{aq})$		$\text{Nb}(\text{OH})_5(\text{aq})$ , $\text{Nb}(\text{OH})_6[-]$ , <b>Nb<sub>2</sub>O<sub>5</sub>(s)</b>

HATCHES			
$\text{Nb}(\text{OH})_5(\text{aq})$ , $\text{Nb}(\text{OH})_4[+]$ , $\text{Nb}(\text{OH})_6[-]$ , <b>Nb<sub>2</sub>O<sub>5</sub>(act)</b>			



☒ 77: Eh-pH diagrams of the system Nb-O-H (1).  $\sum \text{Nb} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 78: Eh-pH diagrams of the system Nb-O-H (2).  $\sum \text{Nb} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





表 48: List of Nd species

FACT	SUPCRT	LLNL	JNC-TDB
Nd[3+], <b>Nd(s)</b> , <b>Nd(s2)</b> , <b>NdH<sub>2</sub>(s)</b> , <b>Nd<sub>2</sub>O<sub>3</sub>(s)</b> , <b>Nd<sub>2</sub>O<sub>3</sub>(s2)</b>	Nd[3+], Nd[4+], Nd[2+], NdOH[2+], NdO[+], NdO <sub>2</sub> H(aq), NdO <sub>2</sub> [-]		Nd[3+]

HATCHES			
Nd[3+], Nd(OH) <sub>2</sub> [+], Nd(OH) <sub>3</sub> (aq), NdOH[2+], <b>Nd(OH)<sub>3</sub></b>			

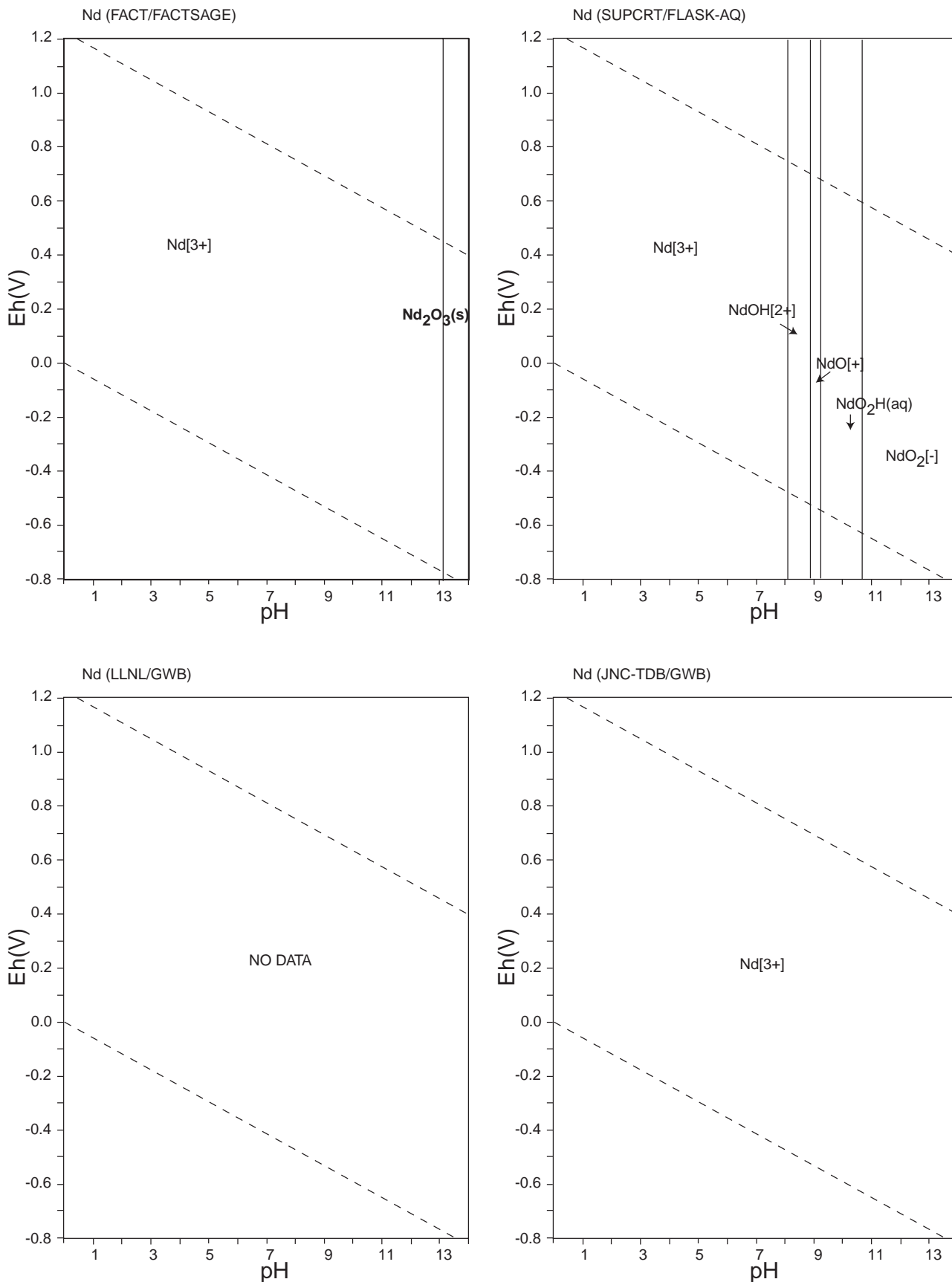


Fig 79: Eh-pH diagrams of the system Nd-O-H (1).  $\sum \text{Nd} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

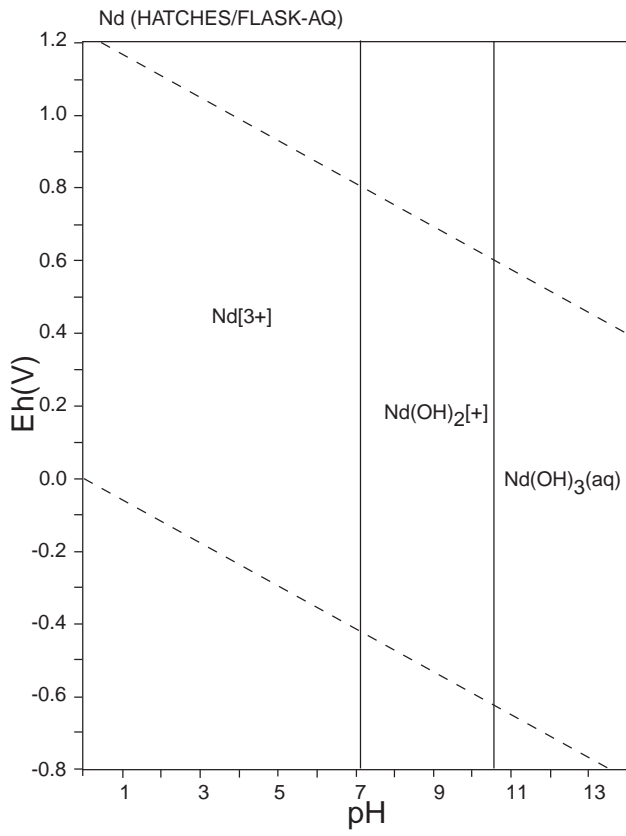


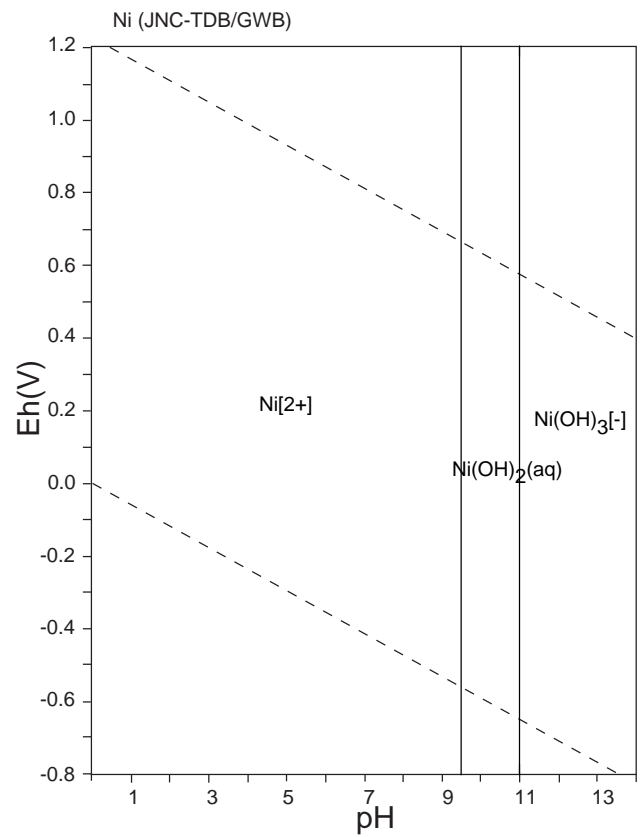
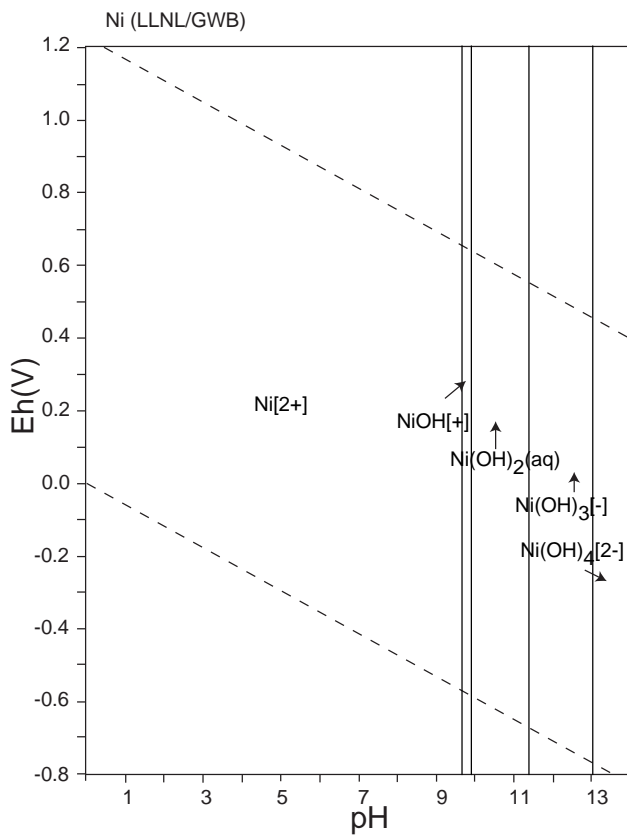
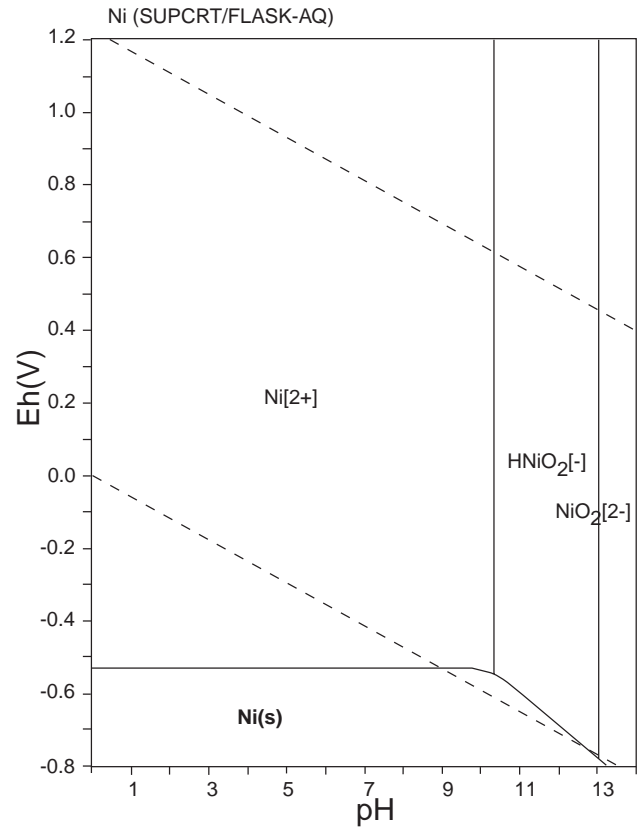
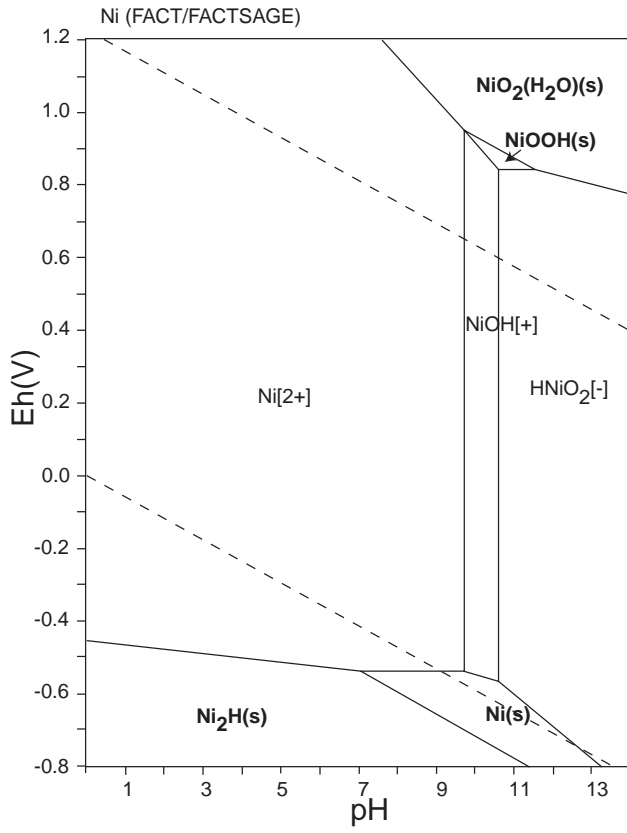
图 80: Eh-pH diagrams of the system Nd-O-H (2).  $\sum Nd = 10^{-10}$ , 298.15K,  $10^5$  Pa.



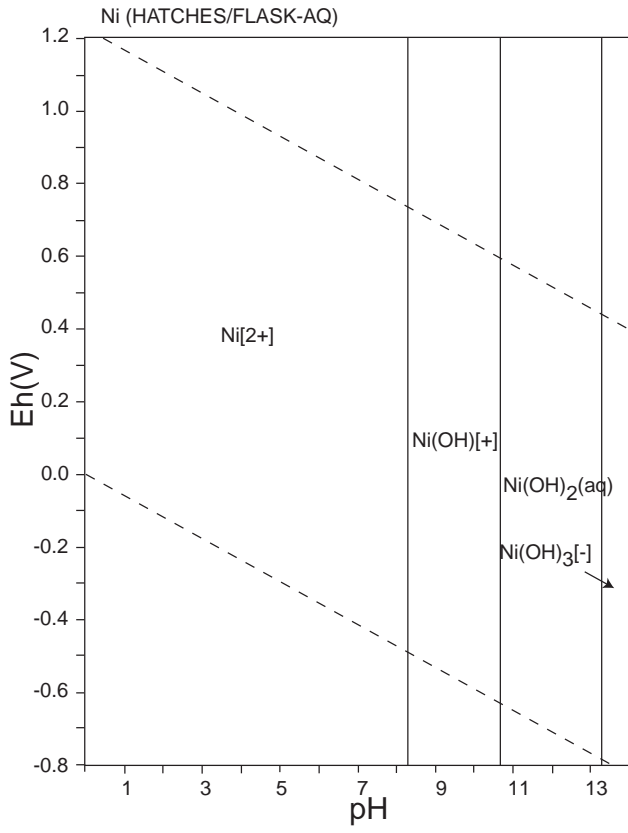
表 49: List of Ni species

FACT	SUPCRT	LLNL	JNC-TDB
Ni[2+], NiOH[+], HNiO <sub>2</sub> [-], <b>Ni<sub>2</sub>H(s)</b> , <b>NiOOH(s)</b> , <b>Ni(OH)<sub>2</sub>(s)</b> , <b>NiO<sub>2</sub>(H<sub>2</sub>O)(s)</b> , <b>Ni(s), NiO(s)</b>	Ni[2+], NiOH[+], HNiO <sub>2</sub> [-], NiO(aq), NiO <sub>2</sub> [2-], <b>Ni(Nickel)</b> , <b>NiO(Bunsenite)</b>	Ni[2+], Ni(OH) <sub>2</sub> , Ni(OH) <sub>3</sub> [-], Ni(OH) <sub>4</sub> [2-], Ni <sub>2</sub> OH[3+], Ni <sub>4</sub> (OH) <sub>4</sub> [4+], NiOH[+], <b>Ni(OH)<sub>2</sub>(s), NiO(s)</b>	Ni[2+], Ni(OH) <sub>2</sub> (aq), Ni(OH) <sub>3</sub> [-], NiOH[+], Ni <sub>2</sub> (OH)[+], Ni <sub>4</sub> (OH)[+], <b>Ni(OH)<sub>2</sub>(s), NiO(c)</b>

HATCHES			
Ni[2+], Ni(OH)[+], Ni(OH) <sub>2</sub> (aq), Ni(OH) <sub>3</sub> [-], Ni <sub>2</sub> (OH)[3+], Ni <sub>4</sub> (OH) <sub>4</sub> [4+], <b>Ni(OH)<sub>2</sub>, NiO</b>			



81: Eh-pH diagrams of the system Ni-O-H (1).  $\sum \text{Ni} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 82: Eh-pH diagrams of the system Ni-O-H (2).  $\sum \text{Ni} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





表 50: List of Np species

FACT	SUPCRT	LLNL	JNC-TDB
<b>Np(s), NpO<sub>2</sub>(s), NpO<sub>3</sub>(H<sub>2</sub>O)(s)</b>		Np[4+], Np[3+], NpO <sub>2</sub> [+], NpO <sub>2</sub> [2+], (NpO <sub>2</sub> ) <sub>2</sub> (OH) <sub>2</sub> [2+], (NpO <sub>2</sub> ) <sub>3</sub> (OH) <sub>5</sub> [+], Np(OH) <sub>2</sub> [2+], Np(OH) <sub>3</sub> [+], Np(OH) <sub>4</sub> (aq), Np(OH) <sub>5</sub> [-], NpO <sub>2</sub> OH(aq), NpO <sub>2</sub> OH[+], NpOH[2+], NpOH[3+], <b>Np(s), Np(OH)<sub>4</sub>(s), Np<sub>2</sub>O<sub>5</sub>(s), NpO<sub>2</sub>(s), NpO<sub>2</sub>(OH)(am), NpO<sub>2</sub>(OH)<sub>2</sub>(s)</b>	Np[4+], Np[3+], NpO <sub>2</sub> [+], NpO <sub>2</sub> OH(am), NpO <sub>2</sub> (OH) <sub>2</sub> [-], NpO <sub>2</sub> [2+], NpOH[3+], <b>Np(OH)<sub>4</sub>(s), NpO<sub>2</sub>(am), NpO<sub>2</sub>OH(am)</b>

HATCHES	OECD-NEA	OECD-NEA update	
Np[4+], Np[3+], NpO <sub>2</sub> [+], NpO <sub>2</sub> [2+], Np(OH) <sub>2</sub> [+], Np(OH) <sub>3</sub> (aq), Np(OH) <sub>4</sub> (aq), Np(OH) <sub>4</sub> [-], Np <sub>2</sub> (OH) <sub>2</sub> [4+], NpO <sub>2</sub> OH <sub>2</sub> [2+], NpO <sub>2</sub> OH <sub>5</sub> [+], NpO <sub>2</sub> OH(aq), NpO <sub>2</sub> OH <sub>2</sub> [-], NpOH[2+], NpOH[3+], <b>Np, Np(OH)<sub>3</sub>, Np(OH)<sub>4</sub>, Np<sub>2</sub>O<sub>5</sub>, NpO<sub>2</sub>, NpO<sub>2</sub>(am), NpO<sub>2</sub>(OH)<sub>2</sub>, NpO<sub>2</sub>OH, NpO<sub>2</sub>OH(am,aged), NpO<sub>2</sub>OH(am,fresh), NpO<sub>3</sub>*H<sub>2</sub>O(cr)</b>	Np[4+], Np[3+], NpO <sub>2</sub> [+], NpO <sub>2</sub> [2+], NpOH[2+], NpOH[3+], NpO <sub>2</sub> OH(aq), NpO <sub>2</sub> OH[+], NpO <sub>2</sub> (OH) <sub>2</sub> [-], Np(OH) <sub>4</sub> (aq), (NpO <sub>2</sub> ) <sub>2</sub> (OH) <sub>2</sub> [2+], (NpO <sub>2</sub> ) <sub>3</sub> (OH) <sub>5</sub> [+], <b>Np(c), NpO<sub>2</sub>(am_hyd), NpO<sub>2</sub>(c), Np<sub>2</sub>O<sub>5</sub>(c), NpO<sub>2</sub>OH(am_aged), NpO<sub>2</sub>OH(am_fresh), NpO<sub>2</sub>(OH)<sub>2</sub>(c), NpO<sub>3</sub>H<sub>2</sub>O(c)</b>	Np[4+], Np[3+], NpO <sub>2</sub> [+], NpO <sub>2</sub> [2+], NpOH[2+], NpOH[3+], Np(OH) <sub>2</sub> [2+], NpO <sub>2</sub> OH(aq), NpO <sub>2</sub> OH[+], NpO <sub>2</sub> (OH) <sub>2</sub> [-], Np(OH) <sub>4</sub> (aq), (NpO <sub>2</sub> ) <sub>2</sub> (OH) <sub>2</sub> [2+], (NpO <sub>2</sub> ) <sub>3</sub> (OH) <sub>5</sub> [+], <b>Np(cr), NpO<sub>2</sub>(cr), Np<sub>2</sub>O<sub>5</sub>(cr), NpO<sub>2</sub>(OH)<sub>2</sub>(cr), NpO<sub>3</sub>H<sub>2</sub>O(cr)</b>	

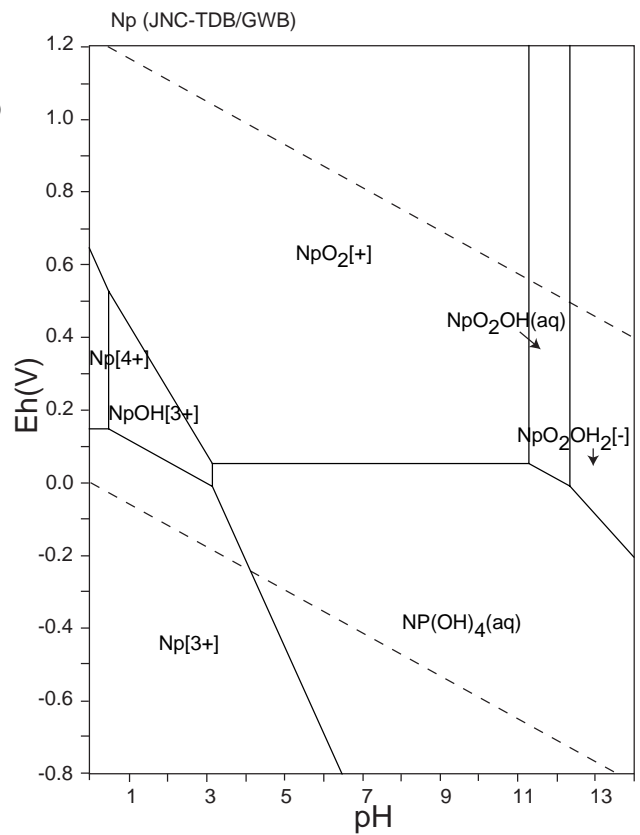
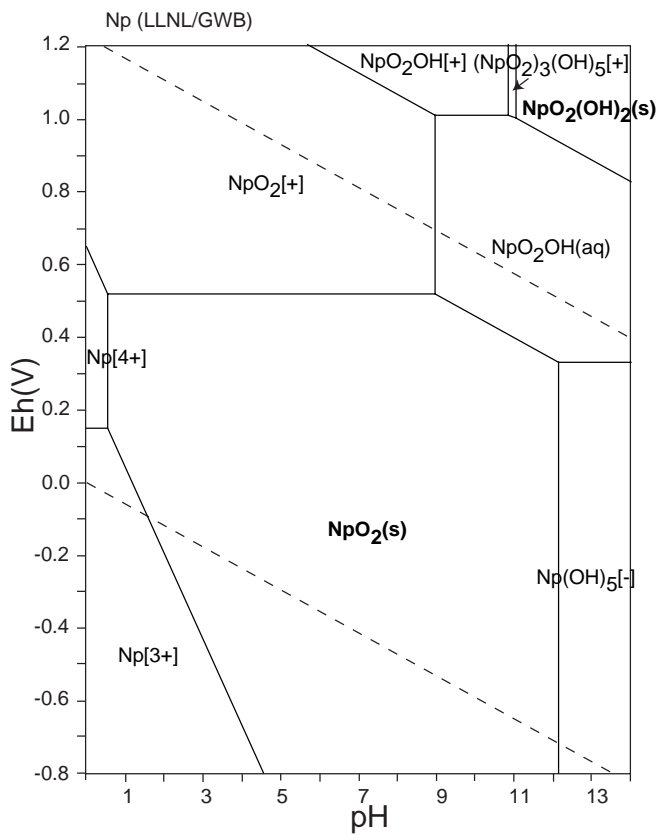
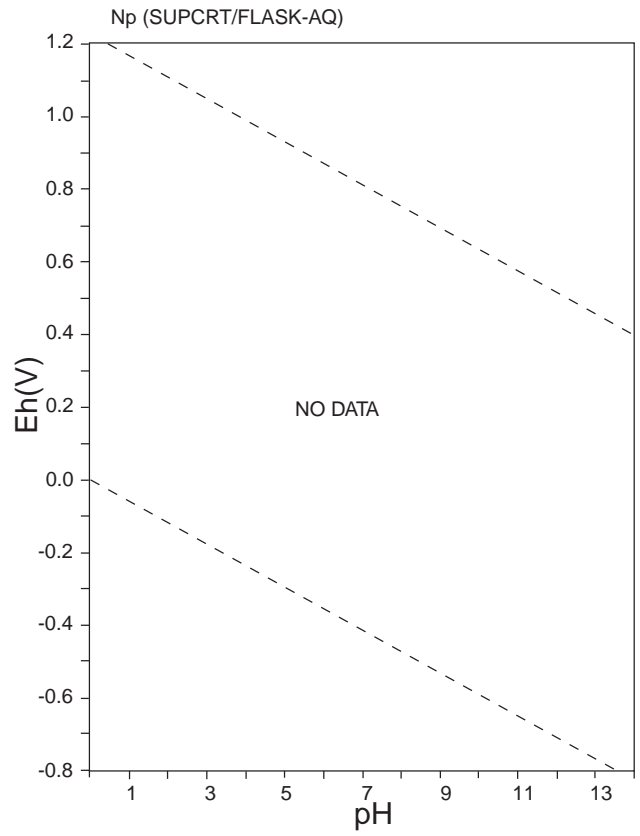
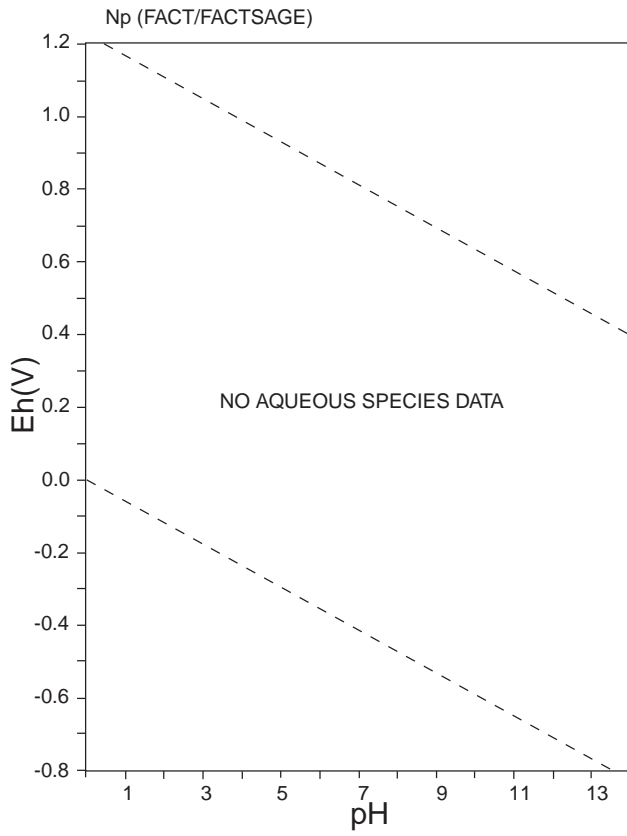
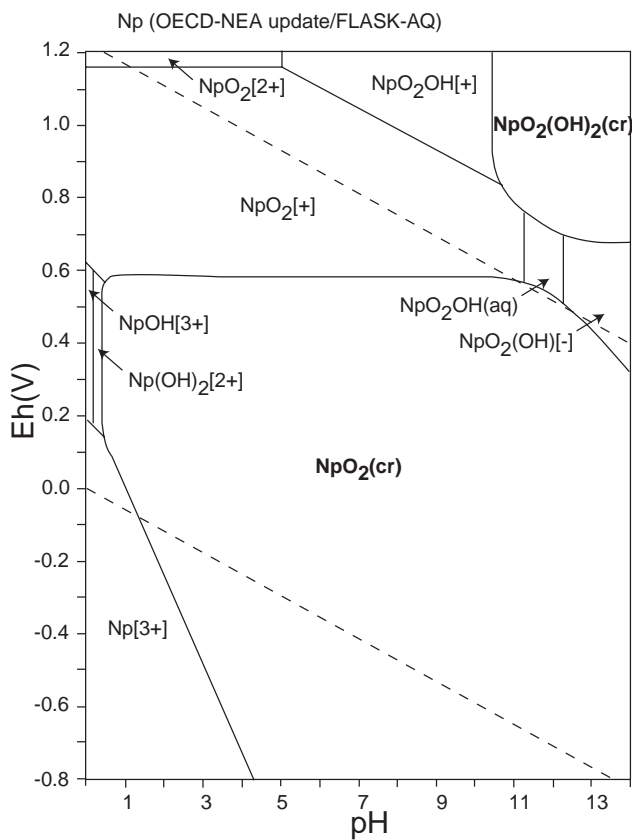
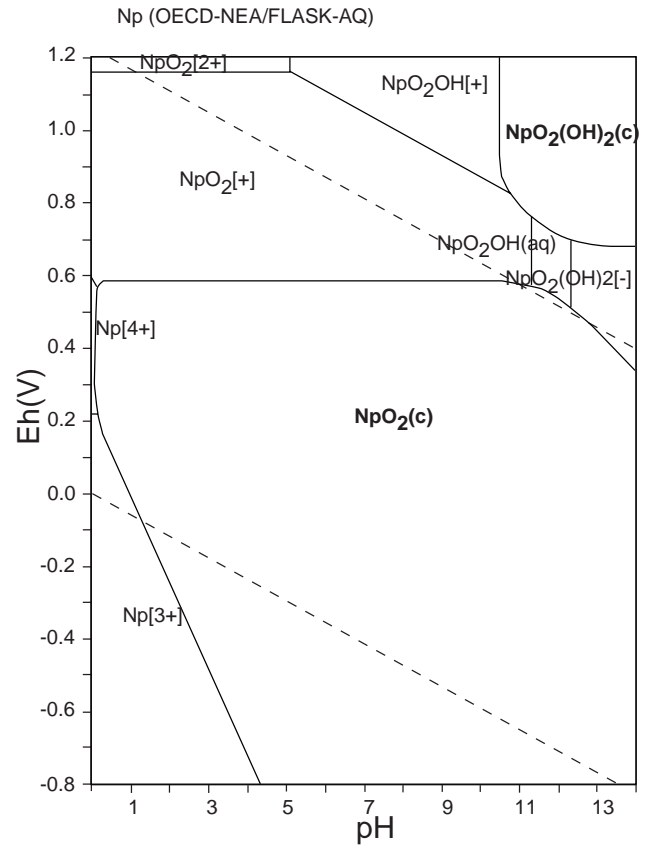
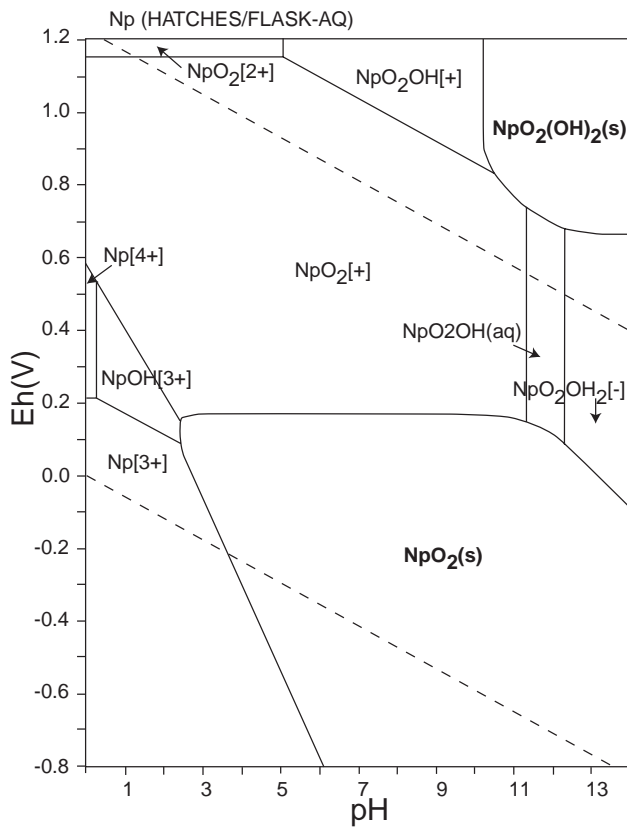


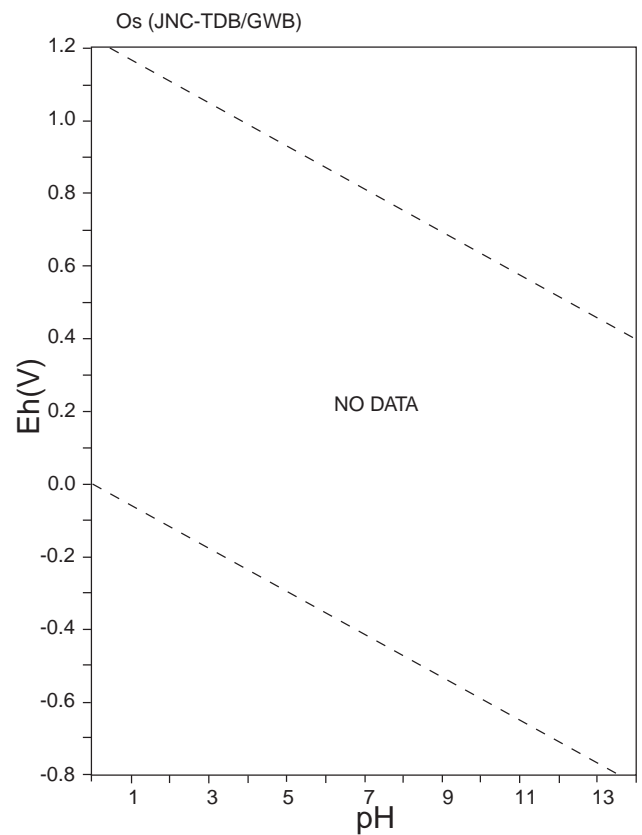
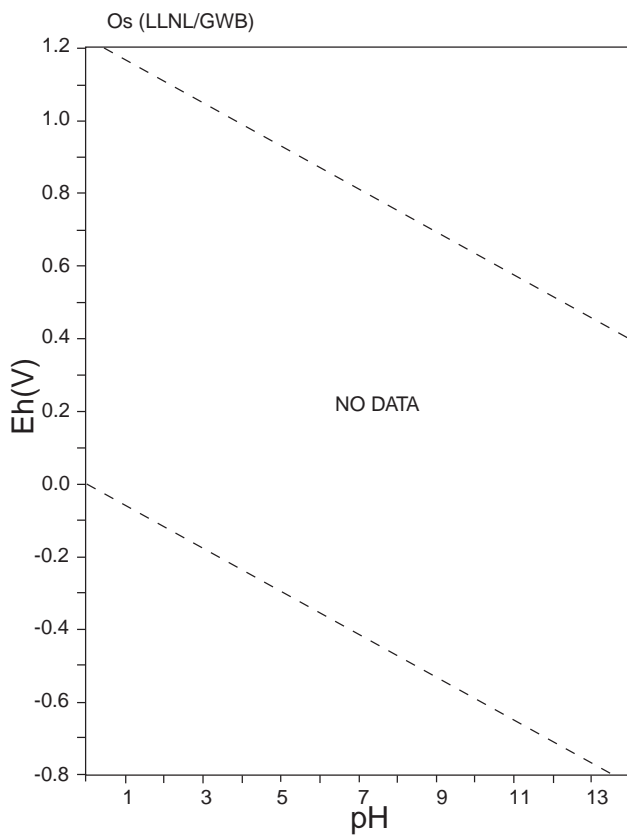
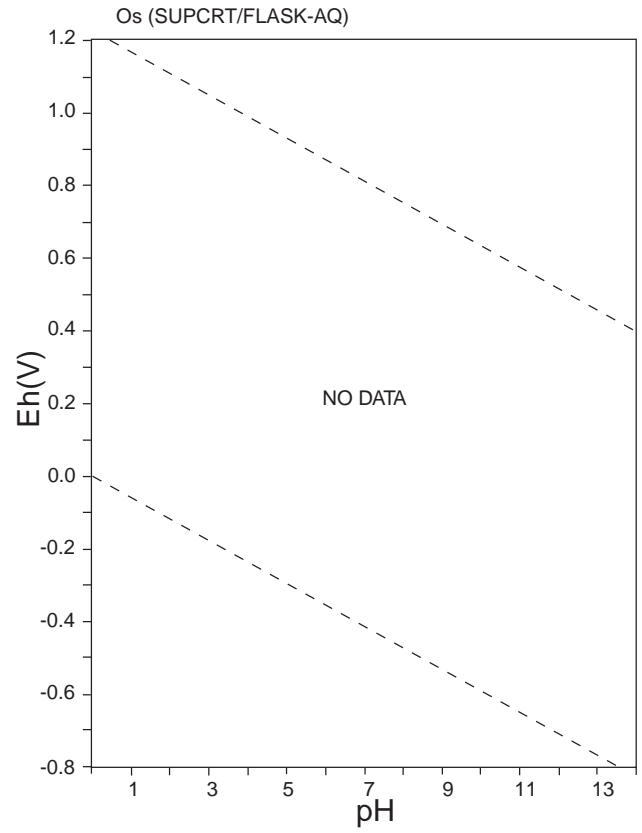
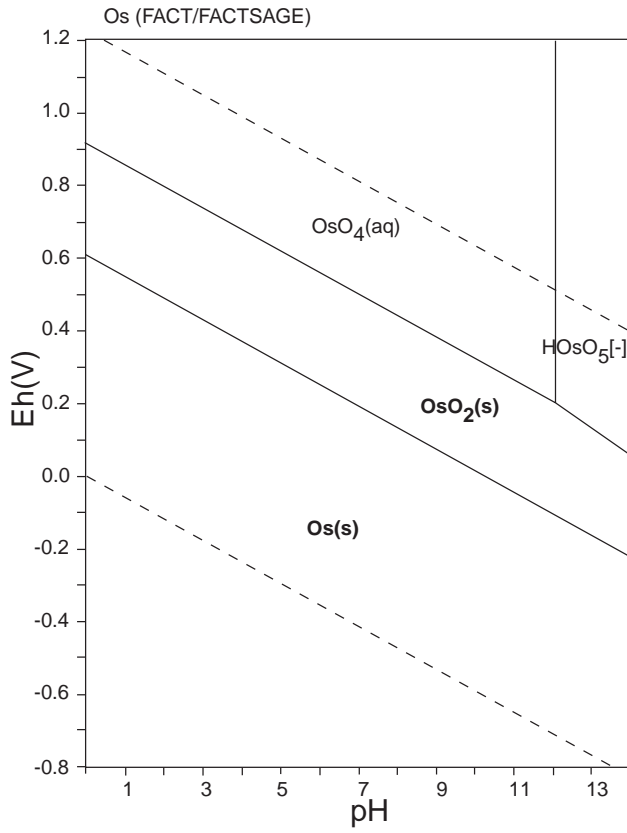
图 83: Eh-pH diagrams of the system Np-O-H (1).  $\sum \text{Np} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 84: Eh-pH diagrams of the system Np-O-H (2).  $\Sigma \text{Np} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 51: List of Os species

FACT	SUPCRT	LLNL	JNC-TDB
$\text{OsO}_4(\text{aq})$ , $\text{HOsO}_5[-]$ , $\text{H}_2\text{OsO}_5[-]$ , $\text{Os}(\mathbf{s})$ , $\text{OsO}_2(\mathbf{s})$ , $\text{OsO}_4(\mathbf{s})$ , $\text{OsO}_4(\mathbf{s2})$ , $\text{Os}(\text{OH})_4(\mathbf{s})$			



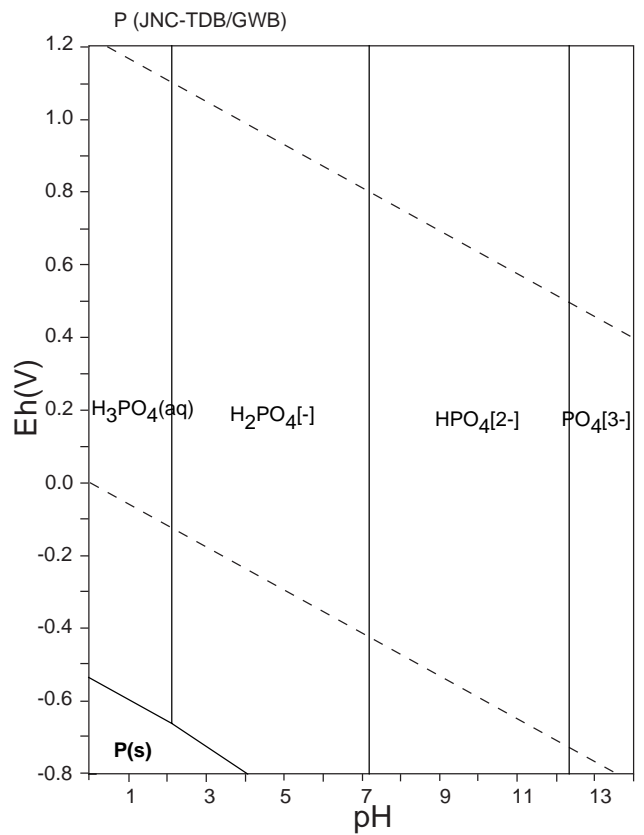
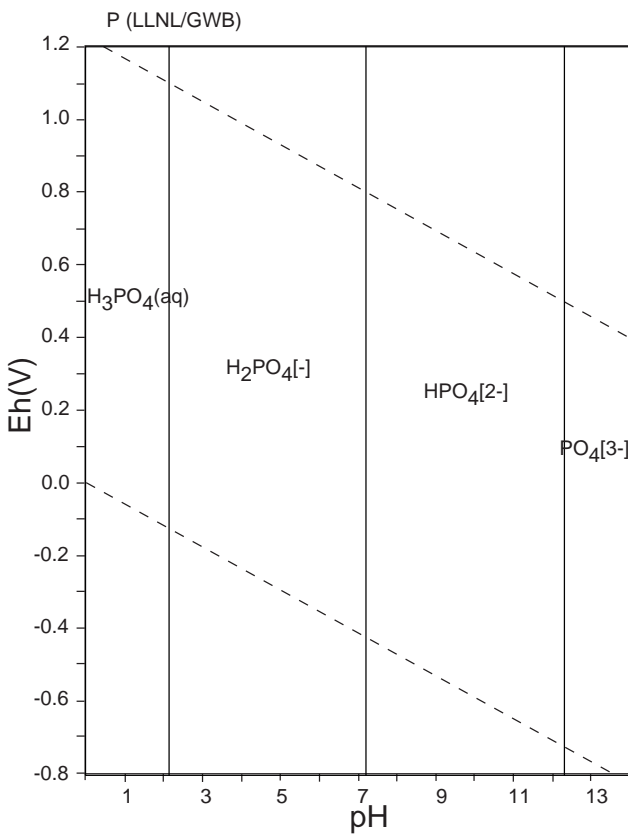
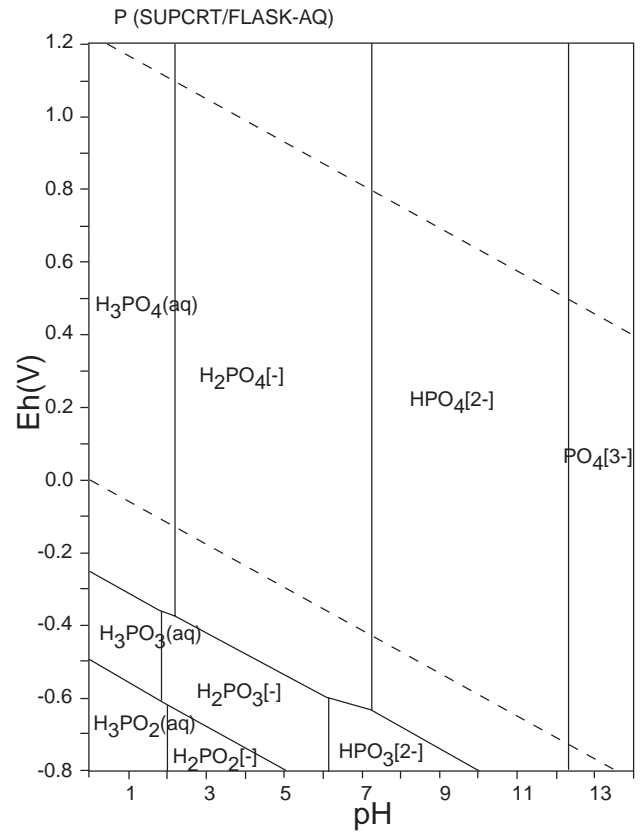
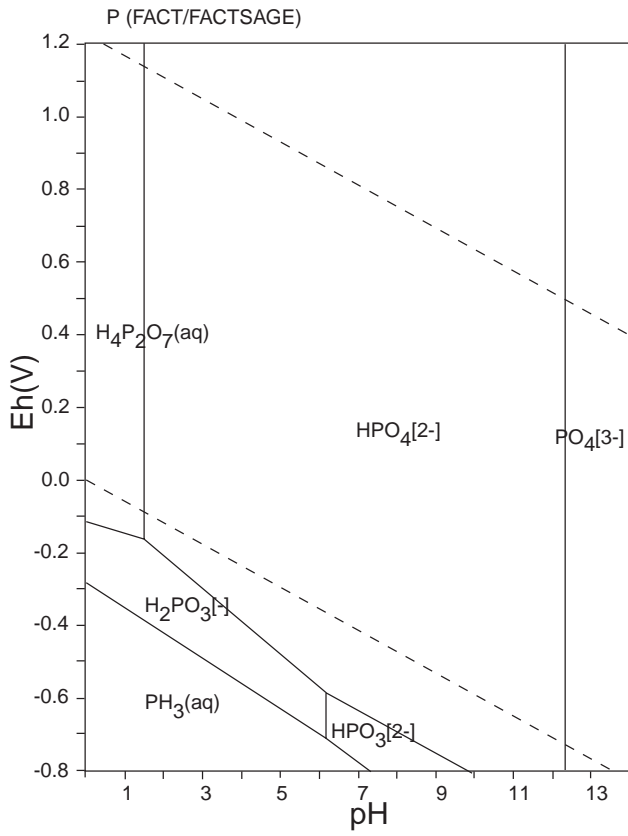
☒ 85: Eh-pH diagrams of the system Os-O-H.  $\sum \text{Os} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 52: List of P species

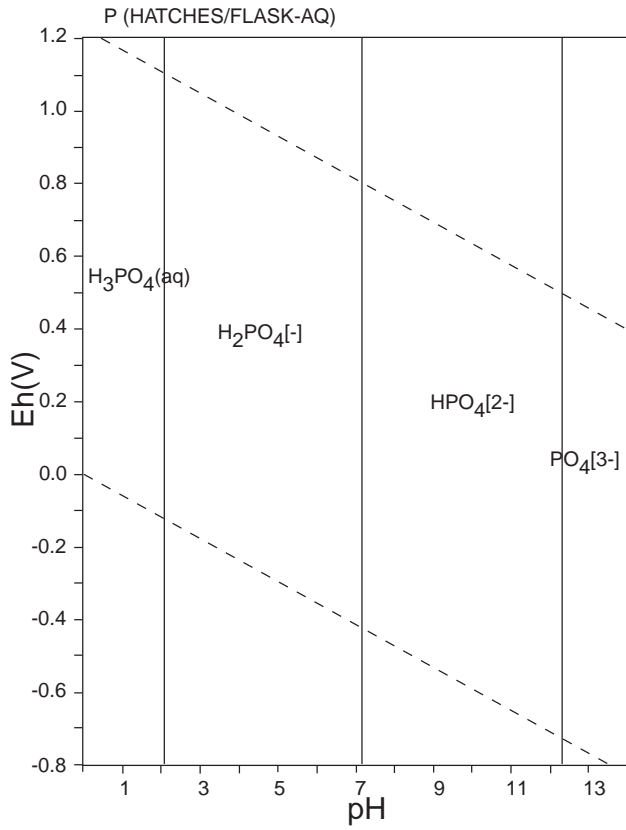
FACT	SUPCRT	LLNL	JNC-TDB
$\text{PO}_4[3-]$ , $\text{P}_2\text{O}_7[4-]$ , $\text{HPO}_3[2-]$ , $\text{H}_2\text{PO}_3[-]$ , $\text{HPO}_4[2-]$ , $\text{H}_2\text{PO}_4[-]$ , $\text{H}_3\text{PO}_4(\text{aq})$ , $\text{HP}_2\text{O}_7[3-]$ , $\text{H}_2\text{P}_2\text{O}_7[2-]$ , $\text{H}_3\text{P}_2\text{O}_7[-]$ , $\text{H}_4\text{P}_2\text{O}_7(\text{aq})$ , $\text{PH}_3(\text{aq})$ , $\text{PH}_4[+]$ , <b>P(s)</b> , <b>P(s2)</b> , <b>P(s3)</b> , <b>P(s4)</b> , <b>(P<sub>2</sub>O<sub>5</sub>)<sub>2</sub>(s)</b> , <b>H<sub>3</sub>PO<sub>4</sub>(s)</b> , <b>(H<sub>3</sub>PO<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)(s)</b>	$\text{PO}_4[3-]$ , $\text{P}_2\text{O}_7[4-]$ , $\text{HPO}_3[2-]$ , $\text{HPO}_4[2-]$ , $\text{H}_2\text{PO}_4[-]$ , $\text{H}_3\text{PO}_4(\text{aq})$ , $\text{HP}_2\text{O}_7[3-]$ , $\text{H}_3\text{P}_2\text{O}_7[-]$ , $\text{H}_4\text{P}_2\text{O}_7(\text{aq})$ , $\text{H}_3\text{PO}_2(\text{aq})$ , $\text{H}_2\text{PO}_2[-]$ , $\text{H}_3\text{PO}_3(\text{aq})$ , $\text{H}_2\text{P}_2\text{O}_7[2-]$ , $\text{H}_2\text{PO}_3[-]$	$\text{HPO}_4[2-]$ , $\text{H}_2\text{P}_2\text{O}_7[2-]$ , $\text{H}_2\text{PO}_4[-]$ , $\text{H}_3\text{P}_2\text{O}_7[-]$ $\text{H}_3\text{PO}_4(\text{aq})$ , $\text{H}_4\text{P}_2\text{O}_7(\text{aq})$ , $\text{HP}_2\text{O}_7[3-]$ , $\text{P}_2\text{O}_7[4-]$ , $\text{PO}_4[3-]$	$\text{PO}_4[3-]$ , $\text{P}_2\text{O}_7[4-]$ , $\text{HPO}_4[2-]$ , $\text{H}_2\text{PO}_4[-]$ , $\text{H}_3\text{PO}_4(\text{aq})$ , $\text{HP}_2\text{O}_7[3-]$ , $\text{H}_2\text{P}_2\text{O}_7[2-]$ , $\text{H}_3\text{P}_2\text{O}_7[-]$ , <b>H<sub>4</sub>P<sub>2</sub>O<sub>7</sub>(am)</b> , <b>P(am)</b> <b>P(c)</b> , <b>P(g)</b> , <b>P<sub>2</sub>(g)</b> , <b>P<sub>4</sub>(g)</b>

HATCHES			
$\text{PO}_4[3-]$ , $\text{H}_2\text{PO}_4[-]$ , $\text{HPO}_4[2-]$ , $\text{H}_2\text{P}_2\text{O}_7[2-]$ , $\text{H}_3\text{P}_2\text{O}_7[-]$ , $\text{H}_3\text{PO}_4(\text{aq})$ , $\text{H}_4\text{P}_2\text{O}_7(\text{aq})$ , $\text{HP}_2\text{O}_7[3-]$ , $\text{P}_2\text{O}_7[3-]$			



86: Eh-pH diagrams of the system P-O-H (1).  $\Sigma P = 10^{-10}$ , 298.15K,  $10^5$  Pa.





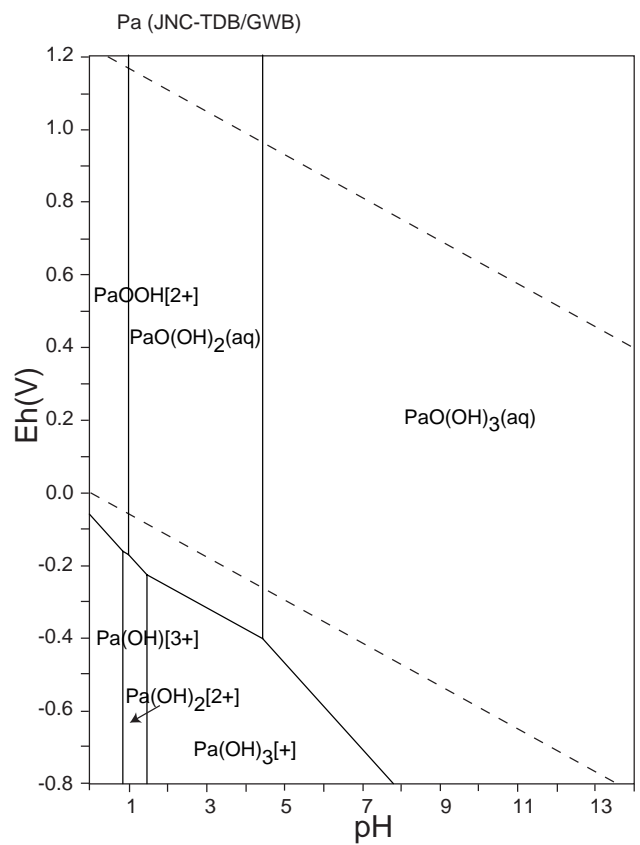
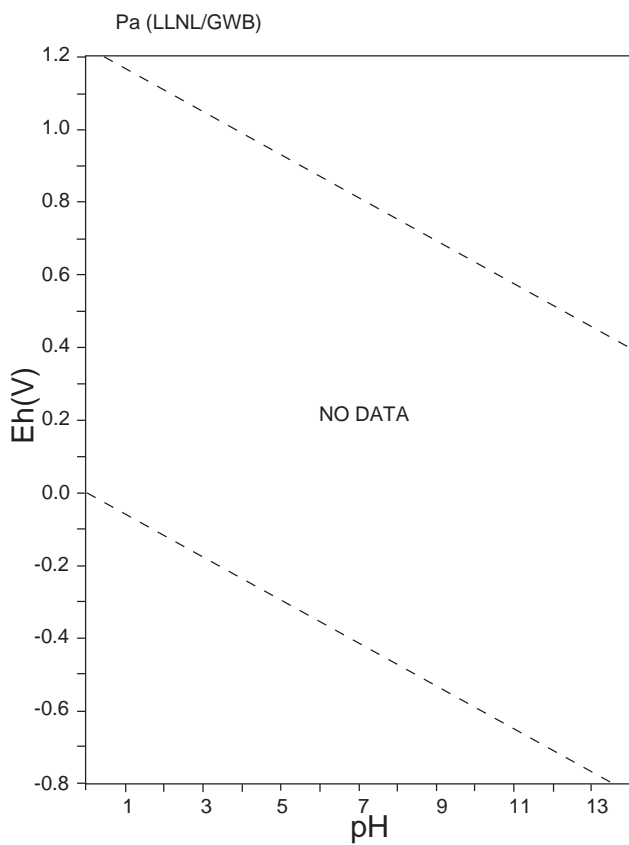
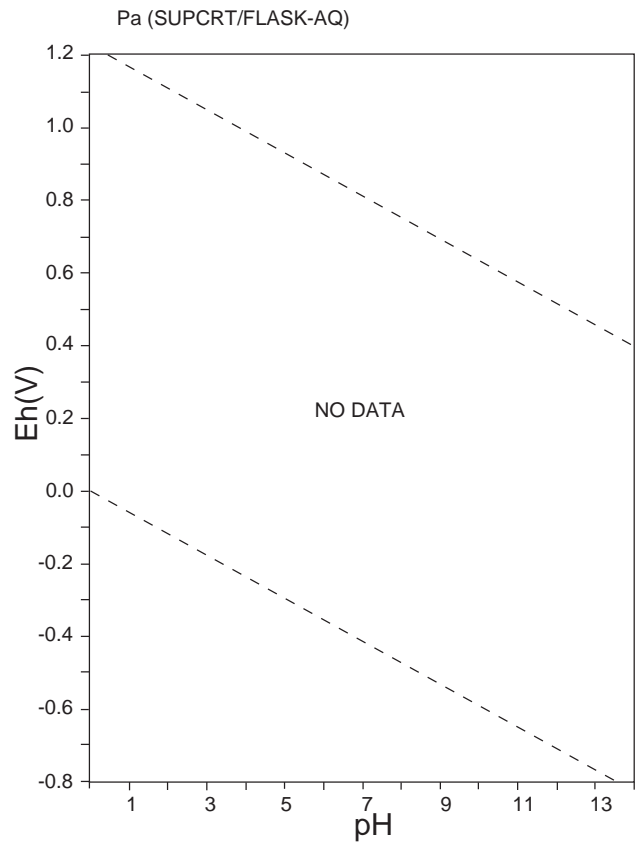
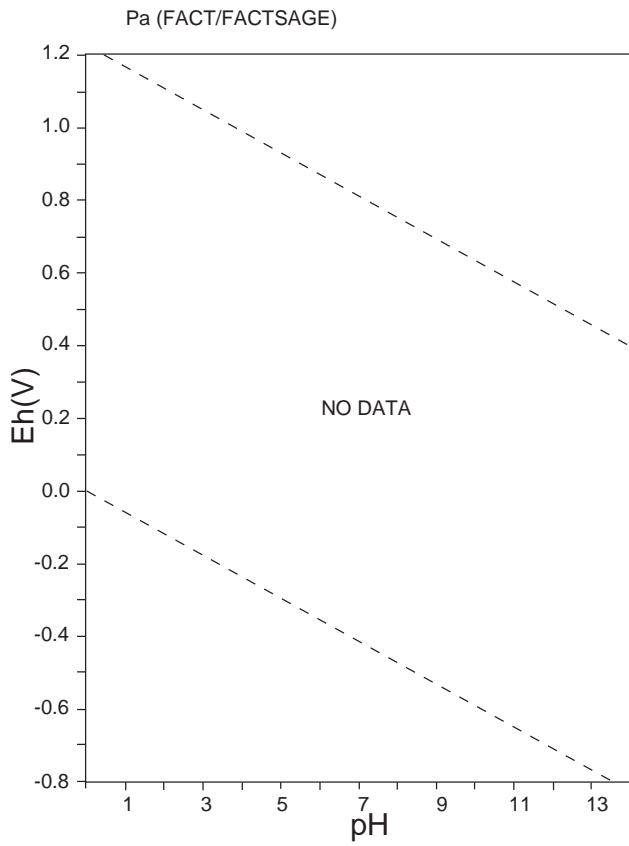
☒ 87: Eh-pH diagrams of the system P-O-H (2).  $\sum \text{P} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



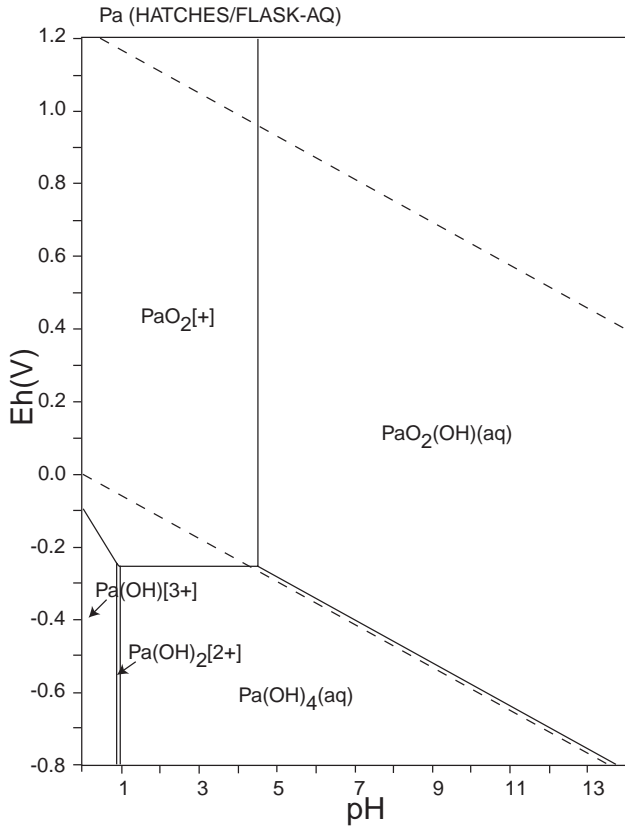
表 53: List of Pa species

FACT	SUPCRT	LLNL	JNC-TDB
			Pa[4+], PaO(OH) <sub>3</sub> (aq) PaO(OH) <sub>2</sub> (aq), PaOOH[2+], Pa(OH)[3+], Pa(OH) <sub>2</sub> [+], Pa(OH) <sub>3</sub> [+], <b>PaO<sub>2</sub>(s),</b> <b>Pa<sub>2</sub>O<sub>5</sub>(s)</b>

HATCHES			
Pa[4+], PaO <sub>2</sub> [+], Pa(OH)[3+], Pa(OH) <sub>2</sub> [2+], Pa(OH) <sub>3</sub> [+], Pa(OH) <sub>4</sub> (aq), PaO(OH)[2+], PaO <sub>2</sub> (OH)(aq), <b>Pa<sub>2</sub>O<sub>5</sub>, PaO<sub>2</sub></b>			



☒ 88: Eh-pH diagrams of the system Pa-O-H (1).  $\sum \text{Pa} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



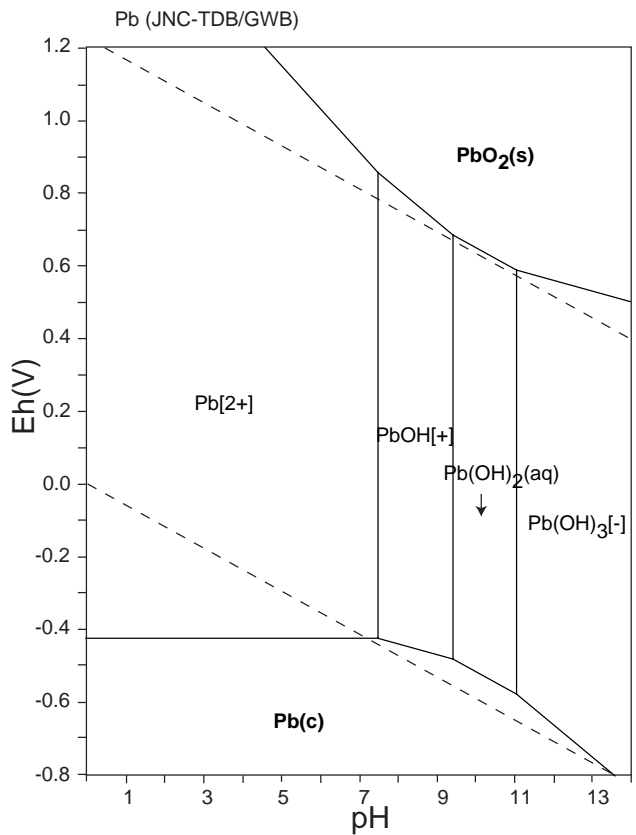
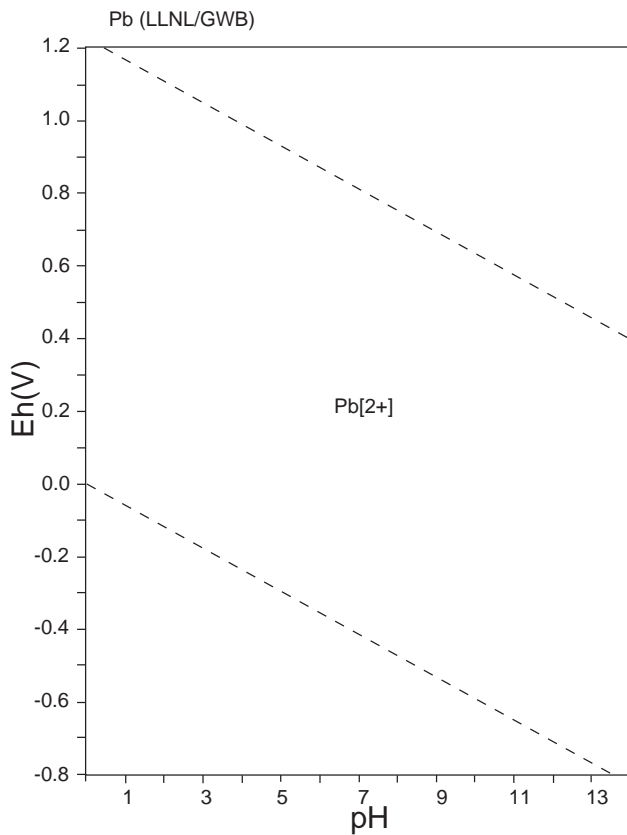
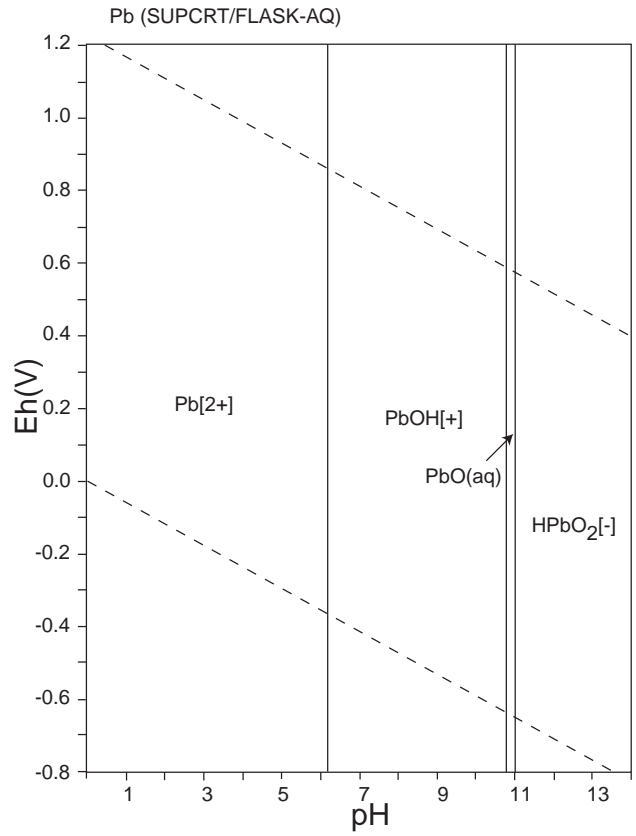
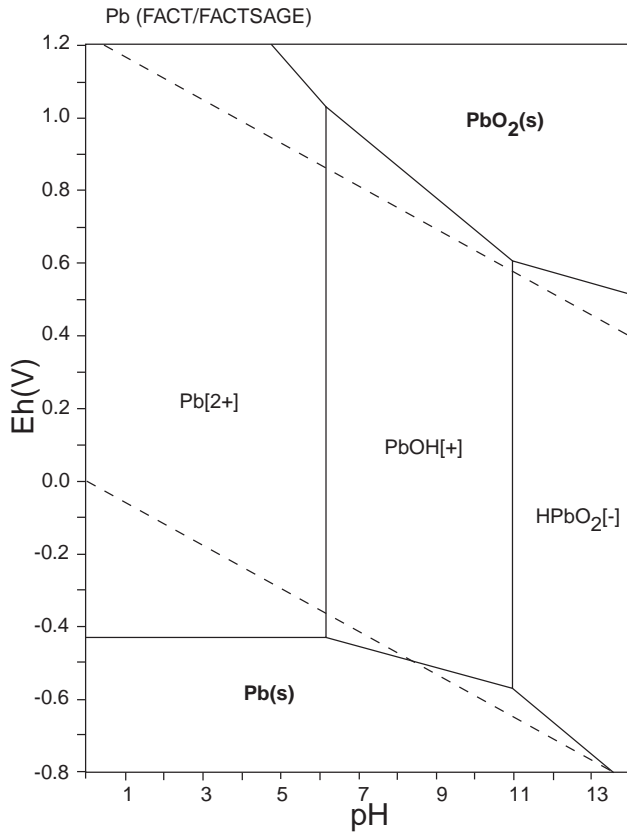
☒ 89: Eh-pH diagrams of the system Pa-O-H (2).  $\sum \text{Pa} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 54: List of Pb species

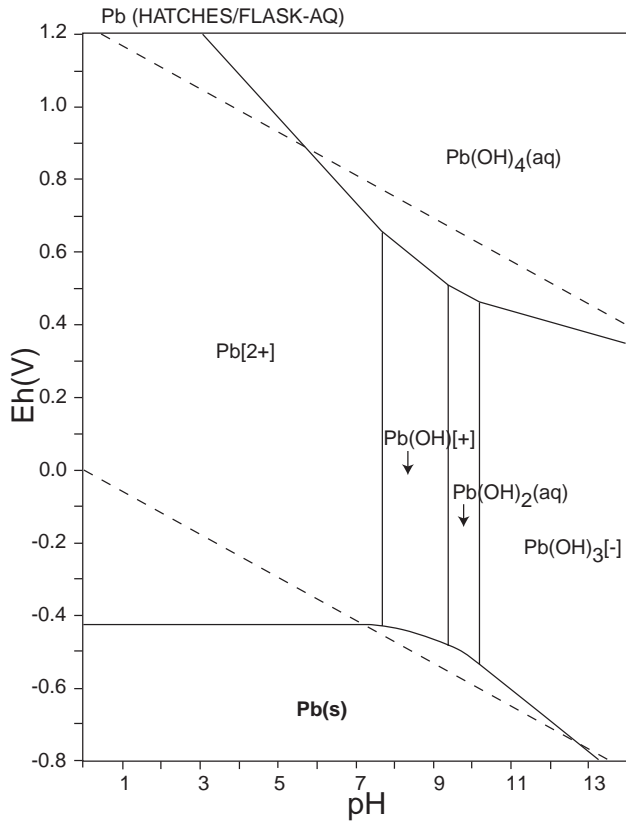
FACT	SUPCRT	LLNL	JNC-TDB
Pb[2+], PbOH[+], HPbO <sub>2</sub> [-], Pb <sub>3</sub> (OH) <sub>4</sub> [2+], Pb <sub>4</sub> (OH) <sub>4</sub> [4+], Pb <sub>6</sub> (OH) <sub>8</sub> [4+], <b>Pb(s), PbO(s2),</b> <b>PbO<sub>2</sub>(s), Pb<sub>3</sub>O<sub>4</sub>(s),</b> <b>Pb(OH)<sub>2</sub>(s),</b> <b>(PbO)<sub>3</sub>(H<sub>2</sub>O)(s),</b> <b>PbO(s)</b>	Pb[2+], PbOH[+], HPbO <sub>2</sub> [-], PbO(aq), <b>PbO(Litharge)</b>	Pb[2+]	Pb[2+], PbOH[+], Pb(OH) <sub>2</sub> (aq), Pb(OH) <sub>3</sub> [-], Pb <sub>2</sub> (OH)[+], Pb <sub>4</sub> (OH) <sub>4</sub> [4+], Pb <sub>3</sub> (OH) <sub>4</sub> [2+], Pb <sub>3</sub> (OH) <sub>5</sub> [+], Pb <sub>6</sub> (OH) <sub>8</sub> [4+], <b>Pb(c)</b> <b>PbO(red),</b> <b>PbO(yellow)</b> <b>Pb(OH)<sub>2</sub>(s),</b> <b>PbO<sub>2</sub>(s),</b> <b>Pb<sub>3</sub>O<sub>4</sub>(s)</b>

HATCHES			
Pb[2+], Pb(iv)[4+], Pb(OH)[+], Pb(OH) <sub>2</sub> (aq), Pb(OH) <sub>3</sub> [+], Pb(OH) <sub>3</sub> [-], Pb(OH) <sub>4</sub> (aq), Pb <sub>2</sub> (OH)[3+], Pb <sub>3</sub> (OH) <sub>4</sub> [2+], Pb <sub>6</sub> (OH) <sub>8</sub> [4+], <b>Pb,</b> <b>Pb(OH)<sub>2</sub>, Pb<sub>3</sub>O<sub>4</sub>, PbO,</b> <b>PbO<sub>2</sub></b>			



☒ 90: Eh-pH diagrams of the system Pb-O-H (1).  $\sum \text{Pb} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

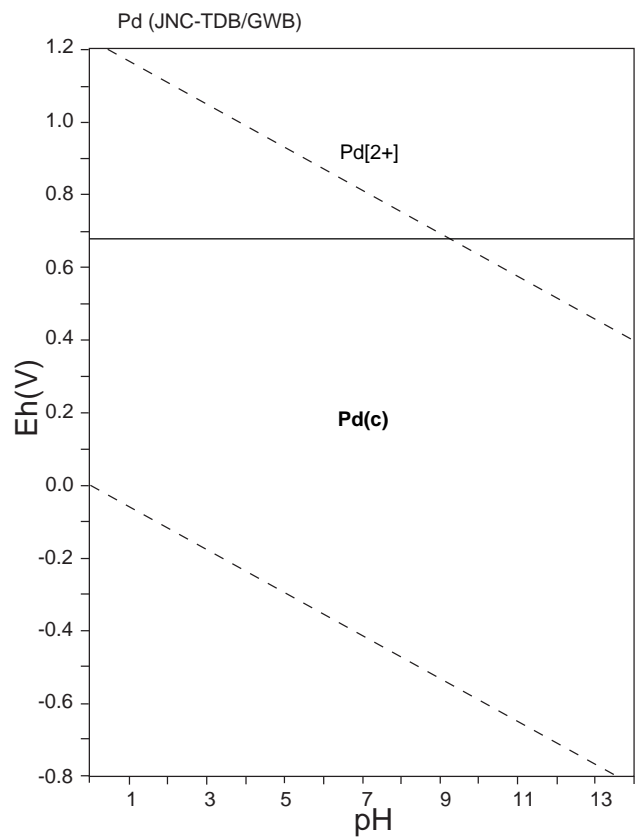
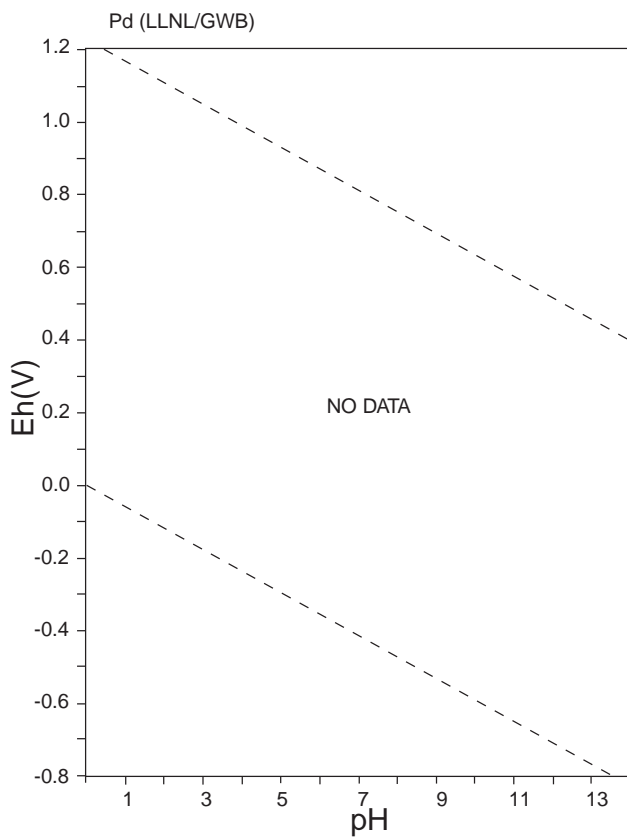
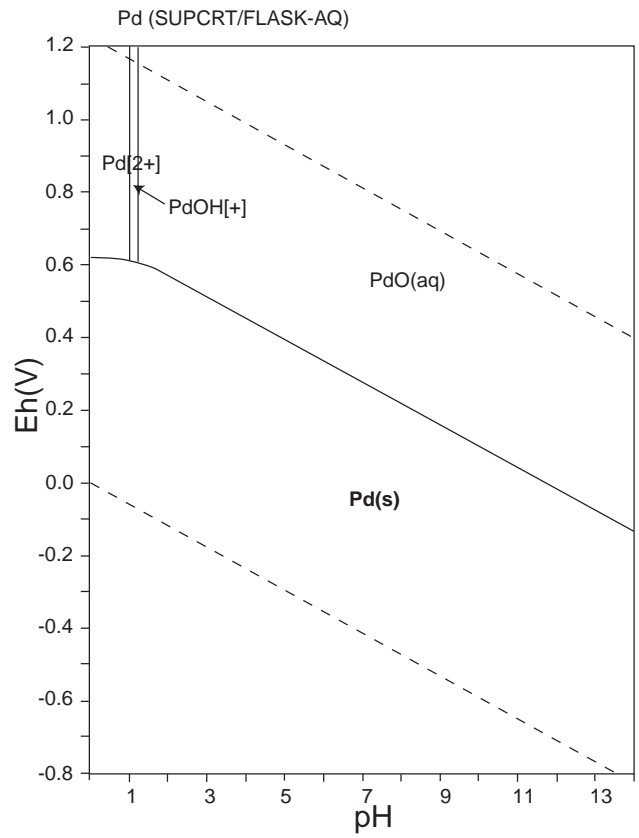
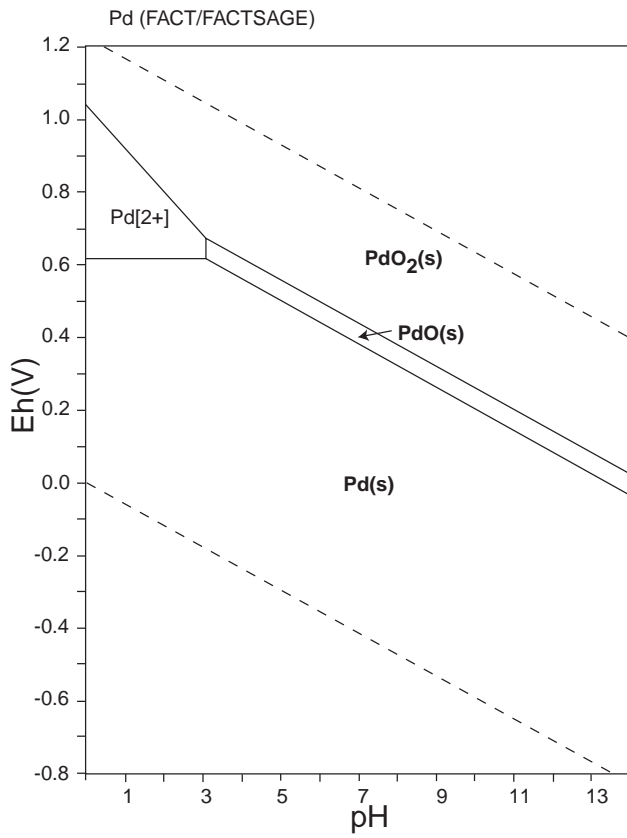




☒ 91: Eh-pH diagrams of the system Pb-O-H (2).  $\sum \text{Pb} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 55: List of Pd species

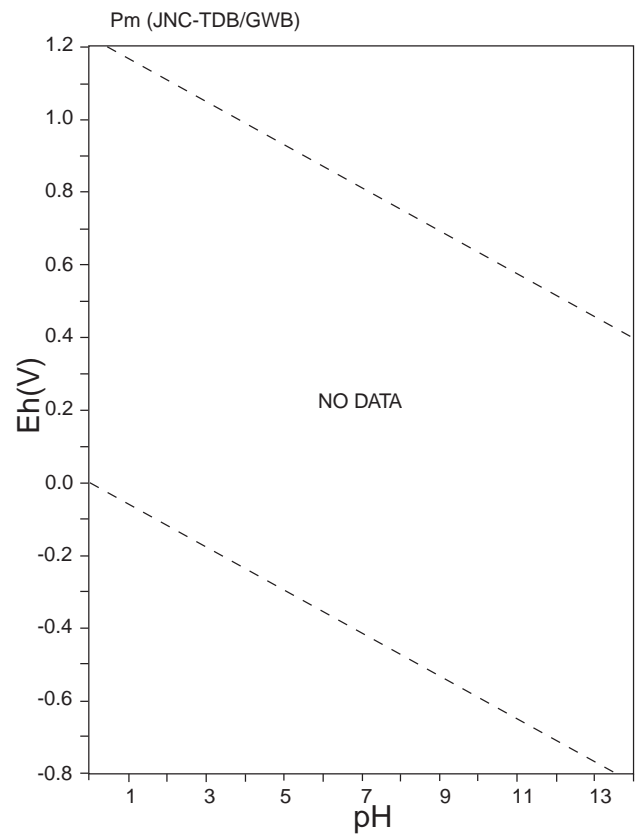
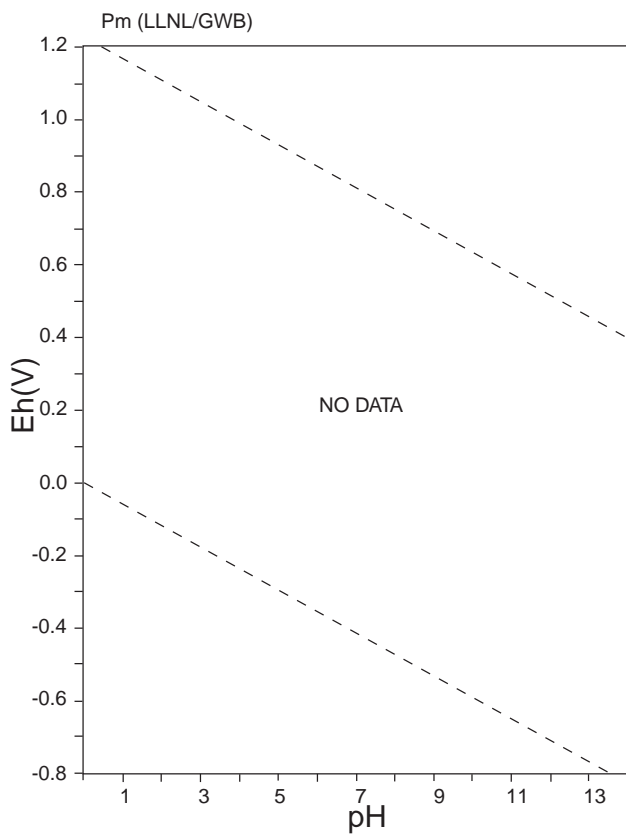
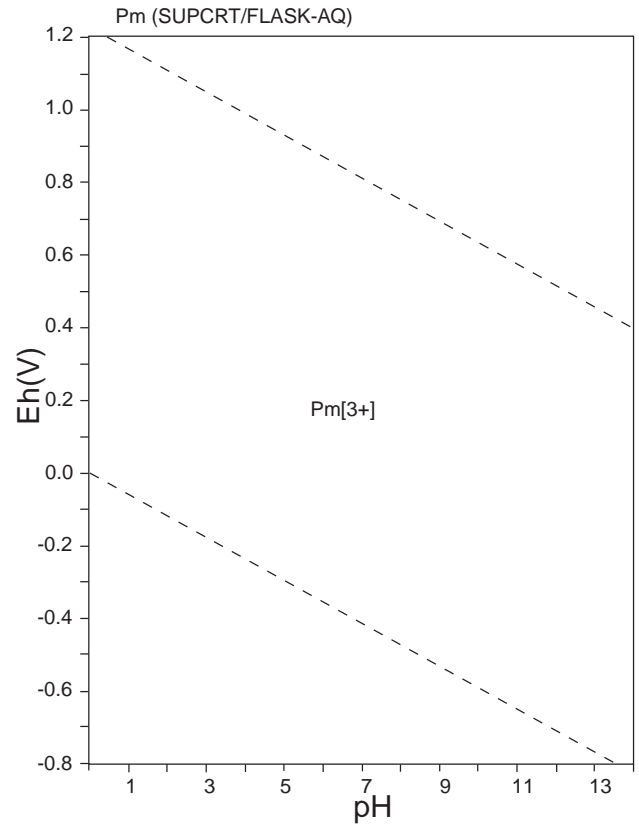
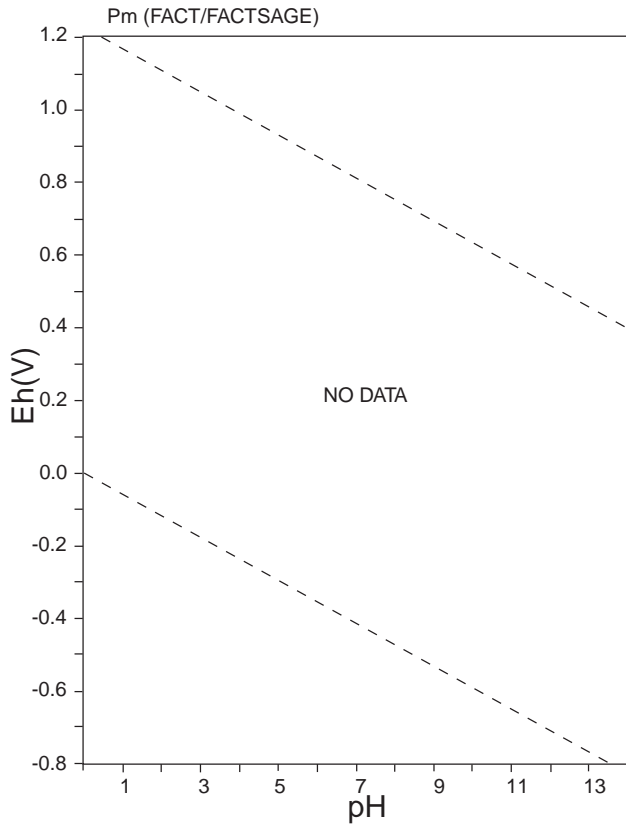
FACT	SUPCRT	LLNL	JNC-TDB
Pd[2+], PdO <sub>2</sub> (s), Pd(s), PdO(s)	Pd[2+], PdOH[+], PdO(aq), Pd(Palladium), PdO(s), Pd(OH) <sub>2</sub> (s)		Pd[2+], Pd(c)



☒ 92: Eh-pH diagrams of the system Pd-O-H.  $\sum \text{Pd} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 56: List of Pm species

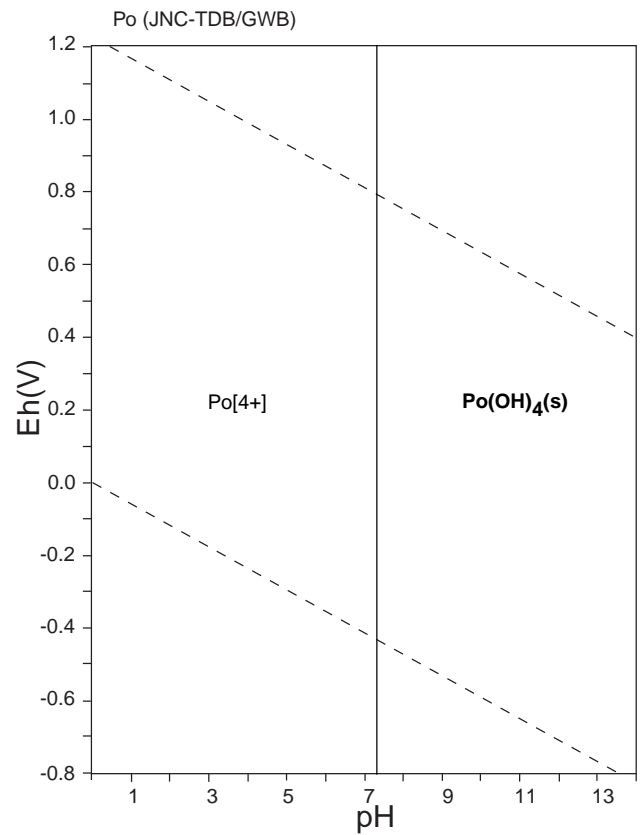
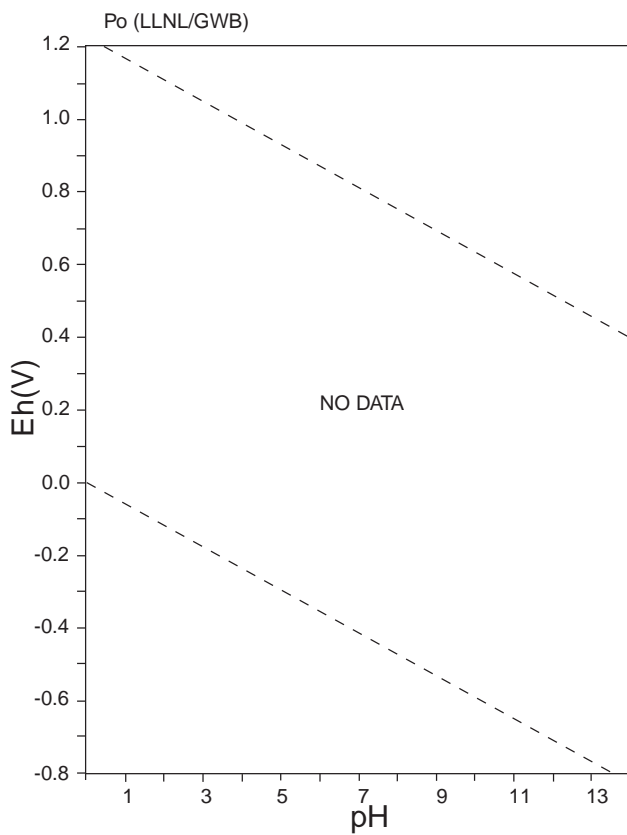
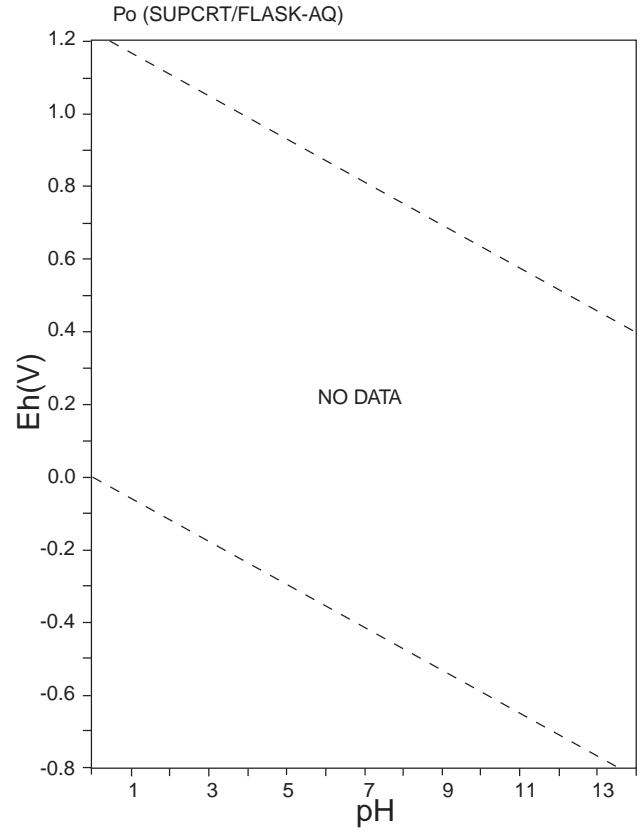
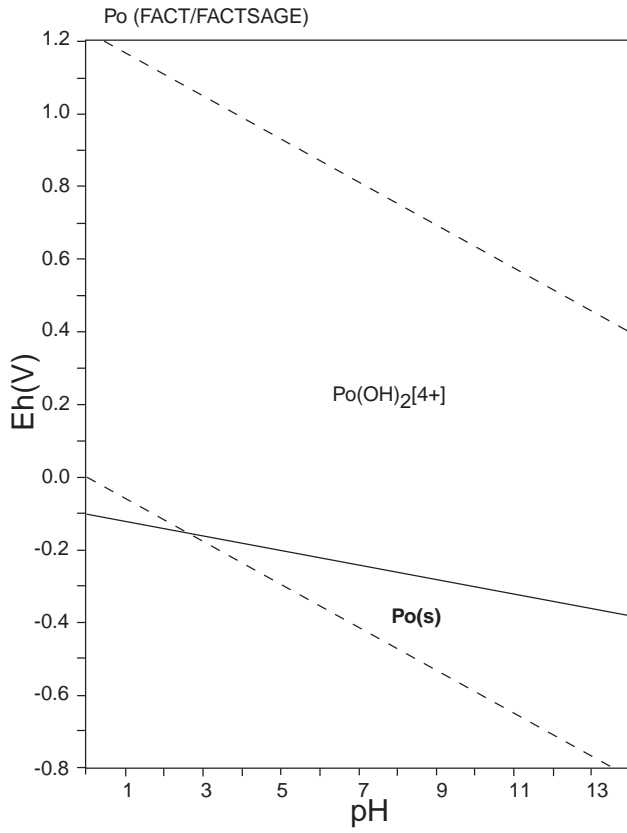
FACT	SUPCRT	LLNL	JNC-TDB
	Pm[4+], Pm[3+], Pm[2+]		



☒ 93: Eh-pH diagrams of the system Pm-O-H.  $\sum Pm = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 57: List of Po species

FACT	SUPCRT	LLNL	JNC-TDB
Po[2+], Po[4+], Po(OH) <sub>2</sub> [4+], <b>Po(s)</b>			Po[4+], <b>Po(OH)<sub>4</sub>(s)</b>

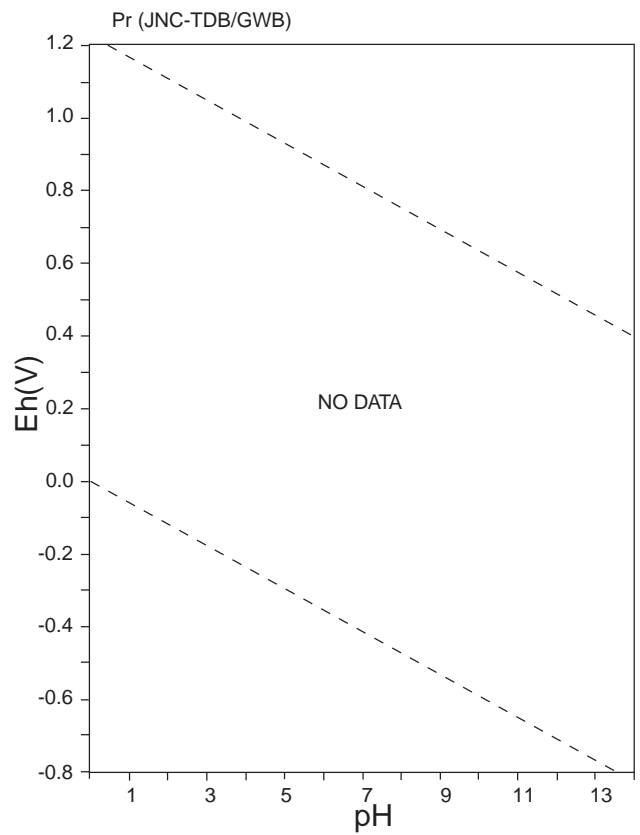
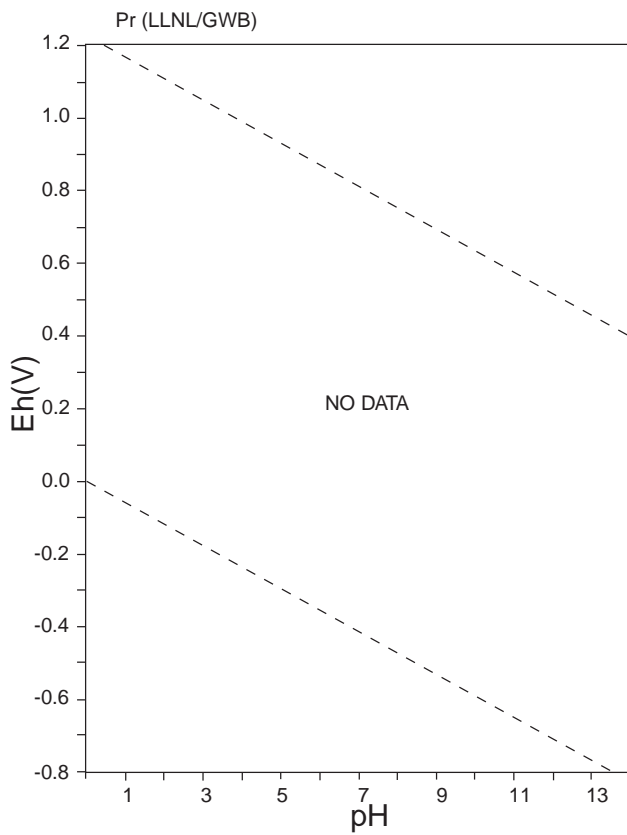
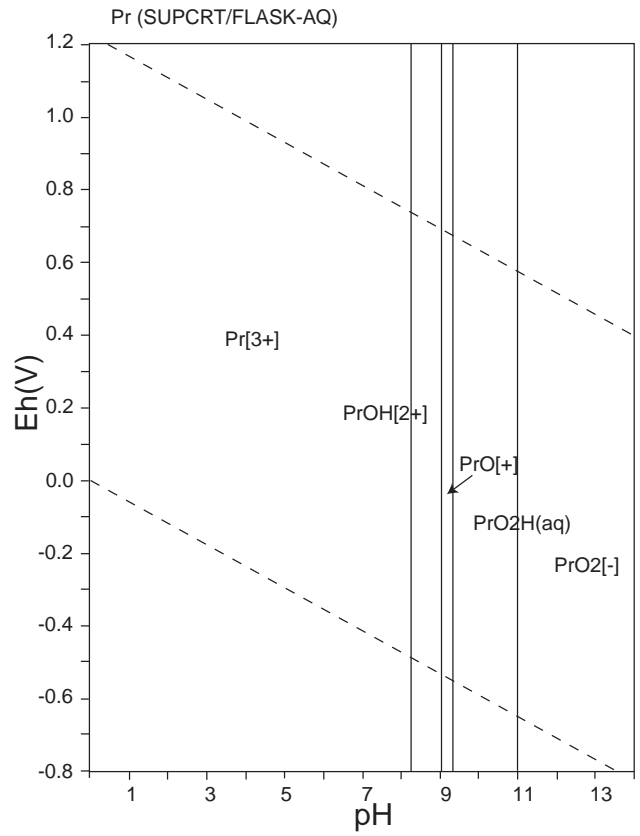
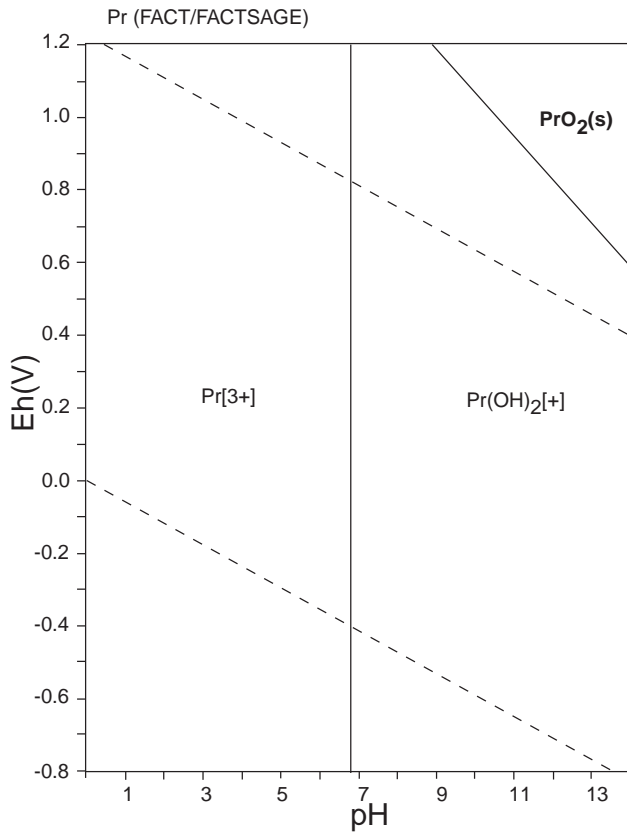


94: Eh-pH diagrams of the system Po-O-H.  $\sum \text{Po} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 58: List of Pr species

FACT	SUPCRT	LLNL	JNC-TDB
Pr[3+], PrOH[2+], Pr(OH) <sub>2</sub> [+], <b>Pr(s)</b> , <b>Pr(s2)</b> , <b>PrH<sub>2</sub>(s)</b> , <b>PrO<sub>2</sub>(s)</b> , <b>Pr<sub>2</sub>O<sub>3</sub>(s)</b> , <b>Pr<sub>6</sub>O<sub>11</sub>(s)</b> , <b>Pr<sub>7</sub>O<sub>12</sub>(s)</b> , <b>PrO<sub>3</sub>H<sub>3</sub>(s)</b>	Pr[3+], PrOH[2+], PrO[+], Pr[4+], Pr[2+], PrO <sub>2</sub> H(aq), PrO <sub>2</sub> [-]		





☒ 95: Eh-pH diagrams of the system Pr-O-H.  $\sum \text{Pr} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 59: List of Pt species

FACT	SUPCRT	LLNL	JNC-TDB
Pt[2+], <b>Pt(s)</b>	Pt[2+], PtOH[+], PtO(aq), <b>Pt(Platinum)</b>		

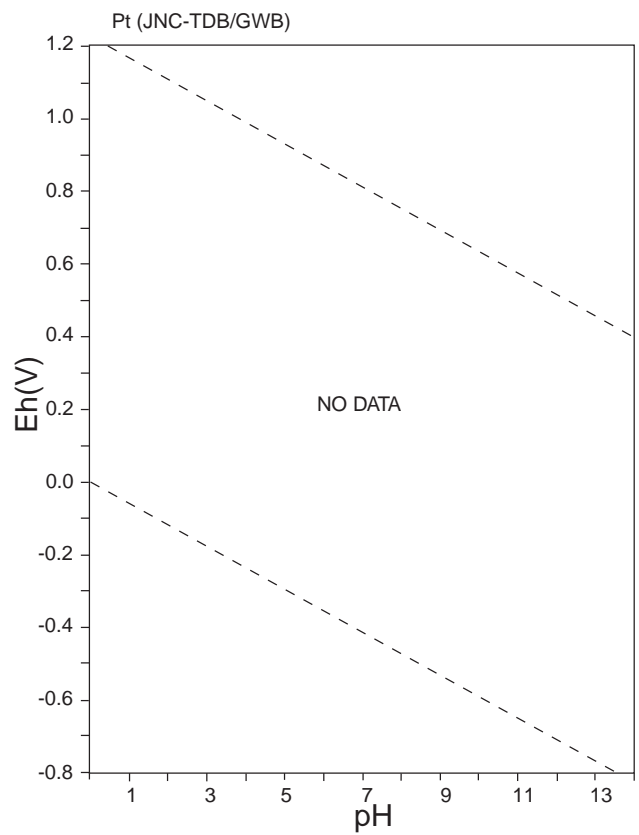
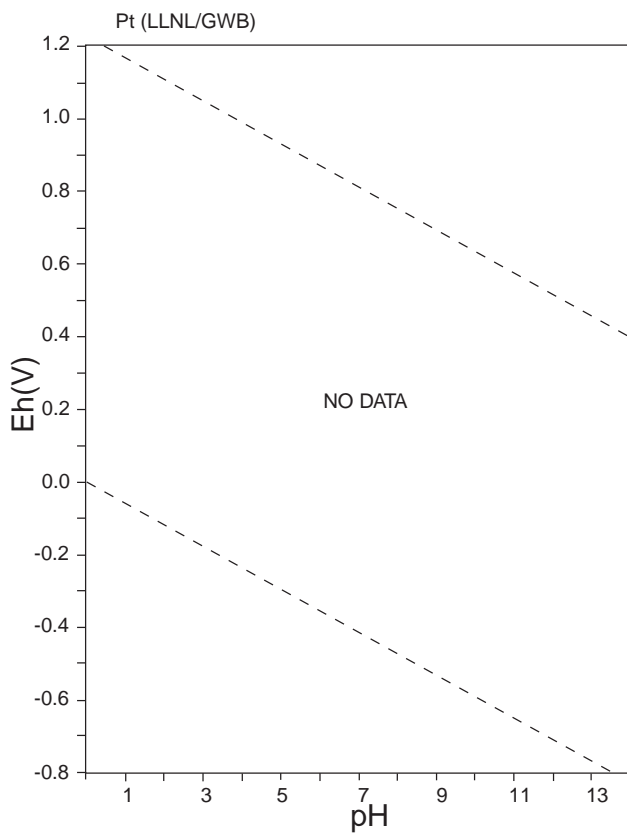
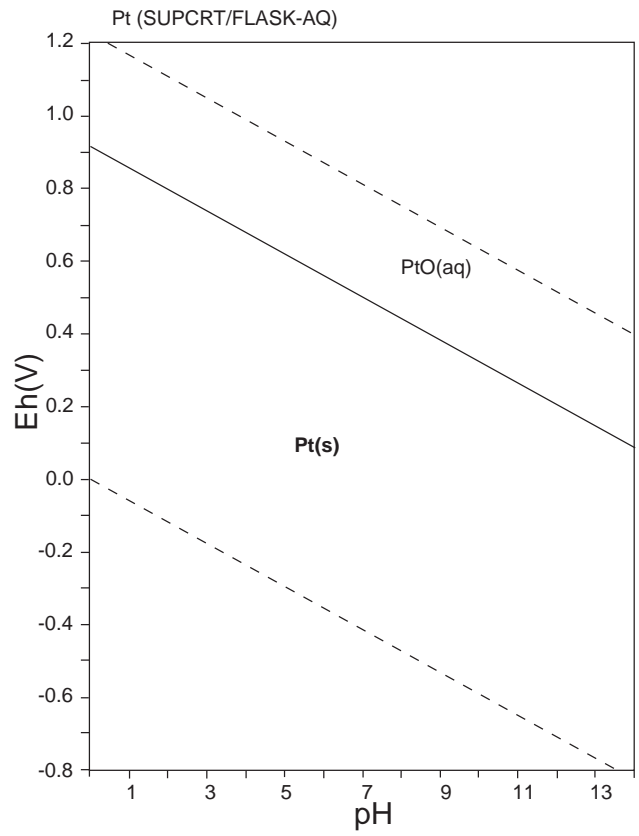
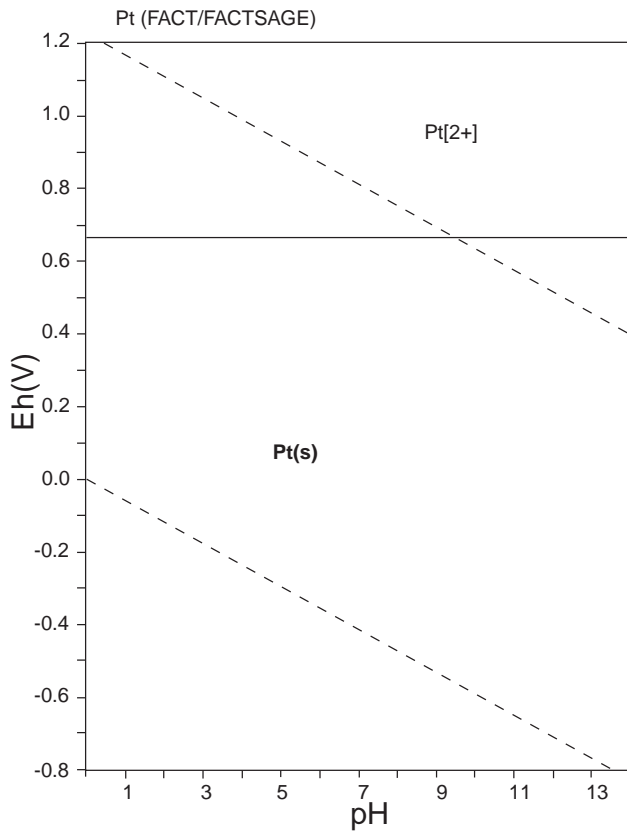


Figure 96: Eh-pH diagrams of the system Pt-O-H.  $\sum \text{Pt} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 60: List of Pu species

FACT	SUPCRT	LLNL	JNC-TDB
Pu[3+], Pu(s), Pu(s2), Pu(s3), Pu(s4), Pu(s5), Pu(s6), PuH <sub>2</sub> (s), PuH <sub>3</sub> (s), PuO <sub>2</sub> (s), Pu <sub>2</sub> O <sub>3</sub> (s), Pu <sub>5</sub> O <sub>8</sub> (s)		PuO <sub>2</sub> [2+], Pu[3+], Pu[4+], PuO <sub>2</sub> [+], (PuO <sub>2</sub> ) <sub>2</sub> (OH) <sub>2</sub> [2+], (PuO <sub>2</sub> ) <sub>3</sub> (OH) <sub>5</sub> [+], Pu(OH) <sub>2</sub> [2+], Pu(OH) <sub>3</sub> [+], Pu(OH) <sub>4</sub> (aq), Pu(OH) <sub>5</sub> [-], PuO <sub>2</sub> OH(aq), PuO <sub>2</sub> OH[+], PuOH[2+], PuOH[3+], Pu(OH) <sub>3</sub> (aq), Pu(OH) <sub>3</sub> (s), Pu(OH) <sub>4</sub> (am), Pu(OH) <sub>4</sub> (s), Pu <sub>2</sub> O <sub>3</sub> (c,beta), PuO <sub>2</sub> (s), PuO <sub>2</sub> (OH) <sub>2</sub> (s), PuO <sub>2</sub> (OH) <sub>2</sub> (c), PuO <sub>2</sub> (c), PuO <sub>2</sub> OH(am)	Pu[4+], Pu[3+], PuOH[2+], PuOH <sub>2</sub> [+], Pu(OH) <sub>3</sub> (aq), PuO <sub>2</sub> [+], PuO <sub>2</sub> OH(aq), PuO <sub>2</sub> (OH) <sub>2</sub> [-], PuO <sub>2</sub> [2+], PuO <sub>2</sub> OH[+], PuO <sub>2</sub> (OH) <sub>2</sub> , PuO <sub>2</sub> OH <sub>3</sub> [-], Pu(OH) <sub>4</sub> (aq), PuOH[3+], Pu(OH) <sub>3</sub> (am), Pu(OH) <sub>3</sub> (c), PuO <sub>2</sub> (am), PuO <sub>2</sub> OH(s)

HATCHES	OECD-NEA	OECD-NEA update	
Pu[4+], Pu[3+], PuO <sub>2</sub> [+], PuO <sub>2</sub> [2+], Pu(OH)[2+], Pu(OH)[3+], Pu(OH) <sub>2</sub> [+], Pu(OH) <sub>2</sub> [2+], Pu(OH) <sub>3</sub> (aq), Pu(OH) <sub>3</sub> [+], Pu(OH) <sub>4</sub> (aq), Pu(OH) <sub>4</sub> [-], Pu <sub>2</sub> (OH) <sub>2</sub> [4+], Pu <sub>2</sub> (OH) <sub>2</sub> [6+], Pu <sub>2</sub> (OH) <sub>3</sub> [5+], Pu <sub>2</sub> (OH) <sub>4</sub> [4+], Pu <sub>2</sub> (OH) <sub>5</sub> [3+], Pu <sub>3</sub> (OH) <sub>5</sub> [4+], PuO <sub>2</sub> (OH) <sub>2</sub> [-], (PuO <sub>2</sub> ) <sub>2</sub> OH <sub>2</sub> [2+], (PuO <sub>2</sub> ) <sub>3</sub> OH <sub>5</sub> [+], PuO <sub>2</sub> OH(aq), PuO <sub>2</sub> OH[+], PuO <sub>2</sub> OH <sub>2</sub> (aq), PuO <sub>2</sub> OH <sub>3</sub> [-], Pu(OH) <sub>3</sub> , Pu(OH) <sub>4</sub> , Pu <sub>2</sub> O <sub>3</sub> , PuO <sub>2</sub> (OH) <sub>2</sub> *H <sub>2</sub> O(c), PuO <sub>2</sub> , PuO <sub>2</sub> (a), PuO <sub>2</sub> (OH) <sub>2</sub> , PuO <sub>2</sub> OH, Pu(OH) <sub>3</sub> (c)	Pu[4+], Pu[3+], PuO <sub>2</sub> [+], PuO <sub>2</sub> [2+], PuOH[2+], PuOH[3+], PuO <sub>2</sub> OH[+], PuO <sub>2</sub> (OH) <sub>2</sub> (aq), (PuO <sub>2</sub> ) <sub>2</sub> (OH) <sub>2</sub> [2+], Pu(c), PuO <sub>1.61</sub> (c_bcc), PuO <sub>2</sub> (c), PuO <sub>2</sub> (hyd_aged), Pu <sub>2</sub> O <sub>3</sub> (c), PuO <sub>2</sub> OH(am), Pu(OH) <sub>3</sub> (c), PuO <sub>2</sub> (OH) <sub>2</sub> H <sub>2</sub> O(c)	Pu[4+], Pu[3+], PuO <sub>2</sub> [+], PuO <sub>2</sub> [2+], PuOH[2+], PuOH[3+], Pu(OH) <sub>2</sub> [2+], Pu(OH) <sub>3</sub> [+], PuO <sub>2</sub> OH(aq), PuO <sub>2</sub> OH[+], PuO <sub>2</sub> (OH) <sub>2</sub> (aq), Pu(OH) <sub>4</sub> (aq), (PuO <sub>2</sub> ) <sub>2</sub> (OH) <sub>2</sub> [2+], Pu(cr), PuO <sub>1.61</sub> (bcc), PuO <sub>2</sub> (cr), Pu <sub>2</sub> O <sub>3</sub> (cr), Pu(OH) <sub>3</sub> (cr), PuO <sub>2</sub> (OH) <sub>2</sub> H <sub>2</sub> O(cr)	

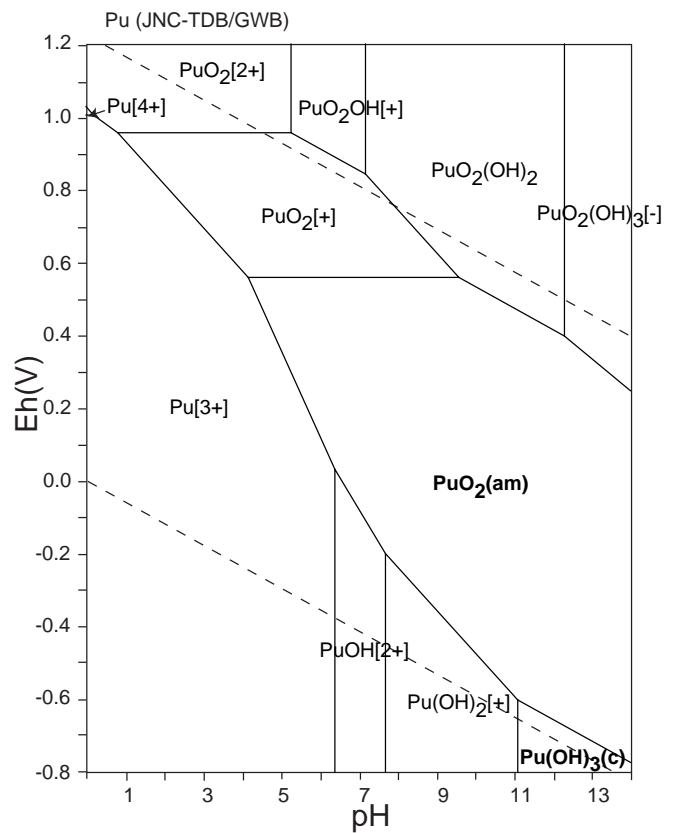
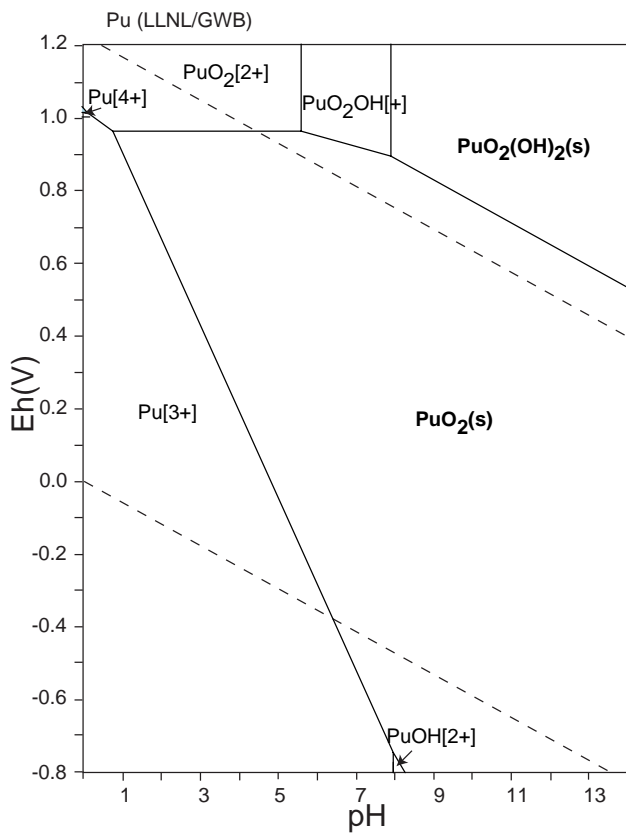
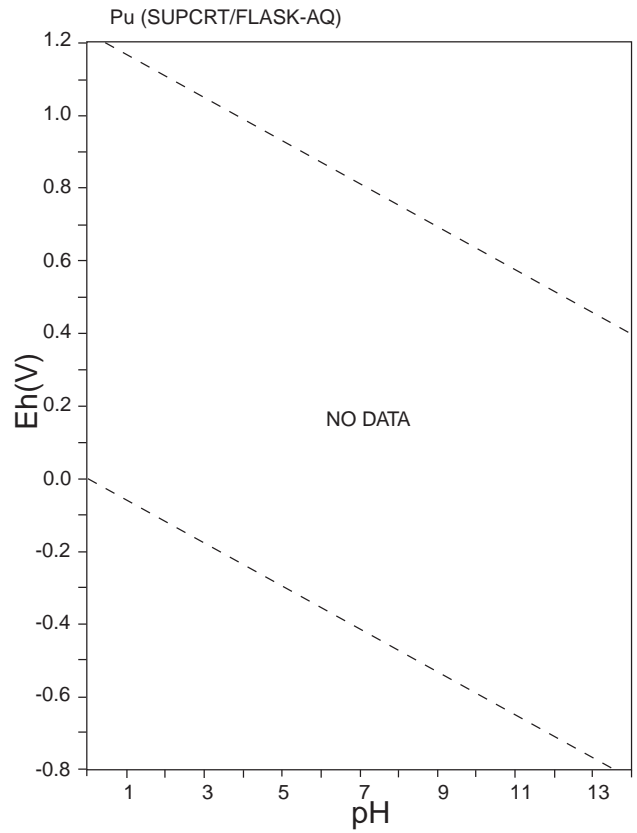
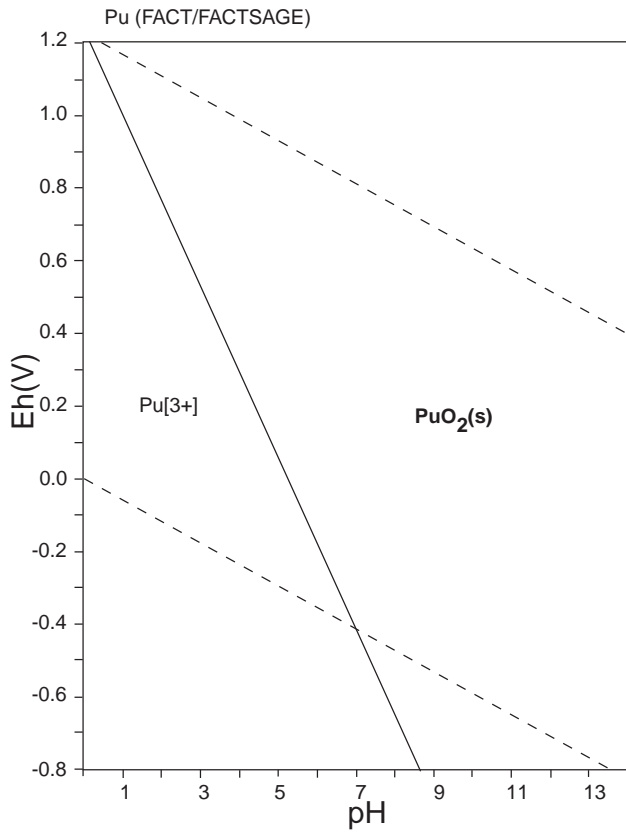
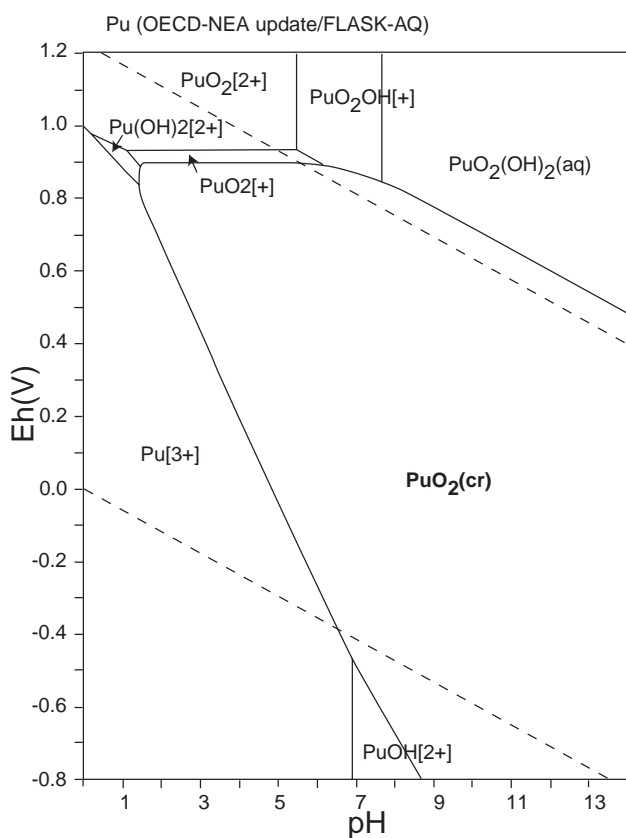
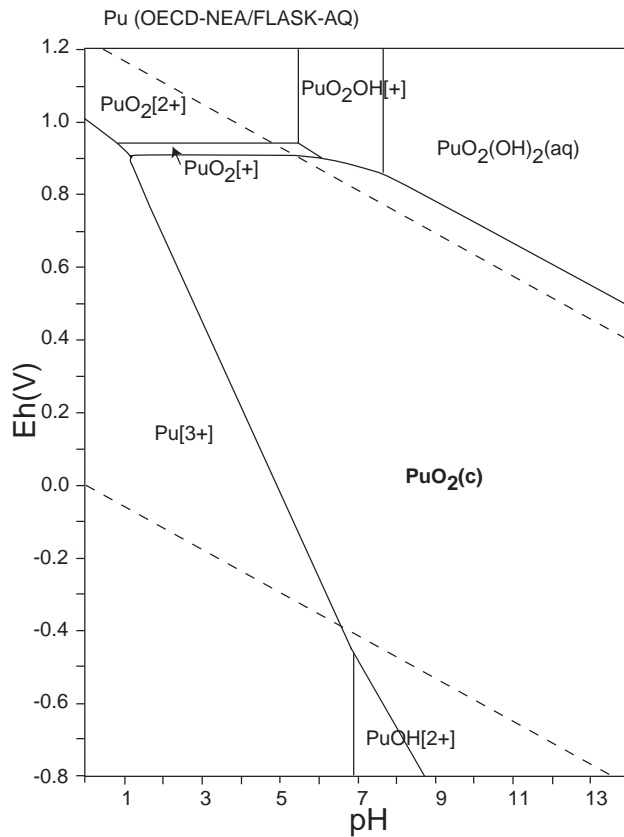
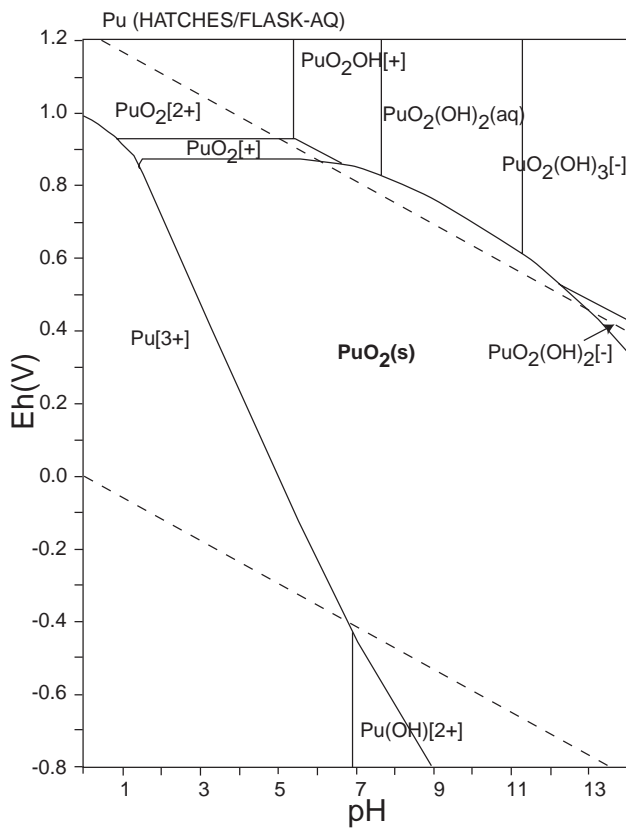


图 97: Eh-pH diagrams of the system Pu-O-H (1).  $\sum \text{Pu} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 98: Eh-pH diagrams of the system Pu-O-H (2).  $\sum \text{Pu} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





表 61: List of Ra species

FACT	SUPCRT	LLNL	JNC-TDB
Ra[2+], <b>Ra(s)</b>	Ra[2+]		Ra[2+], RaOH[+]

HATCHES			
Ra[2+], RaOH[+], <b>Ra(c)</b>			

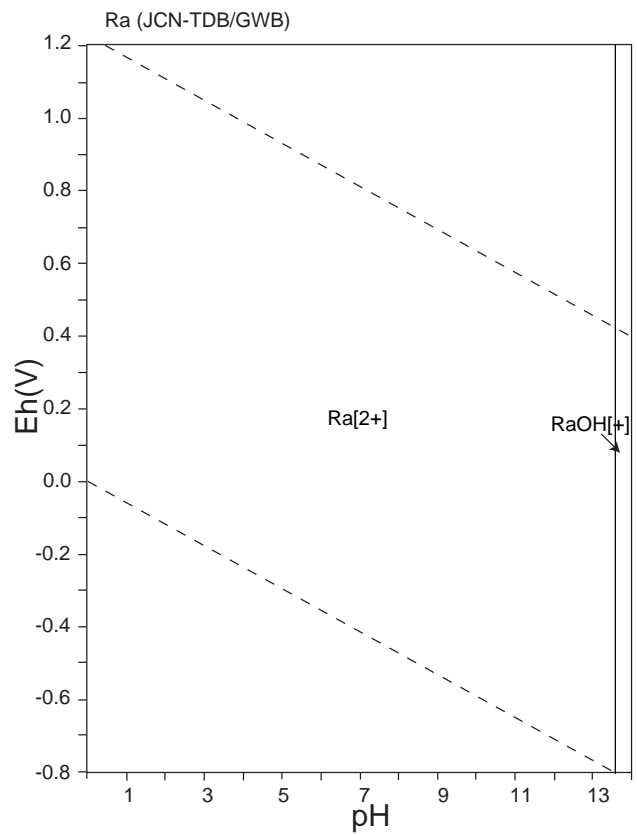
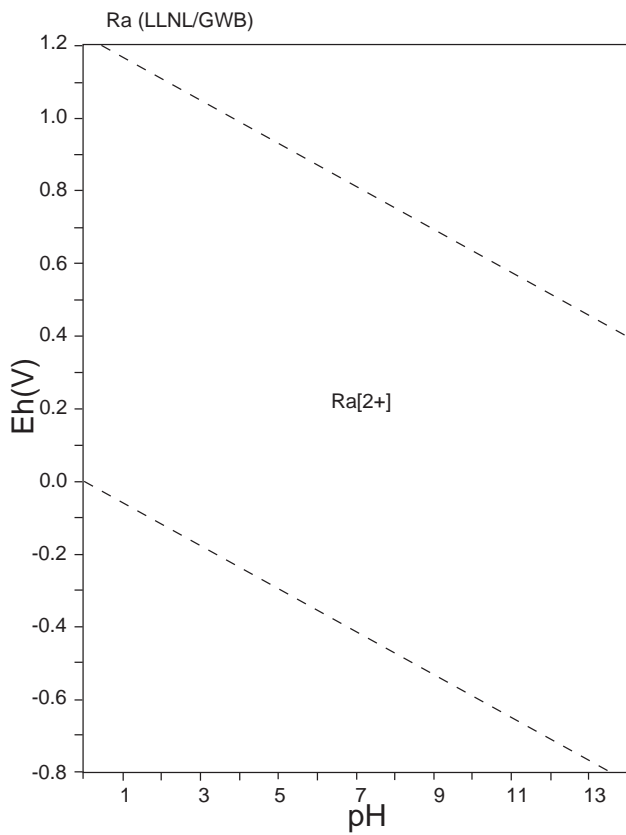
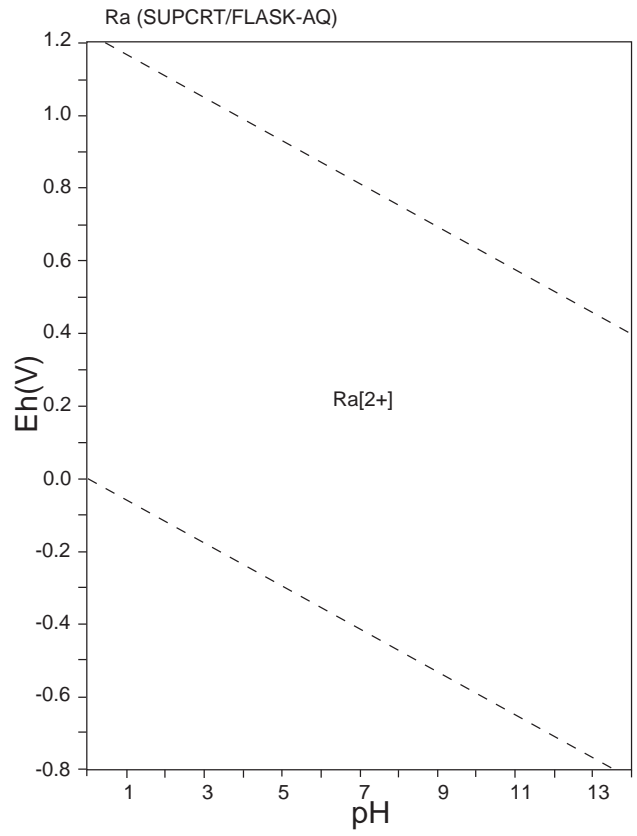
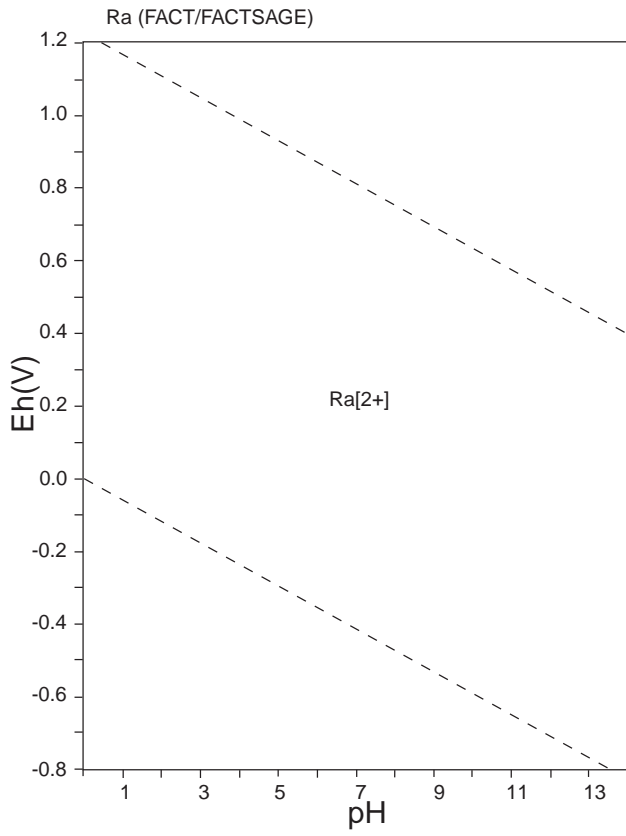


Figure 99: Eh-pH diagrams of the system Ra-O-H (1).  $\sum Ra = 10^{-10}$ , 298.15K,  $10^5$  Pa.

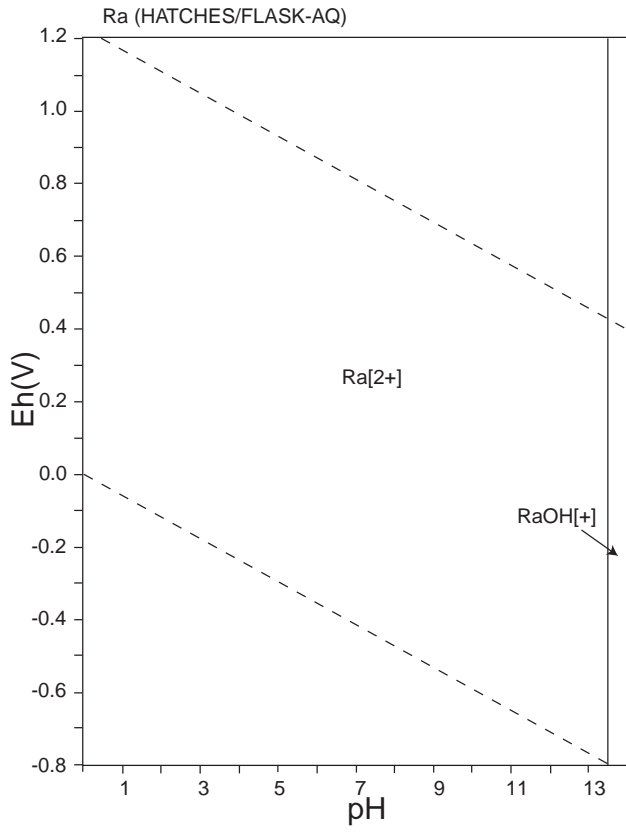
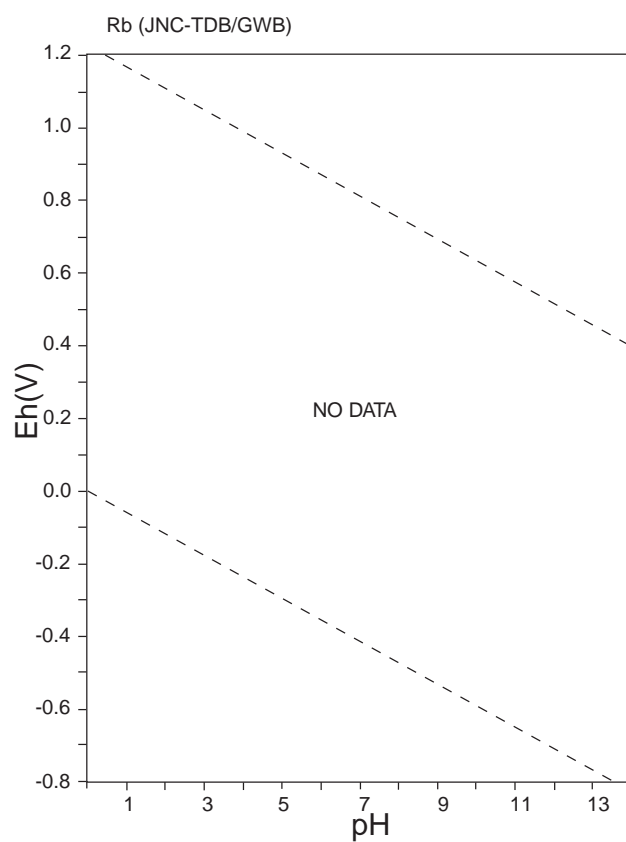
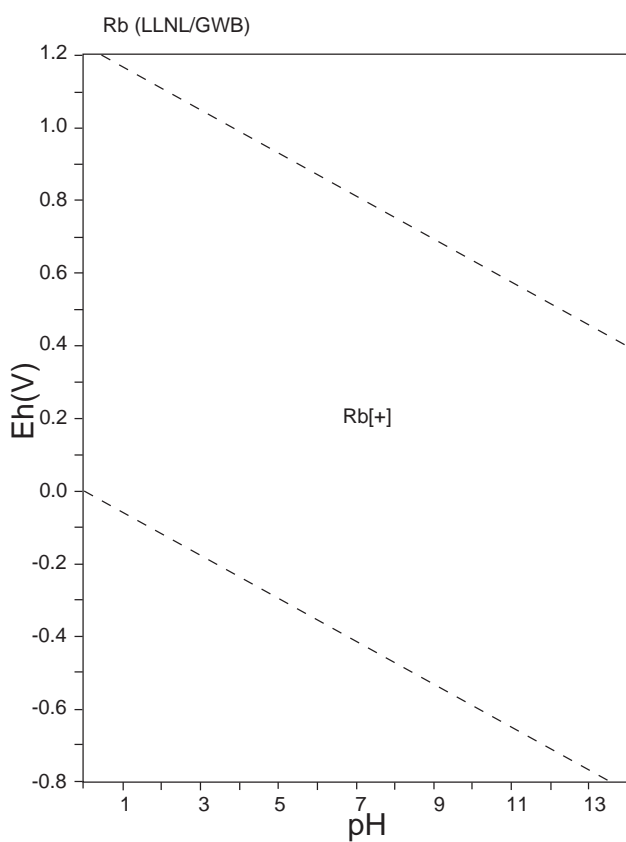
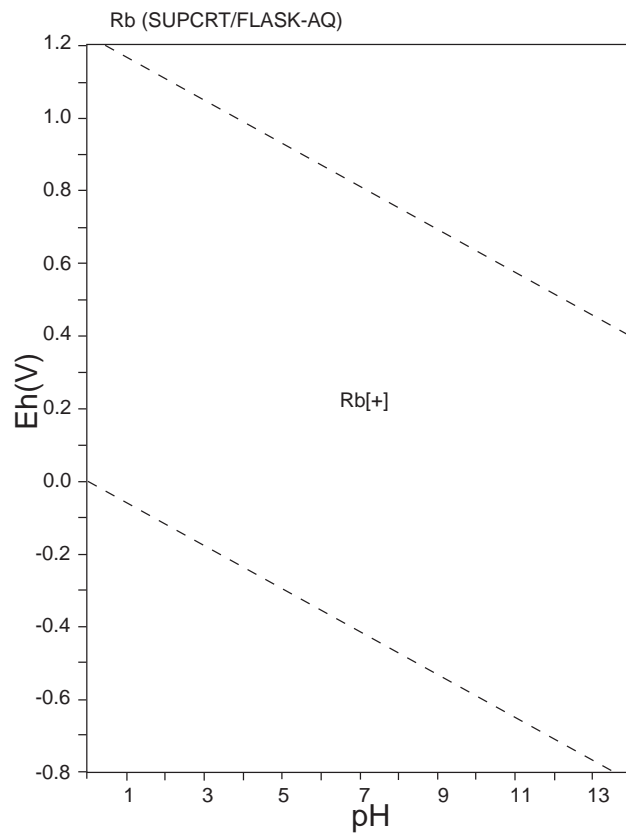
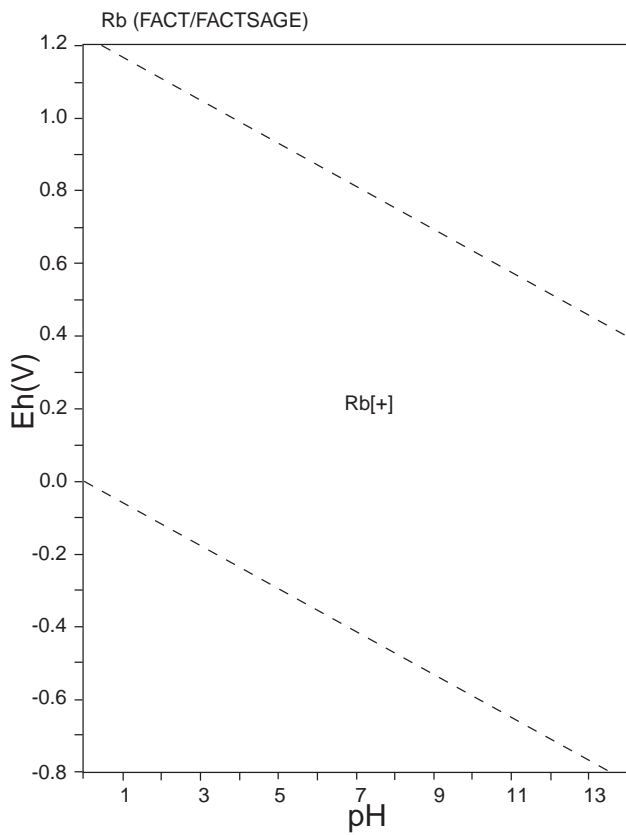


图 100: Eh-pH diagrams of the system Ra-O-H (2).  $\sum Ra = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 62: List of Rb species

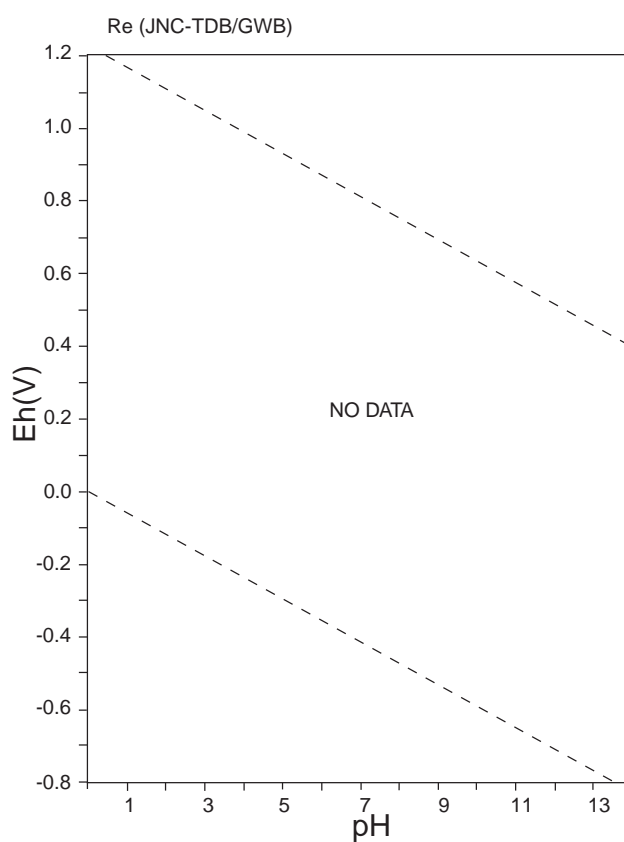
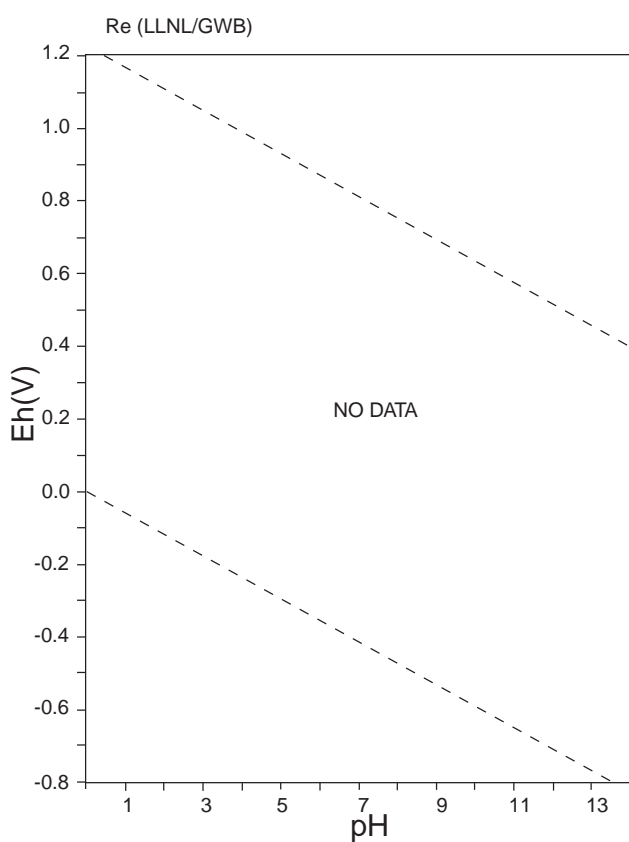
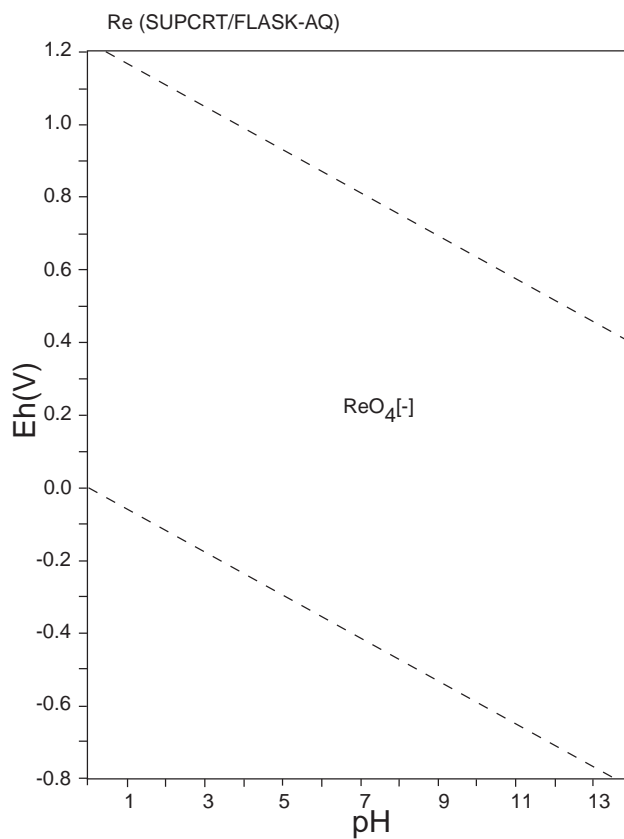
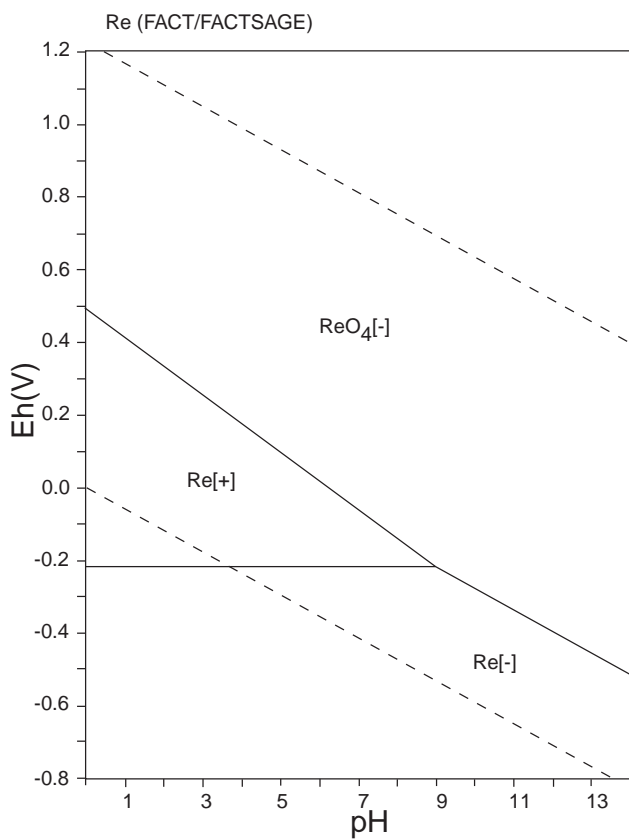
FACT	SUPCRT	LLNL	JNC-TDB
Rb[+], <b>Rb(s)</b> , <b>Rb<sub>2</sub>O(s)</b> , <b>RbOH(s)</b>	Rb[+], RbOH(aq)	Rb[+]	



☒ 101: Eh-pH diagrams of the system Rb-O-H.  $\sum \text{Rb} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 63: List of Re species

FACT	SUPCRT	LLNL	JNC-TDB
$\text{ReO}_4[-]$ , $\text{Re}[-]$ , $\text{Re}[+]$ , $\text{Re}(\mathbf{s})$ , $\text{ReO}_2(\mathbf{s})$ , $\text{ReO}_3(\mathbf{s})$ , $\text{Re}_2\text{O}_7(\mathbf{s})$ , $\text{HReO}_4(\mathbf{s})$	$\text{ReO}_4[-]$		

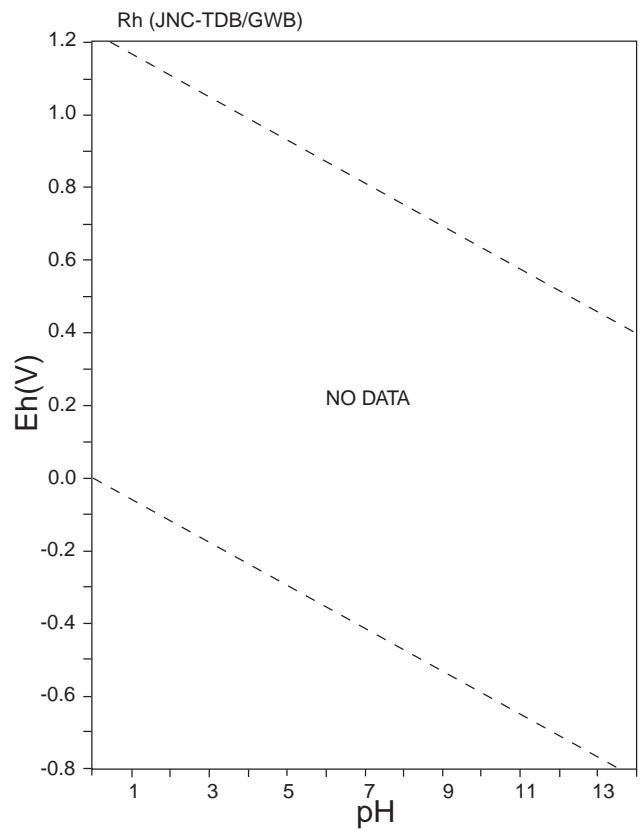
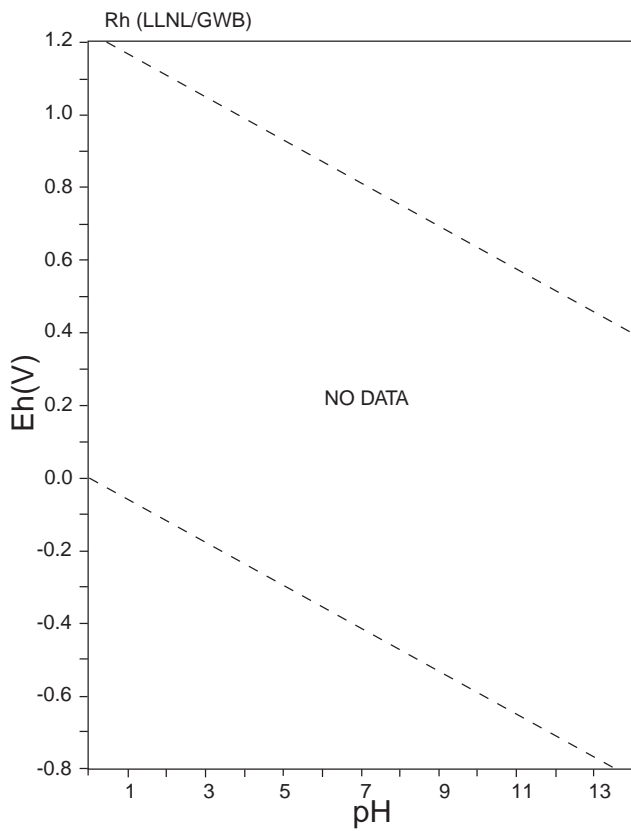
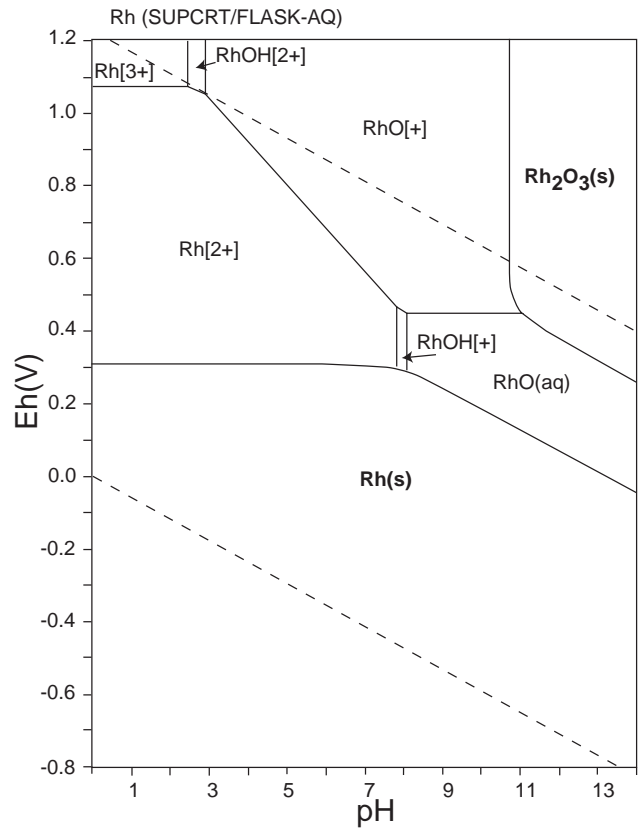
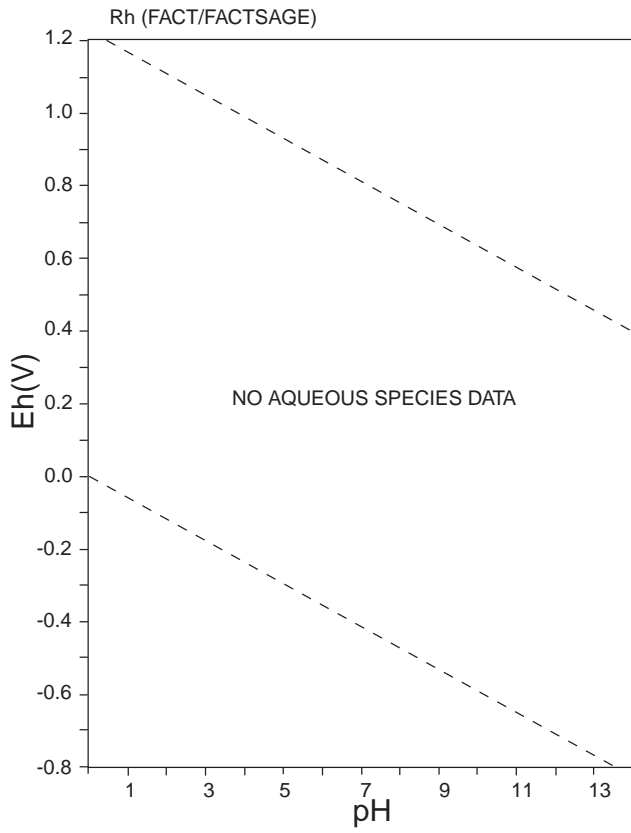


☒ 102: Eh-pH diagrams of the system Re-O-H.  $\sum \text{Re} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 64: List of Rh species

FACT	SUPCRT	LLNL	JNC-TDB
<b>RhO(s), RhO<sub>2</sub>(s), Rh(s), Rh<sub>2</sub>O(s), Rh<sub>2</sub>O<sub>3</sub>(s)</b>	<b>Rh[3+], RhOH[+], RhOH[2+], Rh[2+], RhO(aq), RhO[+], Rh(Rhodium), Rh<sub>2</sub>O(s), Rh<sub>2</sub>O<sub>3</sub>(s)</b>		





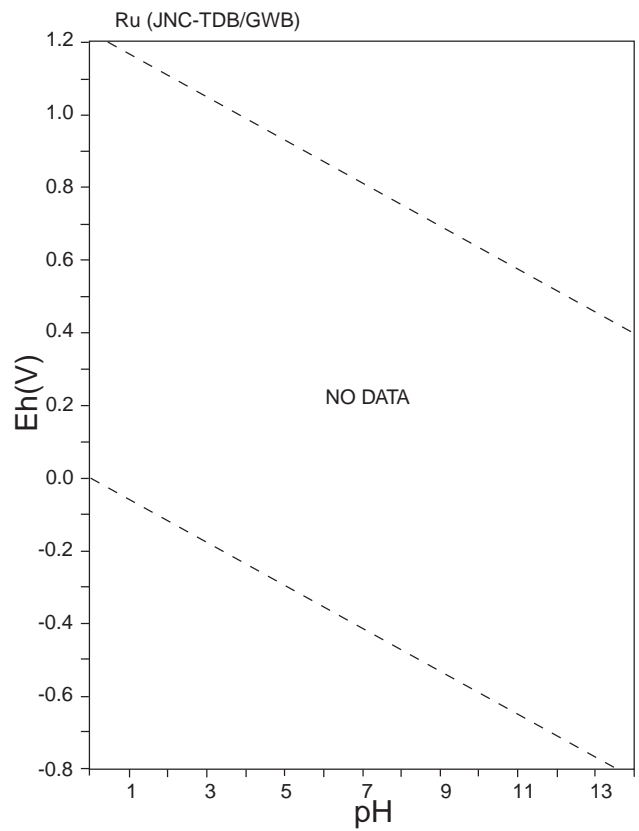
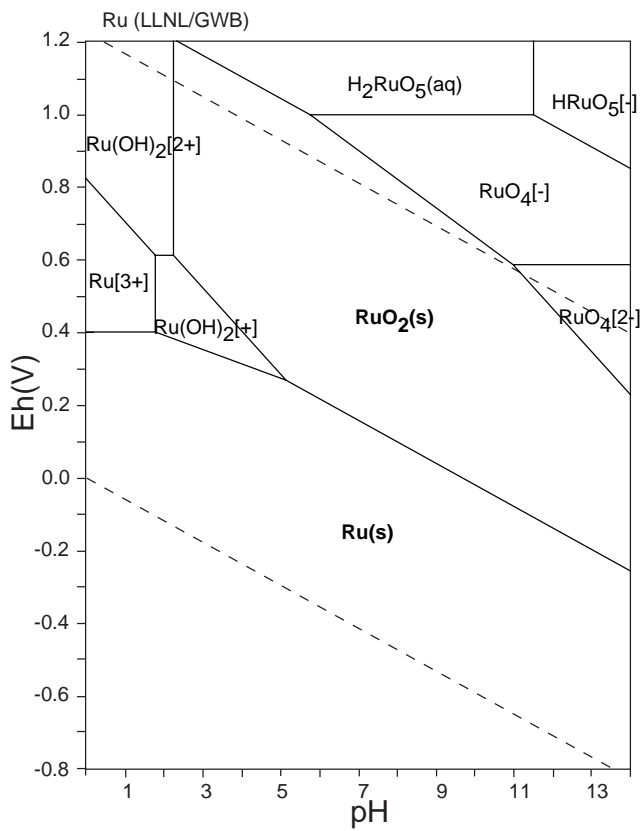
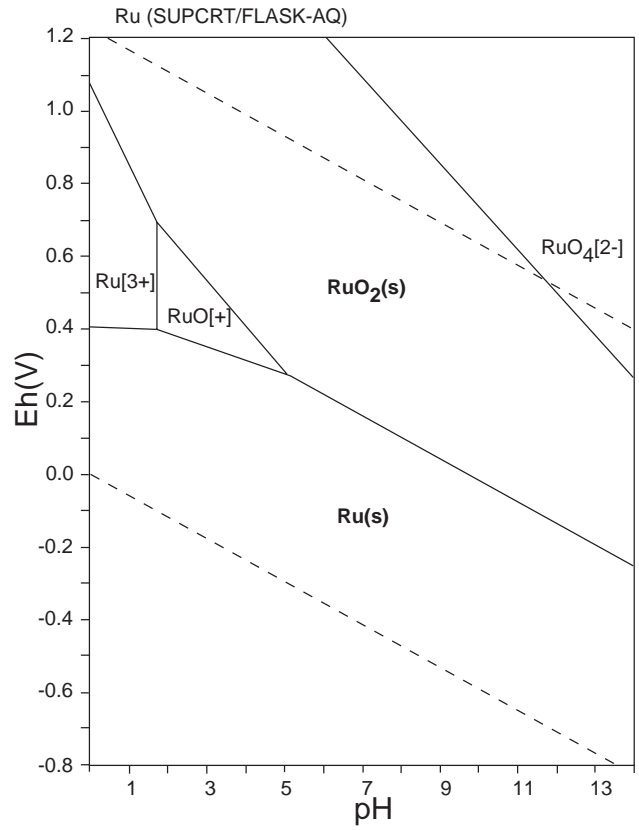
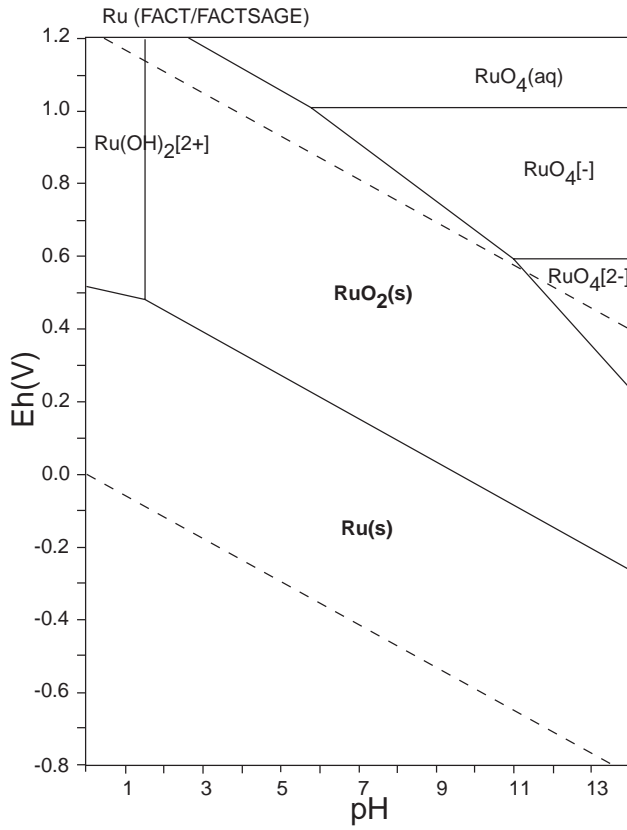
☒ 103: Eh-pH diagrams of the system Rh-O-H.  $\sum \text{Rh} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



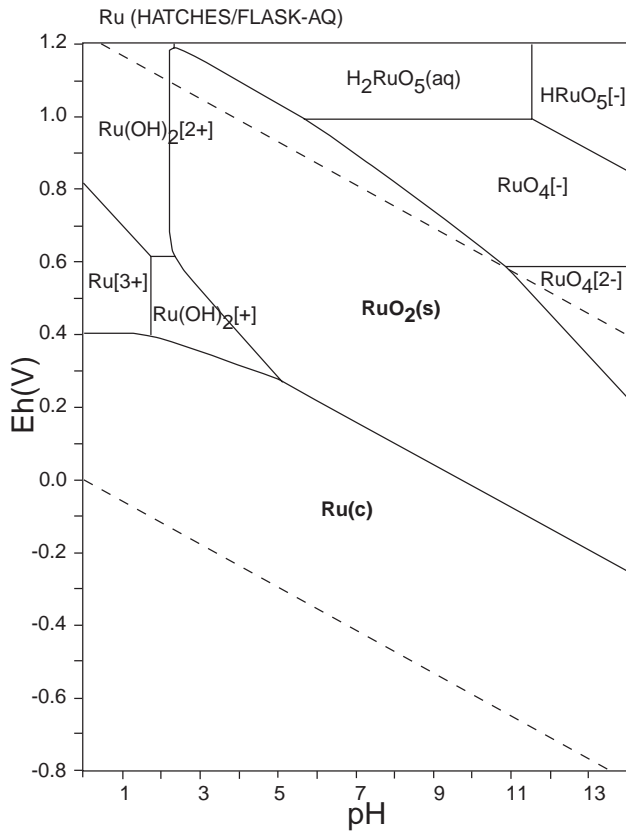
表 65: List of Ru species

FACT	SUPCRT	LLNL	JNC-TDB
<p>RuO<sub>4</sub>[2-], RuO<sub>4</sub>[-],                      RuO<sub>4</sub>(aq),                      Ru(OH)<sub>2</sub>[2+],  <b>RuO<sub>4</sub>(s), Ru(s),                      RuO<sub>2</sub>(s)</b></p>	<p>RuO<sub>4</sub>[2-], Ru[3+],                      Ru[2+], RuOH[+],                      RuOH[2+], RuO(aq),                      RuO[+],  <b>Ru(Ruthenium),                      RuO<sub>2</sub>(s)</b></p>	<p>Ru[3+],                      Ru(OH)<sub>2</sub>[2+],                      Ru[2+], RuO<sub>4</sub>(aq),                      RuO<sub>4</sub>[-], RuO<sub>4</sub>[2-],                      H<sub>2</sub>RuO<sub>5</sub>(aq),                      HRuO<sub>5</sub>[-],                      Ru(OH)<sub>2</sub>[+],                      Ru<sub>4</sub>(OH)<sub>12</sub>[4+],                      RuOH[2+],  <b>Ru(OH)<sub>3</sub>*H<sub>2</sub>O(am),                      Ru(c),                      RuO<sub>2</sub>(s),                      RuO<sub>2</sub>*2H<sub>2</sub>O(am),                      RuO<sub>4</sub>(s), Ru(g),                      RuO<sub>4</sub>(g)</b></p>	

HATCHES			
<p>Ru[3+],                      Ru(OH)<sub>2</sub>[2+],                      Ru[2+], RuO<sub>4</sub>[-],                      RuO<sub>4</sub>[2-],                      H<sub>2</sub>RuO<sub>5</sub>(aq), HRuO<sub>5</sub>[-],                      Ru(OH)[2+],                      Ru(OH)<sub>2</sub>[+],                      Ru<sub>4</sub>(OH)<sub>12</sub>[4+],  <b>Ru(c), Ru<sub>2</sub>O<sub>5</sub>,                      RuO<sub>2</sub>(s), RuO<sub>2</sub>*2H<sub>2</sub>O,                      RuO<sub>4</sub>(s), Ru(OH)<sub>3</sub>*H<sub>2</sub>O</b></p>			



☒ 104: Eh-pH diagrams of the system Ru-O-H (1).  $\Sigma \text{Ru} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



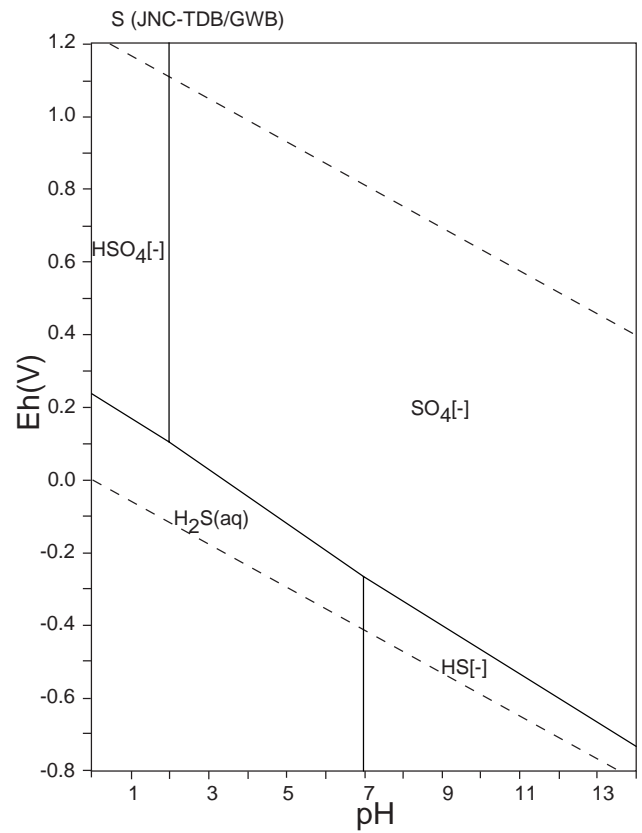
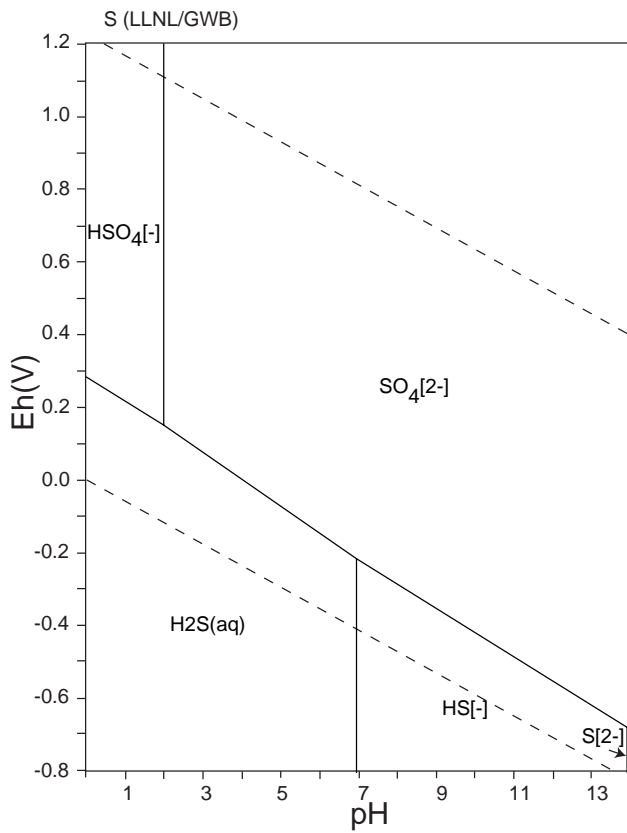
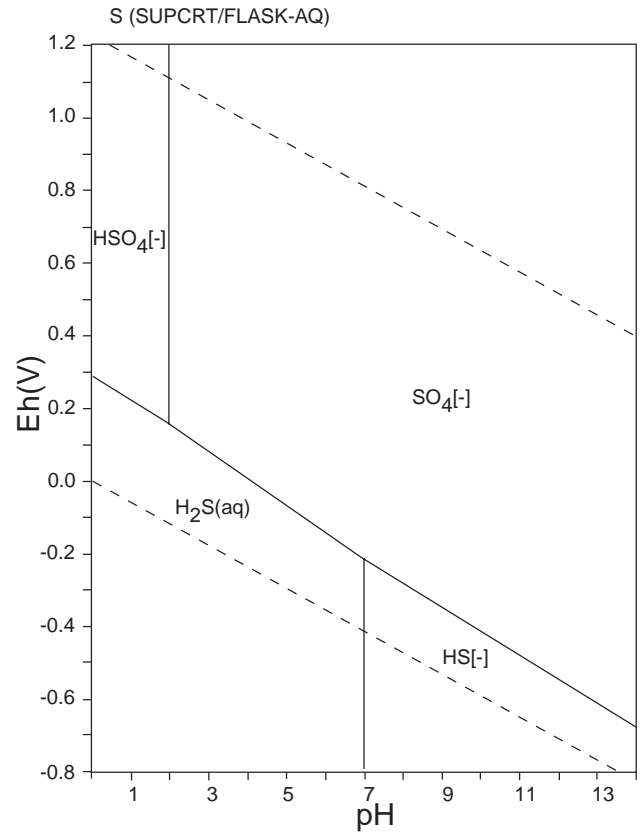
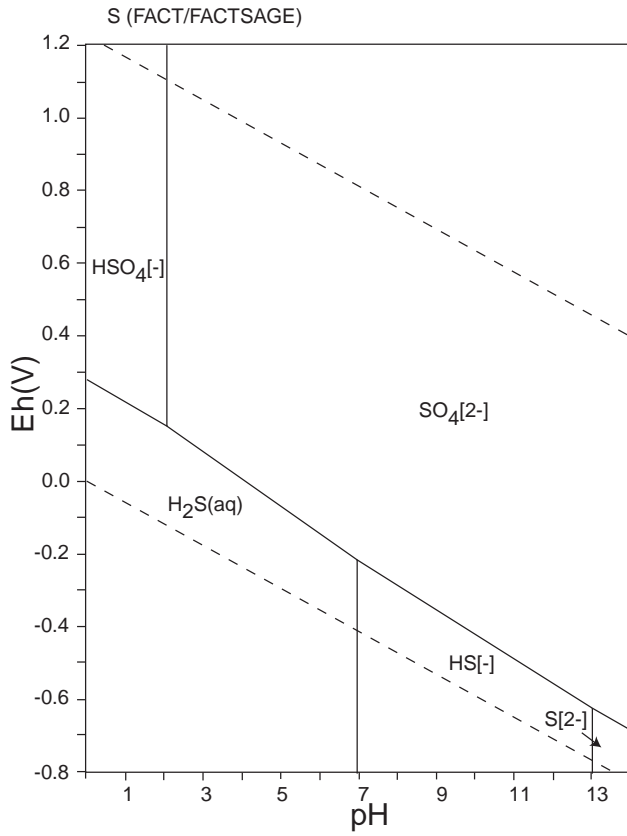
☒ 105: Eh-pH diagrams of the system Ru-O-H (2).  $\sum \text{Ru} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 66: List of S species

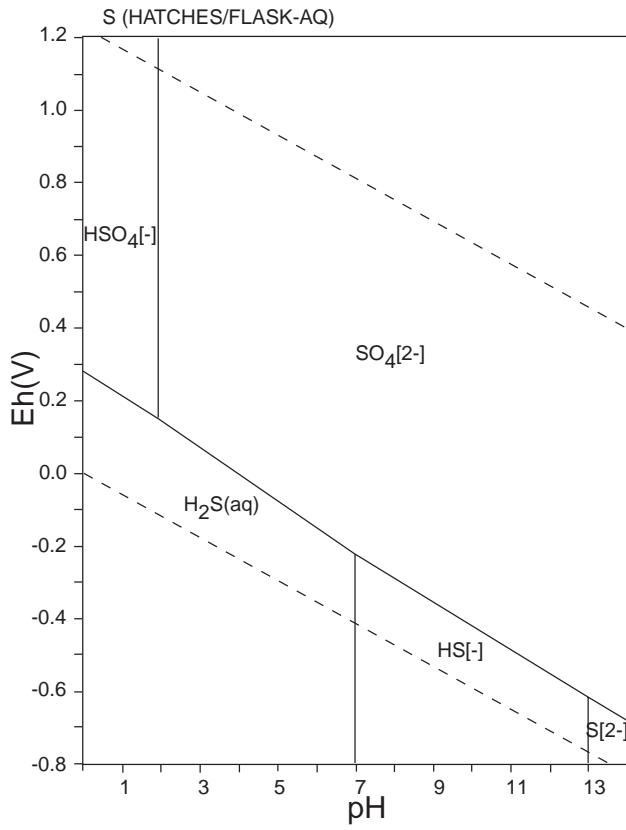
FACT	SUPCRT	LLNL	JNC-TDB
S[2-], S <sub>2</sub> [2-], S <sub>3</sub> [2-], S <sub>4</sub> [2-], S <sub>5</sub> [2-], HS[-], H <sub>2</sub> S(aq), SO <sub>2</sub> (aq), SO <sub>3</sub> [2-], SO <sub>4</sub> [2-], S <sub>2</sub> O <sub>3</sub> [2-], S <sub>2</sub> O <sub>4</sub> [2-], S <sub>2</sub> O <sub>5</sub> [2-], S <sub>2</sub> O <sub>6</sub> [2-], S <sub>2</sub> O <sub>8</sub> [2-], S <sub>3</sub> O <sub>6</sub> [2-], S <sub>4</sub> O <sub>6</sub> [2-], S <sub>5</sub> O <sub>6</sub> [2-], HSO <sub>3</sub> [-], HSO <sub>4</sub> [-], HS <sub>2</sub> O <sub>4</sub> [-], H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> (aq), <b>S(s)</b> , <b>S(s2)</b> , <b>SO<sub>3</sub>(s)</b>	S <sub>2</sub> [2-], S <sub>3</sub> [2-], S <sub>4</sub> [2-], S <sub>5</sub> [2-], HS[-], H <sub>2</sub> S(aq), SO <sub>2</sub> (aq), SO <sub>3</sub> [2-], SO <sub>4</sub> [2-], S <sub>2</sub> O <sub>3</sub> [2-], S <sub>2</sub> O <sub>4</sub> [2-], S <sub>2</sub> O <sub>5</sub> [2-], S <sub>2</sub> O <sub>6</sub> [2-], S <sub>2</sub> O <sub>8</sub> [2-], S <sub>3</sub> O <sub>6</sub> [2-], S <sub>4</sub> O <sub>6</sub> [2-], S <sub>5</sub> O <sub>6</sub> [2-], HSO <sub>3</sub> [-], HSO <sub>4</sub> [-], HS <sub>2</sub> O <sub>4</sub> [-], H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> (aq), HSO <sub>5</sub> [- ], HS <sub>2</sub> O <sub>3</sub> [-], H <sub>2</sub> S <sub>2</sub> O <sub>3</sub> (aq), <b>S(Sulfur)</b>	SO <sub>4</sub> [2-], HS[-], H <sub>2</sub> S(aq), H <sub>2</sub> SO <sub>4</sub> (aq), HSO <sub>4</sub> [-], S[2-], S <sub>2</sub> [2-], S <sub>3</sub> [2-], S <sub>4</sub> [2-], S <sub>5</sub> [2-], S <sub>6</sub> [2-], <b>Sulfur(rhmb)</b> , H <sub>2</sub> S(g), S <sub>2</sub> (g)	SO <sub>4</sub> [2-], S[2-], SO <sub>3</sub> [2-], S <sub>2</sub> O <sub>3</sub> [2-], HS[-], H <sub>2</sub> S(aq), HSO <sub>3</sub> [-], HS <sub>2</sub> O <sub>3</sub> [-], H <sub>2</sub> SO <sub>3</sub> (aq), HSO <sub>4</sub> [-], <b>S(c)</b> , S(g), S <sub>2</sub> (g), SO <sub>2</sub> (g), H <sub>2</sub> S(g)

HATCHES			
SO <sub>4</sub> [2-], HS[-], S <sub>2</sub> [2-], S <sub>3</sub> [2-], S <sub>4</sub> [2-], S <sub>5</sub> [2-], SO <sub>2</sub> (aq), H <sub>2</sub> S(aq), H <sub>2</sub> S <sub>2</sub> O <sub>3</sub> (aq), H <sub>2</sub> S <sub>2</sub> O <sub>4</sub> (aq), H <sub>2</sub> SO <sub>3</sub> (aq), HS <sub>2</sub> O <sub>3</sub> [-], HS <sub>2</sub> O <sub>4</sub> [-], HSO <sub>3</sub> [-], HSO <sub>4</sub> [-], S[2-], S <sub>2</sub> O <sub>3</sub> [2-], S <sub>2</sub> O <sub>4</sub> [2-], S <sub>2</sub> O <sub>5</sub> [2-], S <sub>2</sub> O <sub>6</sub> [2-], S <sub>2</sub> O <sub>8</sub> [2-], S <sub>3</sub> O <sub>6</sub> [2-], S <sub>4</sub> O <sub>6</sub> [2-], S <sub>5</sub> O <sub>6</sub> [2-], SO <sub>3</sub> [2-], <b>S(c)</b> , <b>Sulfur-rhmb</b>			



106: Eh-pH diagrams of the system S-O-H (1).  $\sum S = 10^{-10}$ , 298.15K,  $10^5$  Pa.





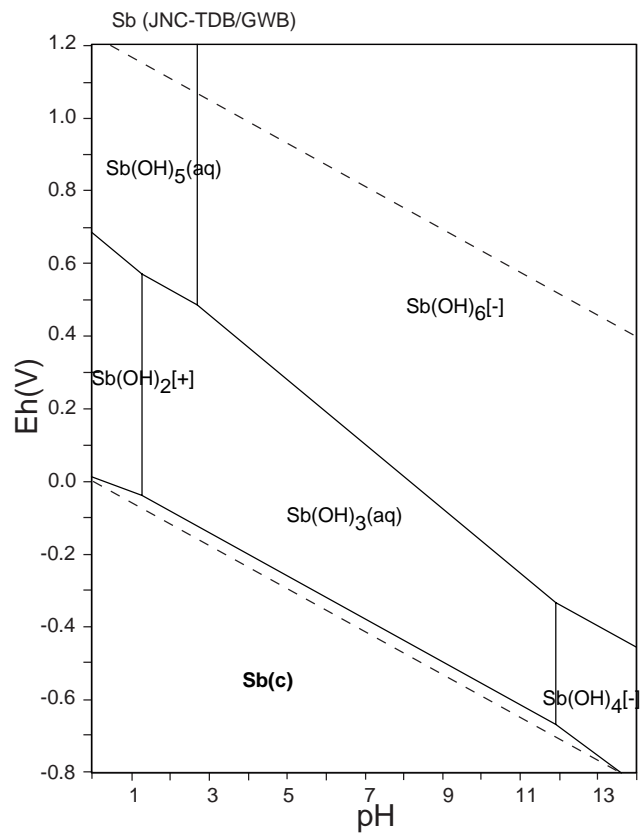
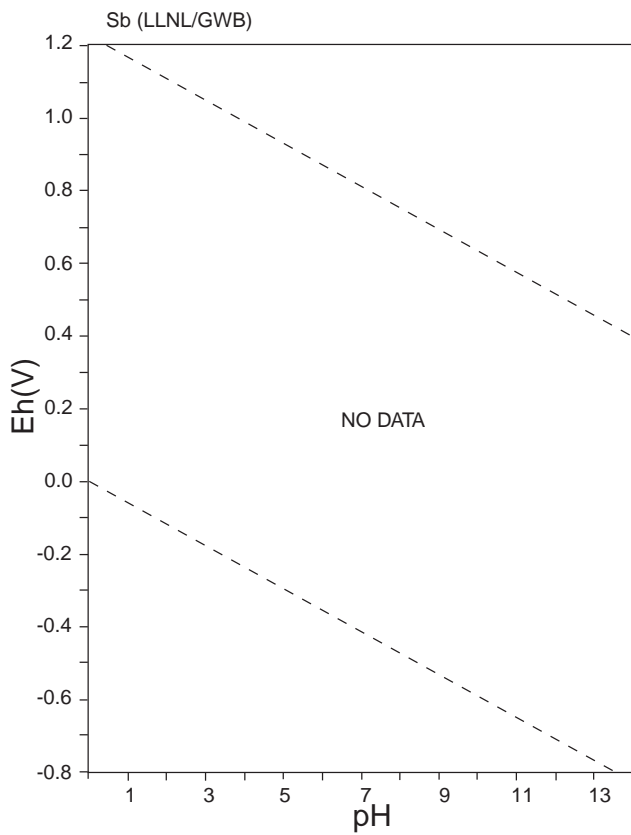
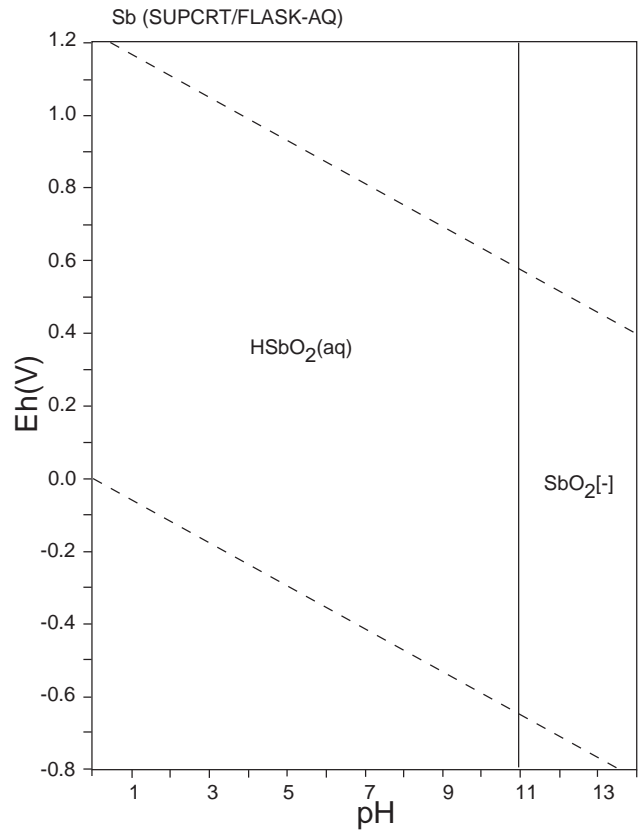
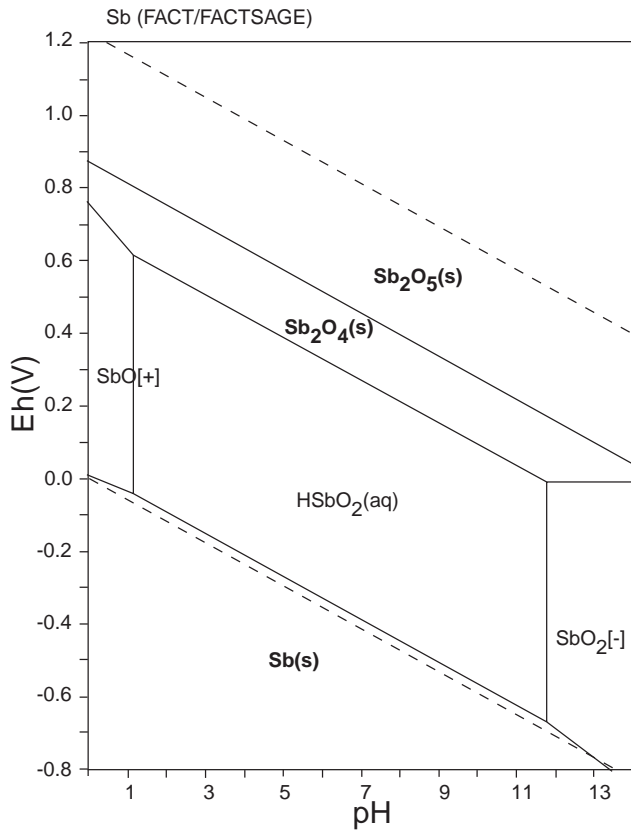
☒ 107: Eh-pH diagrams of the system S-O-H (2).  $\sum S = 10^{-10}$ , 298.15K,  $10^5$  Pa.



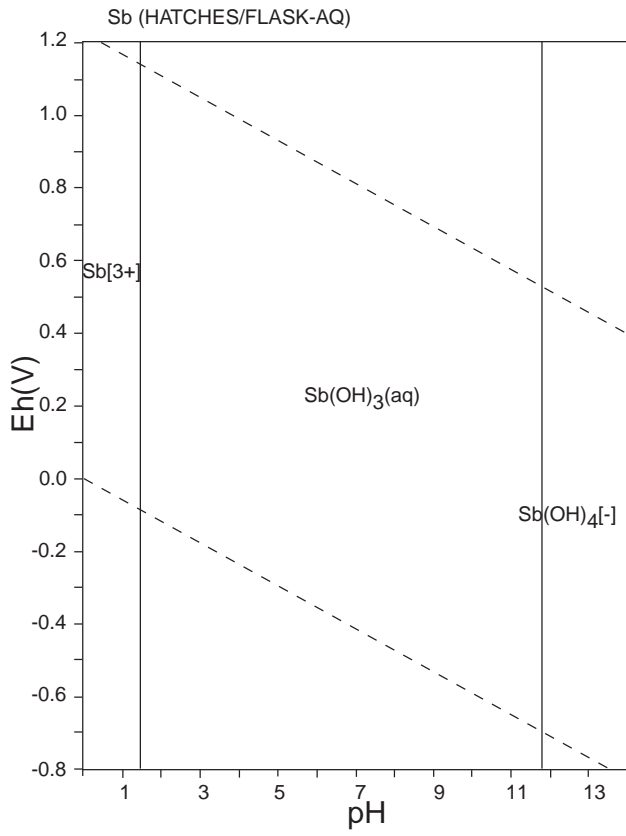
表 67: List of Sb species

FACT	SUPCRT	LLNL	JNC-TDB
$\text{SbO}_2[-]$ , $\text{HSbO}_2(\text{aq})$ , $\text{SbO}[+]$ , <b>Sb(s)</b> , <b>SbO<sub>2</sub>(s)</b> , <b>Sb<sub>2</sub>O<sub>3</sub>(s)</b> , <b>Sb<sub>2</sub>O<sub>3</sub>(s2)</b> , <b>Sb<sub>2</sub>O<sub>4</sub>(s)</b> , <b>Sb<sub>2</sub>O<sub>5</sub>(s)</b>	$\text{SbO}_2[-]$ , $\text{HSbO}_2(\text{aq})$		$\text{Sb}(\text{OH})_3(\text{aq})$ , $\text{Sb}(\text{OH})_5(\text{aq})$ $\text{Sb}(\text{OH})_6[-]$ , $\text{Sb}_{12}(\text{OH})_{64}(\text{aq})$ $\text{Sb}_{12}(\text{OH})_{65}[5-]$ , $\text{Sb}_{12}(\text{OH})_{66}[6-]$ , $\text{Sb}_{12}(\text{OH})_{67}[7-]$ , $\text{Sb}[3+]$ , $\text{SbOH}[2+]$ , $\text{Sb}(\text{OH})_2[+]$ $\text{Sb}(\text{OH})_4[-]$ , <b>Sb<sub>2</sub>(OH)<sub>6</sub>(s)</b> <b>Sb(c)</b> , <b>Valentinite</b> , <b>Sb<sub>2</sub>O<sub>5</sub>(s)</b>

HATCHES			
$\text{Sb}(\text{OH})_3(\text{aq})$ , $\text{Sb}[3+]$ , $\text{Sb}(\text{OH})_2[+]$ , $\text{Sb}(\text{OH})_4[-]$ , <b>Sb<sub>2</sub>O<sub>3</sub></b>			



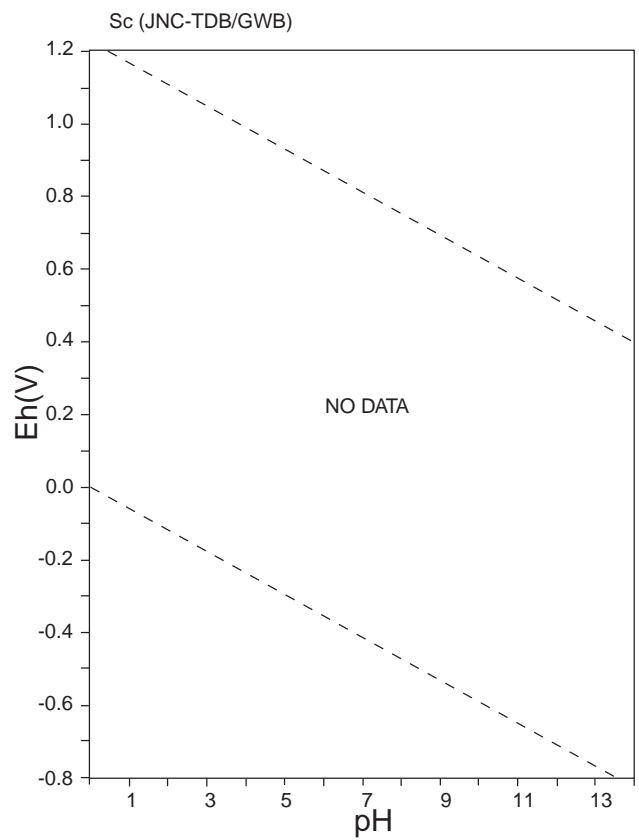
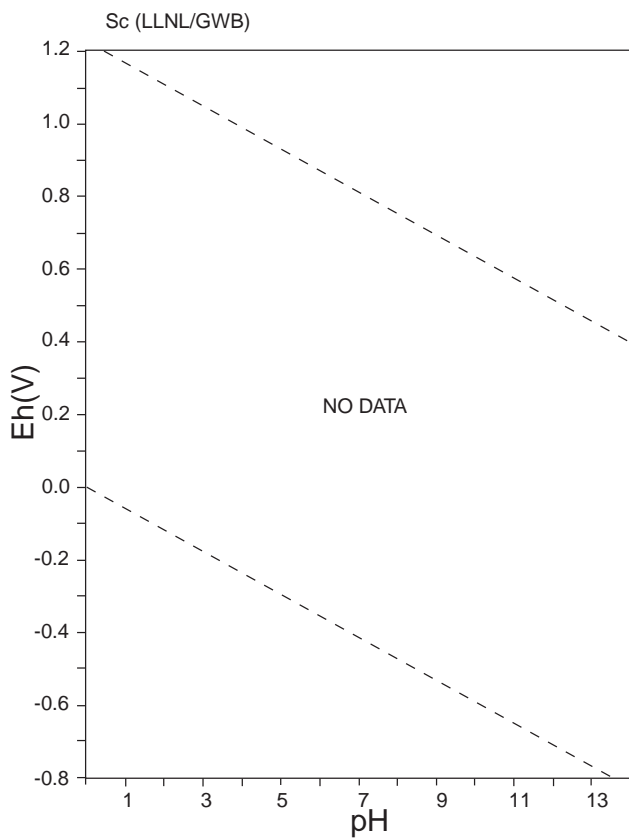
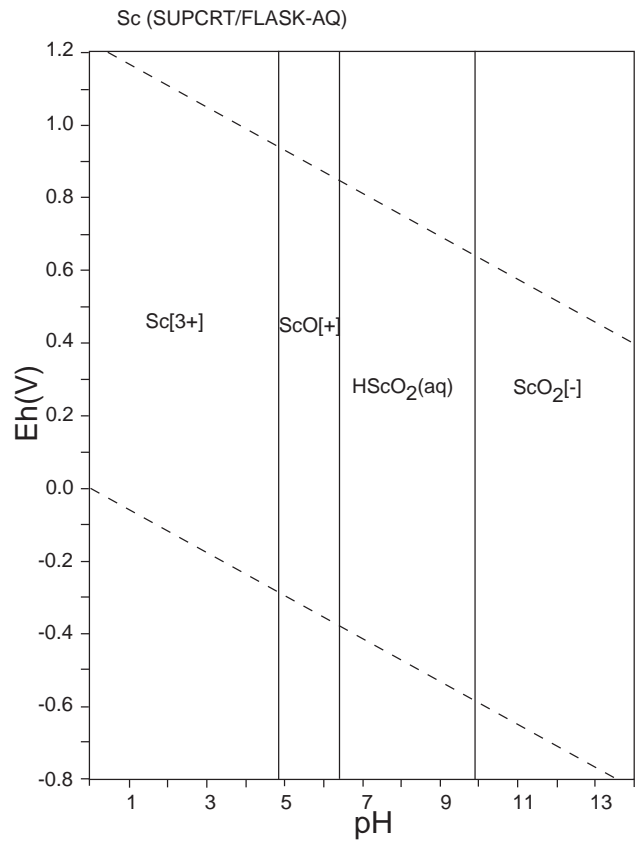
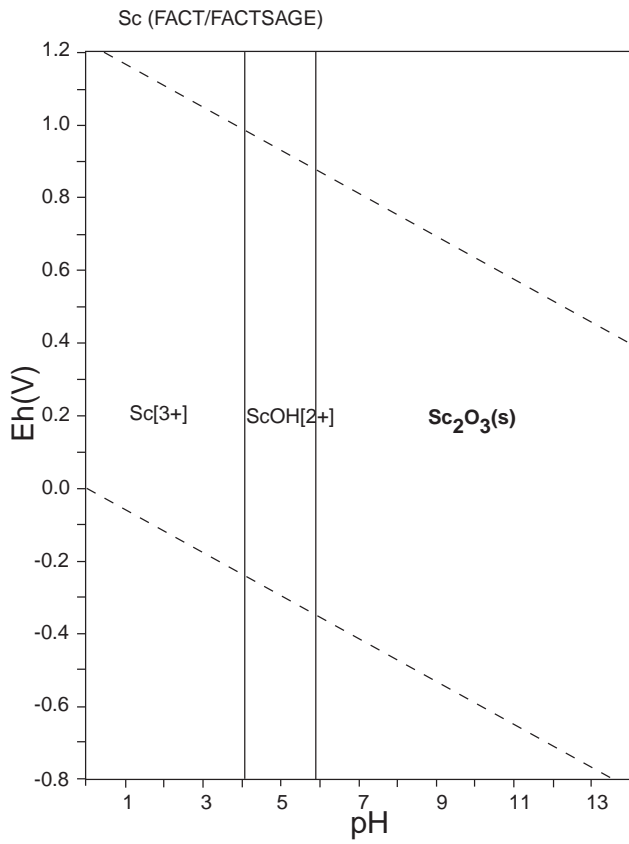
☒ 108: Eh-pH diagrams of the system Sb-O-H (1).  $\sum \text{Sb} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 109: Eh-pH diagrams of the system Sb-O-H (2).  $\sum Sb = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 68: List of Sc species

FACT	SUPCRT	LLNL	JNC-TDB
$\text{Sc}^{3+}$ , $\text{ScOH}^{2+}$ , $\text{Sc}(\text{s})$ , $\text{Sc}(\text{s}2)$ , $\text{Sc}_2\text{O}_3(\text{s})$ , $\text{Sc}(\text{OH})_3(\text{s})$	$\text{Sc}^{3+}$ , $\text{ScOH}^{2+}$ , $\text{ScO}^+$ , $\text{HScO}_2(\text{aq})$ , $\text{ScO}_2^-$		



☒ 110: Eh-pH diagrams of the system Sc-O-H.  $\sum \text{Sc} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





表 69: List of Se species

FACT	SUPCRT	LLNL	JNC-TDB
HSe[-], SeO <sub>3</sub> [2-], SeO <sub>4</sub> [2-], HSeO <sub>3</sub> [-], H <sub>2</sub> SeO <sub>3</sub> (aq), HSeO <sub>4</sub> [-], Se[2-], H <sub>2</sub> Se(aq), <b>Se(s)</b> , <b>SeO<sub>2</sub>(s)</b> , <b>SeO<sub>3</sub>(s)</b> , <b>Se<sub>2</sub>O<sub>5</sub>(s)</b>	HSe[-], SeO <sub>3</sub> [2-], SeO <sub>4</sub> [2-], HSeO <sub>3</sub> [-], H <sub>2</sub> SeO <sub>3</sub> (aq), HSeO <sub>4</sub> [-]	SeO <sub>3</sub> [2-], Se[2-], SeO <sub>4</sub> [2-], H <sub>2</sub> Se(aq), H <sub>2</sub> SeO <sub>3</sub> (aq), HSe[-], HSeO <sub>3</sub> [-], HSeO <sub>4</sub> [-], <b>Se(black)</b> , <b>Se<sub>2</sub>O<sub>5</sub>(s)</b> , <b>SeO<sub>2</sub>(s)</b> , <b>SeO<sub>3</sub>(s)</b>	SeO <sub>4</sub> [2-], Se[2-], HSe[-], H <sub>2</sub> Se(aq), SeO <sub>3</sub> [2-], HSeO <sub>3</sub> [-], H <sub>2</sub> SeO <sub>3</sub> (aq), HSeO <sub>4</sub> [-], <b>Se(s)</b> , <b>SeO<sub>2</sub>(s)</b> , <b>Se<sub>2</sub>O<sub>5</sub>(s)</b> , <b>SeO<sub>3</sub>(s)</b>

HATCHES			
SeO <sub>4</sub> [2-], Se[2-], SeO <sub>3</sub> [2-], H <sub>2</sub> Se(aq), H <sub>2</sub> SeO <sub>3</sub> (aq), HSe[-], HSeO <sub>3</sub> [-], HSeO <sub>4</sub> [-], <b>Se</b> , <b>Se<sub>2</sub>O<sub>5</sub></b> , <b>SeO<sub>2</sub></b> , <b>SeO<sub>3</sub></b>			

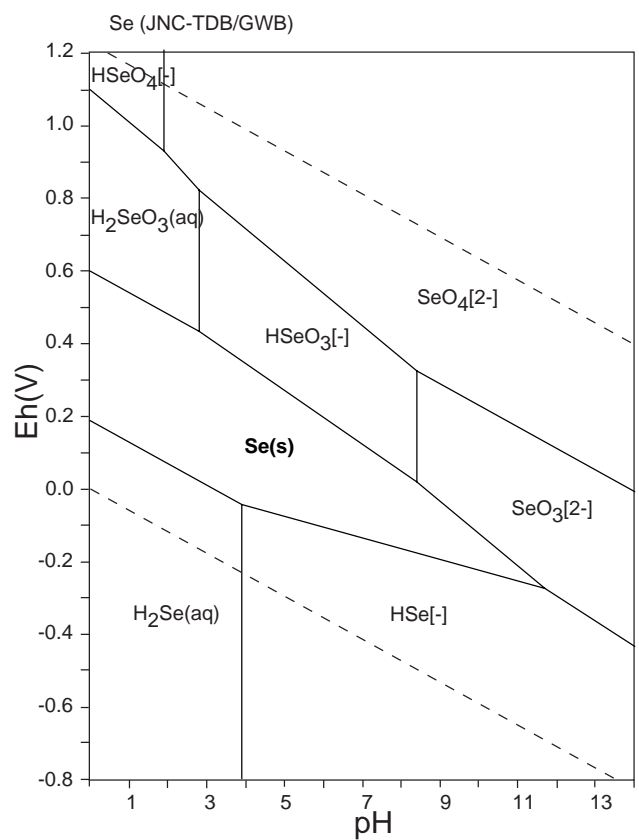
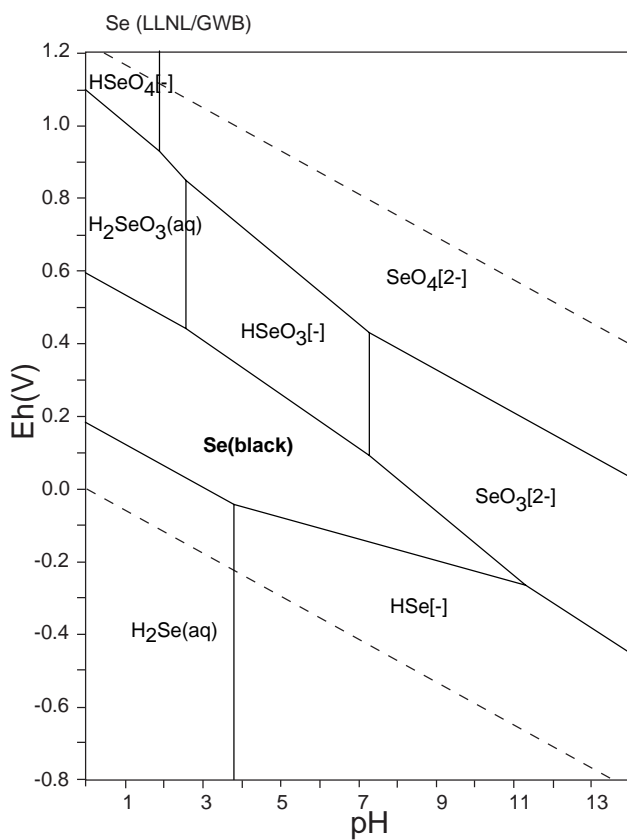
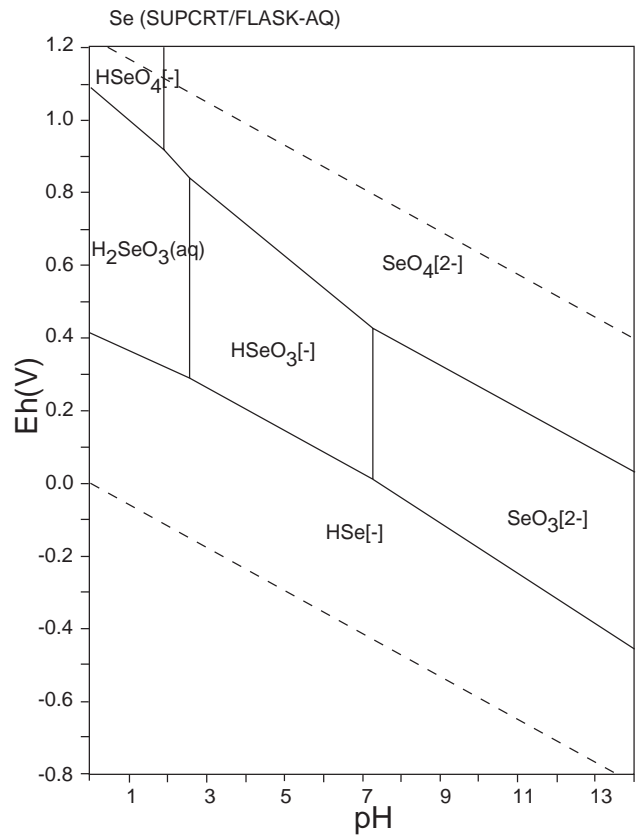
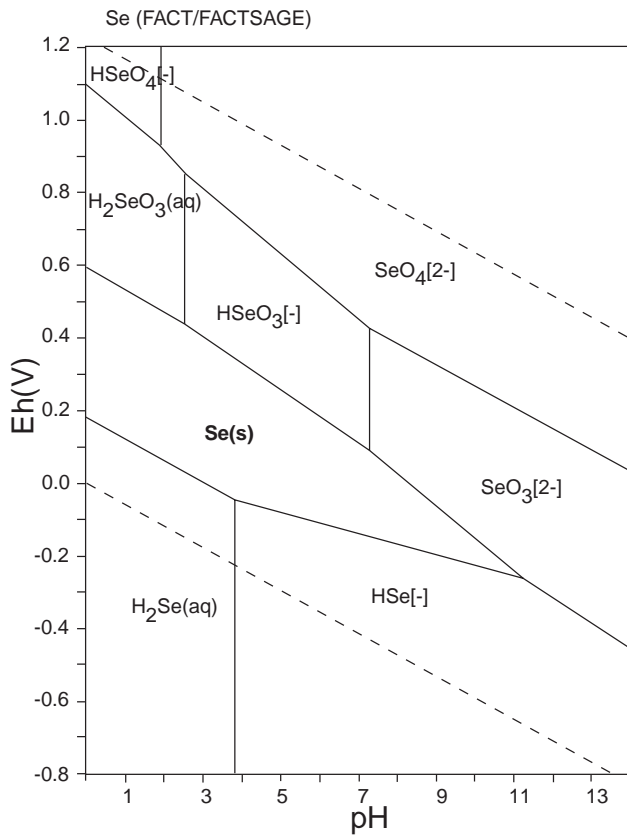
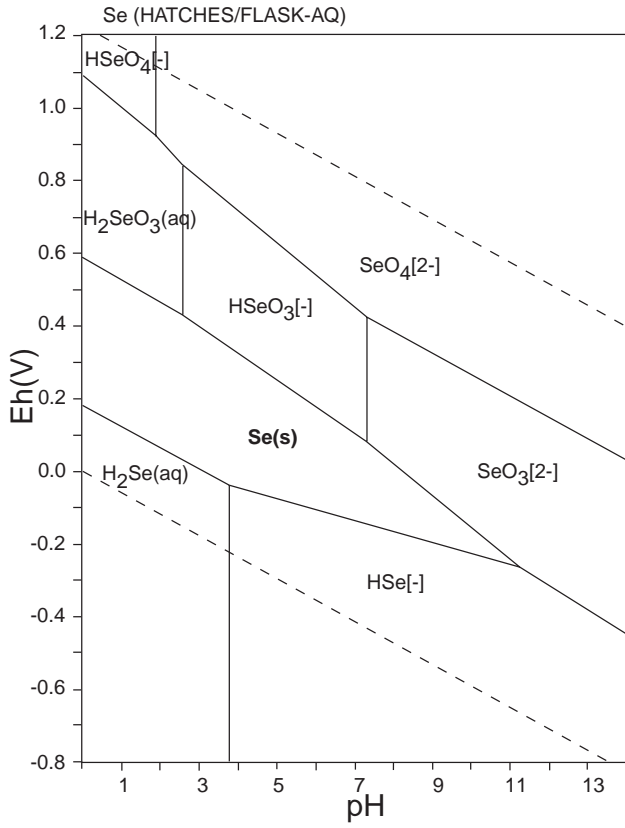


Figure 111: Eh-pH diagrams of the system Se-O-H (1).  $\Sigma \text{Se} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 112: Eh-pH diagrams of the system Se-O-H (2).  $\sum \text{Se} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



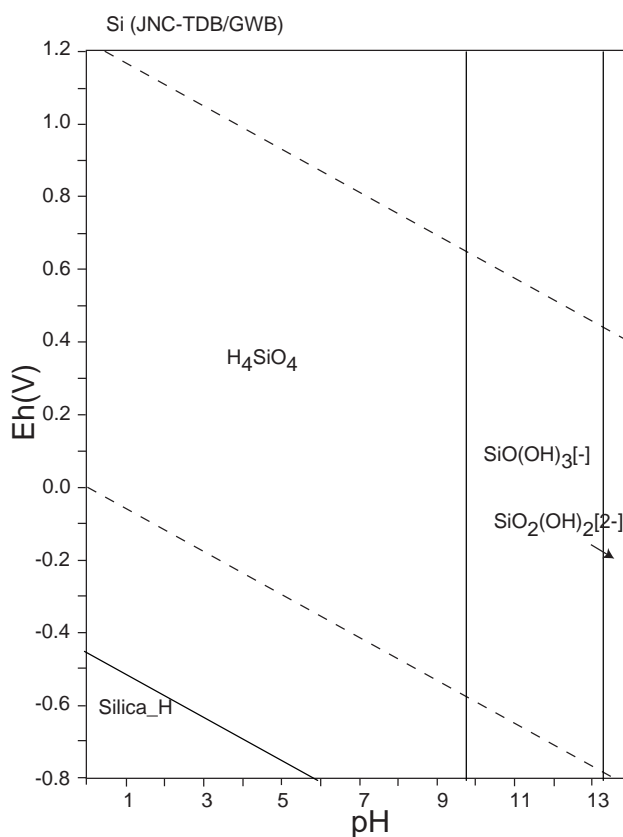
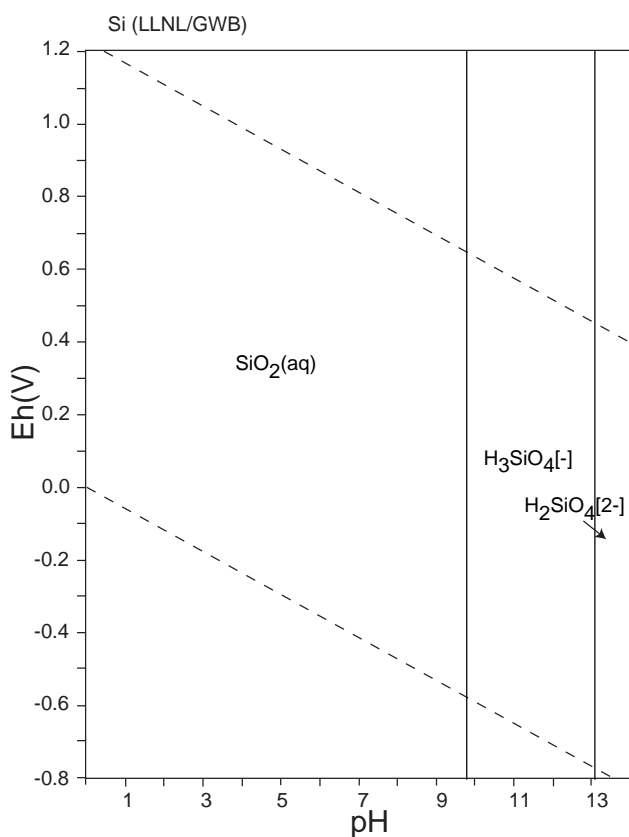
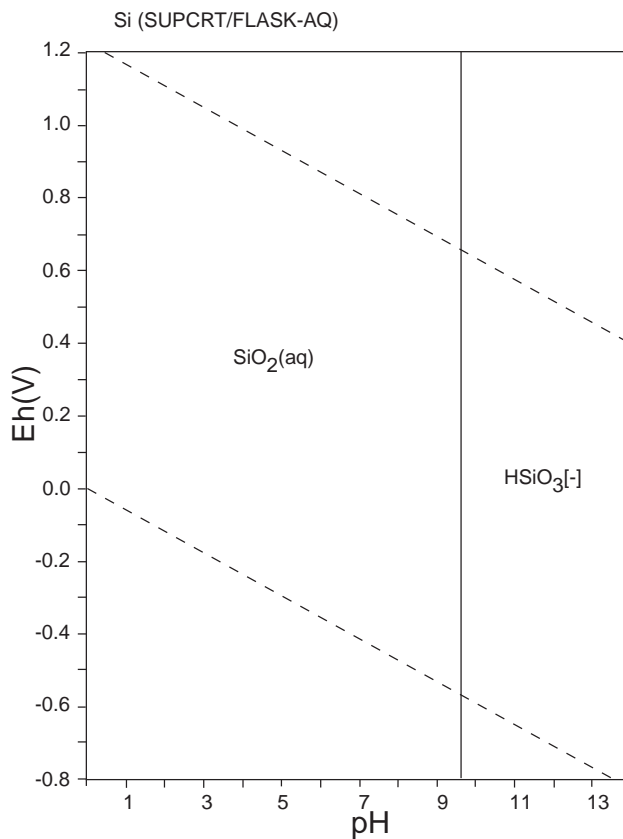
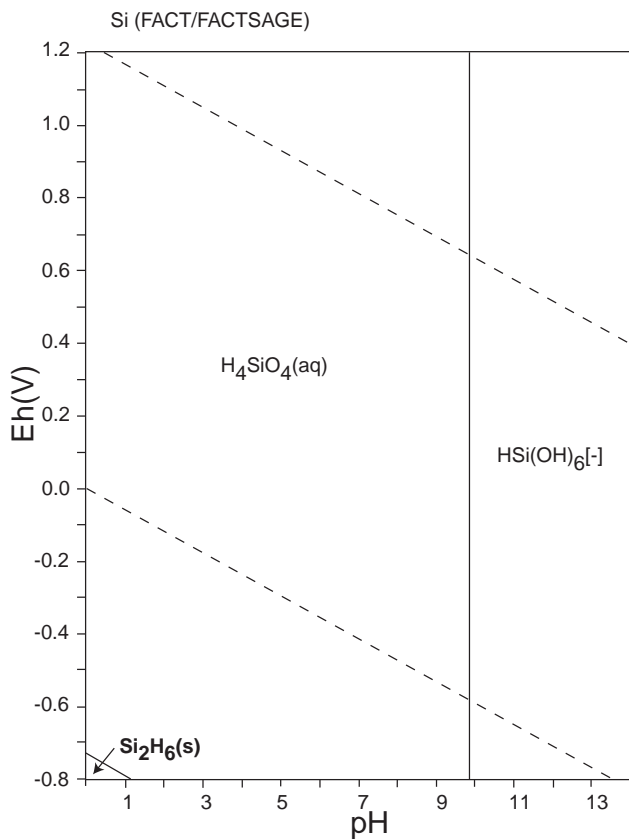
表 70: List of Si species

FACT	SUPCRT	LLNL	JNC-TDB
H <sub>4</sub> SiO <sub>4</sub> (aq), HSi(OH) <sub>6</sub> [-], H <sub>2</sub> SiO <sub>3</sub> (aq), Si(s), Si <sub>2</sub> H <sub>5</sub> (s), H <sub>2</sub> SiO <sub>3</sub> (s), H <sub>4</sub> SiO <sub>4</sub> (s), H <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> (s), H <sub>6</sub> Si <sub>2</sub> O <sub>7</sub> (s), SiO <sub>2</sub> (s), SiO <sub>2</sub> (s2), SiO <sub>2</sub> (s3), SiO <sub>2</sub> (s4), SiO <sub>2</sub> (s5), SiO <sub>2</sub> (s6), SiO <sub>2</sub> (s7), SiO <sub>2</sub> (s8)	SiO <sub>2</sub> (aq), HSiO <sub>3</sub> [-], SiO <sub>2</sub> (Amorpyous- silica), SiO <sub>2</sub> (Chalcedony), SiO <sub>2</sub> (Cristobalite, alpha), SiO <sub>2</sub> (Cristobalite, beta), SiO <sub>2</sub> (Coesite), SiO <sub>2</sub> (Cristobalite), SiO <sub>2</sub> (Quartz)	SiO <sub>2</sub> (aq), H <sub>2</sub> SiO <sub>4</sub> [2- ], H <sub>3</sub> SiO <sub>4</sub> [-], H <sub>4</sub> (H <sub>2</sub> SiO <sub>4</sub> ) <sub>4</sub> [4-], H <sub>6</sub> (H <sub>2</sub> SiO <sub>4</sub> ) <sub>4</sub> [2-], Amrph_silica, Chalcedony, Cristobalite, Quartz, Tridymite	H <sub>4</sub> SiO <sub>4</sub> (aq), SiO <sub>2</sub> (OH)[2-], SiO(OH) <sub>3</sub> [-], Si <sub>2</sub> O <sub>3</sub> (OH) <sub>4</sub> [2-], Si <sub>2</sub> O <sub>2</sub> (OH) <sub>5</sub> [-], Si <sub>3</sub> O <sub>6</sub> (OH) <sub>3</sub> [3-], Si <sub>3</sub> O <sub>5</sub> (OH) <sub>5</sub> [3-], Si <sub>4</sub> O <sub>8</sub> (OH) <sub>4</sub> [4-], Si <sub>4</sub> O <sub>7</sub> (OH) <sub>5</sub> [3-], Si <sub>4</sub> O <sub>3</sub> (OH) <sub>13</sub> [3-], SiO <sub>2</sub> (s,Sil_gel), H <sub>2</sub> SiO <sub>3</sub> (s, Sil_glass), Chalcedony, Quartz, HSiO <sub>2</sub> (s, Silica_H), Sili(am), Si(c), SiO <sub>2</sub> (qua), Si(g)

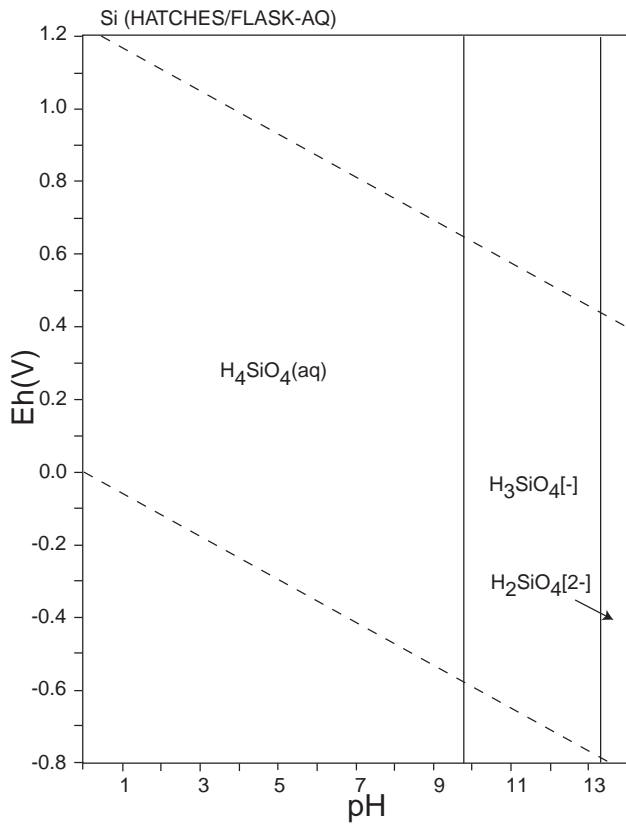
HATCHES			
H <sub>4</sub> SiO <sub>4</sub> (aq), H <sub>2</sub> SiO <sub>4</sub> [2-], H <sub>3</sub> Si <sub>3</sub> O <sub>9</sub> [3-], H <sub>3</sub> SiO <sub>4</sub> [- ], H <sub>4</sub> Si <sub>2</sub> O <sub>7</sub> [2-], H <sub>4</sub> Si <sub>4</sub> O <sub>12</sub> [4-], H <sub>5</sub> Si <sub>2</sub> O <sub>7</sub> [-], H <sub>5</sub> Si <sub>3</sub> O <sub>10</sub> [3-], H <sub>5</sub> Si <sub>4</sub> O <sub>12</sub> [3-], Amrph.silica, Chalcedony, Cristobalite, Crist.beta, Quartz			

Remarks

JNC-TDB: SiO<sub>2</sub>(qua) is not Quartz in the database file, its log<sub>10</sub>K's are different from those of Quartz, but detailed description of SiO<sub>2</sub>(qua) is not given.



☒ 113: Eh-pH diagrams of the system Si-O-H (1).  $\sum \text{Si} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 114: Eh-pH diagrams of the system Si-O-H (2).  $\sum \text{Si} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

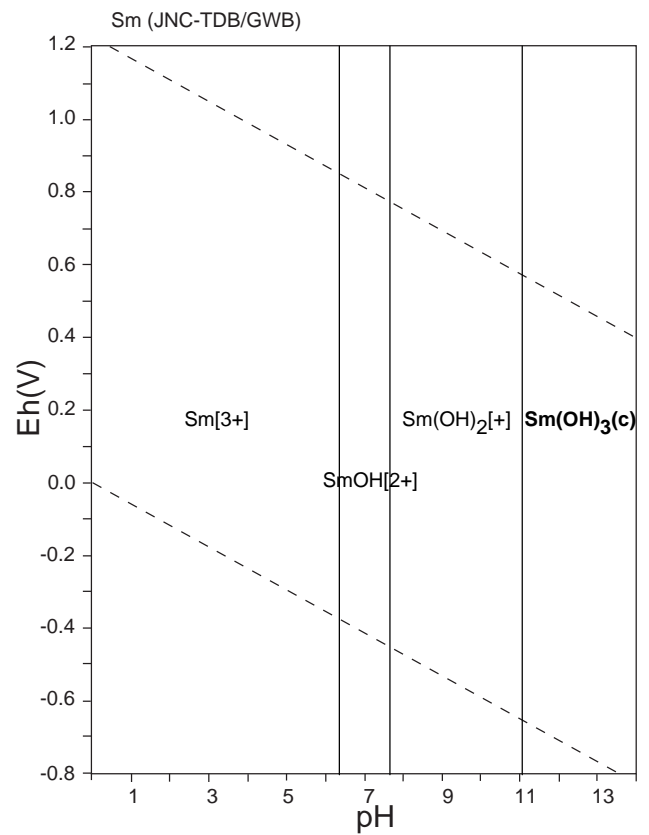
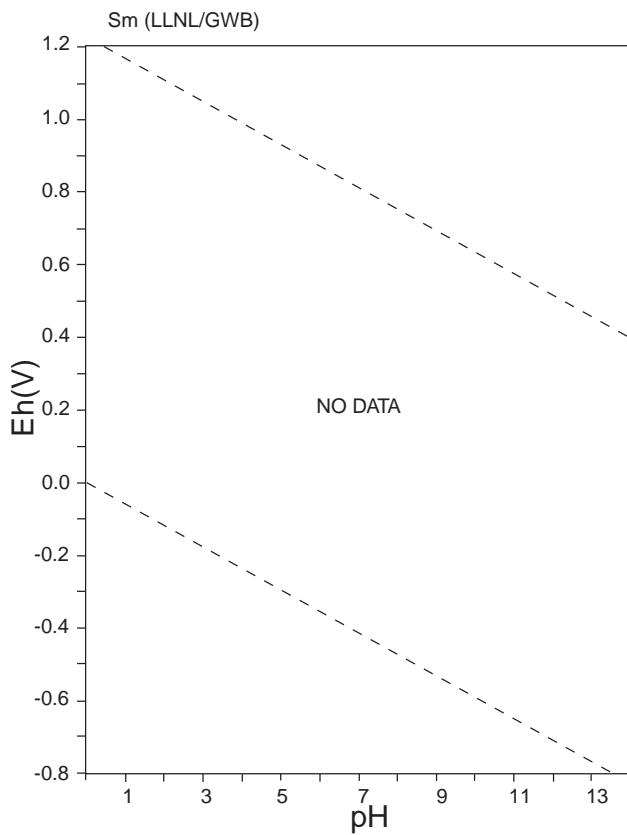
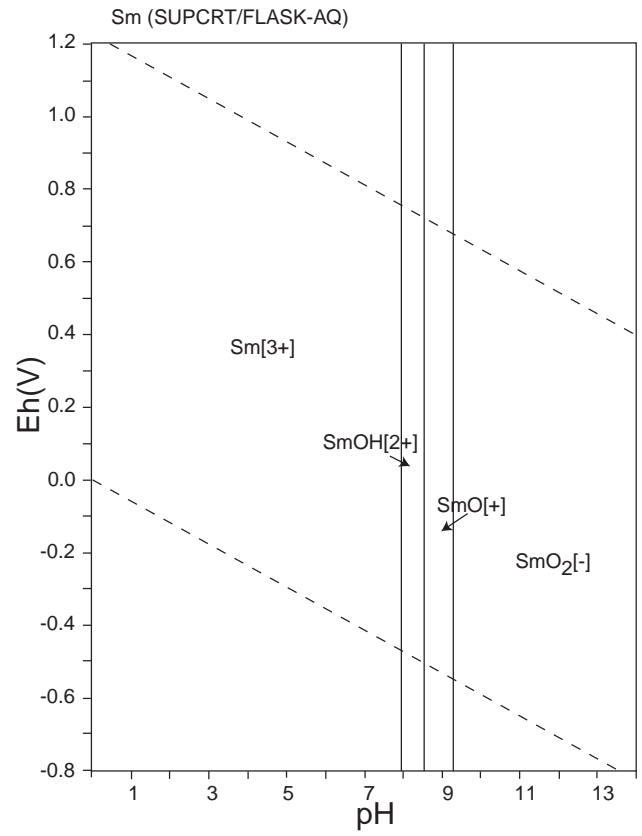
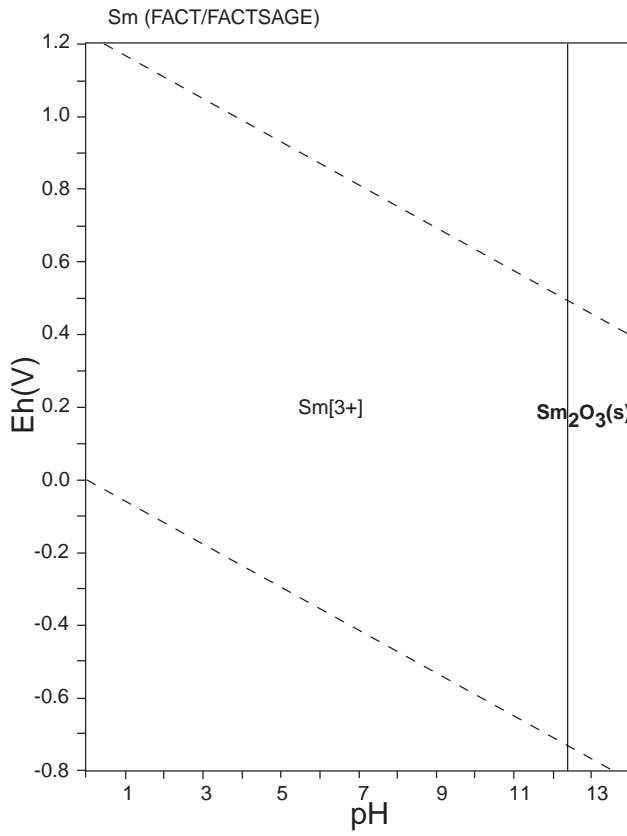




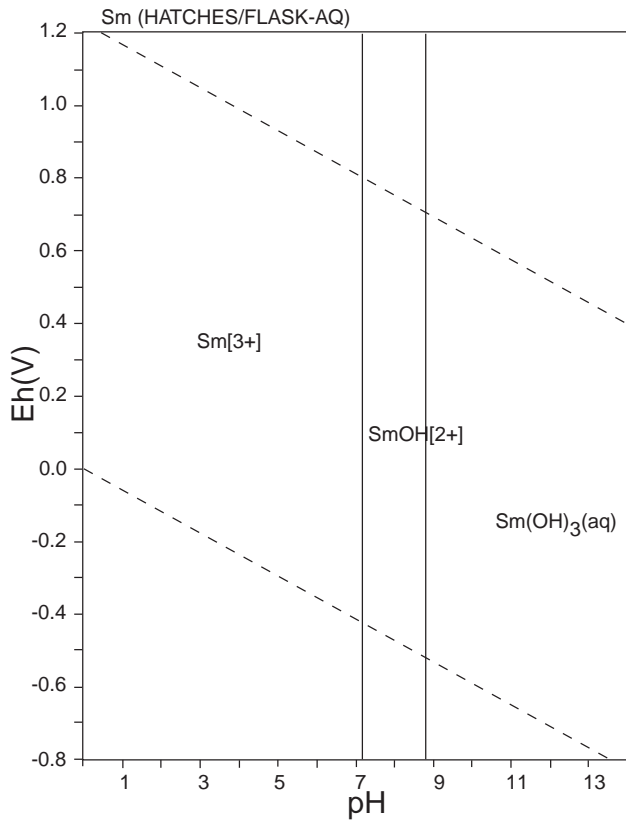
表 71: List of Sm species

FACT	SUPCRT	LLNL	JNC-TDB
Sm[2+], Sm[3+], <b>Sm(s)</b> , <b>Sm(s2)</b> , <b>Sm<sub>2</sub>O<sub>3</sub>(s)</b> , <b>Sm<sub>2</sub>O<sub>3</sub>(s2)</b>	Sm[2+], Sm[3+], Sm[4+], SmOH[2+], SmO[+], SmO <sub>2</sub> H(aq), SmO <sub>2</sub> [-]		Sm[3+], SmOH[2+], Sm(OH) <sub>2</sub> [+], Sm(OH) <sub>3</sub> (aq), <b>Sm(OH)<sub>3</sub>(am)</b> , <b>Sm(OH)<sub>3</sub>(c)</b>

HATCHES			
Sm[3+], Sm(OH) <sub>2</sub> [+], Sm(OH) <sub>3</sub> (aq), SmOH[2+], <b>Sm(OH)<sub>3</sub></b>			



☒ 115: Eh-pH diagrams of the system Sm-O-H (1).  $\sum \text{Sm} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



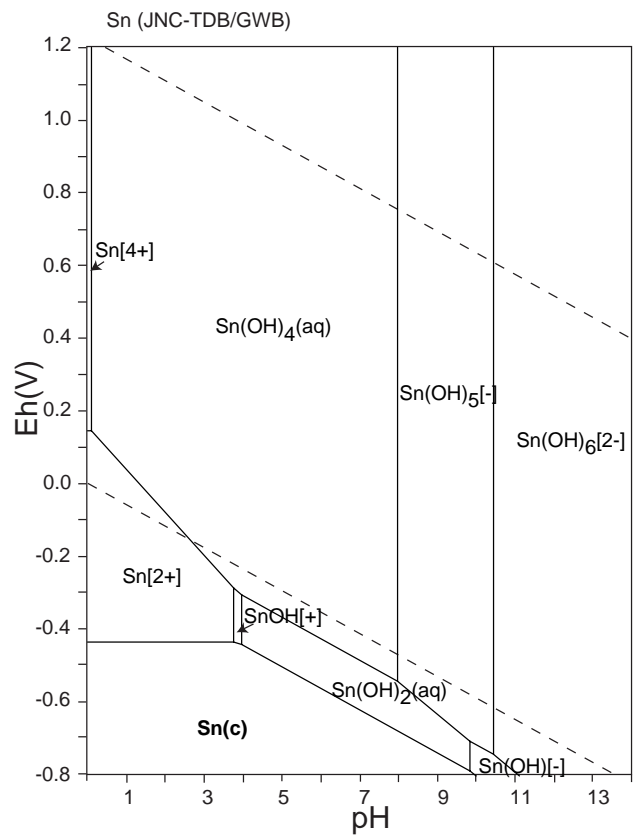
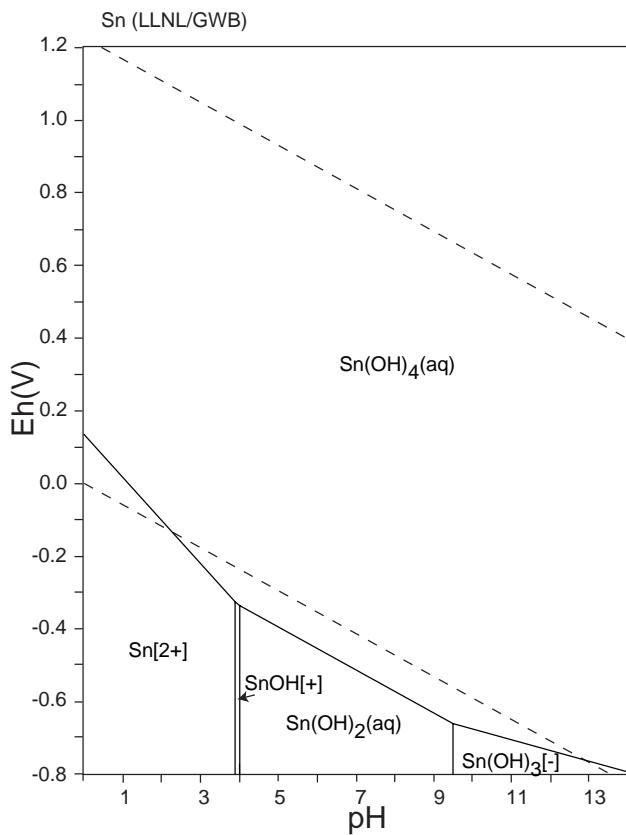
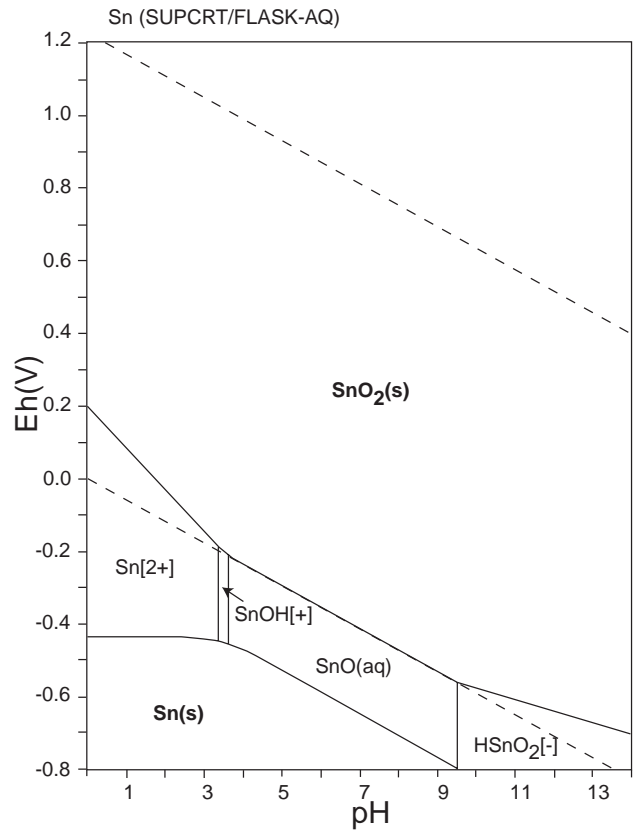
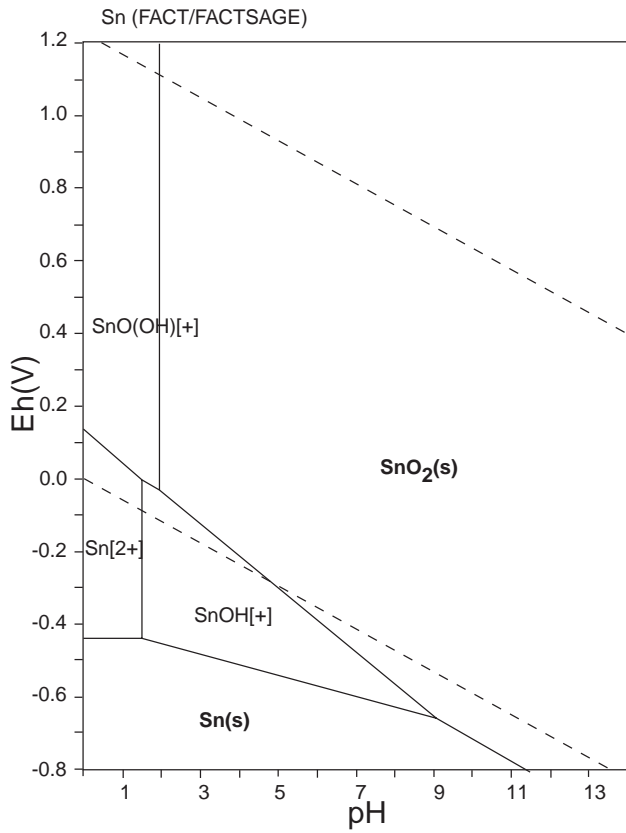
☒ 116: Eh-pH diagrams of the system Sm-O-H (2).  $\sum \text{Sm} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



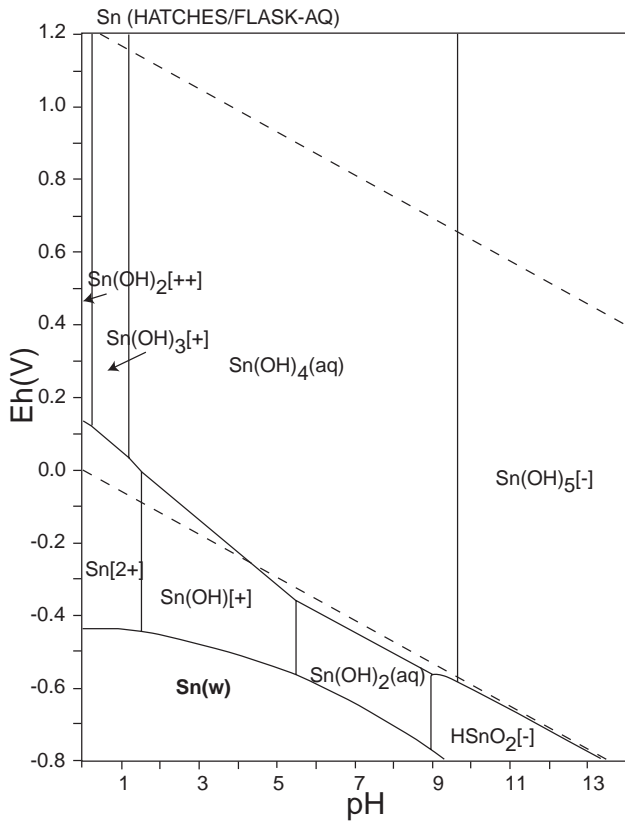
表 72: List of Sn species

FACT	SUPCRT	LLNL	JNC-TDB
Sn[2+], SnOH[+], SnO(OH)[+], <b>Sn(s2)</b> , <b>Sn(s)</b> , <b>SnO(s)</b> , <b>SnO<sub>2</sub>(s)</b>	Sn[2+], SnOH[+], SnO(aq), HSnO <sub>2</sub> [-], <b>Sn(Native tin)</b> , <b>SnO(Romarchite)</b> , <b>SnO<sub>2</sub>(Cassiterite)</b>	Sn[4+], Sn[2+], Sn(OH) <sub>2</sub> (aq), Sn(OH) <sub>2</sub> [2+], Sn(OH) <sub>3</sub> [+], Sn(OH) <sub>3</sub> [-], Sn(OH) <sub>4</sub> (aq), SnOH[+], SnOH[3+], <b>Sn(OH)<sub>2</sub>(s)</b> , <b>SnO(s)</b> , <b>SnO<sub>2</sub>(s)</b>	Sn(OH) <sub>4</sub> (aq), SnOH[+], Sn(OH) <sub>2</sub> (aq), Sn(OH) <sub>3</sub> [-], Sn <sub>3</sub> (OH) <sub>4</sub> [2+], Sn[2+] Sn(OH) <sub>5</sub> [-], Sn(OH) <sub>6</sub> [-], Sn[4+], <b>Sn(c)</b> , <b>Sn(OH)<sub>2</sub>(s)</b> , <b>SnO(c)</b> , <b>SnO<sub>2</sub>(am)</b> <b>SnO<sub>2</sub>(cassiterite)</b>

HATCHES			
Sn[2+], Sn[4+], HSnO <sub>2</sub> [-], Sn(OH)[+], Sn(OH) <sub>2</sub> (aq), Sn(OH) <sub>2</sub> [2+], Sn(OH) <sub>3</sub> [+], Sn(OH) <sub>3</sub> [-], Sn(OH) <sub>4</sub> (aq), Sn(OH) <sub>5</sub> [-], Sn(OH) <sub>6</sub> [2-], Sn <sub>2</sub> (OH) <sub>2</sub> [2+], Sn <sub>3</sub> (OH) <sub>4</sub> [2+], SnOH[3+], <b>H<sub>2</sub>Sn(OH)<sub>6</sub></b> , <b>Sn(OH)<sub>2</sub></b> , <b>Sn(OH)<sub>4</sub></b> , <b>Sn(w)</b> , <b>SnO</b> , <b>SnO<sub>2</sub>(am)</b> , <b>SnO<sub>2</sub>(c)</b> , <b>SnO<sub>2</sub>(pptd)</b>			



☒ 117: Eh-pH diagrams of the system Sn-O-H (1).  $\Sigma \text{Sn} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 118: Eh-pH diagrams of the system Sn-O-H (2).  $\sum Sn = 10^{-10}$ , 298.15K,  $10^5$  Pa.

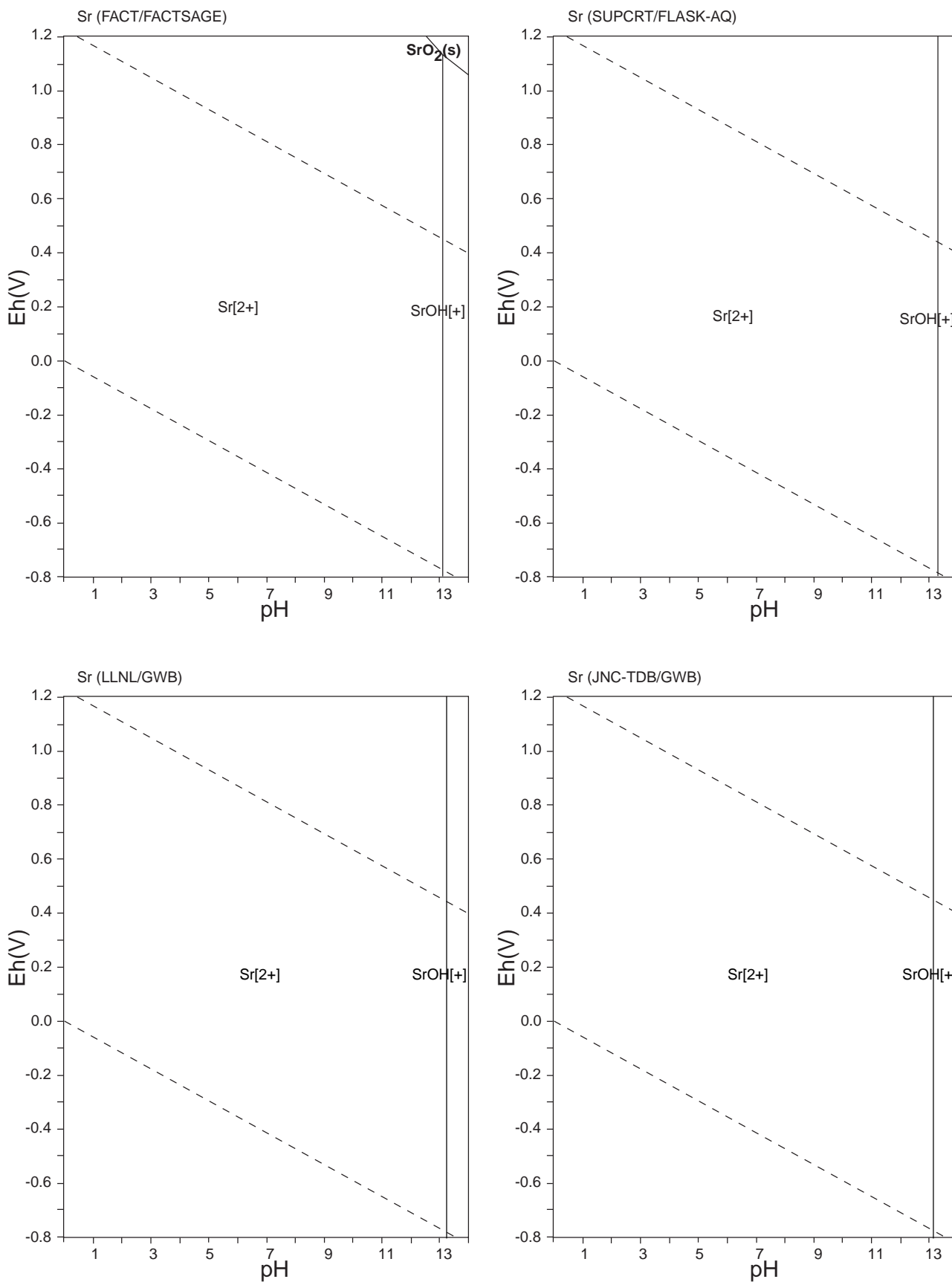




表 73: List of Sr species

FACT	SUPCRT	LLNL	JNC-TDB
Sr[2+], SrOH[+], <b>Sr(s), Sr(s2),</b> <b>SrH<sub>2</sub>(s), SrO(s),</b> <b>SrO<sub>2</sub>(s), Sr(OH)<sub>2</sub>(s)</b>	Sr[2+], SrOH[+]	Sr[2+], SrOH[+], <b>Sr(OH)<sub>2</sub>(c), SrO(c)</b>	Sr[2+], SrOH[+], Sr(OH) <sub>2</sub> (aq), <b>Sr(OH)<sub>2</sub>(s), Sr(c),</b> <b>SrO(c)</b>

HATCHES			
Sr[2+], Sr(OH) <sub>2</sub> (aq), SrOH[+], <b>Sr(OH)<sub>2</sub>,</b> <b>SrO(c)</b>			



☒ 119: Eh-pH diagrams of the system Sr-O-H (1).  $\sum \text{Sr} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

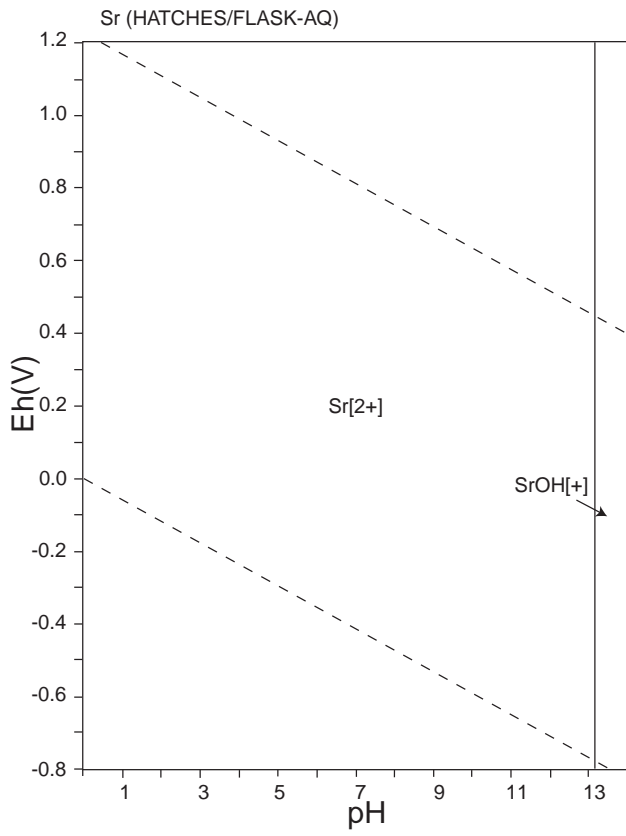
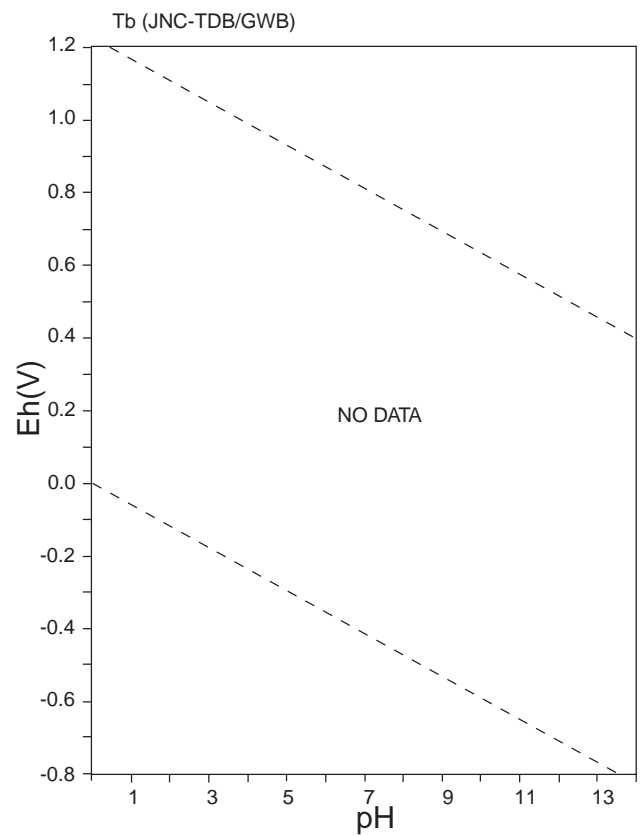
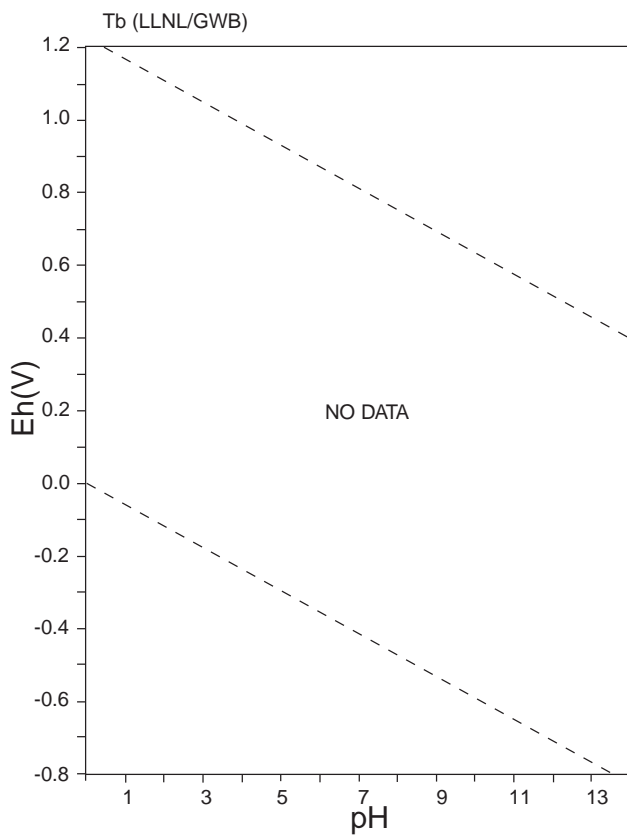
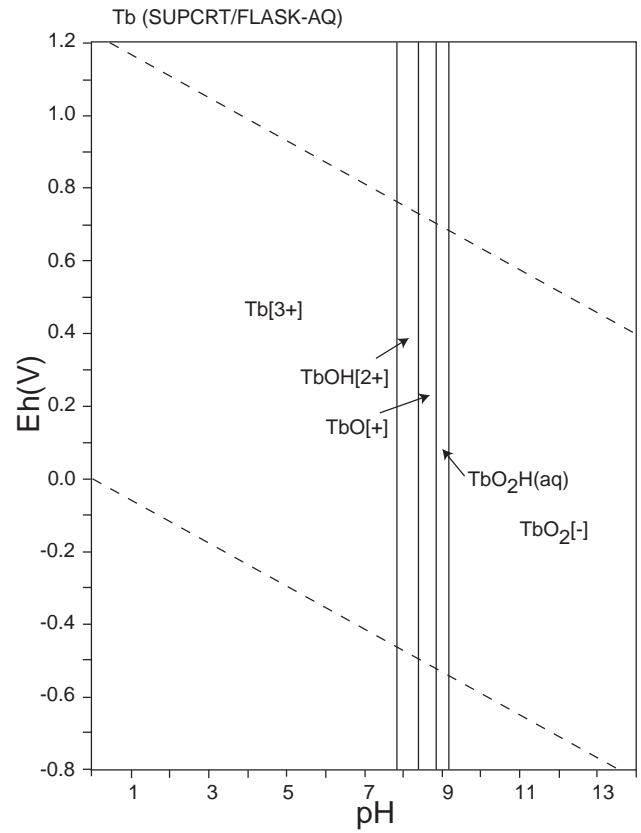
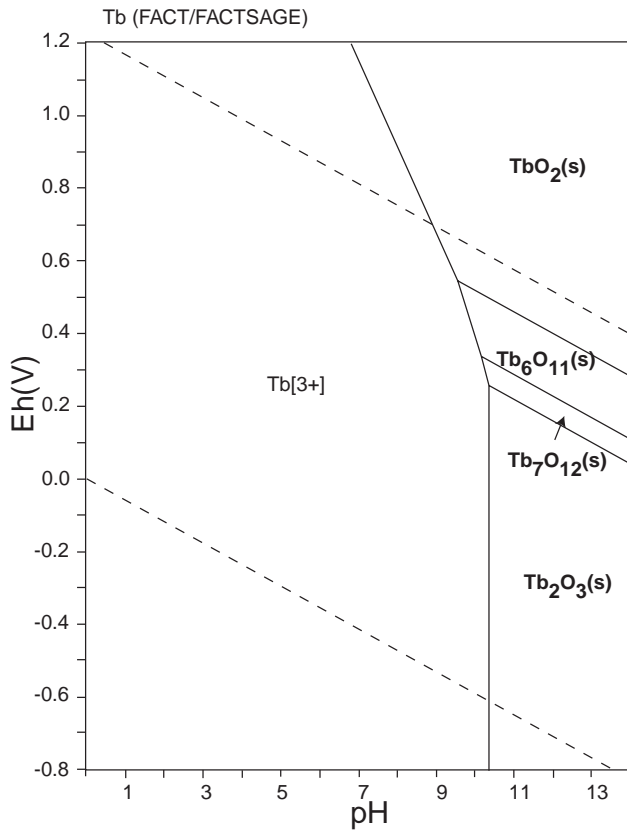


图 120: Eh-pH diagrams of the system Sr-O-H (2).  $\sum \text{Sr} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 74: List of Tb species

FACT	SUPCRT	LLNL	JNC-TDB
<b>Tb[3+]</b> , <b>Tb(s)</b> , <b>Tb(s2)</b> , <b>TbO<sub>2</sub>(s)</b> , <b>Tb<sub>2</sub>O<sub>3</sub>(s)</b> , <b>Tb<sub>6</sub>O<sub>11</sub>(s)</b> , <b>Tb<sub>7</sub>O<sub>12</sub>(s)</b>	<b>Tb[3+]</b> , <b>Tb[4+]</b> , <b>Tb[2+]</b> , <b>TbOH[2+]</b> , <b>TbO[+]</b> , <b>TbO<sub>2</sub>H(aq)</b> , <b>TbO<sub>2</sub>[-]</b>		



☒ 121: Eh-pH diagrams of the system Tb-O-H.  $\sum \text{Tb} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



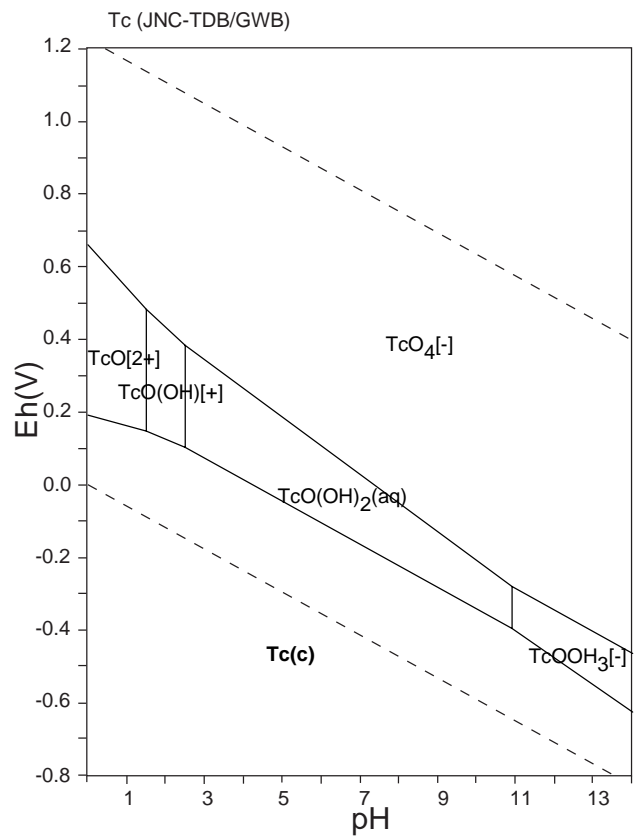
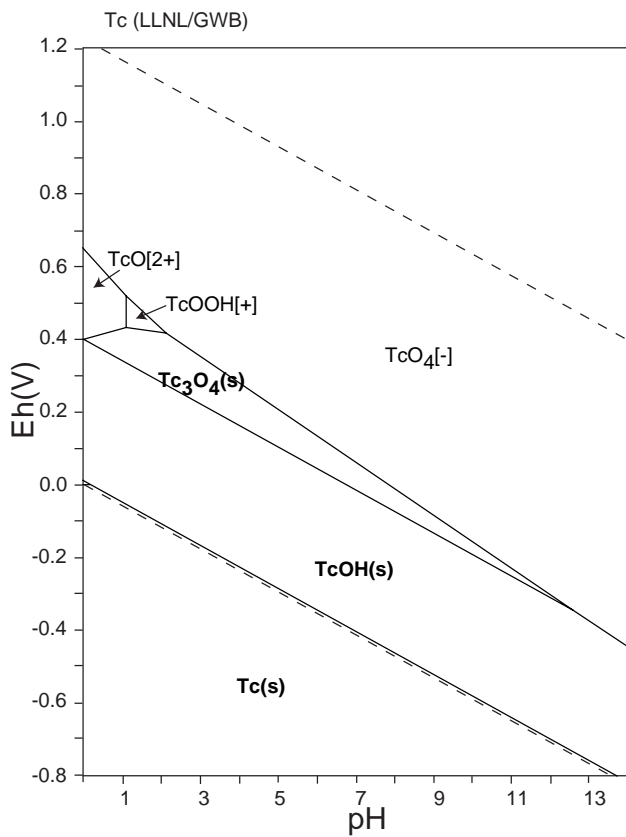
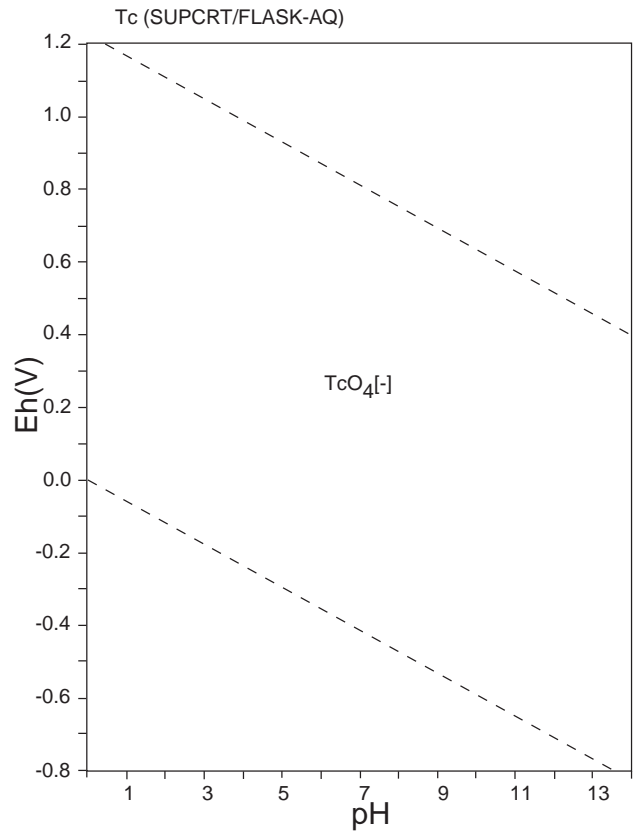
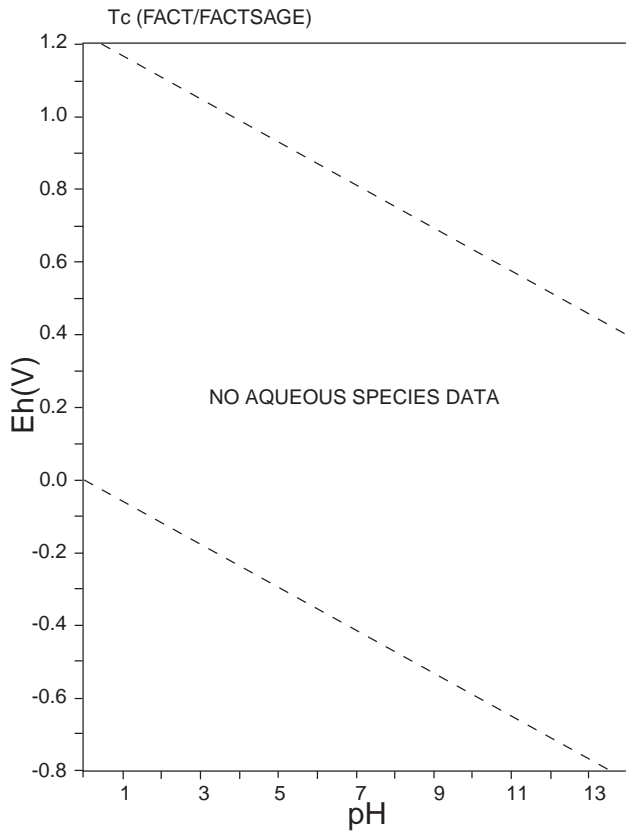
表 75: List of Tc species

FACT	SUPCRT	LLNL	JNC-TDB
<b>Tc(s), TcO<sub>2</sub>(s), TcO<sub>3</sub>(s), Tc<sub>2</sub>O<sub>7</sub>(s)</b>	TcO <sub>4</sub> [-]	TcO <sub>4</sub> [-], Tc[3+], TcO[2+], TcO <sub>4</sub> [2-], TcO <sub>4</sub> [3-], TcO(OH) <sub>2</sub> (aq), TcOOH[+], [TcO(OH) <sub>2</sub> ] <sub>2</sub> (aq), <b>HTcO<sub>4</sub>(s), Tc(OH)<sub>2</sub>(s), Tc(OH)<sub>3</sub>(s), Tc(c), Tc<sub>2</sub>O<sub>7</sub>(s), Tc<sub>3</sub>O<sub>4</sub>(s), Tc<sub>4</sub>O<sub>7</sub>(s), TcO<sub>2</sub>*2H<sub>2</sub>O(am), TcO<sub>3</sub>(s), TcOH(s)</b>	TcO[2+], TcO <sub>4</sub> [2-], TcO <sub>4</sub> [-], TcO(OH)[+], TcO(OH) <sub>2</sub> (aq), TcO(OH) <sub>3</sub> [-], <b>Tc(c), TcO<sub>2</sub>(c), Tc<sub>2</sub>O<sub>7</sub>(c), Tc<sub>2</sub>O<sub>216</sub>H<sub>2</sub>(s), Tc<sub>2</sub>O<sub>7</sub>(s), Tc<sub>2</sub>O<sub>7</sub>H<sub>2</sub>O(s), Tc(g), TcO(g), Tc<sub>2</sub>O<sub>7</sub>(g)</b>

HATCHES	OECD-NEA	OECD-NEA update	
TcO[2+], Tc[3+], TcO <sub>4</sub> [-], TcO(OH)[+], TcO(OH) <sub>2</sub> (aq), TcO(OH) <sub>3</sub> [-], <b>HTcO<sub>4</sub>(s), Tc(c), Tc(OH)<sub>2</sub>, Tc(OH)<sub>3</sub>, Tc<sub>2</sub>O<sub>7</sub>, Tc<sub>2</sub>O<sub>7</sub>*H<sub>2</sub>O, Tc<sub>3</sub>O<sub>4</sub>, Tc<sub>4</sub>O<sub>7</sub>, TcO<sub>2</sub>am, TcO<sub>21</sub>*6H<sub>2</sub>O, TcO<sub>3</sub>, TcOH</b>	TcO <sub>4</sub> [-], TcO <sub>4</sub> [2-], TcO <sub>4</sub> [3-], TcO(OH)[+], TcO(OH) <sub>2</sub> (aq), TcO(OH) <sub>3</sub> [-], <b>Tc(c), TcO<sub>2</sub>(c), Tc<sub>2</sub>O<sub>7</sub>(c), TcO<sub>2</sub>*1.6H<sub>2</sub>O(s), Tc<sub>2</sub>O<sub>7</sub>H<sub>2</sub>O(s)</b>	TcO <sub>4</sub> [-], TcO[2+], TcO <sub>4</sub> [2-], TcO(OH)[+], TcO(OH) <sub>2</sub> (aq), TcO(OH) <sub>3</sub> [-], <b>Tc(cr), TcO<sub>2</sub>(cr), Tc<sub>2</sub>O<sub>7</sub>(cr), TcO<sub>2</sub>*1.6H<sub>2</sub>O(s), Tc<sub>2</sub>O<sub>7</sub>H<sub>2</sub>O(s)</b>	

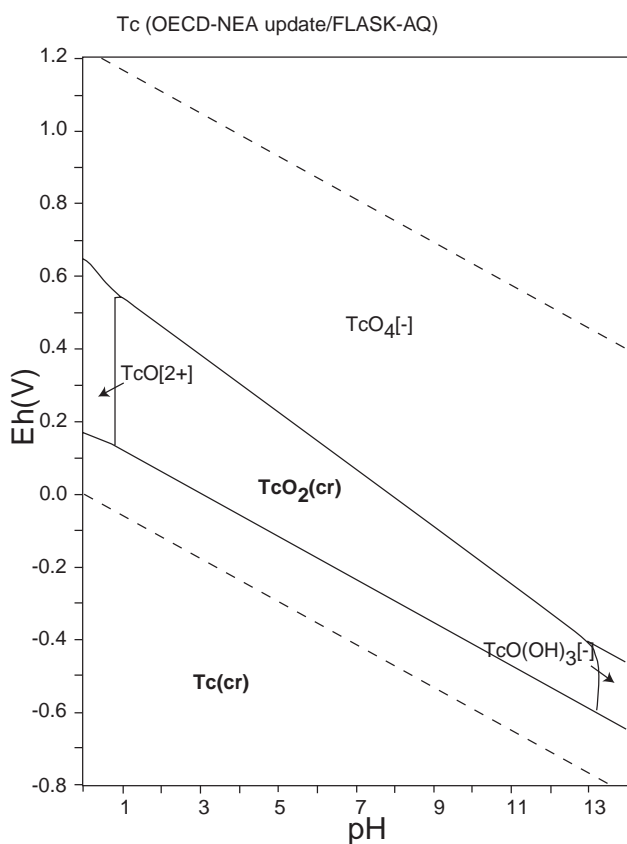
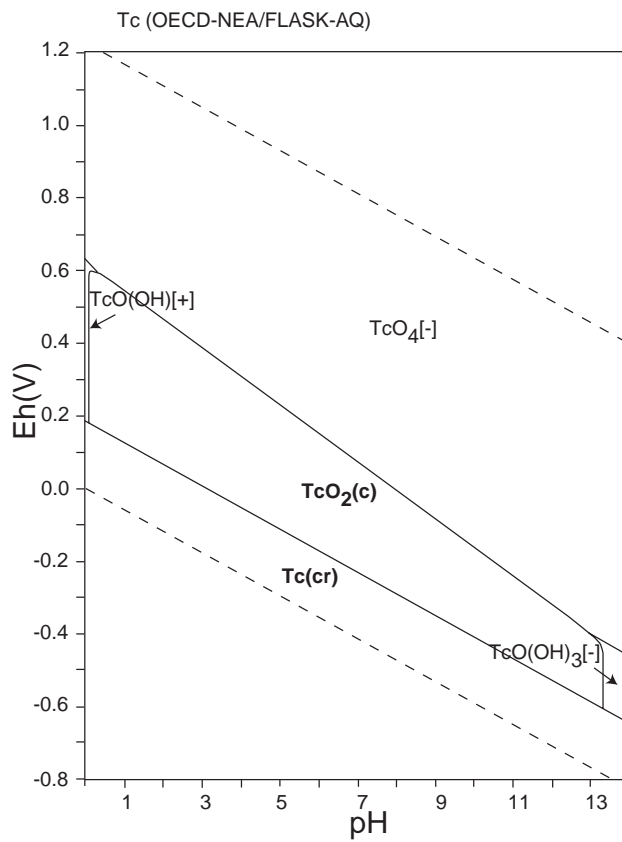
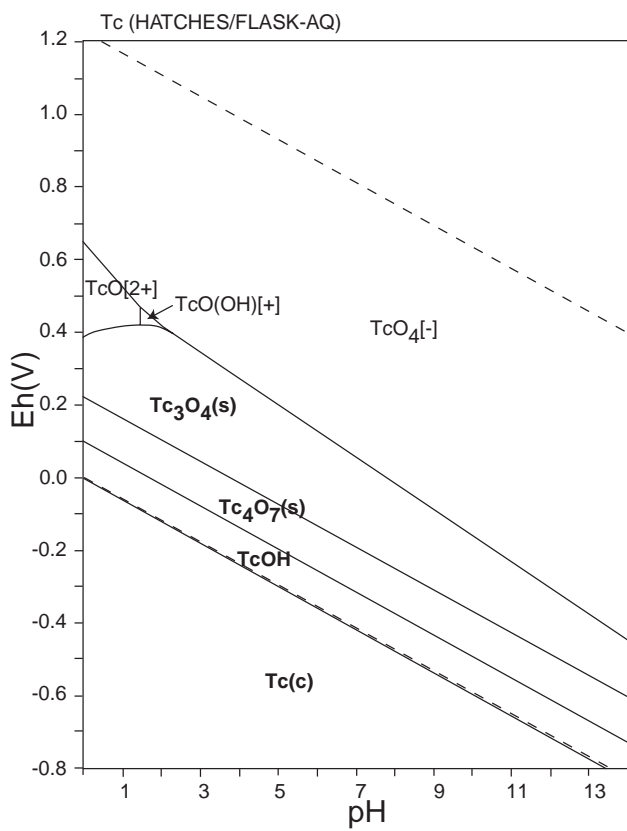
Remarks

JNC-TDB: Given reaction of TcO<sub>216</sub>H<sub>2</sub> in the database file suggests its formula as TcO<sub>3.6</sub>H<sub>3.2</sub>.



☒ 122: Eh-pH diagrams of the system Tc-O-H (1).  $\sum Tc = 10^{-10}$ , 298.15K,  $10^5$  Pa.

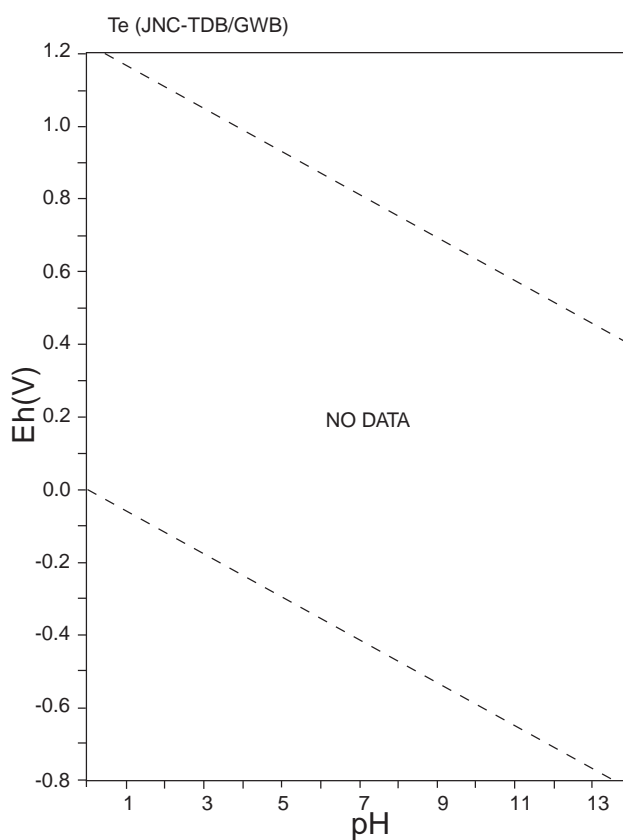
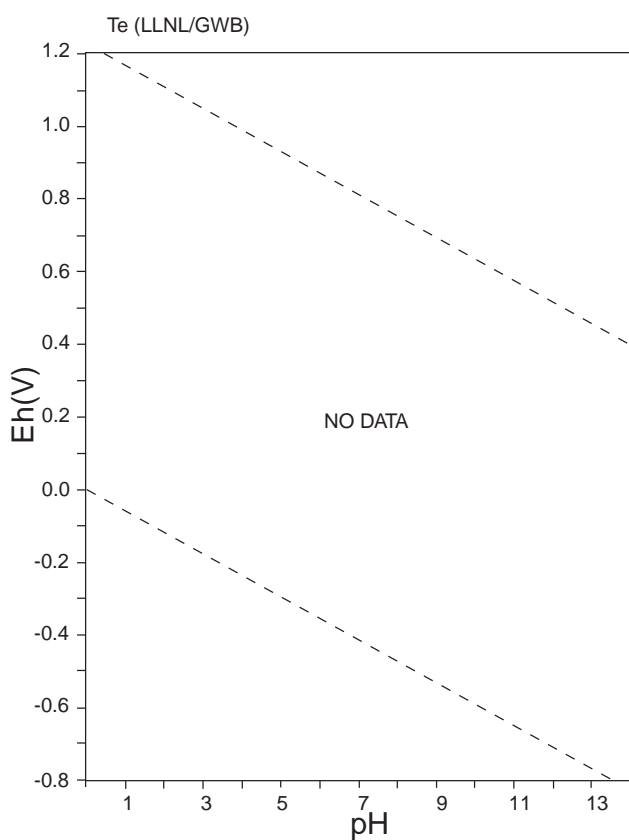
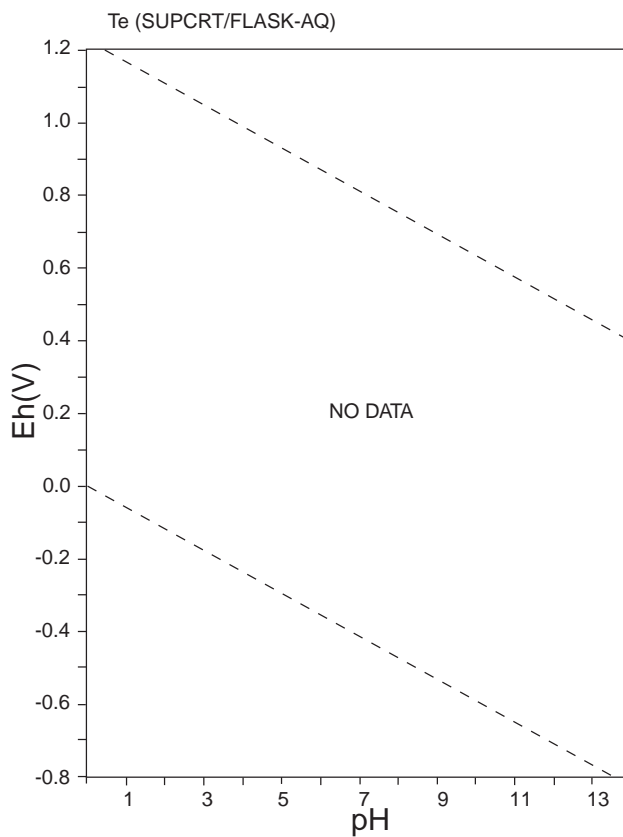
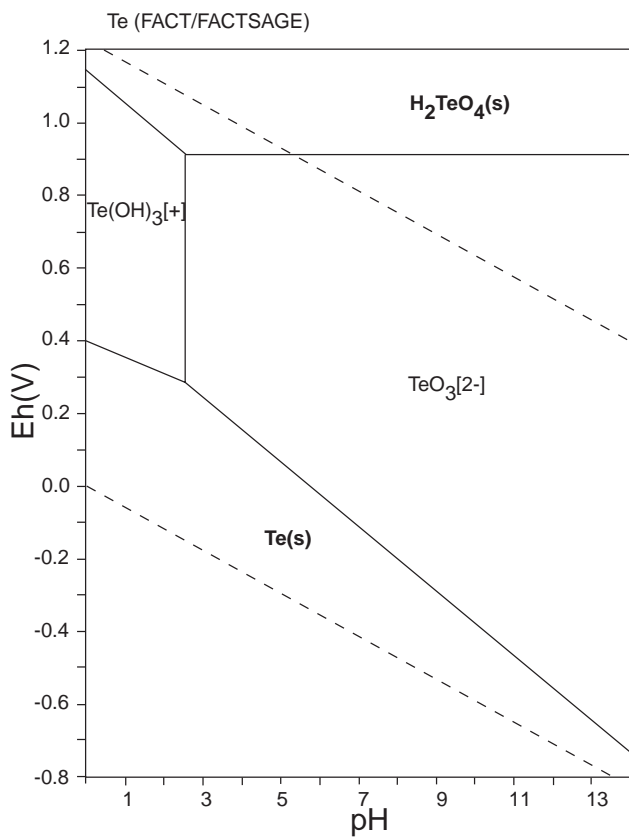




☒ 123: Eh-pH diagrams of the system Tc-O-H (2).  $\sum Tc = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 76: List of Te species

FACT	SUPCRT	LLNL	JNC-TDB
$\text{TeO}_3[2-]$ , $\text{Te}(\text{OH})_3[+]$ , <b>Te(s)</b> , <b>TeO<sub>2</sub>(s)</b> , <b>H<sub>2</sub>TeO<sub>4</sub>(s)</b>			



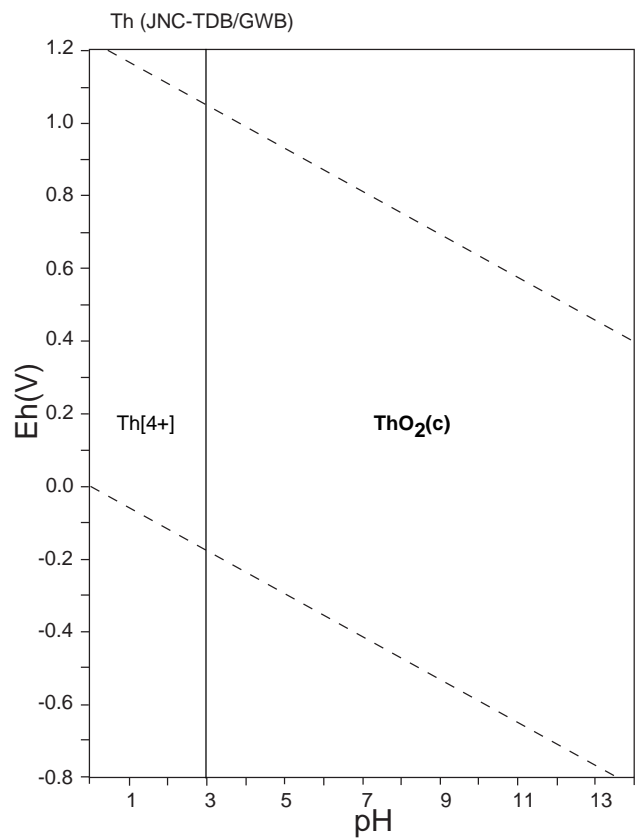
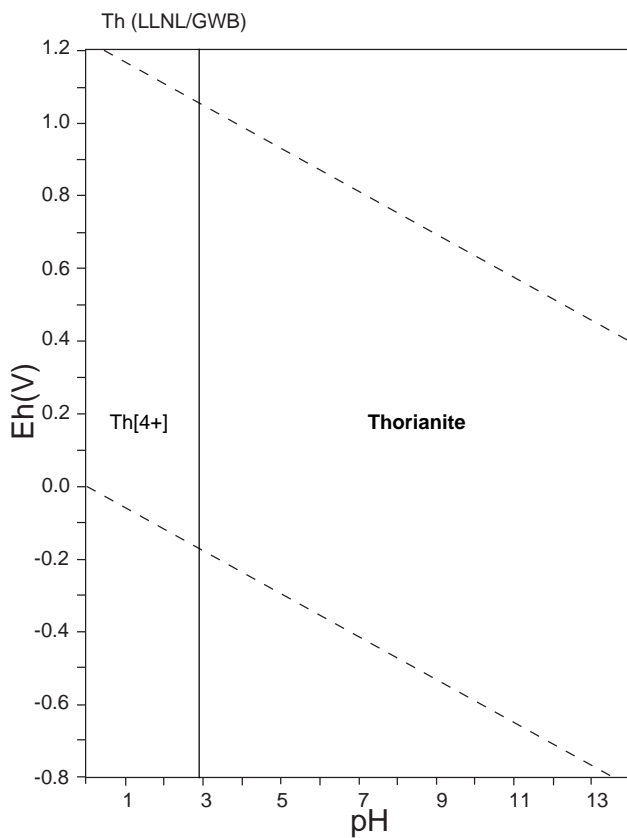
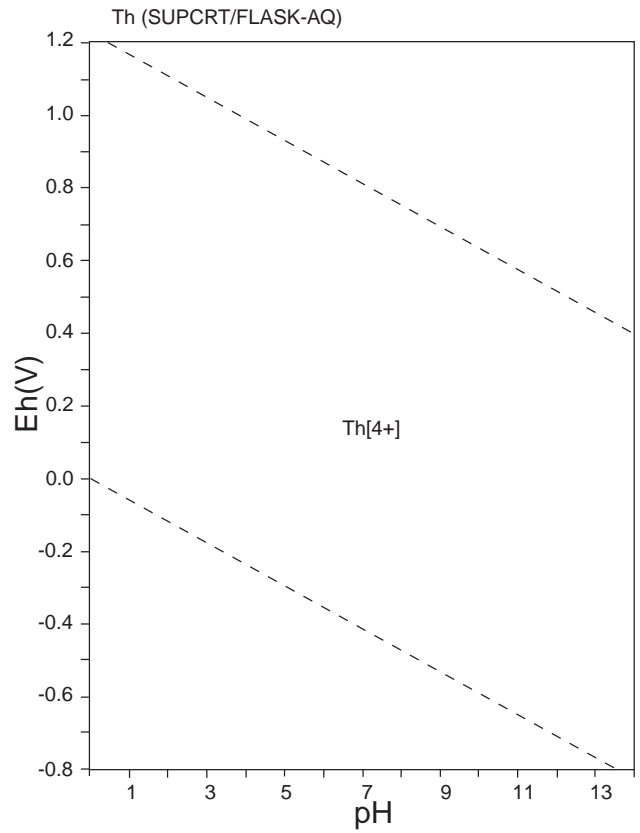
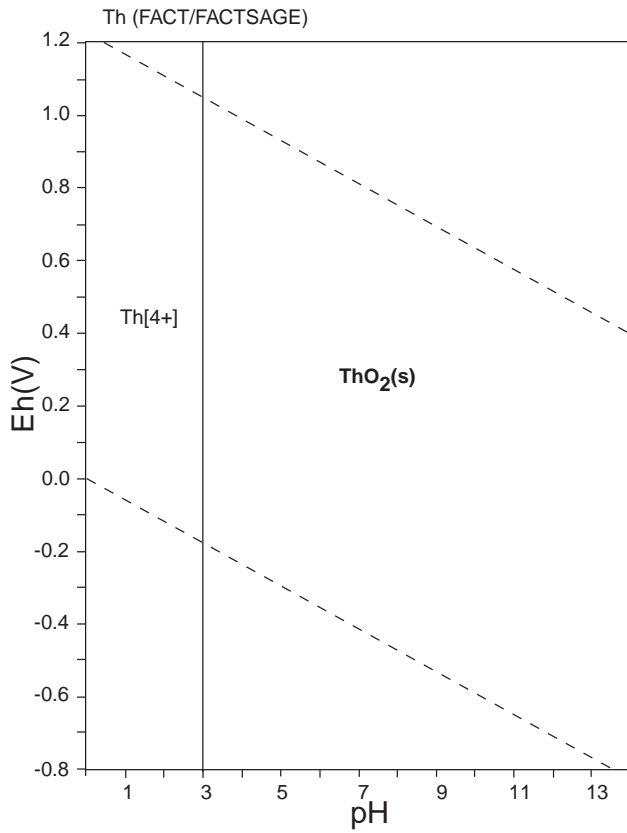
☒ 124: Eh-pH diagrams of the system Te-O-H.  $\sum \text{Te} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



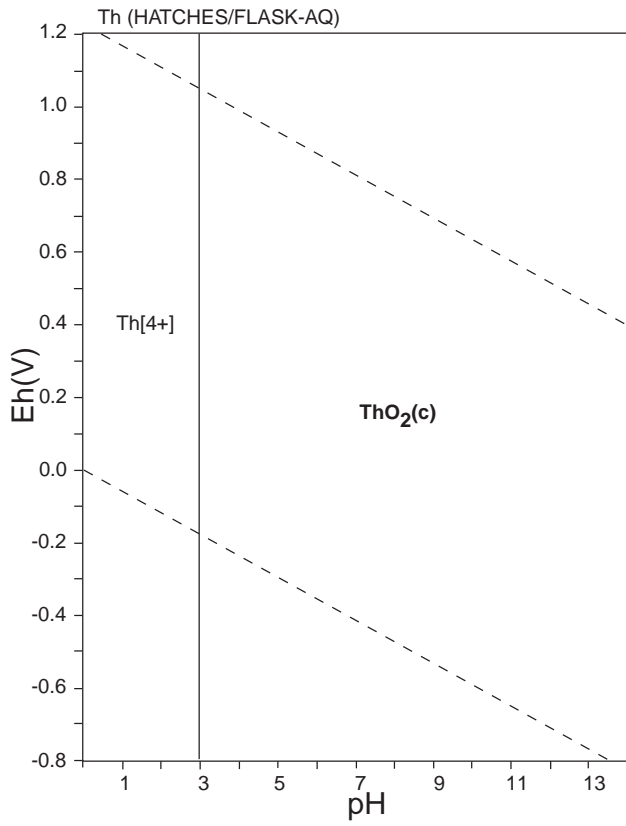
表 77: List of Th species

FACT	SUPCRT	LLNL	JNC-TDB
<b>Th[4+]</b> , <b>Th(s)</b> , <b>Th(s2)</b> , <b>ThH<sub>2</sub>(s)</b> , <b>ThO<sub>2</sub>(s)</b>	Th[4+]	<b>Th[4+]</b> , <b>Th(OH)<sub>2</sub>[2+]</b> , <b>Th(OH)<sub>3</sub>[+]</b> , <b>Th(OH)<sub>4</sub>(aq)</b> , <b>Th<sub>2</sub>(OH)<sub>2</sub>[6+]</b> , <b>Th<sub>4</sub>(OH)<sub>8</sub>[8+]</b> , <b>Th<sub>6</sub>(OH)<sub>15</sub>[9+]</b> , <b>ThOH[3+]</b> <b>Th(OH)<sub>4</sub>(c)</b> , <b>ThO<sub>2</sub>(s)</b> , <b>Thorianite</b>	<b>Th[4+]</b> , <b>Th(OH)<sub>4</sub>(aq)</b> , <b>ThO<sub>2</sub>(am)</b> , <b>ThO<sub>2</sub>(c)</b>

HATCHES			
<b>Th[4+]</b> , <b>Th(OH)[3+]</b> , <b>Th(OH)<sub>2</sub>[2+]</b> , <b>Th(OH)<sub>3</sub>[+]</b> , <b>Th(OH)<sub>4</sub>(aq)</b> , <b>Th<sub>2</sub>(OH)<sub>2</sub>[6+]</b> , <b>Th<sub>4</sub>(OH)<sub>8</sub>[8+]</b> , <b>Th(OH)<sub>4</sub></b> , <b>ThO<sub>2</sub></b> , <b>ThO<sub>2</sub>(c)</b>			



☒ 125: Eh-pH diagrams of the system Th-O-H (1).  $\sum \text{Th} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

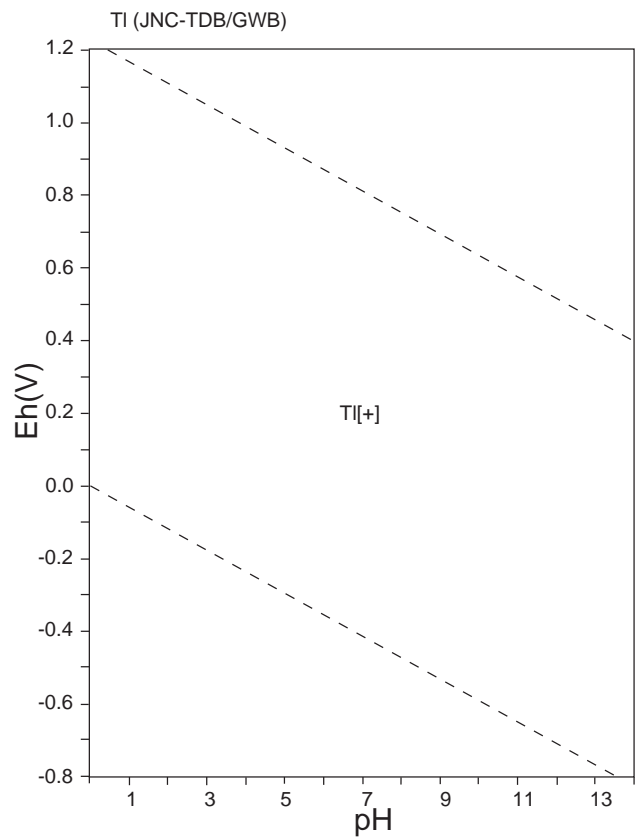
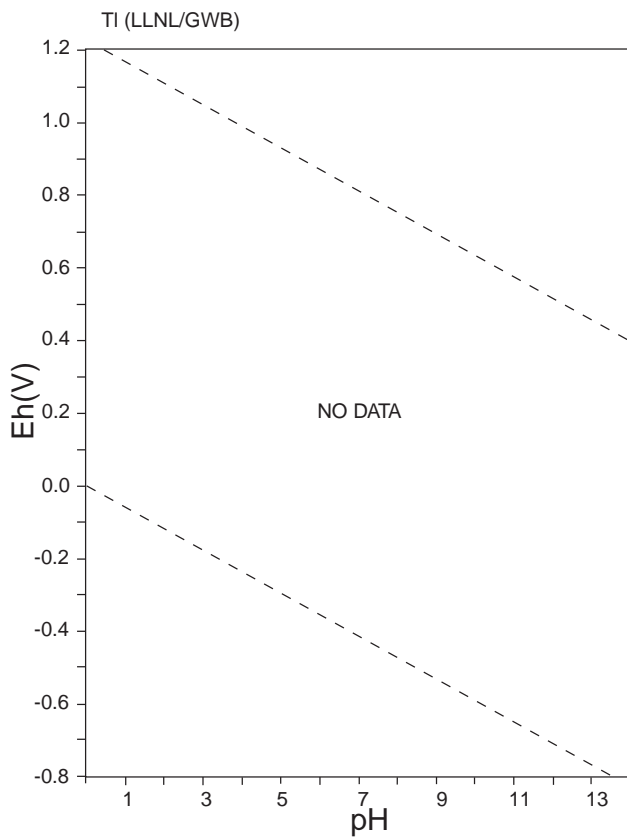
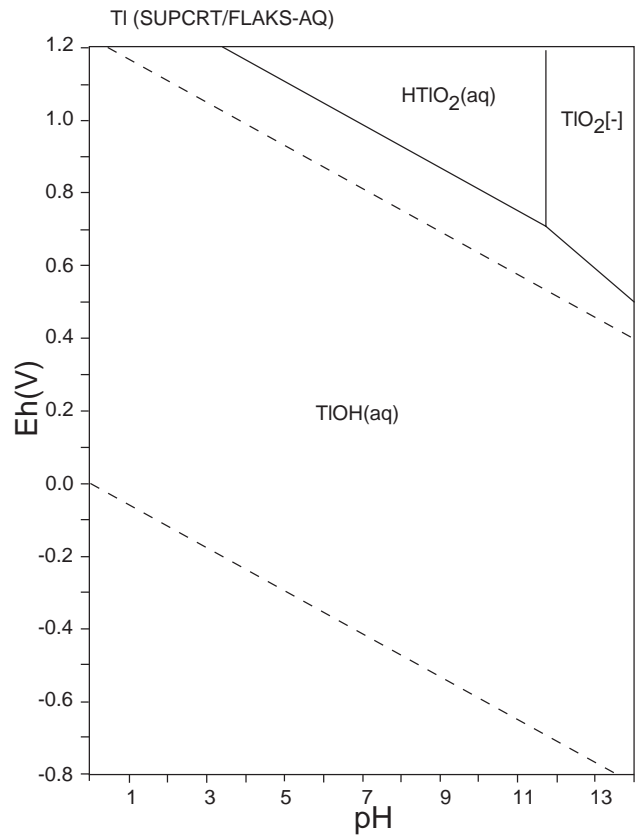
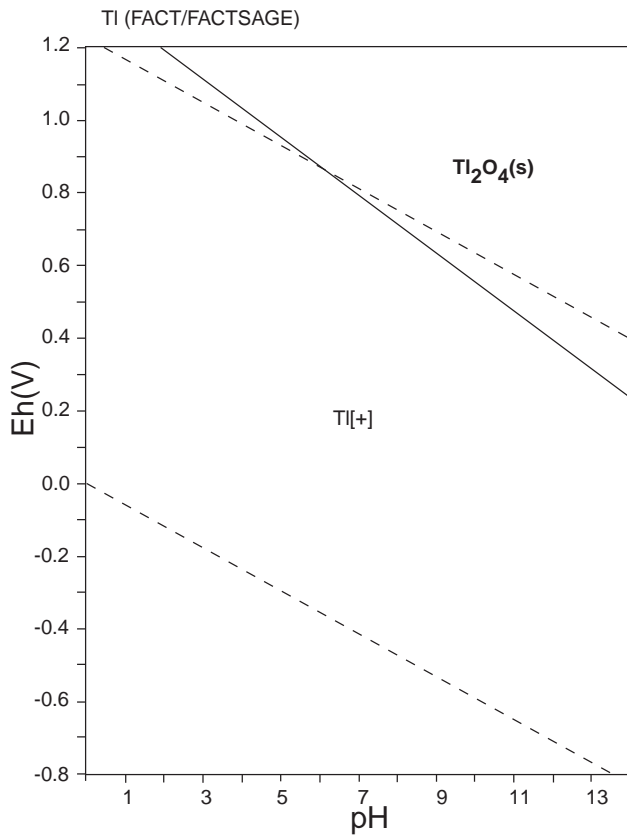


☒ 126: Eh-pH diagrams of the system Th-O-H (2).  $\sum \text{Th} = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 78: List of Tl species

FACT	SUPCRT	LLNL	JNC-TDB
Tl[+], Tl[3+], TlOH(aq), TlOH[2+], Tl(OH) <sub>2</sub> [+], <b>Tl(s)</b> , <b>Tl(s2)</b> , <b>Tl<sub>2</sub>O(s)</b> , <b>Tl<sub>2</sub>O<sub>3</sub>(s)</b> , <b>Tl<sub>2</sub>O<sub>4</sub>(s)</b> , <b>TlOH(s)</b> , <b>Tl(OH)<sub>3</sub>(s)</b>	Tl[+], Tl[3+], TlOH(aq), TlOH[2+], TlO[+], HTlO <sub>2</sub> (aq), TlO <sub>2</sub> [-]		Tl[+]

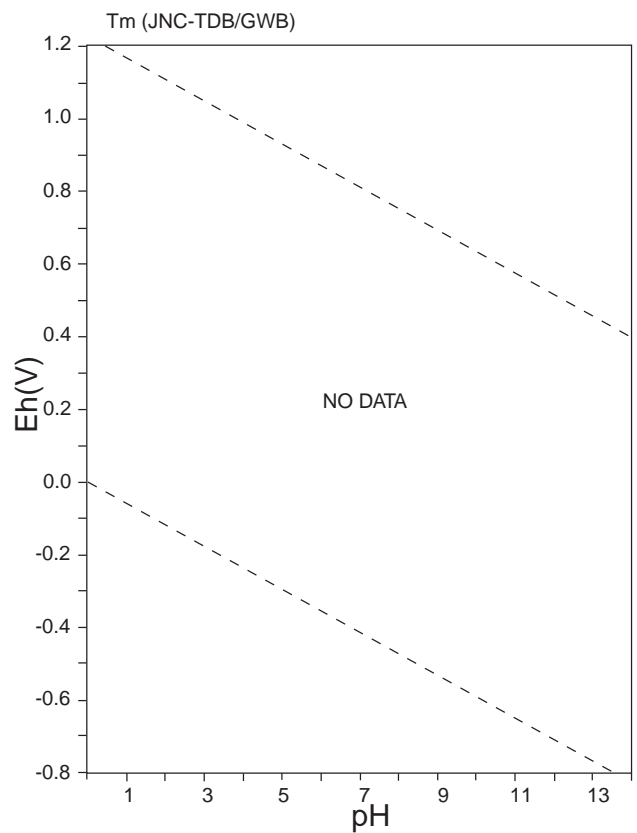
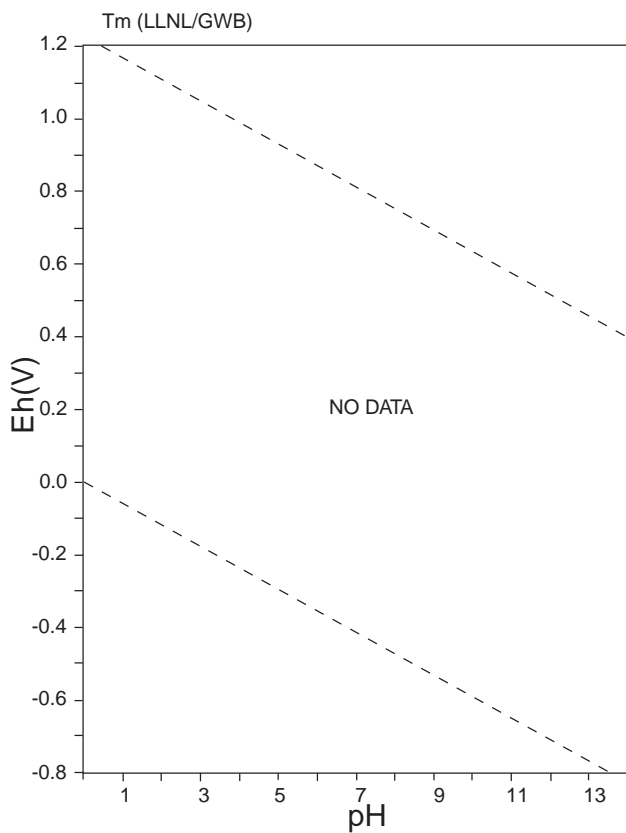
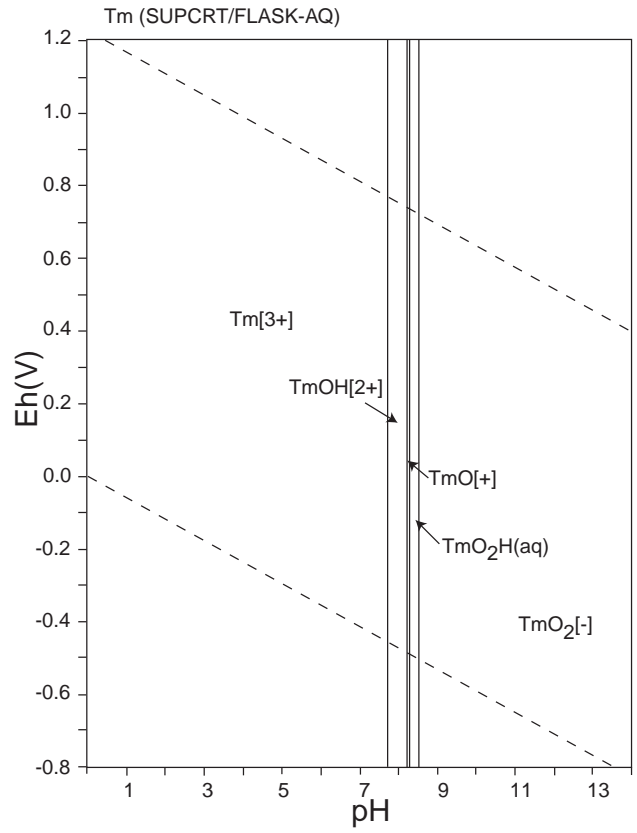
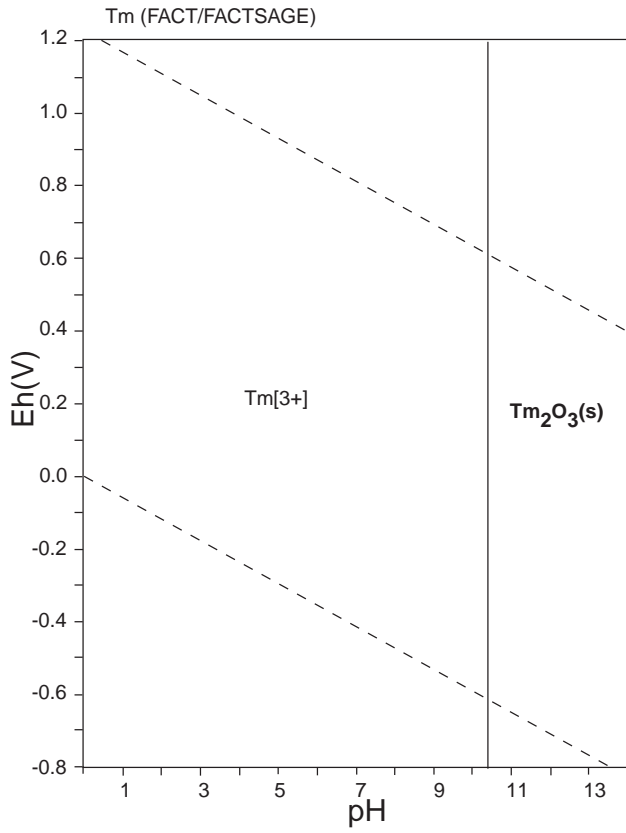




☒ 127: Eh-pH diagrams of the system Ti-O-H.  $\sum Ti = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 79: List of Tm species

FACT	SUPCRT	LLNL	JNC-TDB
Tm[3+], <b>Tm(s)</b> , <b>Tm<sub>2</sub>O<sub>3</sub>(s)</b> , <b>Tm<sub>2</sub>O<sub>3</sub>(s2)</b> , <b>Tm<sub>2</sub>O<sub>3</sub>(s3)</b>	Tm[3+], Tm[4+], Tm[2+], TmOH[2+], TmO[+], TmO <sub>2</sub> H(aq), TmO <sub>2</sub> [-]		



☒ 128: Eh-pH diagrams of the system Tm-O-H.  $\sum Tm = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 80: List of U species

FACT	SUPCRT	LLNL	JNC-TDB
<p>U[3+], U[4+], UO<sub>2</sub>[+], UO<sub>2</sub>[2+], UOH[3+], HO<sub>3</sub>U[+], H<sub>3</sub>O<sub>3</sub>U[+], H<sub>5</sub>O<sub>5</sub>U[-], H<sub>2</sub>O<sub>2</sub>U[2+], H<sub>2</sub>O<sub>6</sub>U<sub>2</sub>[2+], H<sub>5</sub>O<sub>11</sub>U<sub>3</sub>[+], H<sub>7</sub>O<sub>13</sub>U<sub>3</sub>[-], <b>U(s), U(s2), U(s3), UH<sub>3</sub>(s), UO<sub>3</sub>(s), U<sub>3</sub>O<sub>8</sub>(s), U<sub>4</sub>O<sub>9</sub>(s), UO<sub>3</sub>(H<sub>2</sub>O)<sub>2</sub>(s), UO<sub>2</sub>(s)</b></p>	<p>U[3+], U[4+], UO<sub>2</sub>[+], UO<sub>2</sub>[2+], UOH[3+], UO<sub>2</sub>OH[+], HUO<sub>2</sub>[+], HUO<sub>3</sub>[-], UOH[2+], UO[+], HUO<sub>2</sub>(aq), UO[2+], UO<sub>2</sub>(aq), UO<sub>2</sub>OH(aq), UO<sub>3</sub>[-], UO<sub>3</sub>(aq), HUO<sub>4</sub>[-], UO<sub>4</sub>[2-], <b>UO<sub>2</sub>(Uraninite)</b></p>	<p>U[4+], U[3+], UO<sub>2</sub>[+], UO<sub>2</sub>[2+], (UO<sub>2</sub>)<sub>2</sub>(OH)<sub>2</sub>[2+], (UO<sub>2</sub>)<sub>3</sub>(OH)<sub>4</sub>[2+], (UO<sub>2</sub>)<sub>3</sub>(OH)<sub>5</sub>[+], (UO<sub>2</sub>)<sub>3</sub>(OH)<sub>7</sub>[-], (UO<sub>2</sub>)<sub>4</sub>(OH)<sub>7</sub>[+], U(OH)<sub>2</sub>[2+], U(OH)<sub>3</sub>[+], U(OH)<sub>4</sub>(aq), U(OH)<sub>5</sub>[-], U<sub>6</sub>(OH)<sub>15</sub>[9+], UO<sub>2</sub>OH[+], UOH[3+], <b>Gummite, Schoepite, U(c,alph), U<sub>3</sub>O<sub>8</sub>(c,alph), U<sub>4</sub>O<sub>9</sub>(c), UO<sub>2</sub>(OH)<sub>2</sub>(c,bet), UO<sub>2</sub>(am), UO<sub>3</sub>(c,gamma), Uraninite</b></p>	<p>U[4+], U[3+], UO<sub>2</sub>[+], UO<sub>2</sub>[2+], UO<sub>2</sub>(OH)<sub>3</sub>(aq), UO<sub>2</sub>(OH)<sub>4</sub>(aq), (UO<sub>2</sub>)<sub>2</sub>(OH)<sub>2</sub>(aq), (UO<sub>2</sub>)<sub>2</sub>(OH)<sub>2</sub>[2+], (UO<sub>2</sub>)<sub>3</sub>(OH)<sub>4</sub>[2+], (UO<sub>2</sub>)<sub>3</sub>(OH)<sub>5</sub>[+], (UO<sub>2</sub>)<sub>3</sub>(OH)<sub>7</sub>[-], (UO<sub>2</sub>)<sub>4</sub>(OH)<sub>7</sub>[+], UO<sub>2</sub>OH[+], UO<sub>2</sub>(OH)<sub>2</sub>(aq), UOH[3+], U(OH)<sub>4</sub>(aq), <b>UO<sub>2</sub>(am), UO<sub>3</sub>(alpha), UO<sub>3</sub>(beta), UO<sub>3</sub>(gamma), UO<sub>3.0.9</sub>H, UO<sub>3.2</sub>H<sub>2</sub>O, UO<sub>2</sub>(OH)<sub>2</sub>, U(c), UO<sub>2</sub>(c), UO<sub>2.25</sub>(b), UO<sub>2.25</sub>(c), UO<sub>2.3333</sub>, UO<sub>2.6667</sub>, UH<sub>3</sub>(beta), U(g), UO(g), UO<sub>2</sub>(g), UO<sub>3</sub>(g)</b></p>

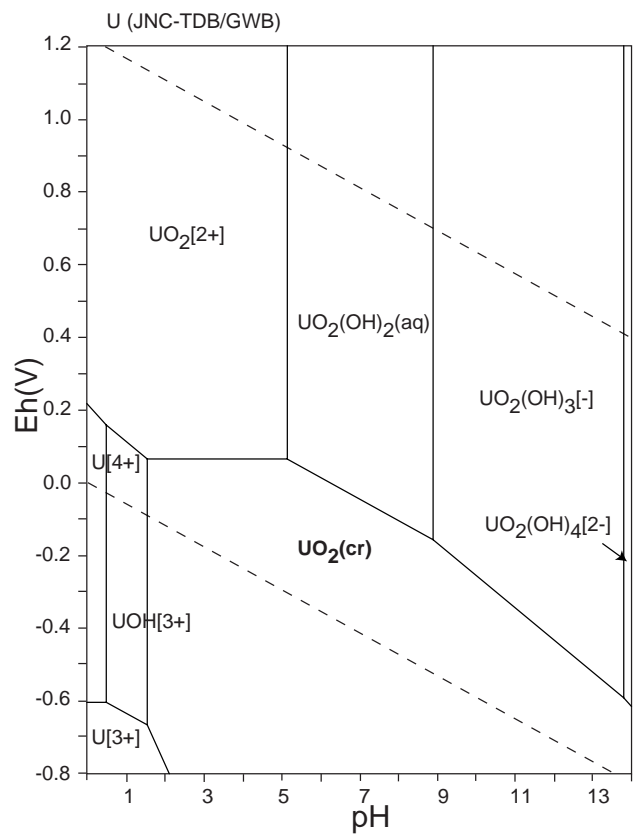
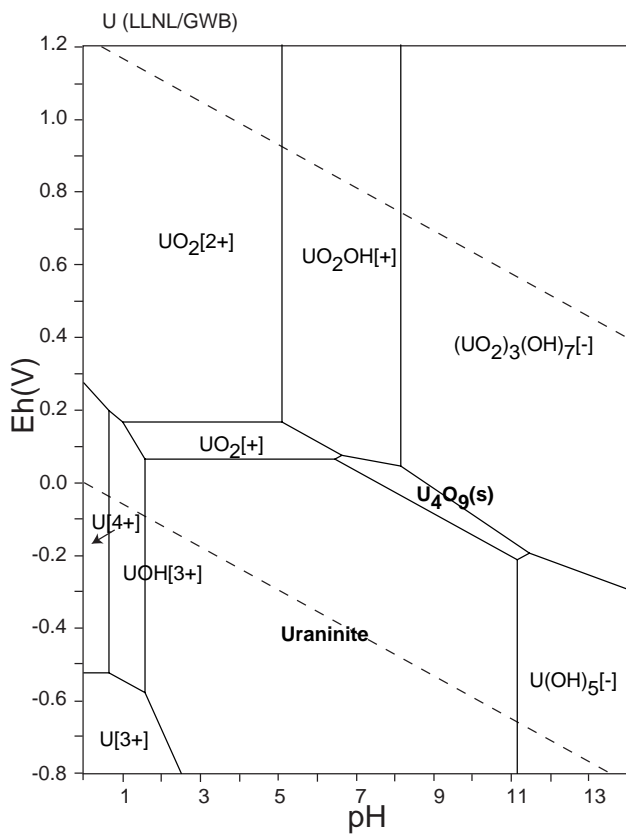
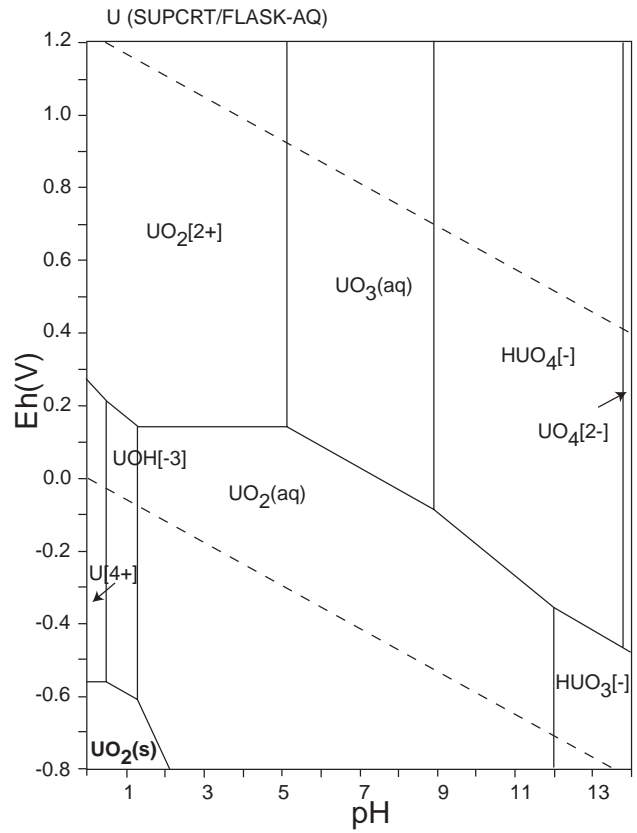
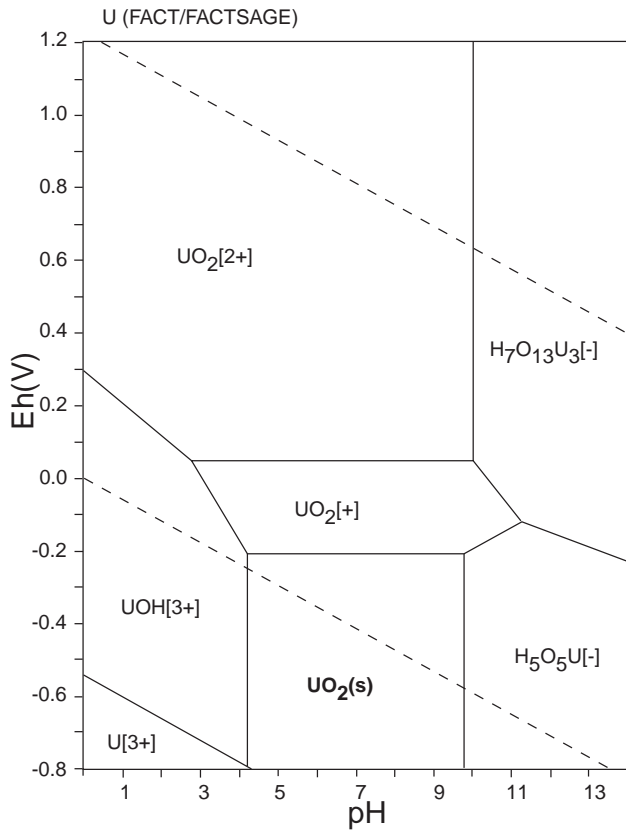
HATCHES	OECD-NEA	OECD-NEA update	
<p>U[4+], UO<sub>2</sub>[+], UO<sub>2</sub>[2+], U(OH)[3+], U(OH)<sub>4</sub>(aq), U<sub>6</sub>(OH)<sub>15</sub>[9+], U<sub>1</sub>(OH)<sub>2</sub>(aq), U<sub>1</sub>(OH)<sub>3</sub>[-], U<sub>1</sub>(OH)<sub>4</sub>[2-], U<sub>12</sub>(OH)<sub>2</sub>[2+], U<sub>12</sub>OH[3+], U<sub>13</sub>(OH)<sub>4</sub>[2+], U<sub>13</sub>(OH)<sub>5</sub>[+], U<sub>13</sub>(OH)<sub>7</sub>[-], U<sub>14</sub>(OH)<sub>7</sub>[+], U<sub>1</sub>OH[+], <b>Gummite, Schoepite, U(c,alph), U<sub>3</sub>O<sub>8</sub>, U<sub>4</sub>O<sub>9</sub>, UO<sub>2</sub>(am), UO<sub>2</sub>(c), UO<sub>2</sub>(OH)<sub>2</sub>, UO<sub>2</sub>OH, UO<sub>3</sub>, UO<sub>3</sub>*2H<sub>2</sub>O, Uraninite</b></p>	<p>U[4+], U[3+], UO<sub>2</sub>[+], UO<sub>2</sub>[2+], UOH[3+], UO<sub>2</sub>OH[+], U(OH)<sub>4</sub>(aq), UO<sub>2</sub>(OH)<sub>3</sub>[-], UO<sub>2</sub>(OH)<sub>4</sub>[2-], (UO<sub>2</sub>)<sub>2</sub>(OH)<sub>2</sub>[2-], (UO<sub>2</sub>)<sub>2</sub>(OH)<sub>2</sub>OH[3+], (UO<sub>2</sub>)<sub>2</sub>(OH)<sub>2</sub>[2+], (UO<sub>2</sub>)<sub>3</sub>(OH)<sub>4</sub>[2+], (UO<sub>2</sub>)<sub>3</sub>(OH)<sub>5</sub>[+], (UO<sub>2</sub>)<sub>3</sub>(OH)<sub>7</sub>[-], (UO<sub>2</sub>)<sub>4</sub>(OH)<sub>7</sub>[+], <b>U(c), UO<sub>2</sub>(c), UO<sub>2.25</sub>(c), UO<sub>2.25</sub>(beta), UO<sub>2.3333</sub>(beta), UO<sub>2.6667</sub>(c), UO<sub>3</sub>(alpha), UO<sub>3</sub>(beta), UO<sub>3</sub>(gamma), UH<sub>3</sub>(beta), UO<sub>3</sub>*0.9H<sub>2</sub>O(alpha), UO<sub>2</sub>(OH)<sub>2</sub>(beta), UO<sub>3</sub>*2H<sub>2</sub>O(c)</b></p>	<p>U[4+], U[3+], UO<sub>2</sub>[+], UO<sub>2</sub>[2+], UOH[3+], UO<sub>2</sub>OH[+], UO<sub>2</sub>(OH)<sub>2</sub>(aq), U(OH)<sub>4</sub>(aq), UO<sub>2</sub>(OH)<sub>3</sub>[-], UO<sub>2</sub>(OH)<sub>4</sub>[2-], (UO<sub>2</sub>)<sub>2</sub>OH[3+], (UO<sub>2</sub>)<sub>2</sub>(OH)<sub>2</sub>[2+], (UO<sub>2</sub>)<sub>3</sub>(OH)<sub>4</sub>[2+], (UO<sub>2</sub>)<sub>3</sub>(OH)<sub>5</sub>[+], (UO<sub>2</sub>)<sub>3</sub>(OH)<sub>7</sub>[-], (UO<sub>2</sub>)<sub>4</sub>(OH)<sub>7</sub>[+], <b>U(cr), UO<sub>2</sub>(cr), UO<sub>2.25</sub>(beta), UO<sub>2.25</sub>(cr), UO<sub>2.3333</sub>(beta), UO<sub>2.6667</sub>(cr), UO<sub>3</sub>(alpha), UO<sub>3</sub>(beta), UO<sub>3</sub>(gamma), UH<sub>3</sub>(beta), UO<sub>3</sub>*0.9H<sub>2</sub>O(alpha), UO<sub>2</sub>(OH)<sub>2</sub>(beta), UO<sub>3</sub>*2H<sub>2</sub>O(cr)</b></p>	

Remarks

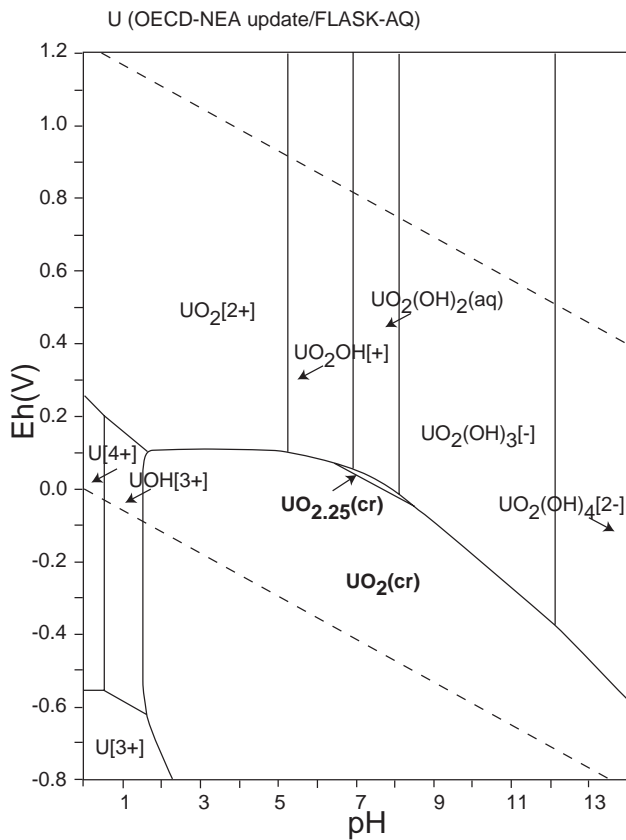
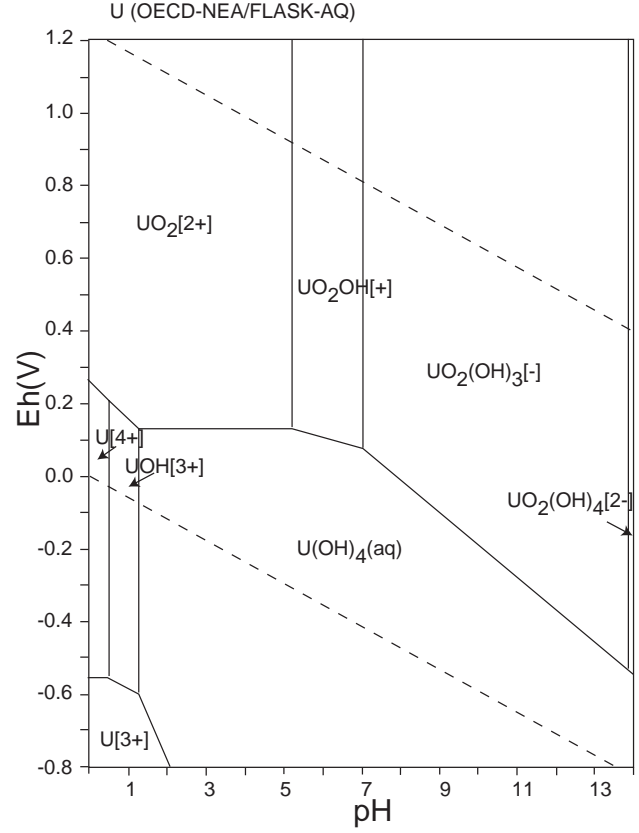
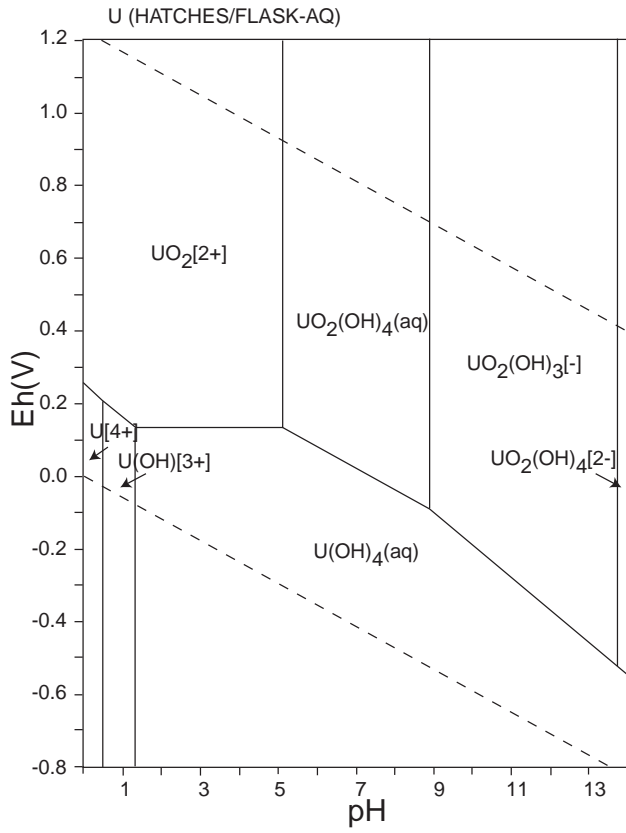
HATCHES: U<sub>1</sub> stands for UO<sub>2</sub>.

JNC-TDB: Given reaction of UO<sub>3.0.9</sub>H in the database file suggests its formula as UO<sub>3</sub>H.

Given reaction of UO<sub>3.2</sub>H<sub>2</sub>O in the database file suggests its formula as UO<sub>3</sub>\*2H<sub>2</sub>O. UO<sub>2.25</sub>(b) may be UO<sub>2.25</sub>(beta)?



☒ 129: Eh-pH diagrams of the system U-O-H (1).  $\Sigma U = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 130: Eh-pH diagrams of the system U-O-H (2).  $\sum U = 10^{-10}$ , 298.15K,  $10^5$  Pa.

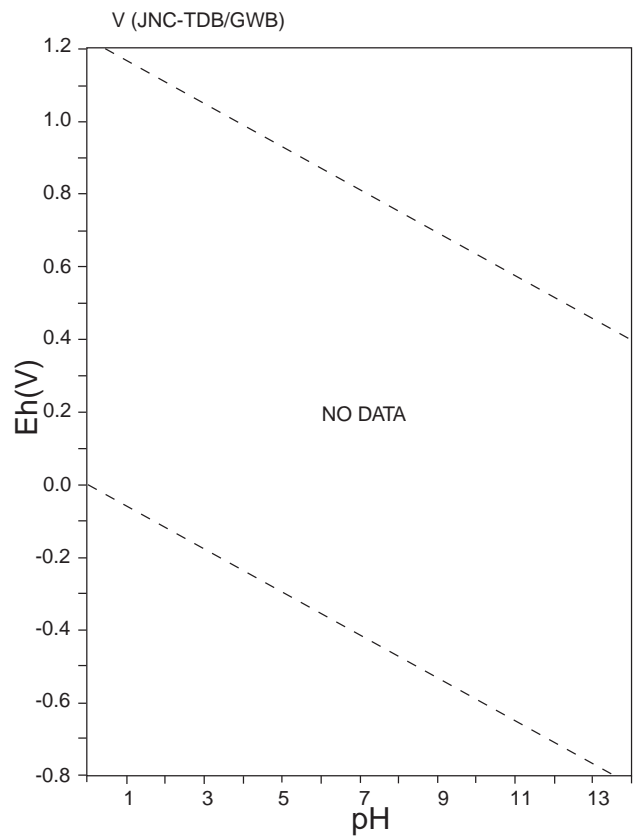
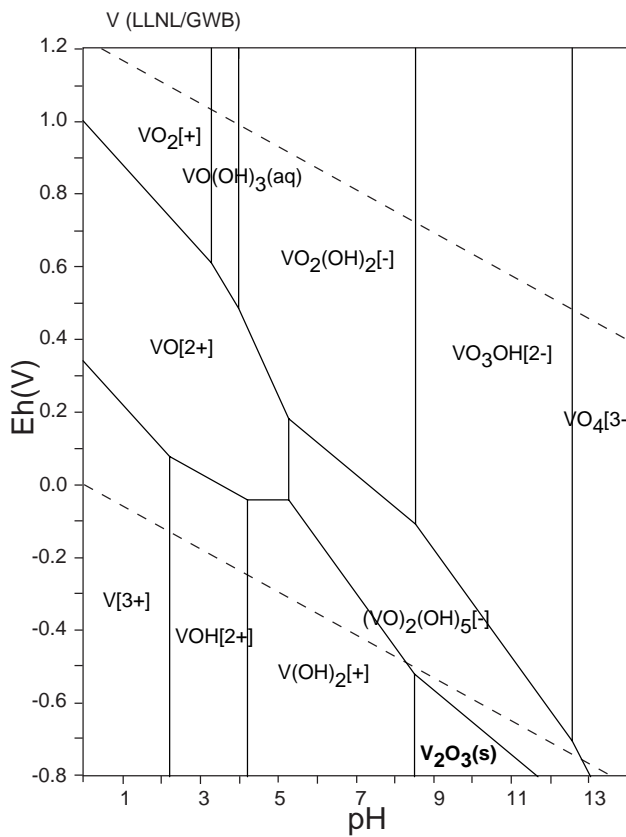
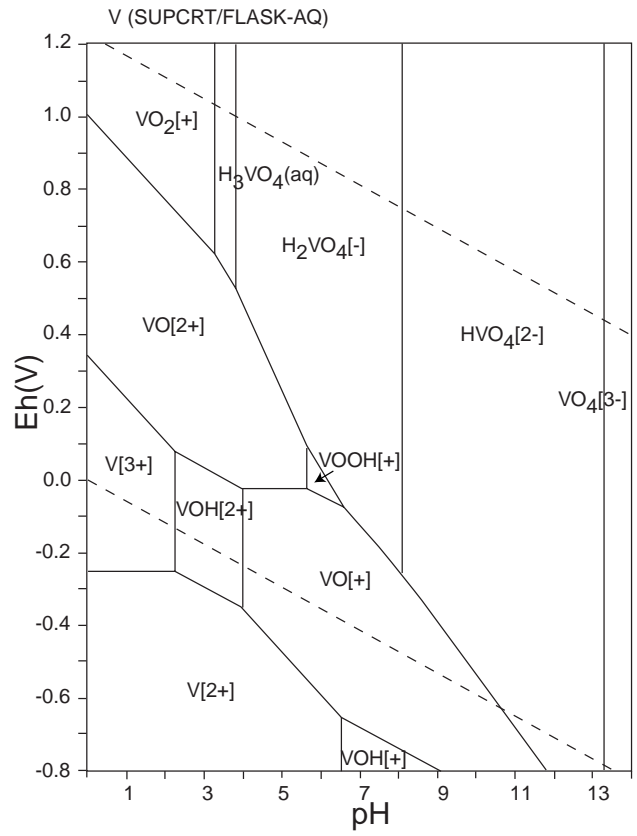
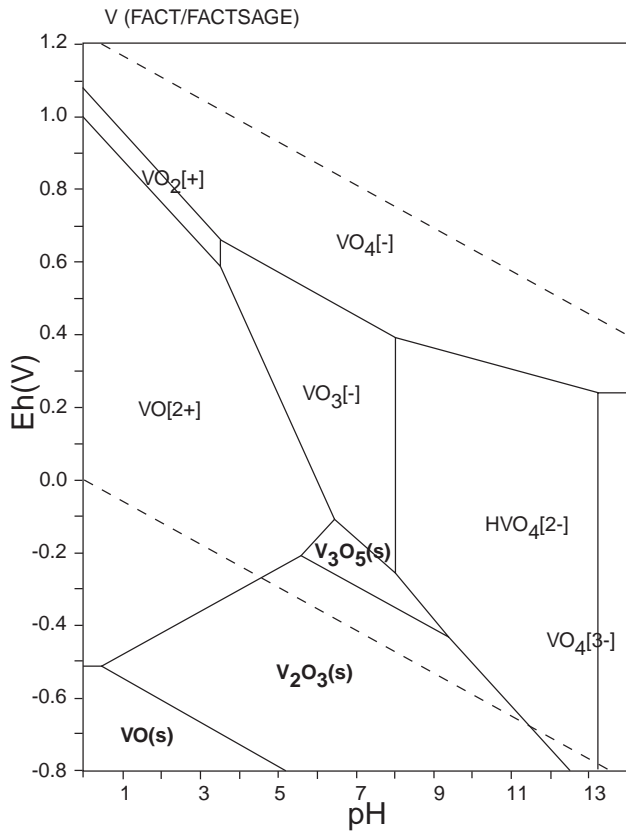




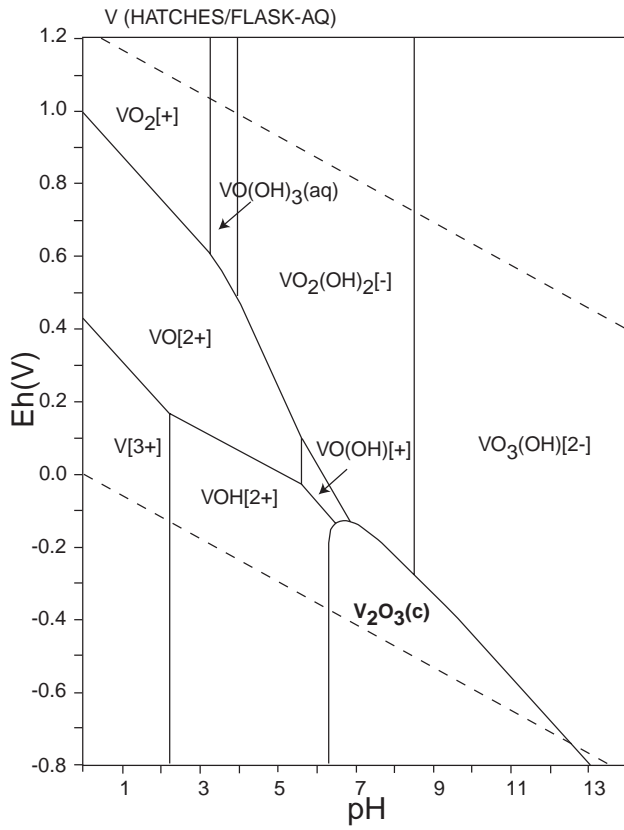
表 81: List of V species

FACT	SUPCRT	LLNL	JNC-TDB
VO[2+], VO <sub>2</sub> [+], VO <sub>4</sub> [3-], HVO <sub>4</sub> [2-], VO <sub>3</sub> [-], VO <sub>4</sub> [-], V <sub>2</sub> O <sub>7</sub> [4-], VOH <sub>2</sub> O <sub>2</sub> [3+], HVO <sub>4</sub> (aq), H <sub>2</sub> VO <sub>4</sub> [+], HV <sub>2</sub> O <sub>7</sub> [3-], H <sub>3</sub> V <sub>2</sub> O <sub>7</sub> [-], HV <sub>10</sub> O <sub>28</sub> [5-], H <sub>2</sub> V <sub>10</sub> O <sub>28</sub> [4-], <b>V(s)</b> , <b>VO(s)</b> , <b>VO<sub>2</sub>(s)</b> , <b>VO<sub>2</sub>(s2)</b> , <b>V<sub>2</sub>O<sub>3</sub>(s)</b> , <b>V<sub>2</sub>O<sub>4</sub>(s)</b> , <b>V<sub>2</sub>O<sub>4</sub>(s2)</b> , <b>V<sub>2</sub>O<sub>5</sub>(s)</b> , <b>V<sub>3</sub>O<sub>5</sub>(s)</b> , <b>V<sub>4</sub>O<sub>7</sub>(s)</b>	VO[2+], VO <sub>2</sub> [+], VO <sub>4</sub> [3-], HVO <sub>4</sub> [2-], V[3+], V[2+], H <sub>3</sub> VO <sub>4</sub> (aq), H <sub>2</sub> VO <sub>4</sub> [-], VO[+], VOH[+], VOH[2+], VOOH[+]	V[3+], VO[2+], VO <sub>4</sub> [3-], (VO) <sub>2</sub> (OH) <sub>2</sub> [2+], (VO) <sub>2</sub> (OH) <sub>5</sub> [-], V(OH) <sub>2</sub> [+], V <sub>2</sub> (OH) <sub>2</sub> [4+], VO(OH) <sub>3</sub> (aq), VO <sub>2</sub> (OH) <sub>2</sub> [-], VO <sub>2</sub> [+], VO <sub>3</sub> OH[2-], VOH[2+], VOOH[+], <b>V<sub>2</sub>O<sub>3</sub>(c)</b> , <b>V<sub>2</sub>O<sub>4</sub>(c)</b> , <b>V<sub>2</sub>O<sub>5</sub>(c)</b> , <b>V<sub>3</sub>O<sub>5</sub>(c)</b> , <b>V<sub>4</sub>O<sub>7</sub>(c)</b>	

HATCHES			
VO[2+], V[3+], VO <sub>2</sub> [+], VO <sub>4</sub> [3-], V <sub>2</sub> (OH) <sub>2</sub> [4+], VO(OH)[+], VO(OH) <sub>3</sub> (aq), VO) <sub>2</sub> (OH) <sub>2</sub> [2+], VO <sub>2</sub> (OH) <sub>2</sub> [-], VO <sub>3</sub> (OH)[2-], VOH[2+], <b>V(OH)<sub>3</sub></b> , <b>V<sub>2</sub>O<sub>3</sub>(c)</b> , <b>V<sub>2</sub>O<sub>4</sub>(c)</b> , <b>V<sub>2</sub>O<sub>5</sub>(c)</b> , <b>V<sub>3</sub>O<sub>5</sub>(c)</b> , <b>V<sub>4</sub>O<sub>7</sub>(c)</b> , <b>VO(OH)<sub>2</sub></b>			



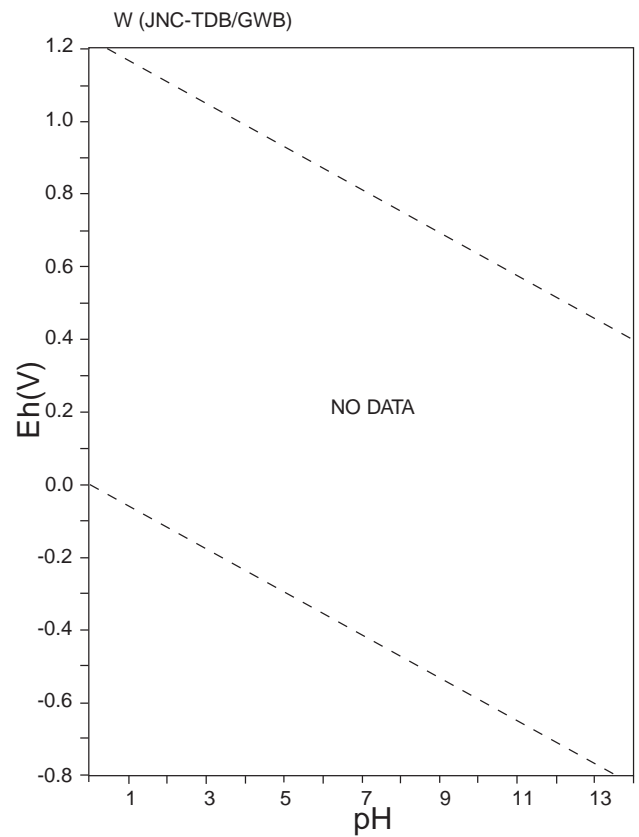
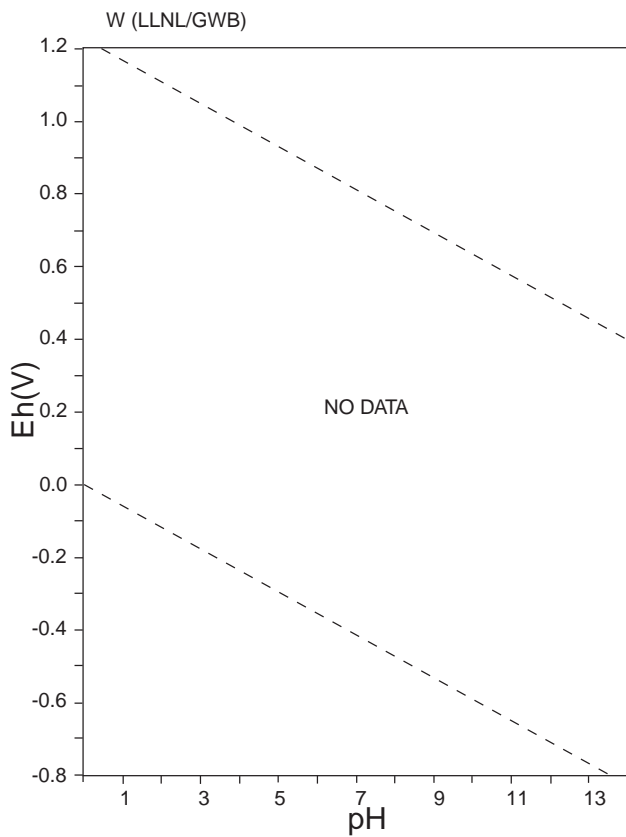
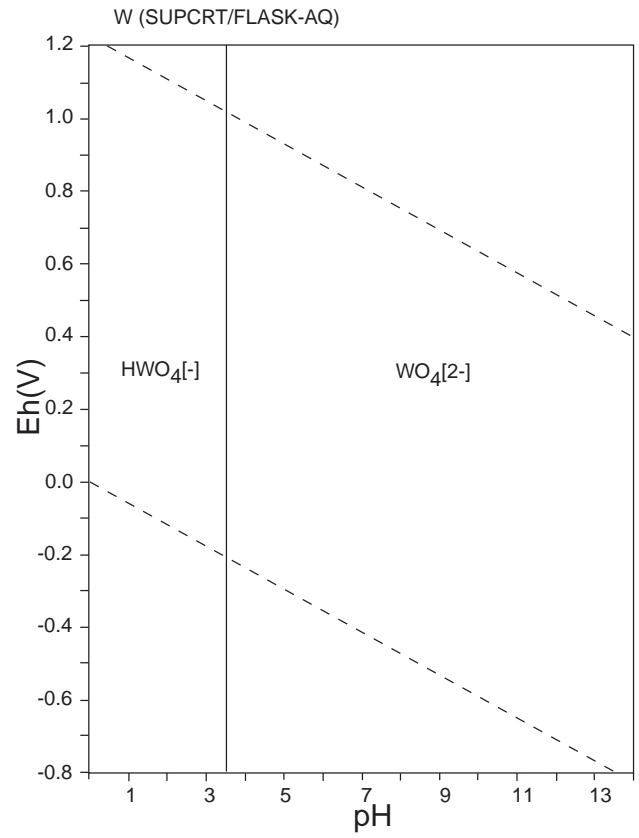
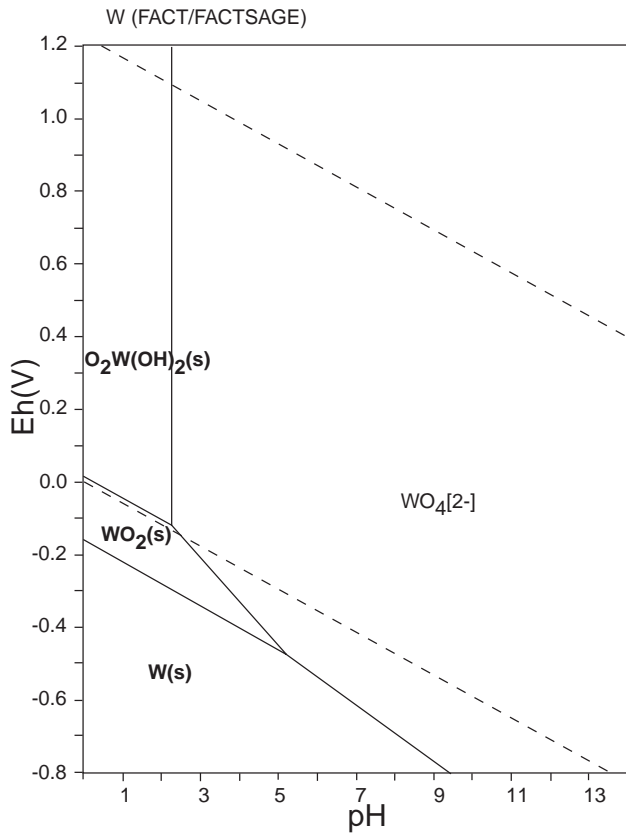
☒ 131: Eh-pH diagrams of the system V-O-H (1).  $\Sigma V = 10^{-10}$ , 298.15K,  $10^5$  Pa.



☒ 132: Eh-pH diagrams of the system V-O-H (2).  $\sum V = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 82: List of W species

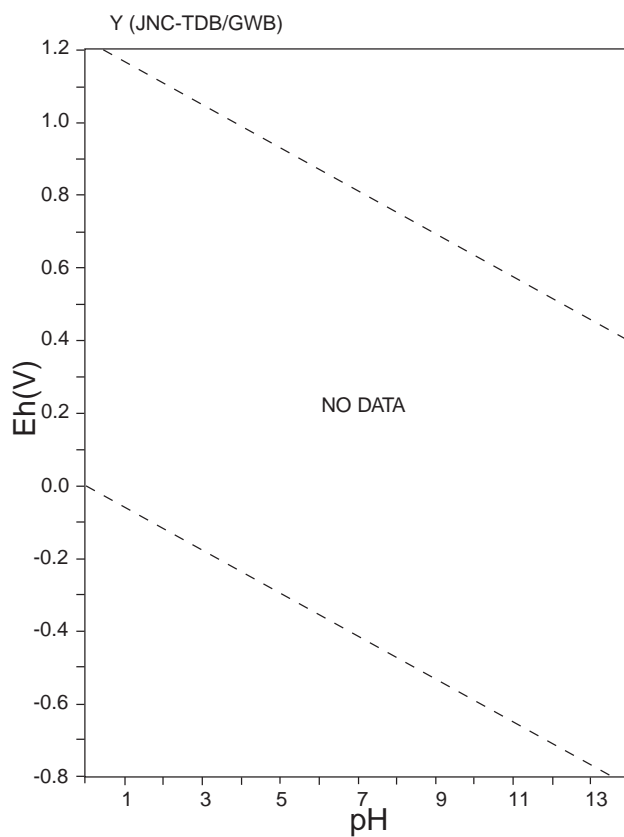
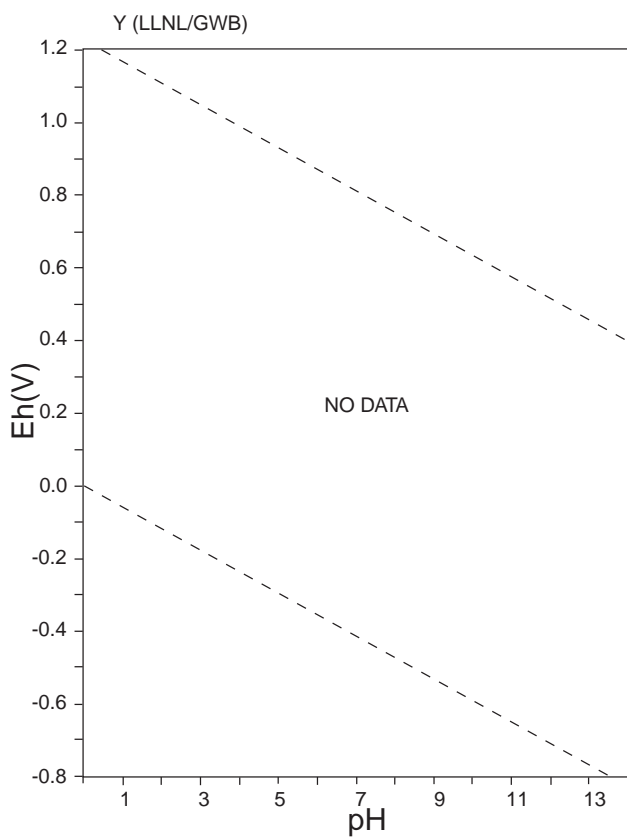
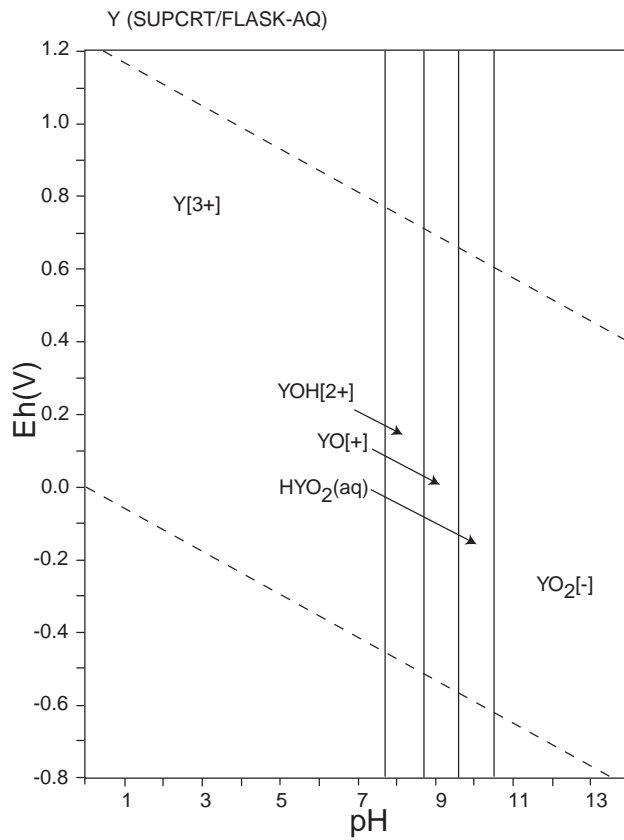
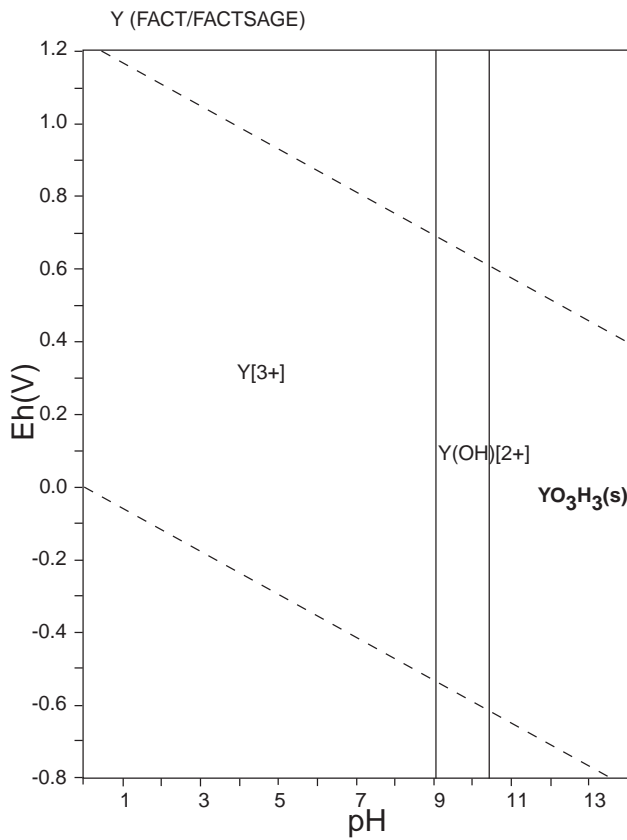
FACT	SUPCRT	LLNL	JNC-TDB
$\text{WO}_4[2-]$ , $\text{W}(\text{s})$ , $\text{WO}_2(\text{s})$ , $\text{WO}_3(\text{s})$ , $\text{WO}_3(\text{s}2)$ , $\text{O}_2\text{W}(\text{OH})_2(\text{s})$	$\text{WO}_4[2-]$ , $\text{HWO}_4[-]$		



☒ 133: Eh-pH diagrams of the system W-O-H.  $\sum W = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 83: List of Y species

FACT	SUPCRT	LLNL	JNC-TDB
$Y[3+]$ , $YOH[2+]$ , $Y_2(OH)_2[4+]$ , $Y(s)$ , $Y(s2)$ , $YH_2(s)$ , $YH_3(s)$ , $Y_2O_3(s)$ , $Y_2O_3(s2)$ , $YO_3H_3(s)$	$Y[3+]$ , $YOH[2+]$ , $YO[+]$ , $HYO_2(aq)$ , $YO_2[-]$		

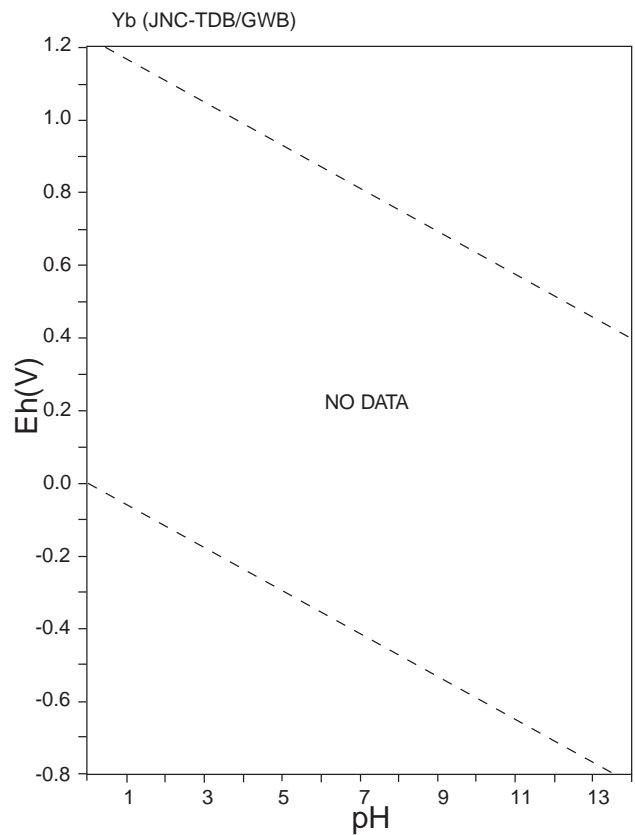
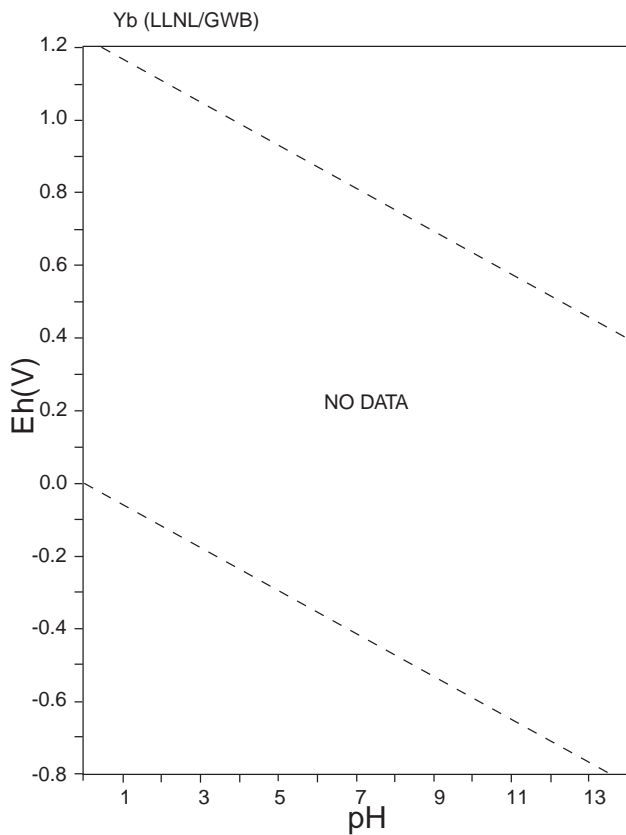
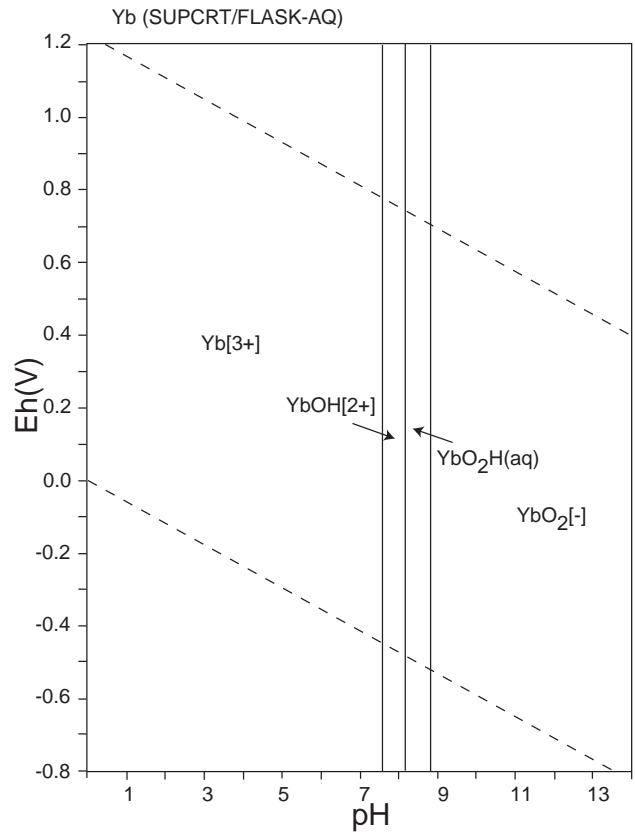
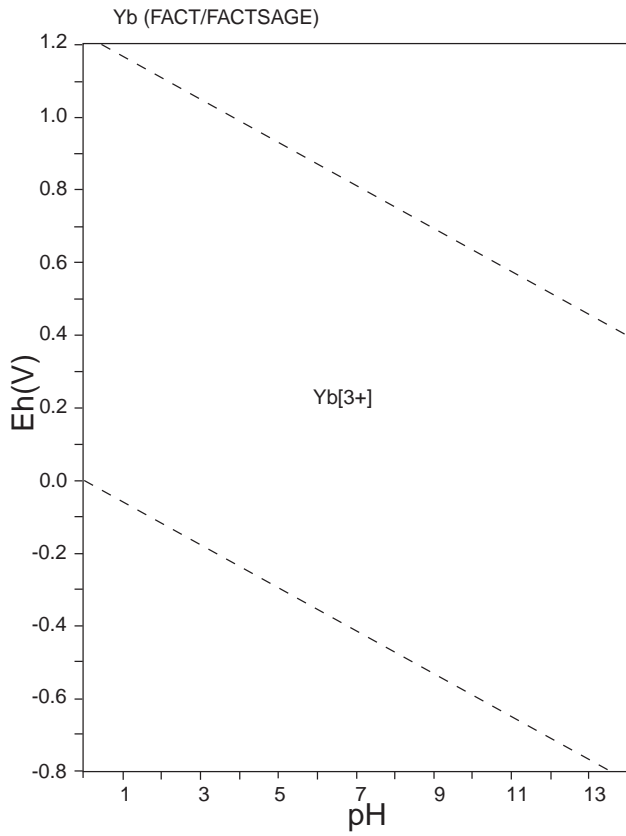


☒ 134: Eh-pH diagrams of the system Y-O-H.  $\sum Y = 10^{-10}$ , 298.15K,  $10^5$  Pa.

表 84: List of Yb species

FACT	SUPCRT	LLNL	JNC-TDB
Yb[2+], Yb[3+], <b>Yb(s), Yb(s2),</b> <b>Yb<sub>2</sub>O<sub>3</sub>(s), Yb<sub>2</sub>O<sub>3</sub>(s2),</b> <b>Yb<sub>2</sub>O<sub>3</sub>(s3)</b>	Yb[2+], Yb[3+], Yb[4+], YbOH[2+], YbO[+], YbO <sub>2</sub> H(aq), YbO <sub>2</sub> [-]		





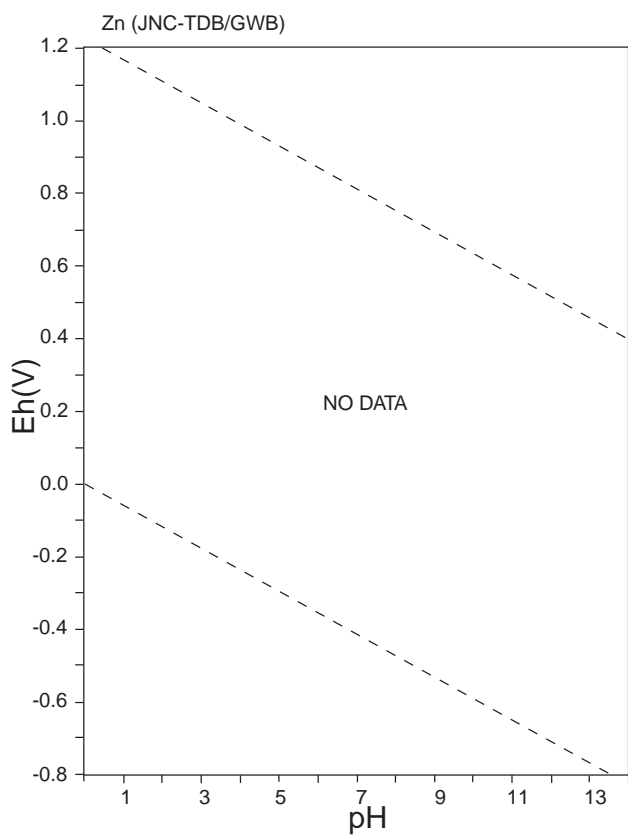
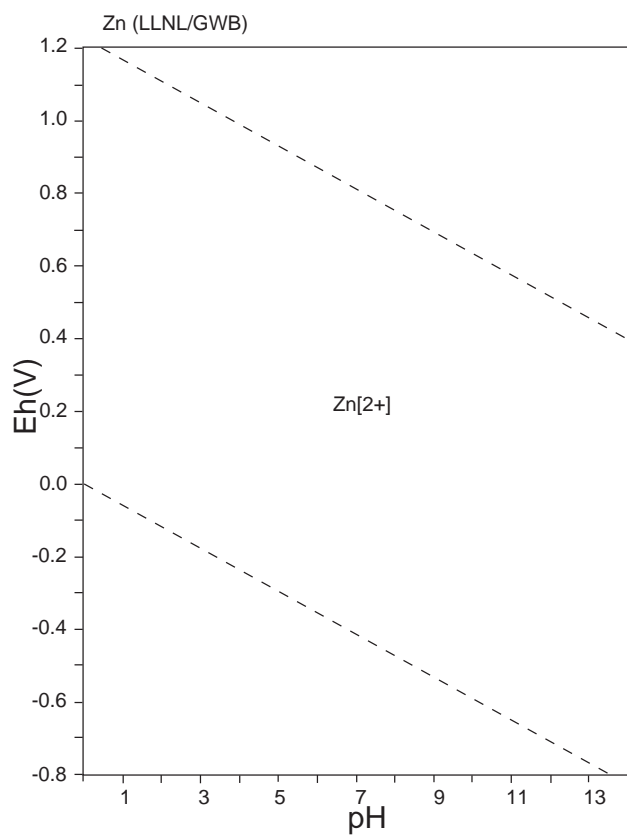
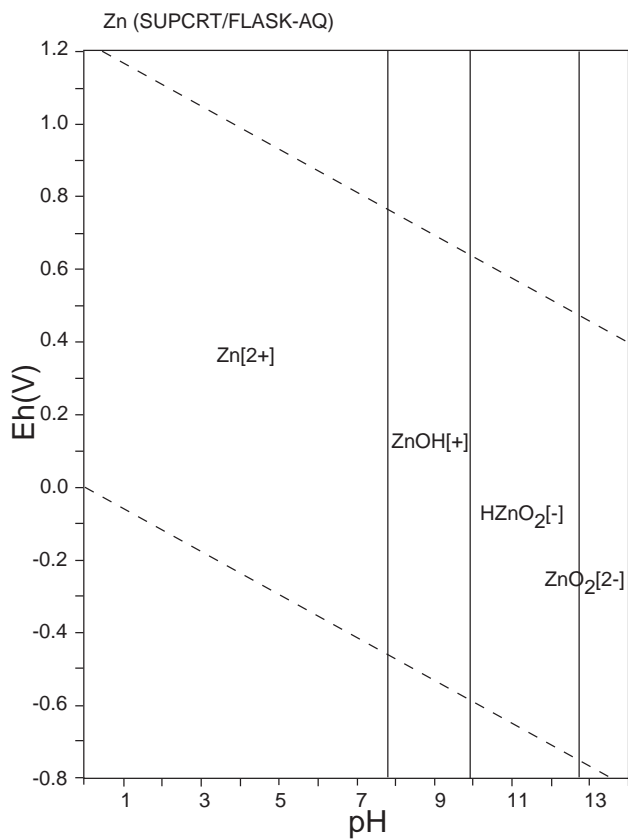
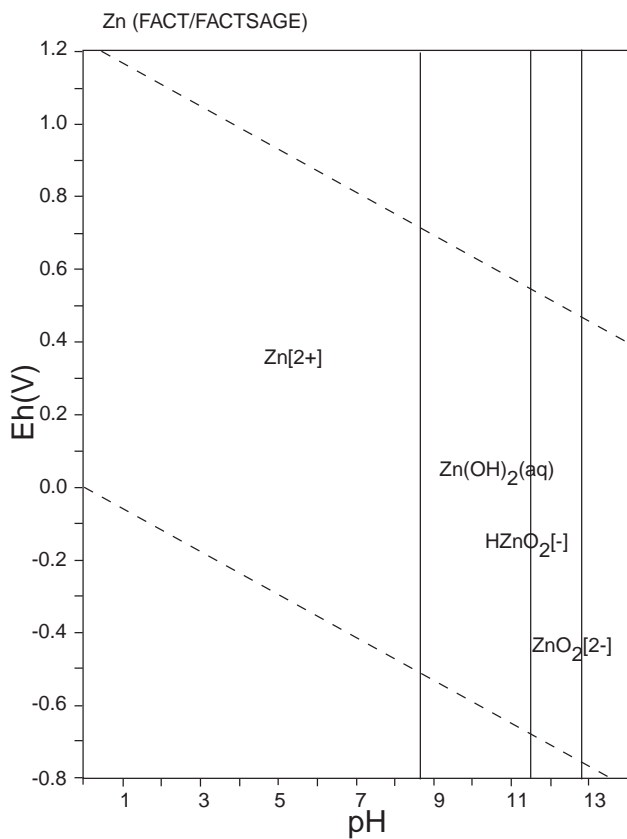
☒ 135: Eh-pH diagrams of the system Yb-O-H.  $\sum \text{Yb} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



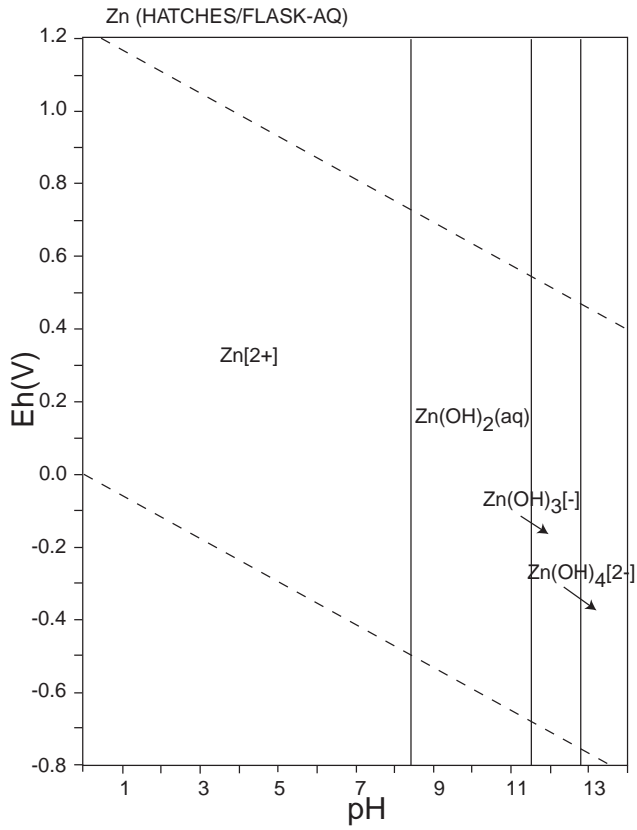
表 85: List of Zn species

FACT	SUPCRT	LLNL	JNC-TDB
Zn[2+], ZnO <sub>2</sub> [2-], ZnOH[+], HZnO <sub>2</sub> [-], Zn(OH) <sub>2</sub> (aq), <b>ZnO(s)</b> , <b>Zn(s)</b> , <b>Zn(OH)<sub>2</sub>(s)</b> , <b>Zn(OH)<sub>2</sub>(s2)</b> , <b>Zn(OH)<sub>2</sub>(s3)</b>	Zn[2+], ZnO <sub>2</sub> [2-], ZnOH[+], HZnO <sub>2</sub> [-], ZnO(aq), <b>ZnO(Zincite)</b>	Zn[2+]	

HATCHES			
Zn[2+], Zn(OH) <sub>2</sub> (aq), Zn(OH) <sub>3</sub> [-], Zn(OH) <sub>4</sub> [2-], Zn <sub>2</sub> (OH) <sub>6</sub> [2-], Zn <sub>2</sub> OH[3+], ZnO <sub>2</sub> [2-], ZnOH[+], <b>Zincite</b> , <b>Zn(OH)<sub>2</sub></b>			



☒ 136: Eh-pH diagrams of the system Zn-O-H (1).  $\sum \text{Zn} = 10^{-10}$ , 298.15K,  $10^5$  Pa.



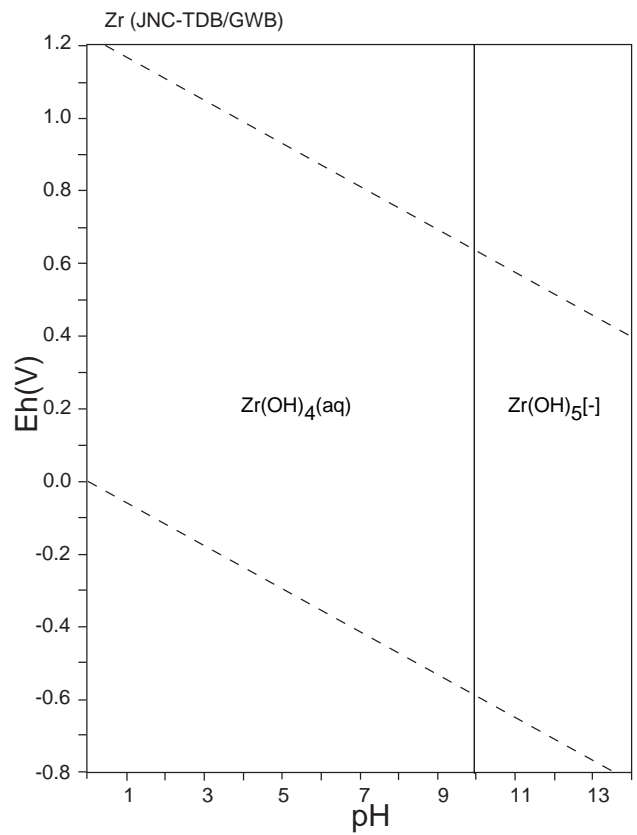
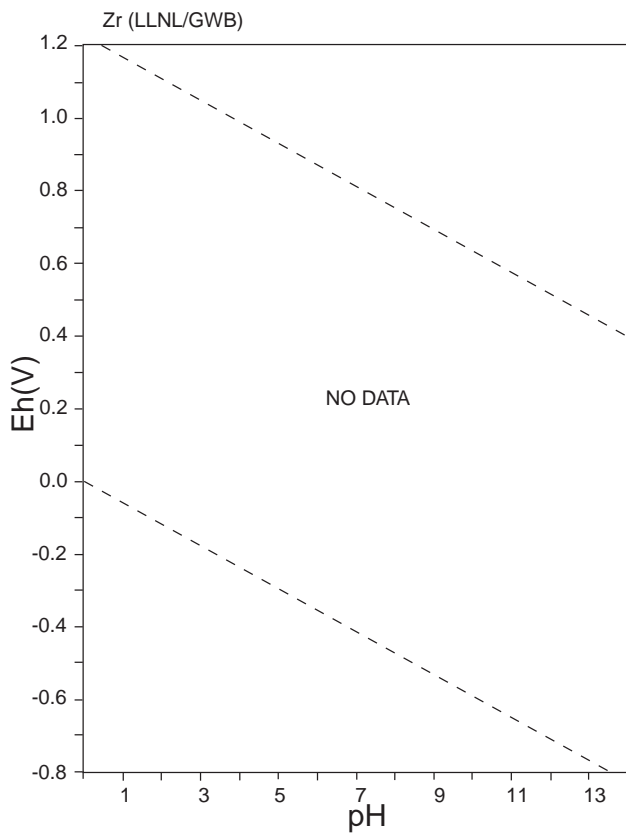
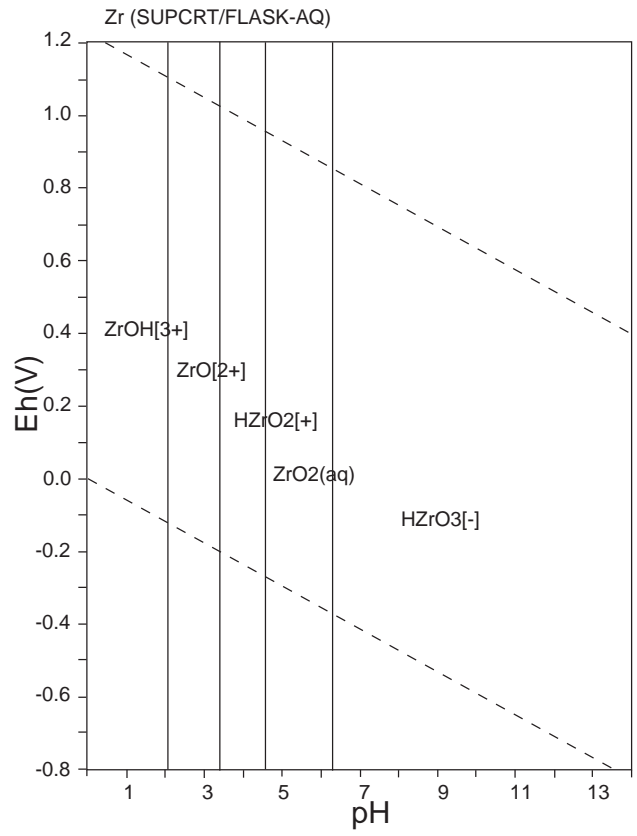
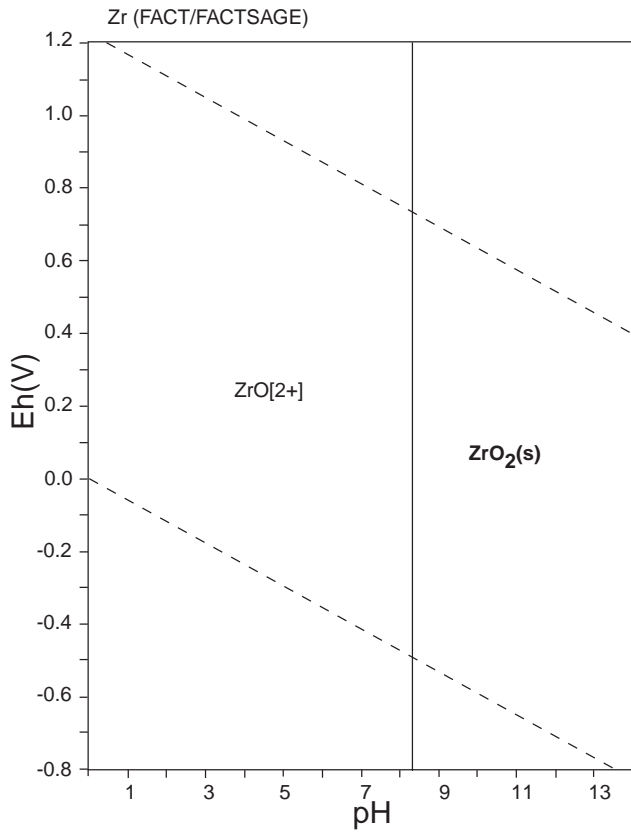
☒ 137: Eh-pH diagrams of the system Zn-O-H (2).  $\sum Zn = 10^{-10}$ , 298.15K,  $10^5$  Pa.



表 86: List of Zr species

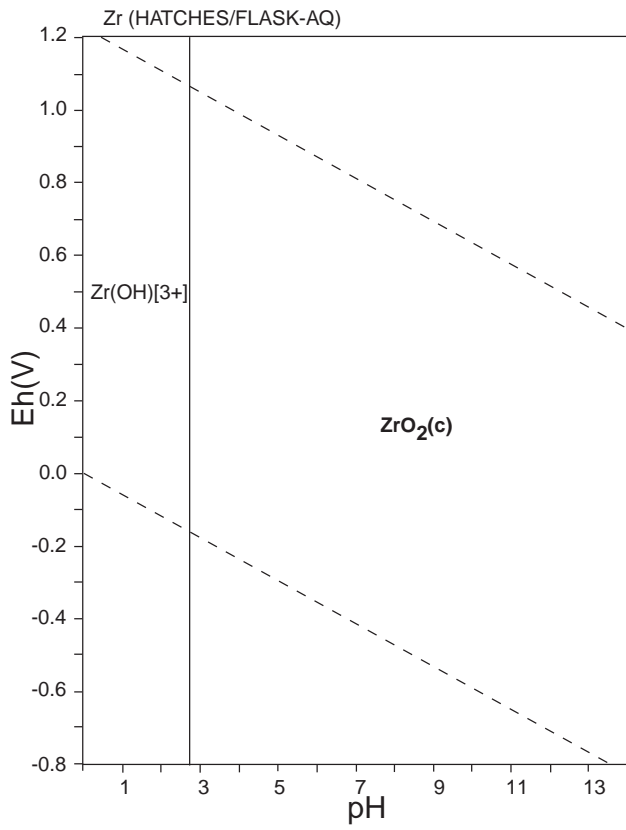
FACT	SUPCRT	LLNL	JNC-TDB
ZrO[2+], <b>Zr(s)</b> , <b>Zr(s2)</b> , <b>ZrH<sub>2</sub>(s)</b> , <b>ZrO<sub>2</sub>(s)</b> , <b>ZrO<sub>2</sub>(s2)</b> , <b>ZrO<sub>2</sub>(s3)</b>	ZrO[2+], Zr[4+], ZrOH[3+], HZrO <sub>2</sub> [+], ZrO <sub>2</sub> (aq), HZrO <sub>3</sub> [-]		Zr(OH) <sub>4</sub> (aq), Zr(OH) <sub>5</sub> [-], <b>ZrO<sub>2</sub>(am)</b>

HATCHES			
Zr[4+], Zr(OH)[3+], Zr(OH) <sub>4</sub> (aq), Zr(OH) <sub>5</sub> [-], Zr <sub>3</sub> (OH) <sub>4</sub> [8+], Zr <sub>4</sub> (OH) <sub>8</sub> [8+], <b>ZrO<sub>2</sub>(am)</b> , <b>ZrO<sub>2</sub>(c)</b>			



☒ 138: Eh-pH diagrams of the system Zr-O-H (1).  $\sum \text{Zr} = 10^{-10}$ , 298.15K,  $10^5$  Pa.





☒ 139: Eh-pH diagrams of the system Zr-O-H (2).  $\sum \text{Zr} = 10^{-10}$ , 298.15K,  $10^5$  Pa.