Atlas of Eh-pH diagrams

Intercomparison of thermodynamic databases

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Contents

List of Tables

List of Figures

1 Introduction

This open file report aims to present an intercomparison of thermodynamic databases by means of Eh-pH diagrams, which are practical and useful for understanding geochemical behavior of elements. An Eh-pH diagram depicts the dominant aqueous species and stable solid phases on a plane defined by the Eh and pH axes. In an Eh-pH diagram, the solid stability area is related to the saturation condition, and dominant aqueous species give us fundamental information on sorption and colloid phenomena as well as surface characteristics of materials. Eh-pH diagrams are thus essential to understanding solute and radionuclide transport in groundwater.

The most well-known studies on comprehensive Eh-pH diagrams are those of Pourbaix (1966) and Brookins (1988). The former discussed corrosion, passivation and immunity of materials, while the latter reported geochemical aspects of the geological disposal of radioactive wastes. These studies have been followed by many thermodynamic databases.

With the ever increasing CPU power of computers, we have started utilizing geochemical codes for calculation of complex chemical reactions. Thus, thermodynamic databases have gained importance from a practical perspective.

Certain geochemical codes enable us to obtain Eh-pH diagrams easily and quickly. With the aid of software, Eh-pH diagrams can provide us with good insight into the state of the art in thermodynamic databases and the differences between them.

It should be noted that this open file report presents the Eh-pH diagrams calculated from databases "as is", without any critical comments. It should also be noted that Eh-pH diagrams represent one aspect of thermodynamic databases and databases are often updated, thus this report is only a snapshot of the present. I would be very pleased if this open file report proves useful in helping the readers use thermodynamic databases.

2 Databases

Let us compare the seven databases listed below. The first database is generic and popular in inorganic chemical engineering. The second and third are generic and popular in geochemistry. The fourth and fifth serve for safety assessment of geological disposal of radioactive wastes, but their coverage of chemical species is sufficiently wide to be suitable for generic use. The sixth and seventh databases mainly cover data on radioactive elements, with incomplete data on other elements. The current report presents only Eh-pH diagrams of radioactive elements included in the sixth and seventh databases.

1. FACT (FACT database) bundled with commercially available software FACTSAGE (FactSage 5.2) (Bale et al., 2002) released by GTT-Technologies.

2. SUPCRT: SUPCRT92 (Johnson et al., 1992) applied with 98 update distributed by Everette Shock from his website on the Internet.

3. Default database "thermo.dat" based on LLNL (Lawrence Livermore National Lab.) data 0.3245r46, bundled with commercially available software GWB (Geochemist's Workbench) written by C. M. Bethke, Illinois University.

4. JNC-TDB (011213g0 and 011213g2) distributed by Japan Nuclear Cycle Organization from their website (http://migrationdb.jnc.go.jp/).

5. HATCHES (ZZ-HATCHES-15) distributed by NEA (Nuclear Energy Agency) Computer Program Services.

6. Databases tabulated in OECD/NEA Chemical Thermodynamics series 1-4 (Grenthe et al., 1992; Silva et al., 1995; Rard et al., 1999; Lemire et al., 2001).

7. Databases tabulated in OECD/NEA Chemical Thermodynamics series 5 (Guillaumont et al., 2003) which is the updated version of the same series 1-4.

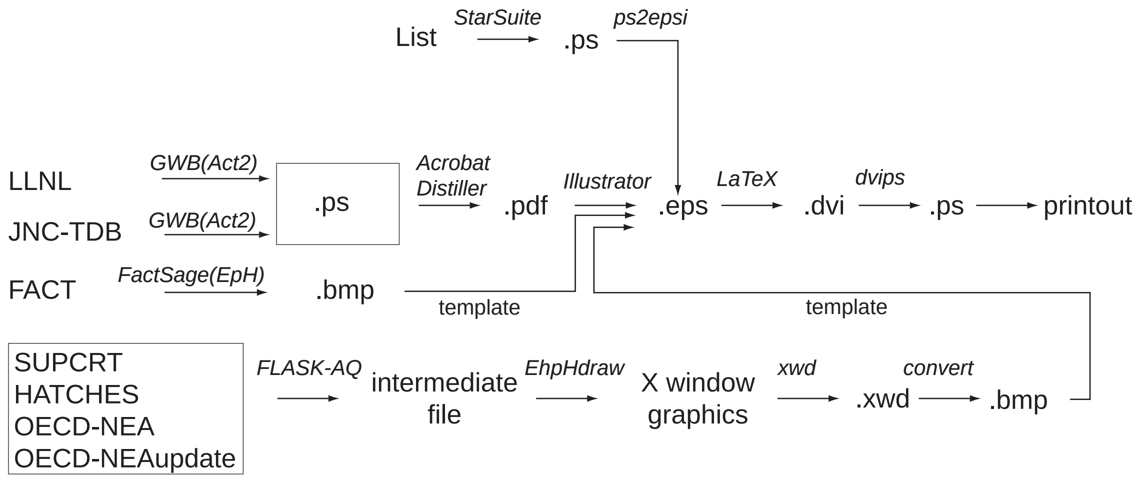

Figure 1: Flow chart of creating this report
Software is in italics. Dot name represents a file with format indicated by extention.

3 Method for constructing Eh-pH diagrams

The present report includes Eh-pH diagrams for the X-H-O system, where X = the symbol of an element like Na, K. This is the most important system for the chemical description of elements in groundwater. To understand the geochemical system of the natural barrier, we took account of not only radioactive elements, but also other elements included in the databases. However, OECD-NEA databases were excluded due to their restricted coverage of the data on non-radioactive elements. Total concentration of elements is 10^{-10} mole/kg for all diagrams. Such a low concentration enables us to safely assume the activity coefficient to be unity and impedes precipitation of the solid phases which hide the area of dominant aqueous species in the Eh-pH diagram.

To avoid unexpected errors during data conversion, databases bundled with commercially available software and databases distributed in the specific format of the software are handled with appropriate software to draw Eh-pH diagrams. Databases of the former type are FACT and LLNL, bundled with FACTSAGE and GWB, respectively. The database of the latter type is JNC-TDB, which is distributed in three formats: EQ3/6, PHREEQC, and GWB. In this report, a version in the GWB format was used. For the other databases, namely SUPCRT, HATCHES, OECD-NEA, and OECD-NEAupdate, the in-house software FLASK-AQ and its companion software EhpHdraw were used to draw the Eh-pH diagrams.

The drawing method for Eh-pH diagrams is well explained in many textbooks of chemical thermodynamics (e.g. Garrels and Christ, 1965). The algorithm for drawing Eh-pH diagrams is not documented in the commercially available software FACTSAGE and GWB.

FLASK-AQ calculates concentration of aqueous species in equilibrium and moles of stable solid (if present) on grids into which Eh and pH are divided, the Eh in 0.005 V increments from -0.8 V to 1.2 V, the pH in increments of 0.04 from 0 to 14, and outputs the dominant species and the stable solid. Companion program EhpHdraw draws Eh-pH diagrams using the output of FLASK-AQ. This method resembles that reported by Anderko et al. (1997). Unfortunately, since Anderko et al. (1997) did not describe their method in detail, I cannot compare the two methods. The accuracy of the present method for drawing boundaries between dominant species or solids depends on the grid size, which inevitably leads to errors as large as 0.0025 V and 0.02 units for Eh and pH, respectively. The following subsections describe the method for drawing Eh-pH diagrams for each database. The database name and software name (both in abbreviation) are concatenated by a slash (Figure 1).

3.1 FACT/FACTSAGE

Eh-pH diagrams are created with EpH of FACTSAGE and saved as a BMP file. This file is used as a template for the line drawing software Illustrator (Adobe Illustrator) and resized to the common axial length.

3.2 SUPCRT/FLASK-AQ

The FLASK-AQ input file was created from the output of SUPCRT92. FLASK-AQ creates an intermediate file from which EhpHdraw draws an Eh-pH diagram on the X window system. This Eh-pH diagram is captured to an X window dump file using ”xwd”, and then converted to a BMP file with ImageMagic. This BMP file is used as a template for Illustrator and resized to the common axial length. An enormous amount of organic species in this database are expressed stoichiometrically in terms of C, H, and O as basis species. Calculations reveal that almost all organic species are decomposed under the stability field of water under ambient conditions.

3.3 LLNL/GWB

The Eh-pH diagram is created with Act2 of GWB and is saved as a PostScript file. This file is converted to a PDF (portable document file) file with Adobe Acrobat Distiller and opened with Illustrator and resized to the common axial length.

3.4 JNC-TDB/GWB

The Eh-pH diagram is created with Act2 of GWB and saved as a PostScript file. This file is converted to a PDF file with Adobe Acrobat Distiller and opened with Illustrator and resized to the common axial length. All diagrams were first created using 011213g0, and S and U data were updated with 011213g2, fixing the erroneous S and U data in the previous version. Visual inspection confirms that all diagrams other than those of S and U are identical between 011213g0 and 011213g2, i.e., that all diagrams from 011213g0 remained unchanged except those of S and U.

3.5 HATCHES/FLASK-AQ

The files of EQ3/6 format data bundled with HATCHES are combined into a single file in which some aux species with the improper keyword ”basis” were corrected. This file is converted to a FLASK-AQ input file using the in-house software AIST TDBCONVERT. FLASK-AQ creates the intermediate file from which EhpHdraw draws an Eh-pH diagram on the X window system. This diagram is captured to an X window dump file using ”xwd”, and then converted to a BMP file with ImageMagic. This BMP file is used as a template for Illustrator and resized to the common axial length.

Organic species are expressed stoichiometrically in terms of the ligand species. Note that this method differs from the case of SUPCRT/FLASK-AQ. However, this difference does not affect the Eh-pH diagrams because ligand species are not included in the X-H-O system.

3.6 OECD/NEA

The tables listing the Standard Gibbs Free Energy of formation for the elements in the OECD-NEA Chemical Thermodynamics vol. 1-4 are entered into a spread sheet and saved as a text file and converted into FLASK-AQ format using in-house software. FLASK-AQ creates the intermediate file from which EhpHdraw draws the Eh-pH diagram in the X window system. This Eh-pH diagram is captured to an X window dump file using ”xwd”, and then converted into a BMP file with ImageMagic. This BMP file is used as a template for Illustrator and resized to the common axial length.

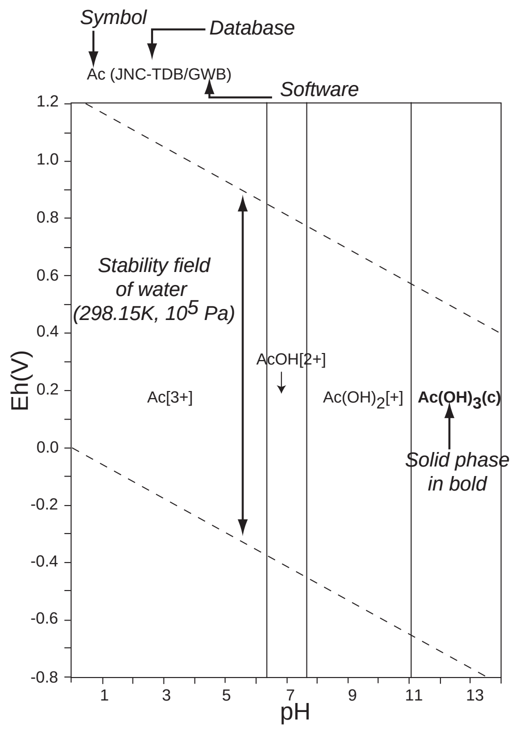

Figure 2: Legend of Eh-pH diagram

3.7 OECD-NEA update

The source database of OECD-NEA Chemical Thermodynamics vol. 5 was processed in the same way as OECD/NEA described above.

4 Explanation of the diagrams and tables

Tables and diagrams are presented in alphabetical order of the chemical symbol of the element. The tables precede the diagrams for each element. The top row of the table contains the database name. The database name and software name (both abbreviation) concatenated with a slash ("/") are found above the diagram next to the chemical symbol of the element (Figure 2). A blank column in the table and NODATA in the diagram mean either "no data for elements" or "no data for aqueous species of elements". The expression of the chemical formula used in the table and diagram is the same as in the source database, namely "as is". This was done to abide by the concept of the database compilers. Consequently, it should be noted that the expression for hydration and the solid phase differs between the databases. The expression for the charge has the same style throughout, while the expression for the solid has many variants: "am" denotes amorphous, "c" or "cr" denotes crystalline, "s" or no index indicates no discrimination for amorphous or crystalline. Some solid phases are labeled with mineral names. FACT database uses "s1", "s2", "s3" notation for polymorph phases, and the present report uses the same notation for the diagram from FACT/FACTSAGE. The names of solid phases in the table and diagram are typed in bold face. The area between the two diagonal lines from the upper left to the lower right in the diagram indicates the stability field of water at 298.15 K and 10^5 Pa. The tables list chemical species whose Eh-pH diagrams can be drawn individually for the database. Certain chemical species do not appear in the diagram because they are unstable or no data is available on them. Thus, it is important to consult the table carefully when using the diagrams.

Table 1: List of softwares used

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

5 Reliability and uncertainty

The reliability and uncertainty of diagrams depend on the following three factors. 1) Reliability of and error in the data in the databases, 2) Uncertainty of the software used for Eh-pH calculation, 3) Fidelity of the drawing. The error is not mentioned in the databases except the OECD-NEA Chemical Thermodynamics Series. The uncertainty in the commercial softwares for drawing Eh-pH diagrams is not described. The uncertainty in FLASK-AQ depends on grid size, as already mentioned. The fidelity of the drawing is confirmed within the grid size of FLASK-AQ by visual inspection. Thus, the overall error excluding errors stemming from the databases and commercial softwares are within ± 0.0025 V for Eh and ± 0.02 units for pH.

6 Description of the softwares and their execution environments

The software used for Eh-pH calculation are GTT-Technologies FactSage 5.2 and Illinois University Geochemist's Workbench 4.0 and the in-house software AIST FLASK-AQ 1.1. FactSage 5.2 and Geochemist's Workbench 4.0 are executed under a Microsoft Windows 2000 Server on a Dell PowerEdge 2600 (Xeon 2.4GHz x2 SMP with 4GB memory). FLASK-AQ 1.1 is executed under SuSE Linux 7.3 (kernel 2.4.20) on HIT PC (Pentium4 2.8 GHz with 1GB memory). FLASK-AQ 1.1 was compiled with Intel C++ 7.0 compiler and executed with batch scheduling software LSF 4.2. To obtain the Eh-pH diagrams from the intermediate file of FLASK-AQ 1.1, the in-house software AIST EhpHdraw was used. ZZ-HATCHES-15 data was converted into the FLASK-AQ format using the in-house software AIST TDBCONVERT coded by Nihon sgi. All in-house software of AIST will be released to the general public in the future.

To obtain snapshots of the Eh-pH diagram drawn by EhpHdraw, the X Window dump software "xwd" was used. To convert from the XWD to BMP format, "convert" of ImageMagic was used. These procedures were carried out under Red Hat Linux 9 or Fedra Core 2 on an IA32 PC.

Conversion from the PostScript file to the PDF file was performed with Adobe Acrobat Distiller 4.0. Trace of the template image, resizing and cosmetics of the diagrams, and outputting to the EPS file were performed using Adobe Illustrator 8.0 under Microsoft Windows 2000 Professional on an IA32 PC.

The lists of chemical species in the tables were created with Sun StarSuite 6.0 and saved as PostScript files and converted into EPS files with "ps2epsi" under Fedra Core 2 on an IA32 PC. The final draft of this report was printed out using LaTeX and "dvips", on a Laser printer under Fedra

Core 2 on an IA32 PC (Table 1).

The names of the software, formats, and hardware are trademarks or registered trademarks and the property of their owners.

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Table 2: List of Ac species

FACT	SUPCRT	LLNL	JNC-TDB
			Ac[3+], AcOH[2+], Ac(OH)$_2$[+], Ac(OH)$_3$(aq), **Ac(OH)$_3$(am)**, **Ac(OH)$_3$(c)**

HATCHES			
Ac[3+], AcOH[2+], **Ac(OH)$_3$**			

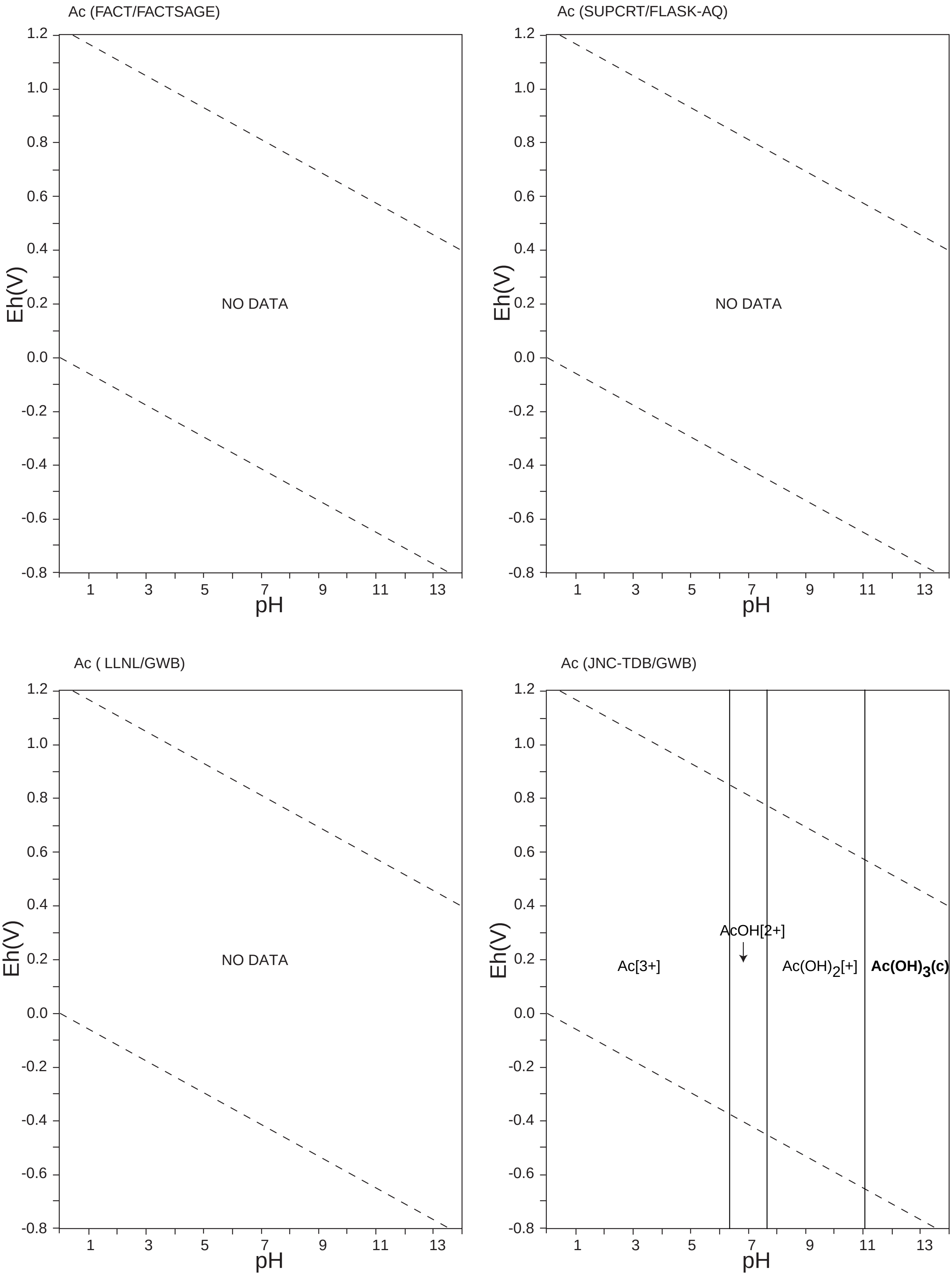

Figure 3: Eh-pH diagrams of the system Ac-O-H (1). $\sum \mathrm{Ac} = 10^{-10}$, 298.15K, 10^5 Pa.

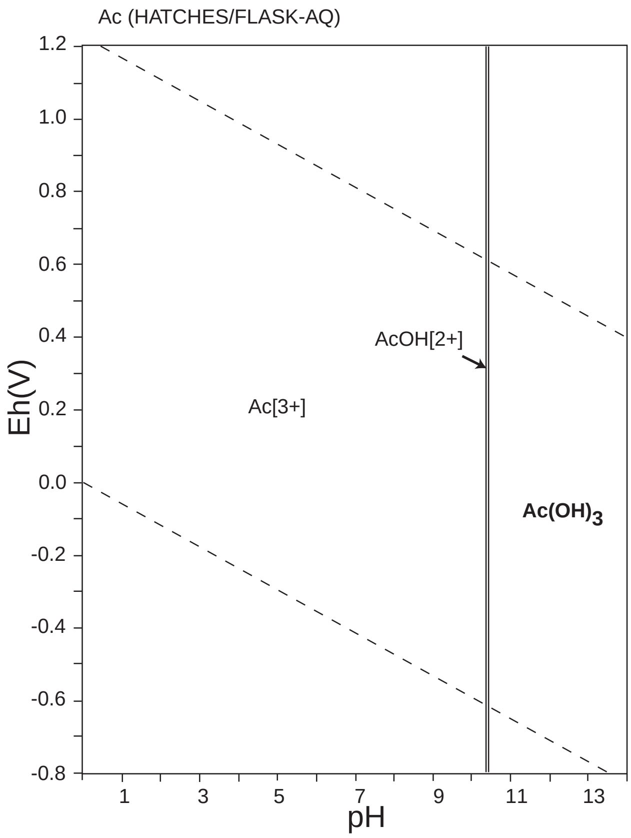

Figure 4: Eh-pH diagrams of the system Ac-O-H (2). $\sum \mathrm{Ac} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 3: List of Ag species

FACT	SUPCRT	LLNL	JNC-TDB
Ag[+], AgOH(aq), $Ag(OH)_2$[-],**Ag_2O(s)**, **Ag_2O_2(s)**, **Ag_2O_3(s)**, **Ag(Native silver)**	Ag[2+], Ag[+], AgOH(aq), AgO[-], **Ag(Native silver)**	Ag[+], **Silver**	Ag[+]
HATCHES			
Ag[+], $Ag(OH)_2$[-], AgOH(aq), **Ag**, **Ag_2O**, **Ag_2O_2**, **Ag_2O_3**			

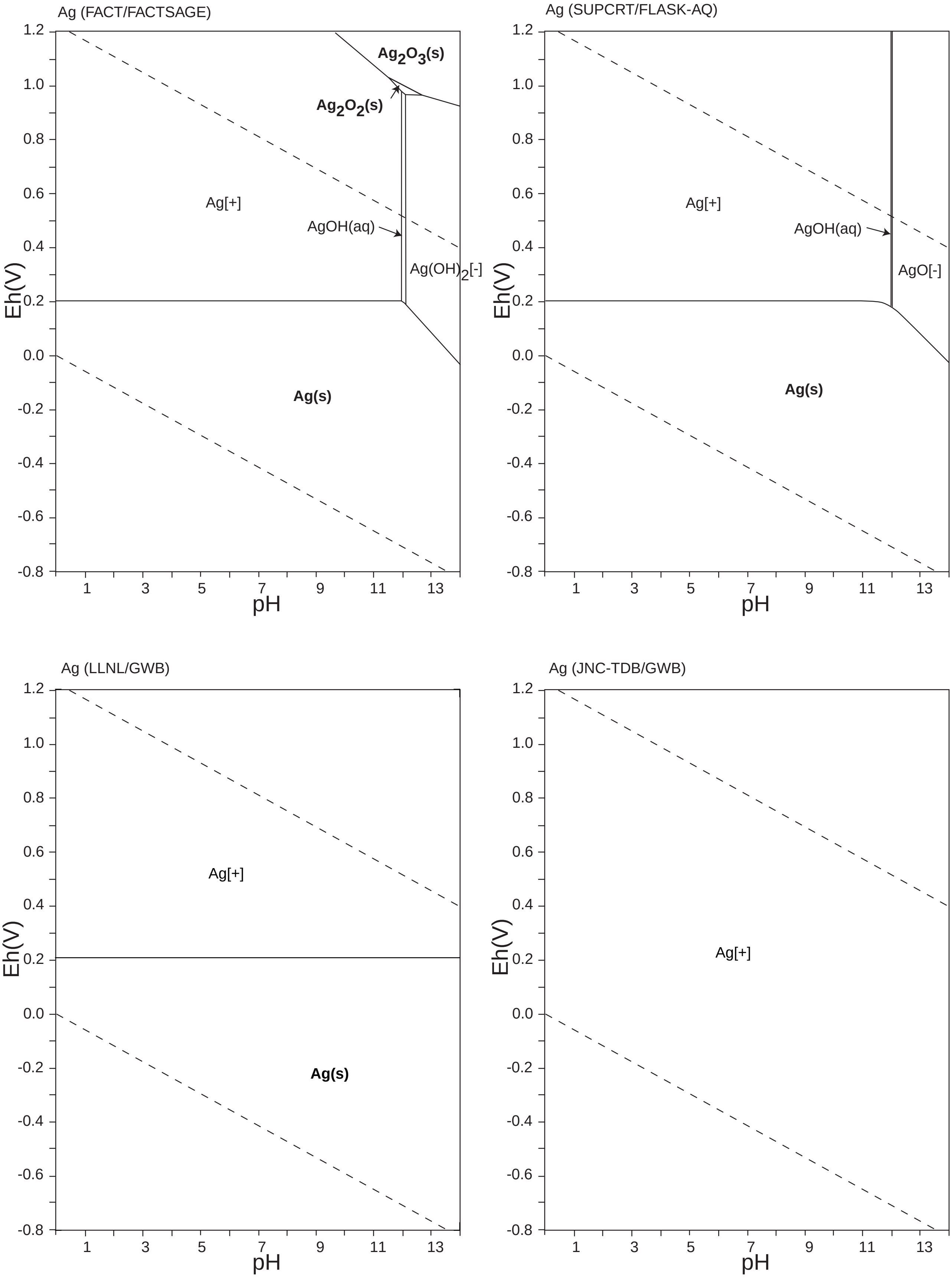

Figure 5: Eh-pH diagrams of the system Ag-O-H (1). $\sum \mathrm{Ag} = 10^{-10}$, 298.15K, 10^5 Pa.

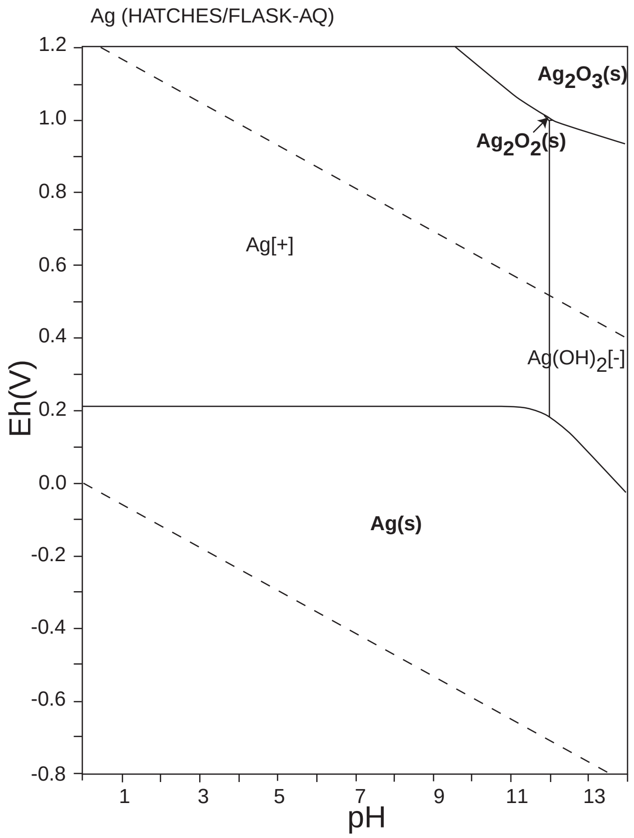

Figure 6: Eh-pH diagrams of the system Ag-O-H (2). $\sum \text{Ag} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 4: List of Al species

FACT	SUPCRT	LLNL	JNC-TDB
$Al^{[3+]}$, $AlO_2[-]$, $AlOH[2+]$, **Al(s)**, **AlH_3(s)**, **Al_2O_3(s)**, **Al_2O_3(s2)**, **Al_2O_3(s3)**, **Al_2O_3(s4)**, **$Al(OH)_3$(s)**, **$Al_2O_3(H_2O)$(s)**, **$Al_2O_3(H_2O)$(s2)**, **$Al_2O_3(H_2O)_3$(s)**	AlO[+], $HAlO_2$(aq), Al[3+], $AlO_2[-]$, AlOH[2+], **Al_2O_3(Corundum)**, **AlO(OH)(Diaspore)**, **AlO(OH)(Boehmite)**, **$Al(OH)_3$(Gibbsite)**, **AlO[+]**, **$HAlO_2$(aq)**	Al[3+], $Al(OH)_2[+]$, $Al(OH)_3$(aq), $Al(OH)_4[-]$ $Al_{13}O_4(OH)_{24}[7+]$, $Al_2(OH)_2[4+]$, $Al_3(OH)_4[5+]$, AlOH[2+], **Boehmite**, **Corundum**, **Diaspore**, **Gibbsite**	Al[3+], AlOH[2+], $Al(OH)_2[+]$, $Al(OH)_3$(aq), $Al(OH)_4[-]$, **Gibbsite**

HATCHES			
Al[3+], Al(OH)[2+], $Al(OH)_2[+]$, $Al(OH)_3$(aq), $Al(OH)_4[-]$, **Boehmite**, **Corundum**, **Diaspore**, **Gibbsite**			

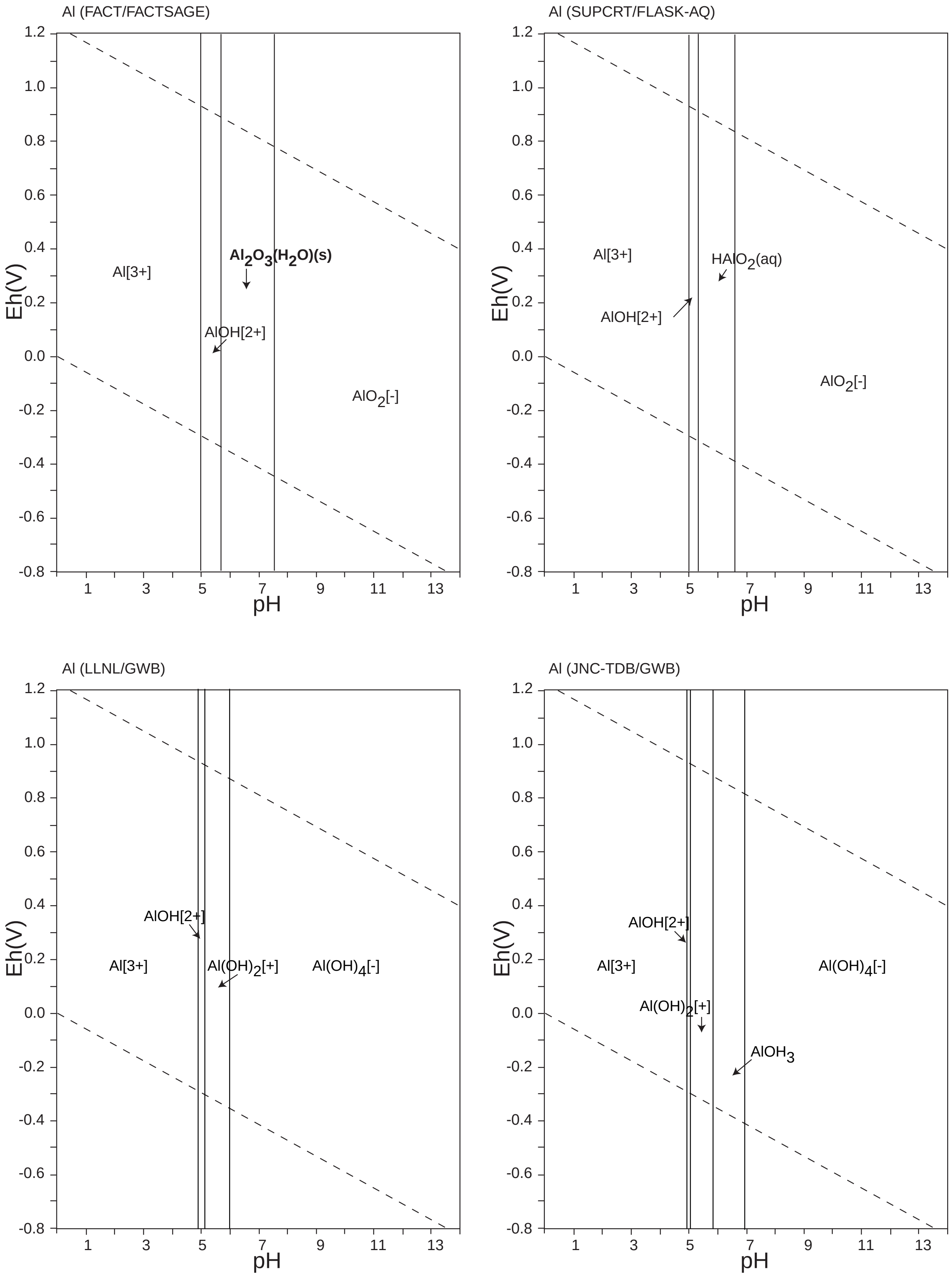

Figure 7: Eh-pH diagrams of the system Al-O-H (1). $\sum \mathrm{Al} = 10^{-10}$, 298.15K, 10^5 Pa.

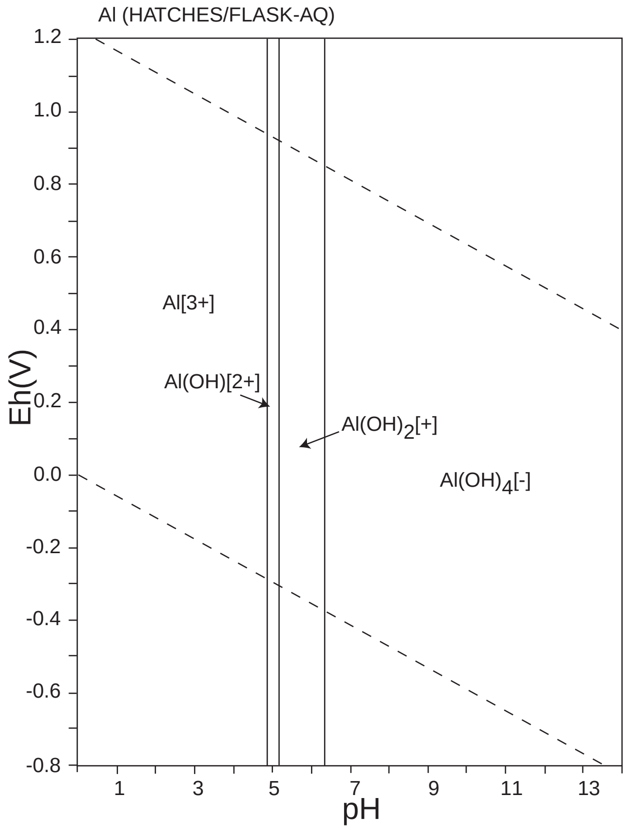

Figure 8: Eh-pH diagrams of the system Al-O-H (2). $\sum \mathrm{Al} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 5: List of Am species

FACT	SUPCRT	LLNL	JNC-TDB
Am(s), Am(s2), Am(s3), AmO_2(s), Am_2O_3(s)		Am^{3+}, Am^{4+}, AmO_2^{+}, AmO_2^{2+}, $Am(OH)_2^{+}$, $Am(OH)_3$(aq), $AmOH^{2+}$, **$Am(OH)_3$(am), $Am(OH)_3$(c)**	Am^{3+}, $AmOH^{2+}$, $Am(OH)_2^{+}$, $Am(OH)_3$(aq), **$Am(OH)_3$(am), $Am(OH)_3$(c)**

HATCHES	OECD-NEA	OECD-NEA update	
Am^{3+}, Am^{4+}, AmO_2^{+}, AmO_2^{2+}, $Am(OH)_2^{+}$, $Am(OH)_3$(aq), $AmOH^{2+}$, **Am, $Am(OH)_3$, Am_2O_3, AmH_2, AmO_2, $Am(OH)_3$(cr)**	Am^{4+}, Am^{2+}, Am^{3+}, AmO_2^{+}, AmO_2^{2+}, $AmOH^{2+}$, $Am(OH)_2^{+}$, $Am(OH)_3$(aq), **Am(c), AmO_2(c), Am_2O_3(c), AmH_2(c), $Am(OH)_3$(am), $Am(OH)_3$(c)**	Am^{4+}, Am^{2+}, Am^{3+}, AmO_2^{+}, AmO_2^{2+}, $AmOH^{2+}$, $Am(OH)_2^{+}$, $Am(OH)_3$(aq), **Am(cr), AmO_2(cr), Am_2O_3(cr), AmH_2(cr), $Am(OH)_3$(cr)**	

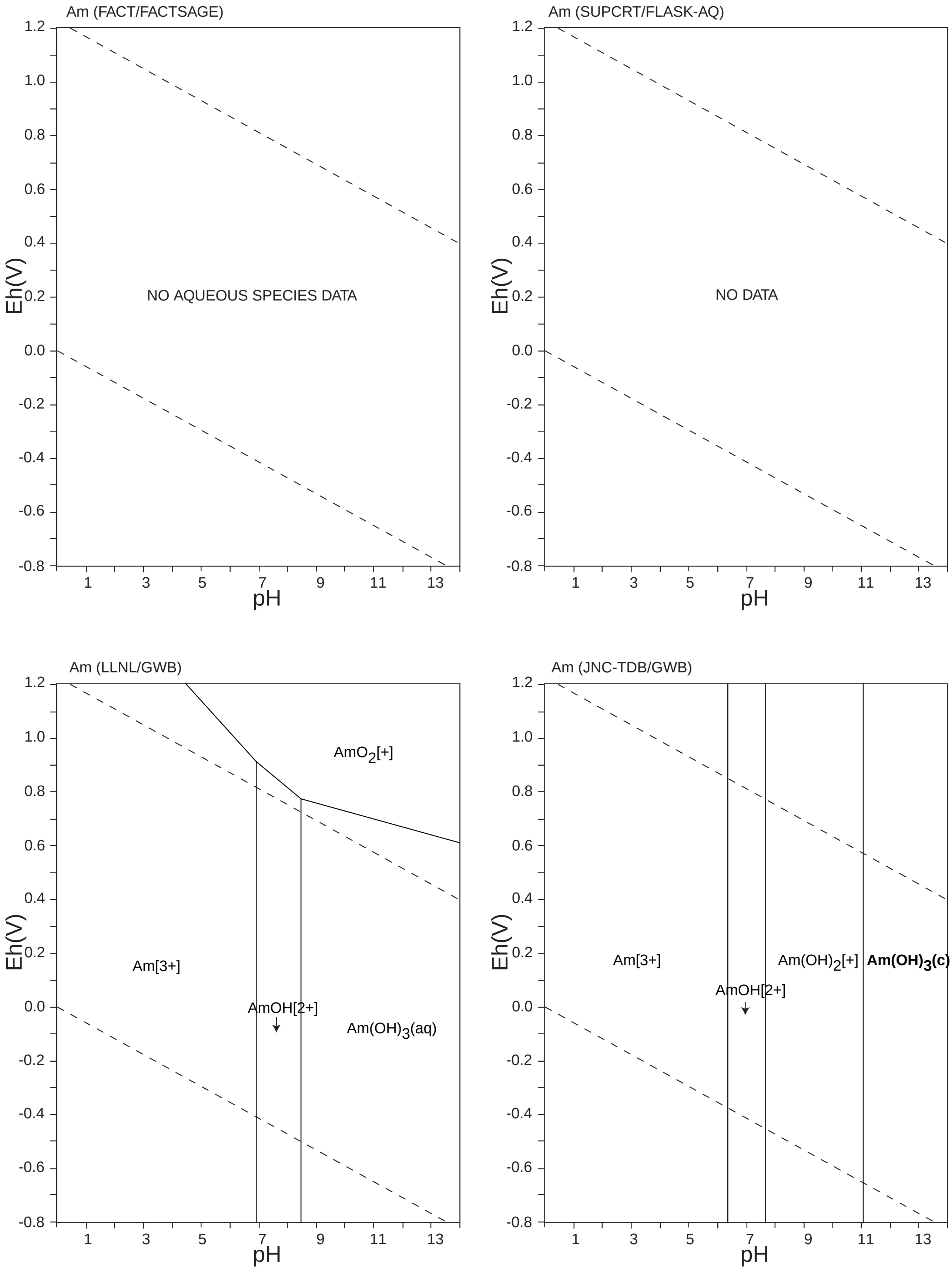

Figure 9: Eh-pH diagrams of the system Am-O-H (1). $\sum \text{Am} = 10^{-10}$, 298.15K, 10^5 Pa.

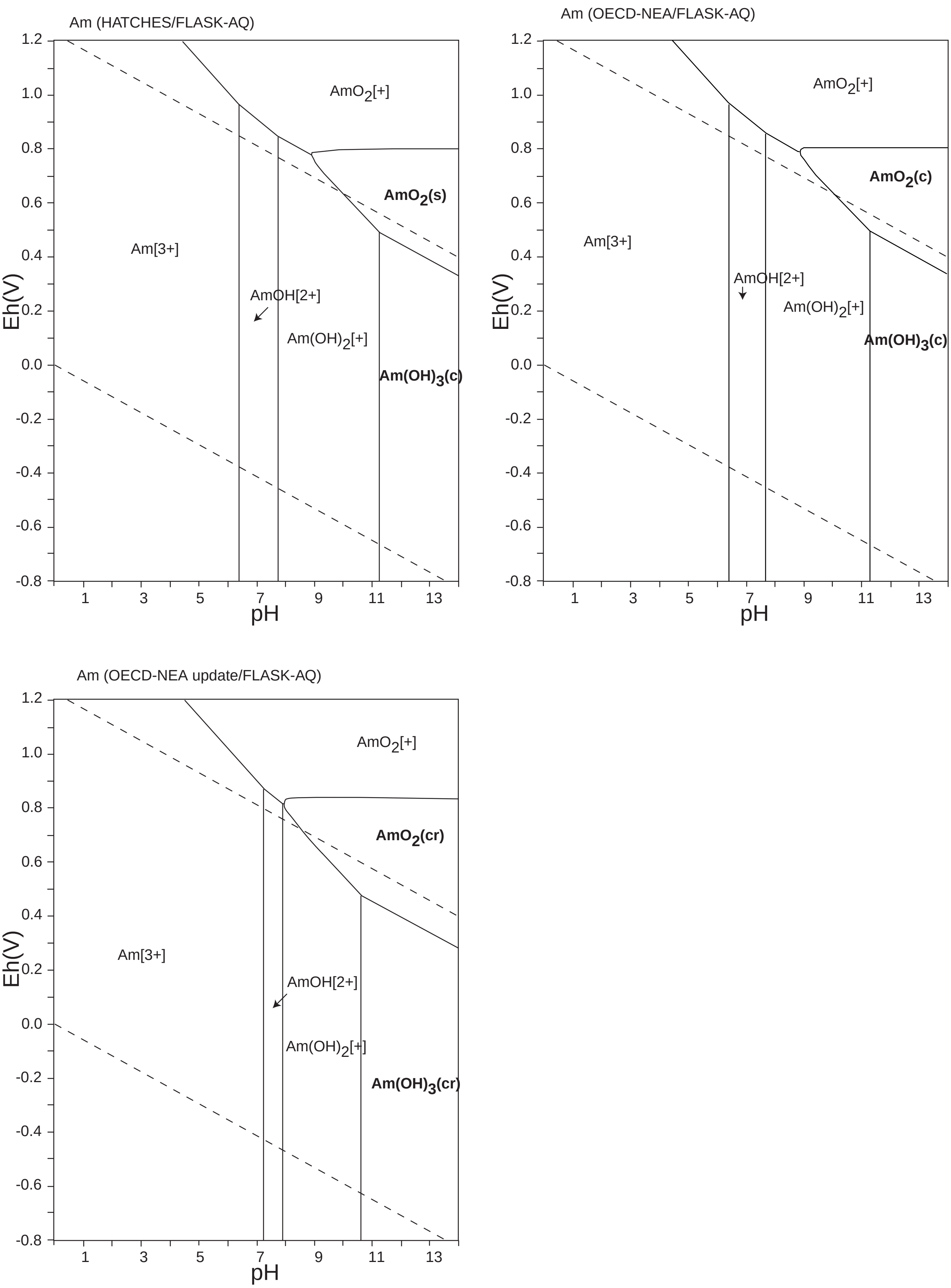

Figure 10: Eh-pH diagrams of the system Am-O-H (2). $\sum \mathrm{Am} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 6: List of As species

FACT	SUPCRT	LLNL	JNC-TDB
AsO_2[-], AsO_4[3-], $HAsO_2$(aq), H_2AsO_3[-], H_2AsO_4[2-], H_2AsO_4[-], H_3AsO_4(aq), AsO[+], **As(s)**, **As_2O_3(s)**, **As_2O_3(s2)**, **As_2O_5(s)**,	AsO_2[-], AsO_4[3-], $HAsO_2$(aq), H_2AsO_3[-], $HAsO_4$[2-], H_2AsO_4[-], H_3AsO_4(aq)	$As(OH)_4$[-], AsH_3(aq), AsO_4[3-], $As(OH)_3$(aq), AsO_2OH[2-], H_2AsO_4[-], H_3AsO_4(aq), $HAsO_4$[2-] **Arsenolite**, **As_2O_5(c)**, **Claudetite**	

HATCHES			
$As(OH)_4$[-], H_2AsO_4[-], $As(OH)_3$(aq), AsO[+], AsO_4[3-], H_3AsO_4(aq), $HAsO_2$(aq), $HAsO_4$[2-], **Arsenolite**, **As_2O_5(c)**, **As_4O_6**, **Claudetite**			

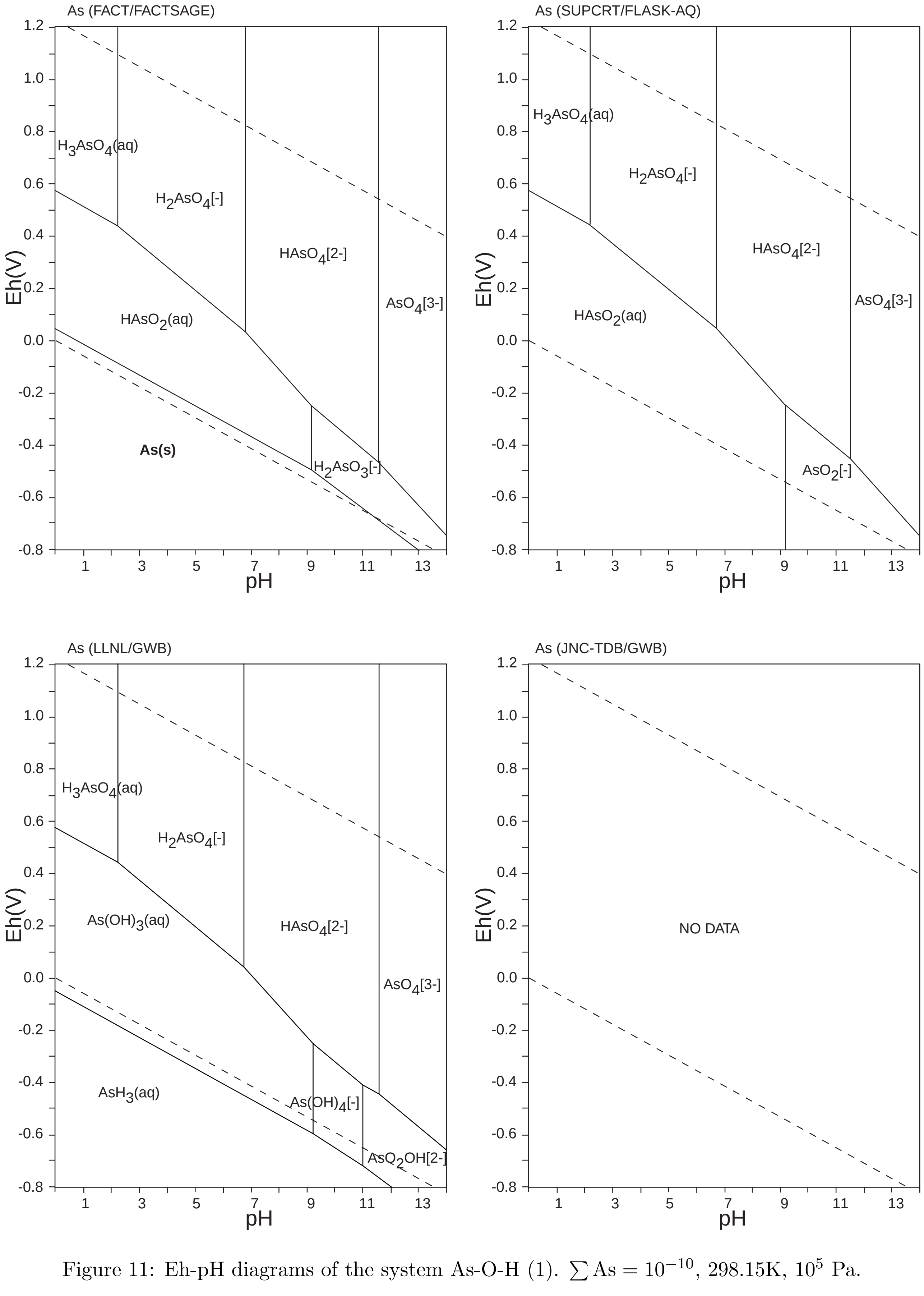

Figure 11: Eh-pH diagrams of the system As-O-H (1). $\sum \text{As} = 10^{-10}$, 298.15K, 10^5 Pa.

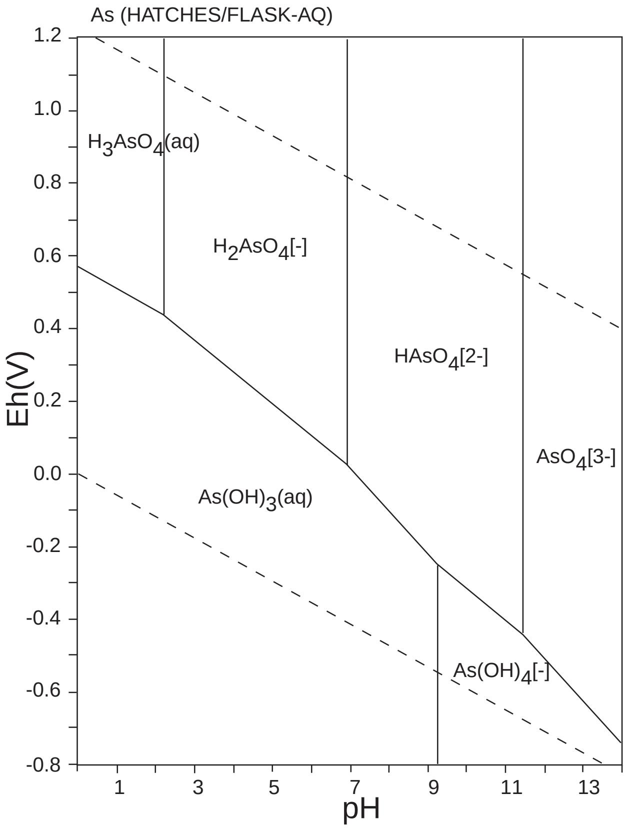

Figure 12: Eh-pH diagrams of the system As-O-H (2). $\sum \text{As} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 7: List of Au species

FACT	SUPCRT	LLNL	JNC-TDB
AuO_3[3-], $HAuO_3$[2-], H_2AuO_3[-], $Au(OH)_3$(aq), **Au_2O_3(s)**, **$Au(OH)_3$(s)**, **Au(s)**	Au[3+], Au[+], **Au(Native gold)**	Au[+], Au[3+], **Gold**	

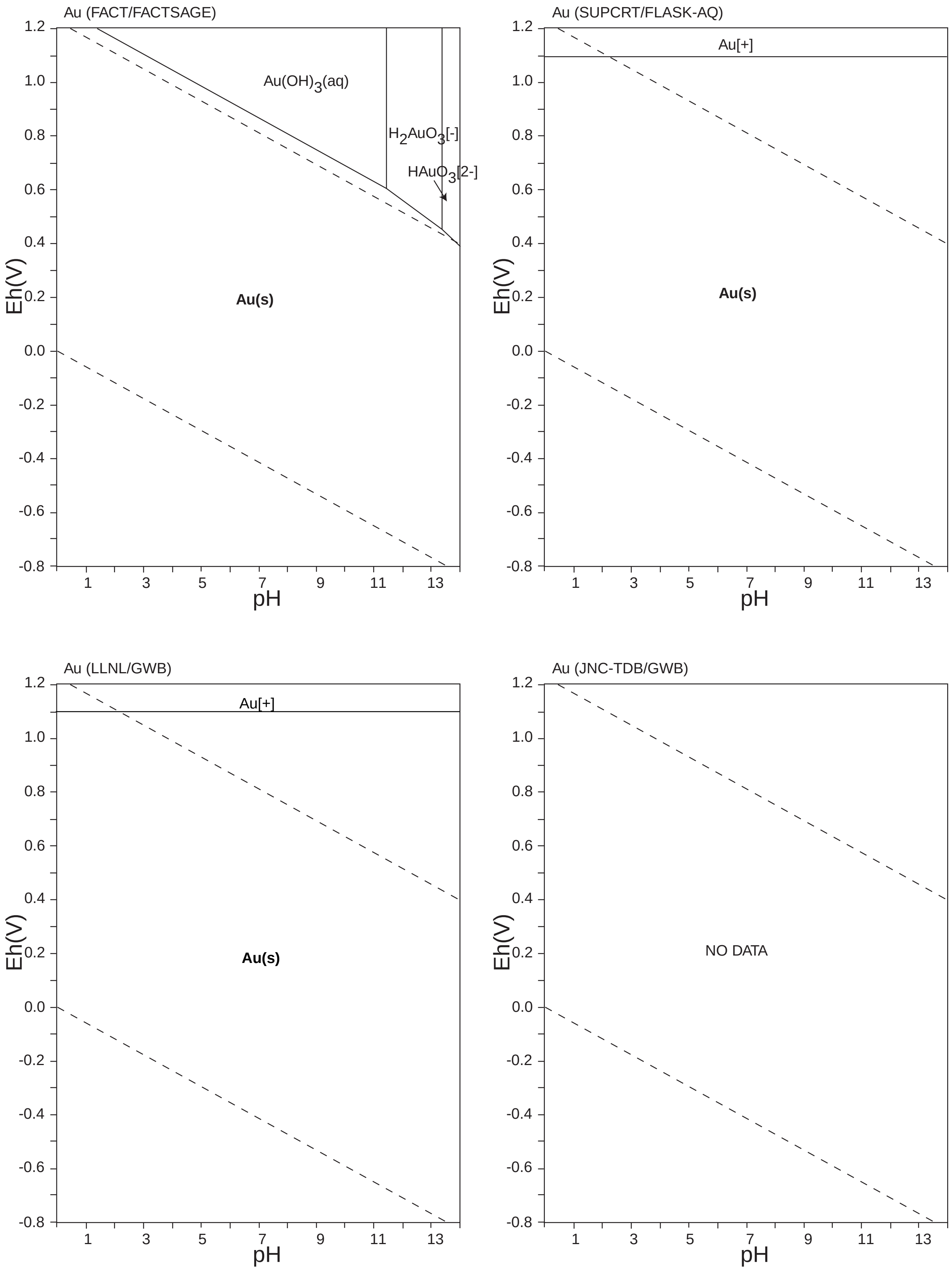

Figure 13: Eh-pH diagrams of the system Au-O-H. $\sum \mathrm{Au} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 8: List of B species

FACT	SUPCRT	LLNL	JNC-TDB
BH_4[-], BO_2[-], B_4O_7[2-], H_2BO_3[-], H_3BO_3(aq), $H_2BO_3(H_2O_2)$[-], HB_4O_7[-], $H_2B_4O_7$(aq), $H_5(BO_3)_2(H_2O_2)_2$[-], **B(s), $B_{10}H_{14}$(s), B_2O_3(s), HBO_2(s), HBO_2(s2), HBO_2(s3), H_3BO_3(s), $B_3H_3O_3$(s), $B_2(OH)_4$(s)**	BO_2[-], $B(OH)_3$(aq)	$B(OH)_3$(aq), $B(OH)_4$[-], $B_2O(OH)_5$[-], $B_3O_3(OH)_4$[-], $B_4O_5(OH)_4$[2-], BH_4[-], **$B(OH)_3$(c,Boric acid)**	$B(OH)_3$(aq), H_2BO_3[-], **B(c), B_2O_3(c), $B(OH)_3$(c)**, B(g)

HATCHES			
$B(OH)_3$(aq), B_4O_7[2-], BH[4-], $H_2B_4O_7$(aq), H_2BO_3[-], HB_4O_7[-], **B_2O_3, Boric Acid, H_3BO_3(c), HBO_2**			

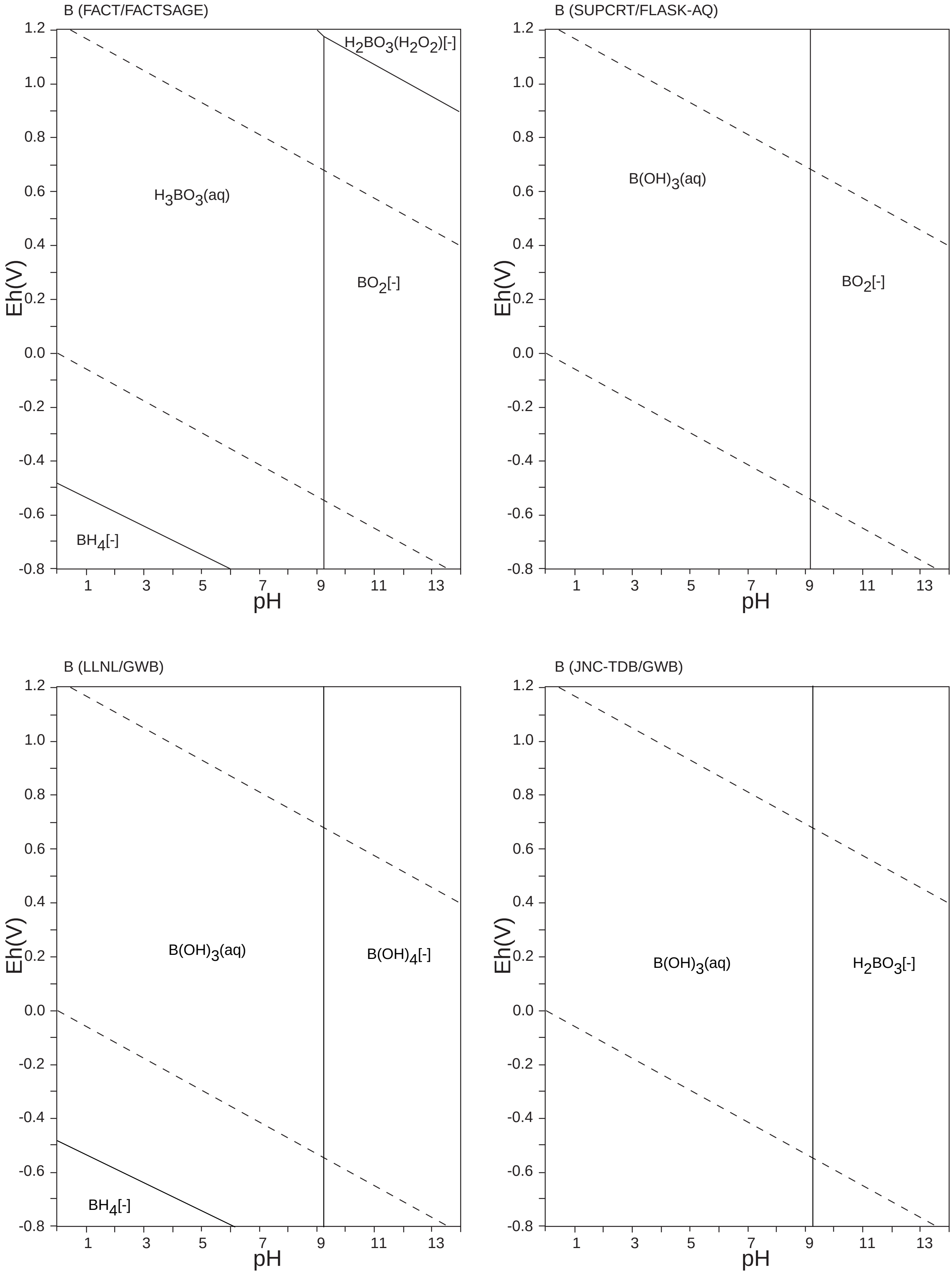

Figure 14: Eh-pH diagrams of the system B-O-H (1). $\sum B = 10^{-10}$, 298.15K, 10^5 Pa.

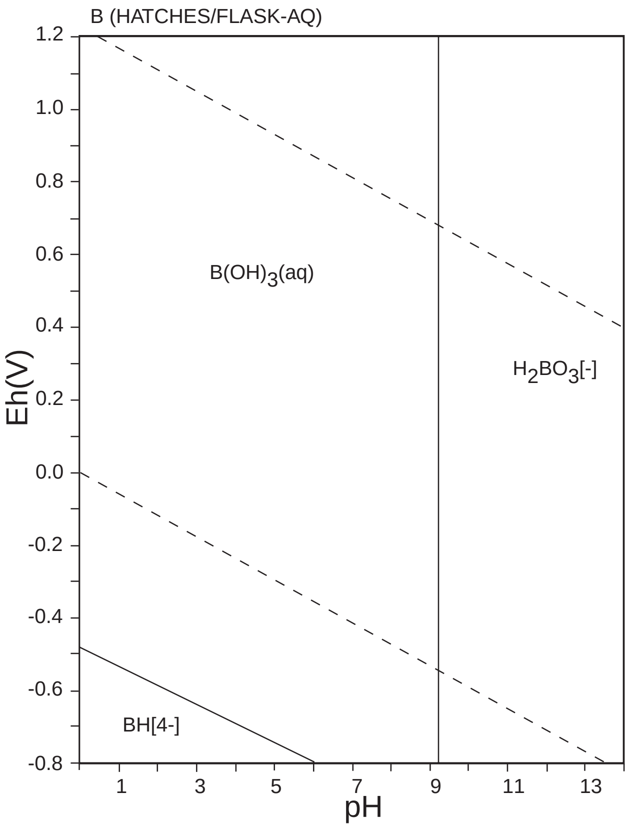

Figure 15: Eh-pH diagrams of the system B-O-H (2). $\sum \mathrm{B} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 9: List of Ba species

FACT	SUPCRT	LLNL	JNC-TDB
Ba[2+], BaOH[+], **Ba(s)**, **BaH_2(s)**, **BaO(s)**, **BaO_2(s)**, **$Ba(OH)_2$(s)**, **$Ba(OH)_2(H_2O)_8$(s)**	Ba[2+], BaOH[+]	Ba[2+], BaOH[+], **$Ba(OH)_2$*$8H_2O$(c)**, **BaO(c)**	Ba[2+], BaOH[+], **Ba(c), BaO(c)**

HATCHES			
Ba[2+], Ba(OH)[+], **$Ba(OH)_2$*$8H_2O$, BaO(c)**			

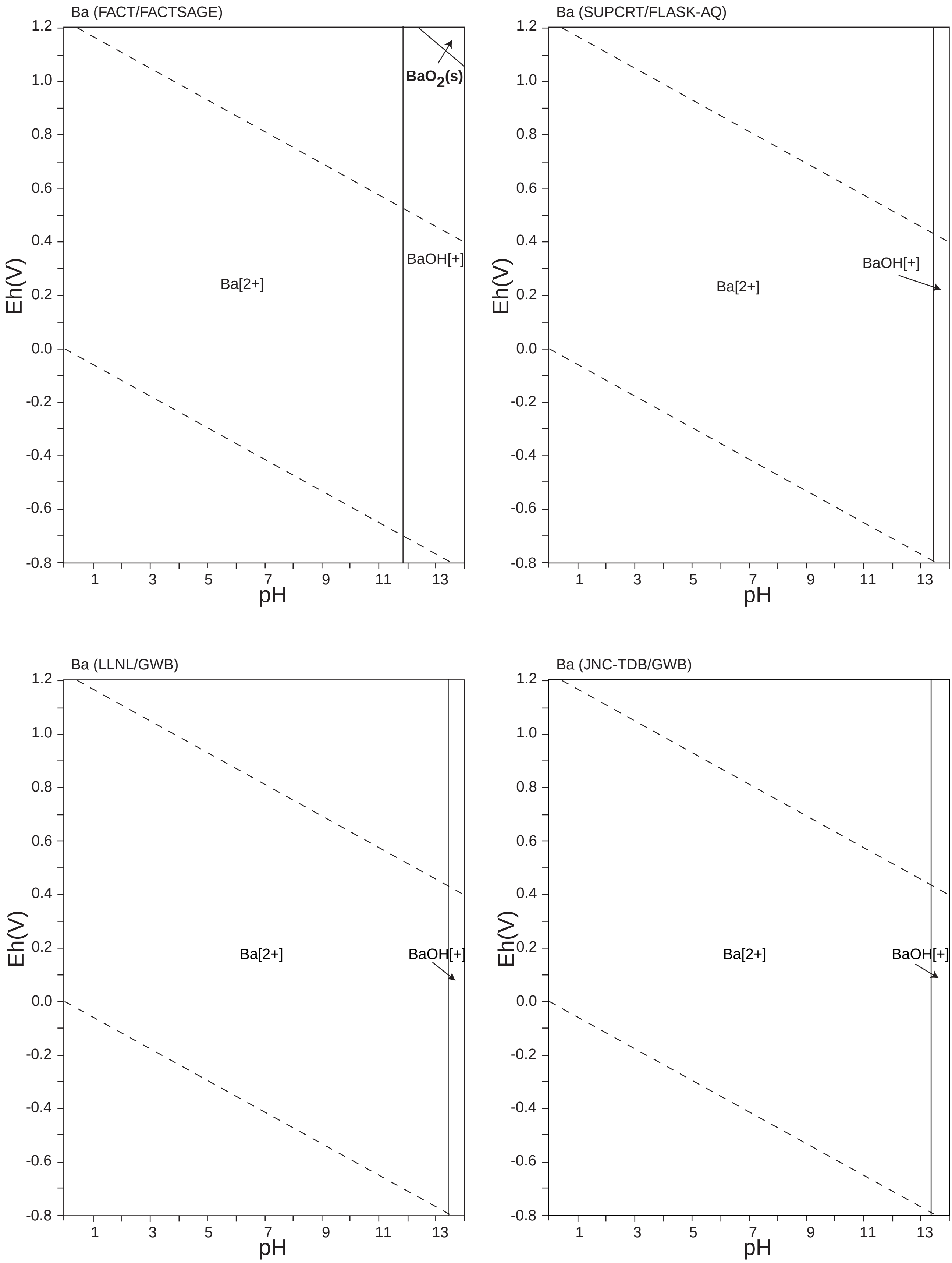

Figure 16: Eh-pH diagrams of the system Ba-O-H (1). $\sum \mathrm{Ba} = 10^{-10}$, 298.15K, 10^5 Pa.

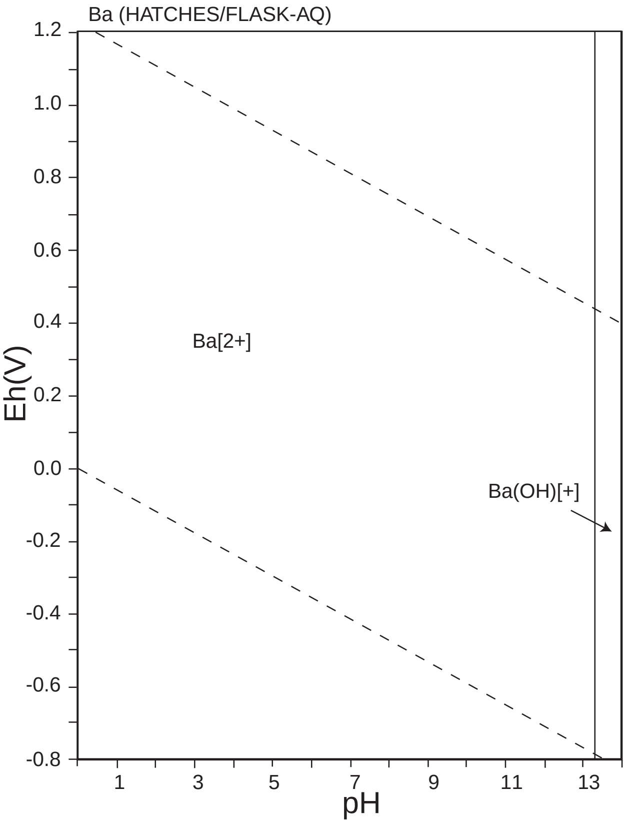

Figure 17: Eh-pH diagrams of the system Ba-O-H (2). $\sum \mathrm{Ba} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 10: List of Be species

FACT	SUPCRT	LLNL	JNC-TDB
Be[2+], BeO_2[2-], $Be_3(OH)_3$[3+], **Be(s)**, **Be(s2)**, **BeO(s)**, **BeO(s2)**, **$Be(OH)_2$(s)**, **$Be(OH)_2$(s2)**	Be[2+], BeO_2[2-], BeOH[+], BeO(aq), $HBeO_2$[-]		

HATCHES			
Be[2+], BeOH[+], $Be(OH)_2$(aq), $Be(OH)_3$[-], $Be(OH)_4$[2-], $Be_2(OH)$[3+], Be_3(OH)3[3+], $Be_5(OH)_6$[4+], $Be_6(OH)_8$[4+], **$Be(OH)_2$(alpha)**, **$Be(OH)_2$(beta)**			

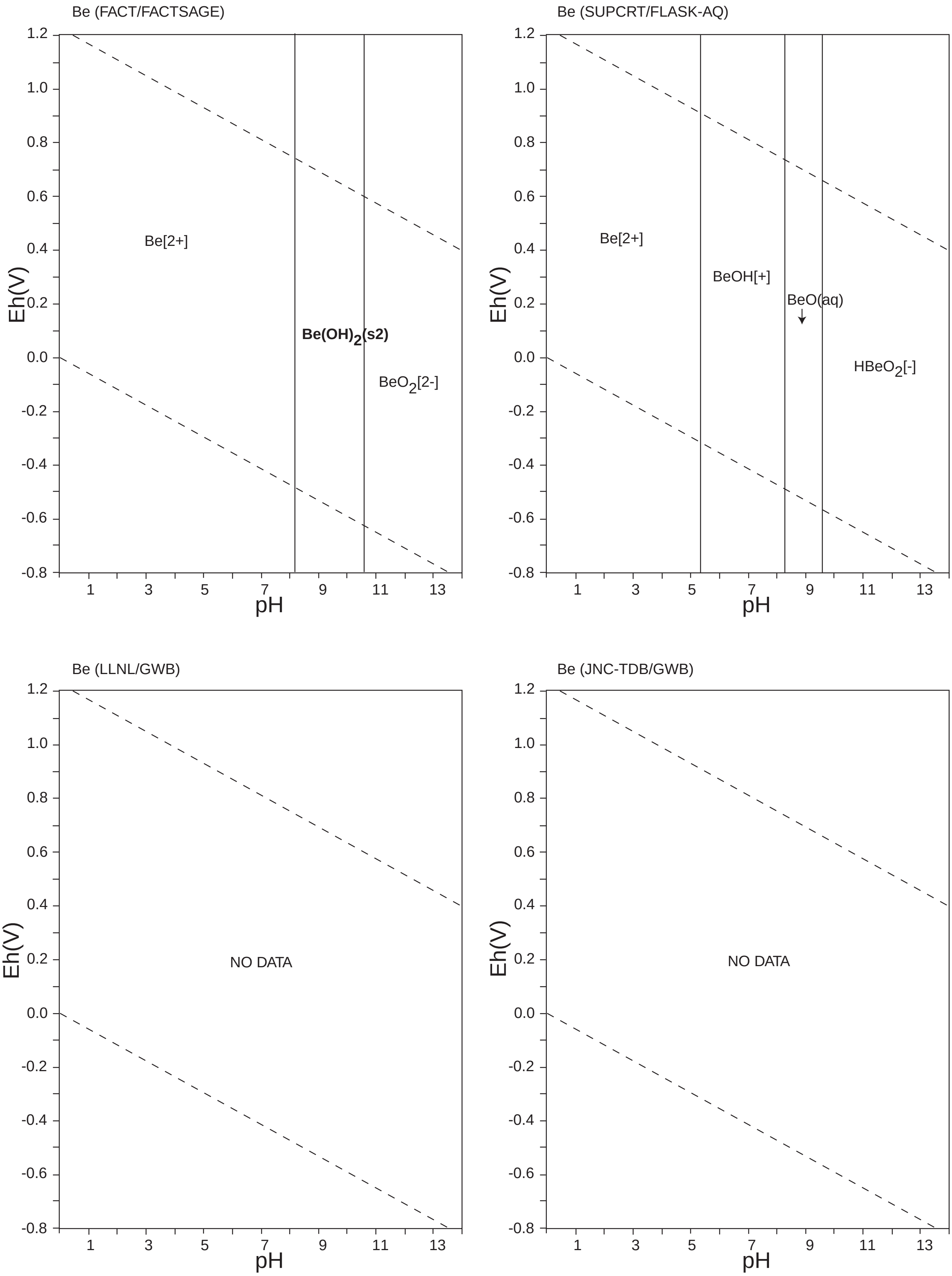

Figure 18: Eh-pH diagrams of the system Be-O-H (1). $\sum \mathrm{Be} = 10^{-10}$, 298.15K, 10^5 Pa.

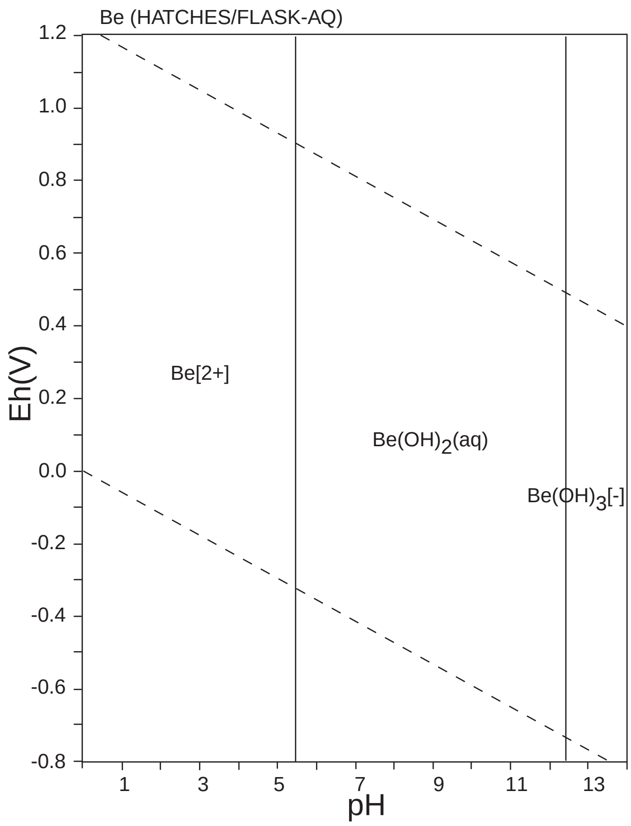

Figure 19: Eh-pH diagrams of the system Be-O-H (2). $\sum \mathrm{Be} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 11: List of Bi species

FACT	SUPCRT	LLNL	JNC-TDB
$Bi[3+]$, $BiO[+]$, $BiOH[2+]$, $Bi_6O_6[6+]$, $Bi_6O_6(OH)_3[3+]$, $Bi_9(OH)_{20}[7+]$, $Bi_9(OH)_{21}[6+]$, $Bi_9(OH)_{22}[5+]$, **Bi(s)**, **Bi_2O_3(s)**, **Bi_2O_3(s2)**, **BiOOH(s)**	$Bi[3+]$, $BiO[+]$, $BiOH[2+]$, $HBiO_2(aq)$, $BiO_2[-]$		$Bi[3+]$, $BiOH[2+]$, $Bi(OH)_2[+]$, $Bi(OH)_3(aq)$, $Bi(OH)_4[-]$, $Bi_6(OH)_{12}[6+]$, $Bi_9(OH)_{20}[7+]$, $Bi_9(OH)_{21}[6+]$, $Bi_9(OH)_{22}[5+]$, $Bi_3(OH)_4[5+]$ **Bi(c)**, **Bi_2O_3(s)**

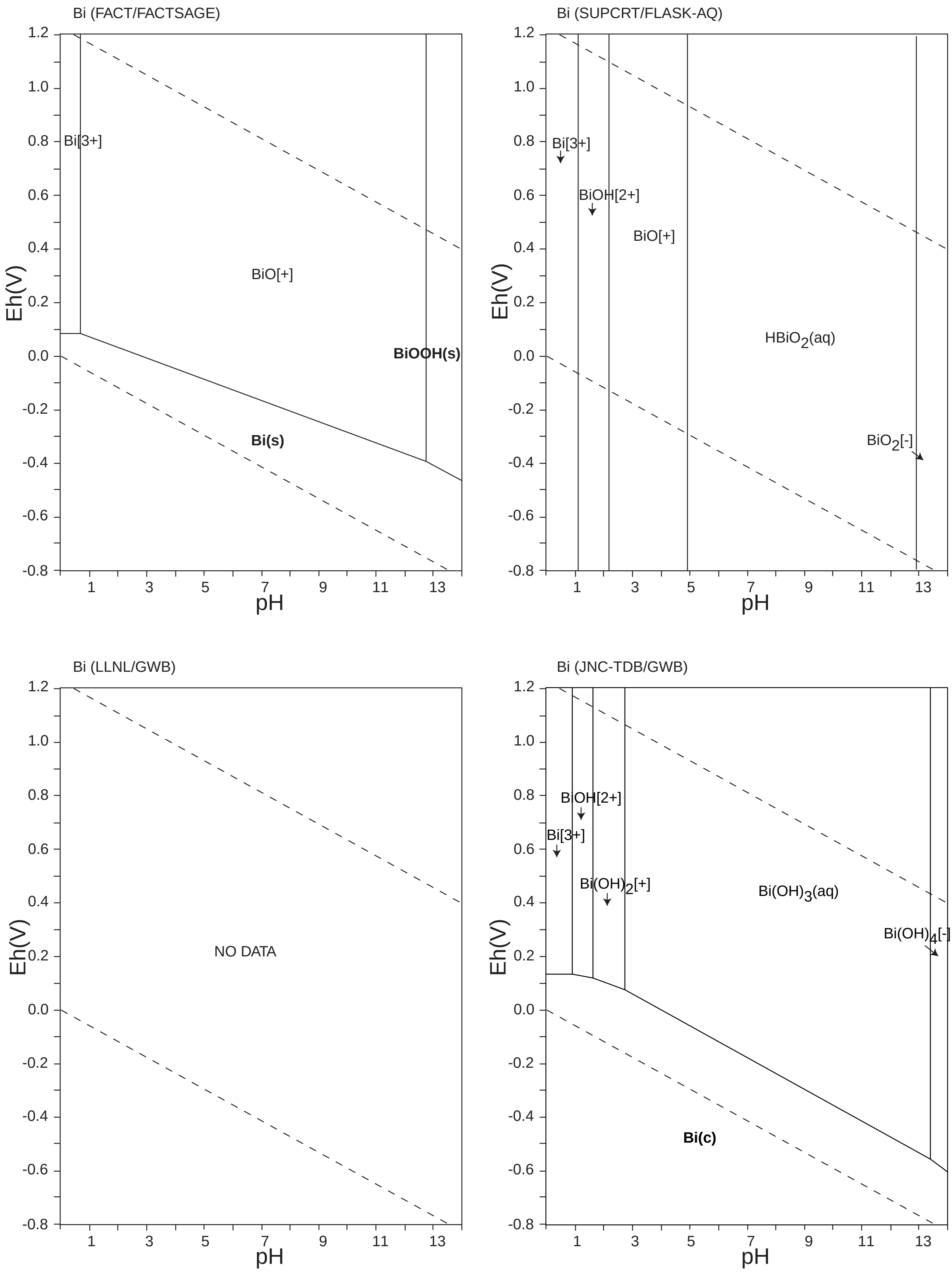

Figure 20: Eh-pH diagrams of the system Bi-O-H. $\sum \mathrm{Bi} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 12: List of Br species

FACT	SUPCRT	LLNL	JNC-TDB
Br[-], Br_2(aq), Br_3[-], Br_5[-], BrO[-], BrO_3[-], HBrO(aq)	Br[-], Br_3[-], BrO[-], BrO_3[-], HBrO(aq), BrO_4[-]	Br[-]	Br[-], Br_2(aq), Br_2(l), BrO[-], BrO_3[-], HBrO(aq), Br(g), Br_2(g), HBr(g)

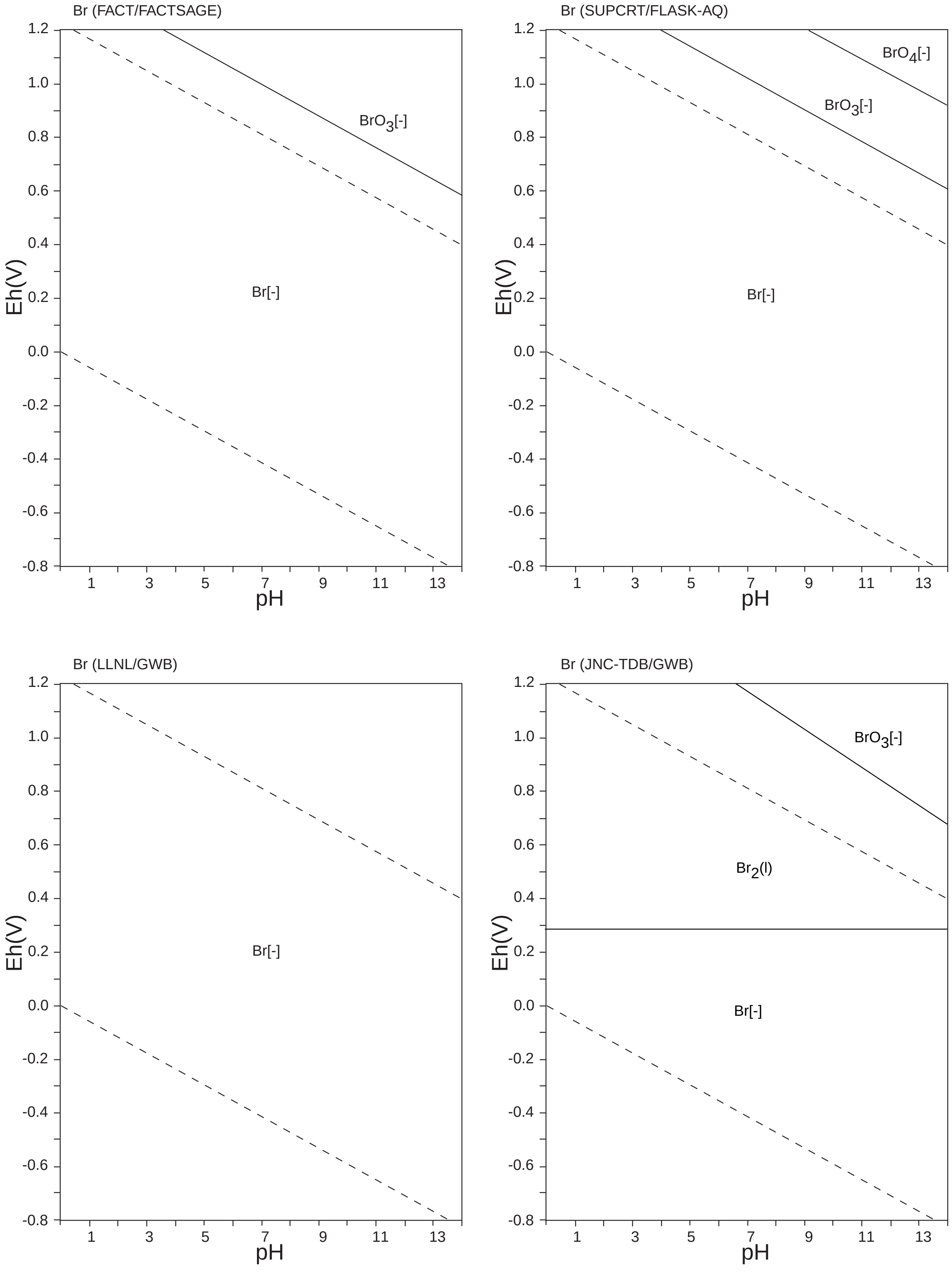

Figure 21: Eh-pH diagrams of the system Br-O-H. $\sum \mathrm{Br} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 13: List of C species (1)

FACT	SUPCRT	LLNL	JNC-TDB
CH_4(aq), C_2H_2(aq), C_2H_4(aq), C_2H_6(aq), CO(aq), CO_2(aq), CO_3[2-], C_2O_4[2-], CH_3OH(aq), C_2H_5O[-], CH_3CH_2OH(aq), HCOO[-], HCOOH(aq), CH_3COO[-], CH_3COOH(aq), HCO_3[-], HC_2O_4[-], **C(s)**, **C(s2)**	CH_4(aq,Methan), C_2H_2 (aq,Ethyne), C_2H_4(aq,Ethylene), C_2H_6(aq,Ethane), CO(aq), CO_2(aq), CO_3[2-], C_2O_4[2-] (Oxalate), CH_3OH(aq,Methanol), C_2H_5OH(aq,Ethanol), HCO_2[-](Formate), H_2CO_2(aq, Formic-acid), $C_2H_3O_2$[-] (Acetate), $C_2H_4O_2$(aq,Acetic-acid), HCO_3[-], C_2HO_4[-](H-Oxalate), C_4H_9OH (aq,1-Butanol), C_4H_8(aq,1-Butene), C_4H_6(aq,1-Butyne), $C_7H_{15}OH$ (aq,1-Heptanol), C_7H_{14}(aq,1-Heptene), C_7H_{12}(aq,1-Heptyne), $C_6H_{13}OH$(aq,1-Hexanol), C_6H_{12}(aq, 1-Hexene), C_6H_{10}(aq, 1-Hexyne), $C_8H_{17}OH$(aq,1-Octanol), C_8H_{16}(aq, 1-Octene), C_8H_{14}(aq, 1-Octyne), $C_5H_{11}OH$(aq,1-Pentanol), C_5H_{10}(aq, 1-Pentene), C_5H_8(aq, 1-Pentyne), C_3H_7OH(aq,1-Propanol), C_3H_6 (aq, 1-Propene), C_3H_4(aq, 1-Propyne), C_4H_8O(aq,2-Butanone), $C_7H_{14}O$ (aq,2-Heptanone), $C_6H_{12}O$(aq,2-Hexanone), $C_4H_7O_3$[-](2-Hydroxybutanoate), $C_4H_8O_3$(aq,2-Hydroxybutanoic), $C_{10}H_{19}O_3$[-] (2-Hydroxydecanoate), $C_{10}H_{20}O_3$(aq,2-Hydroxydecanoic), $C_7H_{13}O_3$[-](2-Hydroxyheptanoate), $C_7H_{14}O_3$(aq,2-Hydroxyheptanoic), $C_6H_{11}O_3$[-](2-Hydroxyhexanoate), $C_6H_{12}O_3$(aq,2-Hydroxyhexanoic), $C_9H_{17}O_3$[-](2-Hydroxynonanoate), $C_9H_{18}O_3$(aq,2-Hydroxynonanoic),	HCO_3[-], (O-phth)[2-], CH_3COO[-], CH_4(aq), CO_2(aq), CO_3[2-], H(O-phth)[-], H_2(O-phth), HCH_3COO, **Graphite**, **O-phth acid(c)**, CH_4(g), CO_2(g)	CO_3[2-], CH_4(aq), HCO_3[-], CO_2(aq), **C(c)**, CH_4(g), C(g), CO(g), CO_2(g)

Table 14: List of C species (2)

C (CONTINUED)

FACT	SUPCRT	LLNL	JNC-TDB
	$C_8H_{15}O_3$[-](2-Hydroxyoctanoate), $C_8H_{16}O_3$(aq,2-Hydroxyoctanoic), $C_5H_9O_3$[-](2-Hydroxypentanoate), $C_5H_{10}O_3$(aq,2-Hydroxypentanoic), $C_8H_{16}O$(aq,2-Octanone), $C_5H_{10}O$(aq,2-Pentanone), C_3H_6O (aq,Acetone), $C_6H_8O_4$[2-] (Adipate), $C_6H_{10}O_4$ (aq,Adipic-acid), $C_9H_{16}O_4$ (aq,Azelaic-acid), $C_9H_{14}O_4$[2-] (Azelate), C_6H_6(aq, Benzene), $C_7H_5O_2$[-] (Benzoate), $C_7H_6O_2$(aq,Benzoic-acid), C_4H_{10}(aq, Butane), $C_4H_8O_2$(aq, Butanoic-acid), $C_6H_4OHCH_3$(aq,o-Cresol), $C_6H_4OHCH_3$(aq,m-Cresol), $C_6H_4OHCH_3$(aq,p-Cresol), $C_{10}H_{19}O_2$[-] (Decanoate), $C_{10}H_{20}O_2$(aq,Decanoic-acid), $C_6H_3OHCH_3CH_3$(aq, 2-3DMP), $C_6H_3OHCH_3CH_3$(aq, 2-4DMP), $C_6H_3OHCH_3CH_3$(aq, 2-5DMP), $C_6H_3OHCH_3CH_3$(aq, 2-6DMP), $C_6H_3OHCH_3CH_3$(aq, 3-4DMP), $C_6H_3OHCH_3CH_3$(aq, 3-5DMP), $C_{12}H_{23}O_2$[-] (Dodecanoate), $C_{12}H_{24}O_2$ (aq,Dodecanoic-acid), $CH_3COOCH_2CH_3$(aq, Ethylacetate), $C_6H_5C_2H_5$(aq, Ethylbenzene), $C_5H_6O_4$[2-](Glutarate), $C_5H_8O_4$ (aq,Glutaric-acid), $C_2H_3O_3$[-](Glycolate), $C_2H_4O_3$ (aq,Glycolic-acid), $C_6H_9O_4$[-](H-Adipate), $C_9H_{15}O_4$[-] (H-Azelate),		

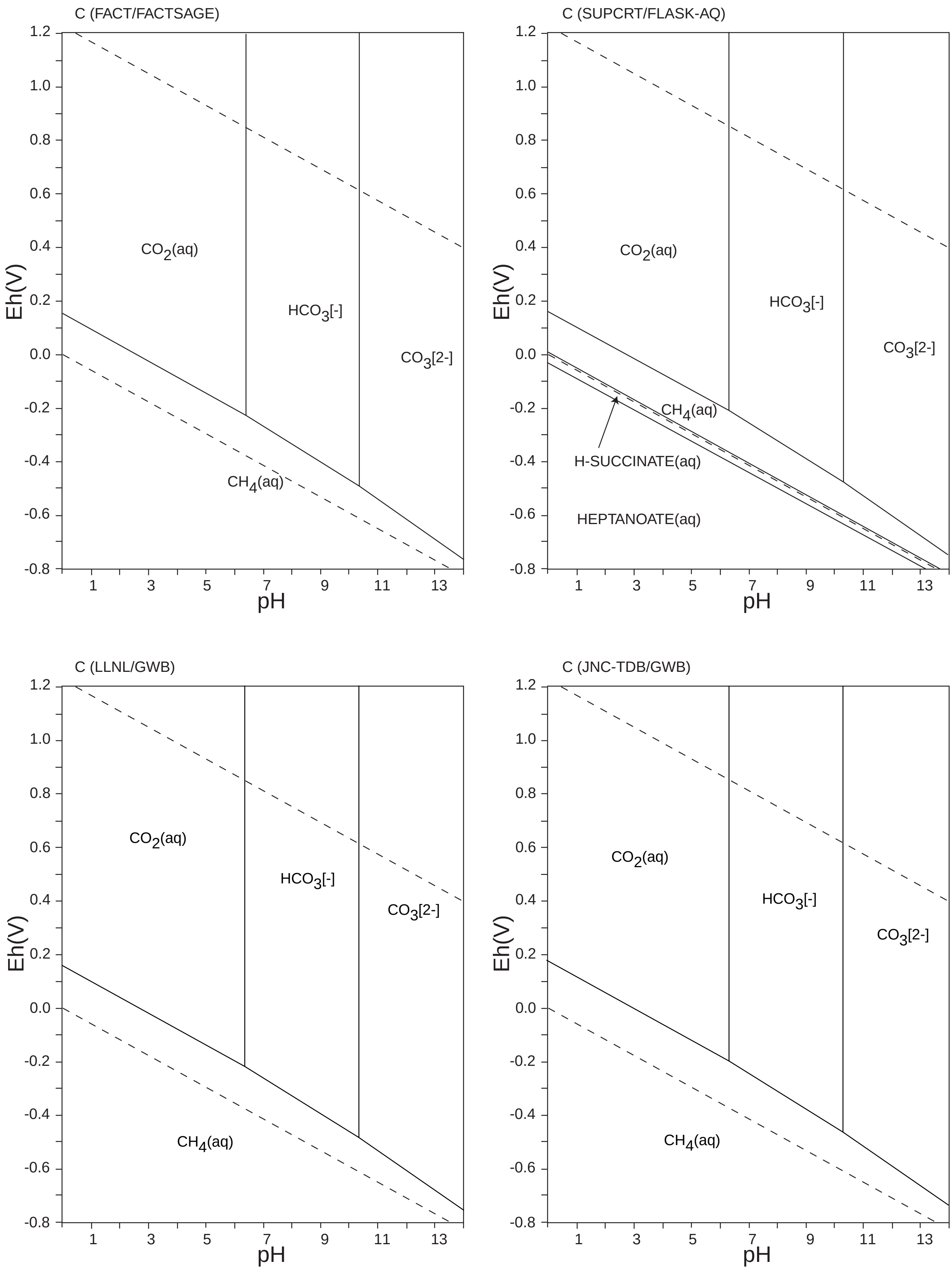

Figure 22: Eh-pH diagrams of the system C-O-H (1). $\sum \mathrm{C} = 10^{-10}$, 298.15K, 10^5 Pa.

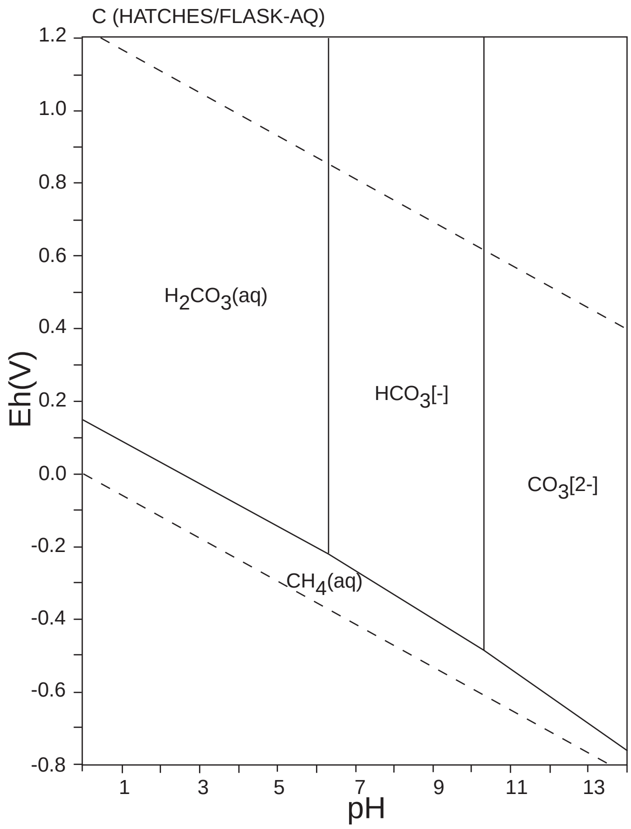

Figure 23: Eh-pH diagrams of the system C-O-H (2). $\sum \mathrm{C} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 15: List of Ca species

FACT	SUPCRT	LLNL	JNC-TDB
Ca[2+], CaOH[+], **Ca(s)**, **Ca(s2)**, **CaH_2(s)**, **CaO_2(s)**, **$Ca(OH)_2$(s)**, **CaO(s)**	Ca[2+], CaOH[+], **CaO(Lime)**	Ca[2+], CaOH[+], **$Ca(OH)_2$(c), Lime, Portlandite**	Ca[2+], CaOH[+], **CaO(s, Lime_qu), Ca(c), CaO(c)**, Ca(g)

HATCHES			
Ca[2+], Ca(OH)[+], **$Ca(OH)_2$, CaO**			

Remarks

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

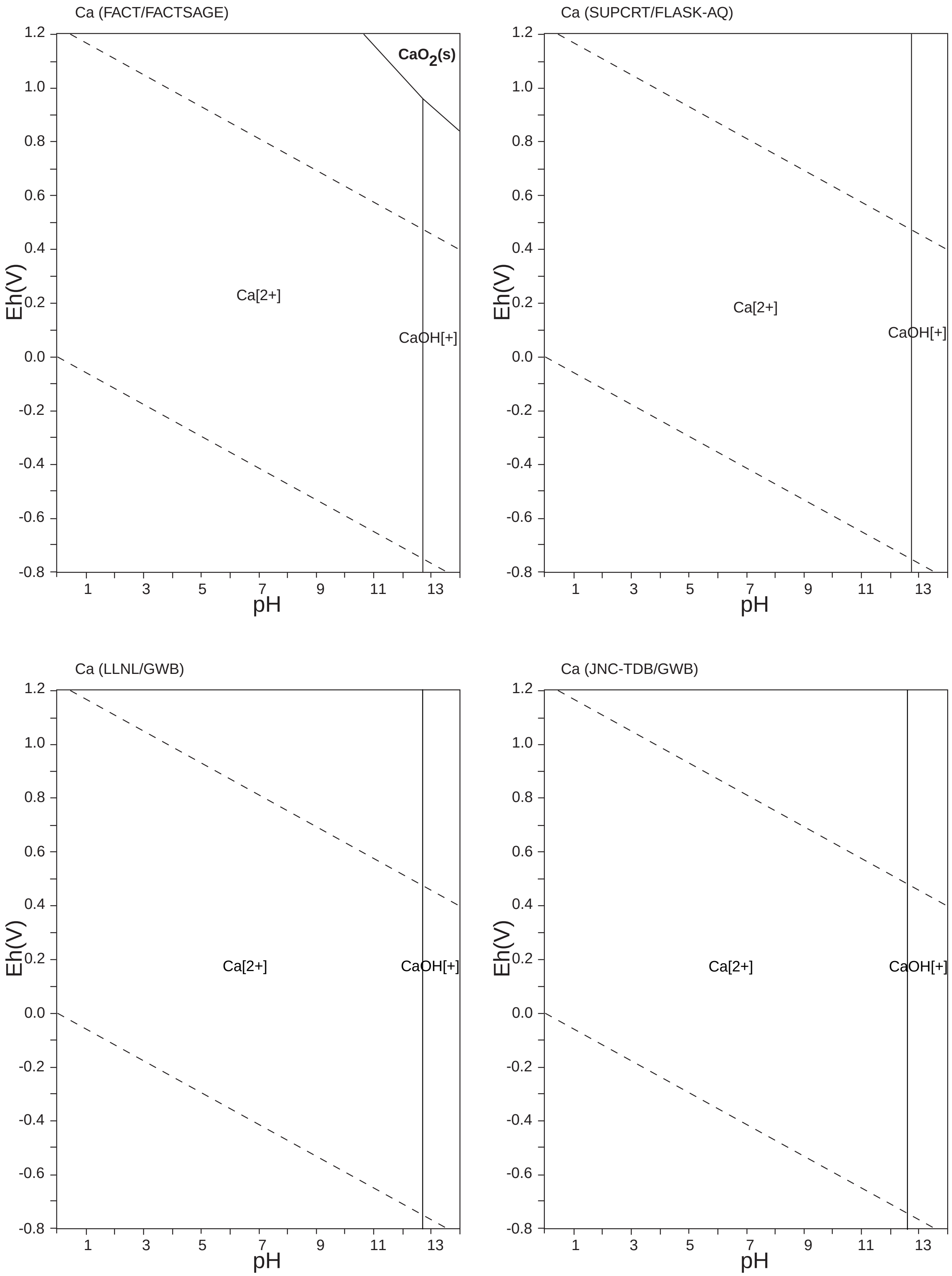

Figure 24: Eh-pH diagrams of the system Ca-O-H (1). $\sum \mathrm{Ca} = 10^{-10}$, 298.15K, 10^5 Pa.

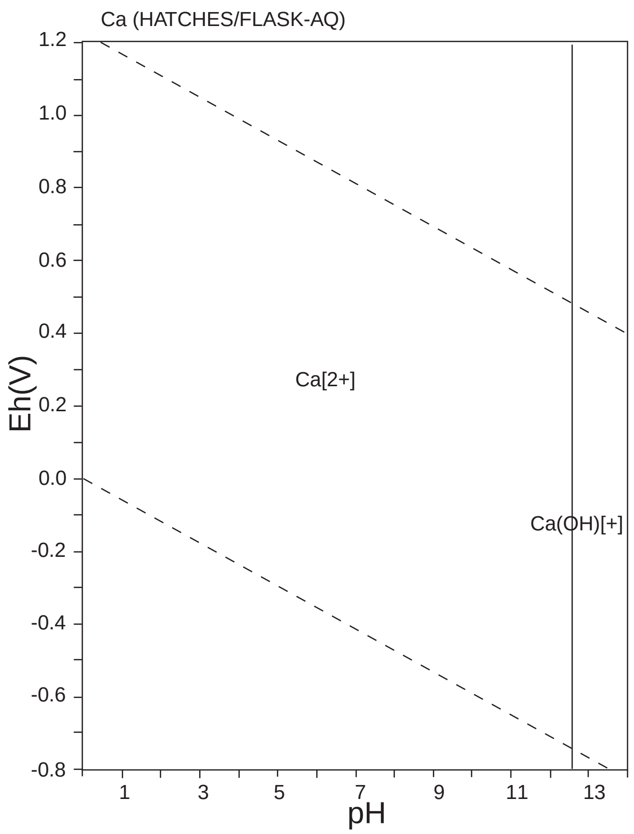

Figure 25: Eh-pH diagrams of the system Ca-O-H (2). $\sum \mathrm{Ca} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 16: List of Cd species

FACT	SUPCRT	LLNL	JNC-TDB
Cd[2+], CdO_2[2-], CdOH[+], $HCdO_2$[-], $Cd(OH)_2$(aq), **Cd(s)**, **CdO(s)**, **$Cd(OH)_2$(s)**	Cd[2+], CdO_2[2-], CdOH[+], $HCdO_2$[-], CdO(aq)		

HATCHES			
Cd[2+], $Cd(OH)_2$(aq), $Cd(OH)_3$[-], $Cd(OH)_4$[2-], Cd_2OH[3+], $Cd_4(OH)_4$[4+], CdOH[+], **$Cd(OH)_2$**			

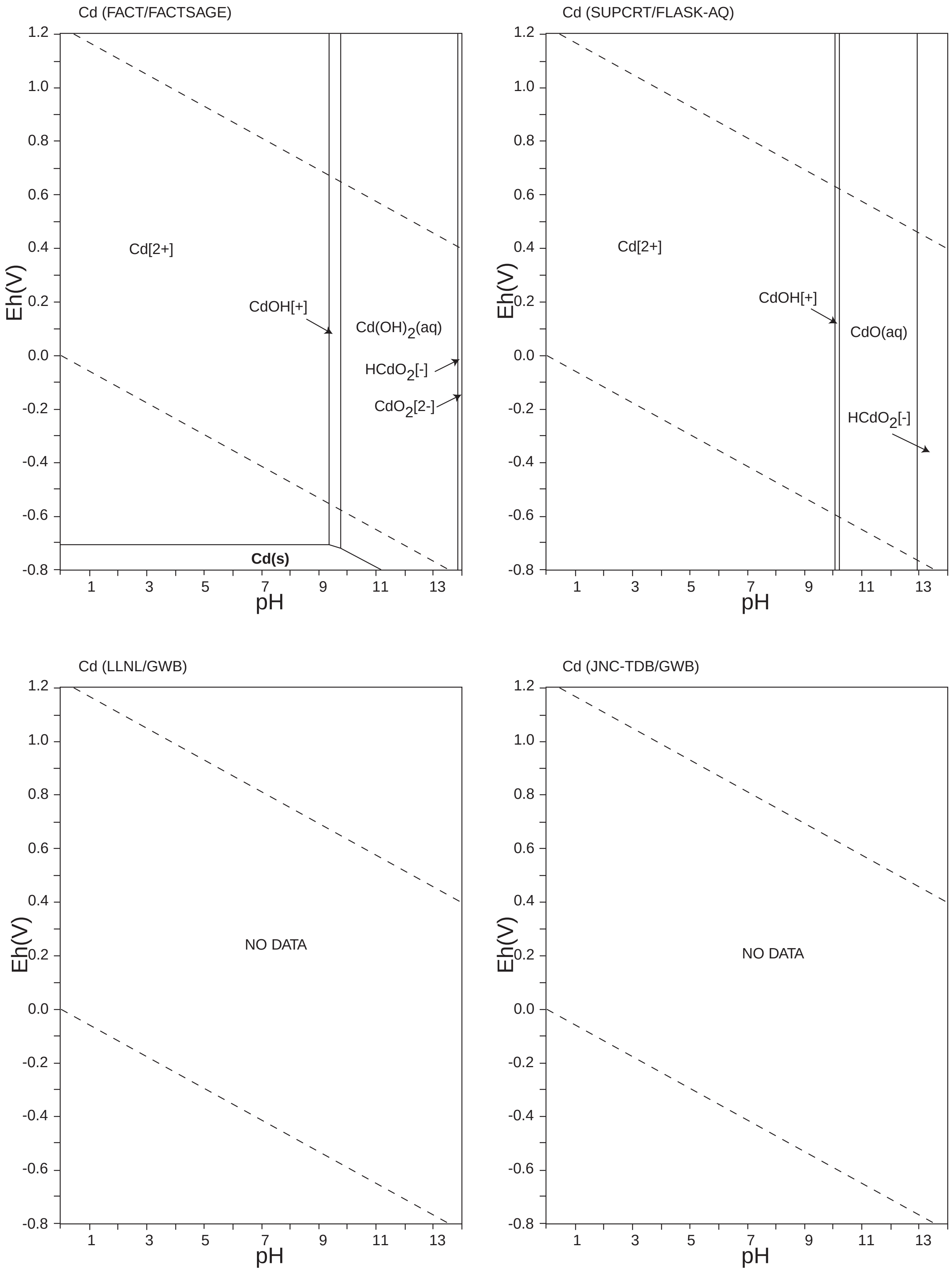

Figure 26: Eh-pH diagrams of the system Cd-O-H (1). $\sum \mathrm{Cd} = 10^{-10}$, 298.15K, 10^5 Pa.

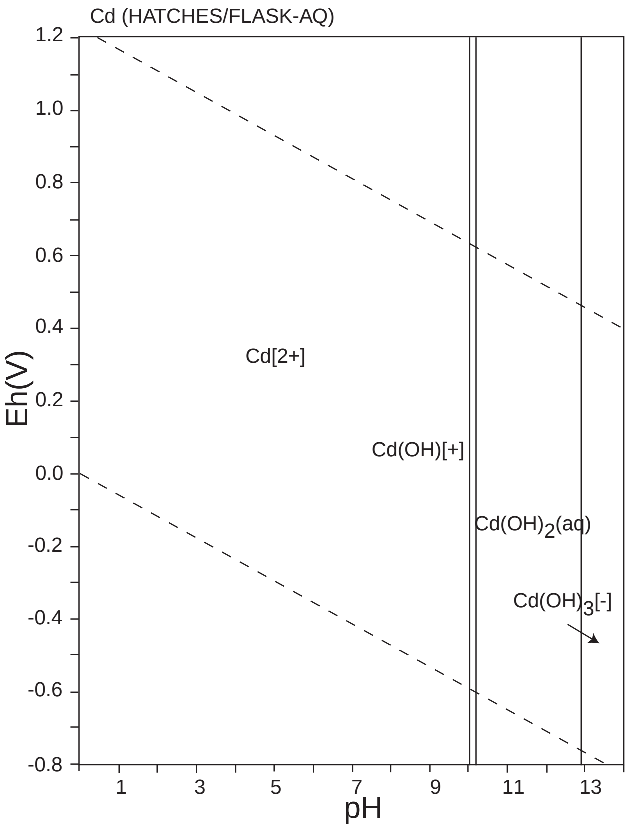

Figure 27: Eh-pH diagrams of the system Cd-O-H (2). $\sum \mathrm{Cd} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 17: List of Ce species

FACT	SUPCRT	LLNL	JNC-TDB
Ce[3+], Ce[4+], **Ce(s)**, **Ce(s2)**, **CeH_2(s)**, **CeO_2(s)**, **Ce_2O_3(s)**, **Ce_6O_{11}(s)**, **$Ce_{18}O_{31}$(s)**	Ce[3+], Ce[4+], Ce[2+], CeOH[2+], CeO[+], CeO_2H (aq), CeO_2[-]		

HATCHES			
Ce[3+], $Ce_2(OH)_2$[4+], $Ce_3(OH)_5$[4+], CeOH[2+], **$Ce(OH)_3$**, **Ce_2O_3**			

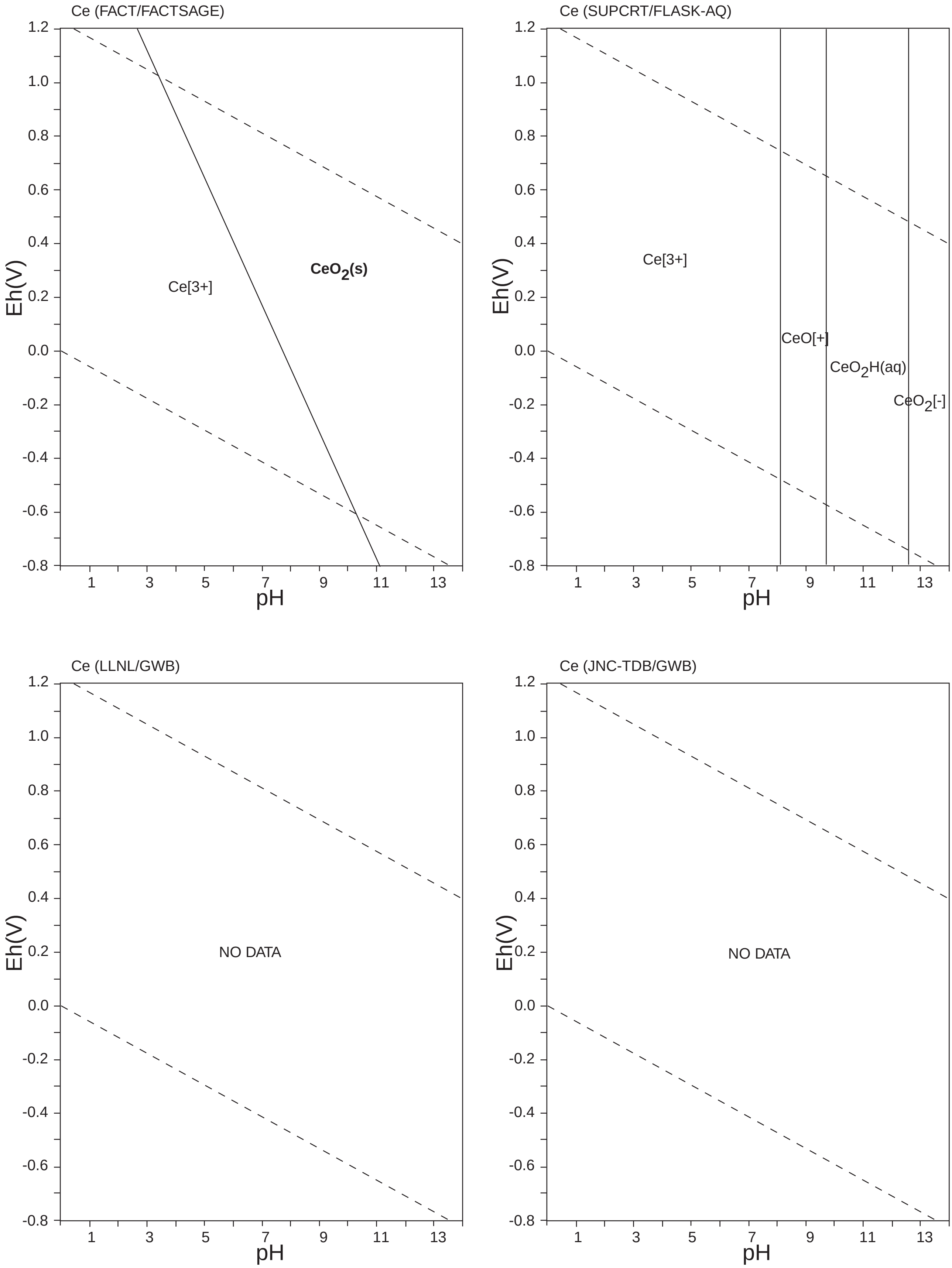

Figure 28: Eh-pH diagrams of the system Ce-O-H (1). $\sum \mathrm{Ce} = 10^{-10}$, 298.15K, 10^5 Pa.

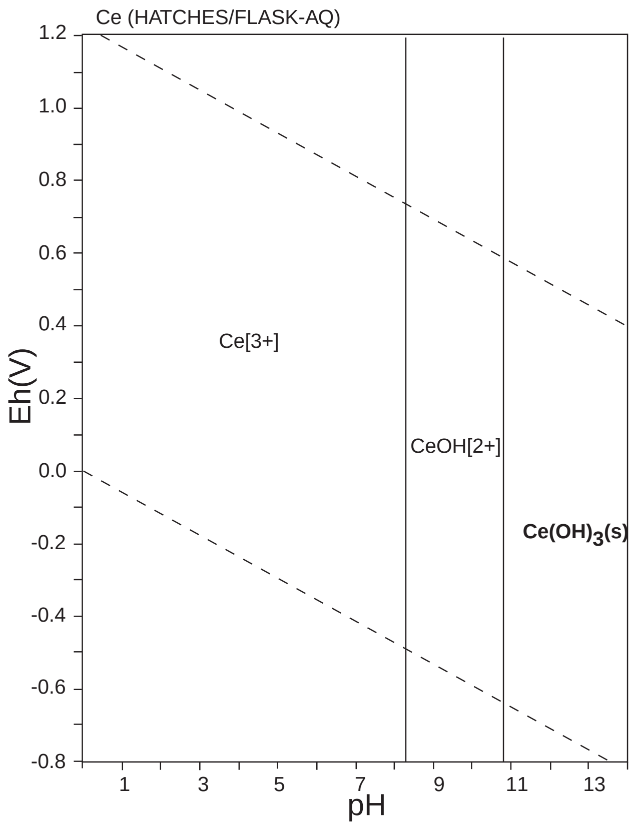

Figure 29: Eh-pH diagrams of the system Ce-O-H (2). $\sum \mathrm{Ce} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 18: List of Cl species

FACT	SUPCRT	LLNL	JNC-TDB
Cl_2(aq), Cl_3[-], ClO_2(aq), Cl[-], ClO[-], ClO_2[-], ClO_3[-], ClO_4[-], HOCl(aq), $HClO_2$(aq)	Cl[-], ClO[-], ClO_2[-], ClO_3[-], ClO_4[-], HClO(aq), $HClO_2$(aq), HCl(aq)	Cl[-], ClO_4[-], HCl(aq)	Cl[-], ClO[-], ClO_2[-], ClO_3[-], ClO_4[-], HClO(aq), $HClO_2$(aq), Cl(g), Cl_2(g), HCl(g)

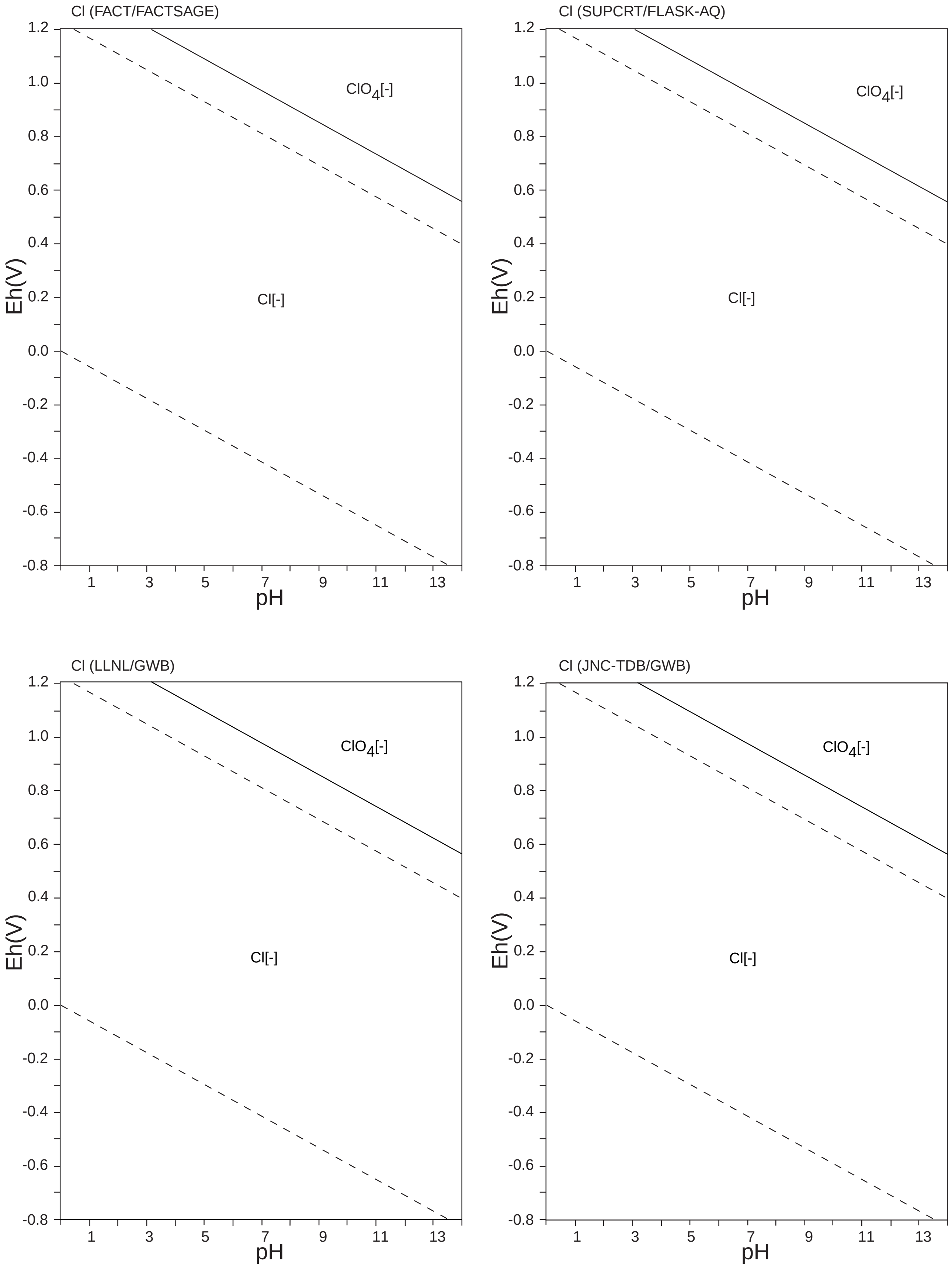

Figure 30: Eh-pH diagrams of the system Cl-O-H. $\sum \mathrm{Cl} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 19: List of Cm species

FACT	SUPCRT	LLNL	JNC-TDB
			Cm^{3+}, $CmOH^{2+}$, $Cm(OH)_2^{+}$, $Cm(OH)_3$(aq), **$Cm(OH)_3$(am)**, **$Cm(OH)_3$(c)**

HATCHES			
Cm^{3+}, Cm^{4+}, $Cm(OH)^{2+}$, $Cm(OH)_2^{+}$, **$Cm(OH)_3$, Cm_2O_3, CmO_2**			

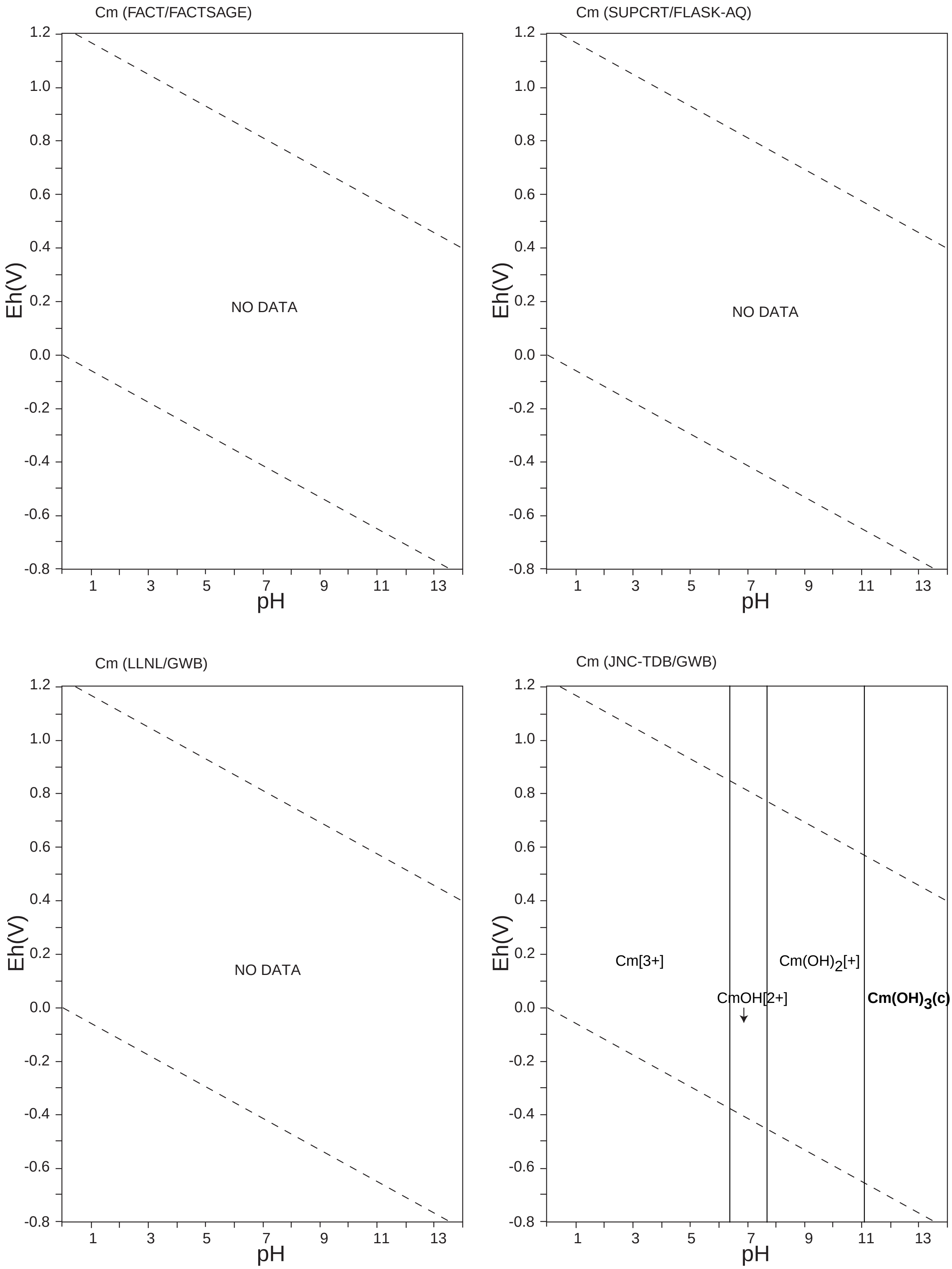

Figure 31: Eh-pH diagrams of the system Cm-O-H (1). $\sum \mathrm{Cm} = 10^{-10}$, 298.15K, 10^5 Pa.

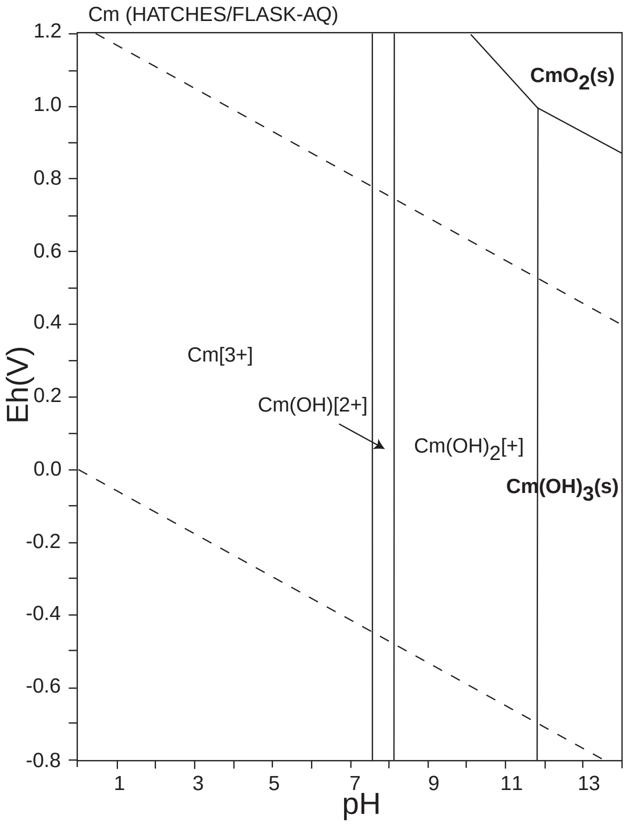

Figure 32: Eh-pH diagrams of the system Cm-O-H (2). $\sum \mathrm{Cm} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 20: List of Co species

FACT	SUPCRT	LLNL	JNC-TDB
Co[2+], Co[3+], $HCoO_2$[-], $Co(OH)_2$(aq), **Co(s)**, **Co(s2)**, **CoO(s)**, **Co_3O_4(s)**, **$Co(OH)_2$(s)**	Co[2+], Co[3+], $HCoO_2$[-], CoO(aq), CoOH[+], CoO2[2-], CoOH[2+]	Co[2+], Co[3+], $Co(OH)_2$(aq), $Co(OH)_3$[-], $Co(OH)_4$[2-], $Co_2(OH)_3$[+], $Co_4(OH)_4$[4+], CoOH[+], $HCoO_2$[-], **$Co(OH)_2$(s,pink)**, **Co_3O_4**, **CoO**	Co[2+], **CoO(s, COBALTO2)**

HATCHES			
Co[2+], Co[3+], $Co(OH)_2$(aq), $Co(OH)_3$[-], $Co(OH)_4$[2-], Co_2OH[3+], $Co_4(OH)_4$[4+], CoOH[+], **$Co(OH)_2$**, **Co_3O_4**, **CoO**			

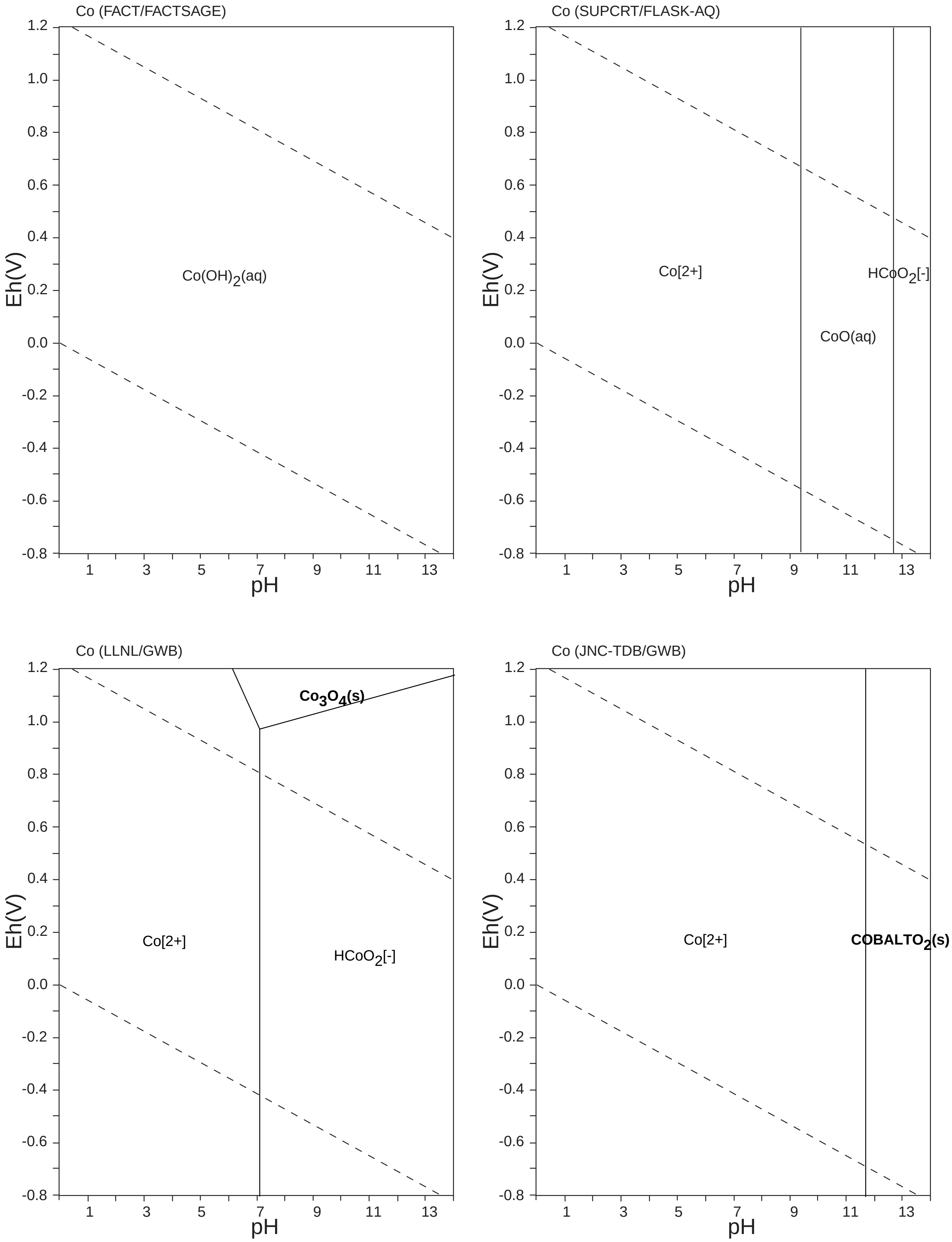

Figure 33: Eh-pH diagrams of the system Co-O-H (1). $\sum \mathrm{Co} = 10^{-10}$, 298.15K, 10^5 Pa.

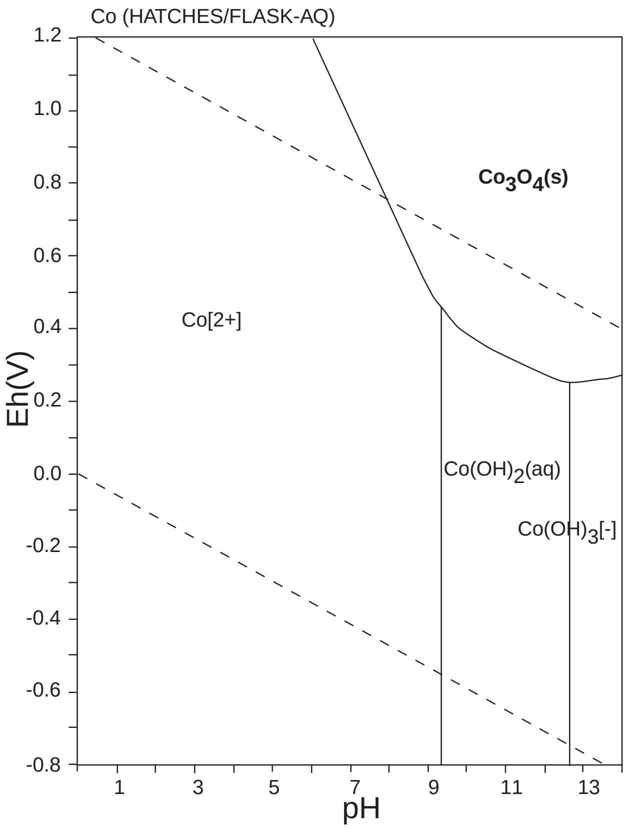

Figure 34: Eh-pH diagrams of the system Co-O-H (2). $\sum \mathrm{Co} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 21: List of Cr species

FACT	SUPCRT	LLNL	JNC-TDB
Cr[2+], Cr[3+], CrO_4[2-], Cr_2O_7[2-], CrOH[2+], $HCrO_4$[-], **Cr(s)**, **CrO_2(s)**, **CrO_3(s)**, **Cr_2O_3(s)**, **Cr_3O_4(s)**, **Cr_5O_{12}(s)**, **Cr_8O_{21}(s)**	Cr[2+], Cr[3+], CrO_4[2-], Cr_2O_7[2-], CrOH[2+], $HCrO_4$[-], $HCrO_2$(aq), CrO_2[-], CrO[+]	Cr[3+], Cr[2+], CrO_4[2-], CrO_4[3-], $Cr(OH)_2$[+], $Cr(OH)_3$(aq), $Cr(OH)_4$[-], $Cr_2(OH)_2$[4+], Cr_2O_7[2-], $Cr_3(OH)_4$[5+], CrOH[2+], H_2CrO_4(aq), $HCrO_4$[-], **Cr_2O_3(s)**, **CrO_2(s)**, **CrO_3(s)**	

HATCHES			
Cr[3+], Cr[2+], CrO_4[2-], $Cr(OH)_2$[+], $Cr(OH)_3$(aq), $Cr(OH)_4$[-], $Cr_2(OH)_2$[4+], Cr_2O_7[2-], $Cr_3(OH)_4$[4+], CrOH[2+], H_2CrO_4(aq), $HCrO_4$[-], **$Cr(OH)_3$**, **Cr_2O_3**, **CrO_2**			

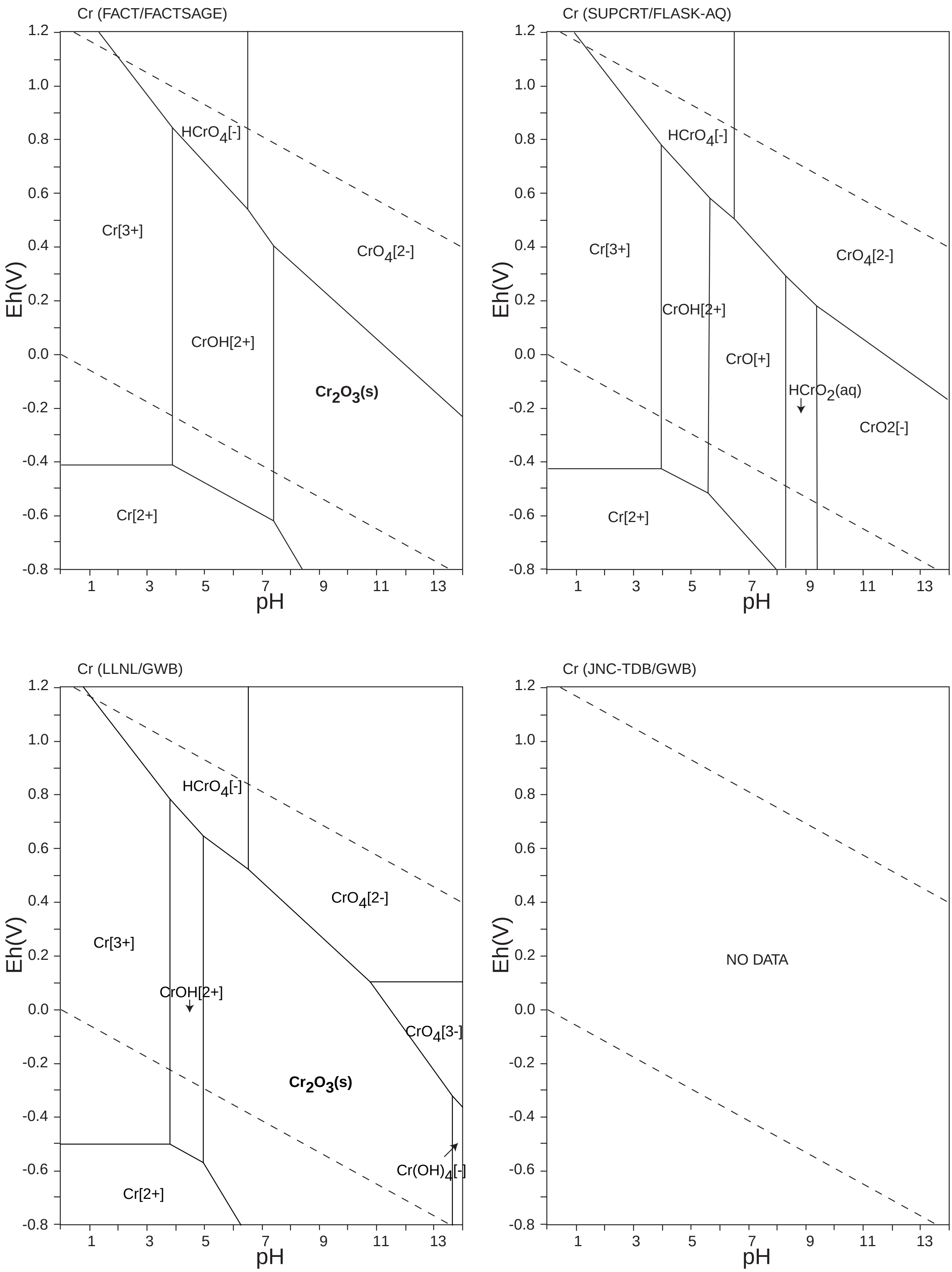

Figure 35: Eh-pH diagrams of the system Cr-O-H (1). $\sum \mathrm{Cr} = 10^{-10}$, 298.15K, 10^5 Pa.

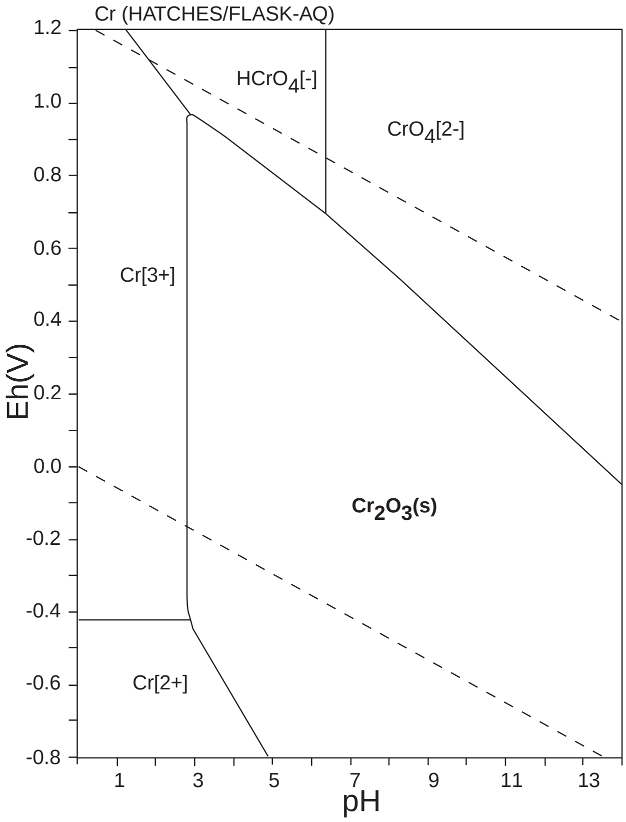

Figure 36: Eh-pH diagrams of the system Cr-O-H (2). $\sum \mathrm{Cr} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 22: List of Cs species

FACT	SUPCRT	LLNL	JNC-TDB
Cs[+], **Cs(s)**, **CsO_2(s)**, **Cs_2O(s)**, **Cs_2O_3(s)**, **CsOH(s)**, **CsOH(s2)**, **CsOH(s3)**	Cs[+], CsOH(aq)	Cs[+]	Cs[+], **Cs(c)**, **Cs_2O(s)**, **CsOH(s)**, Cs(g)

HATCHES			
Cs[+], **CsO**, **CsOH**			

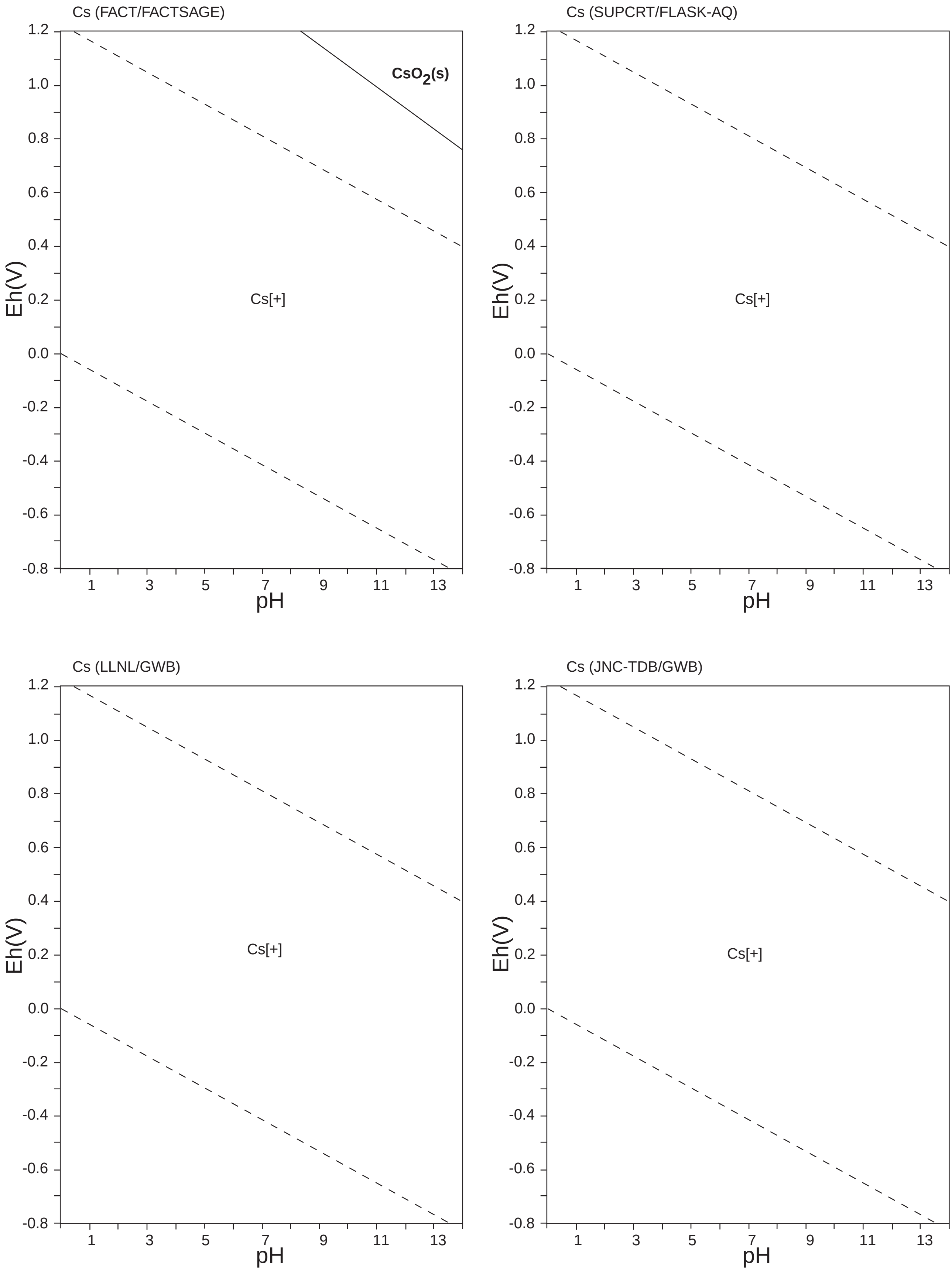

Figure 37: Eh-pH diagrams of the system Cs-O-H (1). $\sum \mathrm{Cs} = 10^{-10}$, 298.15K, 10^5 Pa.

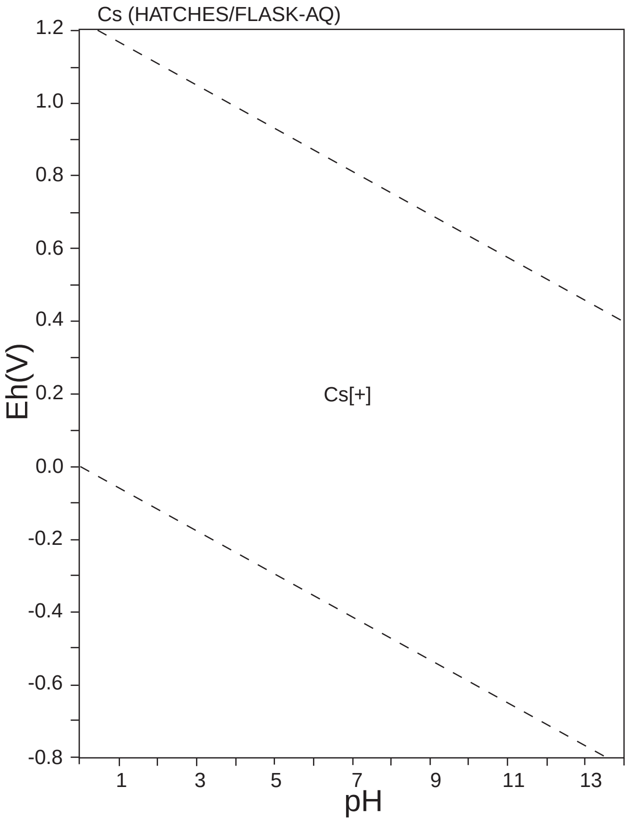

Figure 38: Eh-pH diagrams of the system Cs-O-H (2). $\sum \mathrm{Cs} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 23: List of Cu species

FACT	SUPCRT	LLNL	JNC-TDB
$Cu[+]$, $Cu[2+]$, $CuO_2[2-]$, $HCuO_2[-]$, **$Cu(OH)_2(s)$, Cu (s), CuO(s), $Cu_2O(s)$**	$Cu[+]$, $Cu[2+]$, $CuO_2[2-]$, $HCuO_2[-]$, CuOH[+], CuO(aq), **Cu(Native Copper), CuO(Tenorite), Cu_2O (Cuprite)**	Cu[+], Cu[2+], CuOH[+], **Copper, Cuprite, Tenorite**	

HATCHES			
Cu[2+], Cu[+], $Cu(OH)_4[2-]$, $Cu_2(OH)_2[2+]$, **Copper, Cuprite, Tenorite**			

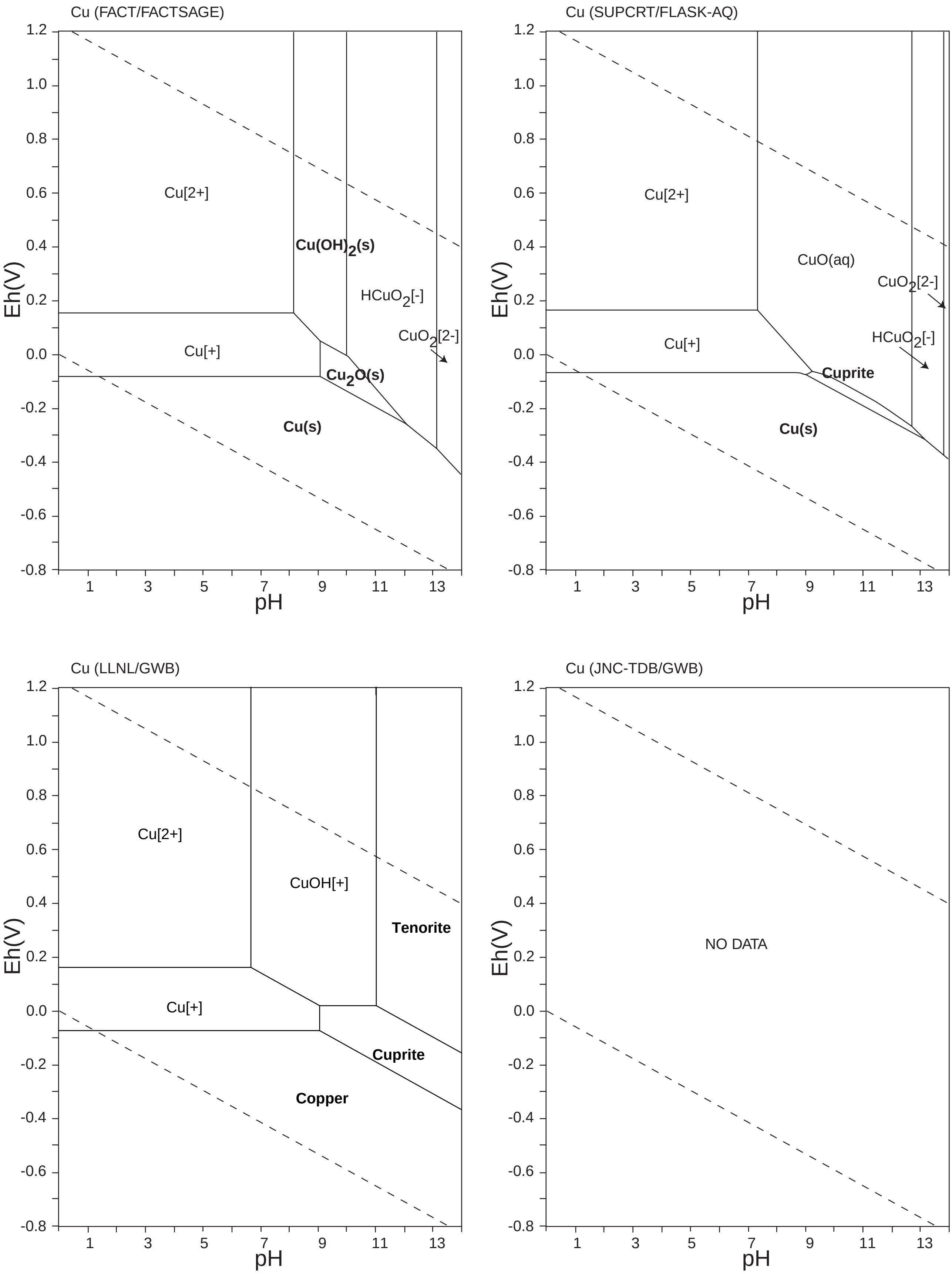

Figure 39: Eh-pH diagrams of the system Cu-O-H (1). $\sum \mathrm{Cu} = 10^{-10}$, 298.15K, 10^5 Pa.

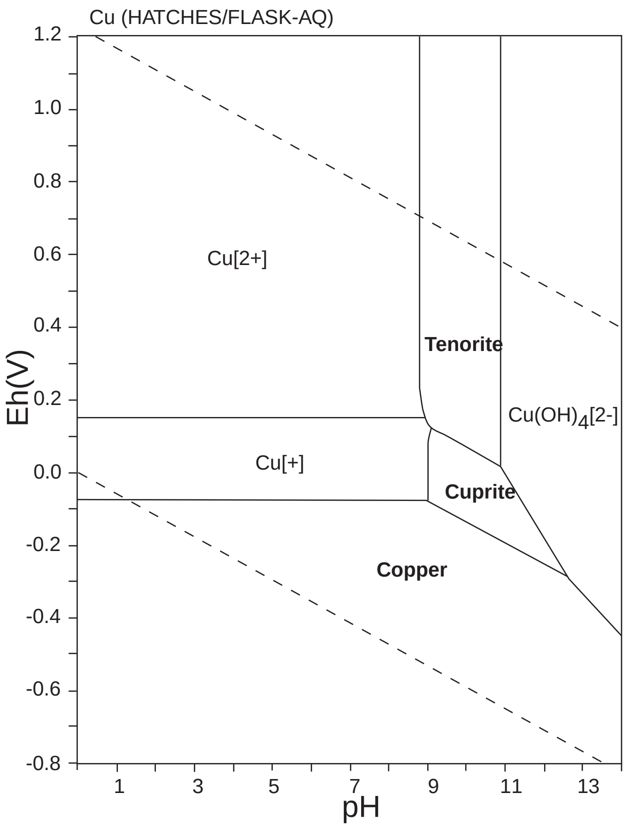

Figure 40: Eh-pH diagrams of the system Cu-O-H (2). $\sum \mathrm{Cu} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 24: List of Dy species

FACT	SUPCRT	LLNL	JNC-TDB
Dy[3+], **Dy(s)**, **Dy(s2)**, **Dy_2O_3(s)**	Dy[3+], Dy[2+], Dy[4+], DyOH[2+], DyO[+], DyO_2H(aq), DyO_2[-]		

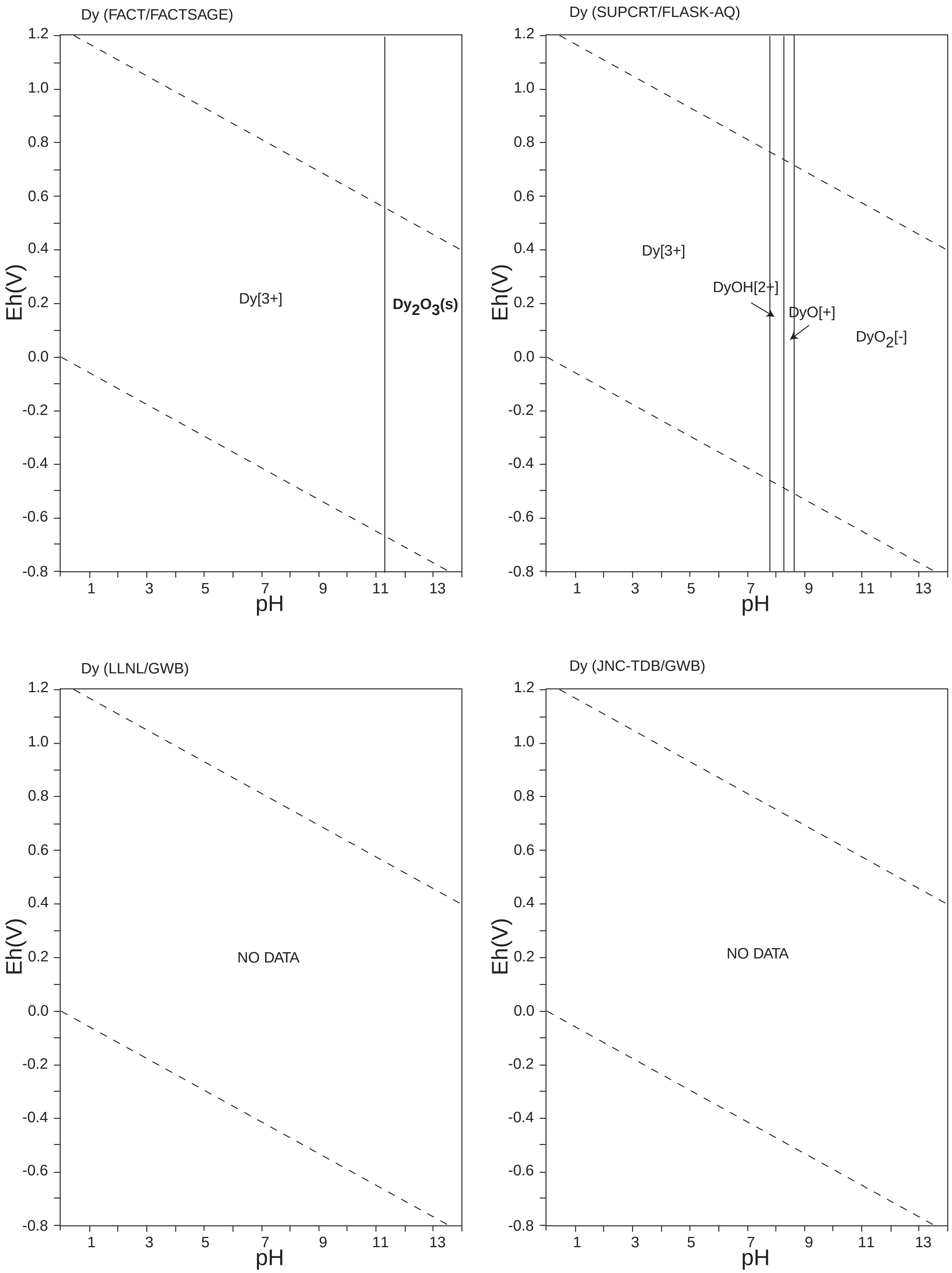

Figure 41: Eh-pH diagrams of the system Dy-O-H. $\sum \mathrm{Dy} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 25: List of Er species

FACT	SUPCRT	LLNL	JNC-TDB
$Er[3+]$, **$Er(s)$**, **$Er_2O_3(s)$**, **$Er_2O_3(s2)$**	$Er[3+]$, $Er[2+]$, $Er[4+]$, $ErOH[2+]$, $ErO[+]$, $ErO_2H(aq)$, $ErO_2[-]$		

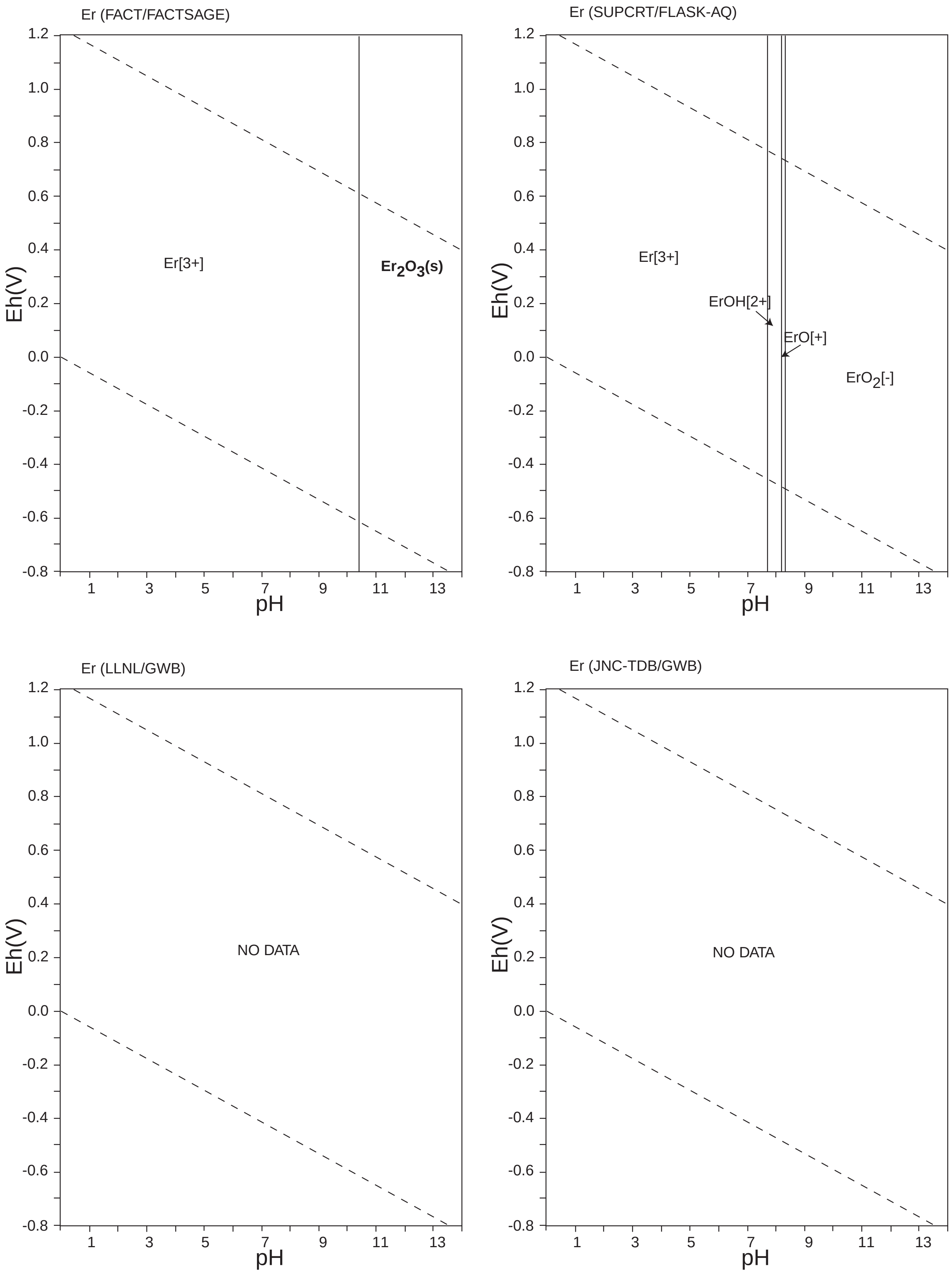

Figure 42: Eh-pH diagrams of the system Er-O-H. $\sum \mathrm{Er} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 26: List of Eu species

FACT	SUPCRT	LLNL	JNC-TDB
Eu[2+], Eu[3+], **Eu(s)**, **EuH_2(s)**, **EuO(s)**, **Eu_2O_3(s)**, **Eu_2O_3(s2)**, **Eu_3O_4(s)**, **EuO_3H_3(s)**	Eu[2+], Eu[3+], Eu[4+], EuOH[2+], EuO[+], EuO_2H(aq), EuO_2[-]	Eu[3+], Eu[2+], $Eu(OH)_2$[+], EuOH[2+], **Eu(s)**, **$Eu(OH)_3$(s)**, **Eu_2O_3(cubic)**, **Eu_2O_3(monoclinic)**, **Eu_3O_4(s)**, **EuO(s)**	

HATCHES			
Eu[3+], Eu(OH)[2+], **Eu**, **$Eu(OH)_3$**, **Eu_2O_3(cubic)**, **Eu_2O_3(monoclinic)**, **Eu_3O_4**, **EuO**			

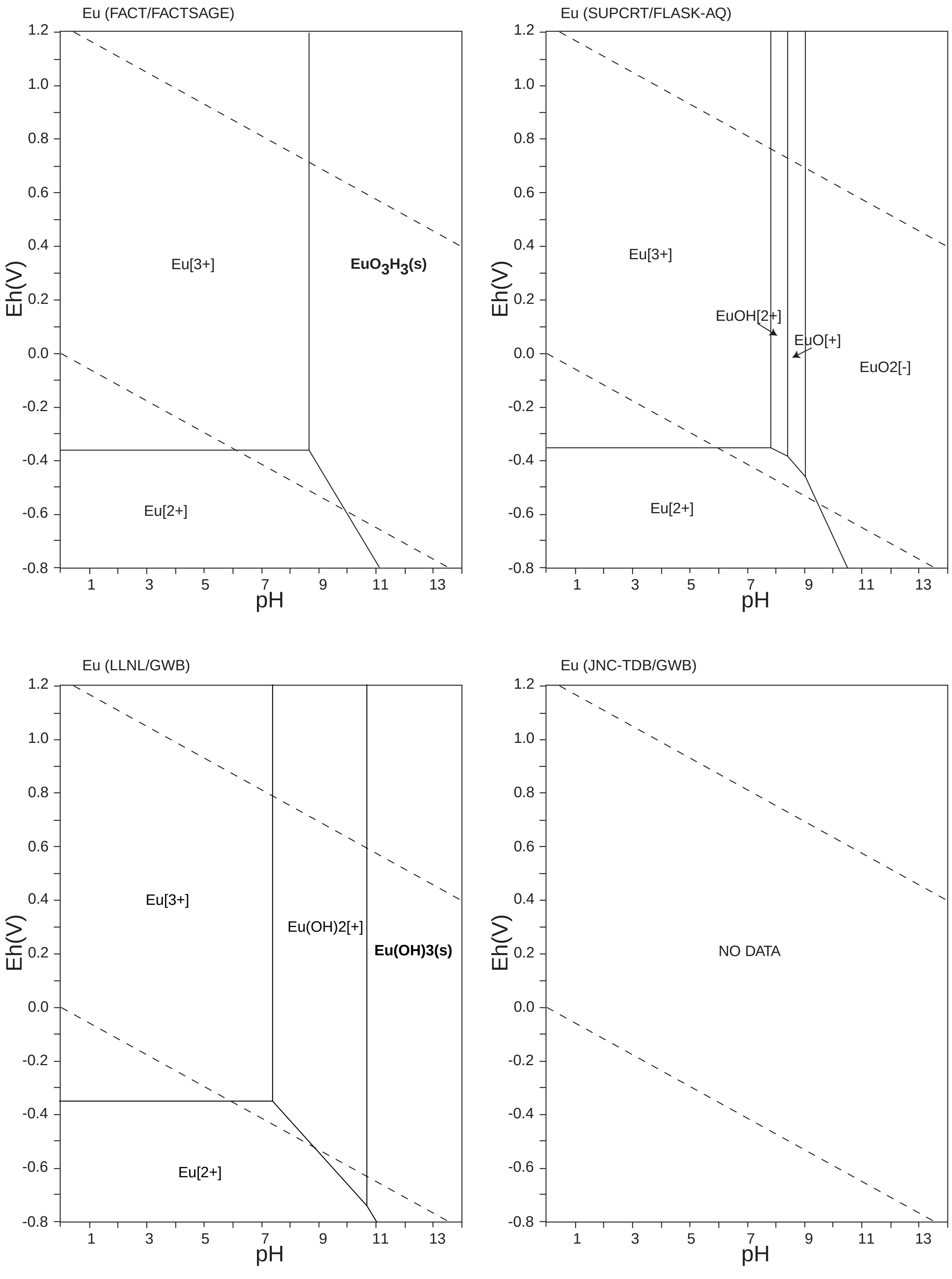

Figure 43: Eh-pH diagrams of the system Eu-O-H (1). $\sum \mathrm{Eu} = 10^{-10}$, 298.15K, 10^5 Pa.

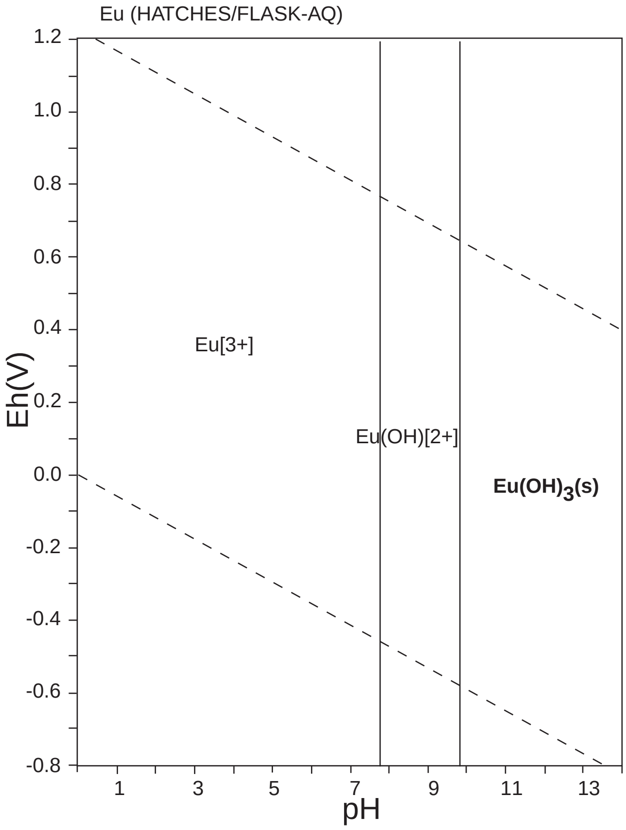

Figure 44: Eh-pH diagrams of the system Eu-O-H (2). $\sum \mathrm{Eu} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 27: List of F species

FACT	SUPCRT	LLNL	JNC-TDB
F[-], HF(aq), HF_2[-]	F[-], HF(aq), HF_2[-]	F[-], H_2F_2, HF, HF_2[-]	F-, HF(aq), HF_2[-], F(g), F_2(g), HF(g)

HATCHES			
F[-], HF(aq), HF_2[-]			

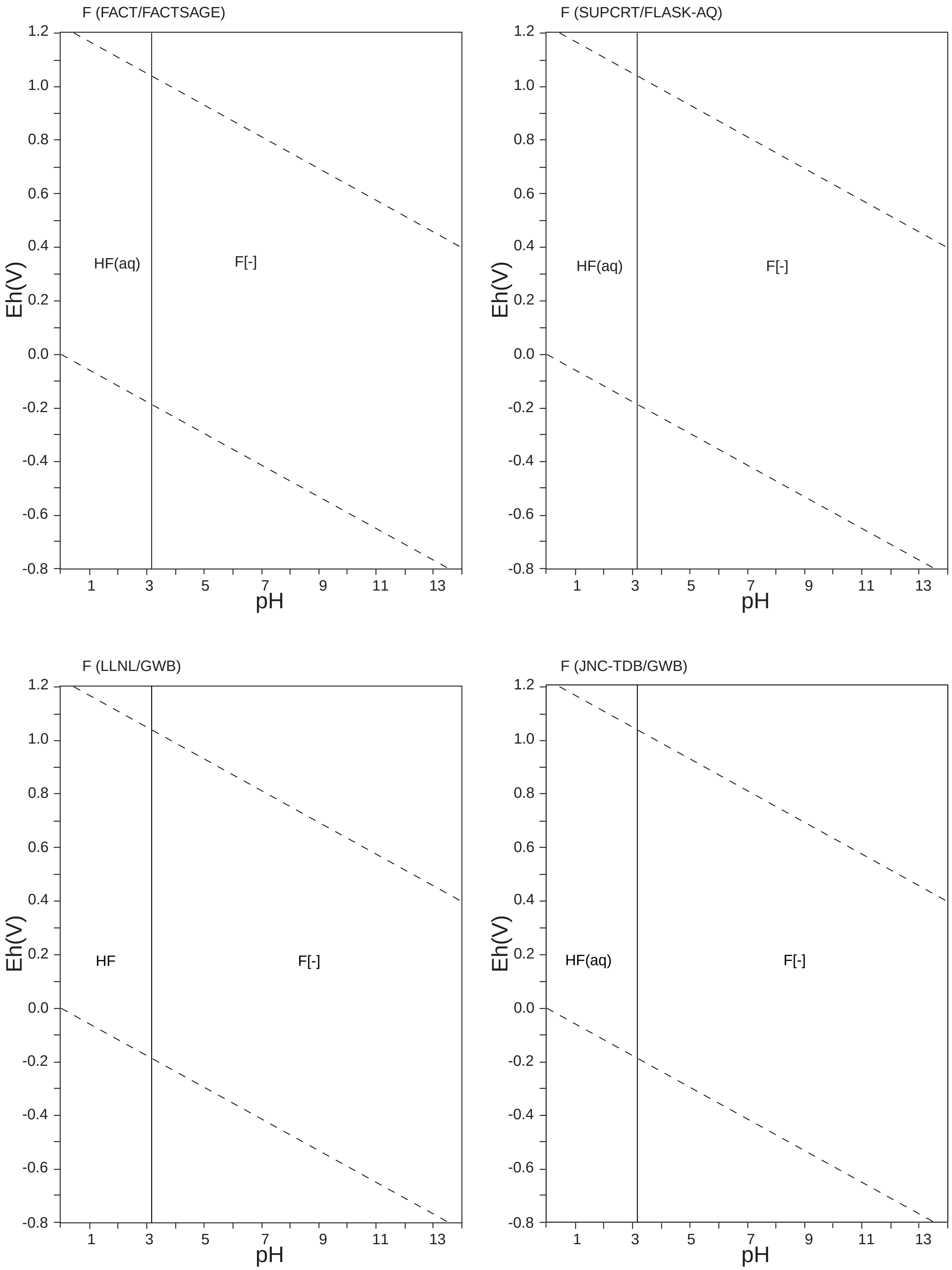

Figure 45: Eh-pH diagrams of the system F-O-H (1). $\sum \mathrm{F} = 10^{-10}$, 298.15K, 10^5 Pa.

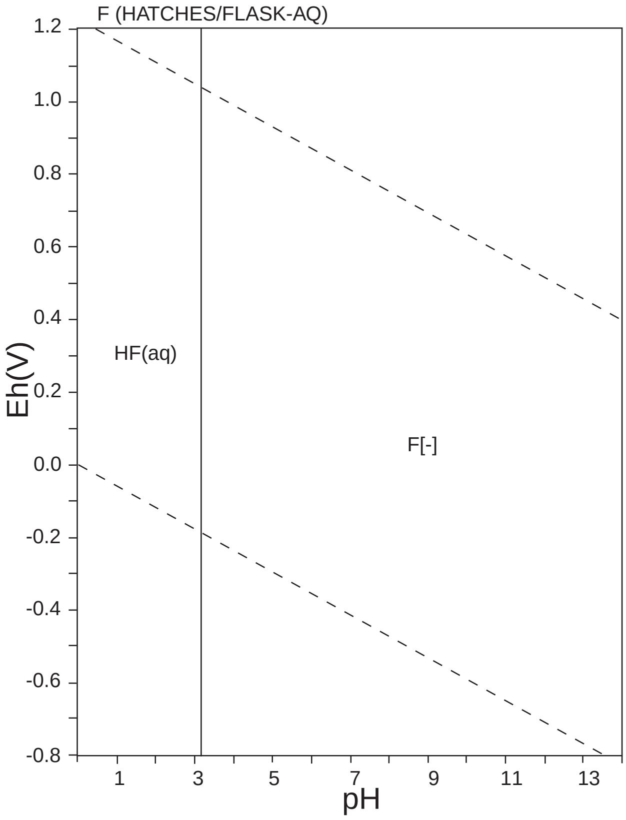

Figure 46: Eh-pH diagrams of the system F-O-H (2). $\sum \mathrm{F} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 28: List of Fe species

FACT	SUPCRT	LLNL	JNC-TDB
$Fe[2+]$, $Fe[3+]$, $FeOH[+]$, $FeOH[2+]$, $HFeO_2[-]$, $Fe(OH)_2[+]$, $FeO_2[2-]$, $Fe(OH)_3(aq)$, $Fe_2(OH)_2[4+]$, **Fe(s)**, **Fe(s2)**, **Fe_2O_3(s2)**, **Fe_2O_3(s3)**, **Fe_3O_4(s2)**, **Fe_3O_4(s3)**, **Fe_3O_4(s4)**, **$Fe(OH)_2$(s)**, **$Fe(OH)_3$(s)**, **$Fe_2O_3(H_2O)$(s)**, **FeO (s)**, **Fe_2O_3(s)**, **Fe_3O_4(s)**	$HFeO_2$(aq), $FeO_2[-]$, FeO(aq), $Fe[2+]$, $Fe[3+]$, $FeOH[+]$, $FeOH[2+]$, $HFeO_2[-]$, $FeO[+]$, **FeO (Ferrous-oxide)**, **Fe_2O_3(Hematite)**, **Fe_3O_4(Magnetite)**	$Fe[2+]$, $Fe[3+]$, $Fe(OH)_2$(aq), $Fe(OH)_2[+]$, $Fe(OH)_3$(aq), $Fe(OH)_3[-]$, $Fe(OH)_4[-]$, $Fe_2(OH)_2[4+]$, $Fe_3(OH)_4[5+]$, $FeOH[+]$, $FeOH[2+]$, **$Fe(OH)_2$(ppd)**, **$Fe(OH)_3$(ppd)**, **FeO(c)** **Goethite**, **Hematite**, **Magnetite**, **Wustite**	$Fe[2+]$, $Fe[3+]$, $FeOH[2+]$, $Fe(OH)_2[+]$, $Fe(OH)_3$(aq), $FeOH_4[-]$, $Fe_2(OH)_2[4+]$, $Fe_3(OH)_4[5+]$, $FeOH[+]$, $Fe(OH)_2$(aq), $Fe(OH)_3[-]$, **$Fe(OH)_3$(a)** **Hematite**, **Magnetite**, **Goethite**

HATCHES			
$Fe[2+]$, $Fe[3+]$, $Fe(OH)[+]$, $Fe(OH)_2$(aq), $Fe(OH)_2[+]$, $Fe(OH)_3$(aq), $Fe(OH)_3[-]$, $Fe(OH)_4[-]$, $Fe(OH)_4[2-]$, $Fe_2(OH)_2[4+]$, $Fe_3(OH)_4[5+]$, $FeOH[2+]$, **$Fe(OH)_2$**, **$Fe(OH)_3$**, **FeO(c)**, **Goethite**, **Hematite**, **Magnetite**, **Wustite**			

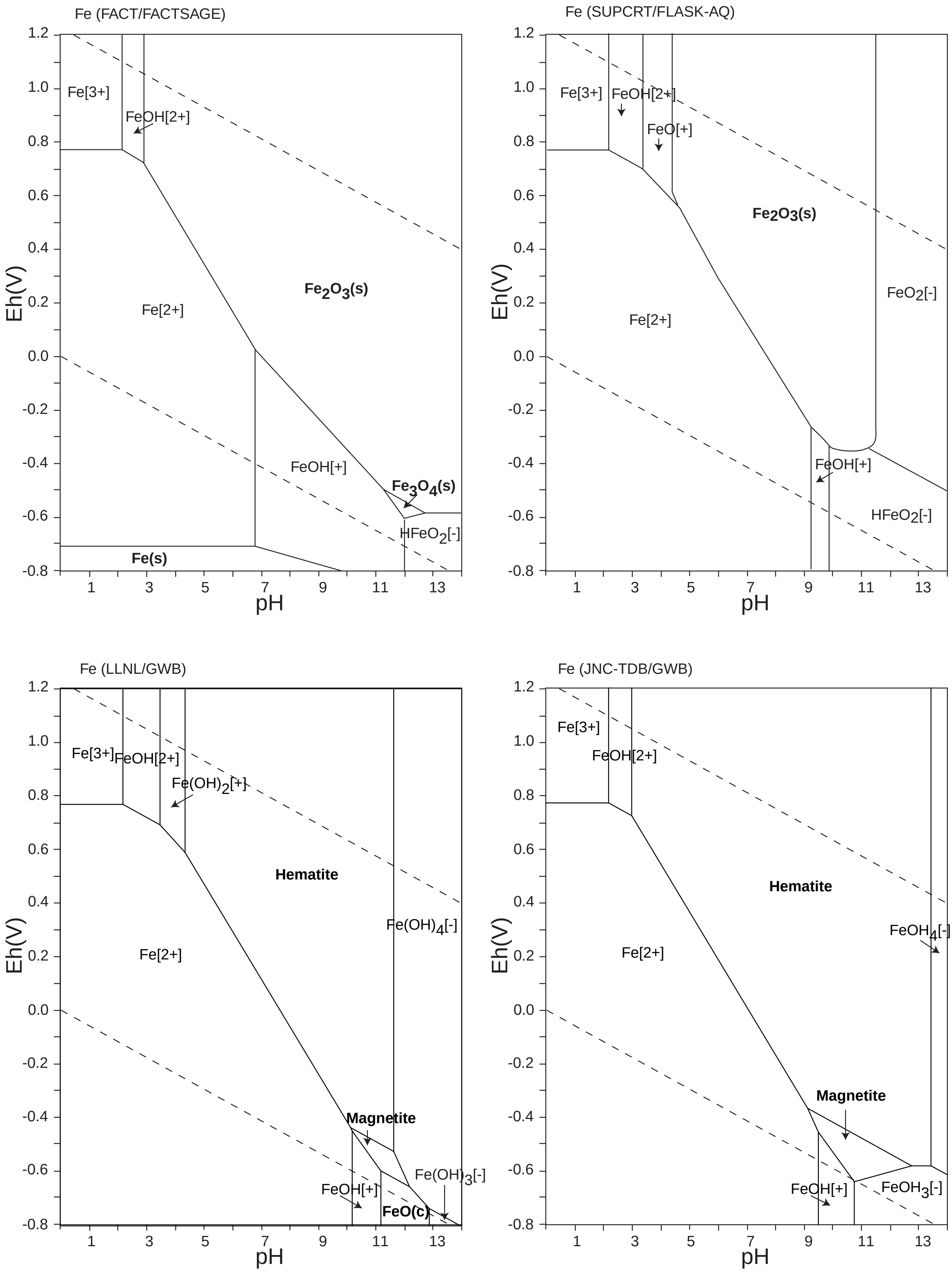

Figure 47: Eh-pH diagrams of the system Fe-O-H (1). $\sum \mathrm{Fe} = 10^{-10}$, 298.15K, 10^5 Pa.

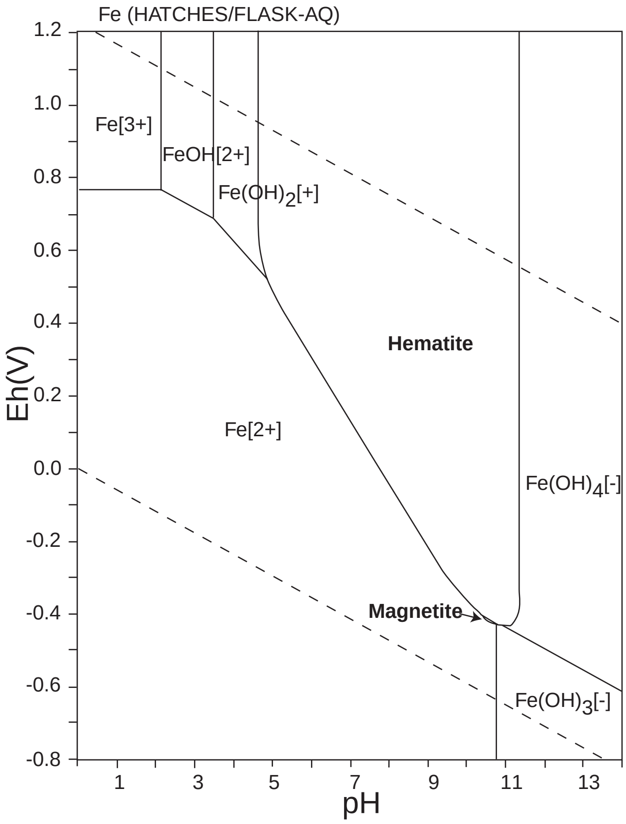

Figure 48: Eh-pH diagrams of the system Fe-O-H (2). $\sum \mathrm{Fe} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 29: List of Fr species

FACT	SUPCRT	LLNL	JNC-TDB
	Fr[+]		

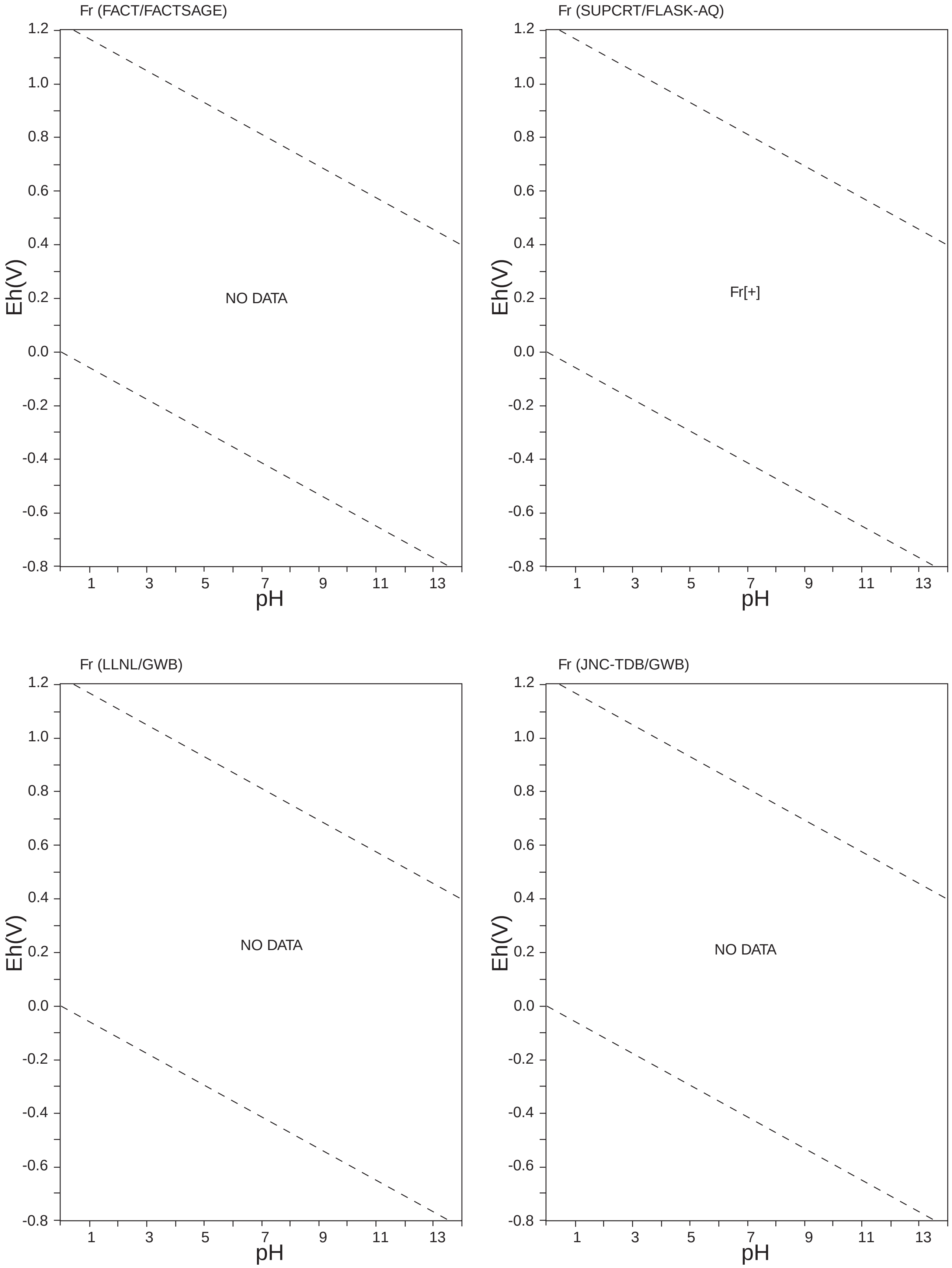

Figure 49: Eh-pH diagrams of the system Fr-O-H. $\sum \mathrm{Fr} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 30: List of Ga species

FACT	SUPCRT	LLNL	JNC-TDB
Ga[3+], GaOH[2+], $Ga(OH)_2$[+], H_2GaO_3[-],Ga[2+], GaO_3[3-], $HGaO_2$[2-], **Ga(s)**, **Ga_2O_3(s)**, **$Ga(OH)_3$(s)**	Ga[3+], GaOH[2+], GaO[+], GaO_2[-], $HGaO_2$(aq)		

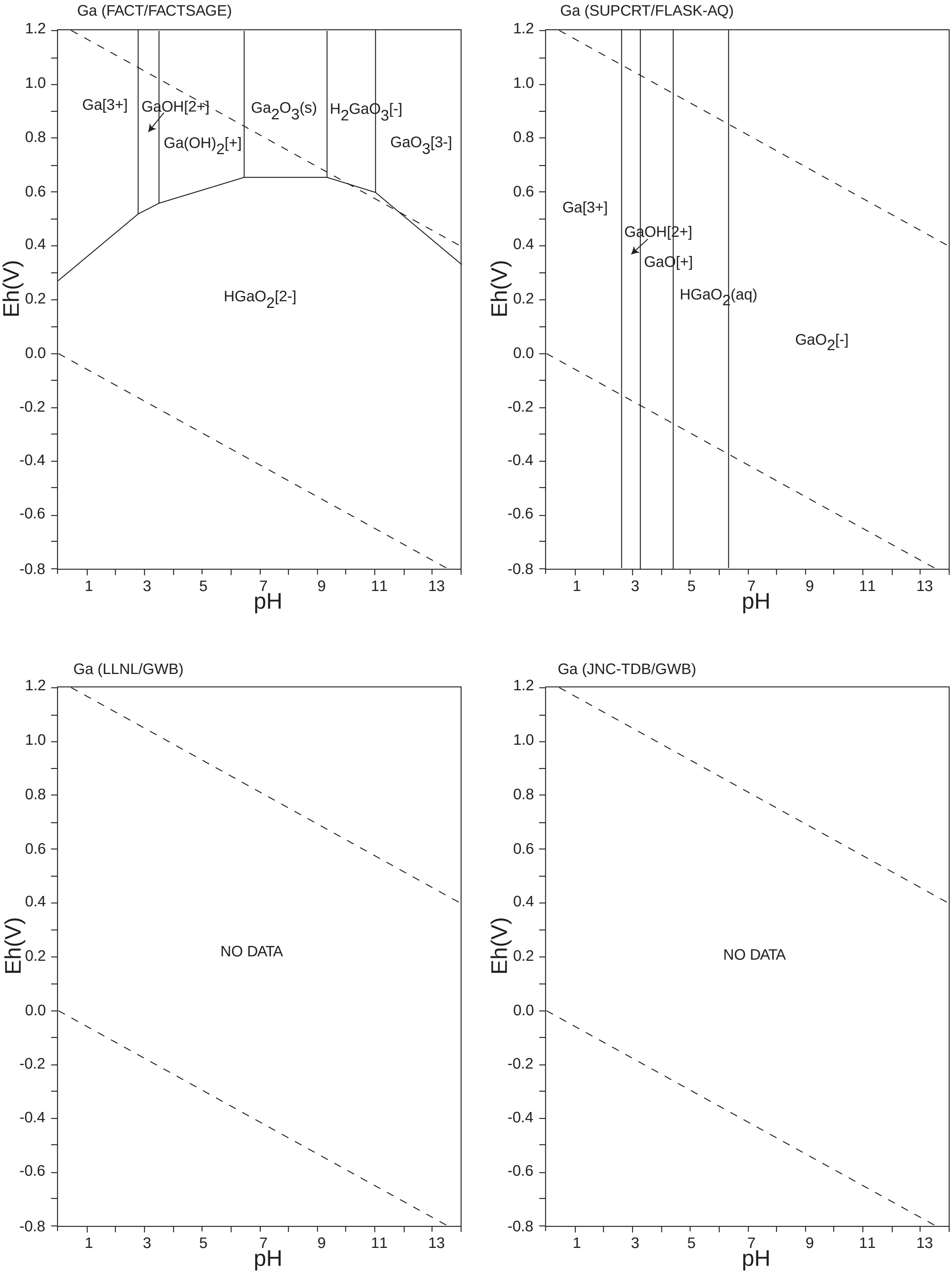

Figure 50: Eh-pH diagrams of the system Ga-O-H. $\sum \mathrm{Ga} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 31: List of Gd species

FACT	SUPCRT	LLNL	JNC-TDB
Gd[3+], **Gd(s)**, **Gd(s2)**, **Gd_2O_3(s)**	Gd[3+], Gd[4+], Gd[2+], GdOH[2+], GdO[+], GdO_2H(aq), GdO_2[-]		

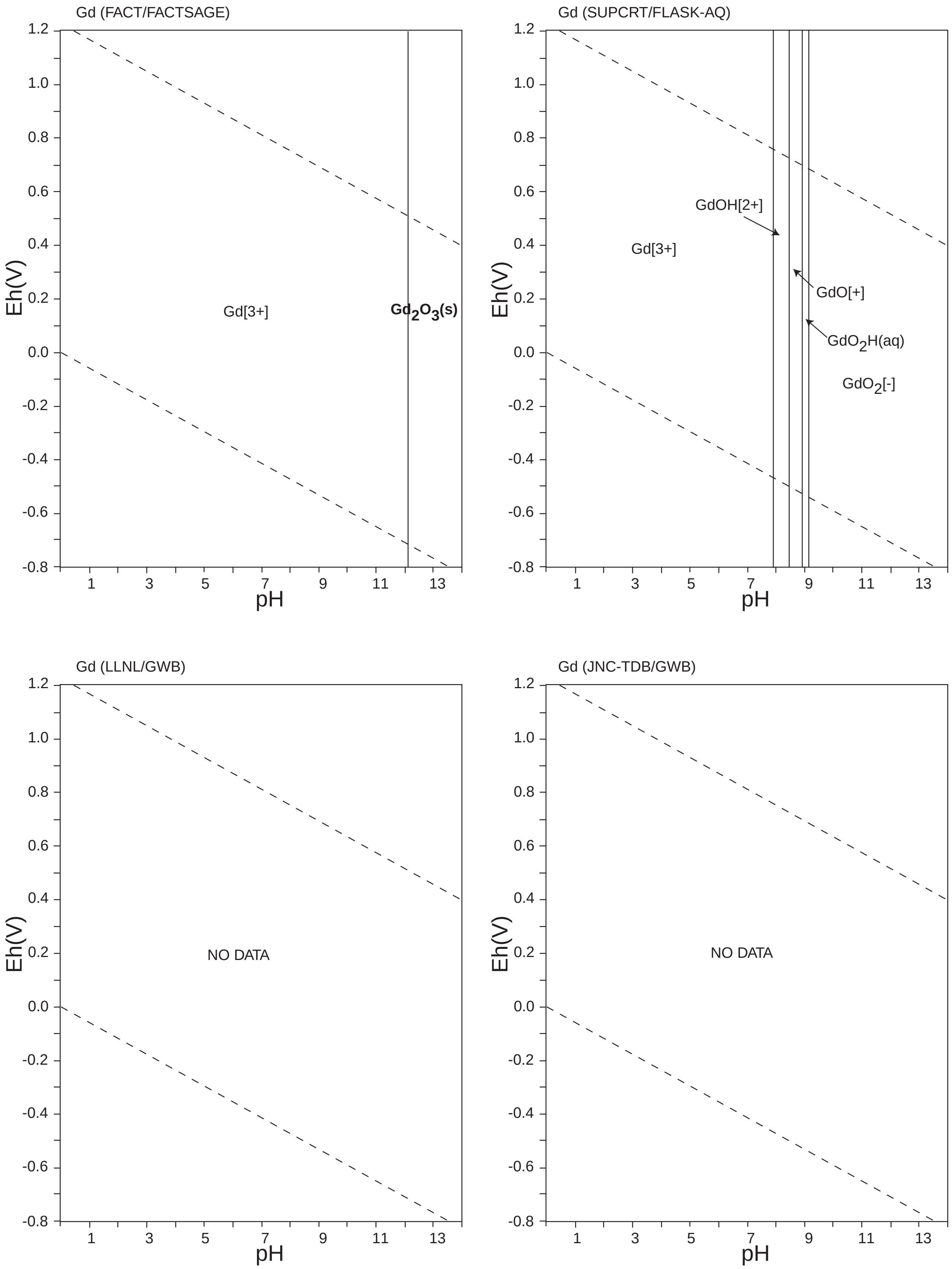

Figure 51: Eh-pH diagrams of the system Gd-O-H. $\sum \mathrm{Gd} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 32: List of Ge species

FACT	SUPCRT	LLNL	JNC-TDB
$HGeO_3$[-], **Ge(s)**, **GeO(s)**, **GeO(s2)**, **GeO_2(s)**, **GeO_2(s2)**			

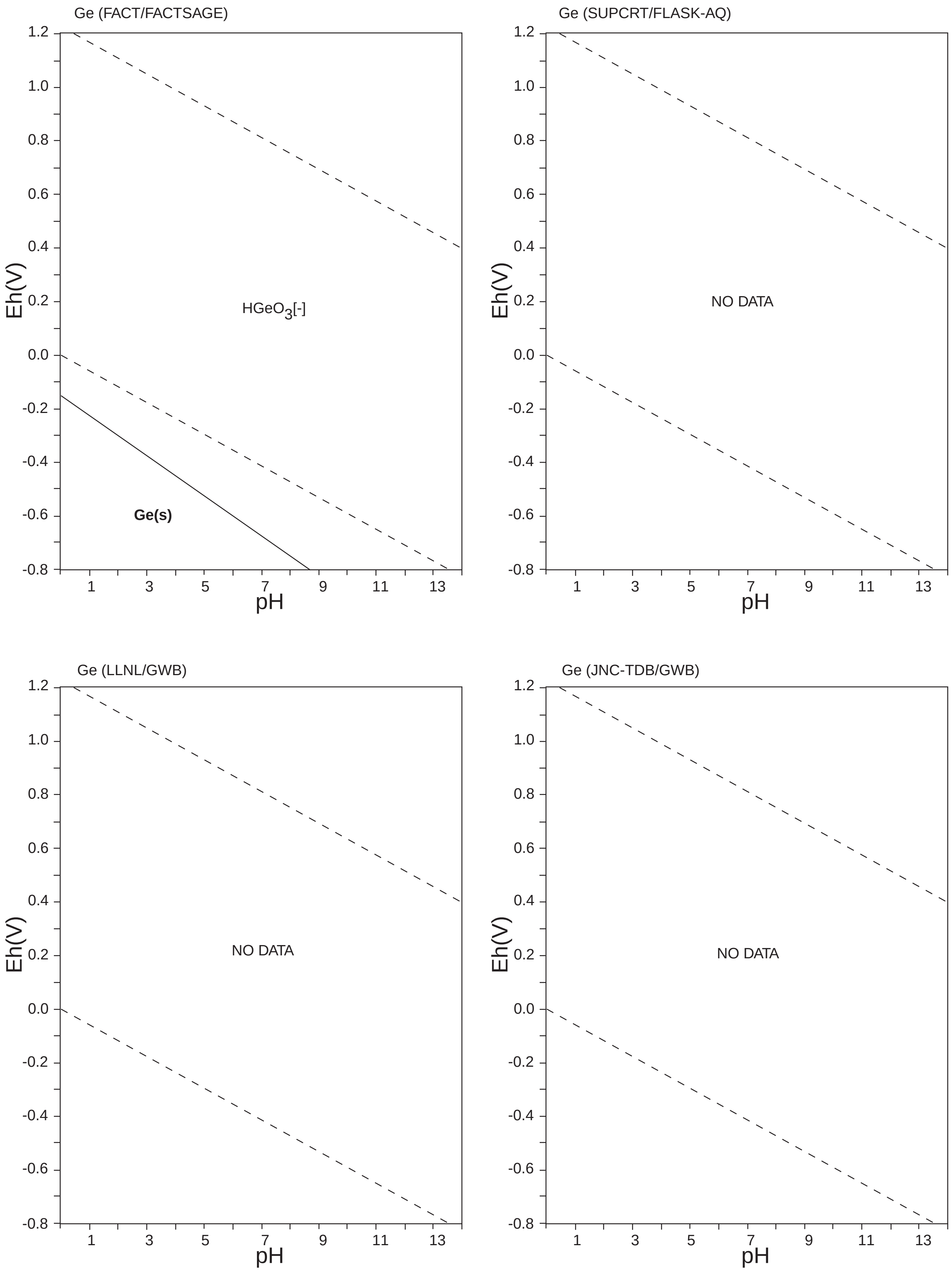

Figure 52: Eh-pH diagrams of the system Ge-O-H. $\sum \mathrm{Ge} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 33: List of Hf species

FACT	SUPCRT	LLNL	JNC-TDB
Hf(s), **Hf(s2)**, **HfO_2(s)**, **HfO_2(s2)**	Hf[4+], HfOH[3+], HfO[2+], $HHfO_2$[+], HfO_2(aq), $HHfO_3$[-]		

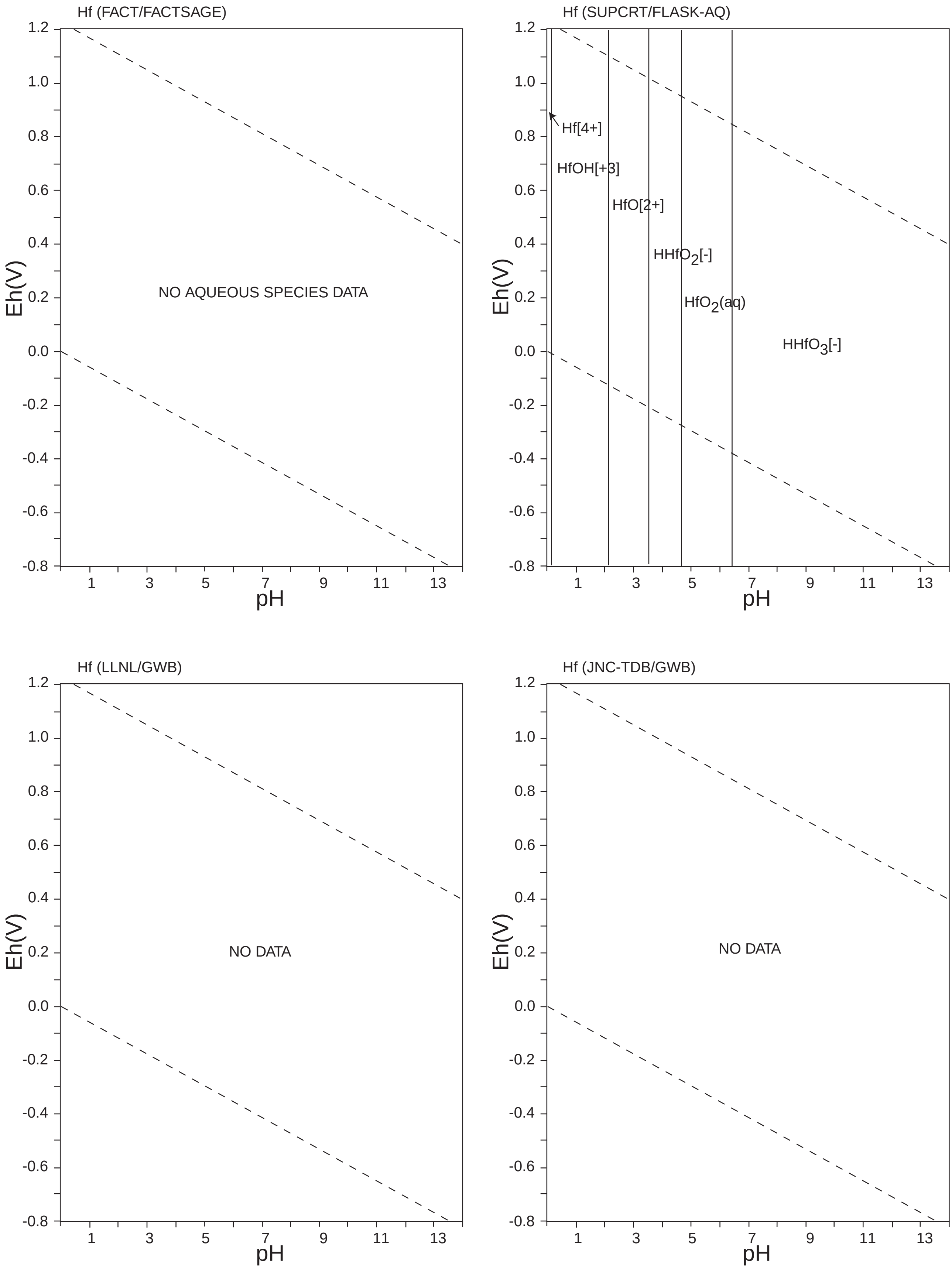

Figure 53: Eh-pH diagrams of the system Hf-O-H. $\sum \mathrm{Hf} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 34: List of Hg species

FACT	SUPCRT	LLNL	JNC-TDB
Hg[2+], Hg_2[2+], HgOH[+], $HHgO_2$[-], $Hg(OH)_2$, Hg(aq), **HgO(s)**	Hg[2+], Hg_2[2+], HgOH[+], $HHgO_2$[-], HgO(aq), **Hg(Quicksilver)**	Hg[2+], Hg_2[2+], **Quicksilver**	

HATCHES			
Hg[2+], $Hg(OH)_2$(aq), $Hg(OH)_3$[-], Hg_2OH[3+], $Hg_3(OH)_3$[3+], HgOH[+], **HgO, Quicksilver**			

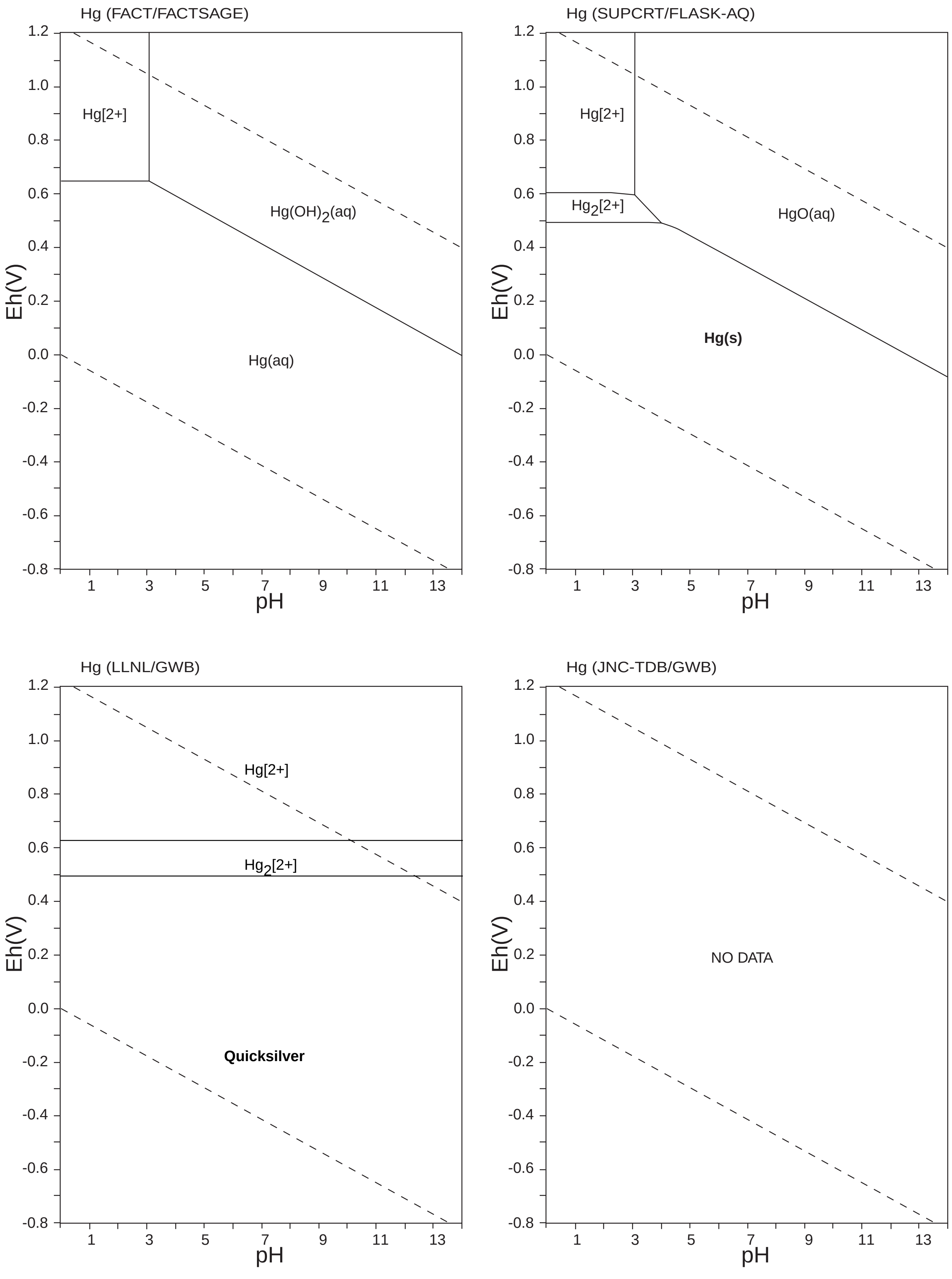

Figure 54: Eh-pH diagrams of the system Hg-O-H (1). $\sum \mathrm{Hg} = 10^{-10}$, 298.15K, 10^5 Pa.

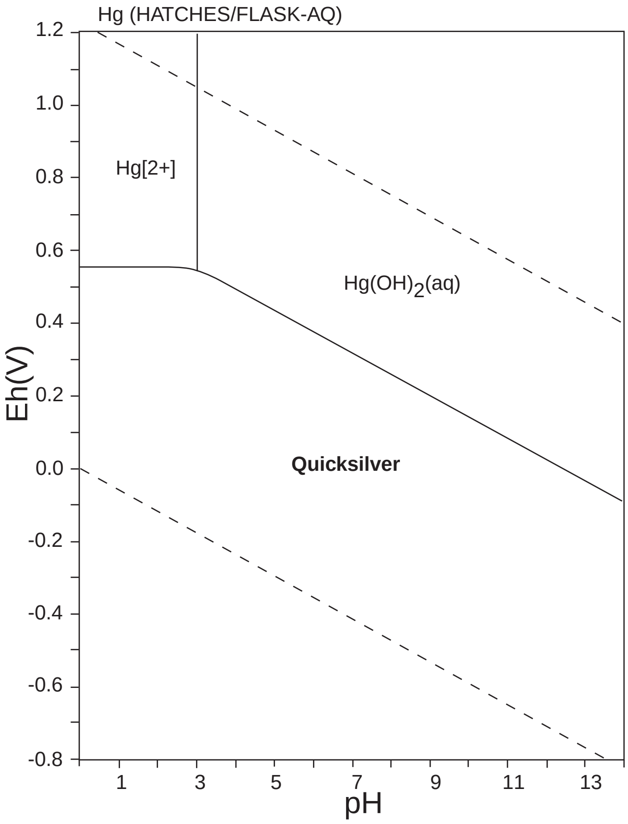

Figure 55: Eh-pH diagrams of the system Hg-O-H (2). $\sum \mathrm{Hg} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 35: List of Ho species

FACT	SUPCRT	LLNL	JNC-TDB
Ho[3+], **Ho(s)** , **Ho(s2)**, **Ho_2O_3(s)**, **Ho_2O_3(s2)**	Ho[3+], Ho[4+], Ho[2+], HoOH[2+], HoO[+], HoO_2H(aq), HoO_2[-]		

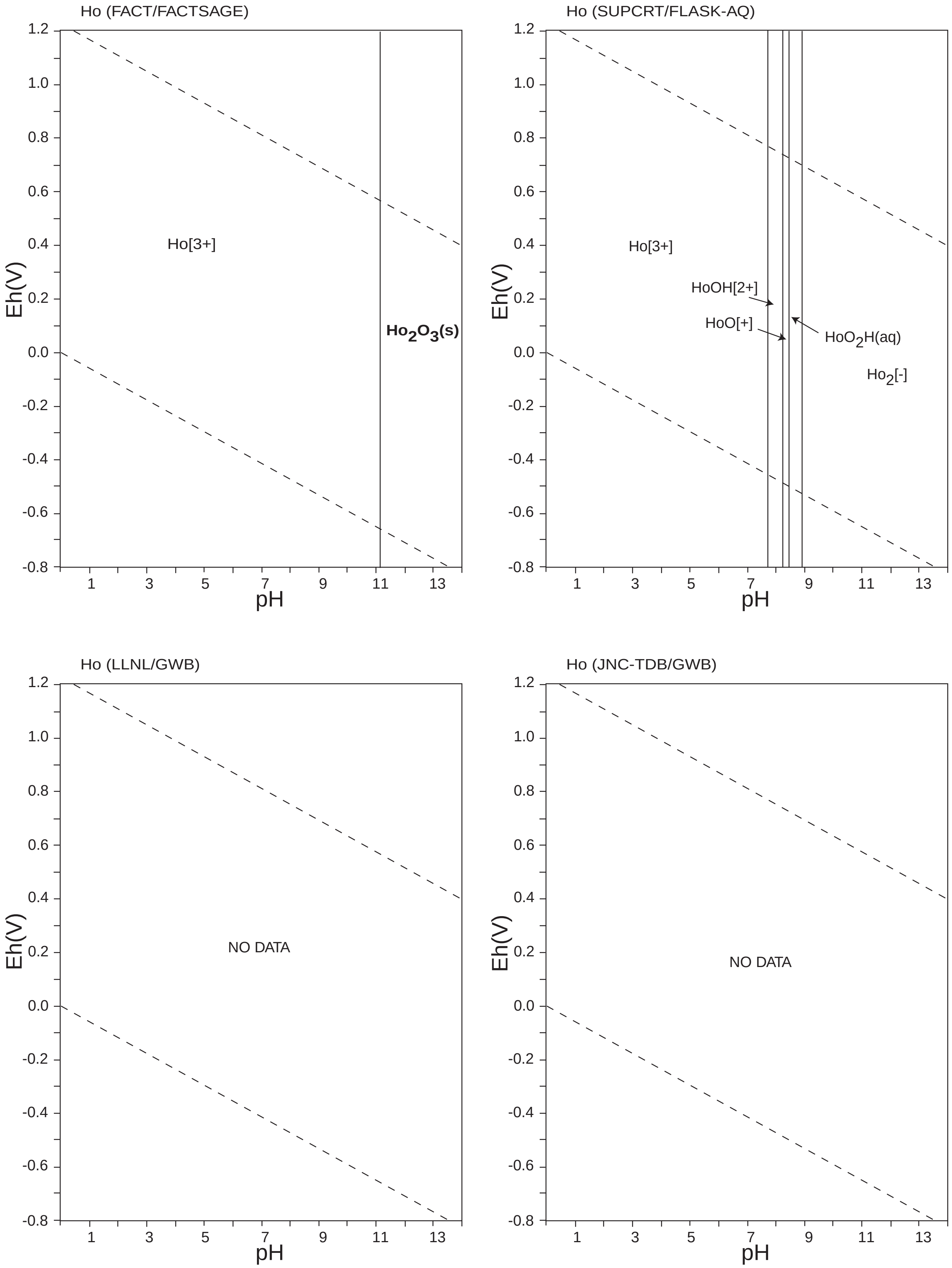

Figure 56: Eh-pH diagrams of the system Ho-O-H. $\sum \mathrm{Ho} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 36: List of I species

FACT	SUPCRT	LLNL	JNC-TDB
I[-], I_3[-], IO[-], IO_3[-], HIO(aq), HIO_3(aq), I_2 (aq), H_2OI[+], I_2OH[-], **I_2(s)**	I[-], I_3[-], IO[-], IO_3[-], HIO(aq), HIO_3(aq), IO_4[-]	I[-]	I[-], IO_3[-], HIO_3(aq), I_3[-], IO[-], IO_4[-], I_2O[2-], HIO(aq), I_2OH[-],I_2(aq), HI(aq), H_2OI[-], **I_2(s), I_2(c),** I(g), I_2(g), HI(g)

HATCHES			
I[-], IO_3[-], H_2IO[+], HI(aq), HIO(aq), HIO_3(aq), I_2(aq), I_2O[2-], I_2OH[-], I_3[-], IO[-], IO_4[-], **I_2**			

Remarks

JNC-TDB: I_2(s) is originally given as I_2 in the database file, but its detailed description is not given. Then (s) is appended to I_2 to avoid confusion with I_2(c).

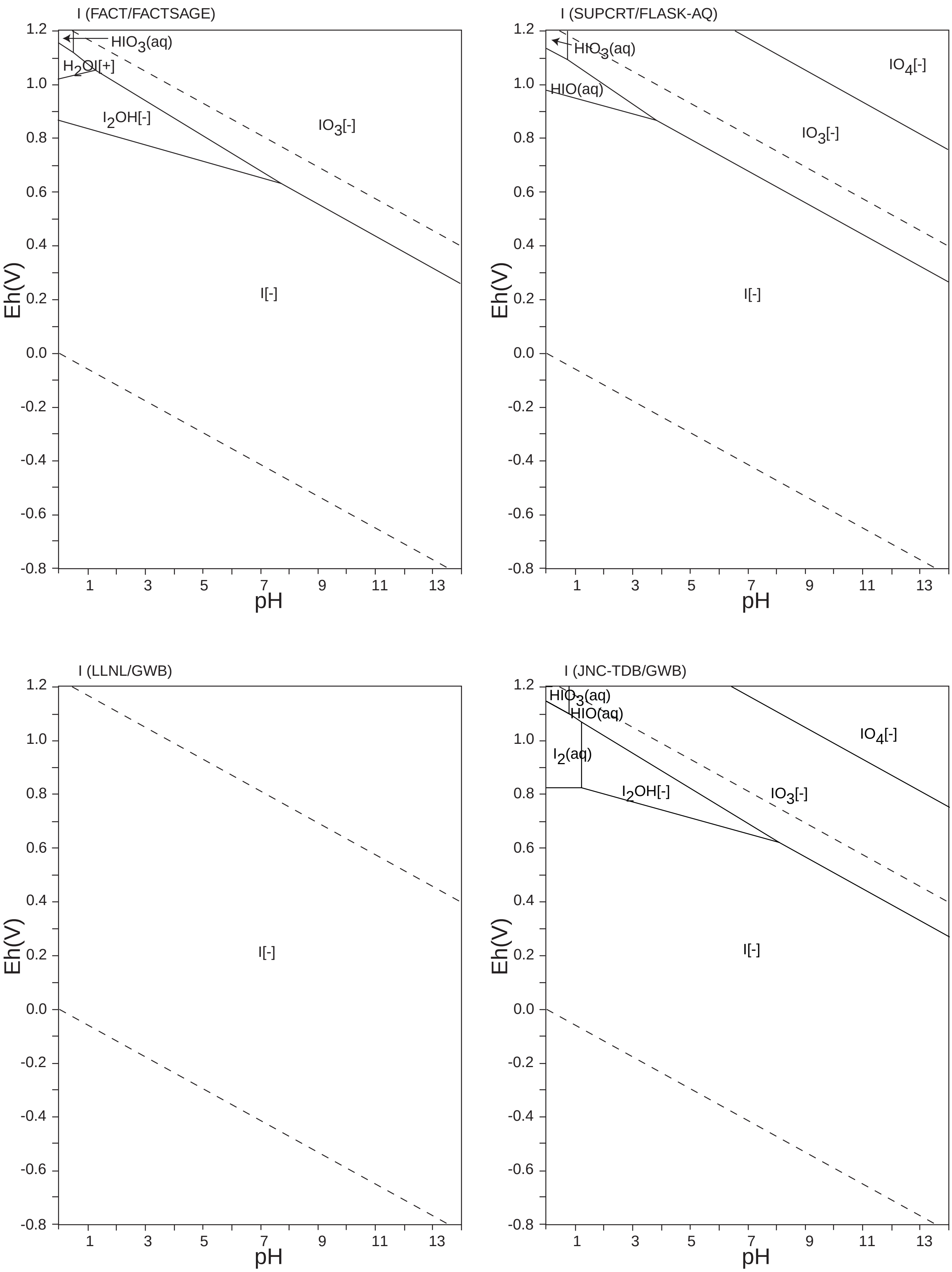

Figure 57: Eh-pH diagrams of the system I-O-H (1). $\sum \mathrm{I} = 10^{-10}$, 298.15K, 10^5 Pa.

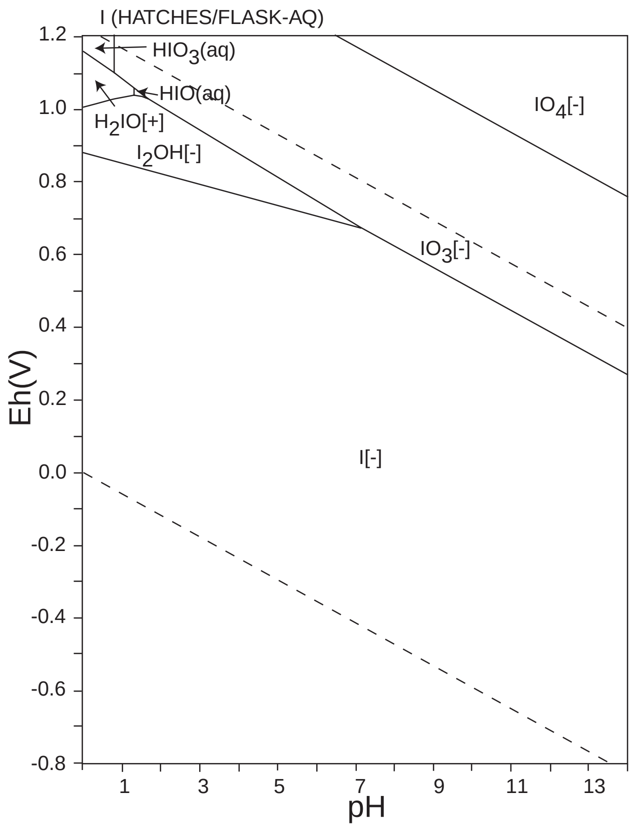

Figure 58: Eh-pH diagrams of the system I-O-H (2). $\sum \mathrm{I} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 37: List of In species

FACT	SUPCRT	LLNL	JNC-TDB
In[3+], InOH[2+], In(OH)$_2$[+], In[+], In[2+], **In(s)**, **In$_2$O$_3$(s)**, **In$_2$O$_3$(s2)**	In[3+], InOH[2+], InO[+], HInO$_2$(aq), InO$_2$[-]		

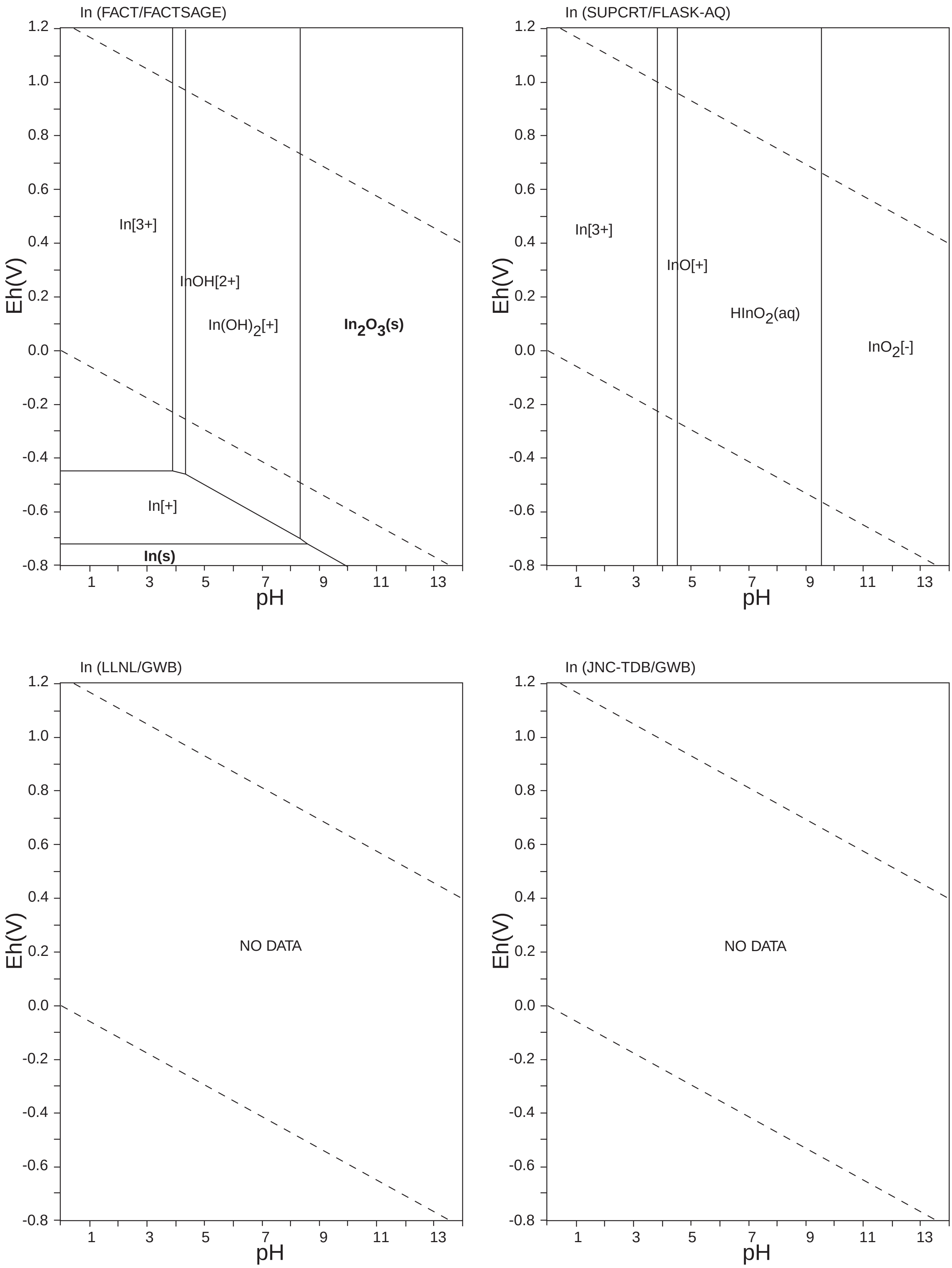

Figure 59: Eh-pH diagrams of the system In-O-H. $\sum \mathrm{In} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 38: List of K species

FACT	SUPCRT	LLNL	JNC-TDB
K[+], **K(s)**, **KH(s)**, **KO_2(s)**, **K_2O(s)**, **K_2O_2(s)**, **KOH(s)**, **KOH(s2)**	K[+], KOH(aq), **K_2O (Potassium-oxide)**	K[+], KOH(aq)	K[+], **K(c)**, K(g)

HATCHES			
K[+], **KOH**			

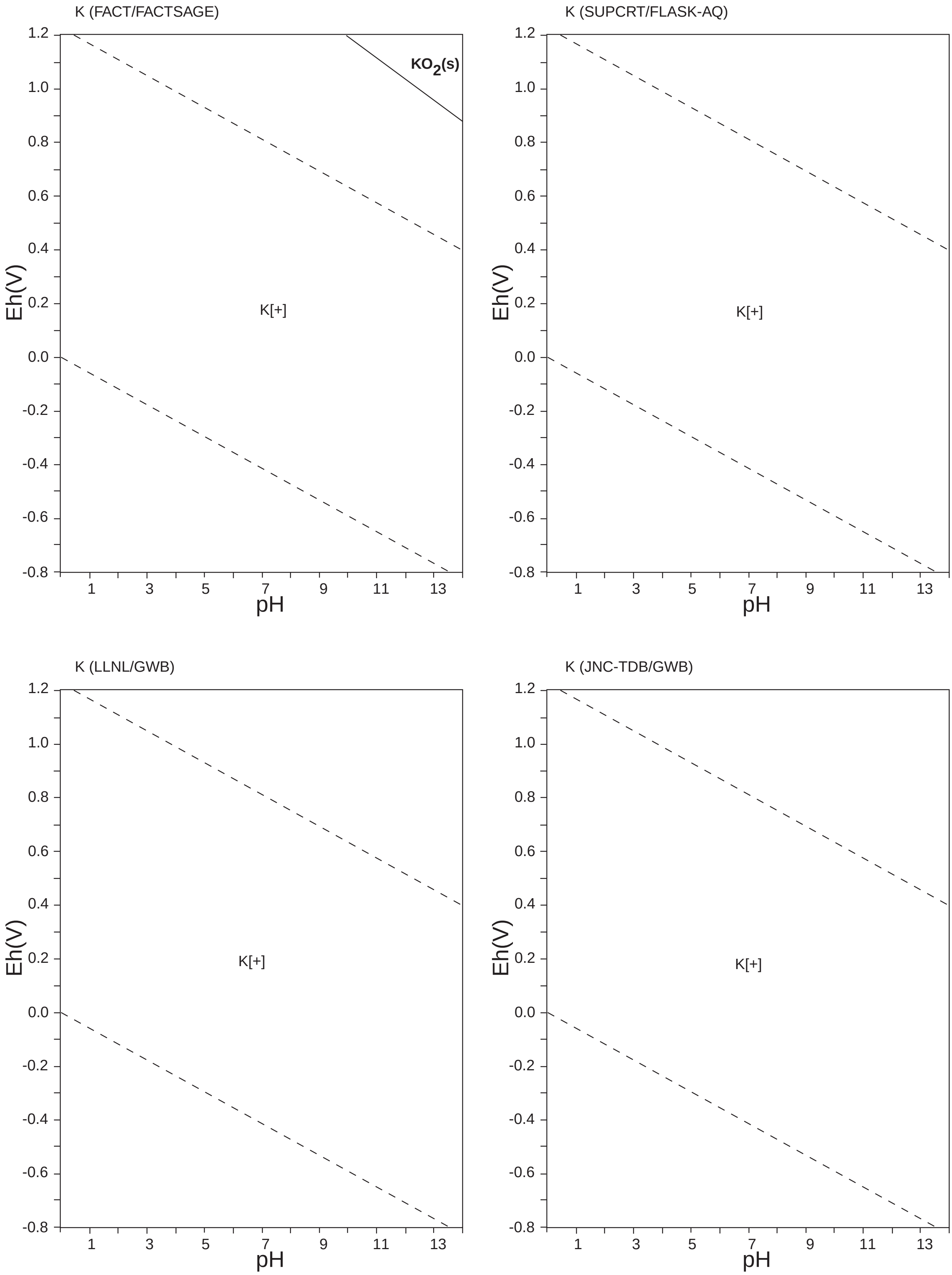

Figure 60: Eh-pH diagrams of the system K-O-H (1). $\sum \mathrm{K} = 10^{-10}$, 298.15K, 10^5 Pa.

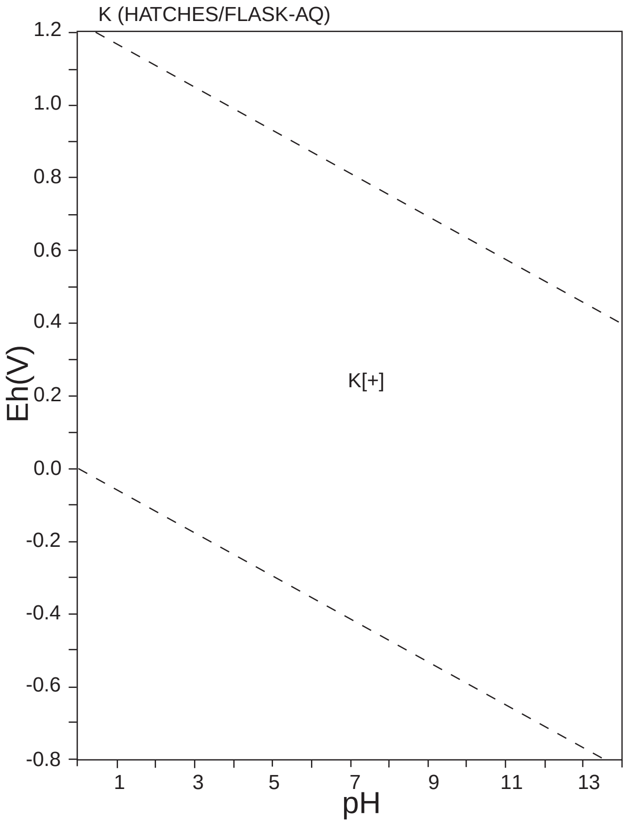

Figure 61: Eh-pH diagrams of the system K-O-H (2). $\sum \mathrm{K} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 39: List of La species

FACT	SUPCRT	LLNL	JNC-TDB
La^{3+}, **La(s)**, **La(s2)**, **La(s3)**, **LaH_2(s)**, **La_2O_3(s)**	La^{3+}, La^{2+}, $LaOH^{2+}$, LaO^{+}, LaO_2H(aq), LaO_2^{-}		

HATCHES			
La^{3+}, La_2OH^{5+}, $La_5(OH)_9^{6+}$, $LaOH^{2+}$, **$La(OH)_3$**			

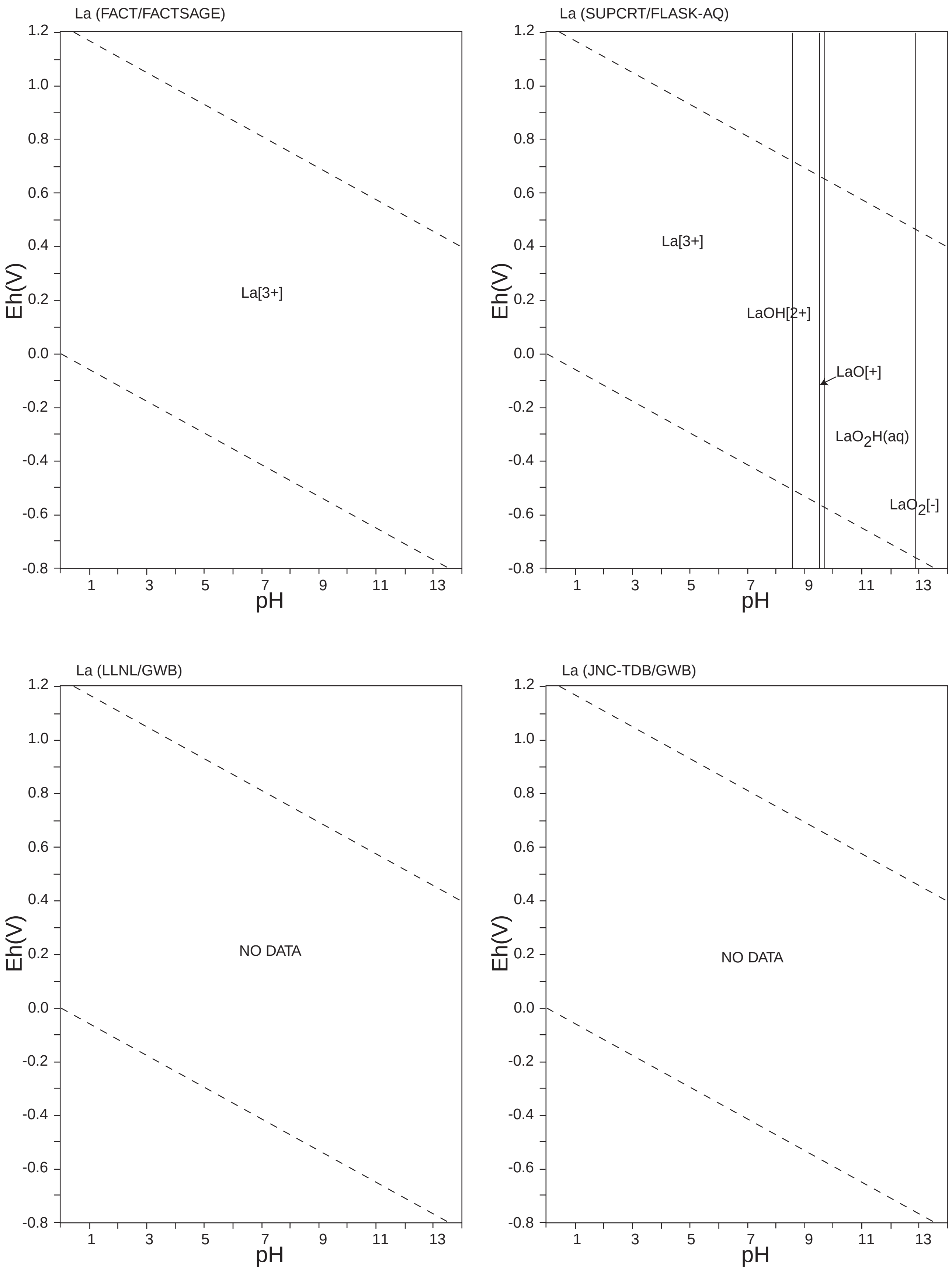

Figure 62: Eh-pH diagrams of the system La-O-H (1). $\sum \mathrm{La} = 10^{-10}$, 298.15K, 10^5 Pa.

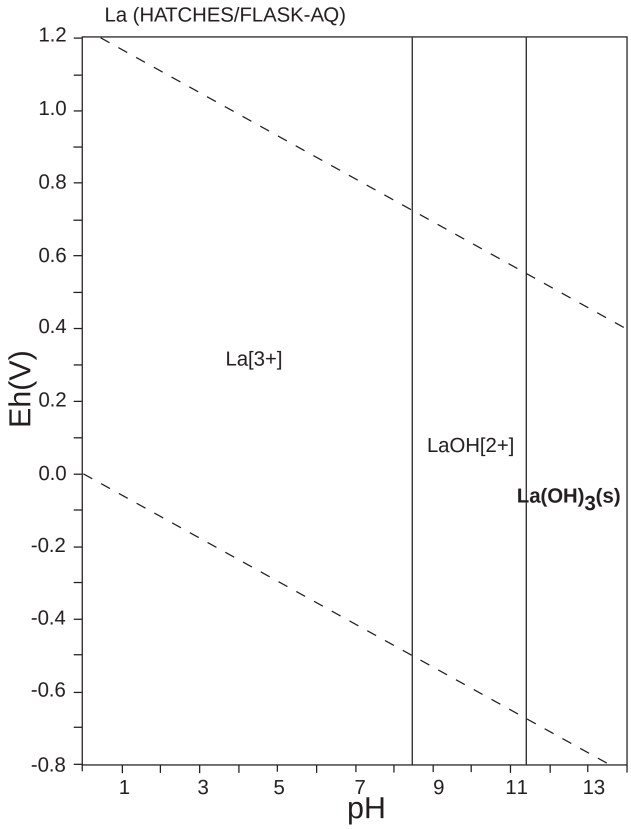

Figure 63: Eh-pH diagrams of the system La-O-H (2). $\sum \mathrm{La} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 40: List of Li species

FACT	SUPCRT	LLNL	JNC-TDB
Li[+], LiOH(aq), **Li(s)**, **LiH(s)**, **Li_2O(s)**, **Li_2O_2(s)**, **LiOH(s)**	Li[+], LiOH(aq)	Li[+], LiOH(aq)	Li[+]

HATCHES			
Li[+]			

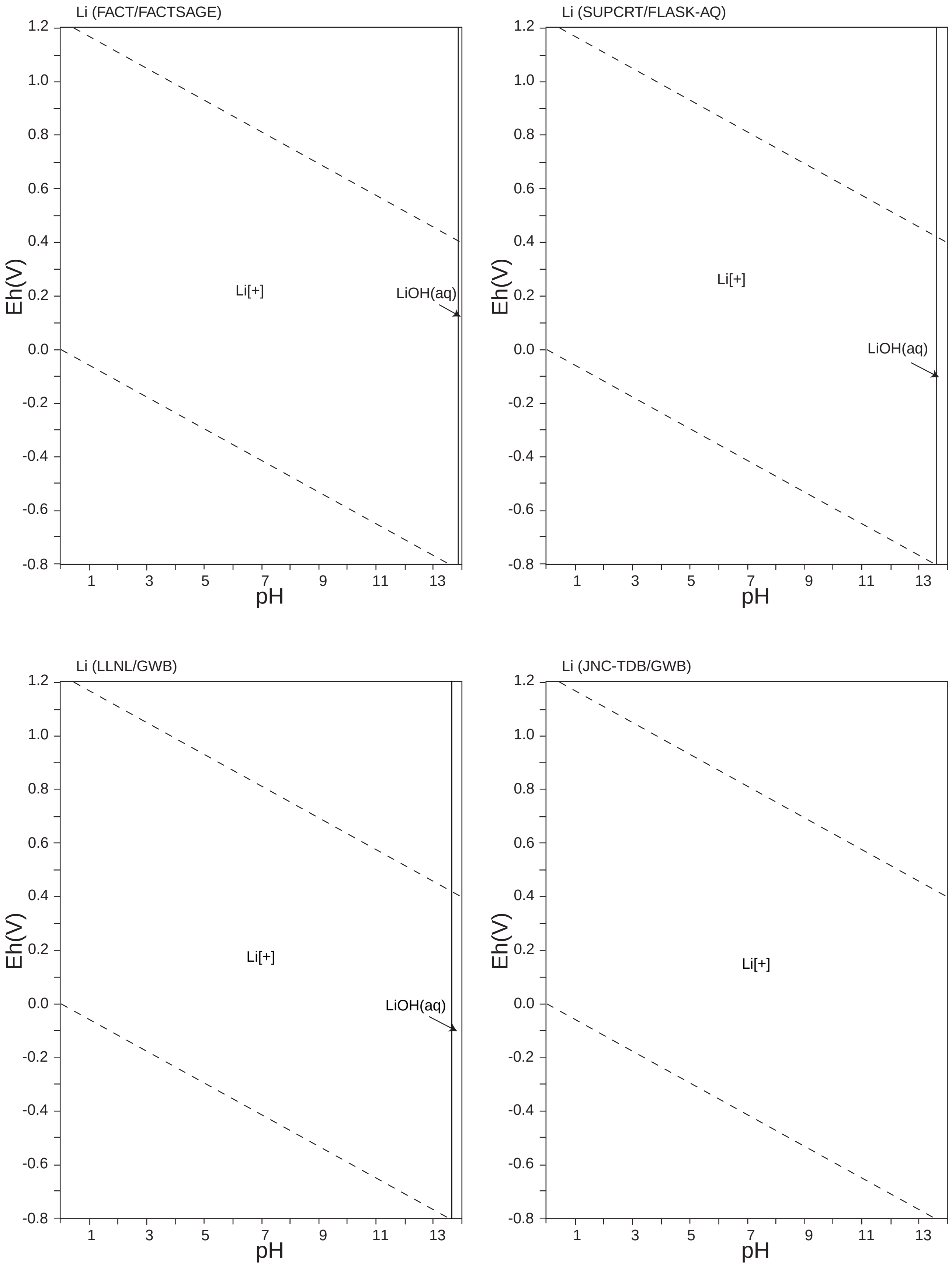

Figure 64: Eh-pH diagrams of the system Li-O-H (1). $\sum \mathrm{Li} = 10^{-10}$, 298.15K, 10^5 Pa.

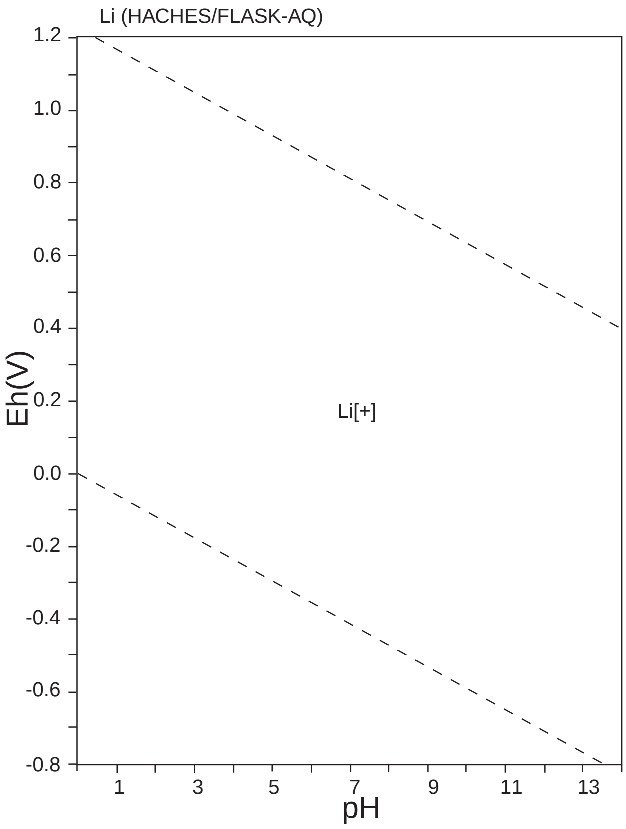

Figure 65: Eh-pH diagrams of the system Li-O-H (2). $\sum \mathrm{Li} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 41: List of Lu species

FACT	SUPCRT	LLNL	JNC-TDB
Lu^{3+}, **Lu(s)**, **Lu_2O_3(s)**	Lu^{3+}, Lu^{4+}, $LuOH^{2+}$, LuO^{+}, LuO_2H(aq), LuO_2^{-}		

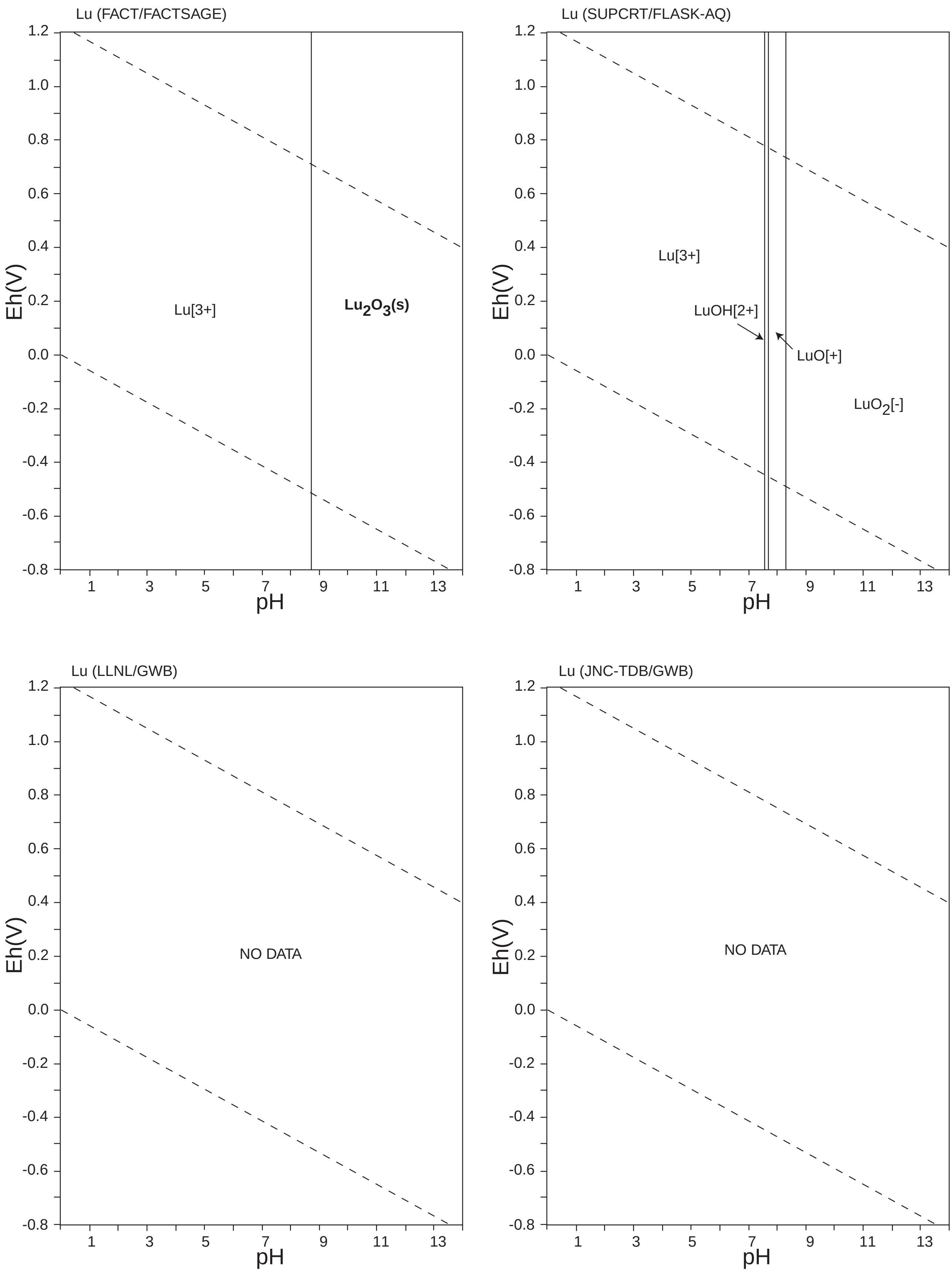

Figure 66: Eh-pH diagrams of the system Lu-O-H. $\sum \text{Lu} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 42: List of Mg species

FACT	SUPCRT	LLNL	JNC-TDB
Mg[2+], MgOH[+], **Mg(s), MgH_2(s), MgO(s), $Mg(OH)_2$(s)**	Mg[2+], MgOH[+], **MgO(Periclase), $Mg(OH)_2$(Brucite)**	Mg[2+], Mg_2OH[3+], $Mg_4(OH)_4$[4+], MgOH[+], **Brucite**	Mg[2+], MgOH[+], **Periclase**

HATCHES			
Mg[2+], MgOH[+], **$Mg(OH)_2$**			

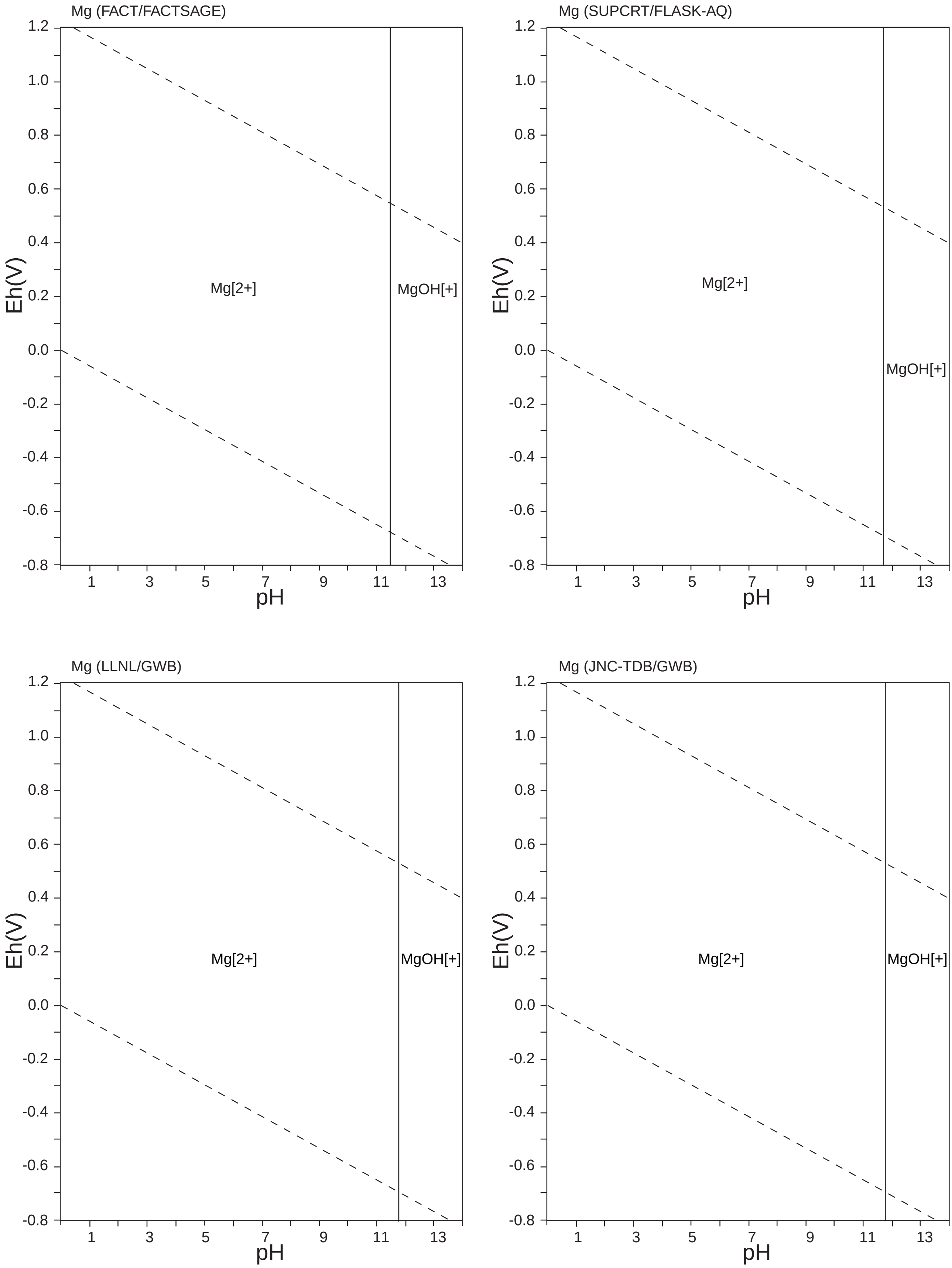

Figure 67: Eh-pH diagrams of the system Mg-O-H (1). $\sum \mathrm{Mg} = 10^{-10}$, 298.15K, 10^5 Pa.

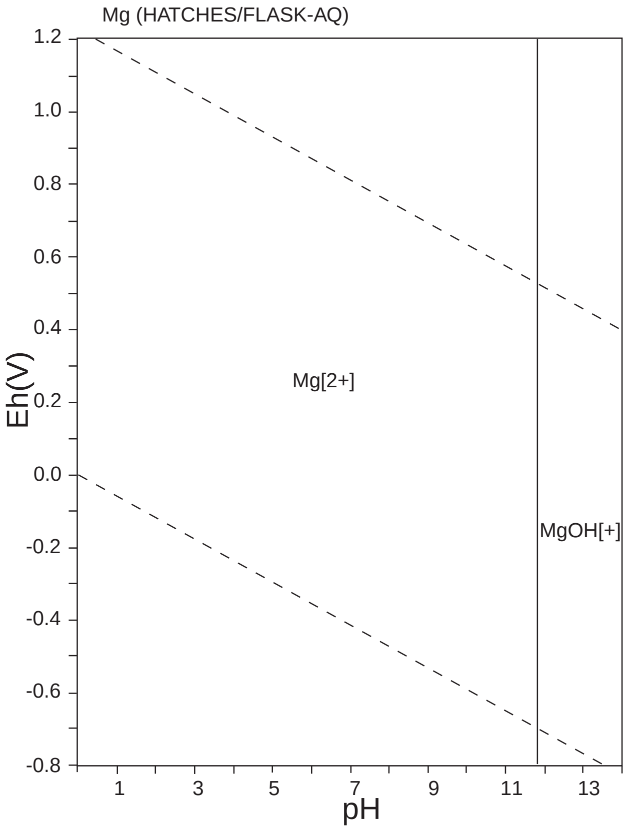

Figure 68: Eh-pH diagrams of the system Mg-O-H (2). $\sum \text{Mg} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 43: List of Mn species

FACT	SUPCRT	LLNL	JNC-TDB
Mn[2+], Mn[3+], MnO_4[2-], MnO_4[-], MnOH[+], $Mn(OH)_3$[-], **Mn(s), Mn(s2), Mn(s3), Mn(s4), MnO_2(s), Mn_2O_3(s), Mn_3O_4(s), Mn_3O_4(s2), MnO(s)**	Mn[2+], Mn[3+], MnO_4[2-], MnO_4[-], MnOH[+], $HMnO_2$[-], MnO(aq), MnO_2[2-], **MnO(Manganosite)**	Mn[2+], MnO_4[-], MnO_4[2-], $Mn(OH)_2$(aq), $Mn(OH)_3$[-], $Mn(OH)_4$[2-], $Mn_2(OH)_3$[+], Mn_2OH[3+], MnOH[+], **Birnessite, Bixbyite, Hausmannite, Manganite, Manganosite, $Mn(OH)_2$(am), $Mn(OH)_3$(c), Pyrolusite, Todorokite**	Mn[2+], Mn[3+], MnO_4[2-], MnO_4[-], MnOH[+], $Mn(OH)_3$[-], **Birnesite, Manganite, Pyrolusite**

HATCHES			
Mn[2+], Mn[3+], MnO_4[2-], $Mn(OH)_2$(aq), $Mn(OH)_3$[-], $Mn(OH)_4$[2-], $Mn_2(OH)_3$[+], Mn_2OH[3+], MnO_4[-], MnOH[+], MnOH[2+], **Birnessite, Bixbyite, Hausmannite, Manganite, Manganosite, $Mn(OH)_2$, $Mn(OH)_3$, $Mn(OH)_3$(c), Mn_3O_4, MnOOH, Pyrolusite, Todorokite**			

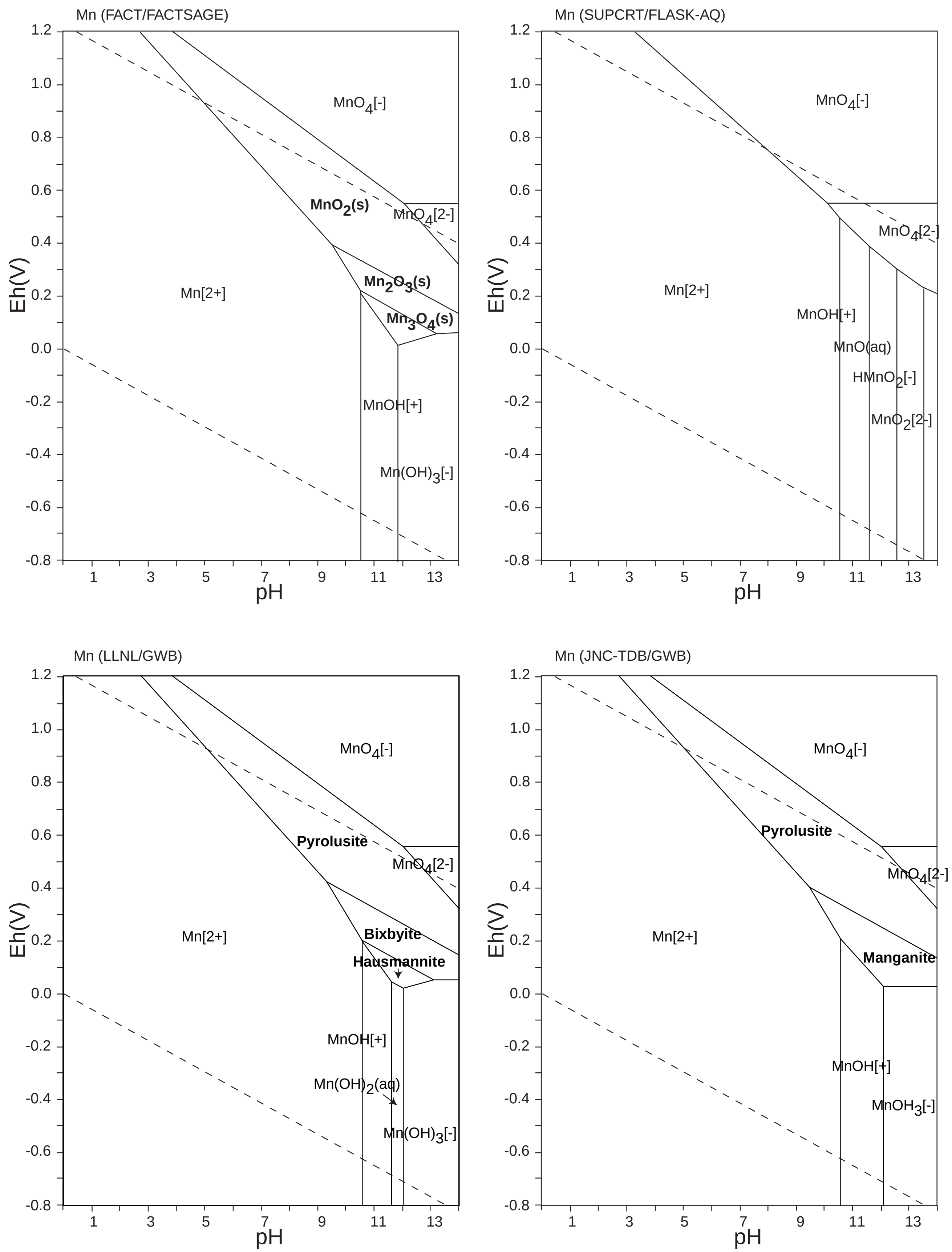

Figure 69: Eh-pH diagrams of the system Mn-O-H (1). $\sum \mathrm{Mn} = 10^{-10}$, 298.15K, 10^5 Pa.

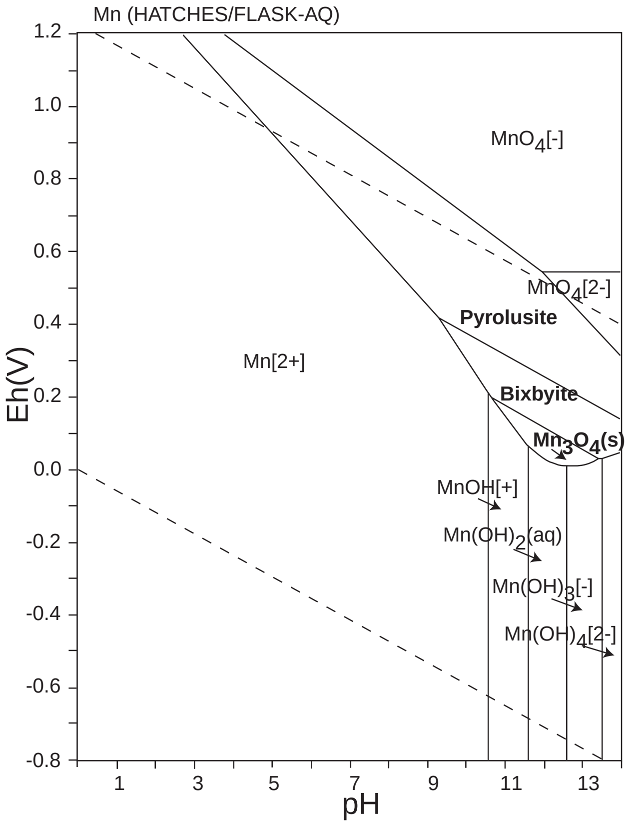

Figure 70: Eh-pH diagrams of the system Mn-O-H (2). $\sum \mathrm{Mn} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 44: List of Mo species

FACT	SUPCRT	LLNL	JNC-TDB
MoO_4[2-], **Mo(s)**, **MoO_2(s)**, **MoO_3(s)**	MoO_4[2-], $HMoO_4$[-]		

HATCHES			
MoO_4[2-], Mo[3+], MoO_2[+], H_2MoO_4(aq), $HMoO_4$[-], $Mo_7O_{21}(OH)_3$[3-], $Mo_7O_{22}(OH)_2$[4-], $Mo_7O_{23}OH$[5-], Mo_7O_{24}[6-], MoO[3+], MoO_2[2+], MoO_2OH[+], **H_2MoO_4**, **Mo**, **MoO_2**, **MoO_3**			

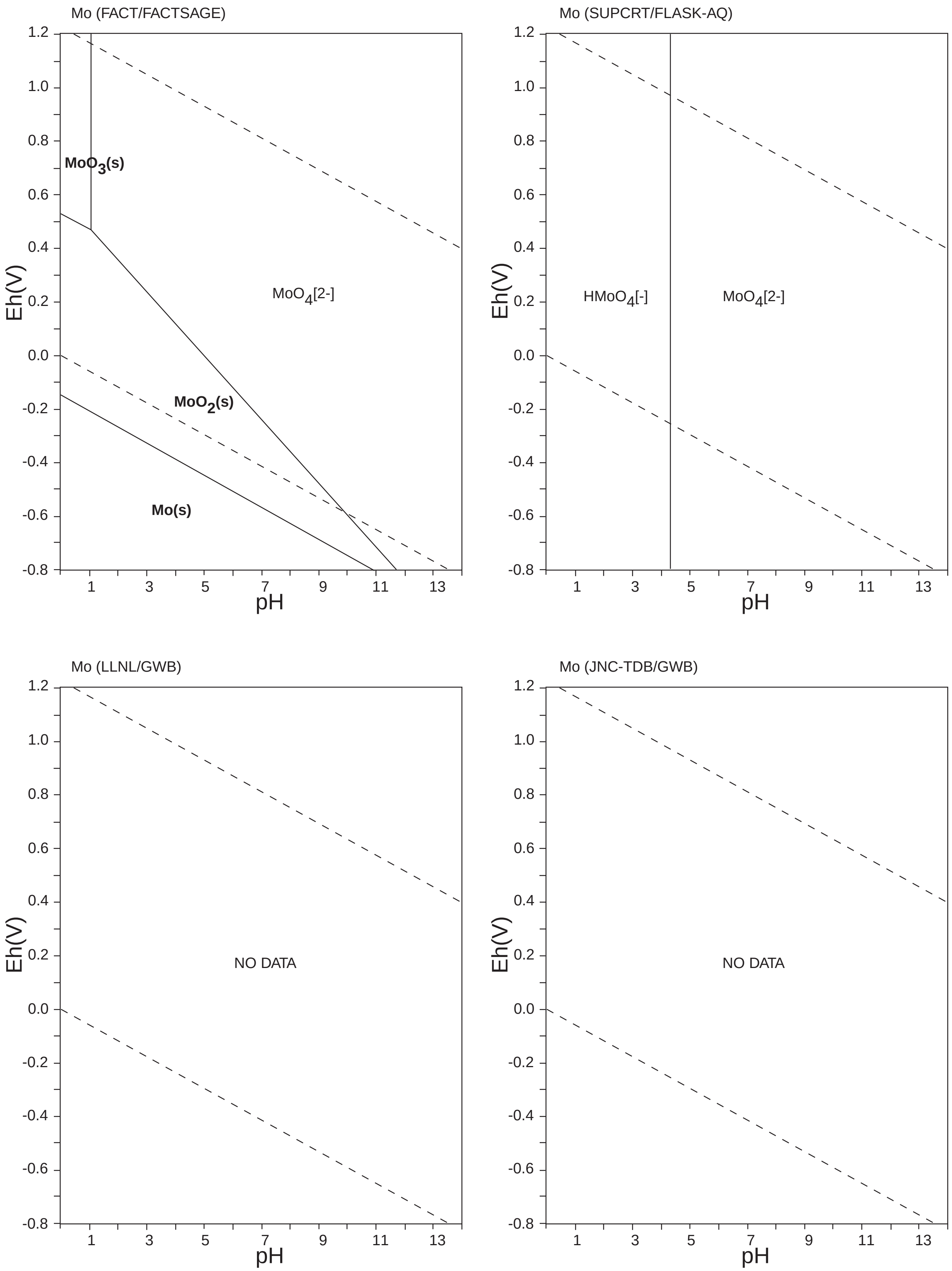

Figure 71: Eh-pH diagrams of the system Mo-O-H (1). $\sum \mathrm{Mo} = 10^{-10}$, 298.15K, 10^5 Pa.

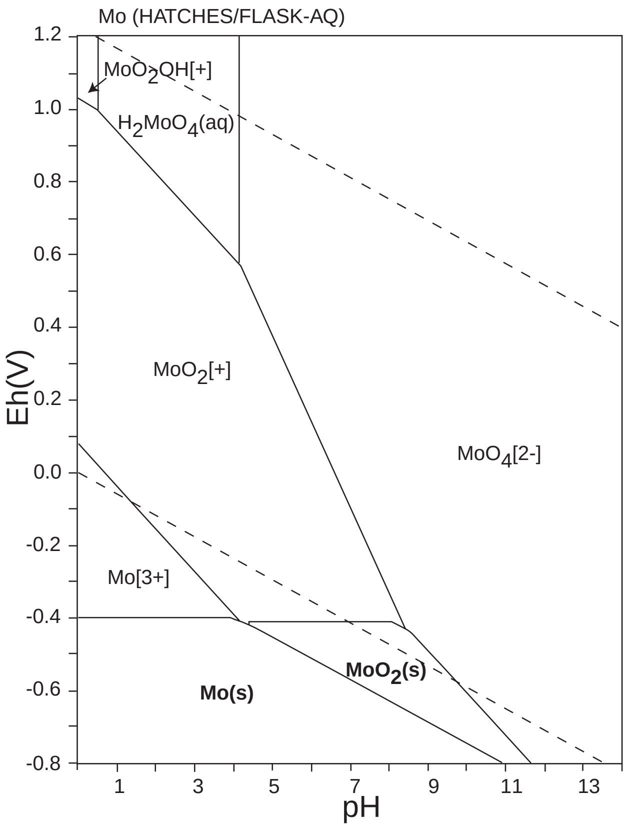

Figure 72: Eh-pH diagrams of the system Mo-O-H (2). $\sum \mathrm{Mo} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 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), **NH_4N_3(s), N_2O_4(s), N_2O_5(s), NH_4NO_3(s)**	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)			

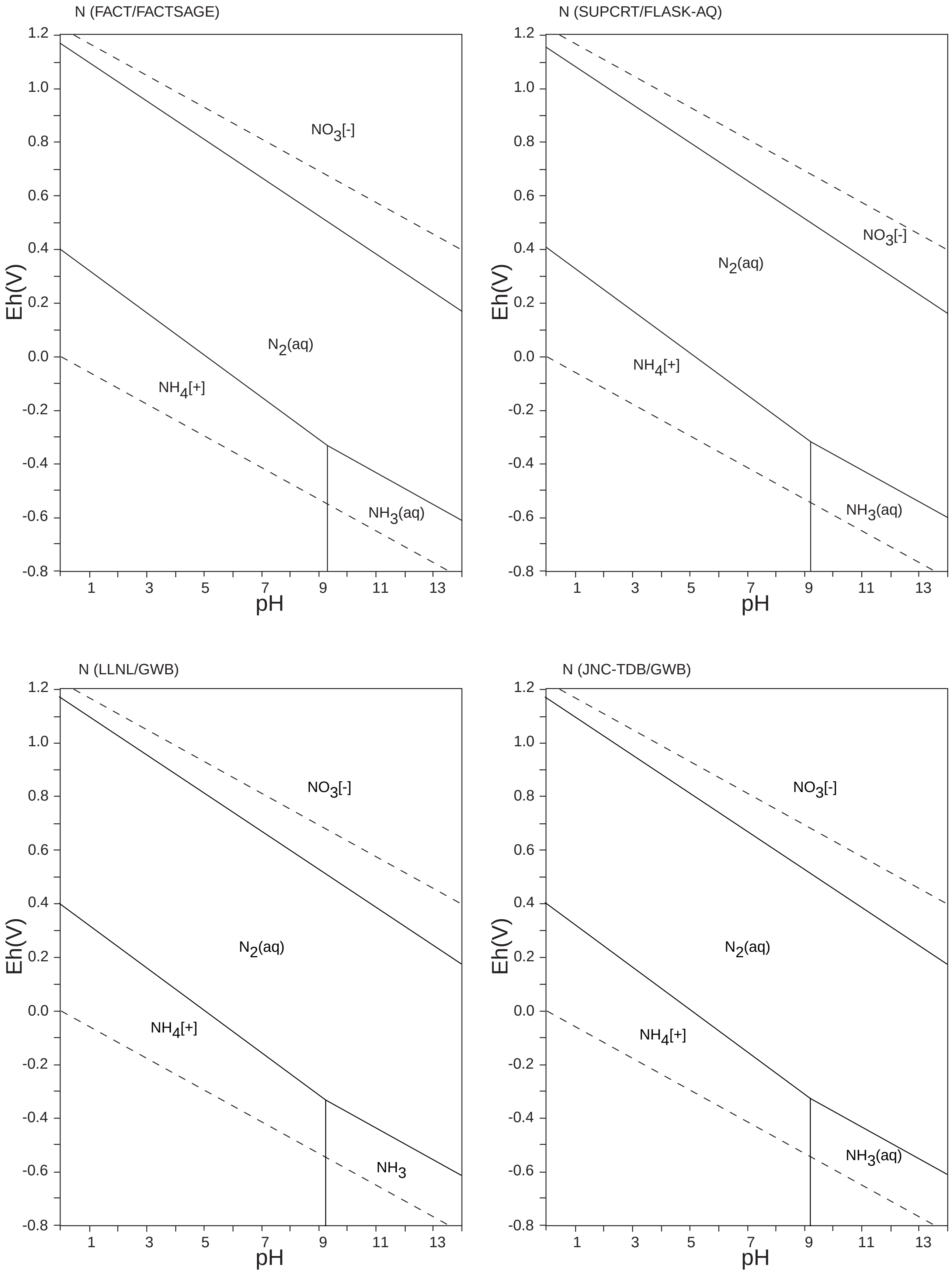

Figure 73: Eh-pH diagrams of the system N-O-H (1). $\sum \mathrm{N} = 10^{-10}$, 298.15K, 10^5 Pa.

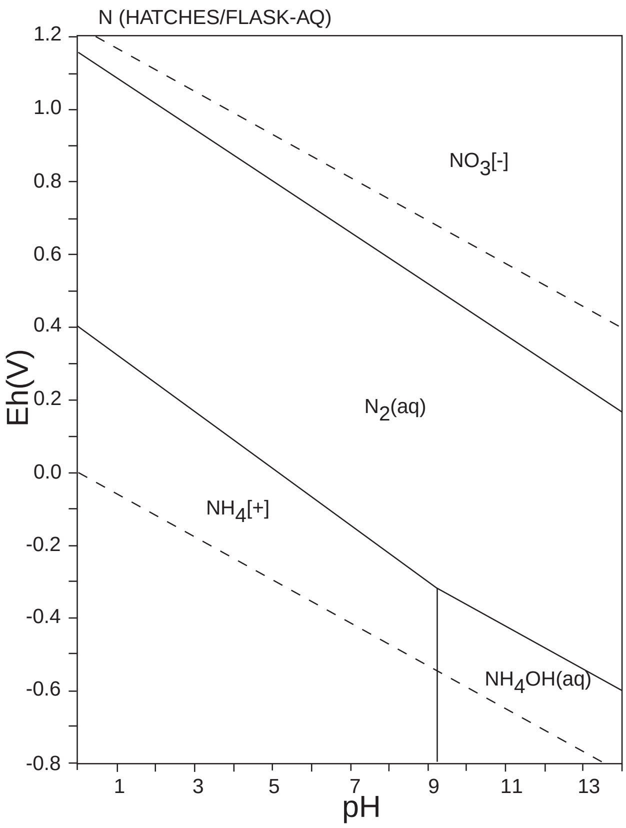

Figure 74: Eh-pH diagrams of the system N-O-H (2). $\sum \mathrm{N} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 46: List of Na species

FACT	SUPCRT	LLNL	JNC-TDB
Na[+], **Na(s), NaH(s), NaO_2(s), Na_2O(s2), Na_2O(s3), Na_2O_2(s), Na_2O_2(s2), NaOH(s), NaOH(s2), Na_2O(s)**	Na[+], NaOH(aq), **Na_2O(Sodium-oxide)**	Na[+], NaOH(aq)	Na+, **Na(c)**, Na(g)

HATCHES			
Na[+]			

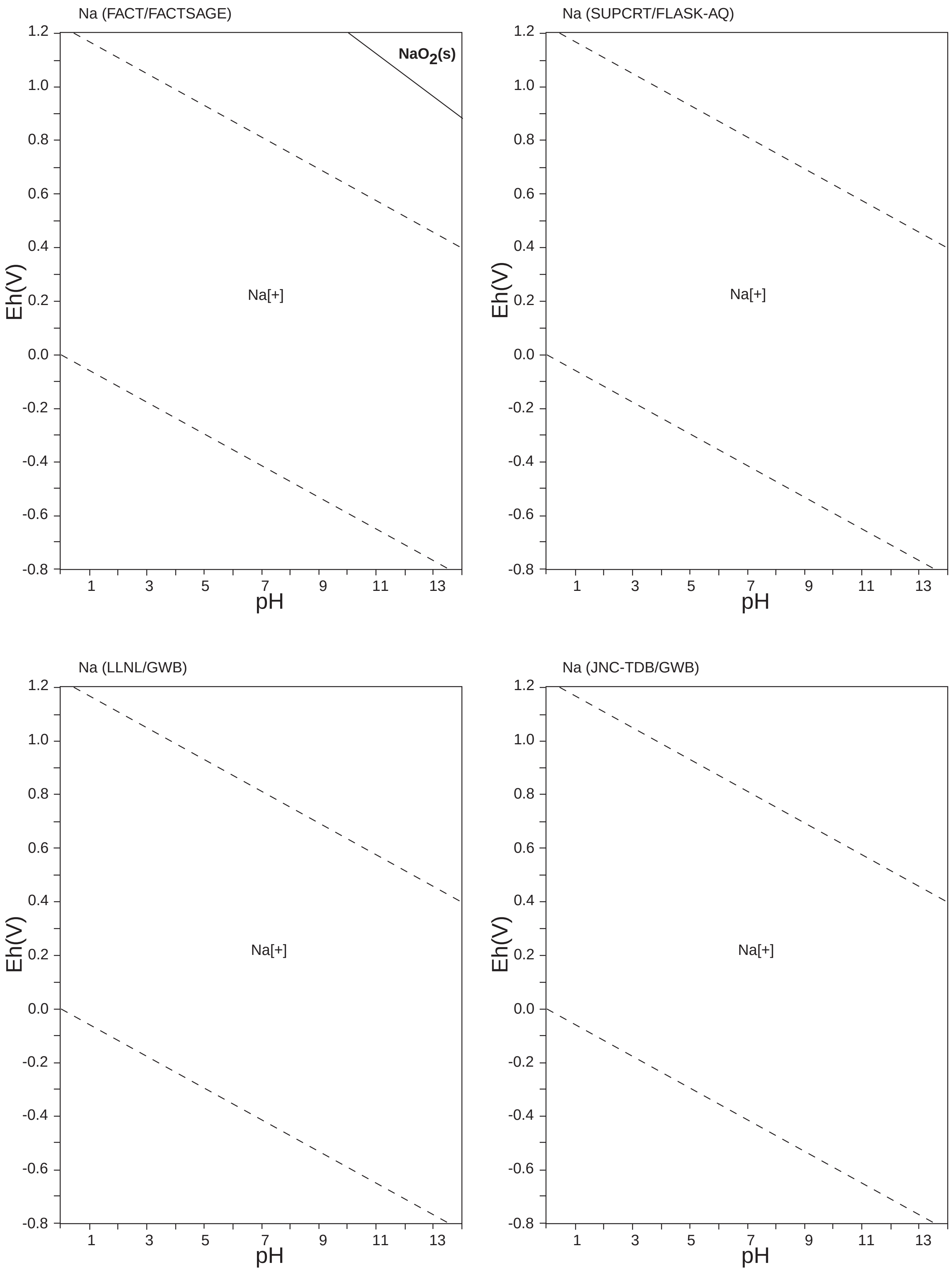

Figure 75: Eh-pH diagrams of the system Na-O-H (1). $\sum \mathrm{Na} = 10^{-10}$, 298.15K, 10^5 Pa.

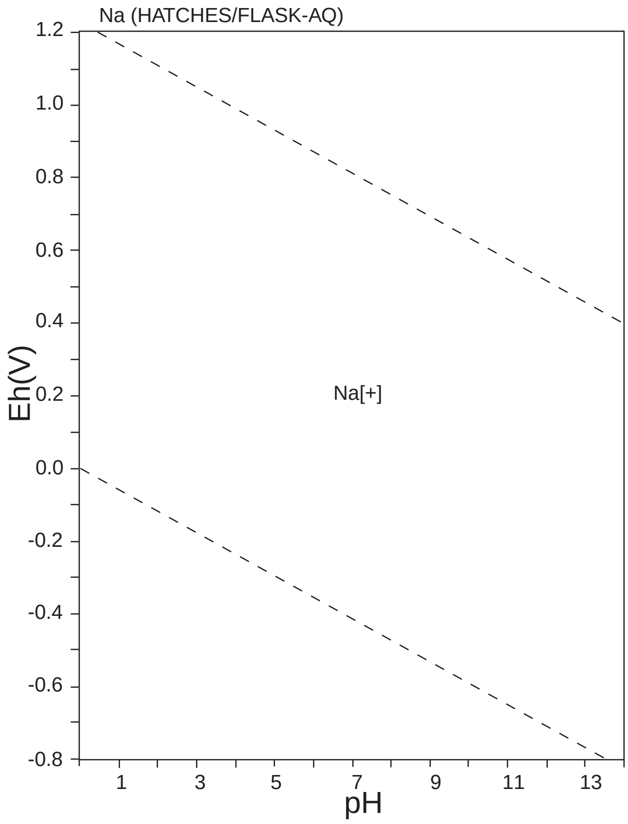

Figure 76: Eh-pH diagrams of the system Na-O-H (2). $\sum \text{Na} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 47: List of Nb species

FACT	SUPCRT	LLNL	JNC-TDB
NbO_3[-], $Nb(OH)_5$(aq), $Nb(OH)_4$[+], **Nb(s), NbO(s), NbO_2(s), NbO_2(s2), NbO_2(s3), Nb_2O_5(s)**	NbO_3[-], $HNbO_3$(aq)		$Nb(OH)_5$(aq), $Nb(OH)_6$[-], **Nb_2O_5(s)**

HATCHES			
$Nb(OH)_5$(aq), $Nb(OH)_4$[+], $Nb(OH)_6$[-], **Nb_2O_5(act)**			

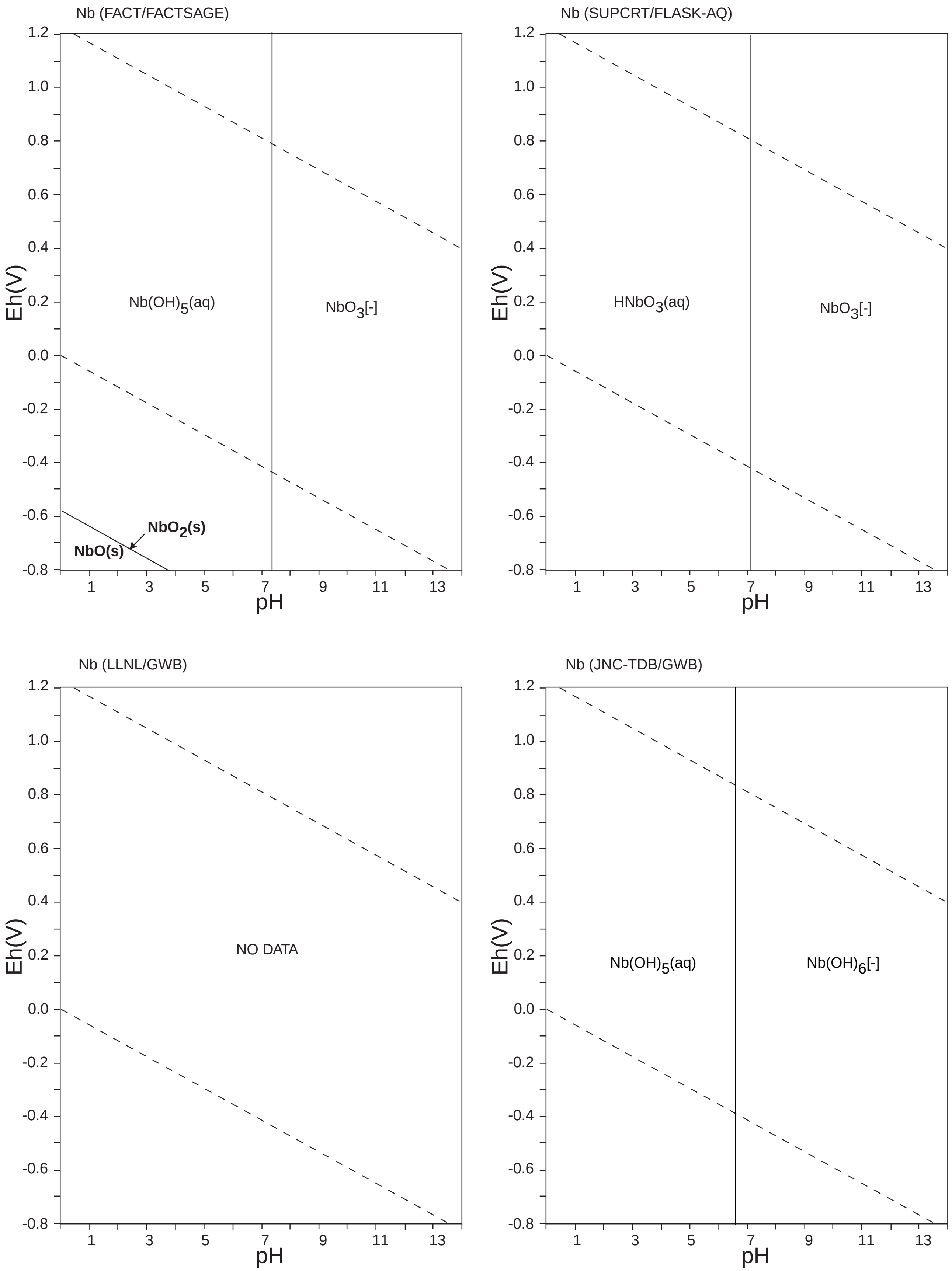

Figure 77: Eh-pH diagrams of the system Nb-O-H (1). $\sum \mathrm{Nb} = 10^{-10}$, 298.15K, 10^5 Pa.

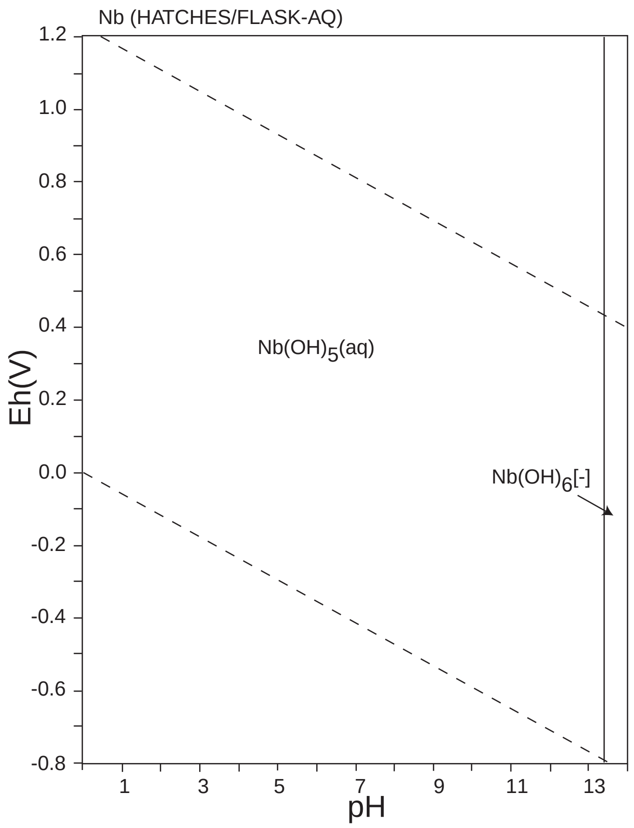

Figure 78: Eh-pH diagrams of the system Nb-O-H (2). $\sum \mathrm{Nb} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 48: List of Nd species

FACT	SUPCRT	LLNL	JNC-TDB
$Nd[3+]$, **$Nd(s)$**, **$Nd(s2)$**, **$NdH_2(s)$**, **$Nd_2O_3(s)$**, **$Nd_2O_3(s2)$**	$Nd[3+]$, $Nd[4+]$, $Nd[2+]$, $NdOH[2+]$, $NdO[+]$, $NdO_2H(aq)$, $NdO_2[-]$		$Nd[3+]$

HATCHES			
$Nd[3+]$, $Nd(OH)_2[+]$, $Nd(OH)_3(aq)$, $NdOH[2+]$, **$Nd(OH)_3$**			

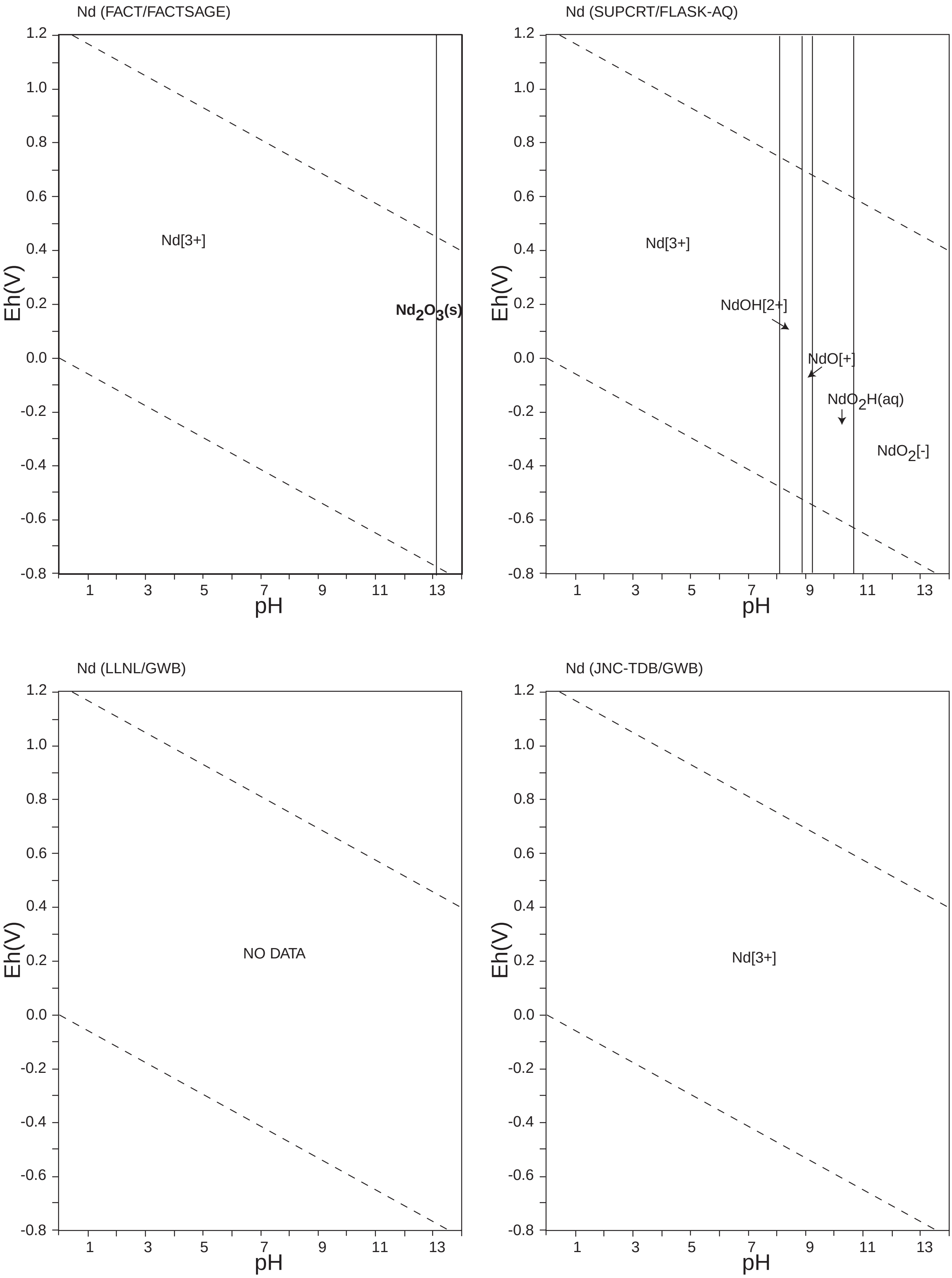

Figure 79: Eh-pH diagrams of the system Nd-O-H (1). $\sum \mathrm{Nd} = 10^{-10}$, 298.15K, 10^5 Pa.

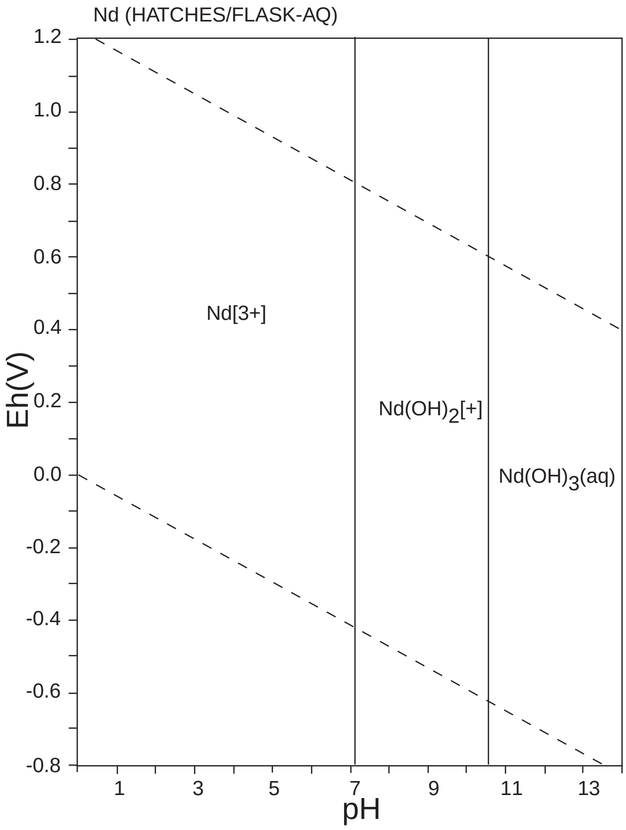

Figure 80: Eh-pH diagrams of the system Nd-O-H (2). $\sum \mathrm{Nd} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 49: List of Ni species

FACT	SUPCRT	LLNL	JNC-TDB
Ni[2+], NiOH[+], $HNiO_2$[-], **Ni_2H(s), NiOOH(s), $Ni(OH)_2$(s), $NiO_2(H_2O)$(s), Ni(s), NiO(s)**	Ni[2+], NiOH[+], $HNiO_2$[-], NiO(aq), NiO_2[2-], **Ni(Nickel), NiO(Bunsenite)**	Ni[2+], $Ni(OH)_2$, $Ni(OH)_3$[-], $Ni(OH)_4$[2-], Ni_2OH[3+], $Ni_4(OH)_4$[4+], NiOH[+], **$Ni(OH)_2$(s), NiO(s)**	Ni[2+], $Ni(OH)_2$(aq), $Ni(OH)_3$[-], NiOH[+], $Ni_2(OH)$[+], $Ni_4(OH)$[+], **$Ni(OH)_2$(s), NiO(c)**

HATCHES			
Ni[2+], Ni(OH)[+], $Ni(OH)_2$(aq), $Ni(OH)_3$[-], $Ni_2(OH)$[3+], $Ni_4(OH)_4$[4+], **$Ni(OH)_2$, NiO**			

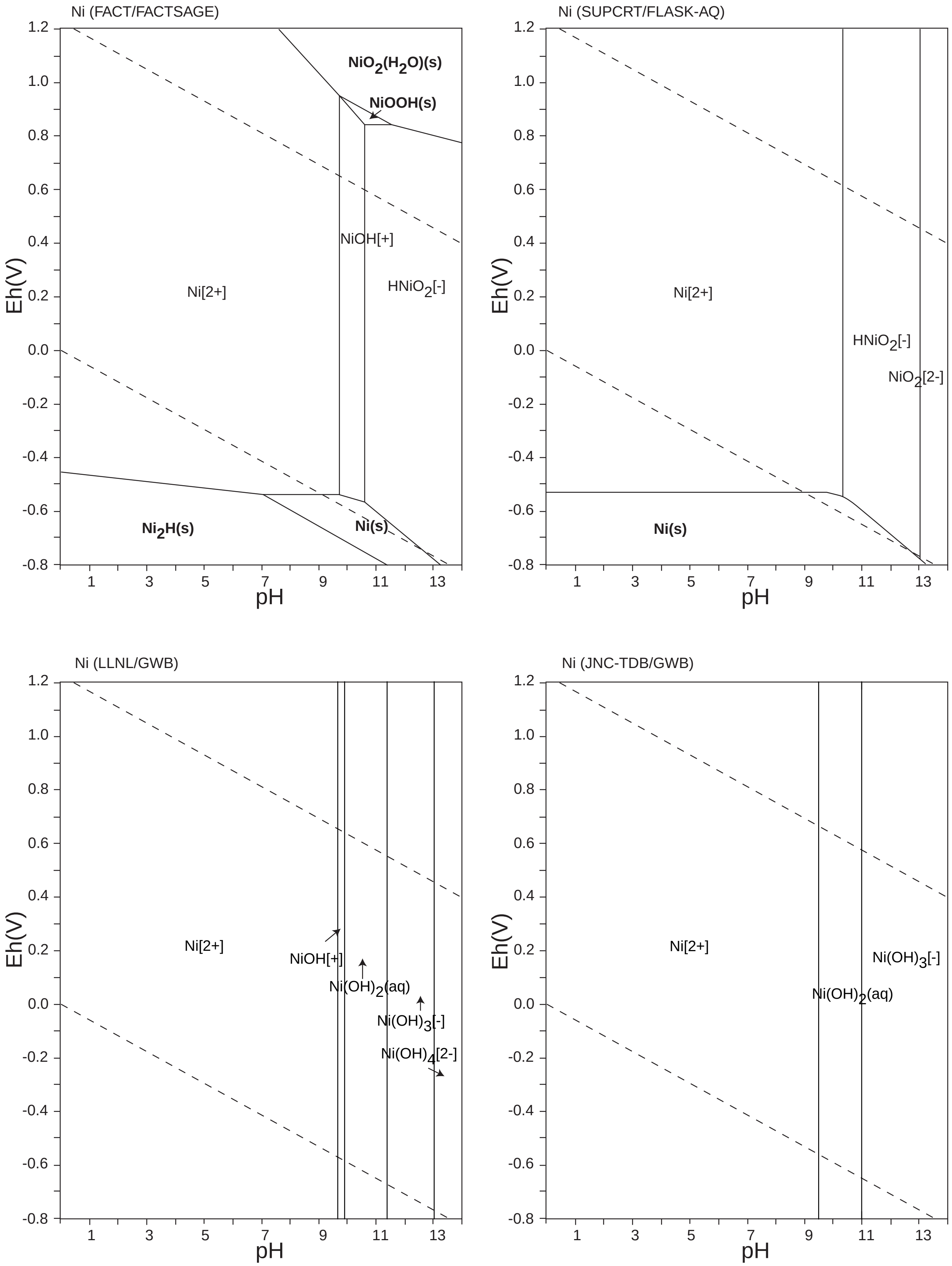

Figure 81: Eh-pH diagrams of the system Ni-O-H (1). $\sum \mathrm{Ni} = 10^{-10}$, 298.15K, 10^5 Pa.

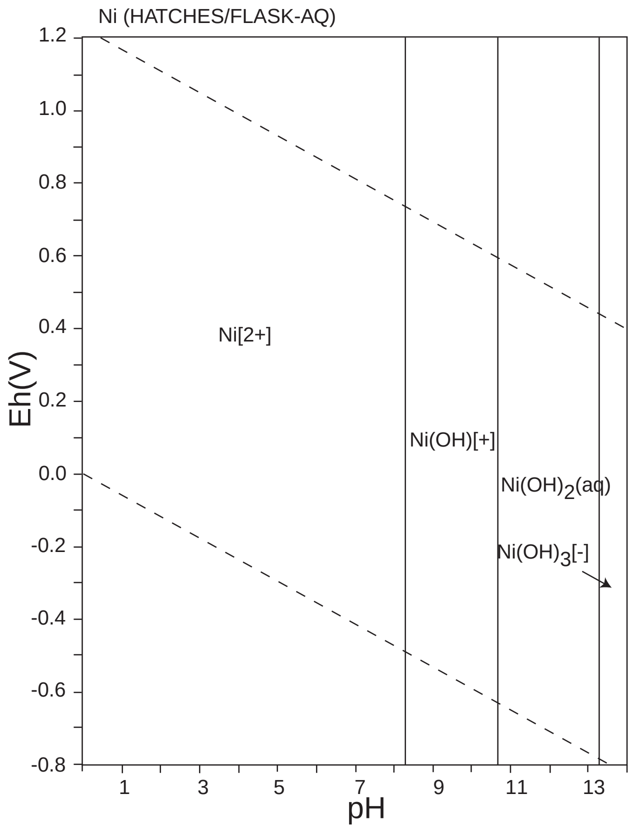

Figure 82: Eh-pH diagrams of the system Ni-O-H (2). $\sum \mathrm{Ni} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 50: List of Np species

FACT	SUPCRT	LLNL	JNC-TDB
Np(s), NpO_2(s), $NpO_3(H_2O)$(s)		Np[4+], Np[3+], NpO_2[+], NpO_2[2+], $(NpO_2)_2(OH)_2$[2+], $(NpO_2)_3(OH)_5$[+], $Np(OH)_2$[2+], $Np(OH)_3$[+], $Np(OH)_4$(aq), $Np(OH)_5$[-], NpO_2OH(aq), NpO_2OH[+], NpOH[2+], NpOH[3+], **Np(s), $Np(OH)_4$(s), Np_2O_5(s), NpO_2(s), NpO_2(OH)(am), $NpO_2(OH)_2$(s)**	Np[4+], Np[3+], NpO_2[+] NpO_2OH(am), $NpO_2(OH)_2$[-] NpO_2[2+], NpOH[3+], **$Np(OH)_4$(s), NpO_2(am), NpO_2OH(am)**

HATCHES	OECD-NEA	OECD-NEA update	
Np[4+], Np[3+], NpO_2[+], NpO_2[2+], $Np(OH)_2$[+], $Np(OH)_3$(aq), $Np(OH)_4$(aq), $Np(OH)_4$[-], $Np_2(OH)_2$[4+], $NpO_{22}OH_2$[2+], $NpO_{23}OH_5$[+], NpO_2OH(aq), NpO_2OH[+], NpO_2OH_2[-], NpOH[2+], NpOH[3+], **Np, $Np(OH)_3$, $Np(OH)_4$, Np_2O_5, NpO_2, NpO_2(am), $NpO_2(OH)_2$, NpO_2OH, NpO_2OH(am,aged), NpO_2OH(am,fresH), NpO_3*H_2O(cr)**	Np[4+], Np[3+], NpO_2[+], NpO_2[2+], NpOH[2+], NpOH[3+], NpO_2OH(aq), NpO_2OH[+], $NpO_2(OH)_2$[-], $Np(OH)_4$(aq), $(NpO_2)_2(OH)_2$[2+], $(NpO_2)_3(OH)_5$[+], **Np(c), NpO_2(am_hyd), NpO_2(c), Np_2O_5(c), NpO_2OH(am_aged), NpO_2OH(am_fresh), $NpO_2(OH)_2$(c), NpO_3H_2O(c)**	Np[4+], Np[3+], NpO_2[+], NpO_2[2+], NpOH[2+], NpOH[3+], $Np(OH)_2$[2+], NpO_2OH(aq), NpO_2OH[+], $NpO_2(OH)_2$[-], $Np(OH)_4$(aq), $(NpO_2)_2(OH)_2$[2+], $(NpO_2)_3(OH)_5$[+], **Np(cr), NpO_2(cr), Np_2O_5(cr), $NpO_2(OH)_2$(cr), NpO_3H_2O(cr)**	

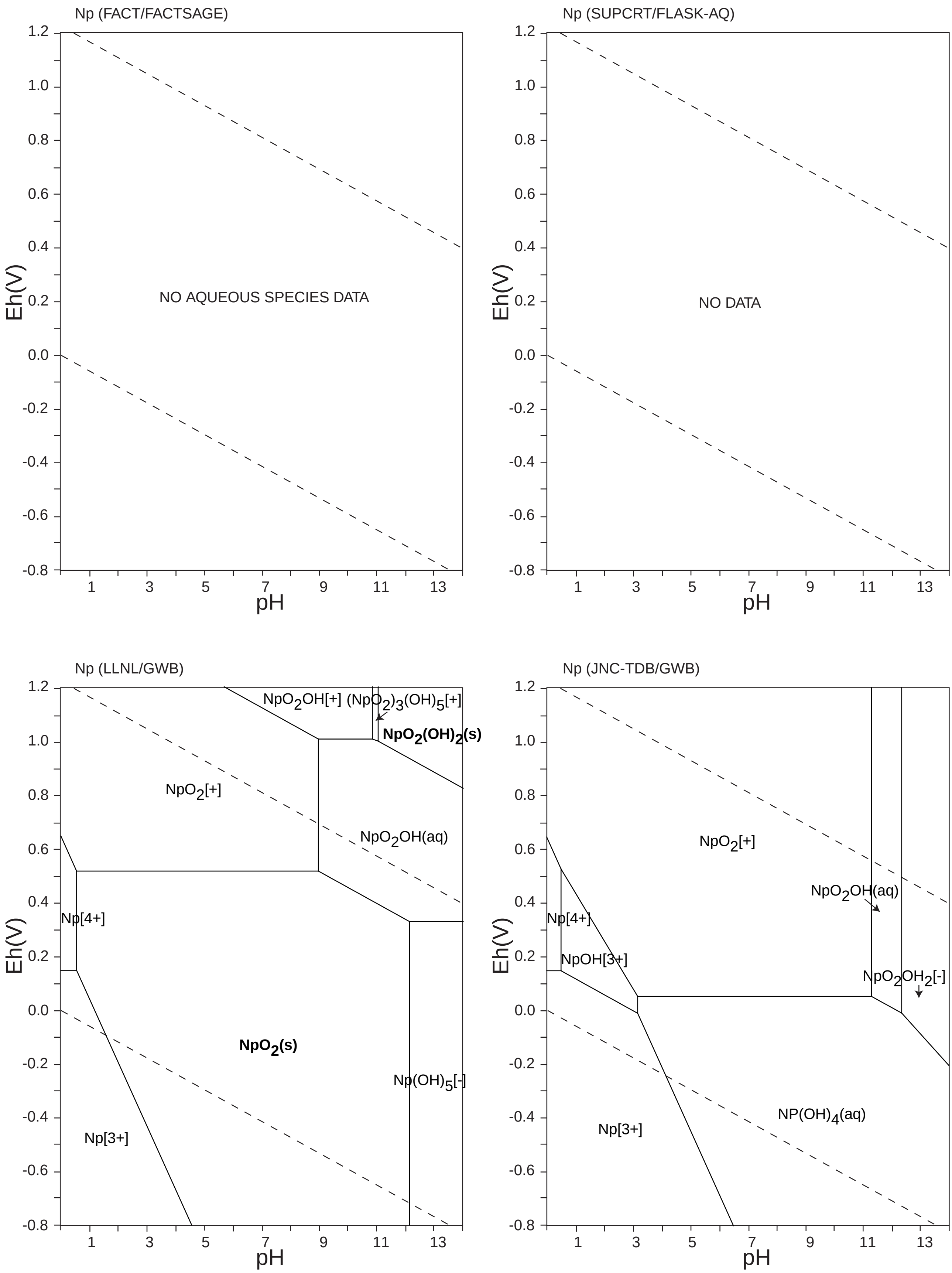

Figure 83: Eh-pH diagrams of the system Np-O-H (1). $\sum \mathrm{Np} = 10^{-10}$, 298.15K, 10^5 Pa.

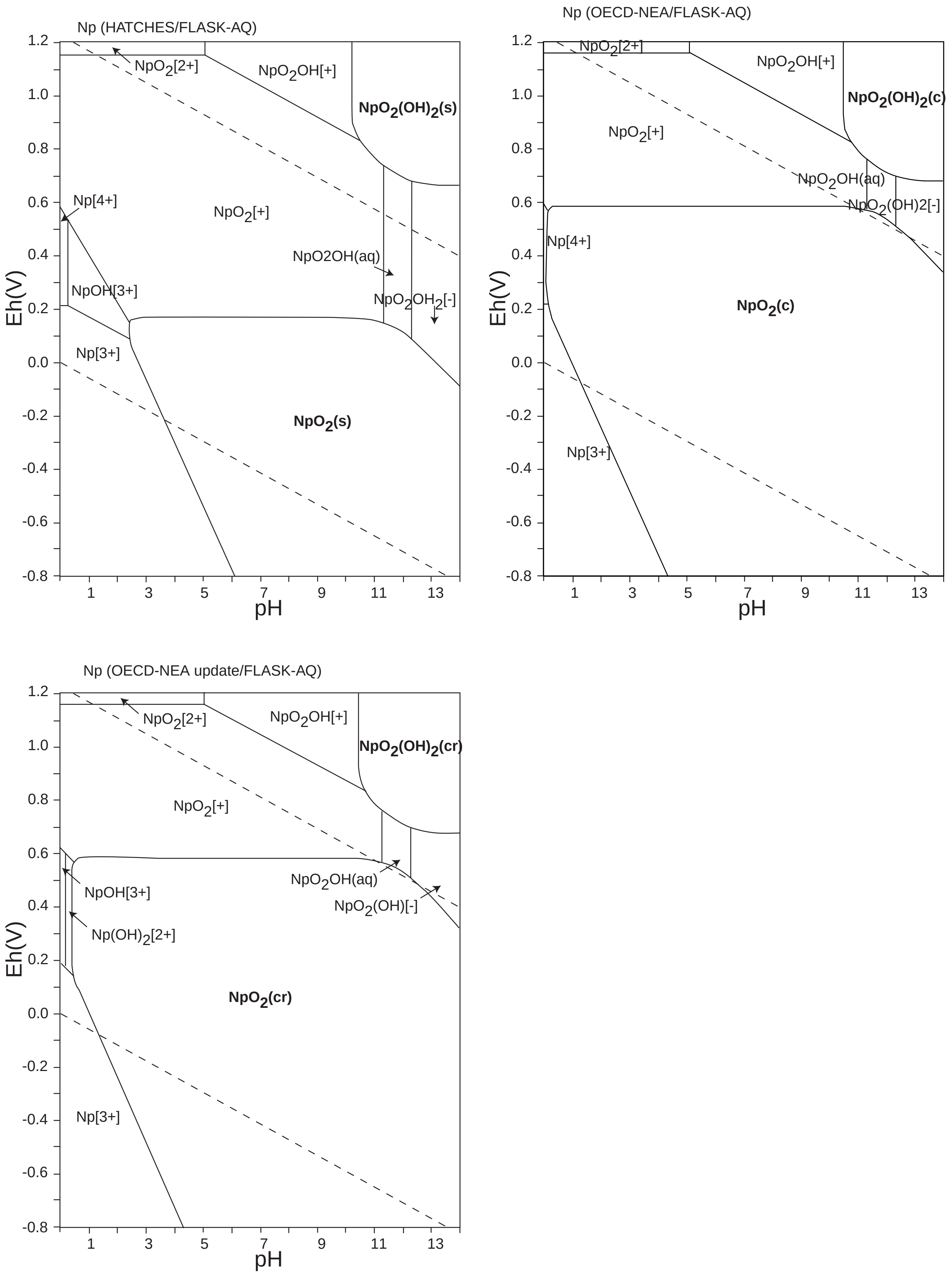

Figure 84: Eh-pH diagrams of the system Np-O-H (2). $\sum \mathrm{Np} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 51: List of Os species

FACT	SUPCRT	LLNL	JNC-TDB
OsO_4(aq), $HOsO_5$[-], H_2OsO_5[-], **Os(s)**, **OsO_2(s)**, **OsO_4(s)**, **OsO_4(s2)**, **$Os(OH)_4$(s)**			

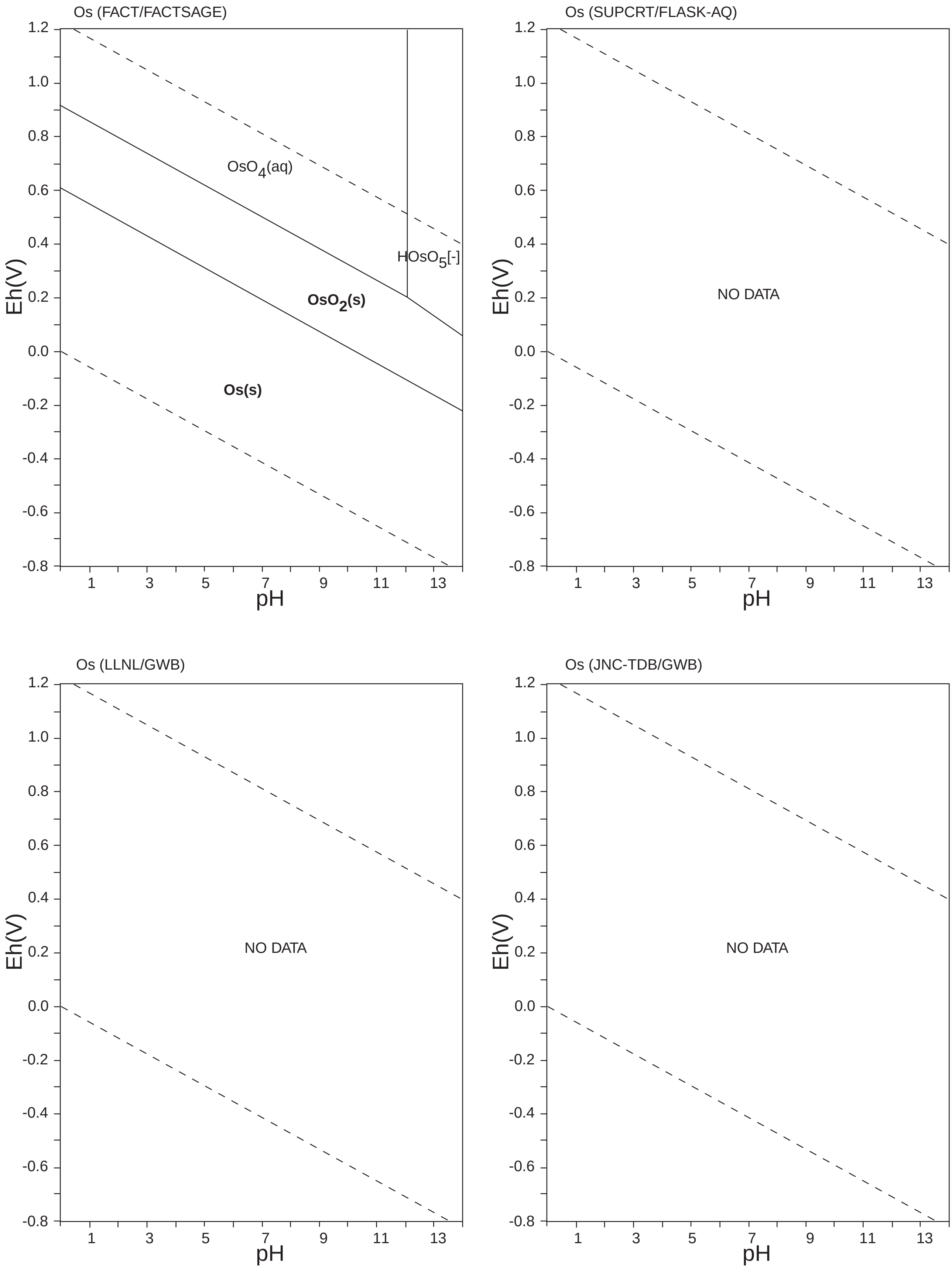

Figure 85: Eh-pH diagrams of the system Os-O-H. $\sum \mathrm{Os} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 52: List of P species

FACT	SUPCRT	LLNL	JNC-TDB
$PO_4[3-]$, $P_2O_7[4-]$, $HPO_3[2-]$, $H_2PO_3[-]$, $HPO_4[2-]$, $H_2PO_4[-]$, $H_3PO_4(aq)$, $HP_2O_7[3-]$, $H_2P_2O_7[2-]$, $H_3P_2O_7[-]$, $H_4P_2O_7(aq)$, $PH_3(aq)$, $PH_4[+]$, **P(s)**, **P(s2)**, **P(s3)**, **P(s4)**, **$(P_2O_5)_2$(s)**, **H_3PO_4(s)**, **$(H_3PO_4)_2(H_2O)$(s)**	$PO_4[3-]$, $P_2O_7[4-]$, $HPO_3[2-]$, $HPO_4[2-]$, $H_2PO_4[-]$, $H_3PO_4(aq)$, $HP_2O_7[3-]$, $H_3P_2O_7[-]$, $H_4P_2O_7(aq)$,$H_3PO_2(aq)$, $H_2PO_2[-]$, $H_3PO_3(aq)$, $H_2P_2O_7[2-]$, $H_2PO_3[-]$	$HPO_4[2-]$, $H_2P_2O_7[2-]$, $H_2PO_4[-]$, $H_3P_2O_7[-]$ $H_3PO_4(aq)$, $H_4P_2O_7(aq)$, $HP_2O_7[3-]$, $P_2O_7[4-]$, $PO_4[3-]$	$PO_4[3-]$, $P_2O_7[4-]$, $HPO_4[2-]$, $H_2PO_4[-]$, $H_3PO_4(aq)$, $HP_2O_7[3-]$, $H_2P_2O_7[2-]$, $H_3P_2O_7[-]$, **$H_4P_2O_7$(am)**, **P(am)** **P(c)**, P(g), P_2(g), P_4(g)

HATCHES			
$PO_4[3-]$, $H_2PO_4[-]$, $HPO_4[2-]$, $H_2P_2O_7[2-]$, $H_3P_2O_7[-]$, $H_3PO_4(aq)$, $H_4P_2O_7(aq)$, $HP_2O_7[3-]$, $P_2O_7[3-]$			

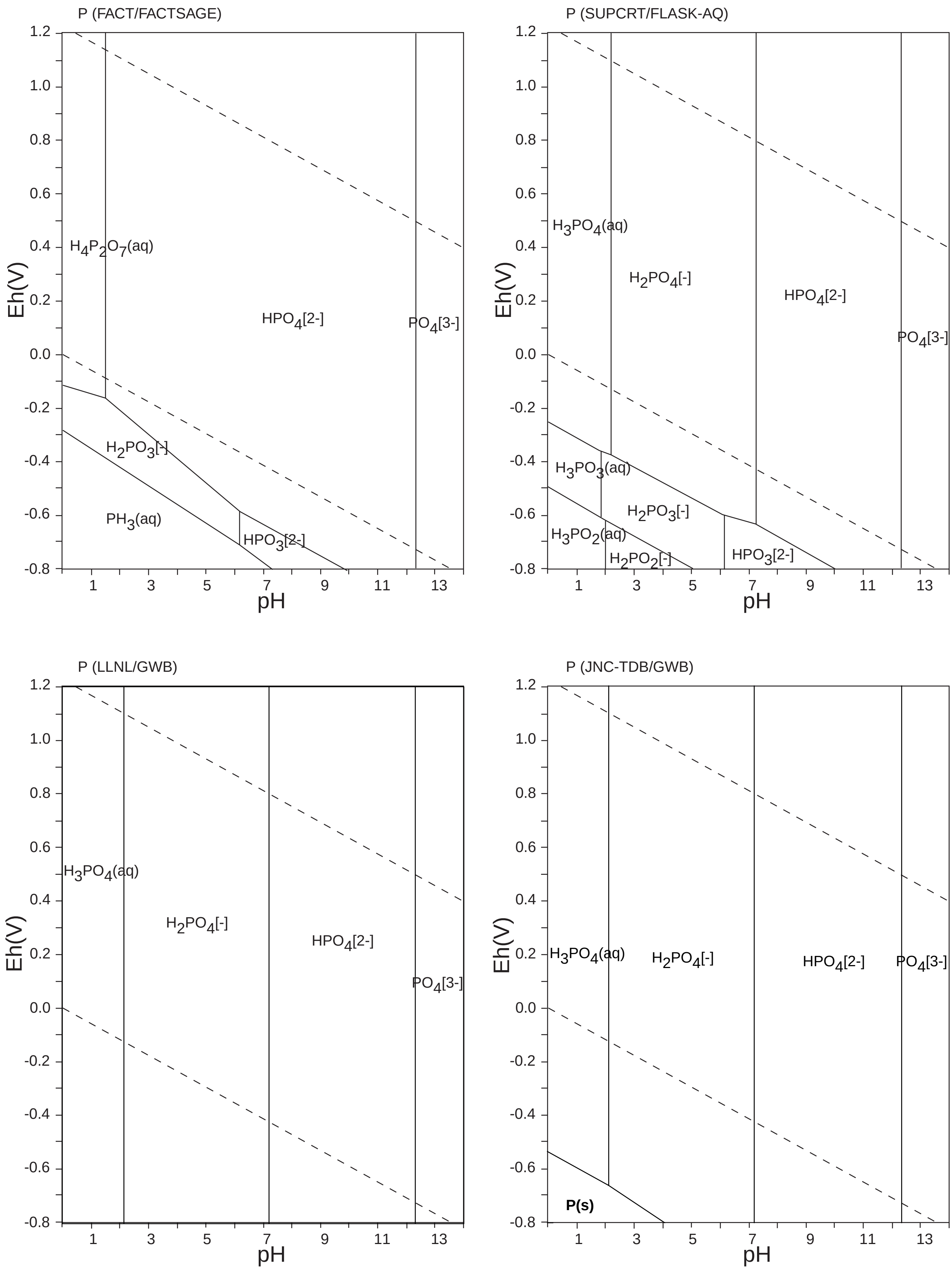

Figure 86: Eh-pH diagrams of the system P-O-H (1). $\sum \mathrm{P} = 10^{-10}$, 298.15K, 10^5 Pa.

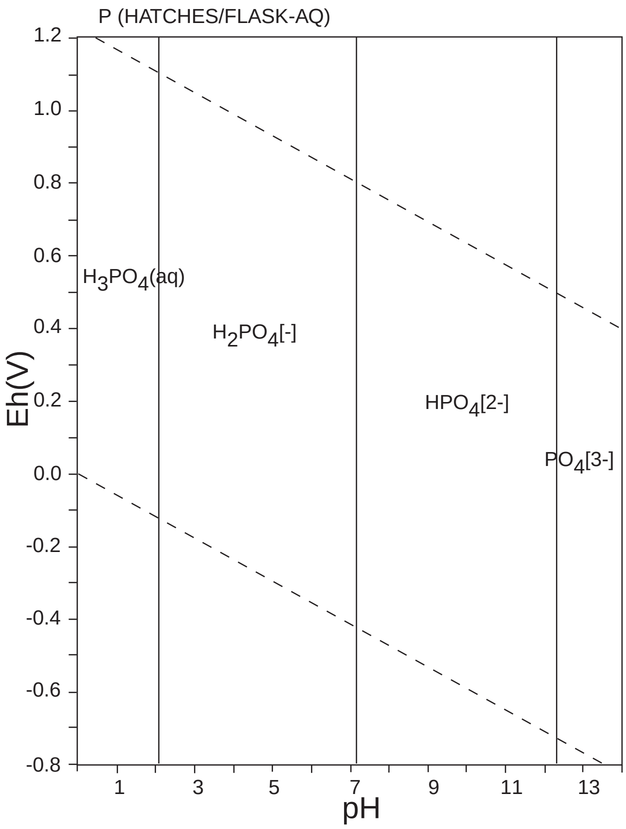

Figure 87: Eh-pH diagrams of the system P-O-H (2). $\sum P = 10^{-10}$, 298.15K, 10^5 Pa.

Table 53: List of Pa species

FACT	SUPCRT	LLNL	JNC-TDB
			$Pa[4+]$, $PaO(OH)_3(aq)$ $PaO(OH)_2(aq)$, $PaOOH[2+]$, $Pa(OH)[3+]$, $Pa(OH)_2[+]$, $Pa(OH)_3[+]$, **$PaO_2(s)$**, **$Pa_2O_5(s)$**

HATCHES			
$Pa[4+]$, $PaO_2[+]$, $Pa(OH)[3+]$, $Pa(OH)_2[2+]$, $Pa(OH)_3[+]$, $Pa(OH)_4(aq)$, $PaO(OH)[2+]$, $PaO_2(OH)(aq)$, **Pa_2O5, PaO_2**			

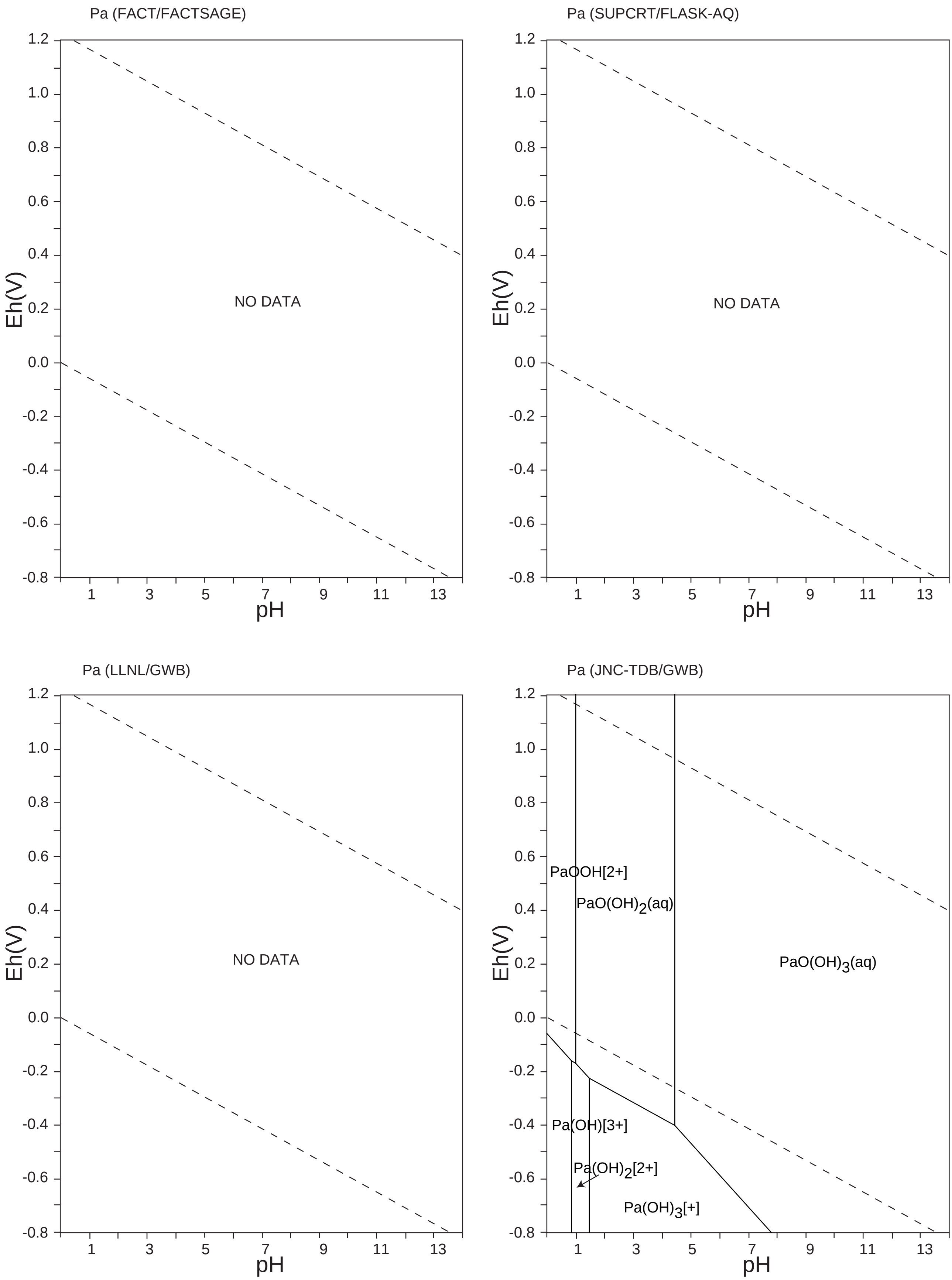

Figure 88: Eh-pH diagrams of the system Pa-O-H (1). $\sum \mathrm{Pa} = 10^{-10}$, 298.15K, 10^5 Pa.

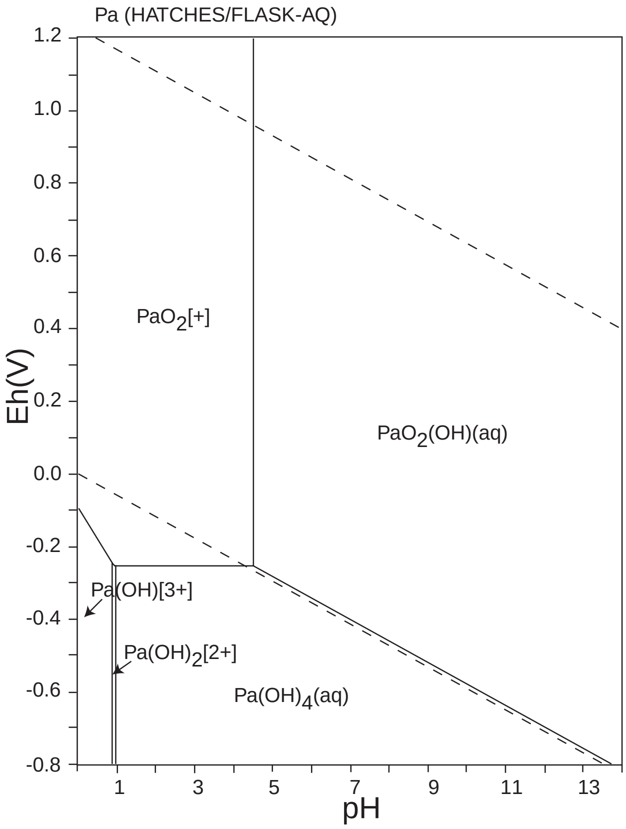

Figure 89: Eh-pH diagrams of the system Pa-O-H (2). $\sum \mathrm{Pa} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 54: List of Pb species

FACT	SUPCRT	LLNL	JNC-TDB
$Pb[2+]$, $PbOH[+]$, $HPbO_2[-]$, $Pb_3(OH)_4[2+]$, $Pb_4(OH)_4[4+]$, $Pb_6(OH)_8[4+]$, **Pb(s)**, **PbO(s2)**, **PbO_2(s)**, **Pb_3O_4(s)**, **$Pb(OH)_2$(s)**, **$(PbO)_3(H_2O)$(s)**, **PbO(s)**	$Pb[2+]$, $PbOH[+]$, $HPbO_2[-]$, PbO(aq), **PbO(Litharge)**	$Pb[2+]$	$Pb[2+]$, $PbOH[+]$, $Pb(OH)_2$(aq), $Pb(OH)_3[-]$, $Pb_2(OH)[+]$, $Pb_4(OH)_4[4+]$, $Pb_3(OH)_4[2+]$, $Pb_3(OH)_5[+]$ $Pb_6(OH)_8[4+]$, **Pb(c)** **PbO(red)**, **PbO(yellow)** **$Pb(OH)_2$(s)**, **PbO_2(s)**, **Pb_3O_4(s)**

HATCHES			
$Pb[2+]$, Pb(iv)[4+], $Pb(OH)[+]$, $Pb(OH)_2$(aq), $Pb(OH)_3[+]$, $Pb(OH)_3[-]$, $Pb(OH)_4$(aq), $Pb_2(OH)[3+]$, $Pb_3(OH)_4[2+]$, $Pb_6(OH)_8[4+]$, **Pb**, **$Pb(OH)_2$**, **Pb_3O_4**, **PbO**, **PbO_2**			

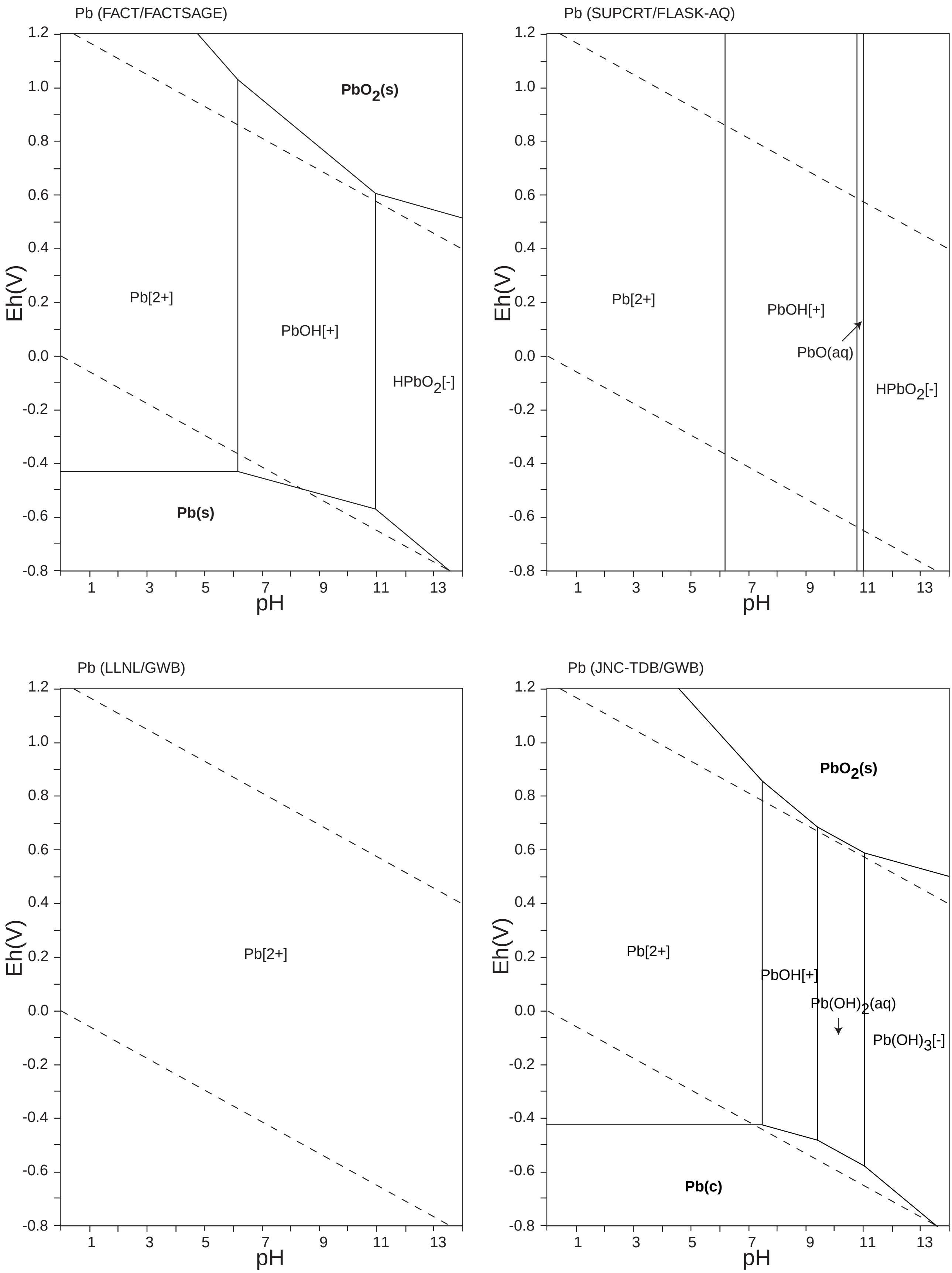

Figure 90: Eh-pH diagrams of the system Pb-O-H (1). $\sum \mathrm{Pb} = 10^{-10}$, 298.15K, 10^5 Pa.

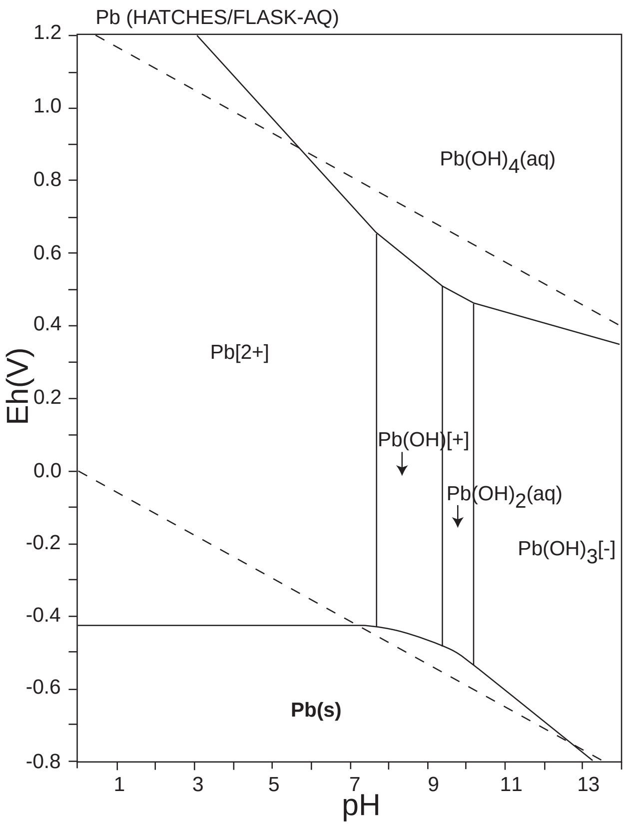

Figure 91: Eh-pH diagrams of the system Pb-O-H (2). $\sum \mathrm{Pb} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 55: List of Pd species

FACT	SUPCRT	LLNL	JNC-TDB
Pd[2+], **PdO_2(s)**, **Pd(s)**, **PdO(s)**	Pd[2+], PdOH[+], PdO(aq), **Pd(Palladium)**, **PdO(s)**, **$Pd(OH)_2$(s)**		Pd[2+], **Pd(c)**

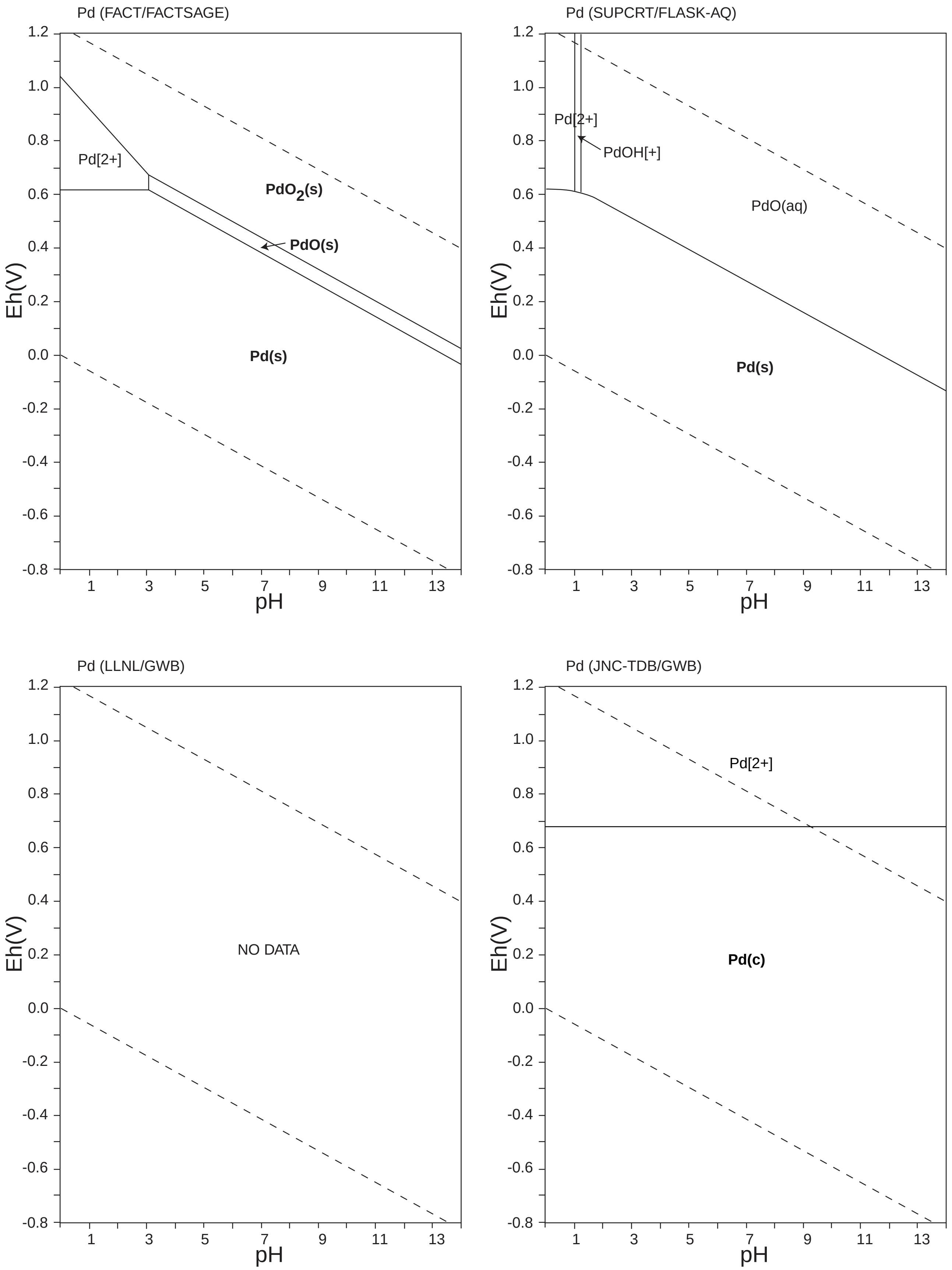

Figure 92: Eh-pH diagrams of the system Pd-O-H. $\sum \mathrm{Pd} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 56: List of Pm species

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

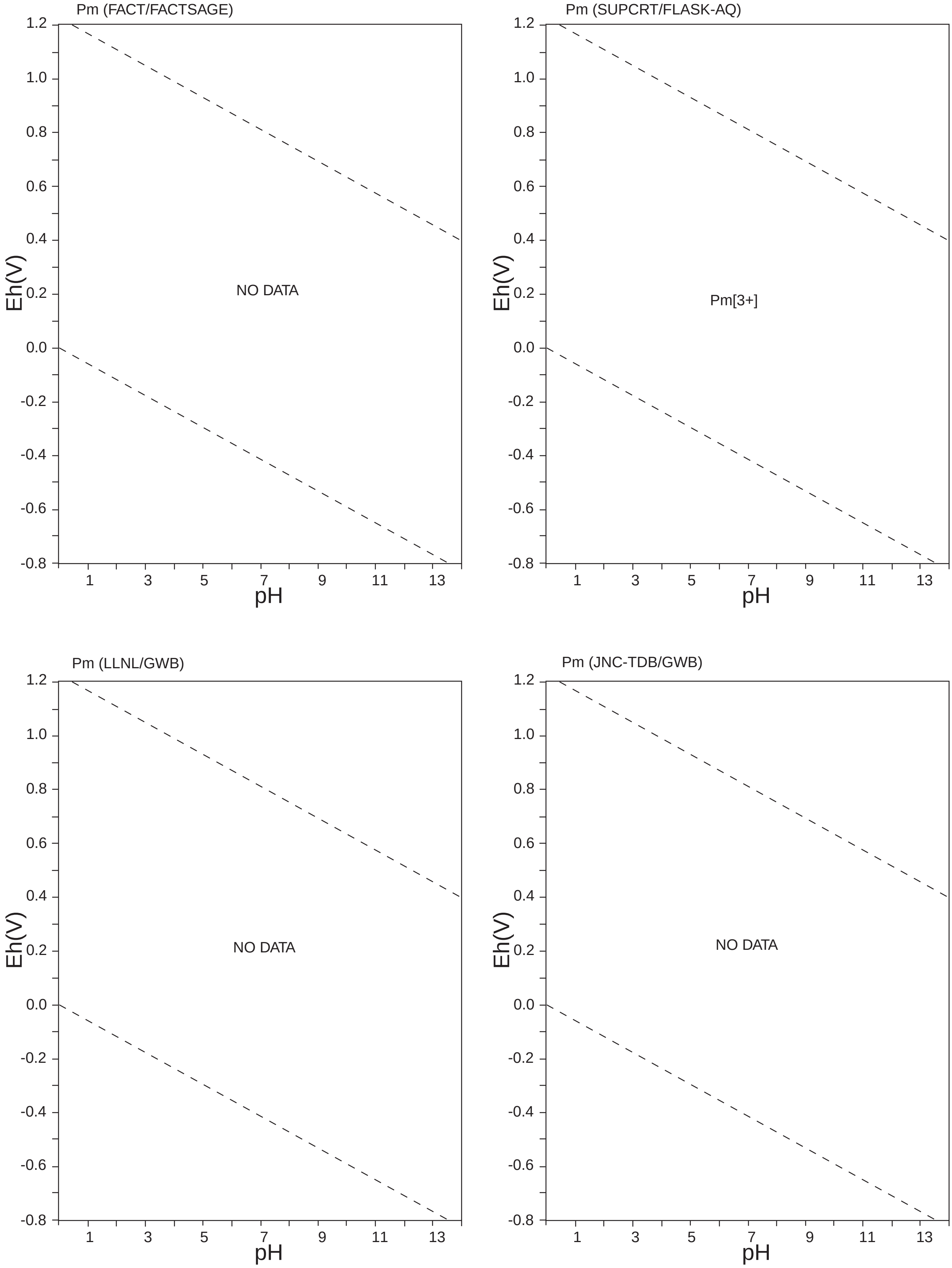

Figure 93: Eh-pH diagrams of the system Pm-O-H. $\sum \mathrm{Pm} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 57: List of Po species

FACT	SUPCRT	LLNL	JNC-TDB
$Po[2+]$, $Po[4+]$, $Po(OH)_2[4+]$, **$Po(s)$**			$Po[4+]$, **$Po(OH)_4(s)$**

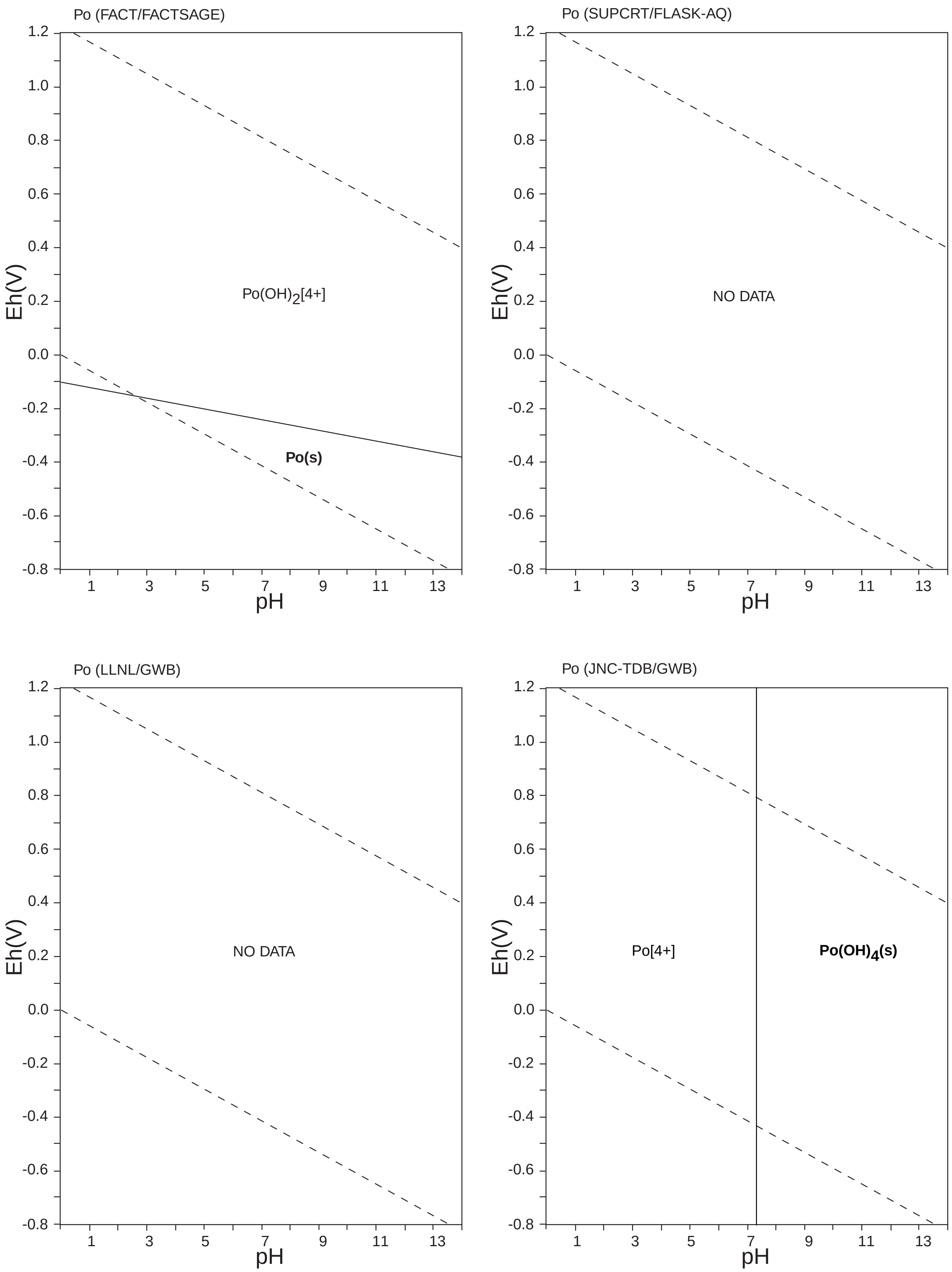

Figure 94: Eh-pH diagrams of the system Po-O-H. $\sum \mathrm{Po} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 58: List of Pr species

FACT	SUPCRT	LLNL	JNC-TDB
Pr[3+], PrOH[2+], Pr(OH)$_2$[+], **Pr(s)**, **Pr(s2)**, **PrH$_2$(s)**, **PrO$_2$(s)**, **Pr$_2$O$_3$(s)**, **Pr$_6$O$_{11}$(s)**, **Pr$_7$O$_{12}$(s)**, **PrO$_3$H$_3$(s)**	Pr[3+], PrOH[2+], PrO[+], Pr[4+], Pr[2+], PrO$_2$H(aq), PrO$_2$[-]		

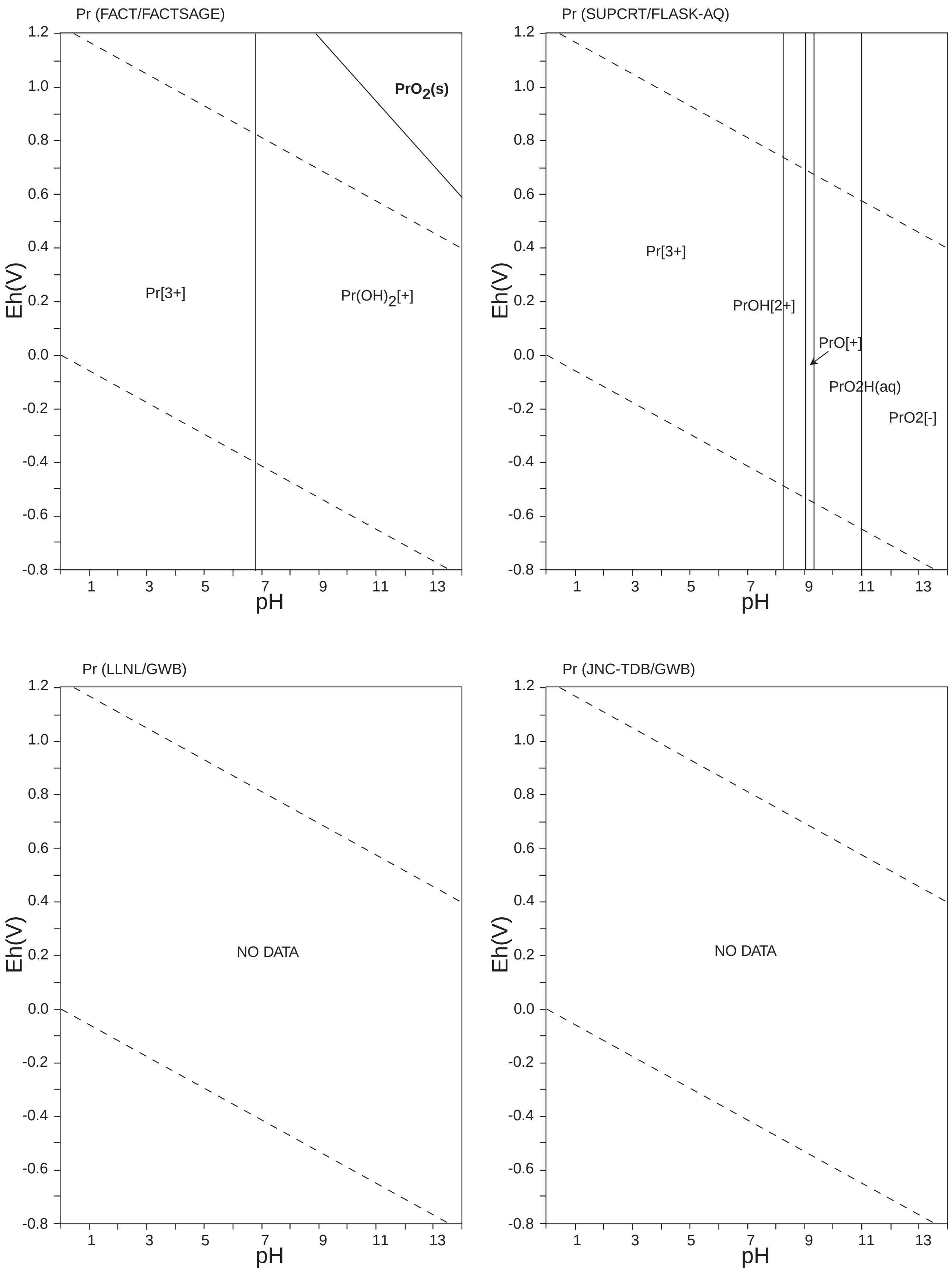

Figure 95: Eh-pH diagrams of the system Pr-O-H. $\sum \mathrm{Pr} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 59: List of Pt species

FACT	SUPCRT	LLNL	JNC-TDB
Pt[2+], **Pt(s)**	Pt[2+], PtOH[+], PtO(aq), **Pt(Platinum)**		

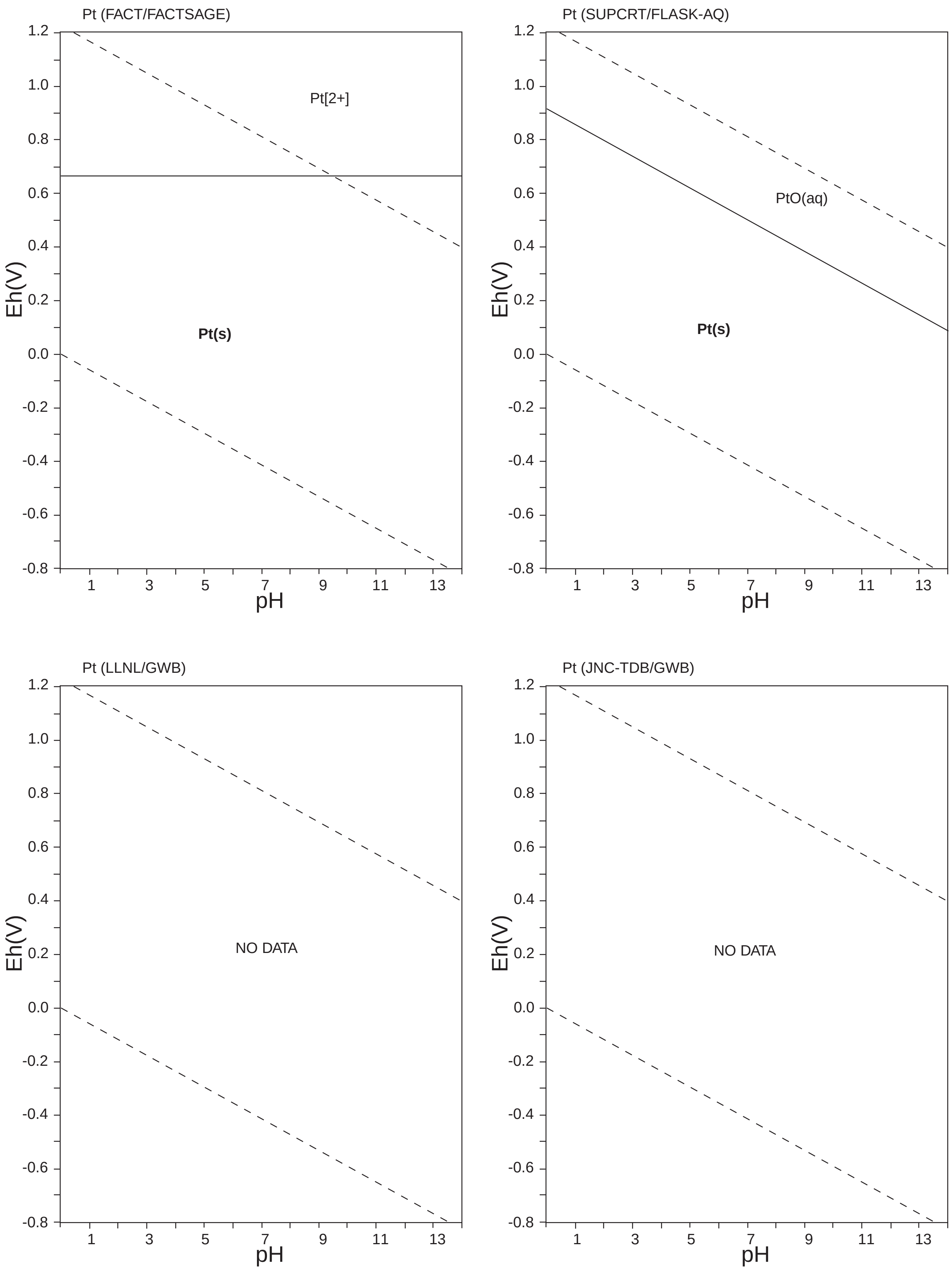

Figure 96: Eh-pH diagrams of the system Pt-O-H. $\sum \mathrm{Pt} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 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_2(s)**, **PuH_3(s)**, **PuO_2(s)**, **Pu_2O_3(s)**, **Pu_5O_8(s)**		PuO_2[2+], Pu[3+], Pu[4+], PuO_2[+], $(PuO_2)_2(OH)_2$[2+], $(PuO_2)_3(OH)_5$[+], $Pu(OH)_2$[2+], $Pu(OH)_3$[+], $Pu(OH)_4$(aq), $Pu(OH)_5$[-], PuO_2OH(aq), PuO_2OH[+], PuOH[2+], PuOH[3+], $Pu(OH)_3$(aq), **$Pu(OH)_3$(s)**, **$Pu(OH)_4$(am)**, **$Pu(OH)_4$(s)**, **Pu_2O_3(c,beta)**, **PuO_2(s)**, **$PuO_2(OH)_2$(s)**, **$PuO_2(OH)_2$(c)**, **PuO_2(c)**, **PuO_2OH(am)**	Pu[4+], Pu[3+], PuOH[2+], $PuOH_2$[+], $Pu(OH)_3$(aq), PuO_2[+], PuO_2OH(aq), $PuO_2(OH)_2$[-], PuO_2[2+], PuO_2OH[+], $PuO_2(OH)_2$, PuO_2OH_3[-], $Pu(OH)_4$(aq), PuOH[3+], **$Pu(OH)_3$(am)**, **$Pu(OH)_3$(c)**, **PuO_2(am)**, **PuO_2OH(s)**

HATCHES	OECD-NEA	OECD-NEA update	
Pu[4+], Pu[3+], PuO_2[+], PuO_2[2+], Pu(OH)[2+], Pu(OH)[3+], $Pu(OH)_2$[+], $Pu(OH)_2$[2+], $Pu(OH)_3$(aq), $Pu(OH)_3$[+], $Pu(OH)_4$(aq), $Pu(OH)_4$[-], $Pu_2(OH)_2$[4+], $Pu_2(OH)_2$[6+], $Pu_2(OH)_3$[5+], $Pu_2(OH)_4$[4+], $Pu_2(OH)_5$[3+], $Pu_3(OH)_5$[4+], $PuO_2(OH)_2$[-], $(PuO_2)_2OH_2$[2+], $(PuO_2)_3OH_5$[+], PuO_2OH(aq), PuO_2OH[+], PuO_2OH_2(aq), PuO_2OH_3[-], **$Pu(OH)_3$**, **$Pu(OH)_4$**, **Pu_2O_3**, **$PuO_2(OH)_2{*}H_2O$(c)**, **PuO_2**, **PuO_2(a)**, **$PuO_2(OH)_2$**, **PuO_2OH**, **$Pu(OH)_3$(c)**	Pu[4+], Pu[3+], PuO_2[+], PuO_2[2+], PuOH[2+], PuOH[3+], PuO_2OH[+], $PuO_2(OH)_2$(aq), $(PuO_2)_2(OH)_2$[2+], **Pu(c)**, **$PuO_{1.61}$(c_bcc)**, **PuO_2(c)**, **PuO_2(hyd_aged)**, **Pu_2O_3(c)**, **PuO_2OH(am)**, **$Pu(OH)_3$(c)**, **$PuO_2(OH)_2H_2O$(c)**	Pu[4+], Pu[3+], PuO2[+], PuO_2[2+], PuOH[2+], PuOH[3+], $Pu(OH)_2$[2+], $Pu(OH)_3$[+], PuO_2OH(aq), PuO_2OH[+], $PuO_2(OH)_2$(aq), $Pu(OH)_4$(aq), $(PuO_2)_2(OH)_2$[2+], **Pu(cr)**, **$PuO_{1.61}$(bcc)**, **PuO_2(cr)**, **Pu_2O_3(cr)**, **$Pu(OH)_3$(cr)**, **$PuO_2(OH)_2H_2O$(cr)**	

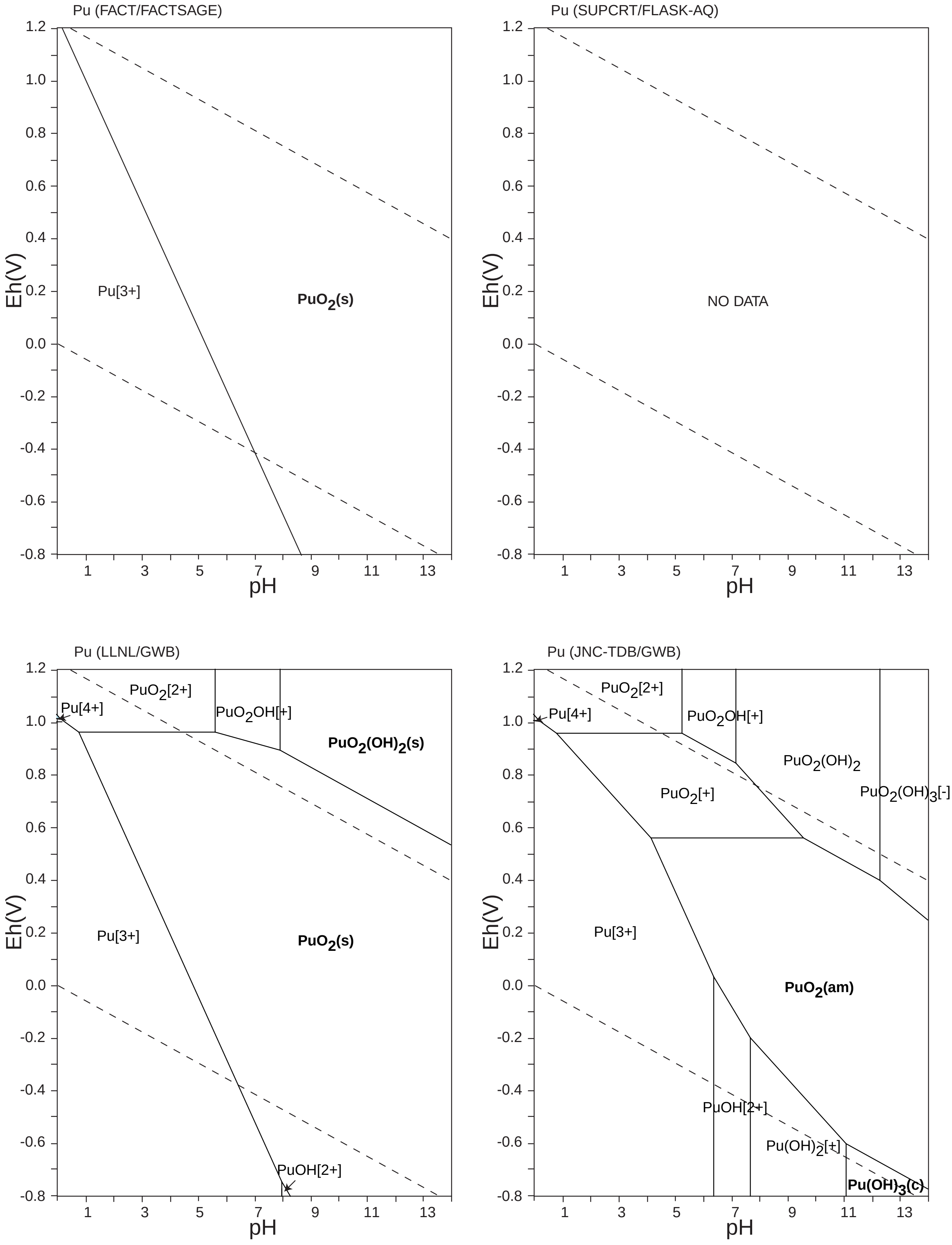

Figure 97: Eh-pH diagrams of the system Pu-O-H (1). $\sum \mathrm{Pu} = 10^{-10}$, 298.15K, 10^5 Pa.

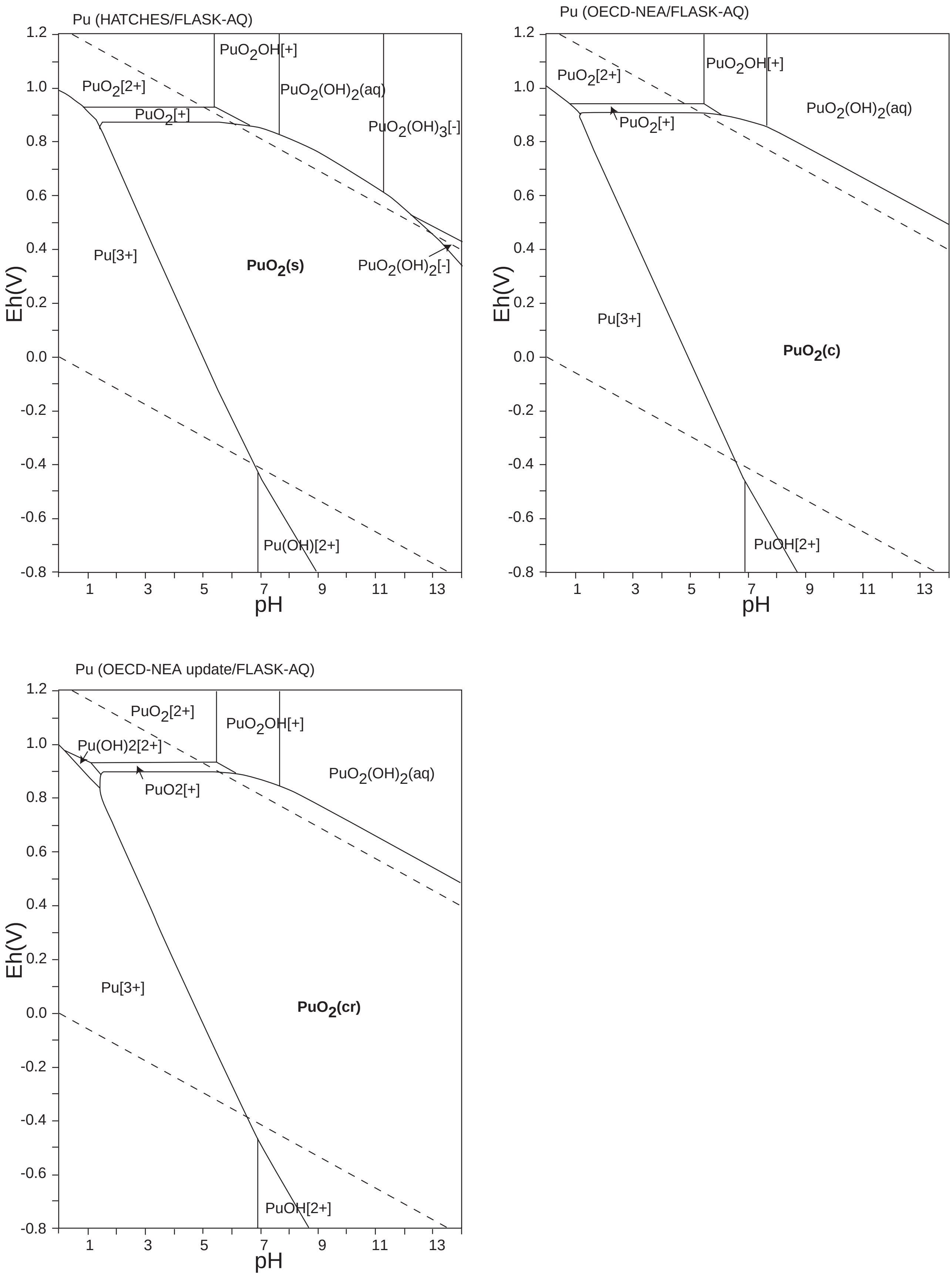

Figure 98: Eh-pH diagrams of the system Pu-O-H (2). $\sum \mathrm{Pu} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 61: List of Ra species

FACT	SUPCRT	LLNL	JNC-TDB
Ra[2+], **Ra(s)**	Ra[2+]		Ra[2+], RaOH[+]

HATCHES			
Ra[2+], RaOH[+], **Ra(c)**			

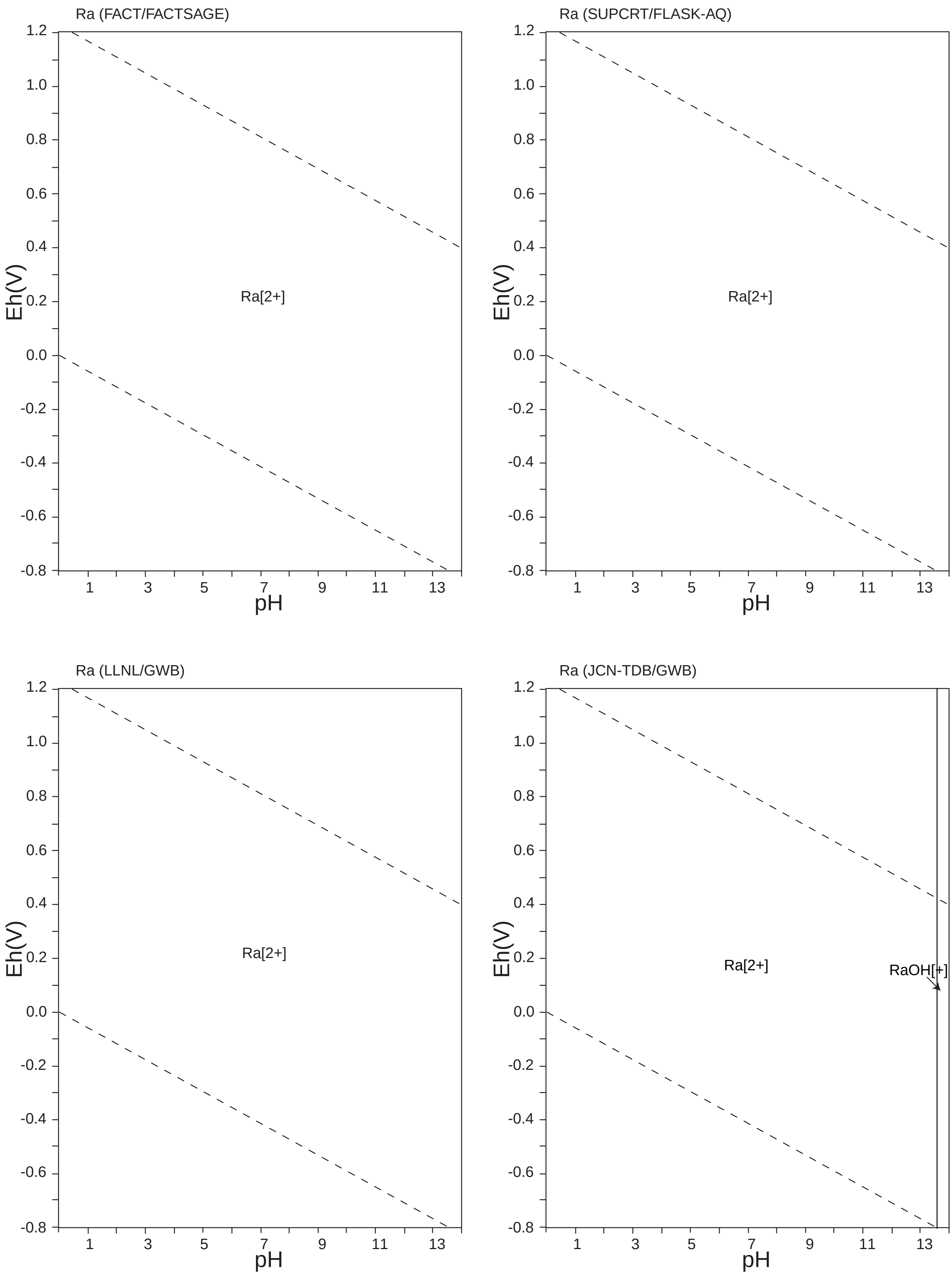

Figure 99: Eh-pH diagrams of the system Ra-O-H (1). $\sum \mathrm{Ra} = 10^{-10}$, 298.15K, 10^5 Pa.

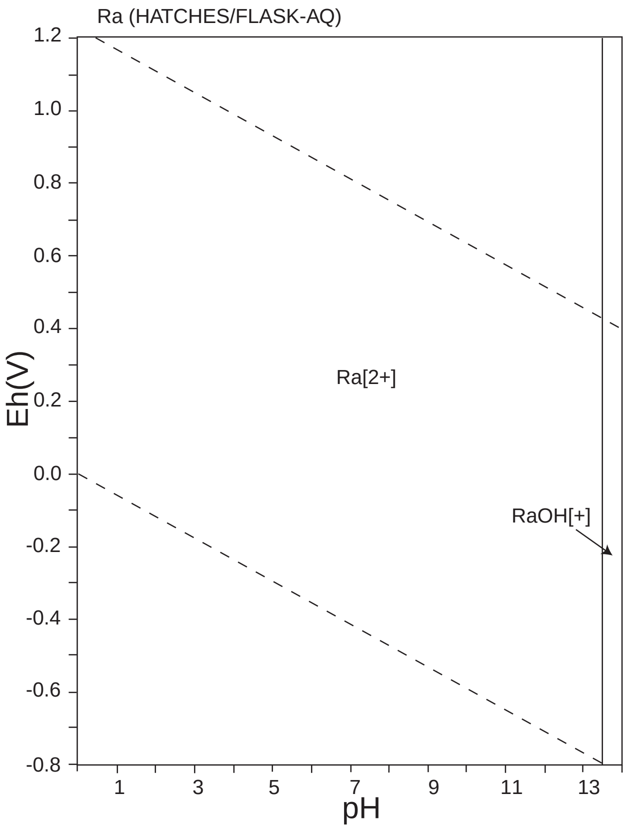

Figure 100: Eh-pH diagrams of the system Ra-O-H (2). $\sum \mathrm{Ra} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 62: List of Rb species

FACT	SUPCRT	LLNL	JNC-TDB
Rb[+], **Rb(s)**, **Rb_2O(s)**, **RbOH(s)**	Rb[+], RbOH(aq)	Rb[+]	

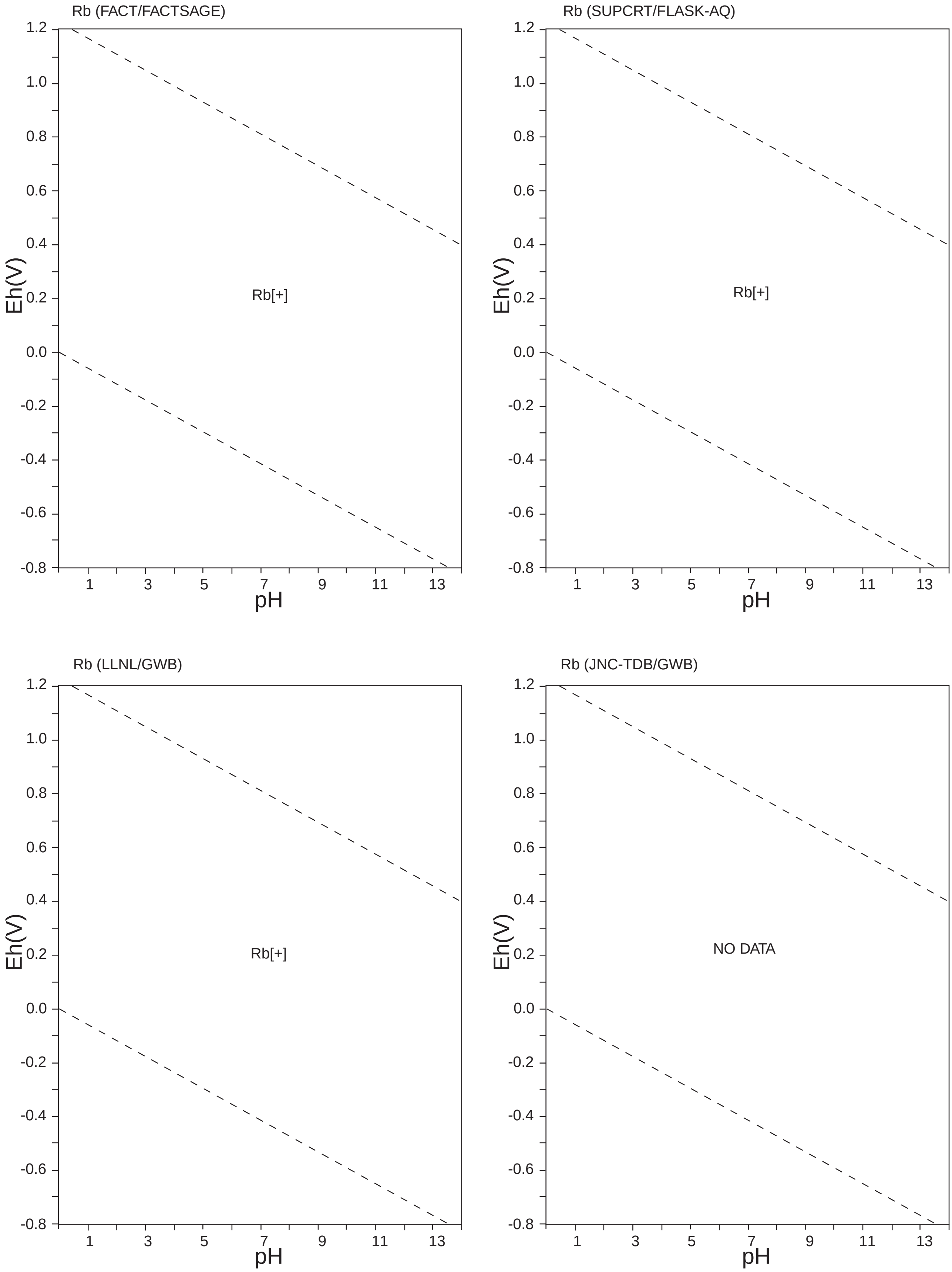

Figure 101: Eh-pH diagrams of the system Rb-O-H. $\sum \mathrm{Rb} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 63: List of Re species

FACT	SUPCRT	LLNL	JNC-TDB
ReO_4[-], Re[-], Re[+], **Re(s)**, **ReO_2(s)**, **ReO_3(s)**, **Re_2O_7(s)**, **$HReO_4$(s)**	ReO_4[-]		

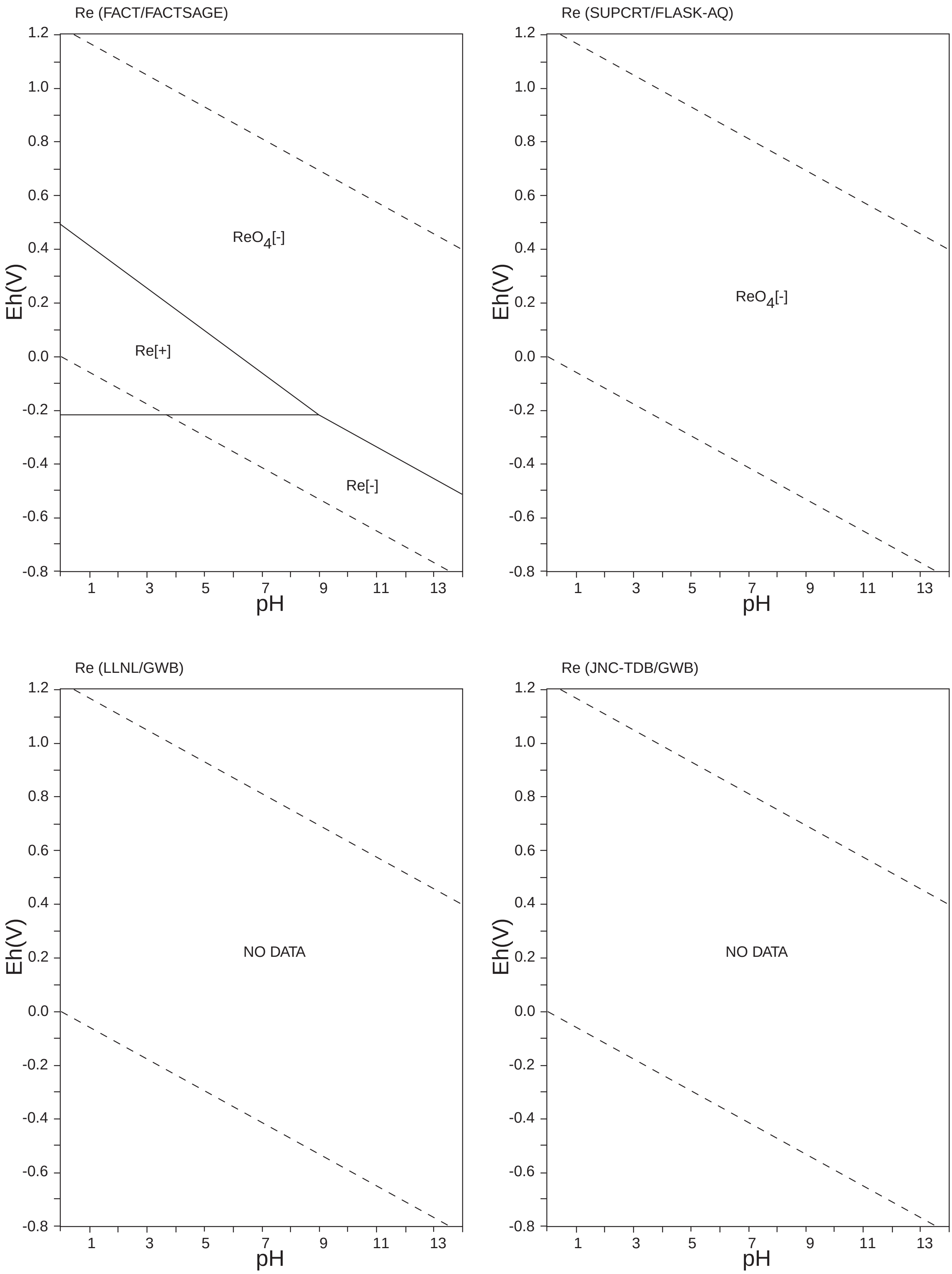

Figure 102: Eh-pH diagrams of the system Re-O-H. $\sum \mathrm{Re} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 64: List of Rh species

FACT	SUPCRT	LLNL	JNC-TDB
$RhO(s)$, **$RhO_2(s)$**, **$Rh(s)$**, **$Rh_2O(s)$**, **$Rh_2O_3(s)$**	Rh[3+], RhOH[+], RhOH[2+], Rh[2+], RhO(aq), RhO[+], **Rh(Rhodium)**, **$Rh_2O(s)$**, **$Rh_2O_3(s)$**		

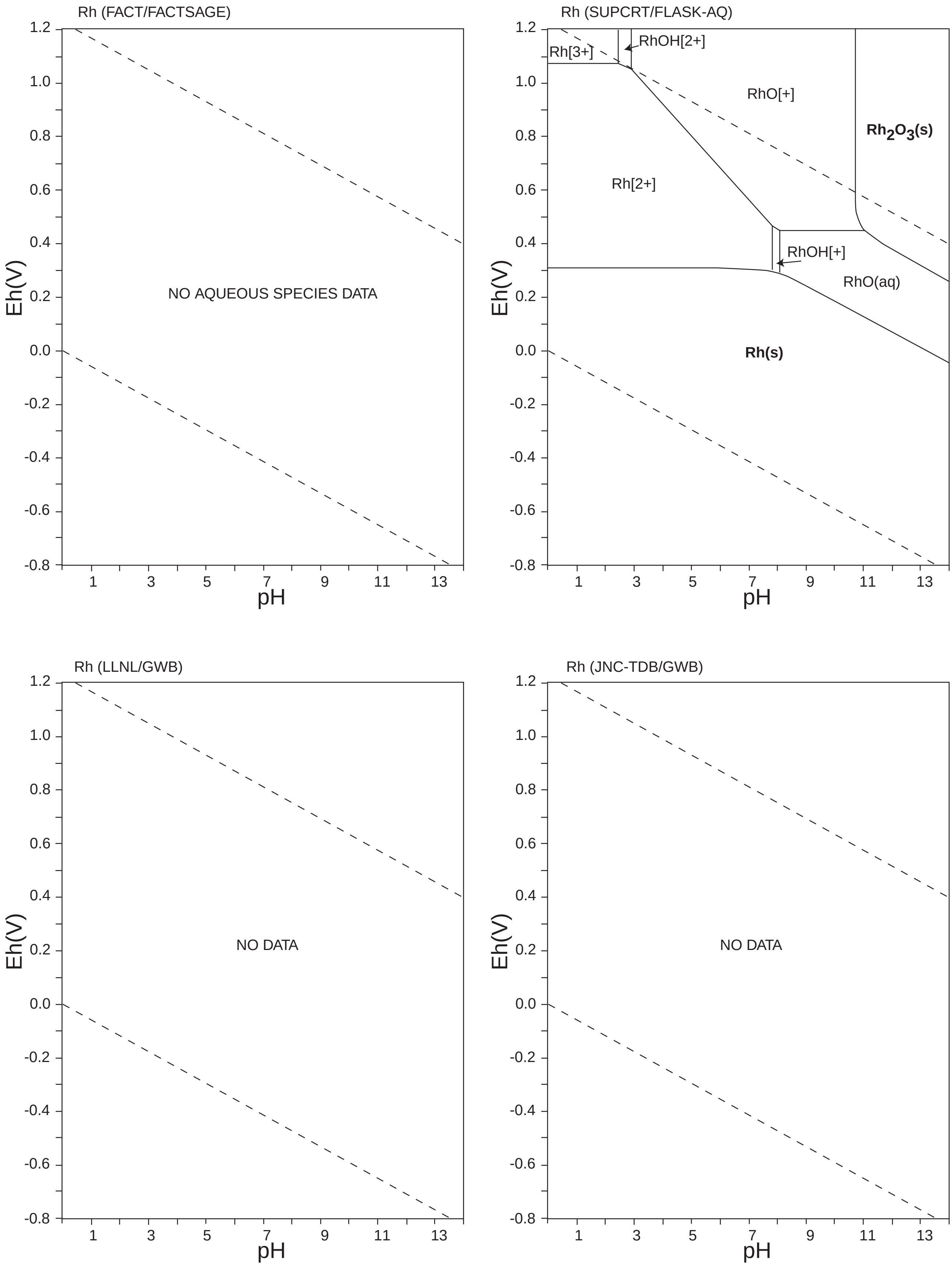

Figure 103: Eh-pH diagrams of the system Rh-O-H. $\sum \mathrm{Rh} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 65: List of Ru species

FACT	SUPCRT	LLNL	JNC-TDB
RuO_4[2-], RuO_4[-], RuO_4(aq), Ru(OH)$_2$[2+], **RuO_4(s), Ru(s), RuO_2(s)**	RuO_4[2-], Ru[3+], Ru[2+], RuOH[+], RuOH[2+], RuO(aq), RuO[+], **Ru(Ruthenium)**, **RuO_2(s)**	Ru[3+], Ru(OH)$_2$[2+], Ru[2+], RuO_4(aq), RuO_4[-], RuO_4[2-], H_2RuO_5(aq), $HRuO_5$[-], Ru(OH)$_2$[+], $Ru_4(OH)_{12}$[4+], RuOH[2+], **Ru(OH)$_3$*H_2O(am), Ru(c), RuO_2(s), RuO_2*2H_2O(am), RuO_4(s)**, Ru(g), RuO_4(g)	

HATCHES			
Ru[3+], Ru(OH)$_2$[2+], Ru[2+], RuO_4[-], RuO_4[2-], H_2RuO_5(aq), $HRuO_5$[-], Ru(OH)[2+], Ru(OH)$_2$[+], $Ru_4(OH)_{12}$[4+], **Ru(c), Ru_2O_5, RuO_2(s), RuO_2*2H_2O, RuO_4(s), Ru(OH)$_3$*H_2O**			

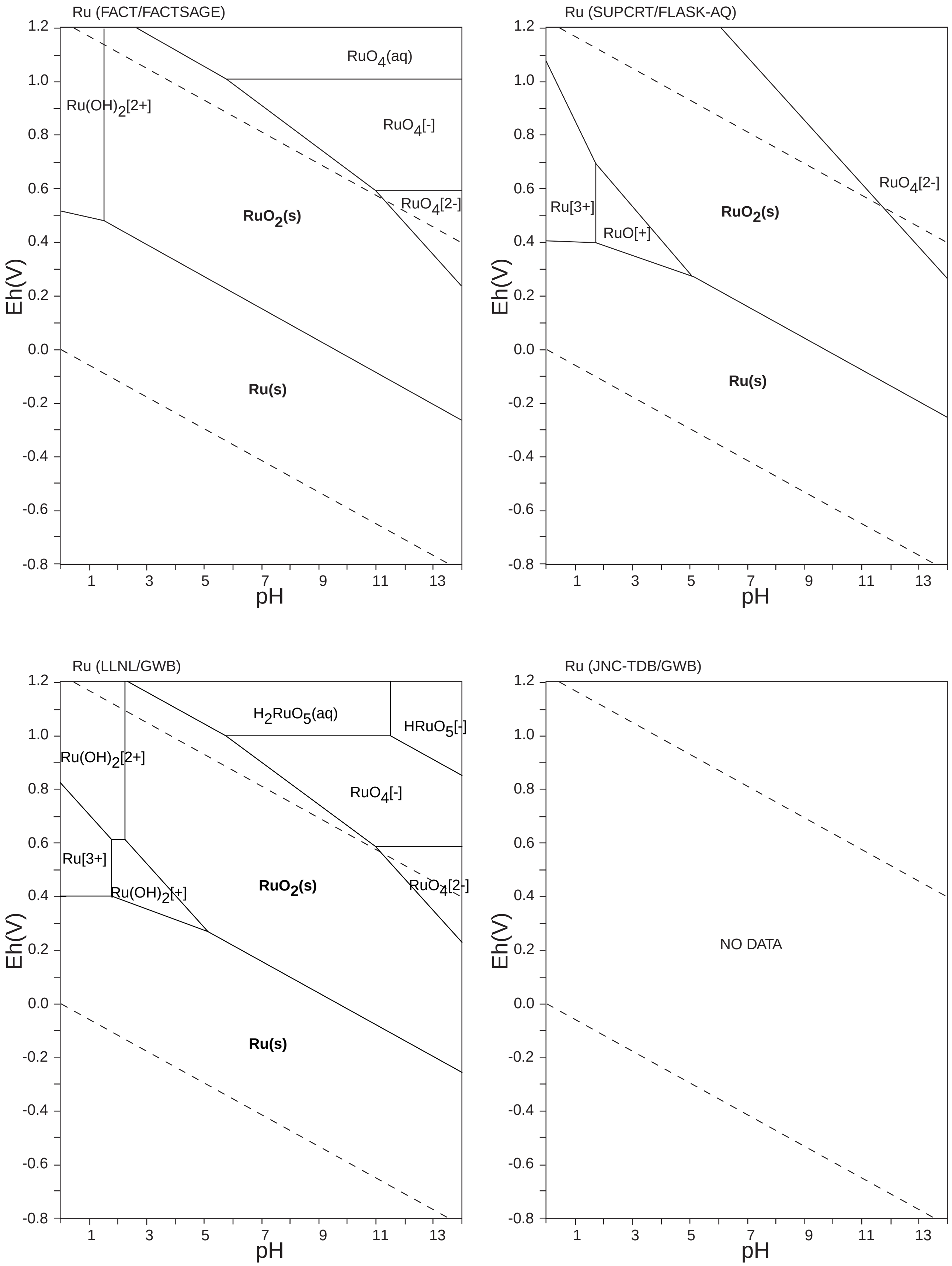

Figure 104: Eh-pH diagrams of the system Ru-O-H (1). $\sum \mathrm{Ru} = 10^{-10}$, 298.15K, 10^5 Pa.

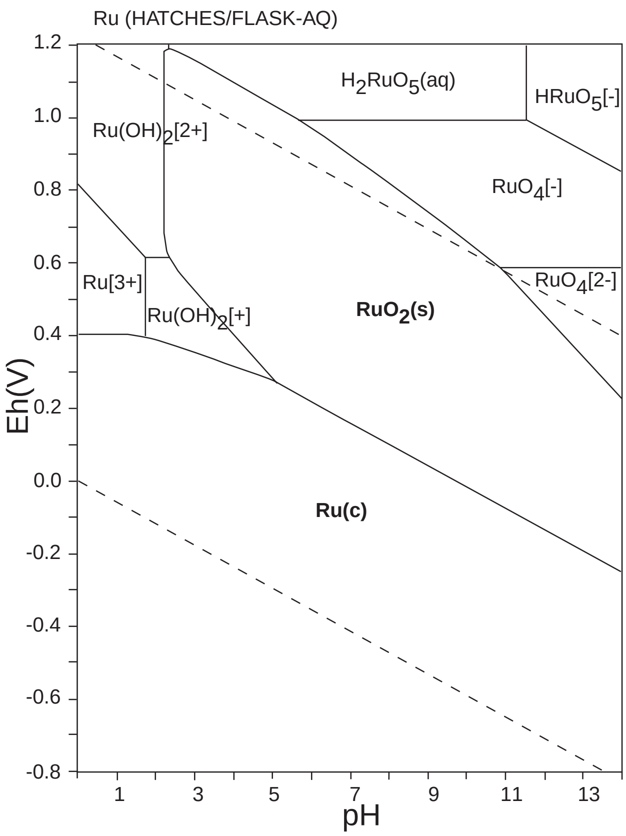

Figure 105: Eh-pH diagrams of the system Ru-O-H (2). $\sum \mathrm{Ru} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 66: List of S species

FACT	SUPCRT	LLNL	JNC-TDB
S[2-], S_2[2-], S_3[2-], S_4[2-], S_5[2-], HS[-], H_2S(aq), SO_2(aq), SO_3[2-], SO_4[2-], S_2O_3[2-], S_2O_4[2-], S_2O_5[2-], S_2O_6[2-], S_2O_8[2-], S_3O_6[2-], S_4O_6[2-], S_5O_6[2-], HSO_3[-], HSO_4[-], HS_2O_4[-], $H_2S_2O_4$ (aq), **S(s)**, **S(s2)**, **SO_3(s)**	S_2[2-], S_3[2-], S_4[2-], S_5[2-], HS[-], H_2S(aq), SO_2(aq), SO_3[2-], SO_4[2-], S_2O_3[2-], S_2O_4[2-], S_2O_5[2-], S_2O_6[2-], S_2O_8[2-], S_3O_6[2-], S_4O_6[2-], S_5O_6[2-], HSO_3[-], HSO_4[-], HS_2O_4[-], $H_2S_2O_4$ (aq), HSO_5[-], HS_2O_3[-], $H_2S_2O_3$(aq), **S(Sulfur)**	SO_4[2-], HS[-], H_2S(aq), H_2SO_4(aq), HSO_4[-], S[2-], S_2[2-], S_3[2-], S_4[2-], S_5[2-], S_6[2-], **Sulfur(rhmb)**, H_2S(g), S_2(g)	SO_4[2-], S[2-], SO_3[2-], S_2O_3[2-], HS[-], H_2S(aq), HSO_3[-], HS_2O_3[-], H_2SO_3(aq), HSO_4[-], **S(c)**, S(g), S_2(g), SO_2(g), H_2S(g)

HATCHES			
SO_4[2-], HS[-], S_2[2-], S_3[2-], S_4[2-], S_5[2-], SO_2(aq), H_2S(aq), $H_2S_2O_3$(aq), $H_2S_2O_4$(aq), H_2SO_3(aq), HS_2O_3[-], HS_2O_4[-], HSO_3[-], HSO_4[-], S[2-], S_2O_3[2-], S_2O_4[2-], S_2O_5[2-], S_2O_6[2-], S_2O_8[2-], S_3O_6[2-], S_4O_6[2-], S_5O_6[2-], SO_3[2-], **S(c)**, **Sulfur-rhmb**			

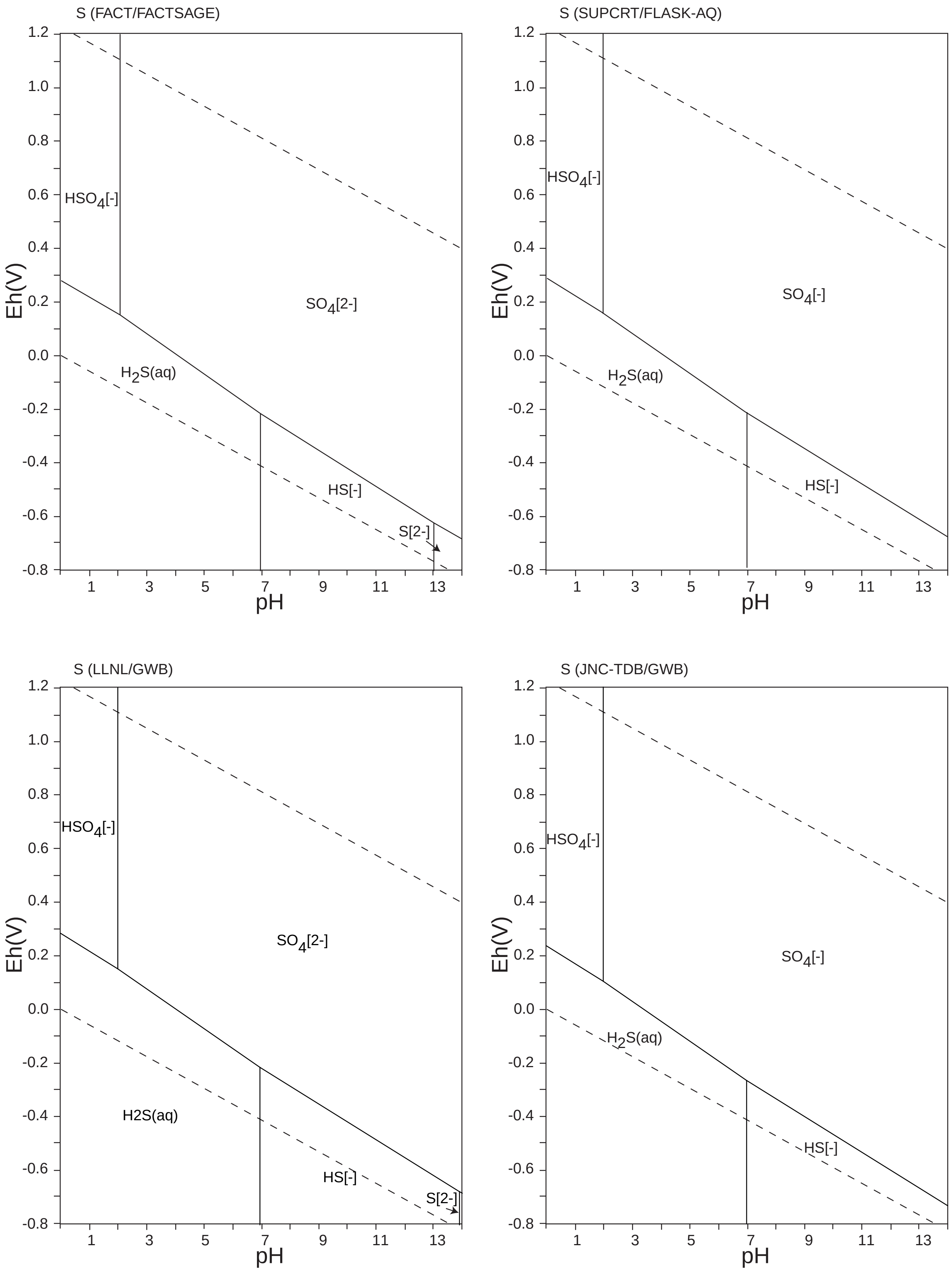

Figure 106: Eh-pH diagrams of the system S-O-H (1). $\sum \mathrm{S} = 10^{-10}$, 298.15K, 10^5 Pa.

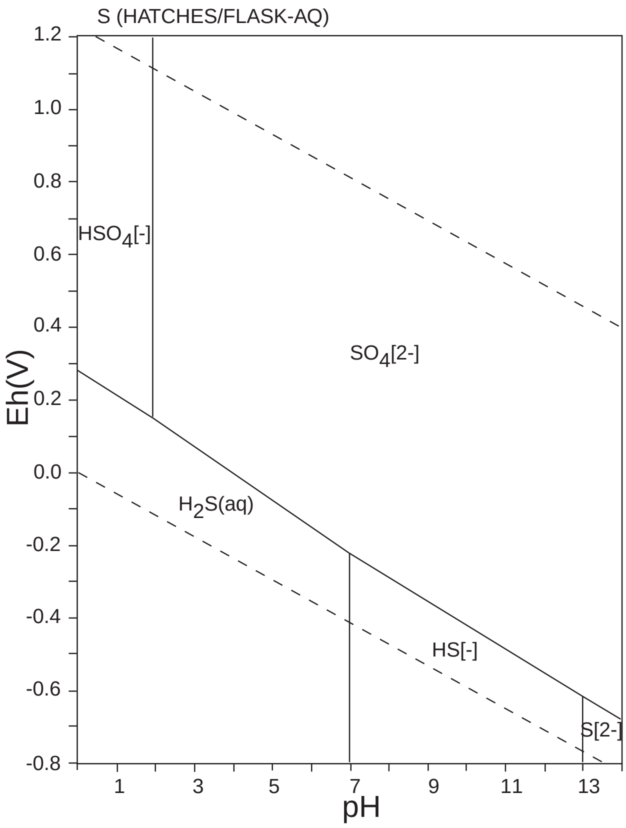

Figure 107: Eh-pH diagrams of the system S-O-H (2). $\sum \mathrm{S} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 67: List of Sb species

FACT	SUPCRT	LLNL	JNC-TDB
SbO_2[-], $HSbO_2$(aq), SbO[+], **Sb(s)**, **SbO_2(s)**, **Sb_2O_3(s)**, **Sb_2O_3(s2)**, **Sb_2O_4(s)**, **Sb_2O_5(s)**	SbO_2[-], $HSbO_2$(aq)		$Sb(OH)_3$(aq), $Sb(OH)_5$(aq) $Sb(OH)_6$[-], $Sb_{12}(OH)_{64}$(aq) $Sb_{12}(OH)_{65}$[5-], $Sb_{12}(OH)_{66}$[6-], $Sb_{12}(OH)_{67}$[7-], Sb[3+], SbOH[2+], $Sb(OH)_2$[+] $Sb(OH)_4$[-], **$Sb_2(OH)_6$(s)** **Sb(c)**, **Valentinite**, **Sb_2O_5(s)**

HATCHES			
$Sb(OH)_3$(aq), Sb[3+], $Sb(OH)_2$[+], $Sb(OH)_4$[-], **Sb_2O_3**			

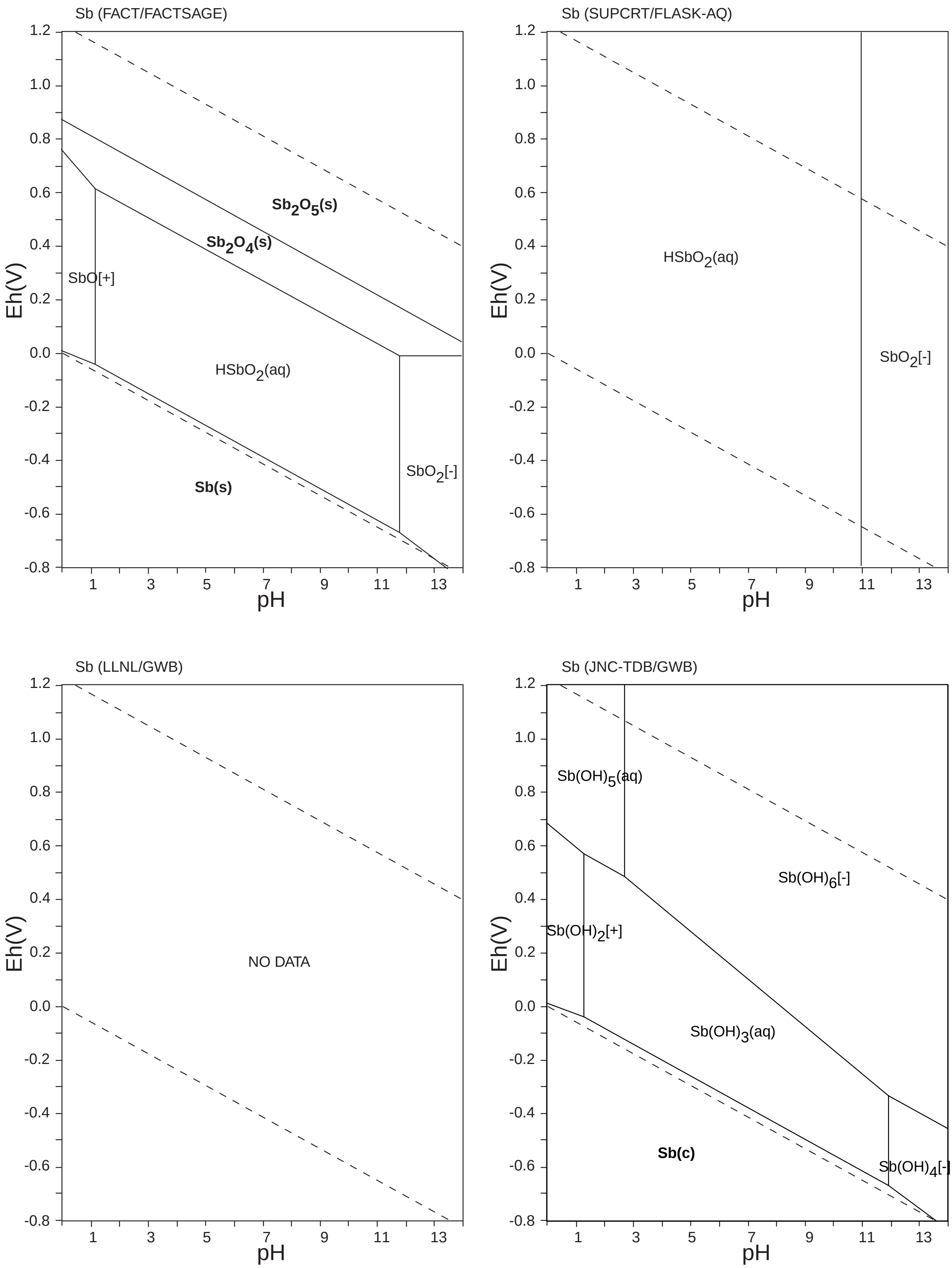

Figure 108: Eh-pH diagrams of the system Sb-O-H (1). $\sum \mathrm{Sb} = 10^{-10}$, 298.15K, 10^5 Pa.

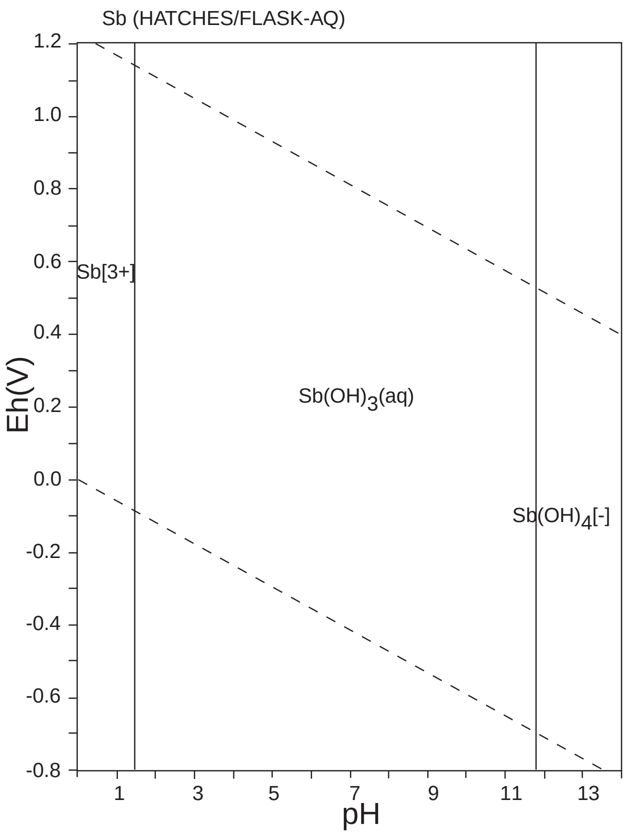

Figure 109: Eh-pH diagrams of the system Sb-O-H (2). $\sum \mathrm{Sb} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 68: List of Sc species

FACT	SUPCRT	LLNL	JNC-TDB
Sc[3+], ScOH[2+], **Sc(s)**, **Sc(s2)**, **Sc_2O_3(s)**, **$Sc(OH)_3$(s)**	Sc[3+], ScOH[2+], ScO[+], $HScO_2$(aq), ScO_2[-]		

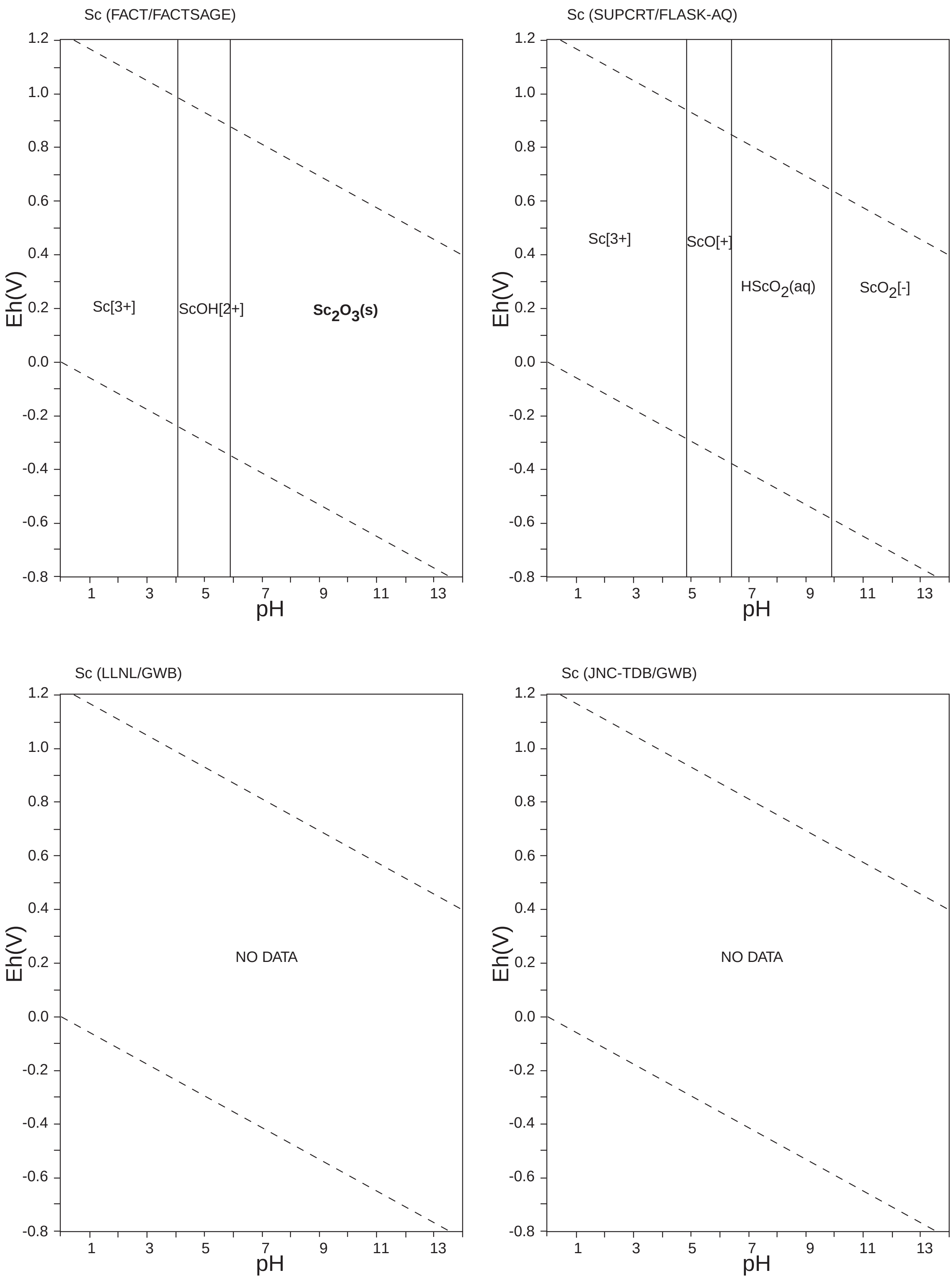

Figure 110: Eh-pH diagrams of the system Sc-O-H. $\sum \mathrm{Sc} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 69: List of Se species

FACT	SUPCRT	LLNL	JNC-TDB
HSe[-], SeO_3[2-], SeO_4[2-], $HSeO_3$[-], H_2SeO_3(aq), $HSeO_4$[-], Se[2-], H_2Se(aq), **Se(s), SeO_2(s), SeO_3(s), Se_2O_5(s)**	HSe[-], SeO_3[2-], SeO_4[2-], $HSeO_3$[-], H_2SeO_3(aq), $HSeO_4$[-]	SeO_3[2-], Se[2-], SeO_4[2-], H_2Se(aq), H_2SeO_3(aq), HSe[-], $HSeO_3$[-], $HSeO_4$[-], **Se(black), Se_2O_5(s), SeO_2(s), SeO_3(s)**	SeO_4[2-], Se[2-], HSe[-], H_2Se(aq), SeO_3[2-], $HSeO_3$[-], H_2SeO_3(aq), $HSeO_4$[-], **Se(s), SeO_2(s), Se_2O_5(s), SeO_3(s)**

HATCHES			
SeO_4[2-], Se[2-], SeO_3[2-], H_2Se(aq), H_2SeO_3(aq), HSe[-], $HSeO_3$[-], $HSeO_4$[-], **Se, Se_2O_5, SeO_2, SeO_3**			

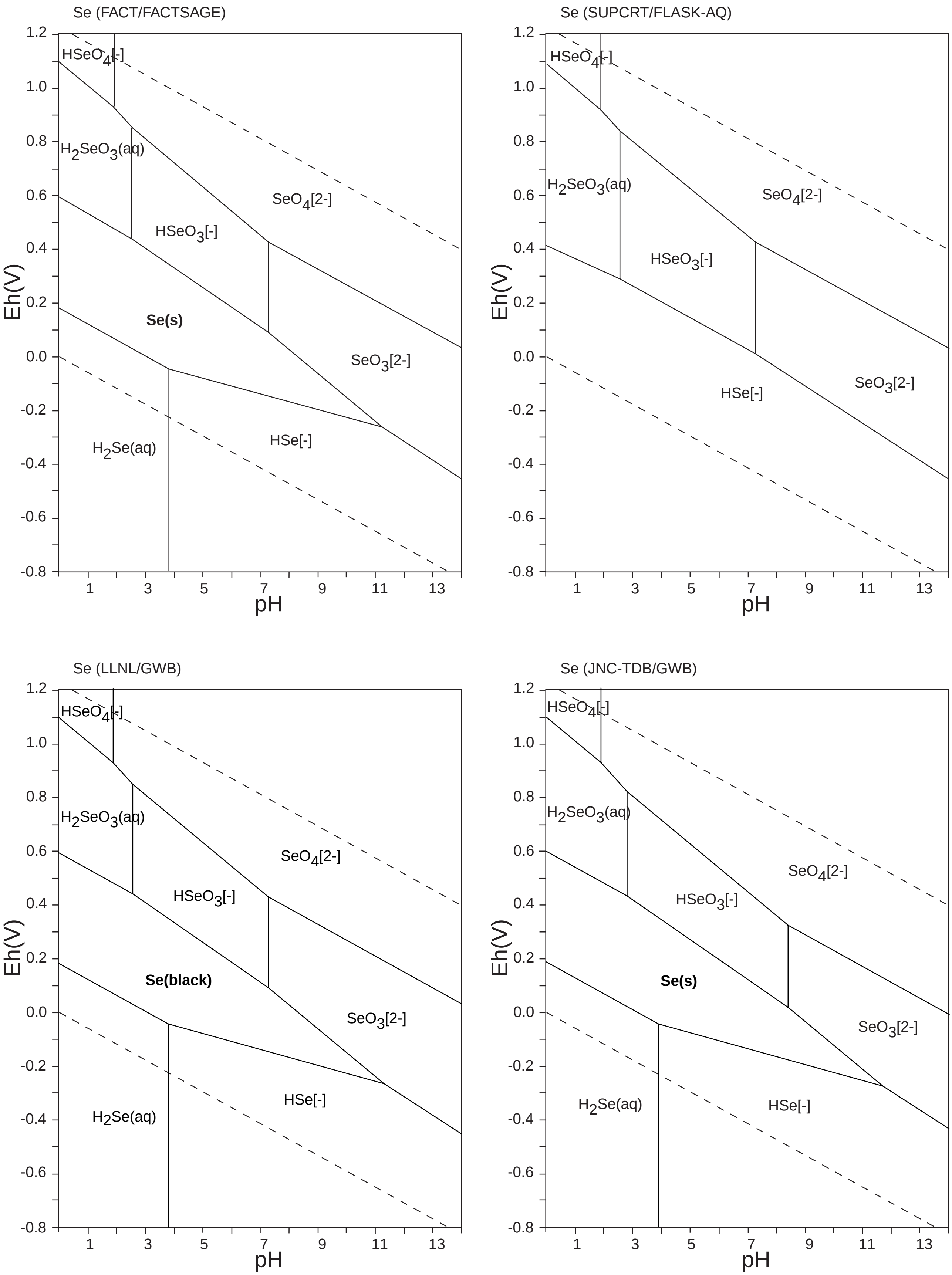

Figure 111: Eh-pH diagrams of the system Se-O-H (1). $\sum Se = 10^{-10}$, 298.15K, 10^5 Pa.

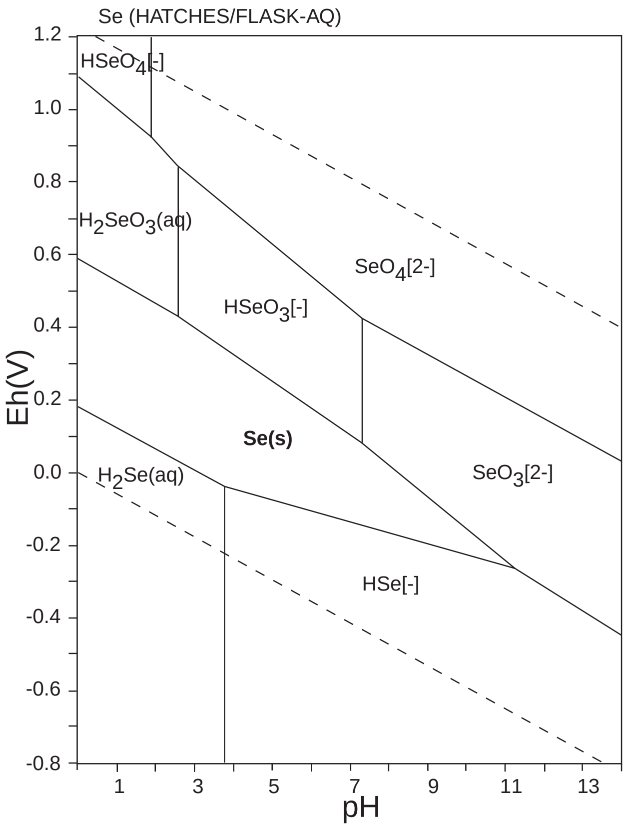

Figure 112: Eh-pH diagrams of the system Se-O-H (2). $\sum \text{Se} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 70: List of Si species

FACT	SUPCRT	LLNL	JNC-TDB
H_4SiO_4(aq), $HSi(OH)_6$[-], H_2SiO_3(aq), **Si(s)**, **Si_2H_5(s)**, **H_2SiO_3(s)**, **H_4SiO_4(s)**, **$H_2Si_2O_5$(s)**, **$H_6Si_2O_7$(s)**, **SiO_2(s)**, **SiO_2(s2)**, **SiO_2(s3)**, **SiO_2(s4)**, **SiO_2(s5)**, **SiO_2(s6)**, **SiO_2(s7)**, **SiO_2(s8)**	SiO_2(aq), $HSiO_3$[-], **SiO_2(Amorpyous-silica)**, **SiO_2(Chalcedony)**, **SiO_2(Cristobalite, alpha)**, **SiO_2(Cristobalite, beta)**, **SiO_2(Coesite)**, **SiO_2(Cristobalite)**, **SiO_2(Quartz)**	SiO_2(aq), H_2SiO_4[2-], H_3SiO_4[-], $H_4(H_2SiO_4)_4$[4-], $H_6(H_2SiO_4)_4$[2-], **Amrph_silica**, **Chalcedony**, **Cristobalite**, **Quartz**, **Tridymite**	H_4SiO_4(aq), $SiO_2(OH)$[2-], $SiO(OH)_3$[-], $Si_2O_3(OH)_4$[2-], $Si_2O_2(OH)_5$[-], $Si_3O_6(OH)_3$[3-], $Si_3O_5(OH)_5$[3-], $Si_4O_8(OH)_4$[4-], $Si_4O_7(OH)_5$[3-], $Si_4O_3(OH)_{13}$[3-], **SiO_2(s,Sil_gel)**, **H2SiO3(s, Sil_glass)**, **Chalcedony**, **Quartz**, **$HSiO_2$(s, Silica_H)**, **Sili(am)**, **Si(c)**, **SiO_2(qua)**, Si(g)

HATCHES			
H_4SiO_4(aq), H_2SiO_4[2-], $H_3Si_3O_9$[3-], H_3SiO_4[-], $H_4Si_2O_7$[2-], $H_4Si_4O_{12}$[4-], $H_5Si_2O_7$[-], $H_5Si_3O_{10}$[3-], $H_5Si_4O_{12}$[3-], **Amrph.silica**, **Chalcedony**, **Cristobalite**, **Crist.beta**, **Quartz**			

Remarks
JNC-TDB: SiO2(qua) is not Quartz in the database file, its log10K's are different from those of Quartz, but detailed description of SiO2(qua) is not given.

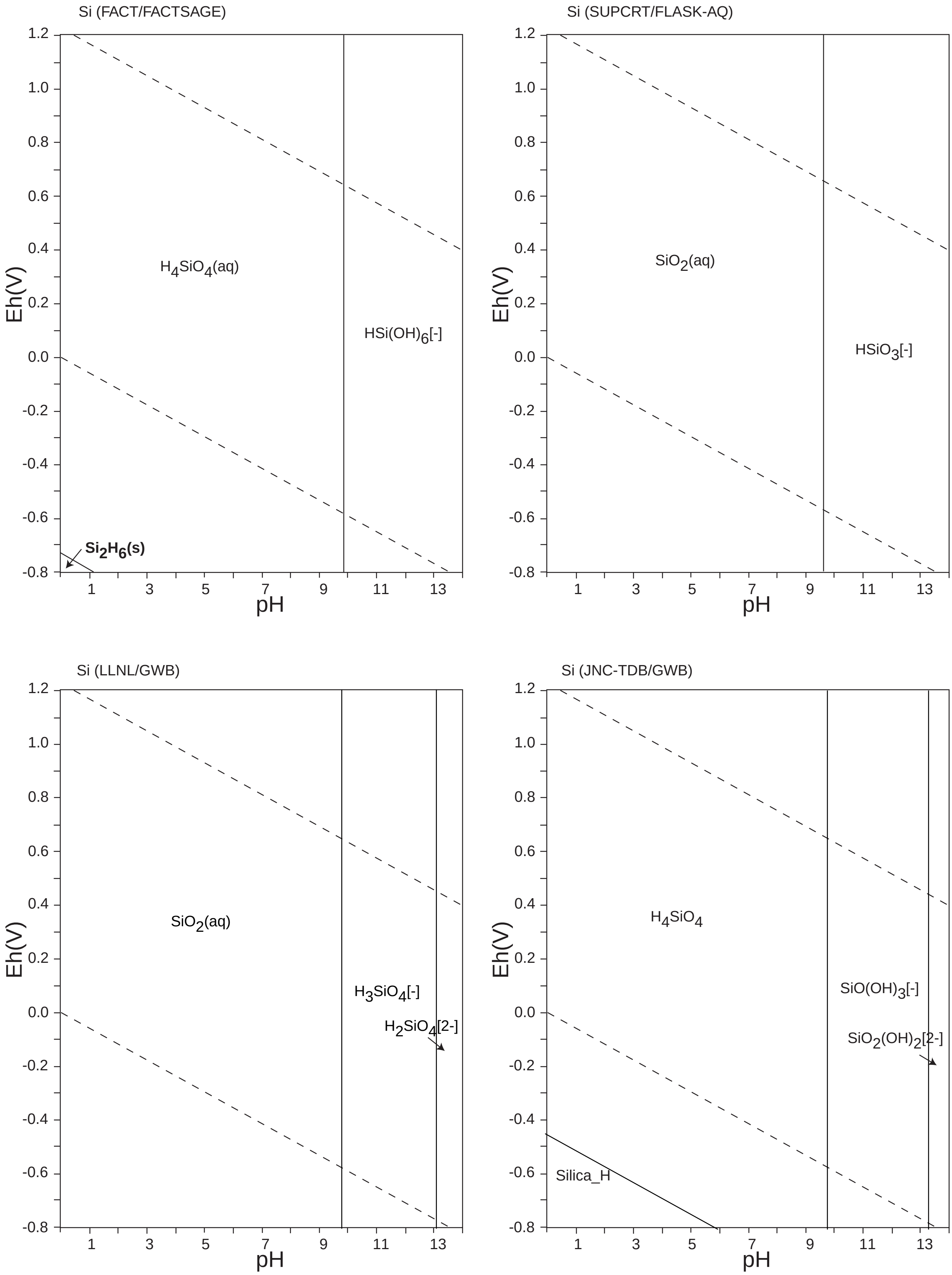

Figure 113: Eh-pH diagrams of the system Si-O-H (1). $\sum \mathrm{Si} = 10^{-10}$, 298.15K, 10^5 Pa.

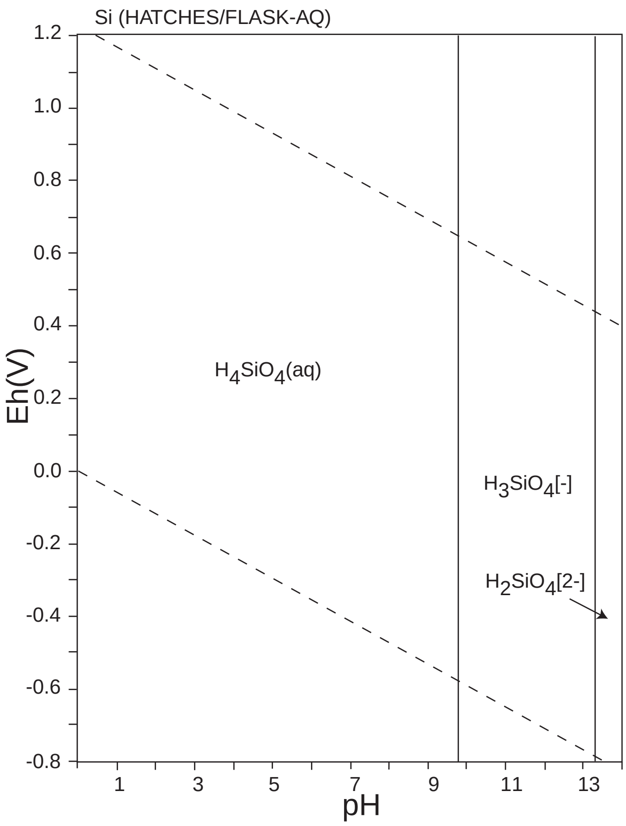

Figure 114: Eh-pH diagrams of the system Si-O-H (2). $\sum \mathrm{Si} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 71: List of Sm species

FACT	SUPCRT	LLNL	JNC-TDB
Sm[2+], Sm[3+], **Sm(s)**, **Sm(s2)**, **Sm_2O_3(s)**, **Sm_2O_3(s2)**	Sm[2+], Sm[3+], Sm[4+], SmOH[2+], SmO[+], SmO_2H(aq), SmO_2[-]		Sm[3+], SmOH[2+], $Sm(OH)_2$[+], $Sm(OH)_3$(aq), **$Sm(OH)_3$(am)**, **$Sm(OH)_3$(c)**

HATCHES			
Sm[3+], $Sm(OH)_2$[+], $Sm(OH)_3$(aq), SmOH[2+], **$Sm(OH)_3$**			

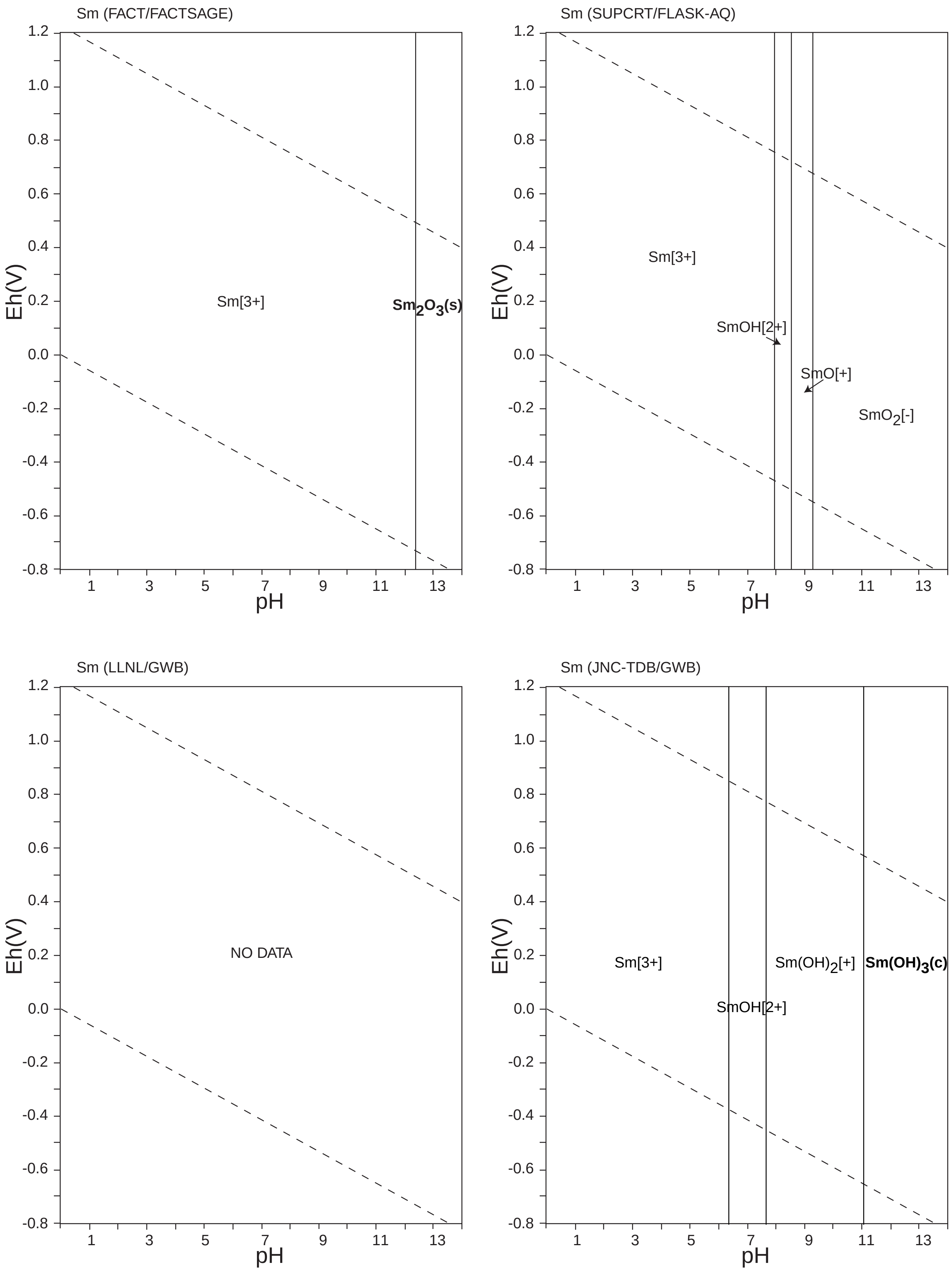

Figure 115: Eh-pH diagrams of the system Sm-O-H (1). $\sum \mathrm{Sm} = 10^{-10}$, 298.15K, 10^5 Pa.

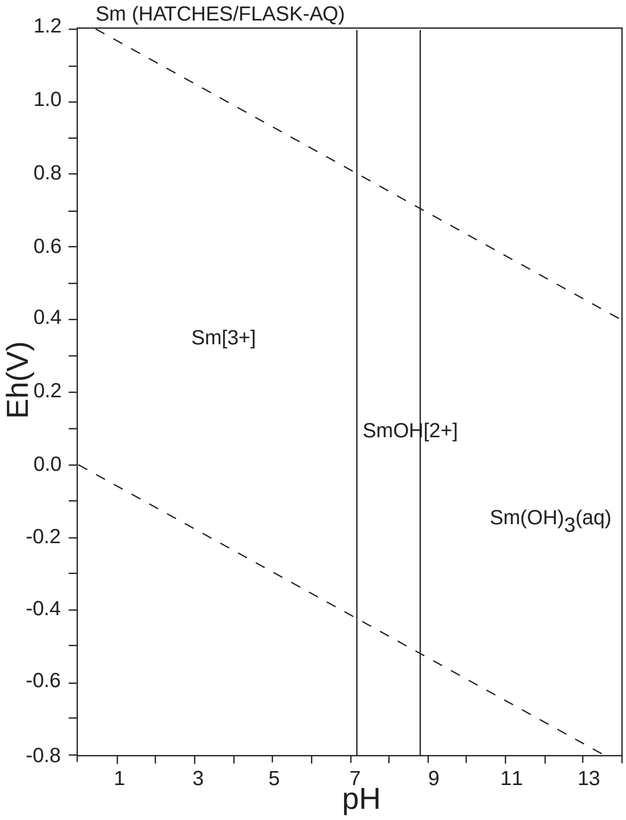

Figure 116: Eh-pH diagrams of the system Sm-O-H (2). $\sum \mathrm{Sm} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 72: List of Sn species

FACT	SUPCRT	LLNL	JNC-TDB
Sn^{2+}, $SnOH^{+}$, $SnO(OH)^{+}$, **Sn(s2), Sn(s), SnO(s), SnO_2(s)**	Sn^{2+}, $SnOH^{+}$, SnO(aq), $HSnO_2^{-}$, **Sn(Native tin)**, **SnO(Romarchite)**, **SnO_2(Cassiterite)**	Sn^{4+}, Sn^{2+}, $Sn(OH)_2$(aq), $Sn(OH)_2^{2+}$, $Sn(OH)_3^{+}$ $Sn(OH)_3^{-}$, $Sn(OH)_4$(aq), $SnOH^{+}$, $SnOH^{3+}$, **$Sn(OH)_2$(s), SnO(s), SnO_2(s)**	$Sn(OH)_4$(aq), $SnOH^{+}$, $Sn(OH)_2$(aq), $Sn(OH)_3^{-}$, $Sn_3(OH)_4^{2+}$, Sn^{2+} $Sn(OH)_5^{-}$, $Sn(OH)_6^{-}$, Sn^{4+}, **Sn(c), $Sn(OH)_2$(s), SnO(c), SnO_2(am) SnO_2(cassiterite)**

HATCHES			
Sn^{2+}, Sn^{4+}, $HSnO2^{-}$, $Sn(OH)^{+}$, $Sn(OH)_2$(aq), $Sn(OH)_2^{2+}$, $Sn(OH)_3^{+}$, $Sn(OH)_3^{-}$, $Sn(OH)_4$(aq), $Sn(OH)_5^{-}$, $Sn(OH)_6^{2-}$, $Sn_2(OH)_2^{2+}$, $Sn_3(OH)_4^{2+}$, $SnOH^{3+}$, **$H_2Sn(OH)_6$, $Sn(OH)_2$, $Sn(OH)_4$, Sn(w), SnO, SnO_2(am), SnO_2(c), SnO_2(pptd)**			

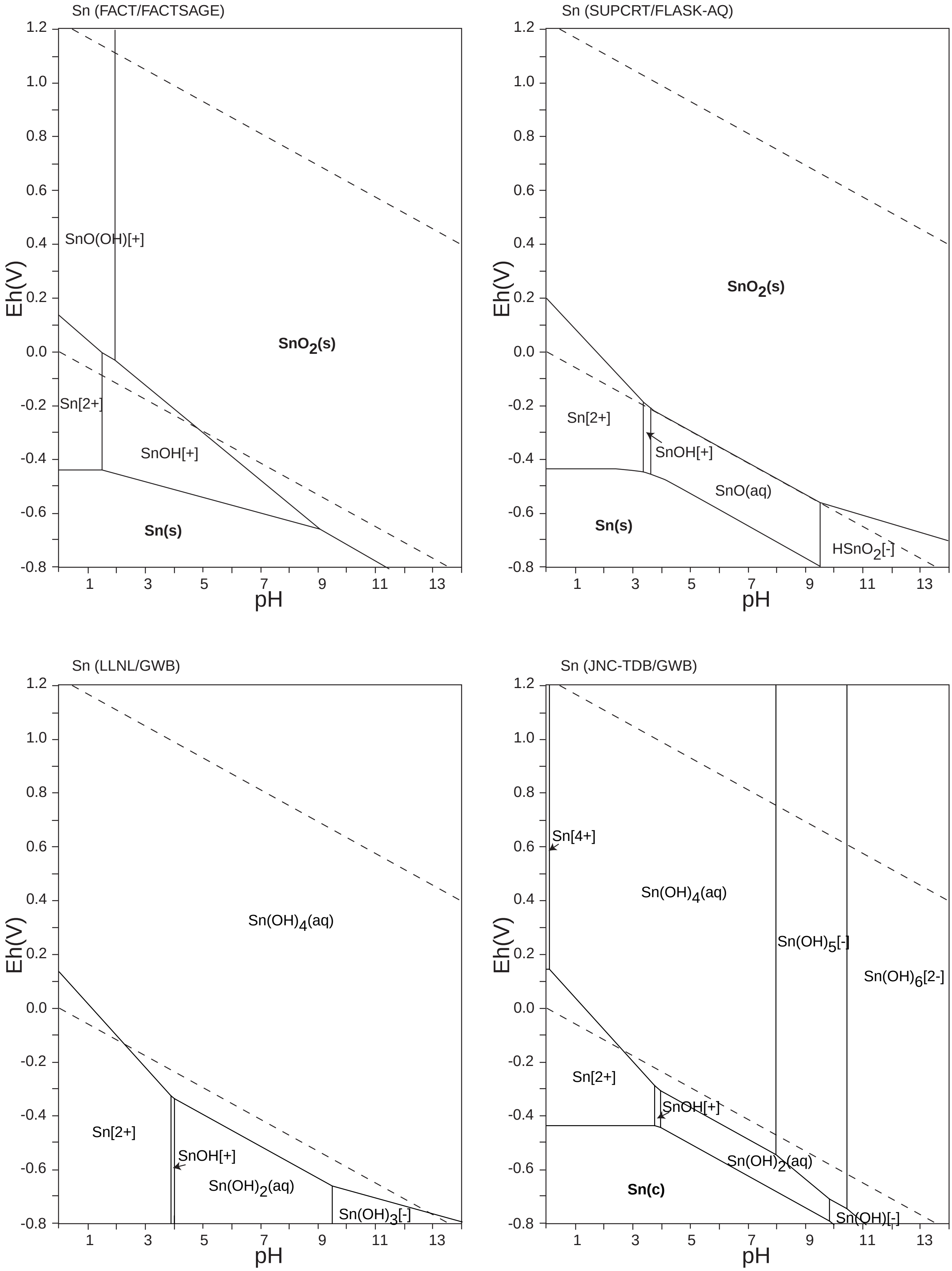

Figure 117: Eh-pH diagrams of the system Sn-O-H (1). $\sum \mathrm{Sn} = 10^{-10}$, 298.15K, 10^5 Pa.

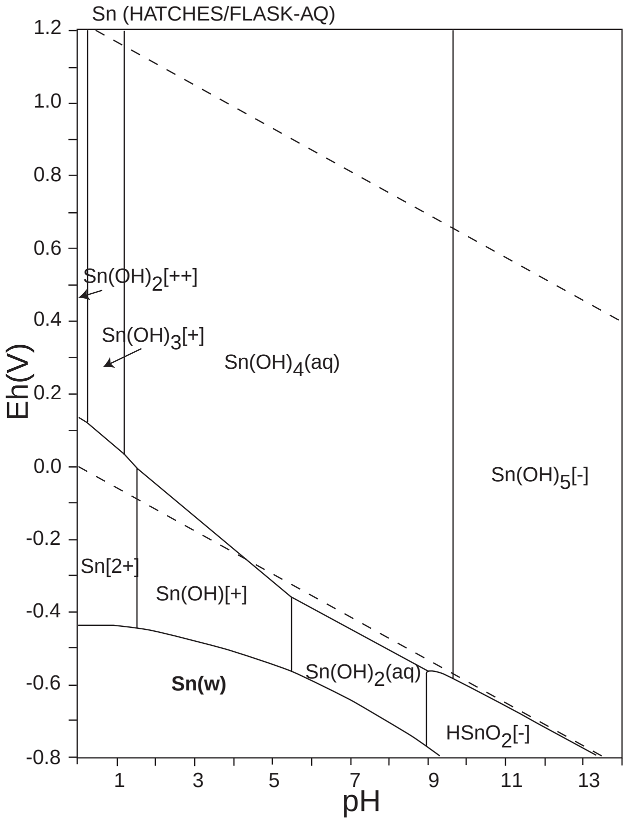

Figure 118: Eh-pH diagrams of the system Sn-O-H (2). $\sum \mathrm{Sn} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 73: List of Sr species

FACT	SUPCRT	LLNL	JNC-TDB
Sr[2+], SrOH[+], **Sr(s)**, **Sr(s2)**, **SrH_2(s)**, **SrO(s)**, **SrO_2(s)**, **$Sr(OH)_2$(s)**	Sr[2+], SrOH[+]	Sr[2+], SrOH[+], **$Sr(OH)_2$(c)**, **SrO(c)**	Sr[2+], SrOH[+], $Sr(OH)_2$(aq), **$Sr(OH)_2$(s)**, **Sr(c)**, **SrO(c)**

HATCHES			
Sr[2+], $Sr(OH)_2$(aq), SrOH[+], **$Sr(OH)_2$**, **SrO(c)**			

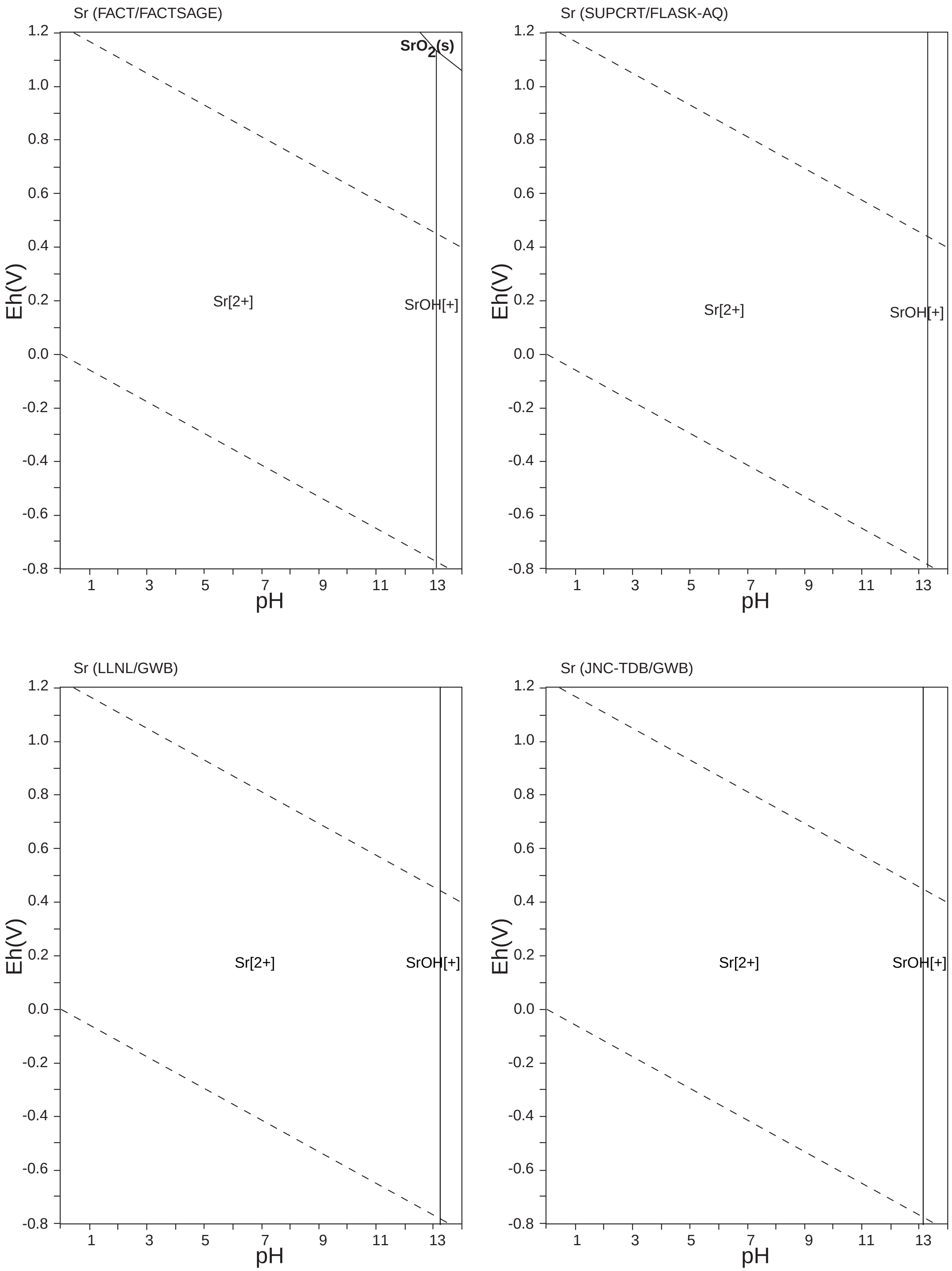

Figure 119: Eh-pH diagrams of the system Sr-O-H (1). $\sum \mathrm{Sr} = 10^{-10}$, 298.15K, 10^5 Pa.

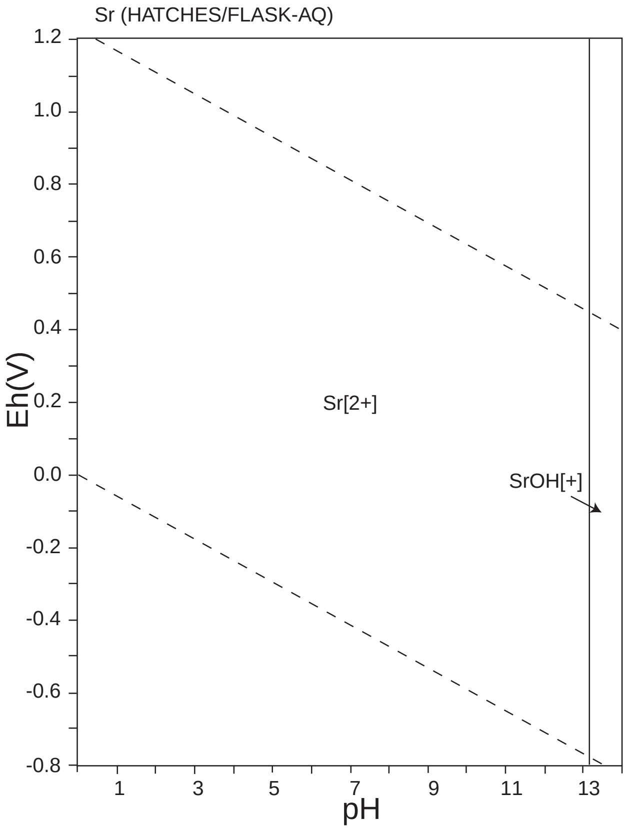

Figure 120: Eh-pH diagrams of the system Sr-O-H (2). $\sum \mathrm{Sr} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 74: List of Tb species

FACT	SUPCRT	LLNL	JNC-TDB
$Tb[3+]$, **$Tb(s)$**, **$Tb(s2)$**, **$TbO_2(s)$**, **$Tb_2O_3(s)$**, **$Tb_6O_{11}(s)$**, **$Tb_7O_{12}(s)$**	$Tb[3+]$, $Tb[4+]$, $Tb[2+]$, $TbOH[2+]$, $TbO[+]$, $TbO_2H(aq)$, $TbO_2[-]$		

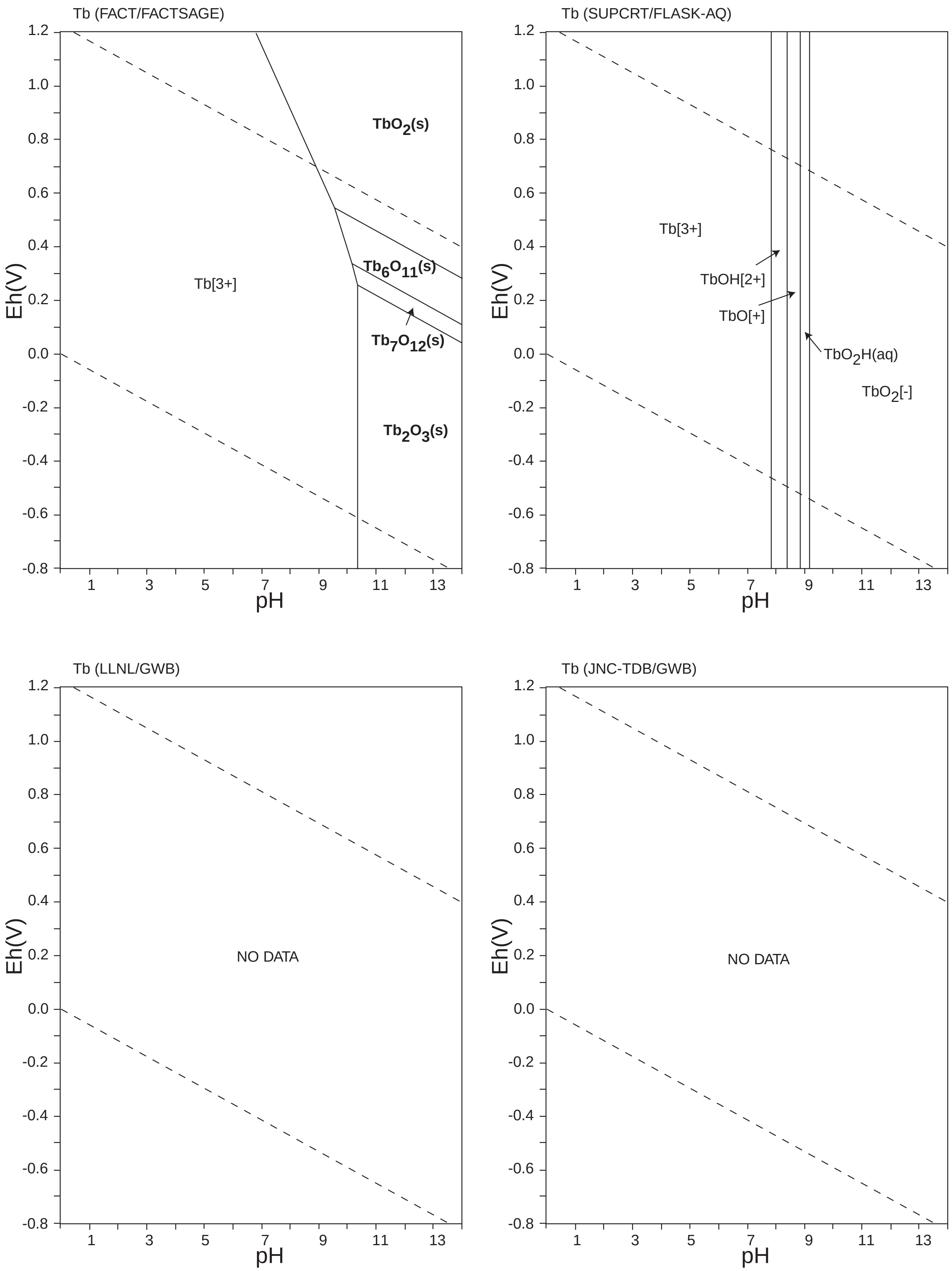

Figure 121: Eh-pH diagrams of the system Tb-O-H. $\sum \mathrm{Tb} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 75: List of Tc species

FACT	SUPCRT	LLNL	JNC-TDB
Tc(s), **TcO_2(s)**, **TcO_3(s)**, **Tc_2O_7(s)**	TcO_4[-]	TcO_4[-], Tc[3+], TcO[2+], TcO_4[2-], TcO_4[3-], $TcO(OH)_2$(aq), TcOOH[+], $[TcO(OH)_2]_2$(aq), **$HTcO_4$(s), $Tc(OH)_2$(s) $Tc(OH)_3$(s), Tc(c) Tc_2O_7(s), Tc_3O_4(s) Tc_4O_7(s), TcO_2*$2H_2O$(am) TcO_3(s), TcOH(s)**	TcO[2+], TcO_4[2-], TcO_4[-], TcO(OH)[+], $TcO(OH)_2$(aq), $TcO(OH)_3$[-], **Tc(c), TcO_2(c), $TcO_{216}H_2$(s), Tc_2O_7(c), $Tc_2O_7H_2O$(s)**, Tc(g), TcO(g), Tc_2O_7(g)

HATCHES	OECD-NEA	OECD-NEA update	
TcO[2+], Tc[3+], TcO_4[-], TcO(OH)[+], $TcO(OH)_2$(aq), $TcO(OH)_3$[-], **$HTcO_4$(s), Tc(c), $Tc(OH)_2$, $Tc(OH)_3$, Tc_2O_7, Tc_2O_7*H_2O, Tc_3O_4, Tc_4O_7, TcO_2am, TcO_{21}*$6H_2O$, TcO_3, TcOH**	TcO_4[-], TcO_4[2-], TcO_4[3-], TcO(OH)[+], $TcO(OH)_2$(aq), $TcO(OH)_3$[-], **Tc(c), TcO_2(c), Tc_2O_7(c), TcO_2*$1.6H_2O$(s), $Tc_2O_7H_2O$(s)**	TcO_4[-], TcO[2+], TcO_4[2-], TcO(OH)[+], $TcO(OH)_2$(aq), $TcO(OH)_3$[-], **Tc(cr), TcO_2(cr), Tc_2O_7(cr), TcO_2*$1.6H_2O$(s), $Tc_2O_7H_2O$(s)**	

Remarks
JNC-TDB: Given reaction of $TcO_{216}H_2$ in the database file suggests its formula as $TcO_{3.6}H_{3.2}$.

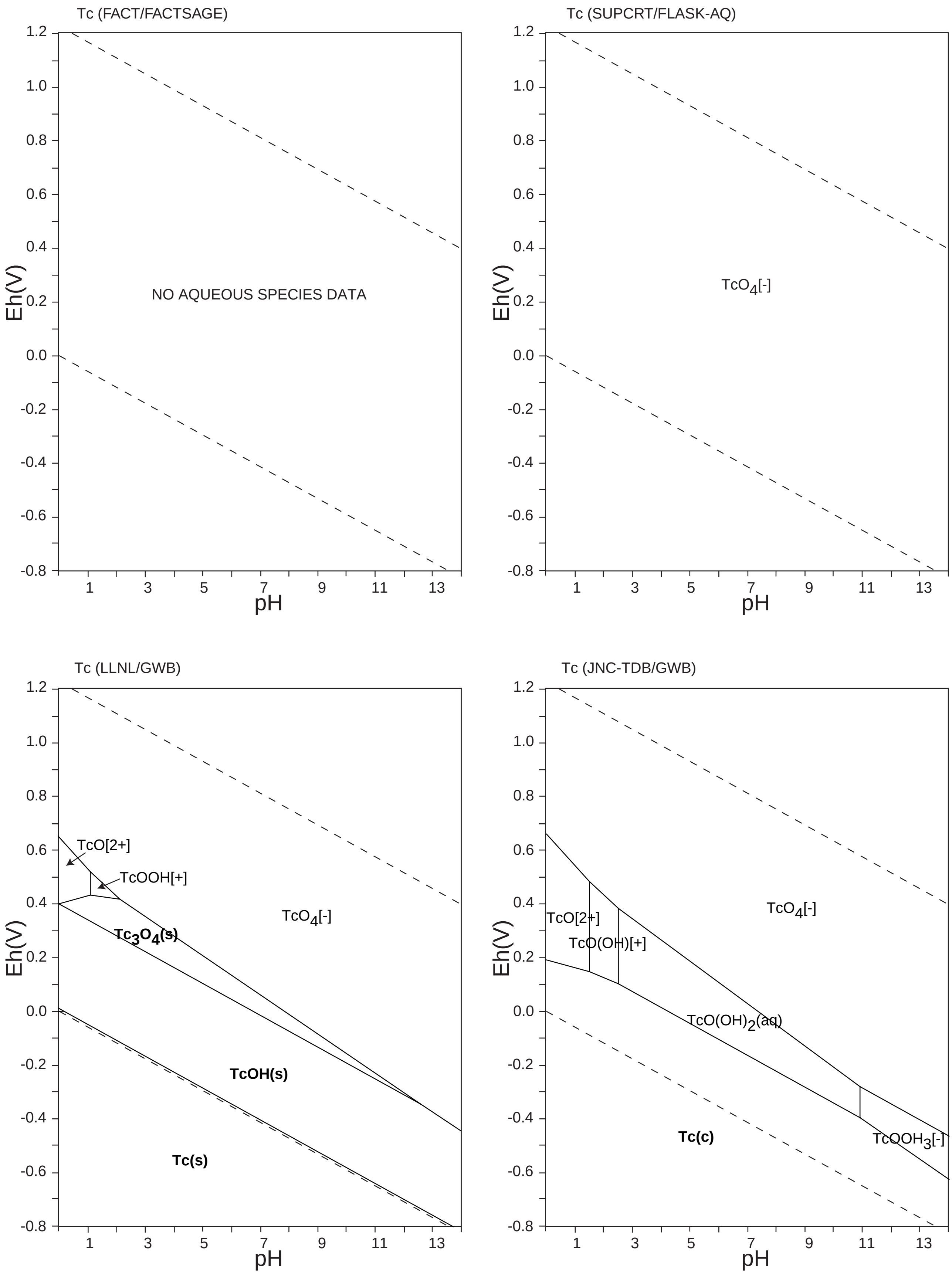

Figure 122: Eh-pH diagrams of the system Tc-O-H (1). $\sum \mathrm{Tc} = 10^{-10}$, 298.15K, 10^5 Pa.

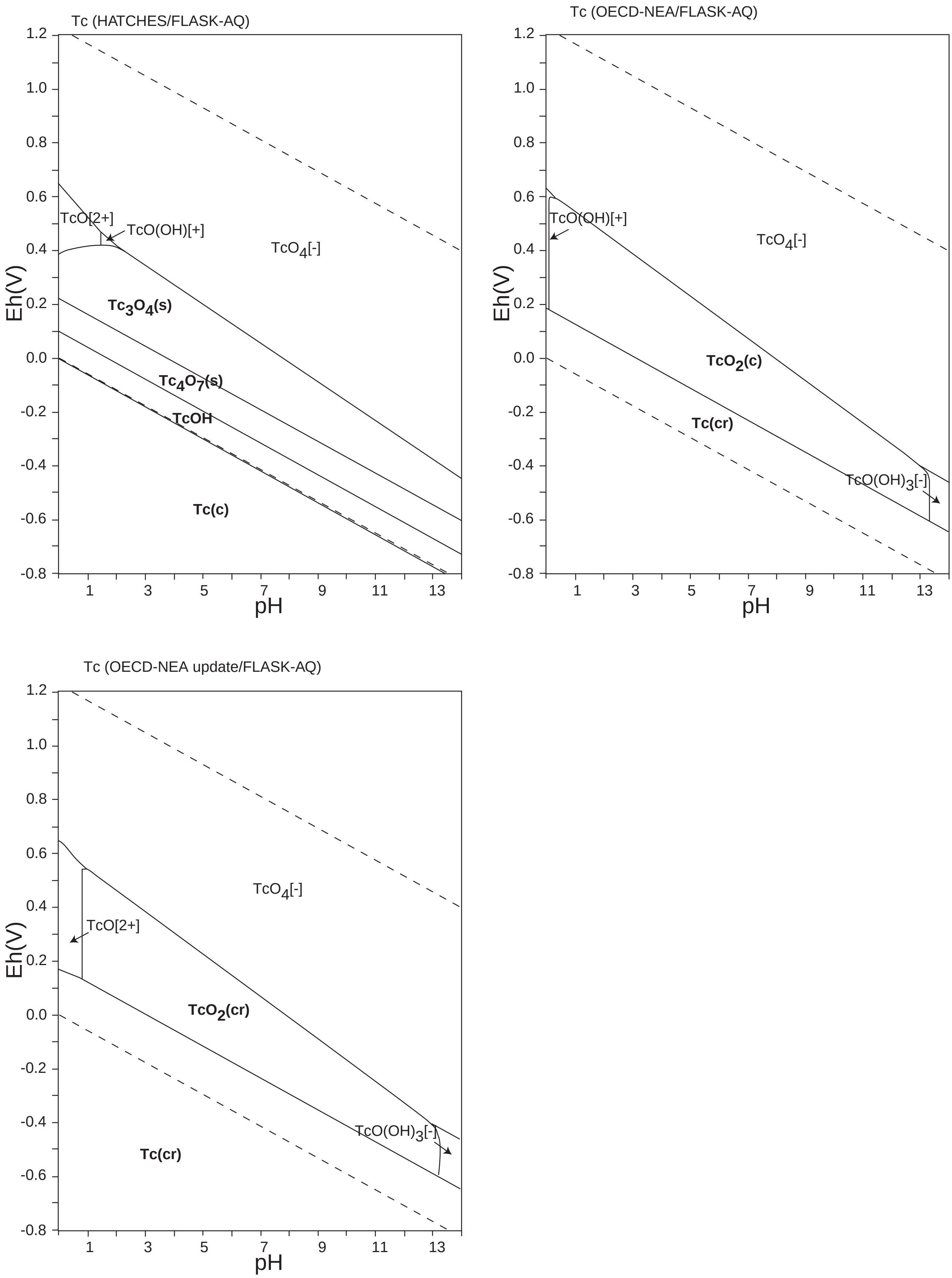

Figure 123: Eh-pH diagrams of the system Tc-O-H (2). $\sum \mathrm{Tc} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 76: List of Te species

FACT	SUPCRT	LLNL	JNC-TDB
TeO_3[2-], $Te(OH)_3$[+], **Te(s)**, **TeO_2(s)**, **H_2TeO_4(s)**			

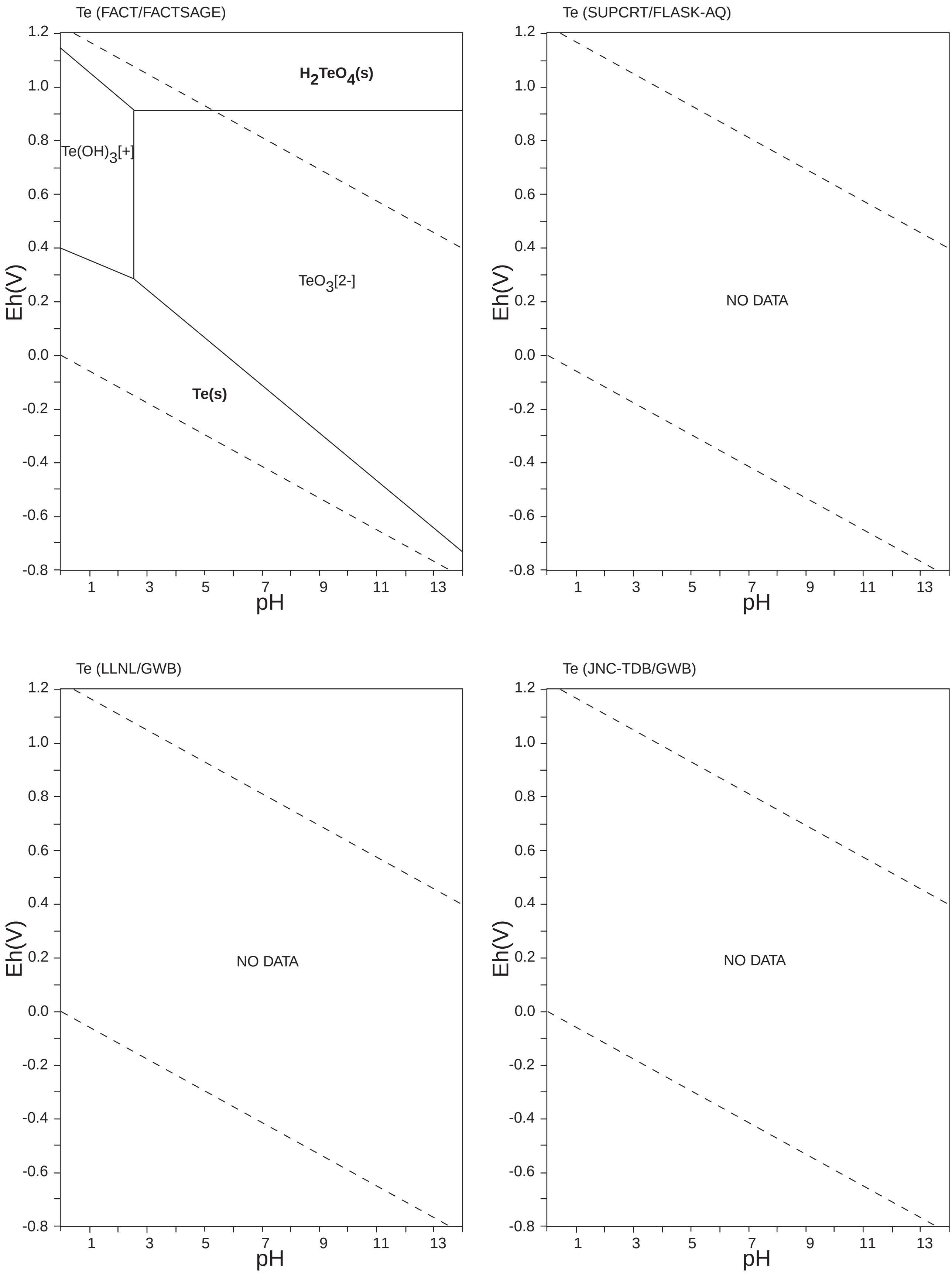

Figure 124: Eh-pH diagrams of the system Te-O-H. $\sum \mathrm{Te} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 77: List of Th species

FACT	SUPCRT	LLNL	JNC-TDB
Th[4+], **Th(s)**, **Th(s2)**, **ThH_2(s)**, **ThO_2(s)**	Th[4+]	Th[4+], $Th(OH)_2$[2+], $Th(OH)_3$[+], $Th(OH)_4$(aq), $Th_2(OH)_2$[6+], $Th_4(OH)_8$[8+], $Th_6(OH)_{15}$[9+], ThOH[3+] **$Th(OH)_4$(c)**, **ThO_2(s)**, **Thorianite**	Th[4+], $Th(OH)_4$(aq), **ThO_2(am)**, **ThO_2(c)**

HATCHES			
Th[4+], Th(OH)[3+], $Th(OH)_2$[2+], $Th(OH)_3$[+], $Th(OH)_4$(aq), $Th_2(OH)_2$[6+], $Th_4(OH)_8$[8+], **$Th(OH)_4$**, **ThO_2**,**ThO_2(c)**			

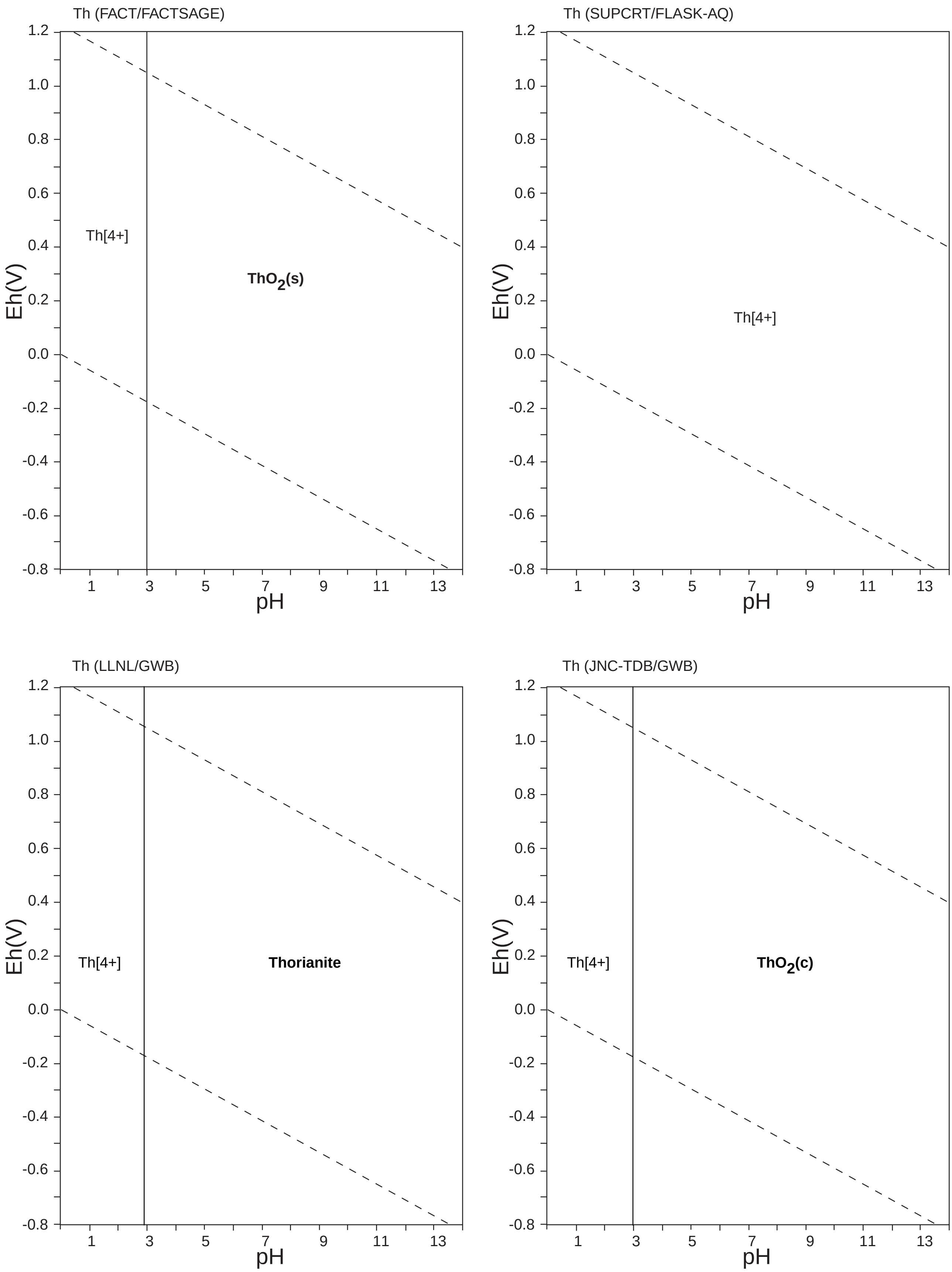

Figure 125: Eh-pH diagrams of the system Th-O-H (1). $\sum \mathrm{Th} = 10^{-10}$, 298.15K, 10^5 Pa.

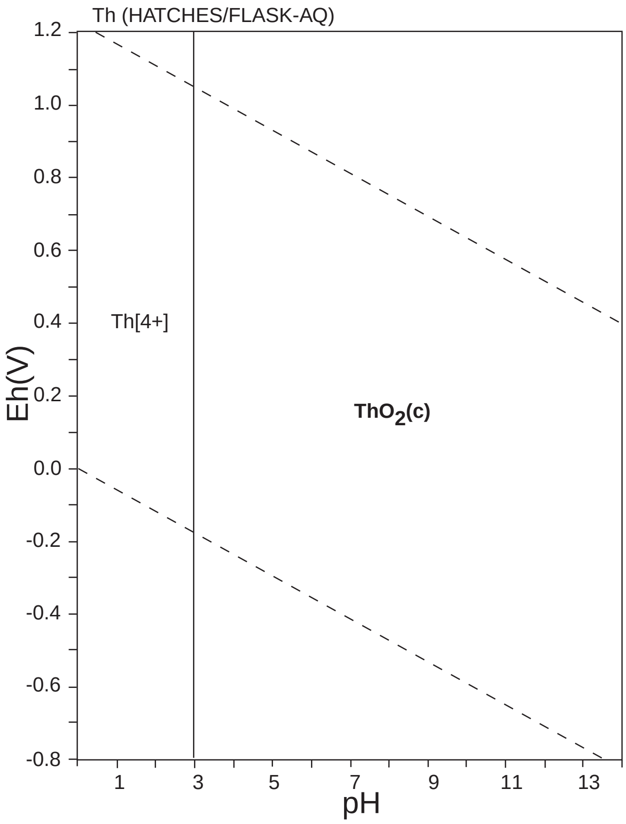

Figure 126: Eh-pH diagrams of the system Th-O-H (2). $\sum \mathrm{Th} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 78: List of Tl species

FACT	SUPCRT	LLNL	JNC-TDB
Tl[+], Tl[3+], TlOH(aq), TlOH[2+], $Tl(OH)_2$[+], **Tl(s)**, **Tl(s2)**, **Tl_2O(s)**, **Tl_2O_3(s)**, **Tl_2O_4(s)**, **TlOH(s)**, **$Tl(OH)_3$(s)**	Tl[+], Tl[3+], TlOH(aq), TlOH[2+], TlO[+], $HTlO_2$(aq), TlO_2[-]		Tl[+]

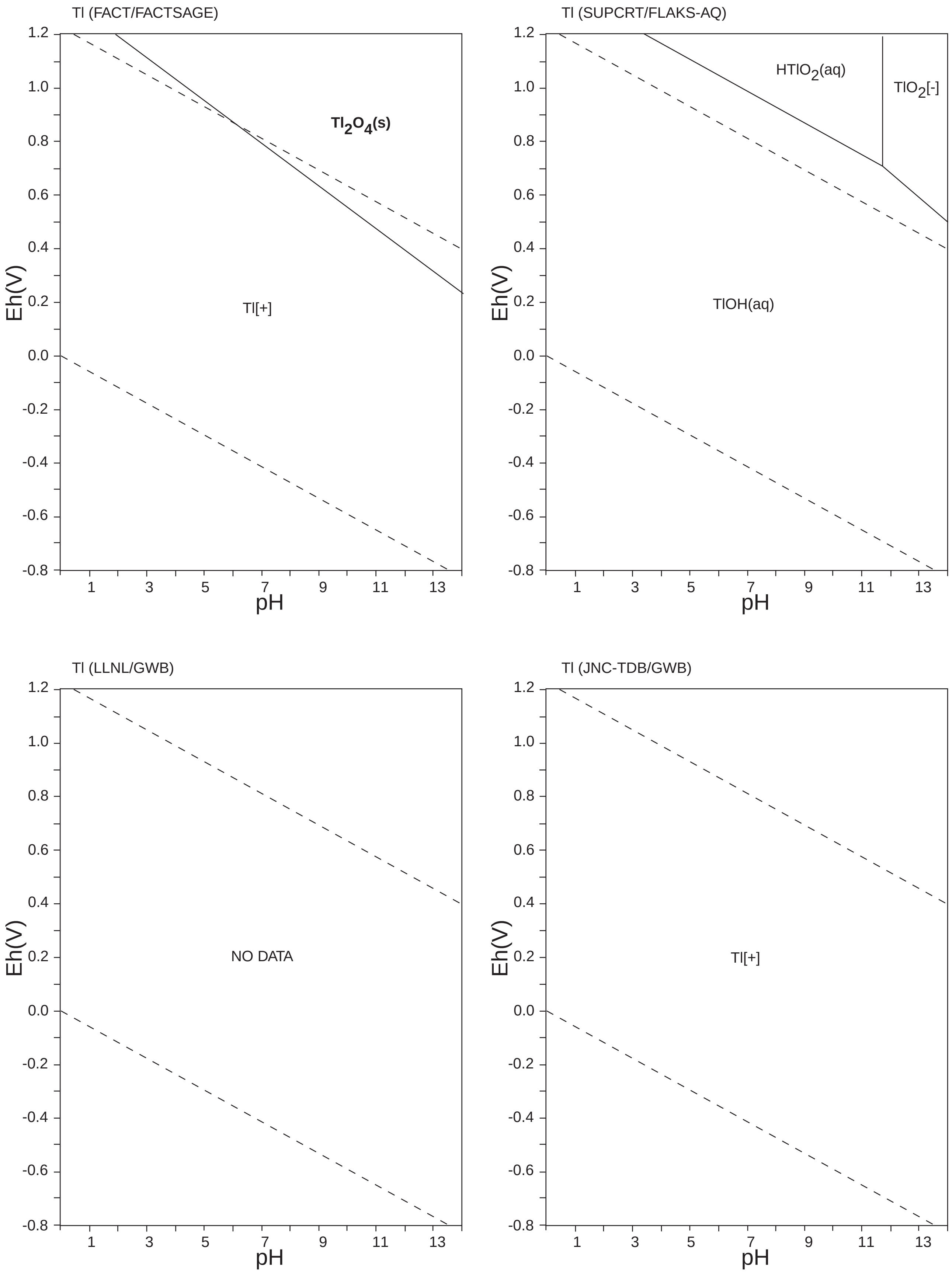

Figure 127: Eh-pH diagrams of the system Tl-O-H. $\sum \mathrm{Tl} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 79: List of Tm species

FACT	SUPCRT	LLNL	JNC-TDB
Tm^{3+}, **Tm(s)**, **Tm_2O_3(s)**, **Tm_2O_3(s2)**, **Tm_2O_3(s3)**	Tm^{3+}, Tm^{4+}, Tm^{2+}, $TmOH^{2+}$, TmO^{+}, TmO_2H(aq), TmO_2^{-}		

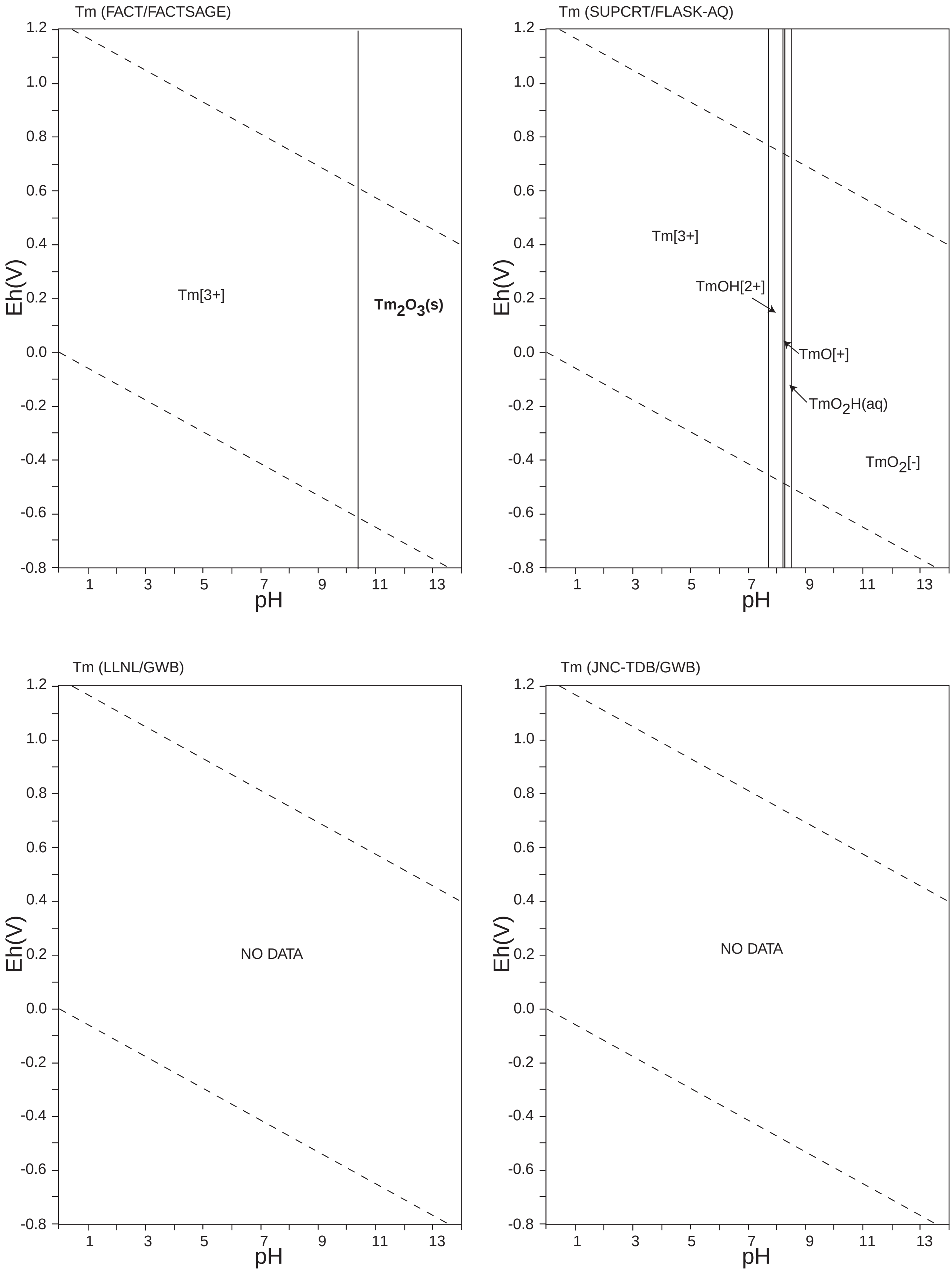

Figure 128: Eh-pH diagrams of the system Tm-O-H. $\sum \mathrm{Tm} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 80: List of U species

FACT	SUPCRT	LLNL	JNC-TDB
$U[3+]$, $U[4+]$, $UO_2[+]$, $UO_2[2+]$, $UOH[3+]$, $HO_3U[+]$, $H_3O_3U[+]$, $H_5O_5U[-]$, $H_2O_2U[2+]$, $H_2O_6U_2[2+]$, $H_5O_{11}U_3[+]$, $H_7O_{13}U_3[-]$, **U(s), U(s2), U(s3), UH_3(s), UO_3(s), U_3O_8(s), U_4O_9(s), $UO_3(H_2O)$(s), $UO_3(H_2O)_2$(s), UO_2(s)**	$U[3+]$, $U[4+]$, $UO_2[+]$, $UO_2[2+]$, $UOH[3+]$, $UO_2OH[+]$, $HUO_2[+]$, $HUO_3[-]$, $UOH[2+]$, $UO[+]$, HUO_2(aq), $UO[2+]$, UO_2(aq), UO_2OH(aq), $UO_3[-]$, UO_3(aq), $HUO_4[-]$, $UO_4[2-]$, **UO_2(Uranitite)**	$U[4+]$, $U[3+]$, $UO_2[+]$ $UO_2[2+]$, $(UO_2)_2(OH)_2[2+]$, $(UO_2)_3(OH)_4[2+]$, $(UO_2)_3(OH)_5[+]$, $(UO_2)_3(OH)_7[-]$, $(UO_2)_4(OH)_7[+]$, $U(OH)_2[2+]$, $U(OH)_3[+]$, $U(OH)_4$(aq), $U(OH)_5[-]$, $U_6(OH)_{15}[9+]$, $UO_2OH[+]$, $UOH[3+]$, **Gummite, Schoepite, U(c,alph), U_3O_8(c,alph), U_4O_9(c), $UO_2(OH)_2$(c,bet), UO_2(am) UO_3(c, gamma), Uraninite**	$U[4+]$, $U[3+]$, $UO_2[+]$, $UO_2[2+]$, $UO_2(OH)_3$(aq), $UO_2(OH)_4$(aq), $(UO_2)_2OH$(aq), $(UO_2)_2(OH)_2[2+]$, $(UO_2)_3(OH)_4[2+]$, $(UO_2)_3(OH)_5[+]$, $(UO_2)_3(OH)_7[-]$, $(UO_2)_4(OH)_7[+]$, $UO_2OH[+]$, $UO_2(OH)_2$(aq), $UOH[3+]$, $U(OH)_4$(aq), **UO_2(am), UO_3(alpha), UO_3(beta), UO_3(gamma), $UO_{3.0.9}$H, $UO_{3.2}$H2O, $UO_2(OH)_2$, U(c), UO_2(c) $UO_{2.25}$(b), $UO_{2.25}$(c), $UO_{2.3333}$, $UO_{2.6667}$, UH_3(beta)**, U(g), UO(g), UO_2(g), UO_3(g)

HATCHES	OECD-NEA	OECD-NEA update	
$U[4+]$, $UO_2[+]$, $UO_2[2+]$, $U(OH)[3+]$, $U(OH)_4$(aq), $U_6(OH)_{15}[9+]$, $Ul(OH)_2$(aq), $Ul(OH)_3[-]$, $Ul(OH)_4[2-]$, $Ul_2(OH)_2[2+]$, $Ul_2OH[3+]$, $Ul_3(OH)_4[2+]$, $Ul_3(OH)_5[+]$, $Ul_3(OH)_7[-]$, $Ul_4(OH)_7[+]$, $UlOH[+]$, **Gummite, Schoepite, U(c,alph), U_3O_8, U_4O_9, UO_2(am), UO_2(c), $UO_2(OH)_2$, UO_2OH, UO_3, UO_3*2H_2O, Uraninite**	$U[4+]$, $U[3+]$, $UO_2[+]$, $UO_2[2+]$, $UOH[3+]$, $UO_2OH[+]$, $U(OH)_4$(aq), $UO_2(OH)_3[-]$, $UO_2(OH)_4[2-]$, $(UO_2)_2OH[3+]$, $(UO2)_2(OH)_2[2+]$, $(UO2)_3(OH)_4[2+]$, $(UO2)_3(OH)_5[+]$, $(UO2)_3(OH)_7[-]$, $(UO2)_4(OH)_7[+]$, **U(c), UO_2(c), $UO_{2.25}$(c), $UO_{2.25}$(beta), $UO_{2.3333}$(beta), $UO_{2.6667}$(c), UO_3(alpha), UO_3(beta), UO_3(gamma), UH_3(beta), UO_3*0.9H_2O(alpha), $UO_2(OH)_2$(beta), UO_3*2H_2O(c)**	$U[4+]$, $U[3+]$, $UO2[+]$, $UO_2[2+]$, $UOH[3+]$, $UO_2OH[+]$, $UO_2(OH)_2$(aq), $U(OH)_4$(aq), $UO_2(OH)_3[-]$, $UO_2(OH)_4[2-]$, $(UO_2)_2OH[3+]$, $(UO_2)_2(OH)_2[2+]$, $(UO_2)_3(OH)_4[2+]$, $(UO_2)_3(OH)_5[+]$, $(UO_2)_3(OH)_7[-]$, $(UO_2)_4(OH)_7[+]$, **U(cr), UO_2(cr), $UO_{2.25}$(beta), $UO_{2.25}$(cr), $UO_{2.3333}$(beta), $UO_{2.6667}$(cr), UO_3(alpha), UO_3(beta), UO_3(gamma), UH_3(beta), UO_3*0.9H_2O(alpa), $UO_2(OH)_2$(beta), UO_3*2H_2O(cr)**	

Rmarks
HATCHES: Ul stands for UO2.
JNC-TDB: Given reaction of $UO_{3.0.9}$H in the database file suggests its formula as UO_3H.
Given reaction of $UO_{3.2}H_2O$ in the database file suggests its formula as UO_3*2H_2O.
$UO_{2.25}$(b) may be $UO_{2.25}$(beta)?

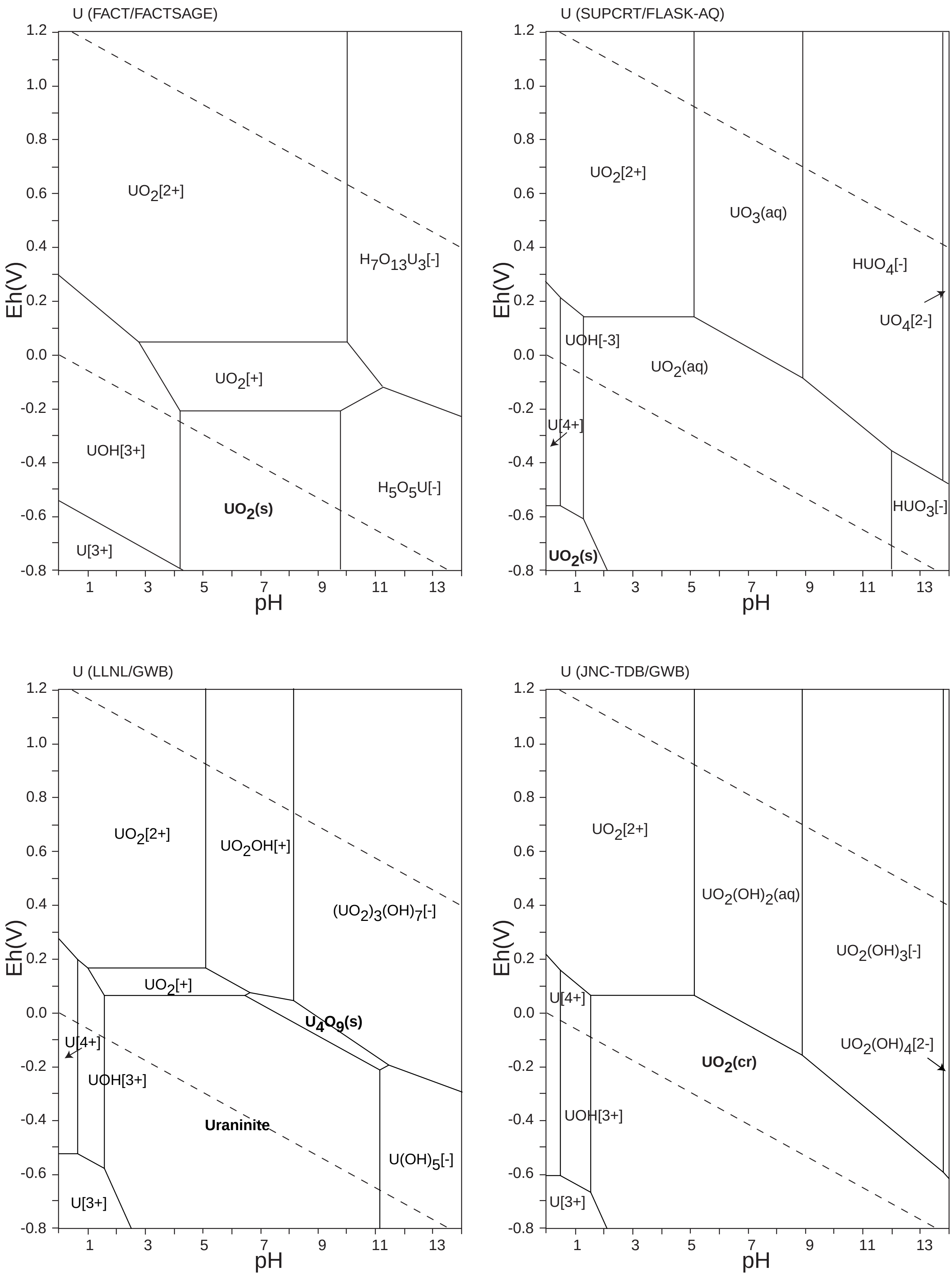

Figure 129: Eh-pH diagrams of the system U-O-H (1). $\sum \mathrm{U} = 10^{-10}$, 298.15K, 10^5 Pa.

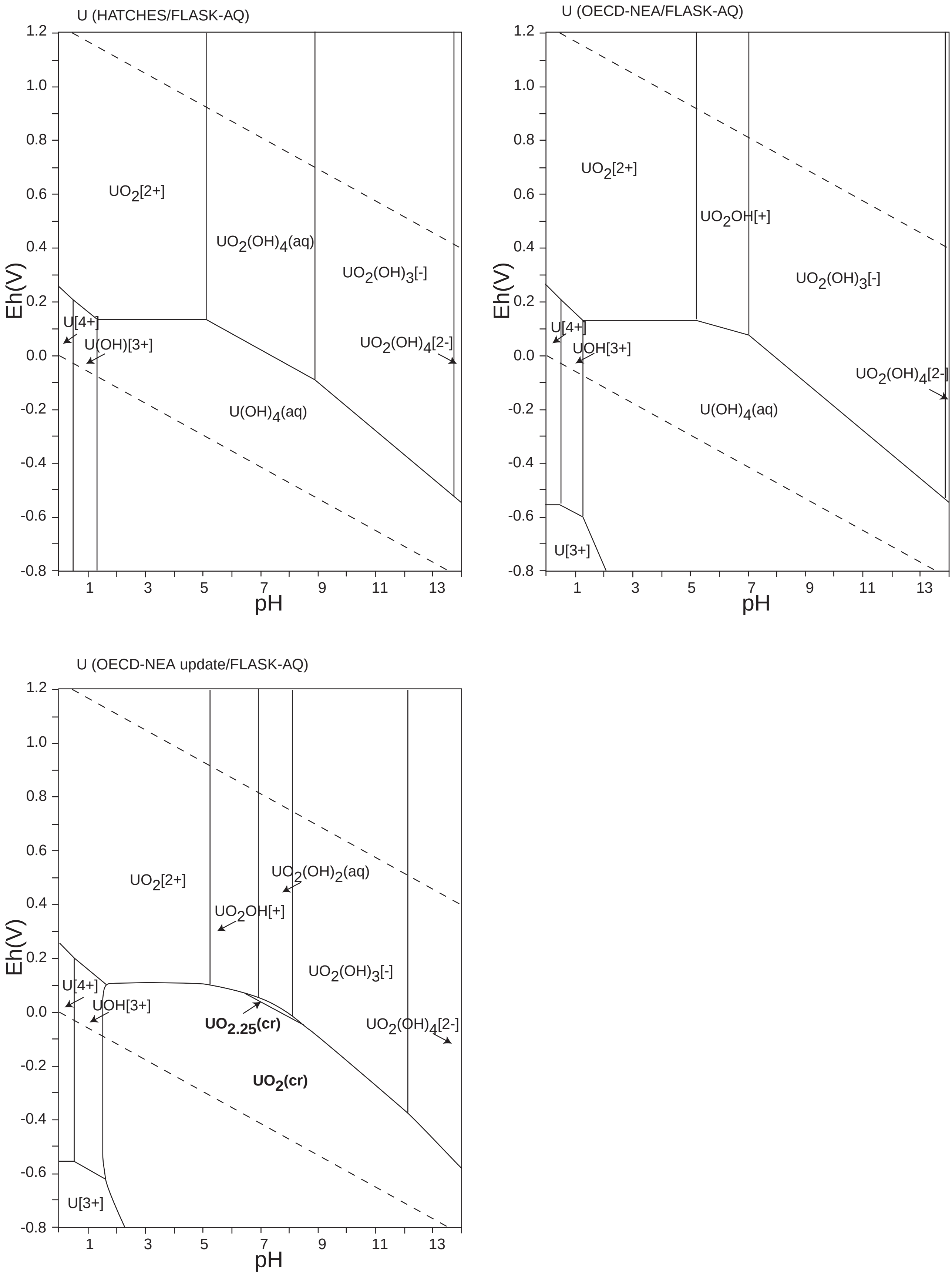

Figure 130: Eh-pH diagrams of the system U-O-H (2). $\sum \mathrm{U} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 81: List of V species

FACT	SUPCRT	LLNL	JNC-TDB
VO[2+], VO_2[+], VO_4[3-], HVO_4[2-], VO_3[-], VO_4[-], V_2O_7[4-], VOH_2O_2[3+], HVO_4(aq), H_2VO_4[+], HV_2O_7[3-], $H_3V_2O_7$[-], $HV_{10}O_{28}$[5-], $H_2V_{10}O_{28}$[4-], **V(s)**, **VO(s)**, **VO_2(s)**, **VO_2(s2)**, **V_2O_3(s)**, **V_2O_4(s)**, **V_2O_4(s2)**, **V_2O_5(s)**, **V_3O_5(s)**, **V_4O_7(s)**	VO[2+], VO_2[+], VO_4[3-], HVO_4[2-], V[3+], V[2+], H_3VO_4(aq), H_2VO_4[-], VO[+], VOH[+], VOH[2+], VOOH[+]	V[3+], VO[2+], VO_4[3-], $(VO)_2(OH)_2$[2+], $(VO)_2(OH)_5$[-], V(OH)2[+], $V_2(OH)_2$[4+], $VO(OH)_3$(aq), $VO_2(OH)_2$[-], VO_2[+], VO_3OH[2-], VOH[2+], VOOH[+], **V_2O_3(c)**, **V_2O_4(c)**, **V_2O_5(c)**, **V_3O_5(c)**, **V_4O_7(c)**	

HATCHES			
VO[2+], V[3+], VO_2[+], VO_4[3-], $V_2(OH)_2$[4+], VO(OH)[+], $VO(OH)_3$(aq), $VO)_2(OH)_2$[2+], $VO_2(OH)_2$[-], VO_3(OH)[2-], VOH[2+], **$V(OH)_3$**, **V_2O_3(c)**, **V_2O_4(c)**, **V_2O_5(c)**, **V_3O_5(c)**, **V_4O_7(c)**, **$VO(OH)_2$**			

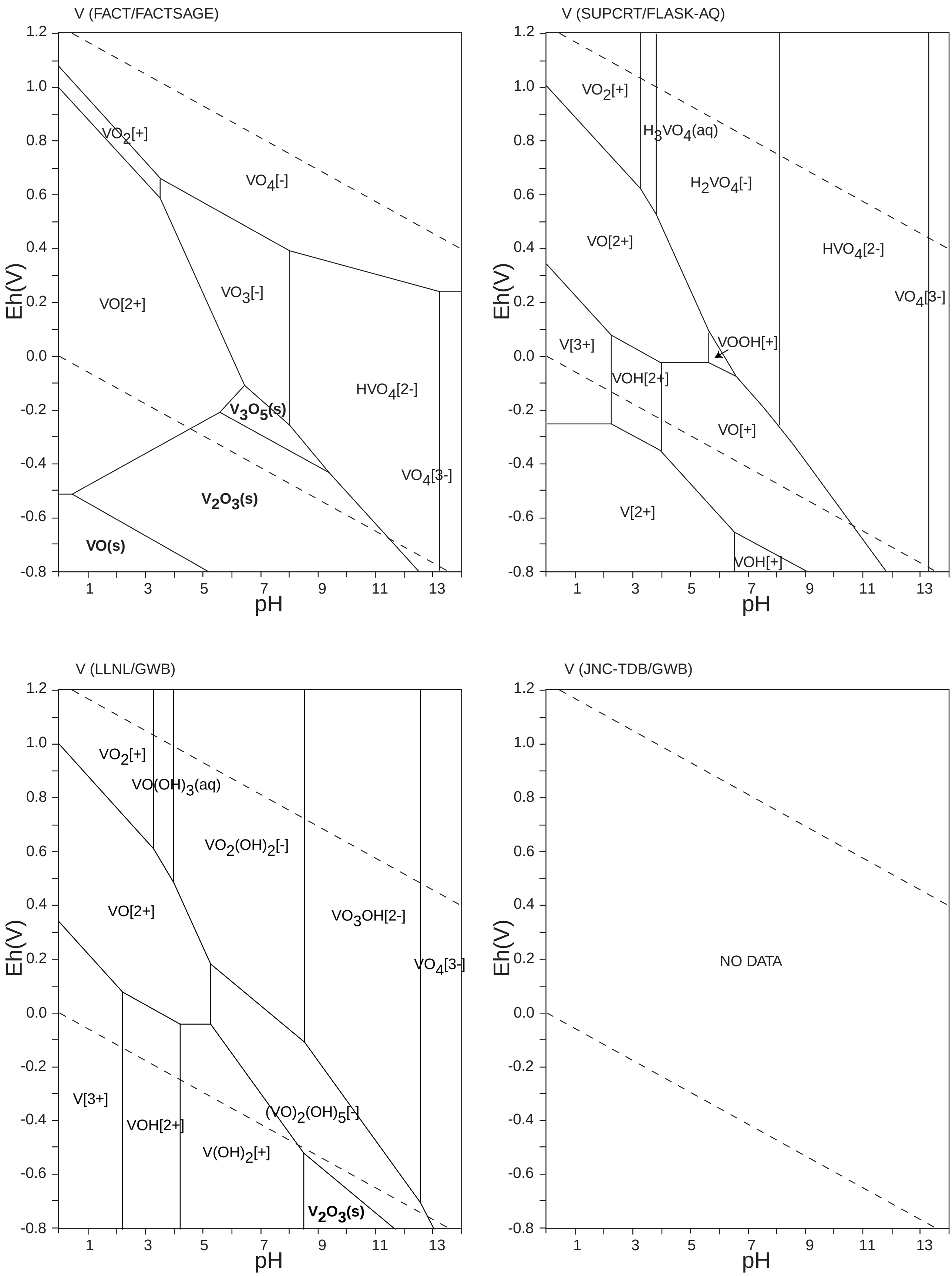

Figure 131: Eh-pH diagrams of the system V-O-H (1). $\sum \mathrm{V} = 10^{-10}$, 298.15K, 10^5 Pa.

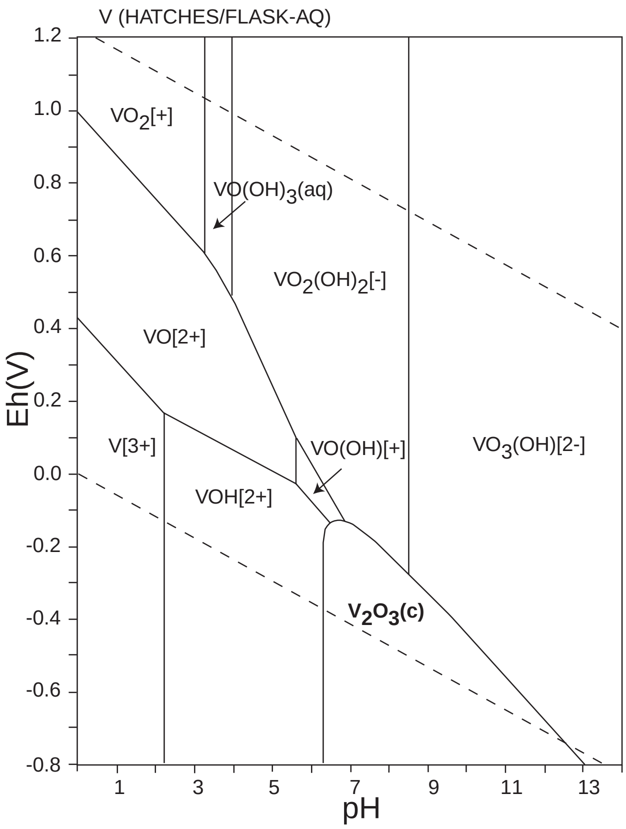

Figure 132: Eh-pH diagrams of the system V-O-H (2). $\sum \mathrm{V} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 82: List of W species

FACT	SUPCRT	LLNL	JNC-TDB
WO_4[2-], **W(s)**, **WO_2(s)**, **WO_3(s)**, **WO_3(s2)**, **$O_2W(OH)_2$(s)**	WO_4[2-], HWO_4[-]		

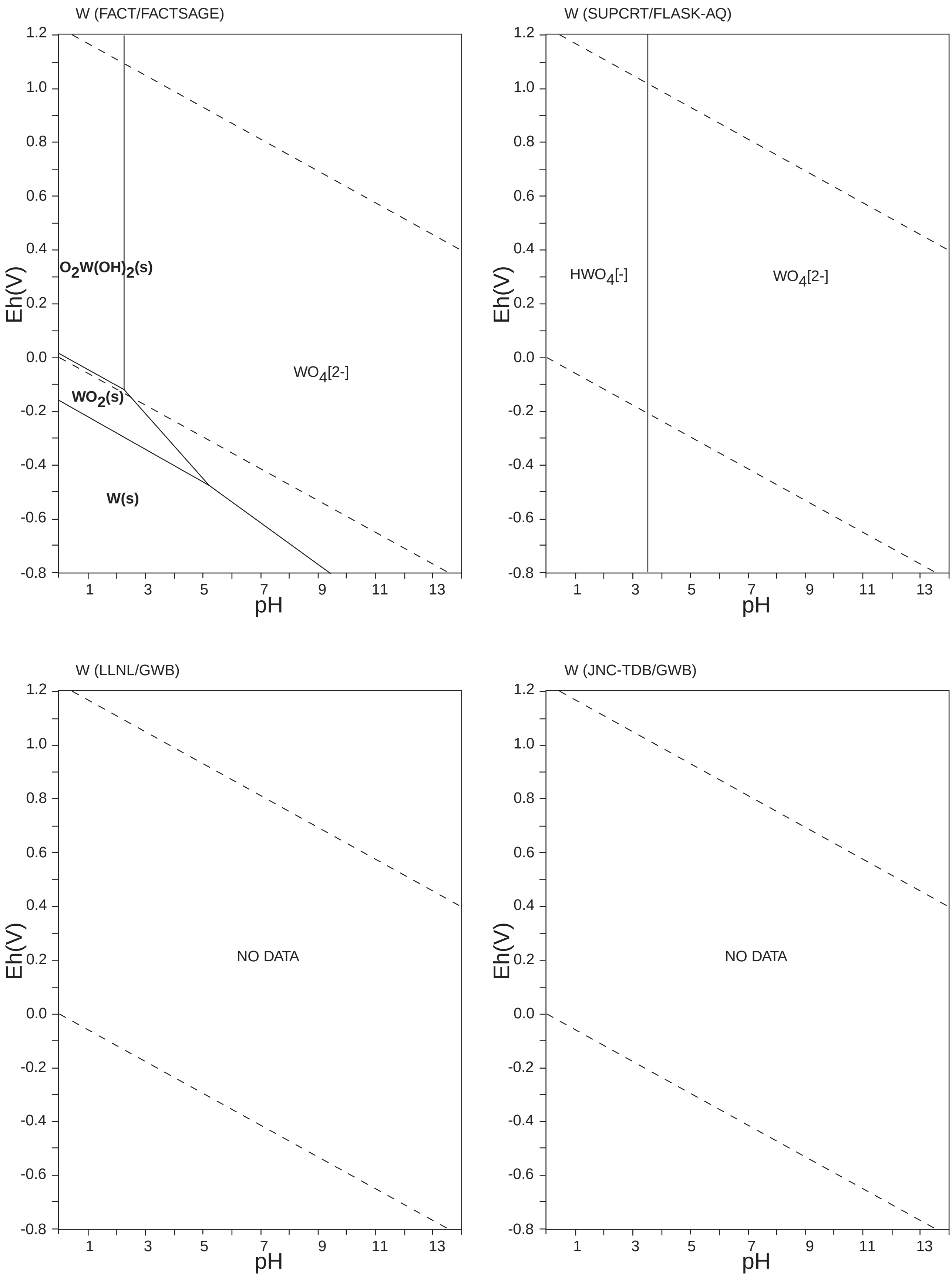

Figure 133: Eh-pH diagrams of the system W-O-H. $\sum \mathrm{W} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 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[-]		

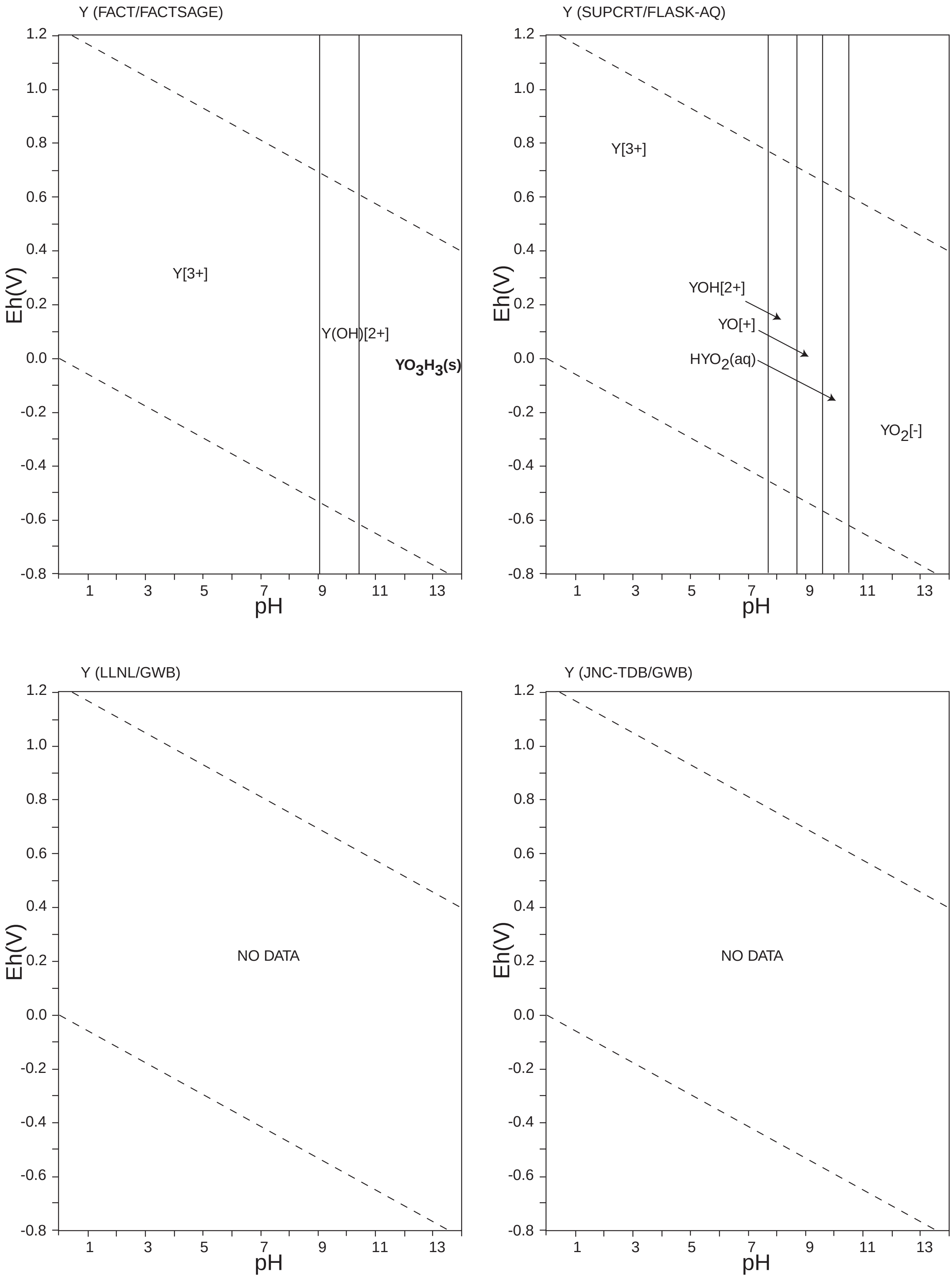

Figure 134: Eh-pH diagrams of the system Y-O-H. $\sum Y = 10^{-10}$, 298.15K, 10^5 Pa.

Table 84: List of Yb species

FACT	SUPCRT	LLNL	JNC-TDB
Yb[2+], Yb[3+], **Yb(s), Yb(s2), Yb_2O_3(s), Yb_2O_3(s2), Yb_2O_3(s3)**	Yb[2+], Yb[3+], Yb[4+], YbOH[2+], YbO[+], YbO_2H(aq), YbO_2[-]		

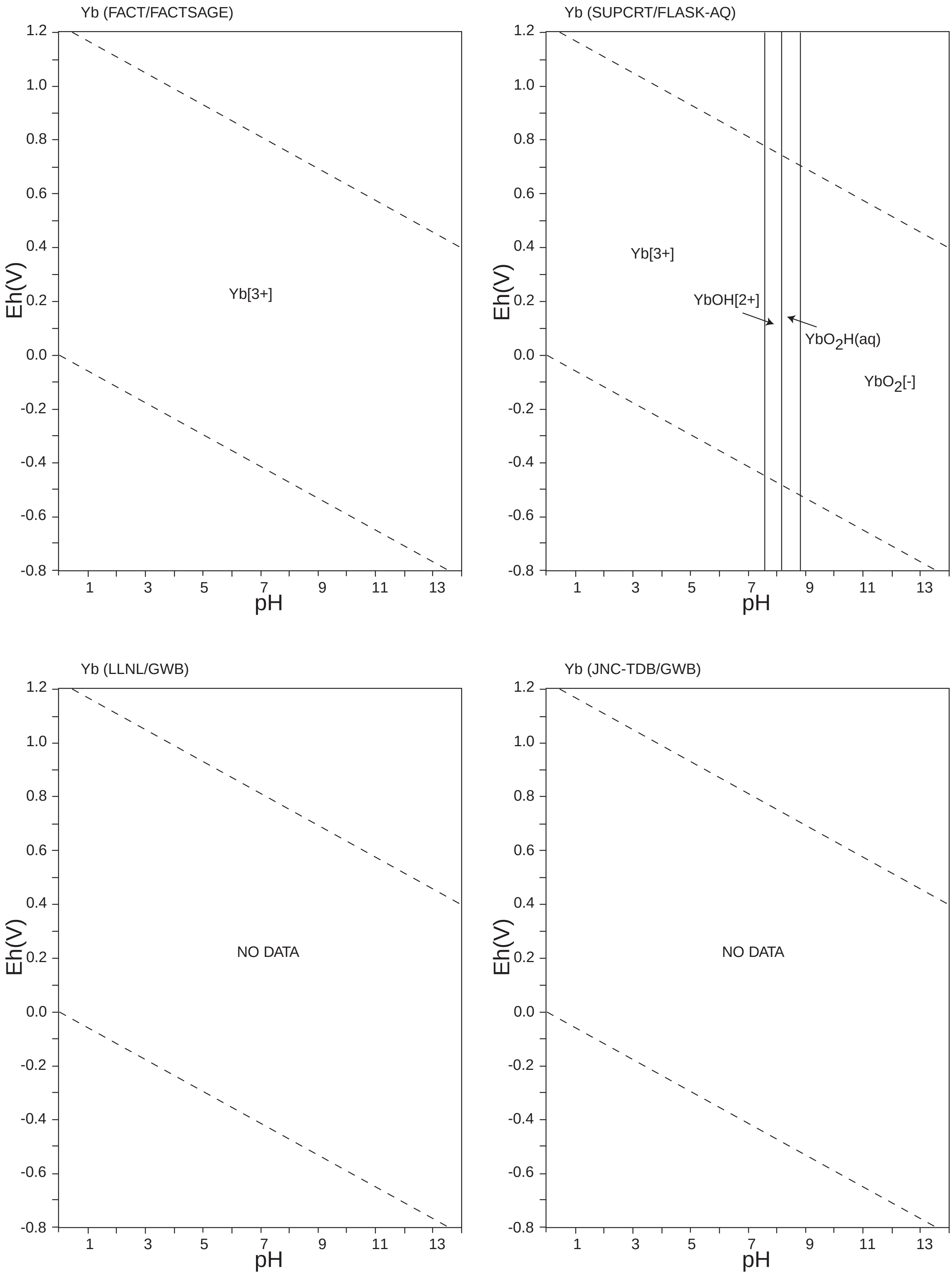

Figure 135: Eh-pH diagrams of the system Yb-O-H. $\sum \mathrm{Yb} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 85: List of Zn species

FACT	SUPCRT	LLNL	JNC-TDB
$Zn^{[2+]}$, $ZnO_2[2-]$, $ZnOH[+]$, $HZnO_2[-]$, $Zn(OH)_2(aq)$, **$ZnO(s)$, $Zn(s)$, $Zn(OH)_2(s)$, $Zn(OH)_2(s2)$, $Zn(OH)_2(s3)$**	Zn[2+], $ZnO_2[2-]$, ZnOH[+], $HZnO_2[-]$, ZnO(aq), **ZnO(Zincite)**	Zn[2+]	

HATCHES			
Zn[2+], $Zn(OH)_2(aq)$, $Zn(OH)_3[-]$, $Zn(OH)_4[2-]$, $Zn_2(OH)_6[2-]$, $Zn_2OH[3+]$, $ZnO_2[2-]$, ZnOH[+],**Zincite, $Zn(OH)_2$**			

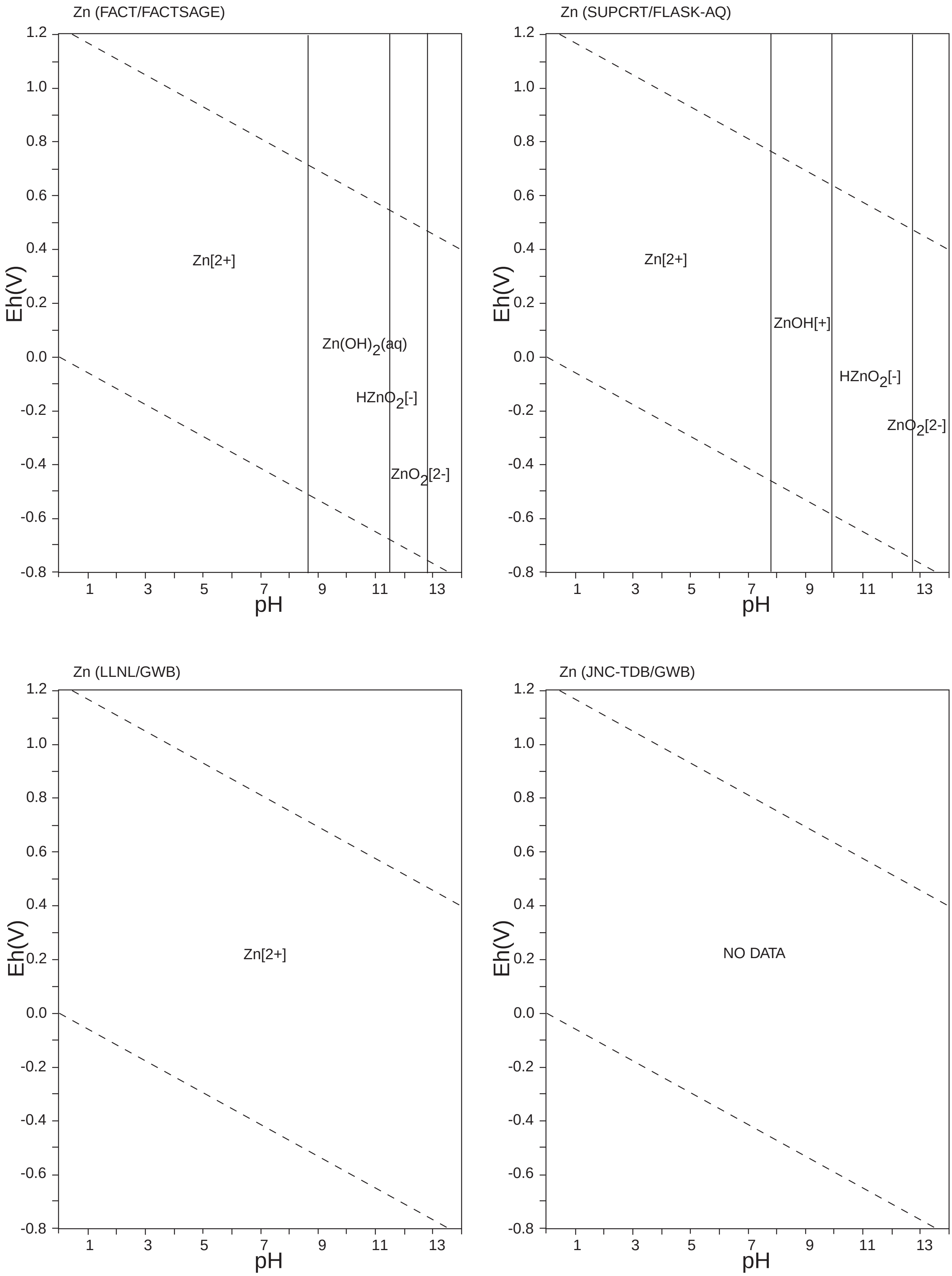

Figure 136: Eh-pH diagrams of the system Zn-O-H (1). $\sum \mathrm{Zn} = 10^{-10}$, 298.15K, 10^5 Pa.

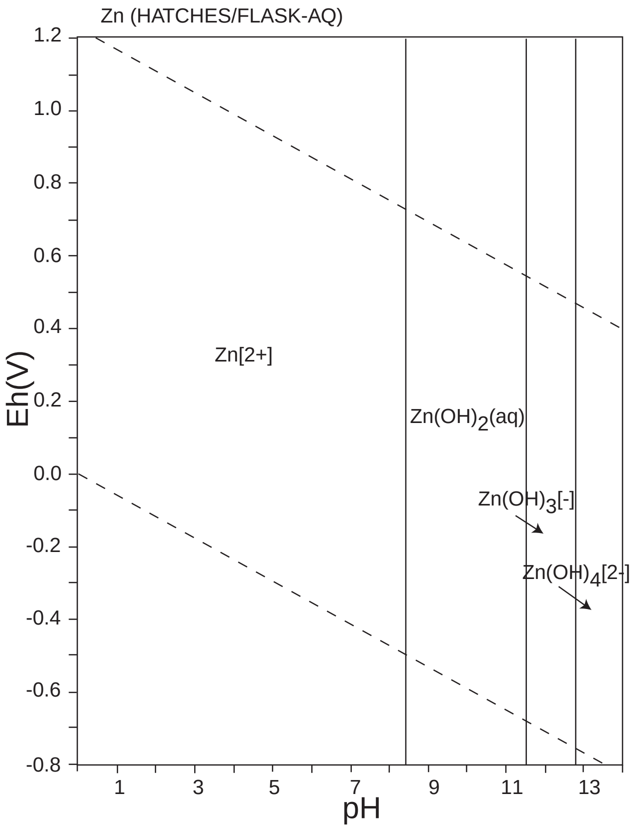

Figure 137: Eh-pH diagrams of the system Zn-O-H (2). $\sum \mathrm{Zn} = 10^{-10}$, 298.15K, 10^5 Pa.

Table 86: List of Zr species

FACT	SUPCRT	LLNL	JNC-TDB
ZrO[2+], **Zr(s)**, **Zr(s2)**, **ZrH_2(s)**, **ZrO_2(s)**, **ZrO_2(s2)**, **ZrO_2(s3)**	ZrO[2+], Zr[4+], ZrOH[3+], $HZrO_2$[+], ZrO_2(aq), $HZrO_3$[-]		$Zr(OH)_4$(aq), $Zr(OH)_5$[-], **ZrO_2(am)**

HATCHES			
Zr[4+], Zr(OH)[3+], $Zr(OH)_4$(aq), $Zr(OH)_5$[-], $Zr_3(OH)_4$[8+], $Zr_4(OH)_8$[8+], **ZrO_2(am)**, **ZrO_2(c)**			

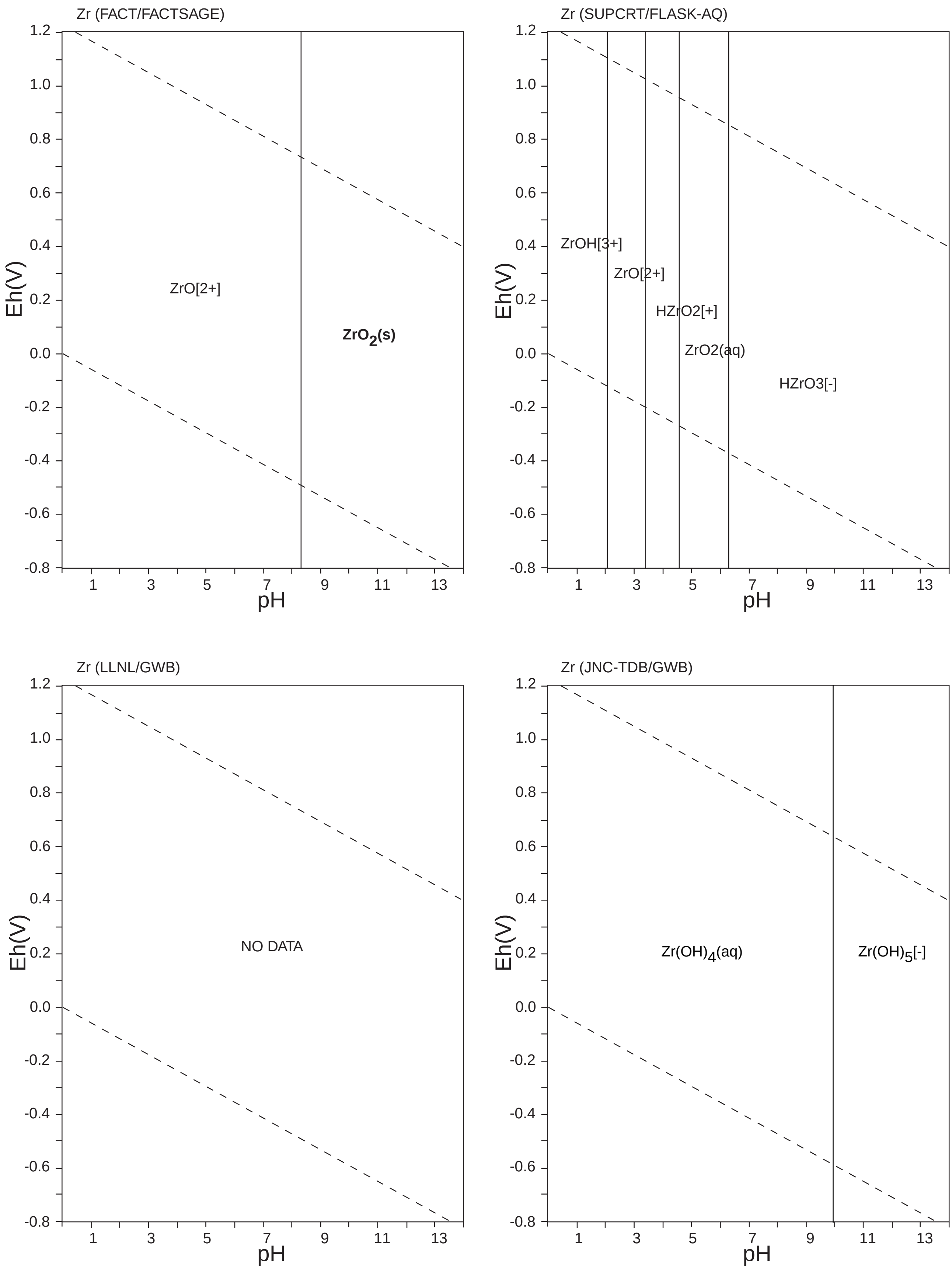

Figure 138: Eh-pH diagrams of the system Zr-O-H (1). $\sum \mathrm{Zr} = 10^{-10}$, 298.15K, 10^5 Pa.

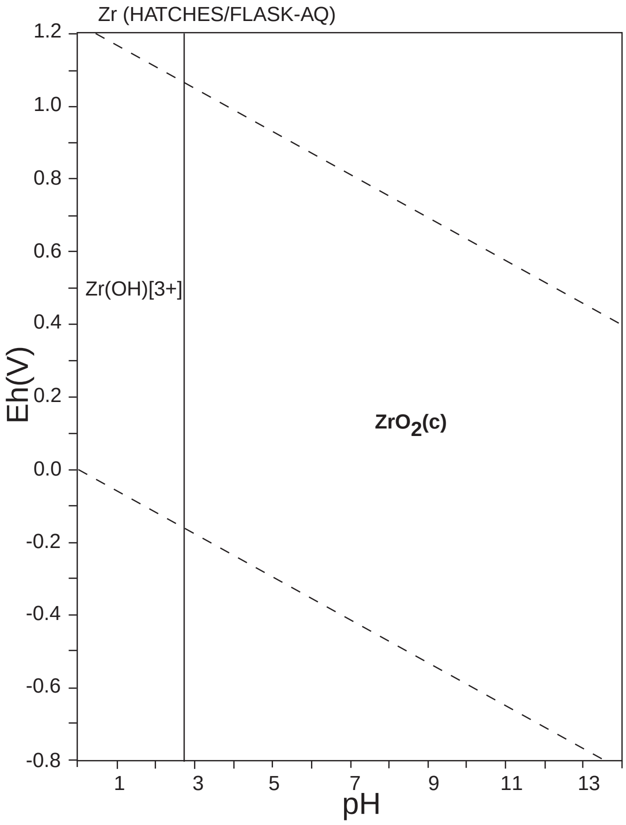

Figure 139: Eh-pH diagrams of the system Zr-O-H (2). $\sum \mathrm{Zr} = 10^{-10}$, 298.15K, 10^5 Pa.