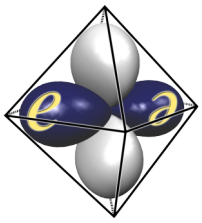


UNIVERSITAT DE BARCELONA

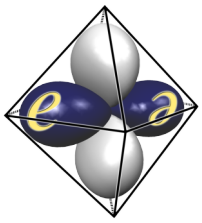
Tables of Coordinating Ability Indices for Anions and Solvents

See: R. Díaz-Torres, S. Alvarez, *Dalton Trans.*, **40**, 10742-10750 (2011).

Table **1.** Coordinating ability indices for anions towards transition metals: number of structures analyzed, coordinating ability index a^{TM} and percentage of structures in which the anion is found coordinated or semicoordinated to a transition metal.

Anion	a^{TM}	%
O^{2-}	3.3	100
CN^-	3.1	100
S^{2-}	2.7	100
PhS^-	2.6	100
N_3^-	2.1	99
PO_4^{3-}	2.1	99
NO_2^-	1.7	98
PhO^-	1.7	98
SCN^-	1.6	97
F^-	1.5	97
$C_2O_4^{2-}$	1.4	96
CH_3COO^-	1.4	96
HPO_4^{2-}	1.4	96
CO_3^{2-}	1.3	95
Cl^-	1.3	95
Br^-	1.0	90
CF_3COO^-	1.0	90
I^-	0.9	90
$H_2PO_4^-$	0.8	87
$CH_3SO_3^-$	0.5	74
SO_4^{2-}	0.3	69
HCO_3^-	0.2	61
NO_3^-	0.1	58
$RCB_{11}H_{11-x}X_x^-$	0.0	48
ReO_4^-	0.0	48
$AlCl_4^-$	-0.1	42
HSO_4^-	-0.3	33
SiF_6^{2-}	-0.3	31
$CF_3SO_3^-$	-0.4	31
ClO_4^-	-0.6	19
$Al(OC(CF_3)_3)_4^-$	-0.6	19
AsF_6^-	-0.6	18
SbF_6^-	-0.9	10
BF_4^-	-1.1	8
PF_6^-	-1.6	3
$B(C_6F_5)_4^-$	-1.7	2
BPh_4^-	-1.8	2
BAr_4^-	-2.3	1

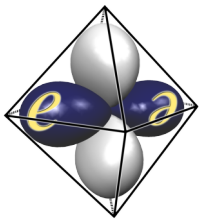
Ar = $(C_6H_3\text{-}3,5(CF_3)_2)$



UNIVERSITAT DE BARCELONA

Table 2. Coordinating ability results for anions towards lanthanides: number of structures analyzed, coordinating ability index a^{Ln} and percentage of structures in which the anion is found coordinated or semicoordinated to a lanthanide. The corresponding coordinating ability indices relative to transition metals are also given for comparison.

Anion	a^{TM}	a^{Ln}	%
F^-	1.5	1.7	98
PhS^-	2.9	1.6	100
$C_2O_4^{2-}$	1.4	1.6	98
SO_4^{2-}	0.3	1.5	97
O^{2-}	3.3	1.4	96
CH_3COO^-	1.6	1.3	95
CN^-	3.1	1.2	94
NO_3^-	0.1	1.1	93
$AlCl_4^-$	-0.1	1.1	93
CF_3COO^-	1.0	1.1	93
CO_3^{2-}	1.3	1.0	91
SCN^-	1.6	0.8	87
Cl^-	1.3	0.8	85
I^-	0.9	0.5	76
Br^-	1.0	0.4	71
N_3^-	2.1	0.3	68
$CF_3SO_3^-$	-0.4	0.1	53
S^{2-}	2.7	-0.3	36
ClO_4^-	-0.6	-0.6	22
BPh_4^-	-1.8	-0.7	17
PF_6^-	-1.6	-0.9	10



UNIVERSITAT DE BARCELONA

Table 3. Coordinating ability results for solvents relative to transition metals: number of structures analyzed, coordinating ability index a^{TM} and percentage of structures in which the anion is found coordinated or semicoordinated to a transition metal.

Solvent	a^{TM}	%
pyridine	1.4	96
formamide	0.3	66
dimethylsulfoxide	0.3	65
hexamethylphosphoramide	0.2	59
triethylamine	0.1	56
n-propanol	0.0	50
water	-0.1	46
dimethoxyethane	-0.2	40
dimethylformamide	-0.2	37
ethylene glycol	-0.2	37
acetonitrile	-0.2	37
trifluoroacetic acid	-0.3	36
i-propanol	-0.3	35
acetic acid	-0.3	34
p-xylene	-0.3	33
diglyme	-0.3	32
tetrahydrofuran	-0.3	32
n-butanol	-0.4	30
methanol	-0.4	30
1,4-dioxane	-0.4	29
carbon disulfide	-0.4	28
t-butanol	-0.4	27
dimethylacetamide	-0.5	26
fluorobenzene	-0.5	26
ethanol	-0.5	24
o-xylene	-0.5	24
benzene	-0.7	17
ethyl acetate	-0.8	13
acetone	-1.0	9
cyclohexane	-1.0	9
nitrobenzene	-1.1	8
toluene	-1.2	6
bromobenzene	-1.2	6
nitromethane	-1.4	4
phenol	-1.4	4
diethyl ether	-1.4	4
o-dichlorobenzene	-1.4	4
chlorobenzene	-1.5	3
1,2-dichloroethane	-1.6	3
dichloromethane	-1.7	2
n-hexane	-1.8	1
carbon tetrachloride	-1.9	1
n-heptane	-1.9	1
n-pentane	-2.1	1
chloroform	-2.2	1

Table 4. Coordinating ability results for solvents relative to lanthanides: number of structures analyzed, coordinating ability index a^{Ln} and percentage of structures in which the anion is found coordinated or semicoordinated to a transition metal. The corresponding indices relative to transition metals are also given for comparison.

Solvent	a^{TM}	a^{Ln}	%
hexamethylphosphoramide	0.2	1.9	100
dimethylacetamide	-0.5	1.3	96
dimethylsulfoxide	0.3	1.1	93
dimethylformamide	-0.2	0.8	86
diglyme	-0.3	0.7	82
water	-0.1	0.6	82
tetrahydrofuran	-0.3	0.4	73
dimethoxyethane	-0.2	0.4	71
i-propanol	-0.3	0.4	71
pyridine	1.4	0.3	66
acetic acid	-0.3	0.0	48
methanol	-0.4	0.0	48
1,4-dioxane	-0.4	-0.1	46
ethanol	-0.5	-0.1	42
acetone	-1.0	-0.5	25
dichloromethane	-1.7	-0.6	19
acetonitrile	-0.2	-0.7	18
triethylamine	0.1	-0.8	14
diethyl ether	-1.4	-0.9	12
cyclohexane	-1.0	-1.0	10
benzene	-0.7	-1.2	6
toluene	-1.2	-1.2	6
nitromethane	-1.5	-1.3	5
chloroform	-2.2	-1.4	4
carbon disulfide	-0.4	-1.4	0
n-pentane	-2.1	-1.7	0
n-hexane	-1.8	-1.7	1