Supplementary Information

Anion polarizabilities and optical basicity in oxynitride glasses. Establishing a common optical basicity scale

Doris Möncke[a,b,c*], Sharafat Ali[b], Bo Jonson[b], Efstratios I. Kamitsos[a*]

[a] *Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation 48 Vassileos Constantinou Avenue, 11635 Athens, Greece*

[b] *Linnæus University, Department of Built Environment and Energy Technology 35195 Växjö, Sweden*

[c] *Inamori School of Engineering at the New York State College of Ceramics, Alfred University, 1 Saxon Drive, Alfred, 14802 New York, USA*

In memoriam to John A. Duffy *1932 -⑤2015

Corresponding authors.
moncke@alfred.edu (D. Möncke), and eikam@eie.gr (E.I. Kamitsos)

Tables S1A-H. Composition in at%, ratio of oxygen over nitrogen N/O, density, molar volume V_m, measured and calculated refractive index n, average polarizability α_m, cation polarizability α_C, average anion polarizability $\alpha_{O\&N}$ and theoretical optical basicity Λ_{th}

Table S1A

Si-O-N Bååk [1]	N/O	Density (g/cm³)	Vm (cm³/mol)	n (@546 nm)	α_m (Å³)	α_C (Å³)	$\alpha_{O\&N}$ (Å³)	Λ_{th}
$Si_{42}N_{58}$	-	3.09	45.40	2.008	9.0	0.099	2.24	0.80
$Si_{42}O_3N_{55}$	18.0	3.00	44.09	1.953	8.5	0.092	2.20	0.75
$Si_{42}O_6N_{52}$	8.0	2.91	42.69	1.898	7.9	0.086	2.16	0.70
$Si_{41}O_{10}N_{49}$	4.7	2.81	41.36	1.842	7.3	0.079	2.12	0.65
$Si_{40}O_{15}N_{45}$	3.0	2.73	39.63	1.787	6.6	0.073	2.05	0.60
$Si_{40}O_{20}N_{40}$	2.0	2.65	37.80	1.732	6.0	0.066	1.98	0.55
$Si_{39}O_{26}N_{35}$	1.3	2.56	36.00	1.676	5.4	0.059	1.90	0.50
$Si_{38}O_{33}N_{29}$	0.9	2.47	34.07	1.621	4.8	0.053	1.81	0.45
$Si_{37}O_{42}N_{21}$	0.5	2.38	31.98	1.566	4.1	0.046	1.70	0.40
$Si_{35}O_{53}N_{12}$	0.2	2.29	29.74	1.511	3.5	0.040	1.59	0.35
$Si_{33}O_{67}$	-	2.20	27.31	1.456	2.9	0.033	1.45	0.30

Values might not add up to 100% due to rounding

[1] T. Bååk, "Silicon oxynitride; a material for GRIN optics", App. Opt. 21 (1982) 1069-1072.

Table S1B

Mg-Si-O-N Ali [2,3]	N/O	Density (g/cm³)	Vm (cm³/mol)	n (@633 nm)	α_m (Å³)	α_C (Å³)	$\alpha_{O\&N}$ (Å³)	Λ_{th}
$Mg_{17}Si_{28}O_{25}N_{30}$	1.200	3.09	653.64	1.893	119.9	0.056	2.13	0.70
$Mg_{19}Si_{26}O_{24}N_{32}$	1.333	3.02	670.27	1.922	125.7	0.059	2.20	0.72
$Mg_{15}Si_{29.5}O_{19.5}N_{36}$	1.846	2.99	673.64	1.896	123.8	0.054	2.19	0.72
$Mg_{17}Si_{29.5}O_{15.5}N_{40}$	2.581	3.01	679.43	1.948	129.9	0.055	2.29	0.74
$Mg_{20}Si_{25}O_{24}N_{31}$	1.292	2.99	671.04	1.994	132.5	0.060	2.36	0.72
$Mg_{25}Si_{22}O_{21}N_{32}$	1.524	3.00	669.09	1.961	129.1	0.065	2.38	0.77
$Mg_{28}Si_{20}O_{22}N_{31}$	1.409	2.99	678.41	1.999	134.4	0.069	2.47	0.78
$Mg_{30}Si_{16}O_{45}N_{9}$	0.200	2.98	679.37	1.748	109.5	0.073	1.97	0.65
$Mg_{25}Si_{21}O_{32}N_{22}$	0.688	2.99	674.76	1.843	118.8	0.066	2.14	0.72
$Mg_{12}Si_{31}O_{33}N_{24}$	0.727	3.05	664.40	1.814	114.0	0.050	1.96	0.69

Values might not add up to 100% due to rounding

[2] S. Ali, B. Paul, R. Magnusson, G. Greczynski, E. Broitman, B. Jonson, P. Eklund, J. Birch, "Novel transparent MgSiON thin films with high hardness and refractive index", Vacuum, 131 (2016) 1-4.
[3] S. Ali, B. Paul, R. Magnusson, E. Ekström, C. Pallier, B. Jonson, P. Eklund, J. Birch, Per Eklund, and Jens Birch "Optical and mechanical properties of Mg-Si-O-N thin films deposited by reactive magnetron sputtering", Surface and Coatings Technology, 2019, 372, p. 9-15.

Table S1C

Ca-Si-O-N Ali [4,5]	N/O	Density (g/cm³)	Vm (cm³/mol)	n (@633 nm)	α_m (Å³)	α_C (Å³)	$\alpha_{O\&N}$ (Å³)	Λ_{th}
$Ca_{13.4}Si_{25.7}O_{56.06}N_{6.4}$	0.11	2.80	311.81	1.62	43.4	0.18	1.69	0.62
$Ca_{12.8}Si_{26.4}O_{53.8}N_{8.5}$	0.16	2.81	300.38	1.65	43.4	0.18	1.75	0.62
$Ca_{20.1}Si_{21.8}O_{48.9}N_{10.6}$	0.22	3.02	355.96	1.70	54.5	0.24	1.85	0.70
$Ca_{16.3}Si_{24.7}O_{48.5}N_{12.1}$	0.25	2.90	319.63	1.69	48.4	0.21	1.85	0.67
$Ca_{23.4}Si_{20.1}O_{44.7}N_{13.3}$	0.30	3.13	382.81	1.74	61.2	0.27	1.94	0.75
$Ca_{26.4}Si_{18.2}O_{42.5}N_{14.3}$	0.34	3.09	435.48	1.75	70.3	0.29	2.05	0.79
$Ca_{24.9}Si_{19.5}O_{41.2}N_{15.8}$	0.39	3.02	412.10	1.74	65.9	0.28	2.06	0.78
$Ca_{21.7}Si_{22.0}O_{39.5}N_{18.3}$	0.46	3.02	356.60	1.72	55.8	0.25	1.97	0.76
$Ca_{25.0}Si_{19.6}O_{40.2}N_{16.7}$	0.41	3.11	399.13	1.75	64.5	0.28	2.02	0.78
$Ca_{20.4}Si_{23.7}O_{34.8}N_{22.8}$	0.65	3.05	325.96	1.83	56.7	0.24	2.18	0.76
$Ca_{24.3}Si_{20.9}O_{34.4}N_{21.9}$	0.64	3.09	374.69	1.85	66.4	0.27	2.27	0.80
$Ca_{25.9}Si_{19.7}O_{34.6}N_{21.3}$	0.61	2.94	421.56	1.76	68.8	0.28	2.22	0.82
$Ca_{22.1}Si_{22.9}O_{31.4}N_{25.2}$	0.80	3.12	333.12	1.92	62.4	0.25	2.36	0.79
$Sr_{22.7}Si_{22.8}O_{29.7}N_{26.5}$	0.89	3.25	323.34	1.94	61.4	0.25	2.32	0.81
$Sr_{23.9}Si_{21.9}O_{29.2}N_{26.5}$	0.91	3.24	339.89	1.95	65.1	0.26	2.37	0.82

Values might not add up to 100% due to rounding

[4] A. Sharafat, J. Grins, S. Esmaeilzadeh, "Hardness and refractive index of Ca–Si–O–N glasses", J. Non-Cryst. Solids 355 (2009) 301-304.
[5] S. Ali, "Preparation, characterization and properties of nitrogen rich glasses in alkaline earth-Si-O-N systems", PhD thesis Stockholm University, Sweden, 2009.

Table S1D

Sr-Si-O-N Ali [6,7]	N/O	Density (g/cm³)	Vm (cm³/mol)	n (@633 nm)	α_m (Å³)	α_C (Å³)	$\alpha_{O\&N}$ (Å³)	Λ_{th}
$Sr_{18.6}Si_{23.4}O_{45.6}N_{13.9}$	0.30	3.80	361.50	1.68	54.2	0.40	1.87	0.73
$Sr_{19.3}Si_{22.9}O_{45.3}N_{14.0}$	0.31	3.72	382.78	1.66	56.0	0.41	1.89	0.74
$Sr_{20.3}Si_{21.8}O_{48.8}N_{10.7}$	0.22	3.69	414.08	1.73	65.5	0.43	2.11	0.74
$Sr_{20.4}Si_{22.3}O_{44.0}N_{14.8}$	0.33	3.86	386.62	1.68	57.9	0.43	1.91	0.76
$Sr_{21.0}Si_{21.2}O_{48.8}N_{10.5}$	0.21	3.90	407.13	1.74	65.1	0.45	2.04	0.75
$Sr_{19.9}Si_{23.1}O_{41.3}N_{17.3}$	0.42	3.83	372.30	1.77	61.3	0.42	2.14	0.77
$Sr_{22.3}Si_{21.6}O_{39.4}N_{18.2}$	0.46	4.01	398.31	1.88	72.3	0.46	2.40	0.80
$Sr_{17.9}Si_{23.6}O_{48.2}N_{11.8}$	0.24	3.59	374.76	1.65	54.2	0.39	1.88	0.72
$Sr_{21.0}Si_{22.3}O_{41.2}N_{17.0}$	0.41	3.90	387.26	1.76	63.2	0.44	2.12	0.78
$Sr_{23.5}Si_{21.1}O_{36.7}N_{20.2}$	0.55	4.00	417.74	1.93	78.8	0.47	2.59	0.83
$Sr_{23.0}Si_{21.0}O_{40.5}N_{17.1}$	0.42	4.07	409.36	1.87	73.7	0.47	2.36	0.80

Values might not add up to 100% due to rounding

[6] S. Ali, Preparation, characterization and properties of nitrogen rich glasses in alkaline earth-Si-O-N systems, PhD thesis Stockholm University, Sweden, 2009.

[7] S. Ali,, B. Forslund, J. Grins, S. Esmaeilzadeh, Formation and properties of nitrogen-rich strontium silicon oxynitride glasses, J. Mat. Science 44 (2009) 664.

Table S1E

Ba-Si-O-N Ali [8]	N/O	Density (g/cm³)	Vm (cm³/mol)	n (@633 nm)	α_m (Å³)	α_C (Å³)	$\alpha_{O\&N}$ (Å³)	Λ_{th}
$Ba_{12.7}Si_{26.0}O_{57.6}N_{5.3}$	0.09	3.27	409.7	1.66	60.0	0.55	2.16	0.68
$Ba_{13.0}Si_{26.0}O_{55.9}N_{6.6}$	0.12	3.31	407.9	1.68	61.1	0.56	2.22	0.69
$Ba_{15.0}Si_{25.0}O_{53.2}N_{8.5}$	0.16	3.49	428.5	1.70	65.7	0.62	2.28	0.72
$Ba_{13.7}Si_{26.3}O_{49.8}N_{11.8}$	0.24	3.42	398.5	1.67	59.0	0.57	2.18	0.72
$Ba_{18.2}Si_{23.0}O_{50.5}N_{9.8}$	0.19	3.68	485.8	1.74	77.7	0.73	2.49	0.78
$Ba_{20.5}Si_{21.8}O_{46.8}N_{12.4}$	0.26	3.92	511.1	1.82	88.2	0.79	2.71	0.83
$Ba_{21.3}Si_{21.8}O_{42.9}N_{15.5}$	0.36	4.05	504.2	1.86	90.0	0.81	2.80	0.86
$Ba_{19.5}Si_{23.6}O_{40.3}N_{18.1}$	0.45	3.79	476.1	1.78	79.2	0.74	2.67	0.84
$Ba_{22.2}Si_{21.3}O_{42.5}N_{15.5}$	0.36	4.18	512.6	1.91	95.3	0.83	2.90	0.88
$Ba_{22.2}Si_{21.7}O_{38.9}N_{18.6}$	0.47	4.13	509.4	1.89	93.2	0.83	2.92	0.89

Values might not add up to 100% due to rounding

[8] S. Ali, B. Jonson, Glasses in the Ba-Si-O-N System, J. Am. Cer. Soc. 94 (2011) 2912-2917.

Table S1F

La-Pr-Si-O-N Ali [9]	N/O	Density (g/cm³)	Vm (cm³/mol)	n (640 nm)	α_m (Å³)	α_C (Å³)	$\alpha_{O\&N}$ (Å³)	Λ_{th}
$La_{23}Si_{19}O_{25}N_{33}$	1.30	5.12	9.13	1.958	92.5	0.60	2.62	1.05
$La_{23}Pr_{0.7}Si_{18}O_{26}N_{33}$	1.25	5.19	9.35	1.962	98.9	0.62	2.59	1.06
$La_{22}Pr_{1.4}Si_{18}O_{29}N_{30}$	1.06	5.22	9.07	1.967	96.9	0.61	2.60	1.05
$La_{21}Pr_{2.3}Si_{18}O_{30}N_{29}$	0.95	5.27	8.92	1.970	95.3	0.61	2.55	1.03
$La_{20}Pr_{4}Si_{18}O_{28}N_{31}$	1.10	5.34	8.96	1.973	97.4	0.61	2.57	1.06
$La_{17}Pr_{7}Si_{18}O_{27}N_{32}$	1.17	5.37	9.01	1.976	99.4	0.62	2.60	1.07
$La_{15}Pr_{10}Si_{18}O_{29}N_{30}$	1.03	5.39	8.91	1.979	98.6	0.61	2.57	1.06
$La_{12}Pr_{11}Si_{18}O_{30}N_{29}$	0.97	5.42	8.69	1.982	93.1	0.59	2.51	1.04
$La_{9}Pr_{14}Si_{19}O_{29}N_{30}$	1.00	5.44	8.52	1.985	88.1	0.57	2.47	1.03
$La_{8}Pr_{17}Si_{17}O_{27}N_{31}$	1.12	5.46	9.02	1.989	103.9	0.61	2.64	1.09
$La_{5}Pr_{19}Si_{18}O_{29}N_{30}$	1.02	5.47	8.83	1.994	99.1	0.59	2.59	1.07
$La_{3}Pr_{21}Si_{18}O_{29}N_{30}$	1.02	5.47	8.66	1.997	93.5	0.57	2.55	1.06
$Pr_{24}Si_{19}O_{30}N_{30}$	1.00	5.49	8.59	1.999	91.1	0.56	2.56	1.05

Values might not add up to 100% due to rounding

[9] A. S. Hakeem, S. Ali, B. Jonson, Preparation and properties of mixed La–Pr silicate oxynitride glasses, J. Non-Cryst. Solids, 368 (2013) 93-97.

Table S1G

Y-Al-Si-O-N Coon [10]	N/O	Density (g/cm³)	Vm (cm³/mol)	n (@550 nm)	α_m (Å³)	α_C (Å³)	$\alpha_{O\&N}$ (Å³)	Λ_{th}
$Y_9Al_{13}Si_{15}O_{63}$ [a]	-	3.38	767	1.658	111.9	0.17	1.68	0.63
$Y_{11}Al_{12}Si_{14}O_{63}$ [a]	-	3.57	764	1.686	115.2	0.20	1.72	0.66
$Y_{13}Al_{6}Si_{19}O_{56}N_{6}$ [b]	0.11	3.82	731.38	1.742	117.2	0.21	1.75	0.68
$Y_{16}Al_{4}Si_{18}O_{54}N_{8}$	0.15	3.87	776.81	1.778	128.9	0.25	1.93	0.72
$Y_{12}Al_{7}Si_{18}O_{53}N_{10}$	0.18	3.70	747.95	1.748	120.5	0.20	1.83	0.70
$Y_{16}Al_{4}Si_{18}O_{52}N_{10}$	0.19	3.99	745.82	1.788	125.0	0.25	1.88	0.74
$Y_{11}Al_{9}Si_{18}O_{51}N_{11}$	0.22	3.67	738.96	1.752	119.6	0.19	1.83	0.70
$Y_{16}Al_{9}Si_{12}O_{50}N_{12}$	0.25	4.06	726.31	1.823	125.6	0.26	1.92	0.80
$Y_{13}Al_{13}Si_{13}O_{48}N_{13}$ [b]	0.29	3.94	722.91	1.834	126.3	0.21	1.96	0.75
$Y_{15}Al_{10}Si_{15}O_{42}N_{18}$	0.44	4.02	736.23	1.853	130.7	0.23	2.04	0.79
Redmington [10]				**(@500 nm)**				
$Y_{10}Al_{22}Si_{7}O_{58}N_{3}$	0.04	3.6	734.2	1.80	124.4	0.17	1.93	0.82
$Y_{11}Al_{20}Si_{9}O_{53}N_{7}$	0.13	3.7	726.3	1.87	130.8	0.18	2.05	0.84

Values might not add up to 100% due to rounding

[a]Value in Coon from Makashima et al. (J. Am. Ceram. Soc.1978, 61 (5-6): 247-249)

[b]Value in Coon from Messier and Deguire (J. Am. Ceram. Soc.1984, 67 (9): 602-605)

[10] D. N. Coon, T. E. Doyle, J. R. Weidner, Refractive indices of glasses in the Y-Al-Si-O-N system, J. Non-Cryst. Solids, 108 (1989) 180-186.

[11] W. Redington, M. Redington, S. Hampshire, M. Serantoni, Properties of some high Al content glasses in various lanthanide–Si–Al–O–N systems, J. Non-Cryst. Solids, 316 (2003) 74-81.

Table S1H

La-Si-O-N Hakeem [12,13]	N/O	Density (g/cm^3)	Vm (cm^3/mol)	n (@633 nm)	α_m (Å^3)	α_C (Å^3)	$\alpha_{O\&N}$ (Å^3)	Λ_{th}
$La_{16}Si_{20}O_{60}N_4$	0.07	4.48	1907	1.75	68.7	0.49	1.92	0.77
$La_{13}Si_{23}O_{57}N_7$	0.12	4.24	1517	1.73	56.6	0.41	1.84	0.73
$La_{16}Si_{21}O_{56}N_7$	0.13	4.44	1853	1.77	68.7	0.48	2.00	0.78
$La_{16}Si_{21}O_{55}N_8$	0.14	4.69	1841	1.79	65.9	0.48	1.92	0.79
$La_{16}Si_{21}O_{55}N_{8.5}$	0.15	4.70	1803	1.78	63.8	0.47	1.88	0.78
$La_{16}Si_{21}O_{54}N_9$	0.16	4.55	1886	1.8	70.3	0.49	2.04	0.80
$La_{16}Si_{21}O_{52}N_{11}$	0.21	4.56	1764	1.84	67.9	0.47	2.09	0.80
$La_{16}Si_{22}O_{50}N_{12}$	0.25	4.44	1696	1.84	67.1	0.45	2.13	0.79
$La_{16}Si_{22}O_{50}N_{12}$	0.244	4.66	1781	1.87	68.8	0.47	2.12	0.81
$La_{17}Si_{21}O_{49}N_{13}$	0.27	4.72	1925	1.88	74.0	0.50	2.19	0.83
$La_{17}Si_{21}O_{44}N_{18}$	0.40	4.68	1864	1.89	72.9	0.49	2.25	0.85
$La_{18}Si_{21}O_{44}N_{17}$	0.39	4.77	1955	1.89	75.0	0.51	2.25	0.86
$La_{21}Si_{18}O_{44}N_{17}$	0.38	5.14	2404	1.92	87.6	0.58	2.28	0.92
$La_{22}Si_{18}O_{43}N_{17}$	0.40	5.15	2496	1.92	90.8	0.59	2.31	0.93
$La_{24}Si_{15}O_{46}N_{15}$	0.32	5.46	3127	1.94	108.8	0.66	2.33	0.97
$La_{21}Si_{19}O_{39}N_{21}$	0.53	4.91	2287	1.94	88.5	0.57	2.47	0.94
$La_{22}Si_{18}O_{37}N_{23}$	0.62	5.28	2440	1.94	87.8	0.59	2.34	0.97
$La_{25}Si_{15}O_{41}N_{19}$	0.47	5.42	3158	1.95	111.5	0.67	2.44	1.00
$La_{24}Si_{17}O_{34}N_{25}$	0.75	5.36	2744	1.94	97.3	0.63	2.43	1.02
$La_{25}Si_{17}O_{31}N_{27}$	0.85	5.27	2826	1.96	103.4	0.64	2.57	1.04
$La_{27}Si_{15}O_{34}N_{24}$	0.70	5.51	3396	1.98	120.5	0.69	2.58	1.07
$La_{24}Si_{18}O_{23}N_{35}$	1.45	4.99	2557	2.31	120.0	0.61	3.44	1.07
$La_{31}Si_{14}O_{14}N_{41}$	2.80	5.51	3856	2.28	161.8	0.73	3.61	1.25

Values might not add up to 100% due to rounding

[12] A. S. Hakeem, J. Grins, S. Esmaeilzadeh, La–Si–O–N glasses: Part I. Extension of the glass forming region, J. Eur. Cer. Soci., 27 (2007) 4773-4781.

[132] A. S. Hakeem, J. Grins, S. Esmaeilzadeh, La-Si-O-N glasses: Part II: Vickers hardness and refractive index, J. Eur. Cer. Soc. 27 (2007) 4783-4787.

Table S1I

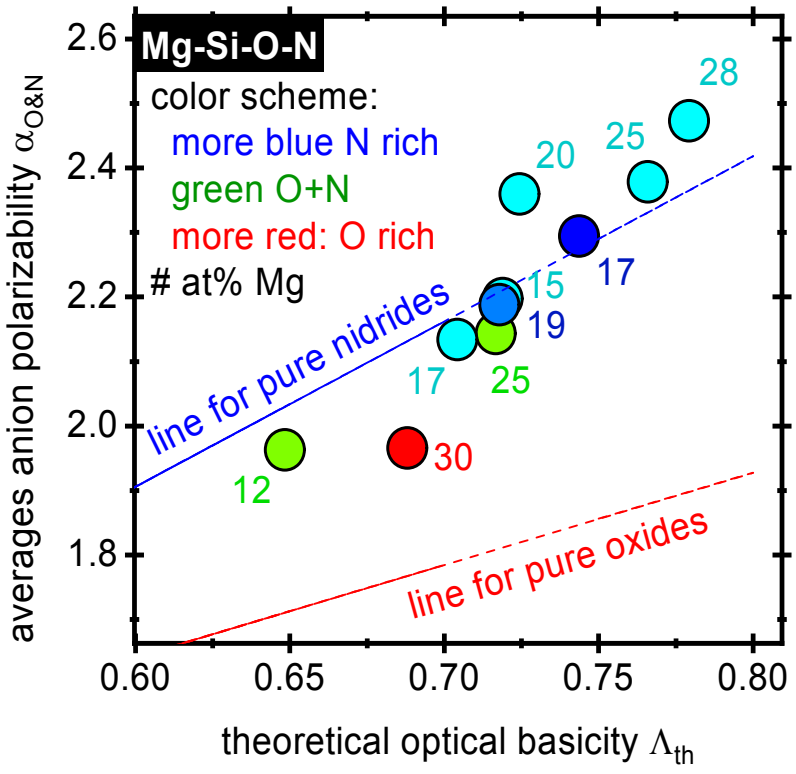
AE-Ca-Si-O-N Ali [14,15]	N/O	Density (g/cm^3)	Vm (cm^3/mol)	n (@640 nm)	α_m (Å^3)	α_C (Å^3)	$\alpha_{O\&N}$ (Å^3)
$Ca_{25}Si_{19}O_{40}N_{15}$	0.38	3.02	795.4	1.74	127.2	0.28	2.06
Mg-Ca-Si-O-N							
$Mg_2Ca_{22}Si_{21}O_{37}N_{19}$	0.52	3.02	781.3	1.75	126.2	0.25	2.07
$Mg_4Ca_{19}Si_{21}O_{38}N_{19}$	0.49	3.00	767.8	1.75	124.0	0.22	2.04
$Mg_6Ca_{18}Si_{21}O_{37}N_{19}$	0.49	2.98	766.7	1.73	121.3	0.21	2.00
$Mg_8Ca_{16}Si_{21}O_{38}N_{18}$	0.48	2.96	763.6	1.70	117.0	0.20	1.94
Sr-Ca-Si-O-N							
$Sr_3Ca_{21}Si_{20}O_{40}N_{16}$	0.41	3.14	813.2	1.77	133.9	0.30	2.16
$Sr_8Ca_{18}Si_{19}O_{37}N_{18}$	0.48	3.35	834.9	1.84	146.6	0.35	2.37
$Sr_{10}Ca_{16}Si_{19}O_{38}N_{17}$	0.47	3.49	830.9	1.86	148.4	0.37	2.39
$Sr_{12}Ca_{14}Si_{19}O_{38}N_{17}$	0.46	3.55	834.3	1.88	151.4	0.38	2.43
Ba-Ca-Si-O-N							
$Ba_4Ca_{20}Si_{20}O_{39}N_{17}$	0.44	3.35	819.4	1.81	140.1	0.37	2.22
$Ba_8Ca_{16}Si_{20}O_{40}N_{16}$	0.41	3.67	848.2	1.86	151.5	0.46	2.34
$Ba_9Ca_{15}Si_{20}O_{40}N_{16}$	0.39	3.84	837.4	1.93	158.0	0.49	2.43
$Ba_{11}Ca_{13}Si_{20}O_{42}N_{15}$	0.36	3.99	869.0	1.97	168.8	0.56	2.56

Values might not add up to 100% due to rounding

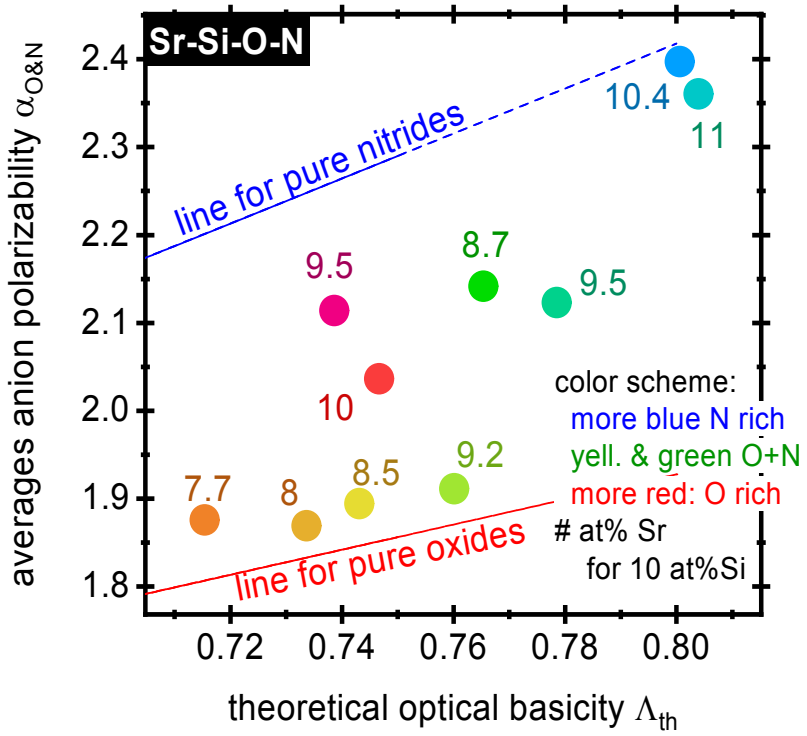
[14] S. Ali, Preparation, characterization and properties of nitrogen rich glasses in alkaline earth-Si-O-N systems, PhD thesis Stockholm University, Sweden, 2009.

[15] S. Ali, et al., Properties of high nitrogen content mixed alkali earth oxynitride glasses $(AE_xCa_{1-x})_{1.2(1)}SiO_{1.9(1)}N_{0.86(6)}$, AE=Mg, Sr, Ba. J. Non-Cryst. Solids 355 (2009) 1259-1263.

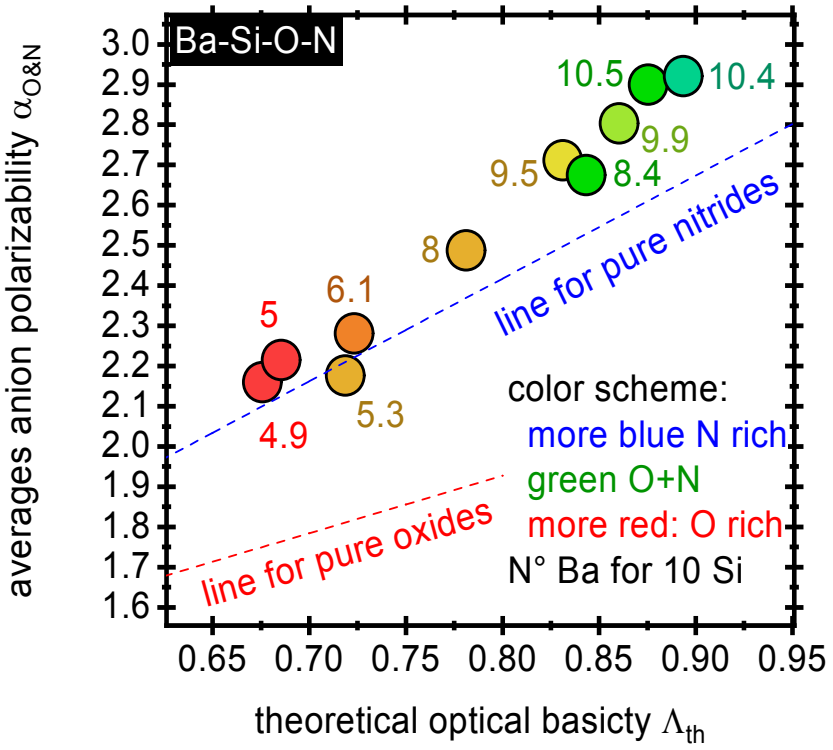
Figures S1 a to f: Experimentally derived average anion polarizability values (in Å^3) from refractive index data, $\alpha_{O/N}$, are plotted versus the calculated theoretical basicities using $\Lambda(M_3N_m) = {}^3/_2\Lambda(M_2O_m)$ for various multi-component systems (see Table 1 for more compositional details). The lines for pure oxides and nitrides follow equations (5) $\alpha_O=(\Lambda+0.547)/0.7$ and (13) $\alpha_N = 0.37 + 2.56\Lambda_{th}$, respectively. The color scheme reflects on the N:O ratio (N-rich: blue, O-rich red) and the numbers give the relative number of modifier atoms (in at% or for every 10 Si-atoms, respectively).



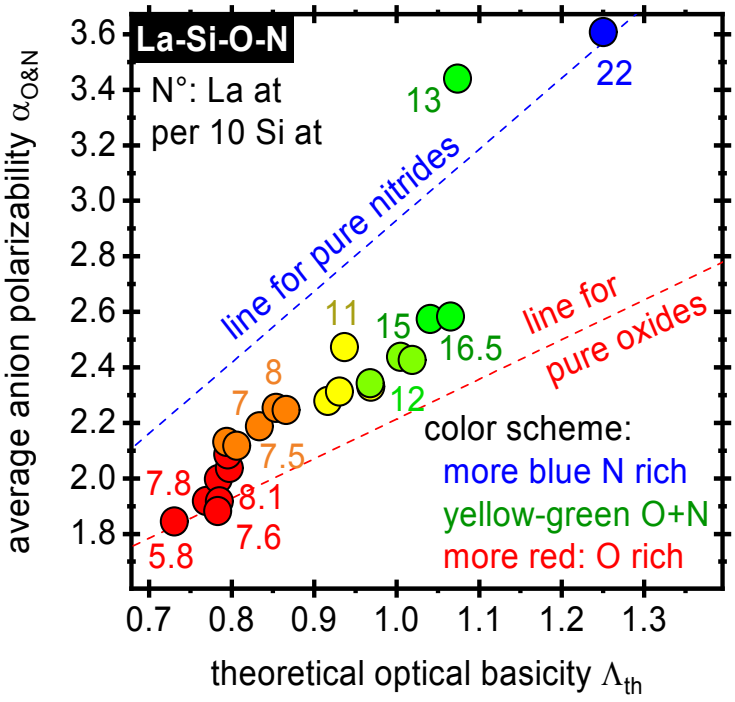
(a)


Sr-Si-O-N
averages anion polarizability $\alpha_{O\&N}$
theoretical optical basicity Λ_{th}
line for pure nitrides
line for pure oxides
10.4
11
8.7
9.5
9.5
10
9.2
8.5
7.7
8
color scheme:
more blue N rich
yell. & green O+N
more red: O rich
at% Sr
for 10 at%Si

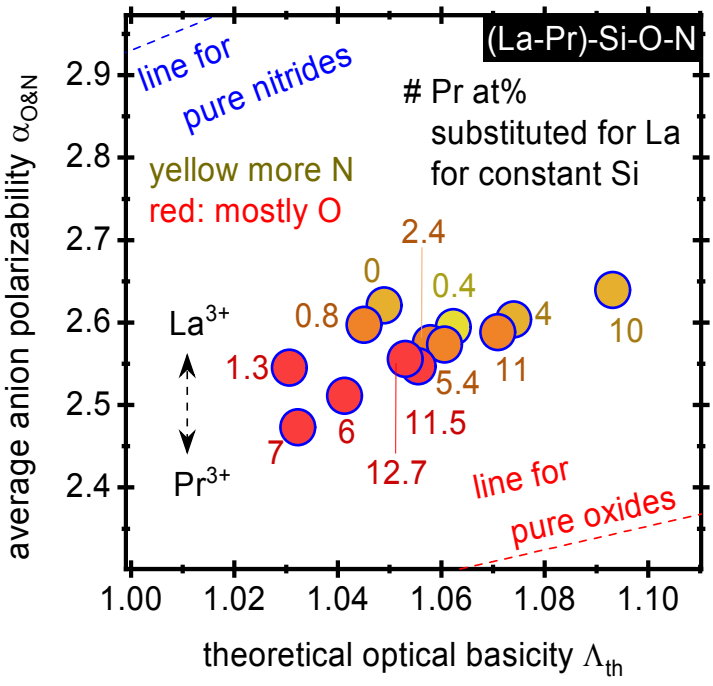
(b)


Ba-Si-O-N
averages anion polarizability $\alpha_{O\&N}$
theoretical optical basicty Λ_{th}
line for pure nitrides
line for pure oxides
10.5
10.4
9.9
9.5
8.4
8
6.1
5
4.9
5.3
color scheme:
more blue N rich
green O+N
more red: O rich
N° Ba for 10 Si

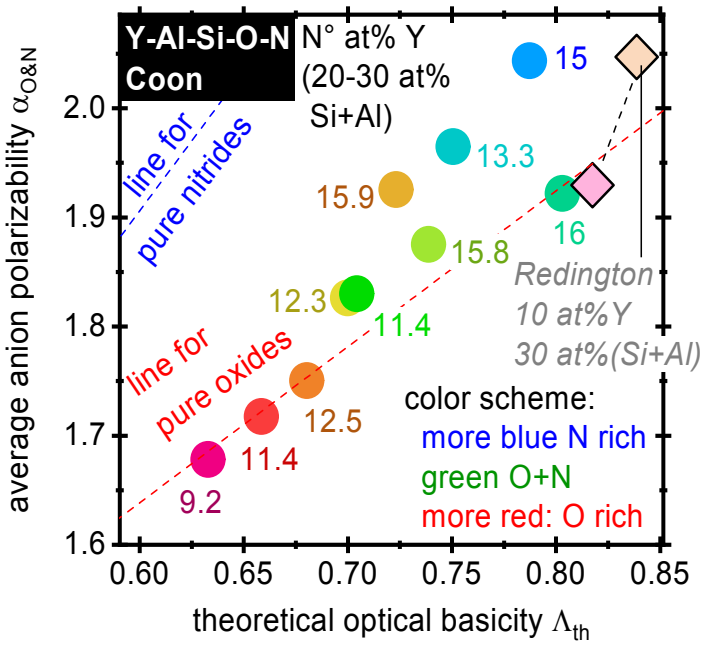
(c)


La-Si-O-N
N°: La at
per 10 Si at
22
13
line for pure nitrides
11
15
16.5
line for
pure oxides
8
7
12
7.5
color scheme:
more blue N rich
yellow-green O+N
7.8
8.1
more red: O rich
7.6
5.8
average anion polarizability $\alpha_{O\&N}$
theoretical optical basicity Λ_{th}
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
0.7
0.8
0.9
1.0
1.1
1.2
1.3

(d)


(La-Pr)-Si-O-N
line for
pure nitrides
Pr at%
substituted for La
for constant Si
yellow more N
red: mostly O
2.4
0
0.4
0.8
4
10
La^{3+}
1.3
11
5.4
11.5
6
7
12.7
Pr^{3+}
line for
pure oxides
average anion polarizability $\alpha_{O\&N}$
theoretical optical basicity Λ_{th}
2.9
2.8
2.7
2.6
2.5
2.4
1.00
1.02
1.04
1.06
1.08
1.10

(e)


Y-Al-Si-O-N
Coon
N° at% Y
(20-30 at%
Si+Al)
15
13.3
15.9
16
15.8
12.3
11.4
12.5
11.4
9.2
line for
pure nitrides
line for
pure oxides
Redington
10 at%Y
30 at%(Si+Al)
color scheme:
more blue N rich
green O+N
more red: O rich
average anion polarizability $\alpha_{O\&N}$
theoretical optical basicity Λ_{th}
2.0
1.9
1.8
1.7
1.6
0.60
0.65
0.70
0.75
0.80
0.85

(f)