Electronic Supplementary Information

Table S1: Solvent phase stabilization energy (in kcal mol^{-1}) in different solvents (single point calculations) obtained at the B3LYP/6-31++G(d,p) level of theory

System	SE (Carbon Tetrachloride) ε = 2.2	SE (Ethanol) ε = 24.3	SE (Acetonitrile) ε = 37.5	SE(DMSO) ε = 46.7	SE (Water) ε = 80.4
1-O_2-1-Li	104.74	114.68	115.05	115.25	115.51
1-O_2-1-Na	86.17	100.43	100.93	101.21	101.57
1-O_2-1-K	87.48	100.33	100.77	101.02	101.33
1-O_2-1-Be	118.09	135.97	136.67	137.07	137.58
1-O_2-1-Mg	56.59	98.00	99.57	100.44	101.57
1-O_2-1-Ca	76.98	125.96	127.76	128.74	130.03
2-O_2-1-Li	111.04	111.45	111.52	111.56	111.61
2-O_2-1-Na	94.85	100.61	100.84	100.98	101.15
2-O_2-1-K	96.61	102.25	102.46	102.58	102.73
2-O_2-1-Be	168.31	168.63	168.66	168.68	168.70
2-O_2-1-Mg	111.51	123.71	124.26	124.56	124.96
2-O_2-1-Ca	136.08	155.30	156.08	156.51	157.07
3-O_2-2-Li	207.95	204.58	204.52	204.49	204.45
3-O_2-2-Na	170.41	176.89	177.16	177.31	177.51
3-O_2-2-K	169.74	176.94	177.21	177.36	177.56
3-O_2-2-Be	358.37	358.50	358.55	358.57	358.61
3-O_2-2-Mg	251.89	267.79	268.49	268.87	269.38
3-O_2-2-Ca	291.06	315.92	316.92	317.48	318.21
4-O_2-3-Li	392.26	392.05	392.00	391.97	391.94
4-O_2-3-Na	340.10	350.05	350.54	350.82	351.20
4-O_2-3-K	339.58	348.07	348.41	346.74	350.43
4-O_2-3-Be	555.61	555.35	555.40	555.42	555.46
4-O_2-3-Mg	394.85	413.22	414.03	414.47	415.06
4-O_2-3-Ca	447.36	477.08	478.28	478.94	479.82
5-O_2-4-Li	422.42	413.53	413.32	413.20	413.05
5-O_2-4-Na	344.36	353.31	353.69	353.90	354.18
5-O_2-4-K	339.12	349.93	350.34	350.57	350.86
5-O_2-4-Be	753.80	752.91	752.95	752.97	753.00
5-O_2-4-Mg	539.18	561.63	562.61	563.16	563.88
5-O_2-4-Ca	604.23	639.57	641.00	641.78	642.81
6-O_2-5-Li	649.00	634.36	639.23	639.14	633.88
6-O_2-5-Na	557.37	567.89	568.35	568.61	568.95
6-O_2-5-K	558.20	568.40	565.99	566.24	566.58
6-O_2-5-Be	952.26	950.58	950.59	950.60	950.62
6-O_2-5-Mg	682.63	707.22	708.31	708.92	709.71
6-O_2-5-Ca	760.85	801.29	802.93	803.83	805.01

TABLE S2 Wave length of transitions, ΔE values {E_{HOMO}(Complex)– E_{HOMO}(O_2)}, oscillator strengths, major MOs involved in the transition and contribution of the MOs. (obtained at CAM-B3LYP/6-31++G (d,p) level of theory).

System	Wavelength (in nm)	ΔE (in au)	Oscillator Strength	Contributing MO	Expansion Co-efficient
1-O_2-1-Li	350.02	0.0524	0.0067	HOMO⟶LUMO	0.94372
1-O_2-1-Na	476.73	0.0988	0.0043	HOMO⟶LUMO	0.96014
1-O_2-1-K	477.88	0.1234	0.0014	HOMO⟶LUMO	0.94384
1-O_2-1-Be	309.77	0.0406	0.0067	HOMO–1⟶LUMO	0.69802
1-O_2-1-Mg	404.81	0.0935	0.0122	HOMO–2⟶LUMO	0.25584
1-O_2-1-Ca	573.53	0.1521	0.0095	HOMO–2⟶LUMO	0.10365

TABLE S3 Wave length of transitions, oscillator strengths, major MOs involved in the transition and contribution of the MOs compared with Li in all systems (obtained at CAM-B3LYP/6-31++G (d,p) level of theory).

System	Wavelength (In nm)	Oscillator Strength	Contributing MO	Expansion Co-Efficient
1-O_2-1-Li	350.02	0.0666	HOMO⟶LUMO	0.89997
2-O_2-1-Li	154.21	0.0449	HOMO⟶LUMO	0.42705
3-O_2-2-Li	176.72	0.0182	HOMO⟶LUMO+4	0.11783
4-O_2-3-Li	281.63	0.0001	HOMO⟶LUMO+2	0.97025
5-O_2-4-Li	243.13	0.0000	HOMO⟶LUMO+4	0.47662
6-O_2-5-Li	254.45	0.0012	HOMO⟶LUMO+4	0.97302

Fig. **S1** Dispersal of π- electron cloud in the benzene ring against a concentrated electron cloud in O_2 molecule