SUPPLEMENTARY MATERIAL

Potential Energy Surfaces for Noble Gas (Ar, Kr, Xe, Rn) – Propylene Oxide Systems: Analytical Formulation and Binding

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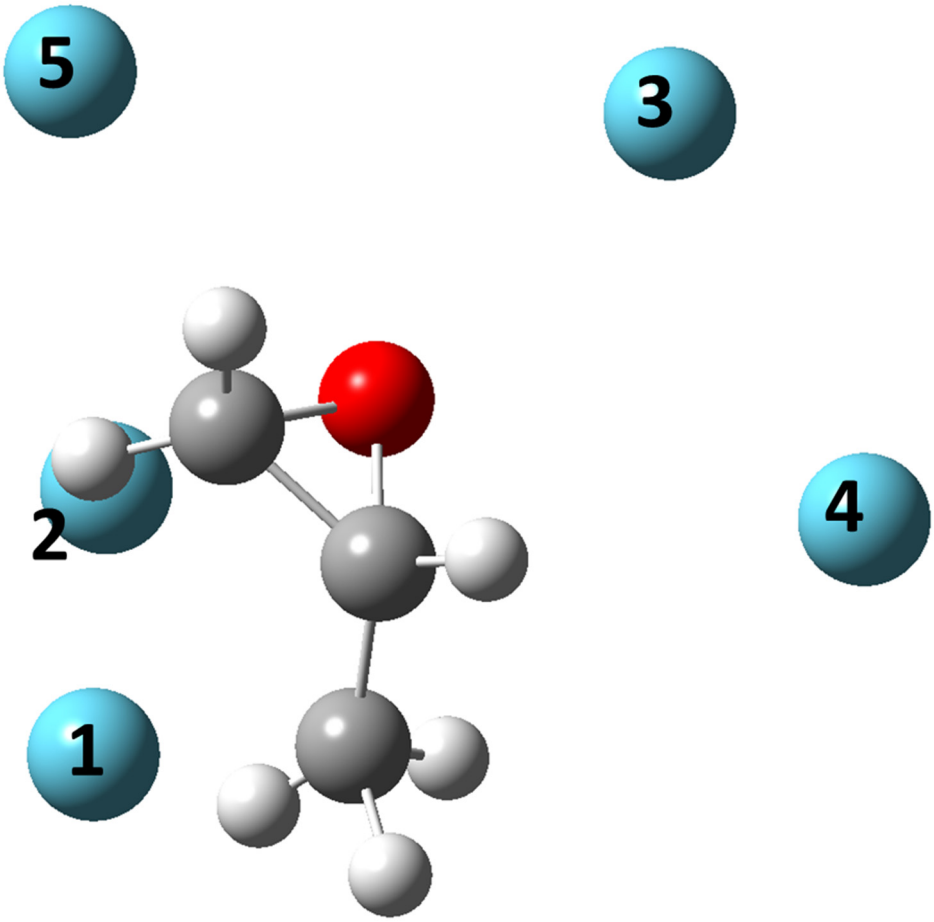

Figure S1. Minima geometries for Kr – propylene oxide identified on the present PES. The numbering of the Kr atom corresponds to the minima reported in Table 6.

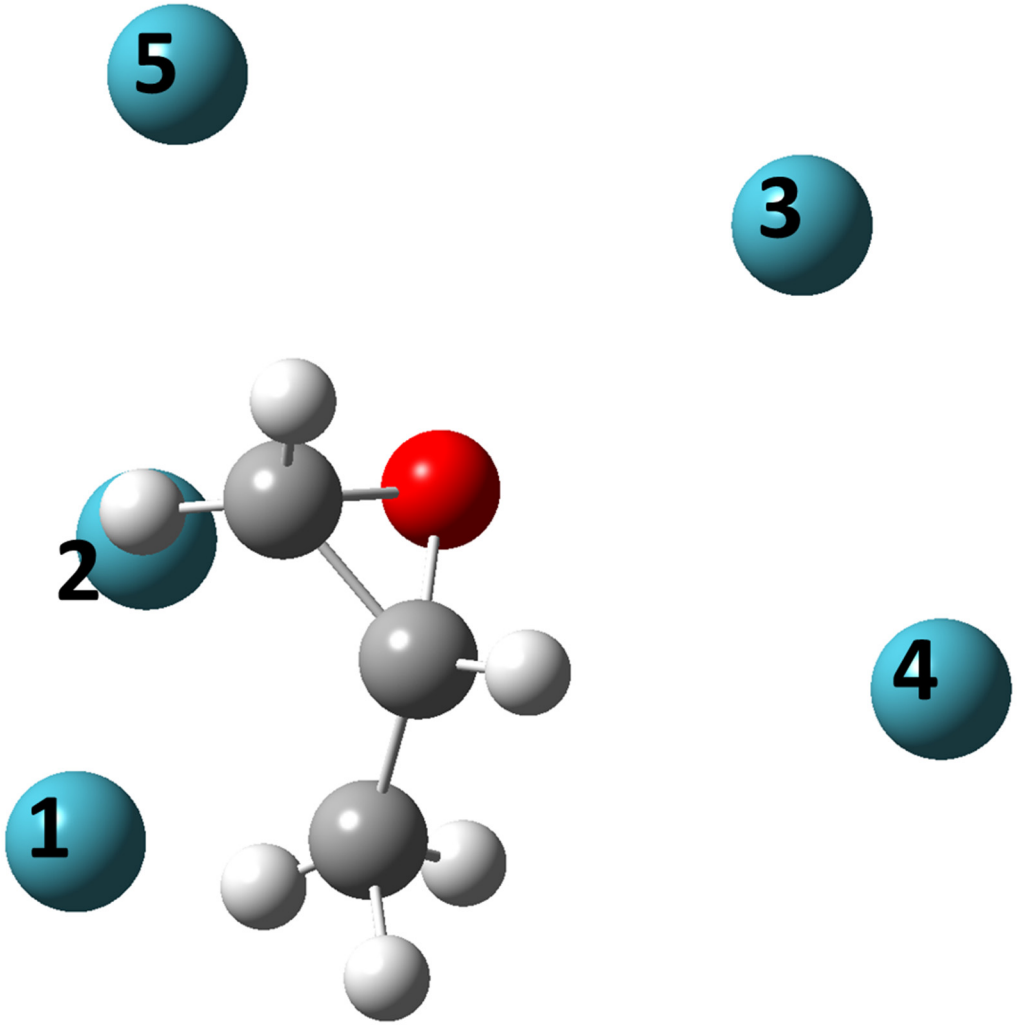

Figure S2. Minima geometries for Xe – propylene oxide identified on the present PES. The numbering of the Xe atom corresponds to the minima reported in Table 7.

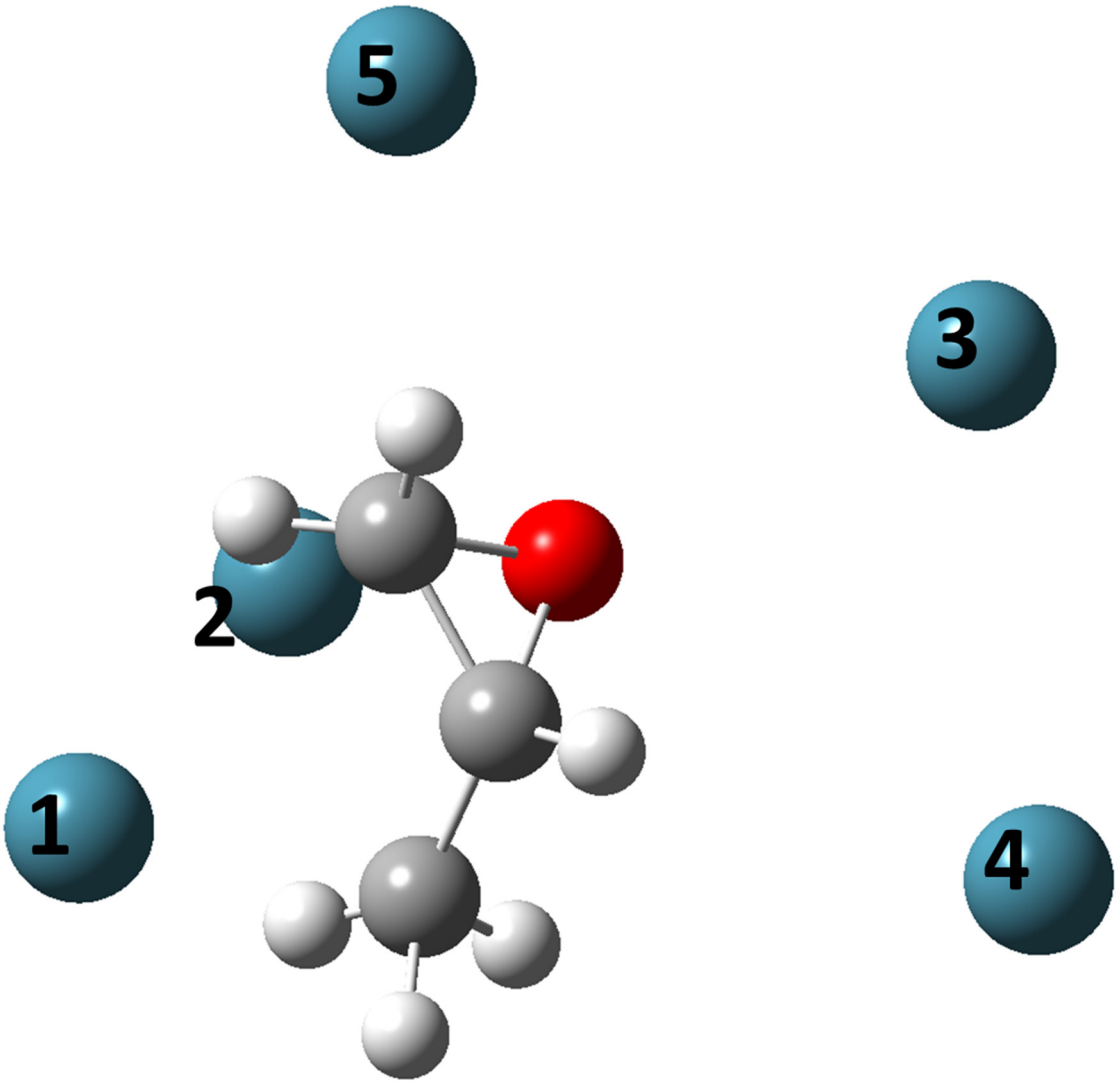

Figure S3. Minima geometries for Rn – propylene oxide identified on the present PES. The numbering of the Rn atom corresponds to the minima reported in Table 8.

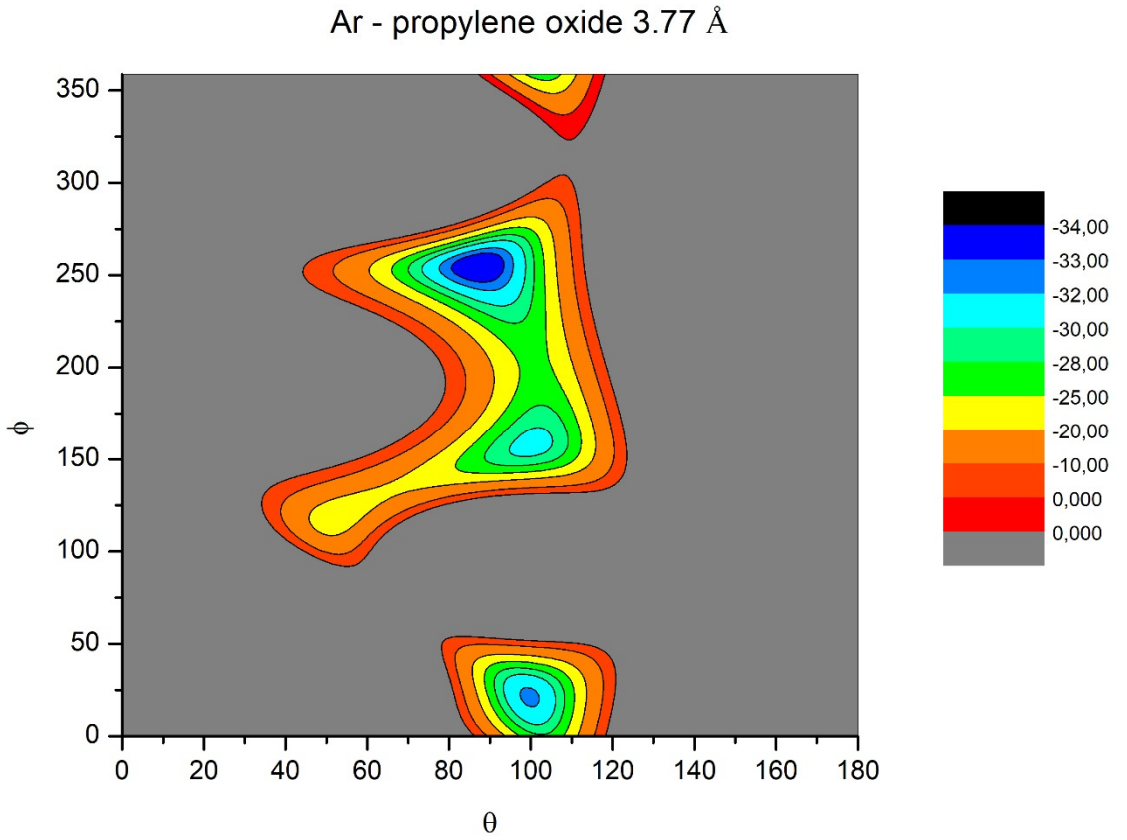

Figure S4. Color contour map for the Ar – propylene oxide system at R=3.77 Å (left panel). The axes report the angles θ and ϕ in degrees, while a color scale reports the potential energy in meV.

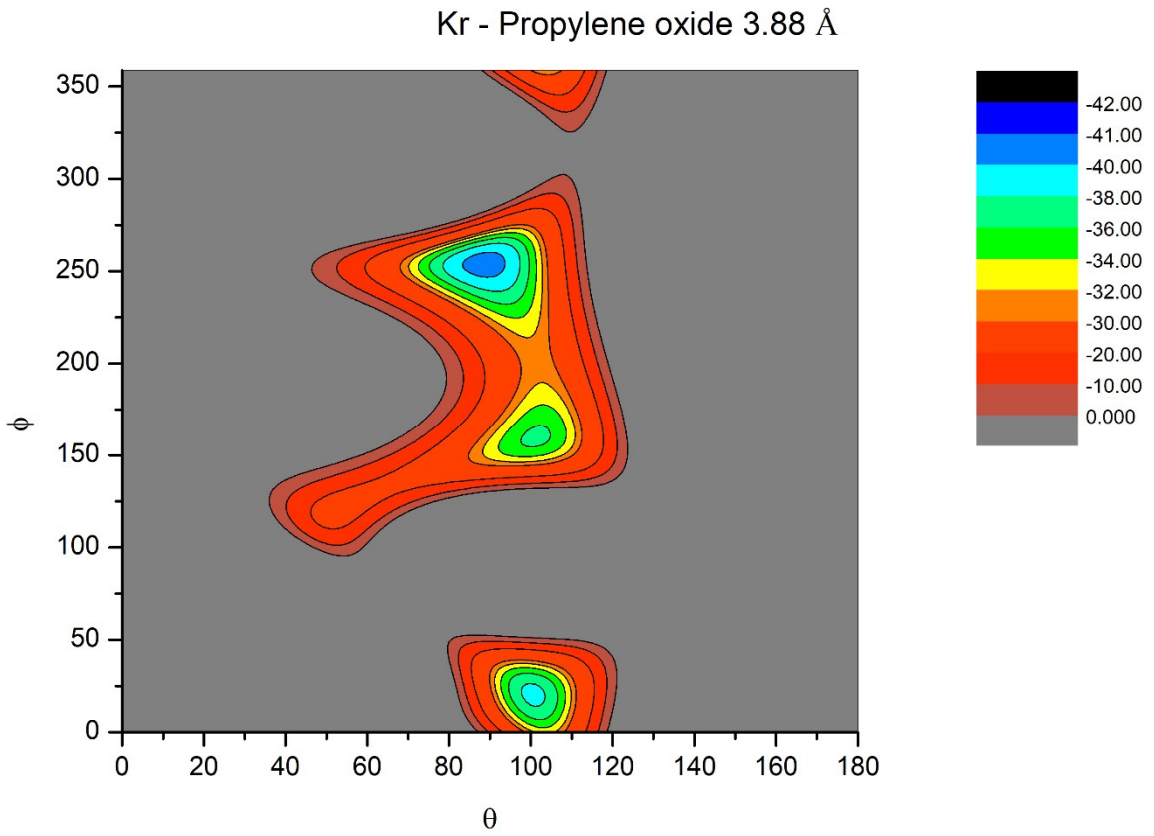

Figure S5. Color contour map for the Kr – propylene oxide system at R=3.88 Å (left panel). The axes report the angles θ and ϕ in degrees, while a color scale reports the potential energy in meV.

Table S1: Binding energies for Ar-propylene oxide system calculated at different levels of theory, MP2/CBS extrapolation and CCSD(T) correction.

	MP2/aug-cc-pVDZ	**MP2/aug-cc-pVTZ**	**MP2/aug-cc-pVQZ**	**CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ**	**$\Delta CCSD(T)$**	**MP2/CBS**	**CCSD(T)/CBS**
MIN 1	-28.2	-35.1	-38.2	-31.2	+3.9	-40.7	-36.8
MIN 2	-26.0	-33.8	-36.8	-31.2	+2.6	-38.6	-36.0
MIN 3	-28.2	-36.9	-40.3	-34.7	+2.2	-42.4	-40.2
MIN 4	-31.2	-39.8	-43.3	-34.7	+5.1	-45.4	-40.3
MIN 5	-24.7	-31.7	-34.7	-28.2	+3.5	-36.5	-33.0

Table S2: Binding energies for Kr-propylene oxide system calculated at different levels of theory, MP2/CBS extrapolation and CCSD(T) correction.

	MP2/aug-cc-pVDZ	**MP2/aug-cc-pVTZ**	**MP2/aug-cc-pVQZ**	**CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ**	**$\Delta CCSD(T)$**	**MP2/CBS**	**CCSD(T)/CBS**
MIN 1	-34.3	-44.7	-48.6	-38.0	+6.7	-50.9	-44.2
MIN 2	-32.5	-43.4	-47.3	-38.6	+4.8	-49.4	-44.6
MIN 3	-38.0	-49.9	-54.6	-41.6	+8.3	-57.5	-49.2
MIN 4	-34.7	-46.8	-51.2	-42.0	+4.8	-53.8	-49.0
MIN 5	-30.4	-39.9	-43.4	-34.3	+5.6	-45.4	-39.8

Table S3: Binding energies for Xe-propylene oxide system calculated at different levels of theory, MP2/CBS extrapolation and CCSD(T) correction.

	MP2/aug-cc-pVDZ	**MP2/aug-cc-pVTZ**	**MP2/aug-cc-pVQZ**	**CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ**	**$\Delta CCSD(T)$**	**MP2/CBS**	**CCSD(T)/CBS**
MIN 1	-39.9	-54.2	-59.8	-44.2	+10.0	-63.2	-53.2
MIN 2	-38.2	-53.3	-59.4	-45.5	+7.8	-63.0	-55.2
MIN 3	-40.8	-57.2	-63.7	-49.9	+7.3	-67.5	-60.2
MIN 4	-42.9	-59.8	-67.8	-48.6	+11.2	-70.9	-59.7
MIN 5	-35.1	-49.0	-54.6	-40.3	+8.7	-57.9	-49.2

Table S4: Binding energies for Rn-propylene oxide system calculated at different levels of theory, MP2/CBS extrapolation and CCSD(T) correction.

	MP2/aug-cc-pVDZ	**MP2/aug-cc-pVTZ**	**MP2/aug-cc-pVQZ**	**CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ**	$\Delta CCSD(T)$	**MP2/CBS**	**CCSD(T)/CBS**
MIN 1	-41.6	-59.8	-67.2	-48.1	+11.7	-71.6	-59.9
MIN 2	-40.8	-59.4	-67.2	-50.3	+9.1	-71.8	-63.7
MIN 3	-45.1	-65.9	-74.1	-52.7	+11.4	-79.0	-67.6
MIN 4	-42.9	-63.3	-71.6	-53.8	+9.3	-76.4	-67.1
MIN 5	-49.0	-54.2	-61.1	-43.8	+10.4	-65.6	-55.2