Supporting Information for:

Ping-Pong Protons: How Hydrogen Bonding Networks Facilitate
Heterolytic Bond Cleavages in Peptide Radical Cations

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Table S1. Energies of relevant species. Absolute electronic energies, computed at the $\omega B97X$ -D/6-31G(d) level, given in hartree. Relative energies (in comparison to first transition state barrier height) given in kcal/mol.

Figure 1 c4/22 Cleavage TS c4/22 Cleavage Products -1734.126637 -13.72 Figure2 c4/22 Cleavage Products -1734.128694 -1734.128694 -10.00 c4/22 Cleavage TS -1734.128694 -10.00 -1734.146870 -11.41 □ Proton Transfer TS □ 1.734.148596 -10.85 □ 1.85	Species	Electronic Energy	Relative Energy
C4/z2 Cleavage Products	Figure 1		
Figure 2 c4/z2 Cleavage TS c4/z2 Cleavage TS c4/z2 Cleavage Products l³ Proton Transfer TS l³ Proton Transfer Products -1734.148541 -12.45 Figure 3 c3/z3 Cleavage Products l³ Proton Transfer TS (H44 to O32) l³ Proton Transfer Products -1734.128318 -0.46 l³ Proton Transfer Products -1734.128318 -0.46 l³ Proton Transfer TS (H44 to O32) l³ Proton Transfer Products -1734.127159 0.27 l³ Proton Transfer Products -1734.078510 0.00 c3/z3 Cleavage TS -1734.078510 0.00 c3/z3 Cleavage TS -1734.093216 -9.23 l³ Proton Transfer TS (H3 to O12) l³ Proton Transfer Products -1734.093216 -9.23 l³ Proton Transfer Products -1734.095743 -1.081 2nd Proton Transfer Products -1734.095743 -1.081 2nd Proton Transfer Products -1734.099397 -13.11 Figure 5 c2/z2 Cleavage TS -1-239.574084 0.00 c2/z2 Cleavage TS -1-239.596992 -1-4.37 l³ Proton Transfer Products -1-239.636658 -39.27 Figure 6 c3/z2 Cleavage TS -1-486.80329 0.00 c3/z2 Cleavage TS -1-486.839048 -22.44 l³ Proton Transfer Products -1-486.852781 -31.06 Figure 7 c3/z2 Cleavage TS -1-486.85299 0.00 c3/z2 Cleavage TS -1-486.850099 -1-4.88 l³ Proton Transfer Products -1-486.850099 -1-4.88 l³ Proton Transfer Products -1-486.850099 -1-4.88 l³ Proton Transfer TS (H3 to O12) -1-486.850009 -1-4.88 l³ Proton Transfer Products -1-486.850009 -1-4.88 l³ Proton Transfer TS (H3 to O12) -1-486.851214 -1-5.63 -1-1.82 l³ Proton Transfer Products -1-1.486.8444601 -1-1.48	c4/z2 Cleavage TS	-1734.104771	0.00
c4/z2 Cleavage TS -1734.128694 0.00 c4/z2 Cleavage Products -1734.146870 -11.41 1st Proton Transfer TS -1734.145986 -10.85 1st Proton Transfer Products -1734.148541 -12.45 Figure 3 c3/z3 Cleavage TS -1734.127586 0.00 c3/z3 Cleavage Products -1734.127159 0.27 1st Proton Transfer TS (H44 to O32) -1734.127159 0.27 1st Proton Transfer Products -1734.078510 0.00 c3/z3 Cleavage TS -1734.078510 0.00 c3/z3 Cleavage Products -1734.093216 -9.23 1st Proton Transfer TS (H3 to O12) -1734.086236 -7.19 1st Proton Transfer Products -1734.086236 -4.85 2nd Proton Transfer Products -1734.086236 -4.85 2nd Proton Transfer TS (H14 to O22) -1734.088383 -6.20 3rd Proton Transfer Products -1734.089397 -13.11 Figure 5 c2/z2 Cleavage TS -1239.574084 0.00 c2/z2 Cleavage Products -1239.596836 <t< td=""><td>c4/z2 Cleavage Products</td><td>-1734.126637</td><td>-13.72</td></t<>	c4/z2 Cleavage Products	-1734.126637	-13.72
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1st Proton Transfer TS	c4/z2 Cleavage TS	-1734.128694	0.00
1st Proton Transfer TS	c4/z2 Cleavage Products	-1734.146870	-11.41
Figure 3 c3/z3 Cleavage TS c3/z3 Cleavage Products l³¹ Proton Transfer TS (H44 to O32) l³¹ Proton Transfer Products -1734.127159 0.27 l³¹ Proton Transfer Products -1734.137502 -6.22 Figure 4 c3/z3 Cleavage TS -1734.078510 0.00 c3/z3 Cleavage Products -1734.093216 -9.23 l³¹ Proton Transfer TS (H3 to O12) -1734.089965 -7.19 l³¹ Proton Transfer TS (H14 to O22) -1734.089965 -7.19 l³¹ Proton Transfer TS (H14 to O22) -1734.086236 -4.85 2n⁴ Proton Transfer TS (H24 to O32) -1734.088383 -6.20 3r⁴ Proton Transfer TS (H24 to O32) -1734.089397 -13.11 Figure 5 c2/z2 Cleavage TS -1239.574084 0.00 c2/z2 Cleavage Products -1239.596836 -14.28 l³¹ Proton Transfer TS (H4 to O38) -1239.596836 -14.28 l³¹ Proton Transfer Products -1239.636658 -39.27 Figure 6 c3/z2 Cleavage Products -1486.89329 0.00 c3/z2 Cleavage Products -1486.89048 -22.44 l³¹ Proton Transfer TS (H44 to N33) -1486.89048 -22.44 l³¹ Proton Transfer Products -1486.852781 -31.06 Figure 7 c3/z2 Cleavage Products -1486.850009 -14.88 l³¹ Proton Transfer TS (H3 to O12) -1486.845121 -1486.851214 -15.63 2n⁴ Proton Transfer Products -1486.851214 -15.63 2n⁴ Proton Transfer Products -1486.844601 -11.48		-1734.145986	-10.85
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13	Figure 3		
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1st Proton Transfer Products	c3/z3 Cleavage Products	-1734.128318	-0.46
1st Proton Transfer Products		-1734.127159	0.27
Figure 4 c3/z3 Cleavage TS c3/z3 Cleavage Products -1734.093216 -9.23 1st Proton Transfer TS (H3 to O12) -1734.089965 -7.19 1st Proton Transfer Products -1734.095743 -10.81 2nd Proton Transfer TS (H14 to O22) -1734.086236 -4.85 2nd Proton Transfer Products -1734.091955 -8.44 3rd Proton Transfer TS (H24 to O32) -1734.088383 -6.20 3rd Proton Transfer Products -1734.099397 -13.11 Figure 5 c2/z2 Cleavage TS -1239.574084 0.00 c2/z2 Cleavage Products -1239.596992 -14.37 1st Proton Transfer TS (H4 to O38) -1239.596836 -14.28 1st Proton Transfer Products -1239.636658 -39.27 Figure 6 c3/z2 Cleavage Products -1486.80329 0.00 c3/z2 Cleavage Products -1486.849489 -28.99 1st Proton Transfer TS (H44 to N33) -1486.852781 -31.06 Figure 7 c3/z2 Cleavage TS -1486.85209 0.00 c3/z2 Cleavage TS -1486.85209 -1486.852781 -31.06		-1734.137502	-6.22
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Tigure 5 C2/z2 Cleavage TS -1239.574084 0.00		-1734.091955	-8.44
Figure 5 c2/z2 Cleavage TS -1239.574084 0.00 c2/z2 Cleavage Products -1239.596992 -14.37 1st Proton Transfer TS (H4 to O38) -1239.596836 -14.28 1st Proton Transfer Products -1239.636658 -39.27 Figure 6 c3/z2 Cleavage TS -1486.80329 0.00 c3/z2 Cleavage Products -1486.849489 -28.99 1st Proton Transfer TS (H44 to N33) -1486.839048 -22.44 1st Proton Transfer Products -1486.852781 -31.06 Figure 7 c3/z2 Cleavage TS -1486.8526299 0.00 c3/z2 Cleavage TS -1486.850009 -14.88 1st Proton Transfer TS (H3 to O12) -1486.845132 -11.82 1st Proton Transfer Products -1486.851214 -15.63 2nd Proton Transfer TS (H14 to O49) -1486.84601 -11.48	3 rd Proton Transfer TS (H24 to O32)	-1734.088383	-6.20
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Figure 6 c3/z2 Cleavage TS -1486.80329 0.00 c3/z2 Cleavage Products -1486.849489 -28.99 1st Proton Transfer TS (H44 to N33) -1486.839048 -22.44 1st Proton Transfer Products -1486.852781 -31.06 Figure 7 c3/z2 Cleavage TS -1486.826299 0.00 c3/z2 Cleavage Products -1486.850009 -14.88 1st Proton Transfer TS (H3 to O12) -1486.845132 -11.82 1st Proton Transfer Products -1486.851214 -15.63 2nd Proton Transfer TS (H14 to O49) -1486.844601 -11.48	1st Proton Transfer TS (H4 to O38)	-1239.596836	-14.28
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Figure 7 c3/z2 Cleavage TS	1st Proton Transfer TS (H44 to N33)	-1486.839048	-22.44
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1st Proton Transfer Products -1486.851214 -15.63 2nd Proton Transfer TS (H14 to O49) -1486.844601 -11.48	c3/z2 Cleavage Products	-1486.850009	-14.88
2 nd Proton Transfer TS (H14 to O49) -1486.844601 -11.48	1 st Proton Transfer TS (H3 to O12)	-1486.845132	-11.82
	1st Proton Transfer Products	-1486.851214	-15.63
2 nd Proton Transfer Products -1486.854263 -17.55	2 nd Proton Transfer TS (H14 to O49)	-1486.844601	-11.48
	2 nd Proton Transfer Products	-1486.854263	-17.55