

$\text{H}_3\text{C}-\text{C}(=\text{O})\text{NHPH}$	-440.281003	97.5
$\text{H}_3\text{C}-\text{C}(\text{OH})=\text{NPh}$	-440.261258	97.3
$\text{H}_2\text{C}=\text{CH}_2$	-78.593808	32.1
CH_4	-40.524020	28.3

¹ SCRF=SCI-PCM, $\epsilon=1.92$. ² SCRF=SCI-PCM, $\epsilon=78.39$.

Table S11. Selected Optimized Dihedral Angles (in degrees) of the Calculated Species

	12a	12b	12c	12d	12e
C _A -C _B -C _C -O _D	-6.5	-7.5	-16.7	-7.9	-15.0
C _B -C _C -O _D -C _E	-18.8	-16.3	-14.1	-17.3	-14.2
C _C -O _D -C _E -O _F	43.4	41.3	41.9	42.9	42.0
O _D -C _E -O _F -C _A	-45.1	-45.6	-40.2	-46.6	-42.1
C _E -O _F -C _A -C _B	21.6	23.3	11.0	23.3	14.2
O _F -C _A -C _B -C _C	5.2	4.4	18.1	5.3	15.2
C _B =C-N-H	-4.9; -176.5	-5.9; -176.1	17.5; 172.0	-0.7	-179.3
C _C -C _B =C-N	177.2	177.7	166.4	173.9	-123.6
C _B =C-O _H -H	2.9			177.3	-16.5
C _C -C _B =C-O _H	-3.1	-2.5	-12.7	-6.2	57.2
C-C _B =C _C -O _G		0.7		-1.4	
C _B =C _C -O _G -H		0.2		0.4	

